



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 04:41 PM UTC

PDB ID : 5E7C / pdb_00005e7c
Title : Macromolecular diffractive imaging using imperfect crystals - Bragg data
Authors : Ayer, K.; Yefanov, O.; Oberthuer, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffner, A.; Doerner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Robinson, J.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on : 2015-10-12
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

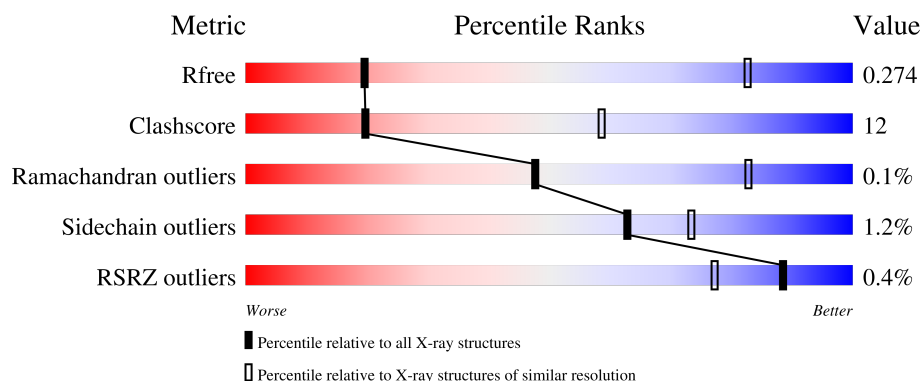
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

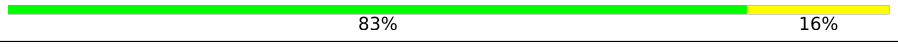
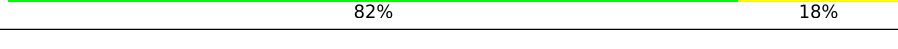
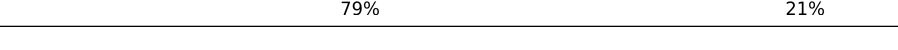
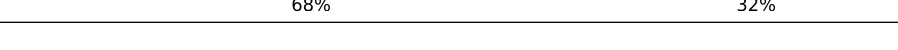
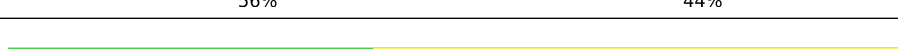
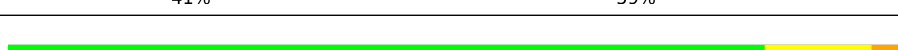
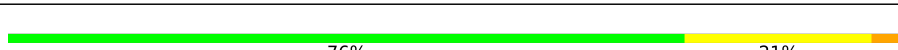
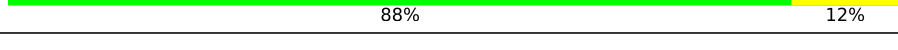
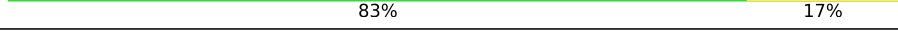
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	334	78% 22%
1	a	334	79% 21%
2	B	504	81% 18%

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

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Mol	Chain	Length	Quality of chain
2	b	504	% 
3	C	451	
3	c	451	
4	D	342	% 
4	d	342	2% 
5	E	81	
5	e	81	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	38	
9	j	38	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	3% 
12	m	34	
13	O	243	
13	o	243	
14	T	30	
14	t	30	

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Mol	Chain	Length	Quality of chain
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	29	
17	y	29	
18	X	39	
18	x	39	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL	u	201	-	-	-	X
22	BCT	A	604	-	X	-	-
22	BCT	a	603	-	X	-	-
23	CLA	A	605	X	-	-	-
23	CLA	A	606	X	-	-	-
23	CLA	A	608	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607[A]	X	-	-	-
23	CLA	B	607[B]	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	604	X	-	-	-
23	CLA	a	605	X	-	-	-
23	CLA	a	607	X	-	-	-
23	CLA	a	613	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609[A]	X	-	-	-
23	CLA	b	609[B]	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	BCR	A	609	-	X	-	-
25	BCR	B	618	-	X	X	-
25	BCR	B	619	-	X	X	-
25	BCR	B	620	-	X	X	-
25	BCR	C	514	-	X	-	-
25	BCR	C	515	-	X	-	-
25	BCR	C	521	-	X	-	-
25	BCR	F	101	-	X	-	-
25	BCR	H	101	-	X	-	-
25	BCR	K	101	-	X	X	-
25	BCR	T	101	-	X	X	-
25	BCR	a	608	-	X	-	-
25	BCR	b	620	-	X	X	-
25	BCR	b	621	-	X	X	-
25	BCR	b	622	-	X	-	-
25	BCR	c	515	-	X	-	-
25	BCR	c	516	-	X	-	-
25	BCR	c	522	-	X	-	-
25	BCR	f	101	-	X	X	-
25	BCR	h	101	-	X	-	-
25	BCR	k	101	-	X	X	-
25	BCR	t	101	-	X	X	-
26	PL9	A	610	-	X	-	-
26	PL9	D	405	-	X	-	-
26	PL9	a	609	-	X	-	-
26	PL9	d	404	-	X	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 49966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	13			
2	b	504	Total	C	N	O	S	6	10	0
			4024	2641	668	702	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			
3	c	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	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	81	Total	C	N	O		0	2	0
			668	436	107	125				
5	e	81	Total	C	N	O		0	2	0
			668	436	107	125				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			
8	i	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	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	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	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
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			
14	t	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

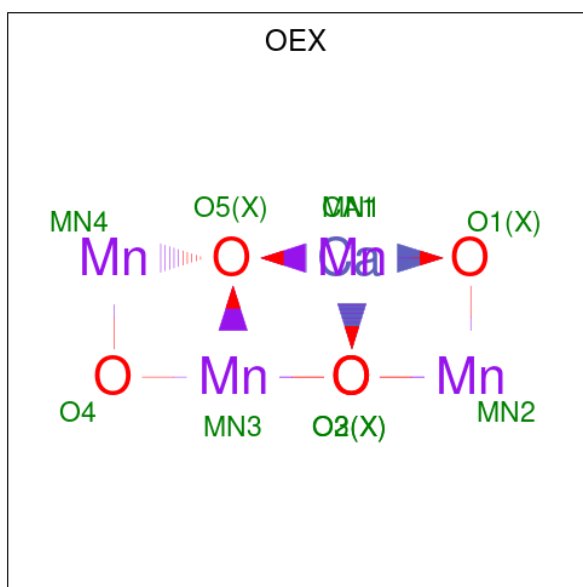
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	1	0
			292	196	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
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

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

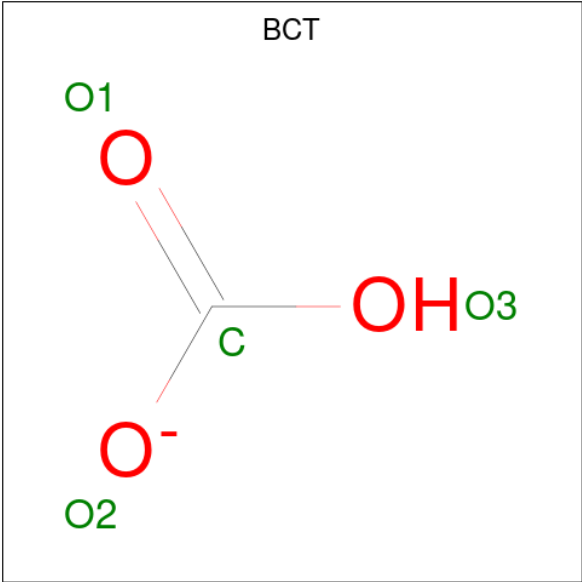


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

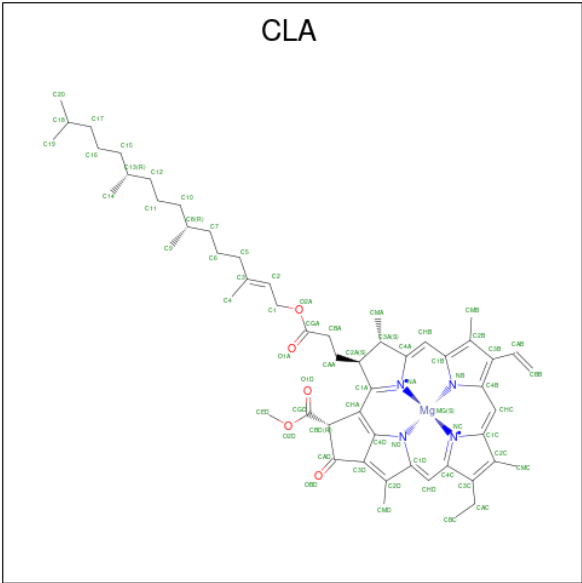
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	0
			2	2		
21	V	1	Total	Cl	0	0
			1	1		
21	a	1	Total	Cl	0	0
			1	1		
21	c	1	Total	Cl	0	0
			1	1		
21	u	1	Total	Cl	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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

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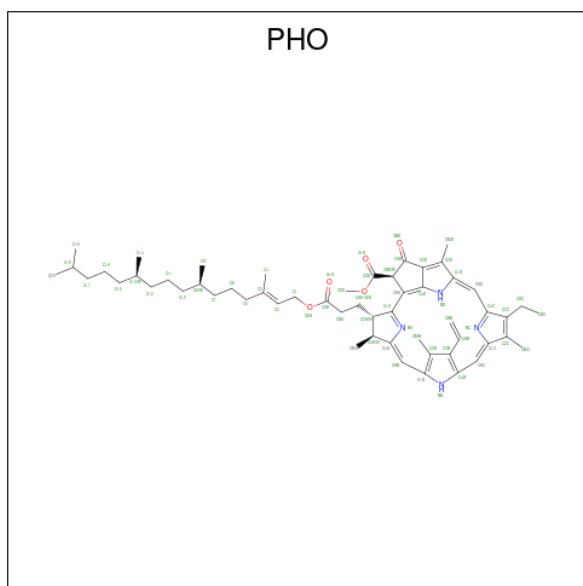
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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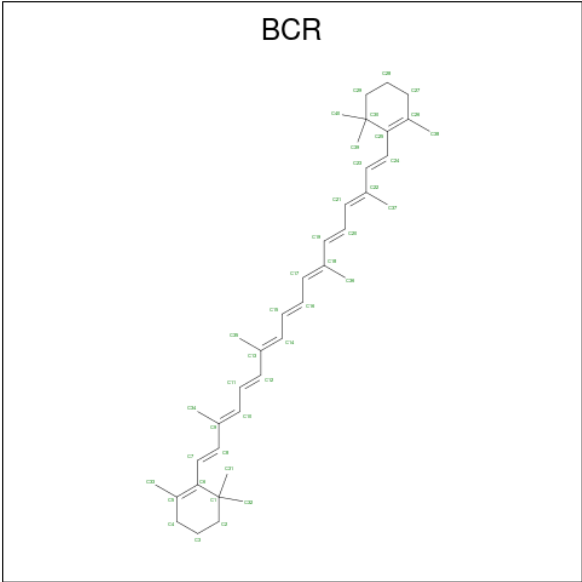
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



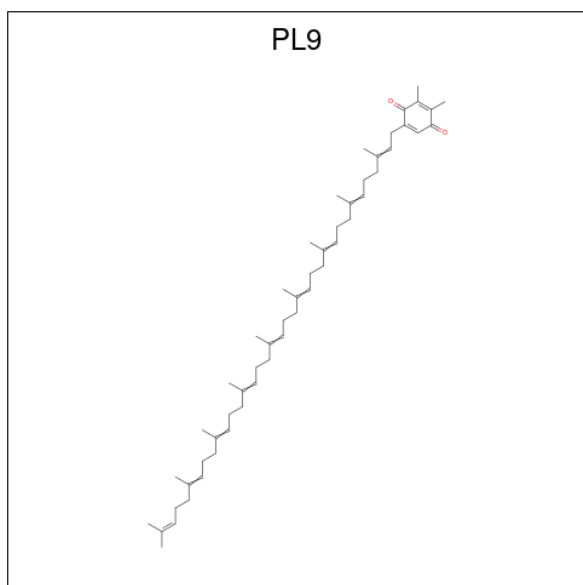
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total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

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

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



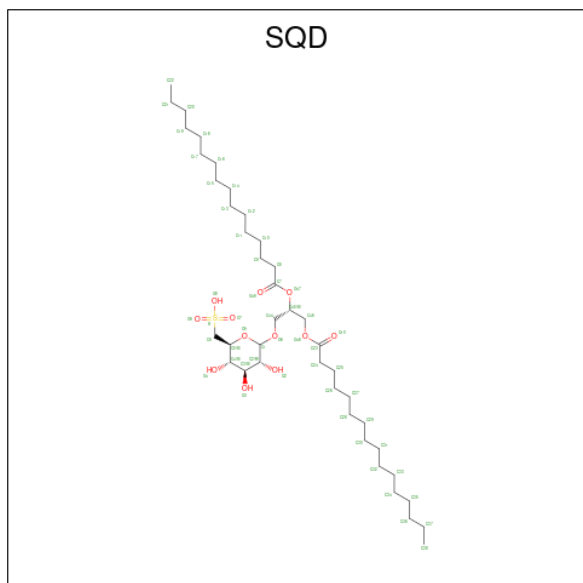
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 55 53 2	0	0
26	D	1	Total C O 55 53 2	0	0

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

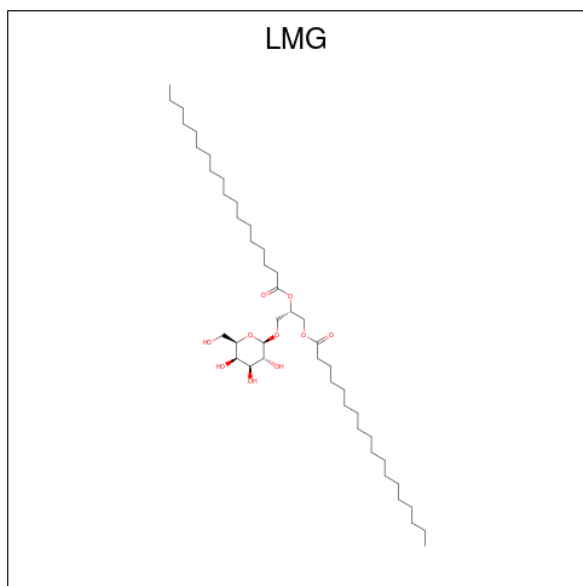
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	X	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	x	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	J	1	Total	C	O	0	0
			51	41	10		
28	Z	1	Total	C	O	0	0
			37	27	10		
28	a	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	j	1	Total	C	O	0	0
			51	41	10		
28	z	1	Total	C	O	0	0
			37	27	10		

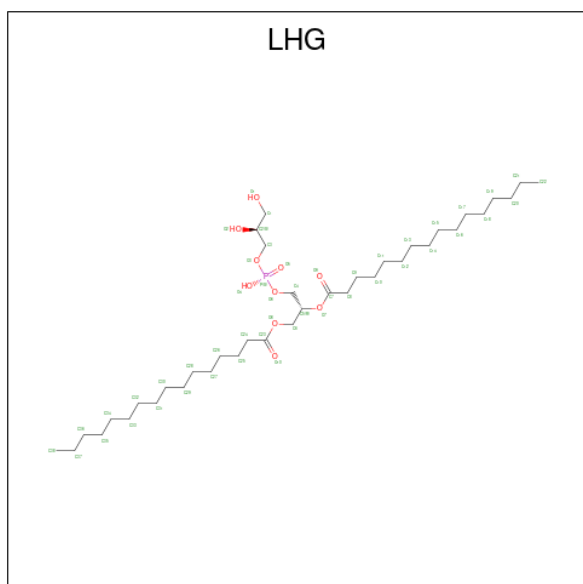
- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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



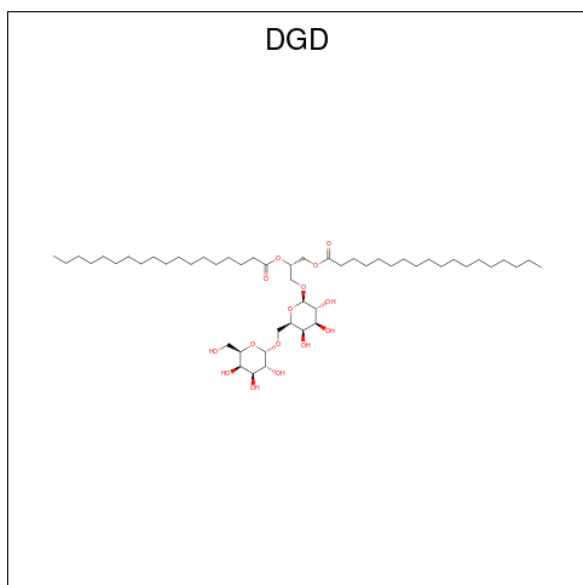
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O P 49 38 10 1	0	0

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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



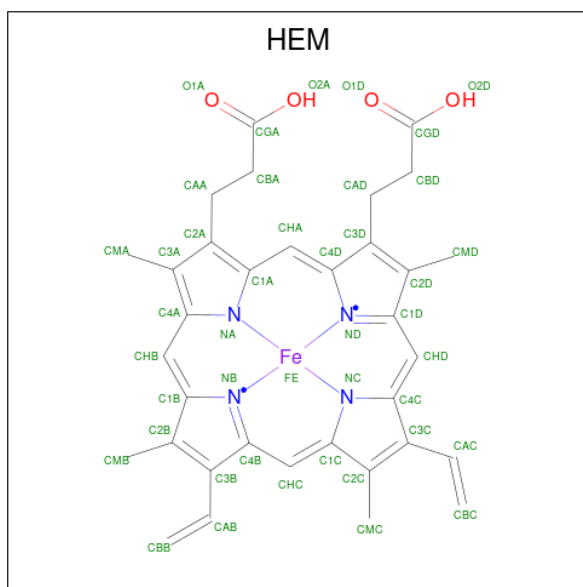
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		

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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

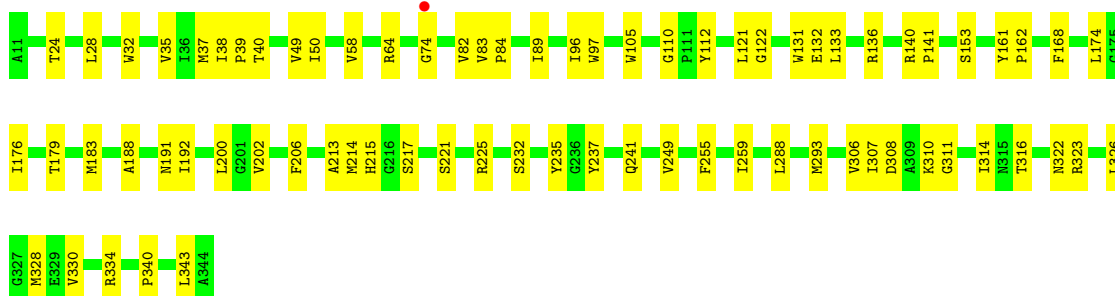
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

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

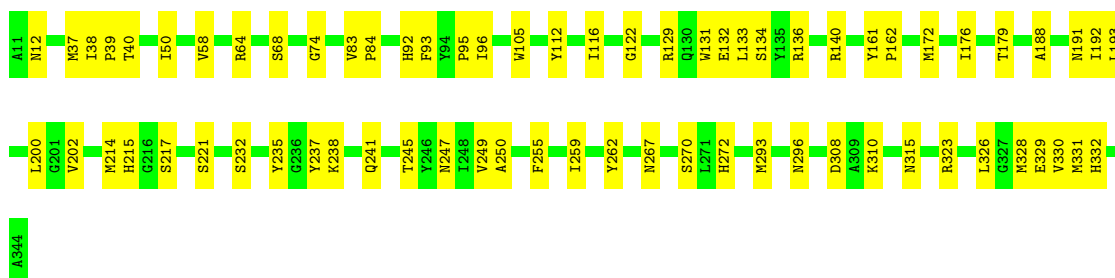
- Molecule 1: Photosystem II protein D1 1

Chain A:  78% 22%



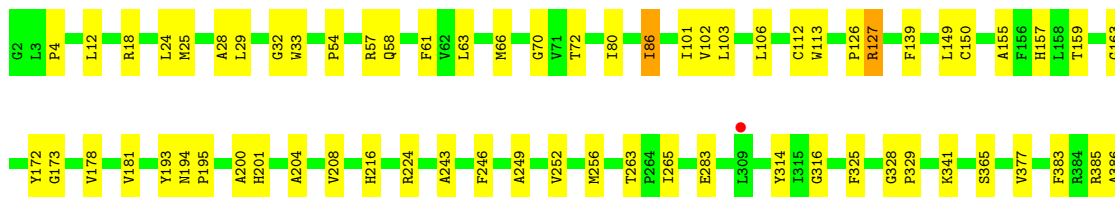
- Molecule 1: Photosystem II protein D1 1

Chain a:  79% 21%



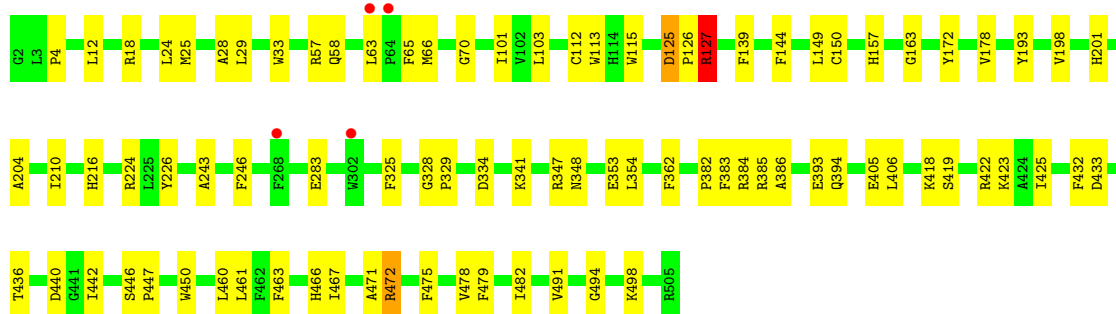
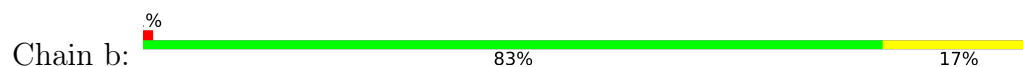
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  81% 18%

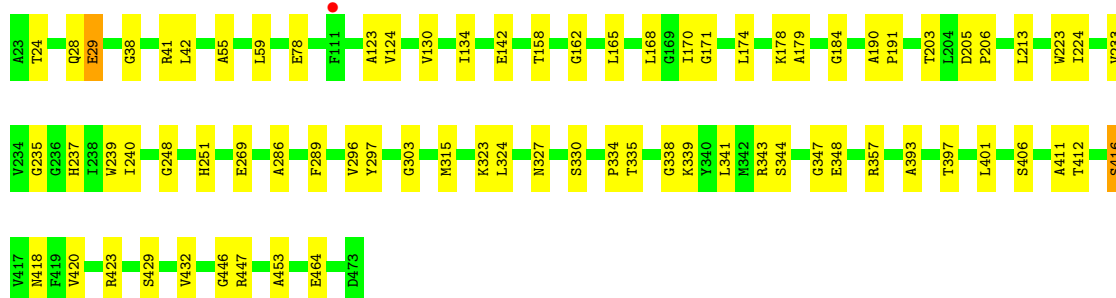
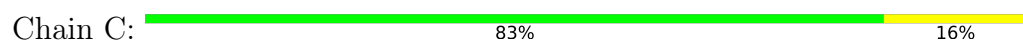




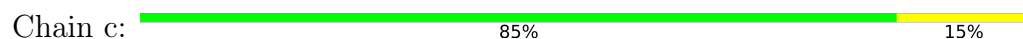
• Molecule 2: Photosystem II CP47 reaction center protein



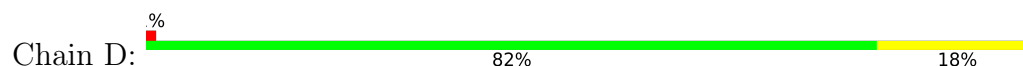
• Molecule 3: Photosystem II CP43 reaction center protein

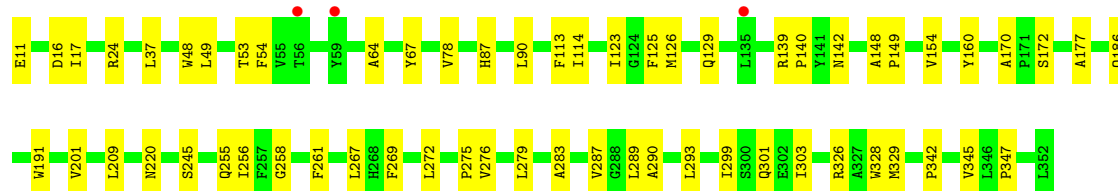


• Molecule 3: Photosystem II CP43 reaction center protein

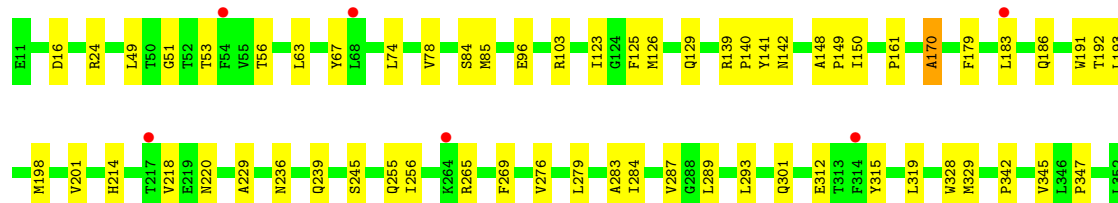
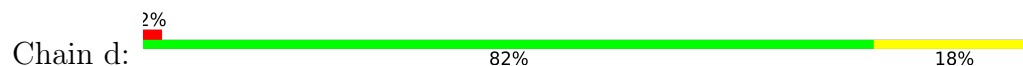


• Molecule 4: Photosystem II D2 protein

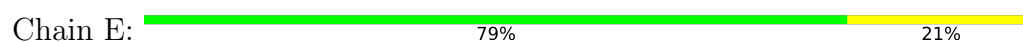




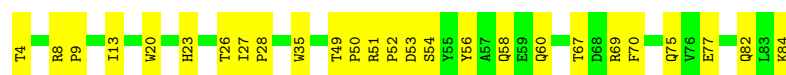
• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



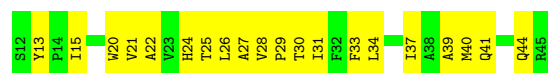
• Molecule 5: Cytochrome b559 subunit alpha



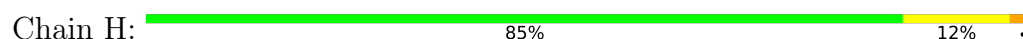
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H





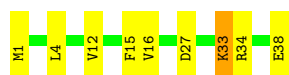
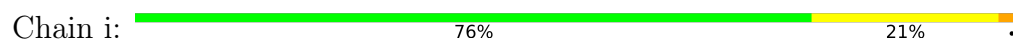
- Molecule 7: Photosystem II reaction center protein H



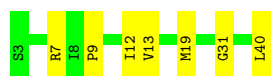
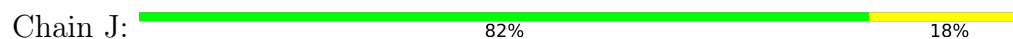
- Molecule 8: Photosystem II reaction center protein I



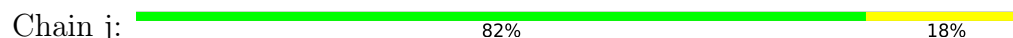
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

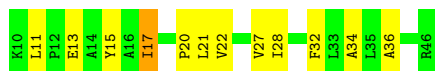


- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K





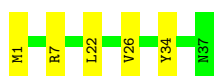
- Molecule 11: Photosystem II reaction center protein L

Chain L: 84% 16%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 14%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 3% 85% 15%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 88% 12%



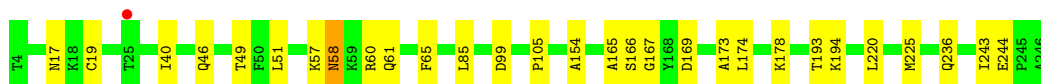
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 87% 13%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 88% 12%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 83% 17%



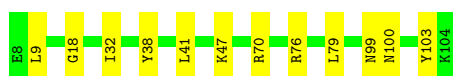
- Molecule 14: Photosystem II reaction center protein T

Chain t: 83% 17%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 88% 12%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 87% 13%



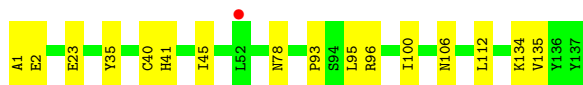
- Molecule 16: Cytochrome c-550

Chain V: 90% 10%



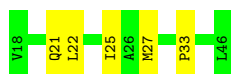
- Molecule 16: Cytochrome c-550

Chain v: 88% 12%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 83% 17%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 76% 24%



- Molecule 18: Photosystem II reaction center X protein

Chain X: 85% 15%



- Molecule 18: Photosystem II reaction center X protein

Chain x: 77% 23%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 92% 8%



- Molecule 19: Photosystem II reaction center protein Z

Chain z: 85% 11% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.25Å 226.26Å 307.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 4.50 29.93 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.93-4.50) 99.5 (29.93-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 4.44Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.246 , 0.275 0.254 , 0.274	Depositor DCC
R_{free} test set	2721 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	211.4	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 11.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	49966	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PL9, DGD, CL, FE2, LMG, LHG, BCT, HEM, SQD, PHO, CA, MG, OEX, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/2734	0.84	0/3727
1	a	0.44	0/2734	0.84	0/3727
2	B	0.38	0/4194	0.80	5/5713 (0.1%)
2	b	0.40	0/4194	0.83	6/5713 (0.1%)
3	C	0.39	0/3634	0.82	0/4947
3	c	0.41	0/3634	0.84	3/4947 (0.1%)
4	D	0.37	0/2821	0.79	3/3844 (0.1%)
4	d	0.38	0/2821	0.79	2/3844 (0.1%)
5	E	0.42	0/693	0.79	0/944
5	e	0.42	0/693	0.86	0/944
6	F	0.54	0/284	0.82	0/387
6	f	0.61	0/284	1.39	4/387 (1.0%)
7	H	0.38	0/544	0.80	1/739 (0.1%)
7	h	0.39	0/544	0.81	0/739
8	I	0.38	0/327	0.82	0/439
8	i	0.39	0/327	0.91	1/439 (0.2%)
9	J	0.36	0/278	0.84	0/376
9	j	0.39	0/278	0.84	0/376
10	K	0.44	0/303	0.86	0/416
10	k	0.44	0/303	0.82	0/416
11	L	0.36	0/319	0.76	0/433
11	l	0.36	0/319	0.74	0/433
12	M	0.46	0/278	0.90	0/378
12	m	0.45	0/278	0.88	0/378
13	O	0.36	0/1926	0.77	0/2611
13	o	0.39	0/1926	0.84	2/2611 (0.1%)
14	T	0.36	0/282	0.76	0/382
14	t	0.39	0/282	0.77	0/382
15	U	0.35	0/785	0.74	0/1064
15	u	0.39	0/785	0.84	0/1064
16	V	0.39	0/1096	0.78	0/1487
16	v	0.38	0/1096	0.87	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.44	0/216	0.85	0/289
17	y	0.50	0/216	1.01	0/289
18	X	0.38	0/298	0.79	0/403
18	x	0.45	0/298	0.89	0/403
19	Z	0.44	0/490	0.89	0/669
19	z	0.56	0/490	1.10	2/669 (0.3%)
All	All	0.40	0/43004	0.83	30/58496 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	15	ILE	CA-C-N	-9.18	110.91	122.84
6	f	15	ILE	C-N-CA	-9.18	110.91	122.84
19	z	35	ARG	CB-CG-CD	7.49	128.53	111.30
19	z	5	PHE	N-CA-C	6.30	117.81	111.07
16	v	35	TYR	N-CA-C	5.99	117.48	111.07
3	c	25	ASN	CA-C-N	-5.83	113.73	122.24
3	c	25	ASN	C-N-CA	-5.83	113.73	122.24
2	B	478	VAL	N-CA-C	5.76	117.64	112.17
2	B	328	GLY	CA-C-N	5.70	125.60	119.85
2	B	328	GLY	C-N-CA	5.70	125.60	119.85
6	f	26	LEU	N-CA-C	5.66	118.39	111.82
2	b	125	ASP	CA-C-N	5.64	125.49	119.28
2	b	125	ASP	C-N-CA	5.64	125.49	119.28
3	c	26	ARG	N-CA-C	5.50	117.58	110.65
2	B	194	ASN	CA-C-N	5.48	125.13	119.05
2	B	194	ASN	C-N-CA	5.48	125.13	119.05
4	d	170	ALA	CA-C-N	-5.44	114.32	119.76
4	d	170	ALA	C-N-CA	-5.44	114.32	119.76
7	H	52	THR	N-CA-C	-5.33	105.92	112.90
8	i	33	LYS	CB-CA-C	-5.29	108.81	116.54
6	f	27	ALA	N-CA-C	5.28	119.64	112.04
2	b	328	GLY	CA-C-N	5.27	125.17	119.85
2	b	328	GLY	C-N-CA	5.27	125.17	119.85
2	b	127	ARG	CG-CD-NE	5.19	123.42	112.00
4	D	170	ALA	CA-C-N	-5.18	114.58	119.76
4	D	170	ALA	C-N-CA	-5.18	114.58	119.76
4	D	37	LEU	N-CA-C	5.03	116.46	110.97
2	b	478	VAL	N-CA-C	5.02	116.94	112.17
13	o	244	GLU	CA-C-N	5.01	125.25	119.83
13	o	244	GLU	C-N-CA	5.01	125.25	119.83

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	2637	0	2551	69	0
1	a	2637	0	2551	60	0
2	B	4024	0	3901	91	0
2	b	4024	0	3901	83	0
3	C	3506	0	3439	70	0
3	c	3506	0	3439	60	0
4	D	2726	0	2627	52	0
4	d	2726	0	2627	61	0
5	E	668	0	658	14	0
5	e	668	0	658	24	0
6	F	275	0	282	11	0
6	f	275	0	282	19	0
7	H	525	0	558	9	0
7	h	525	0	558	6	0
8	I	320	0	339	10	0
8	i	320	0	339	8	0
9	J	272	0	279	7	0
9	j	272	0	279	6	0
10	K	293	0	305	11	0
10	k	293	0	305	12	0
11	L	309	0	327	6	0
11	l	309	0	327	6	0
12	M	272	0	300	5	0
12	m	272	0	300	6	0
13	O	1883	0	1865	26	0
13	o	1883	0	1865	22	0
14	T	270	0	278	8	0
14	t	270	0	278	9	0
15	U	774	0	773	11	0
15	u	774	0	773	11	0
16	V	1072	0	1088	13	0
16	v	1072	0	1088	12	0
17	Y	215	0	246	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	y	215	0	246	9	0
18	X	292	0	328	8	0
18	x	292	0	328	9	0
19	Z	479	0	516	3	0
19	z	479	0	516	4	0
20	A	10	0	0	1	0
20	a	10	0	0	1	0
21	A	2	0	0	0	0
21	V	1	0	0	0	0
21	a	1	0	0	0	0
21	c	1	0	0	0	0
21	u	1	0	0	0	0
22	A	4	0	1	0	0
22	a	4	0	1	0	0
23	A	195	0	216	15	0
23	B	1105	0	1224	53	0
23	C	845	0	936	46	0
23	D	195	0	216	7	0
23	a	260	0	288	13	0
23	b	1105	0	1224	49	0
23	c	845	0	936	40	0
23	d	130	0	144	7	0
24	A	64	0	74	1	0
24	D	64	0	74	8	0
24	a	64	0	74	0	0
24	d	64	0	74	6	0
25	A	40	0	55	16	0
25	B	120	0	165	74	0
25	C	120	0	164	44	0
25	F	40	0	54	16	0
25	H	40	0	55	10	0
25	K	40	0	55	25	0
25	T	40	0	55	28	0
25	a	40	0	55	14	0
25	b	120	0	165	71	0
25	c	120	0	165	48	0
25	f	40	0	55	24	0
25	h	40	0	55	15	0
25	k	40	0	55	22	0
25	t	40	0	55	30	0
26	A	55	0	80	16	0
26	D	55	0	80	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	a	55	0	80	10	0
26	d	55	0	80	3	0
27	A	54	0	78	4	0
27	B	54	0	78	9	0
27	X	43	0	53	3	0
27	a	108	0	156	3	0
27	b	108	0	156	15	0
27	x	43	0	53	4	0
28	A	51	0	72	2	0
28	B	51	0	72	4	0
28	C	102	0	144	1	0
28	J	51	0	72	3	0
28	Z	37	0	44	1	0
28	a	51	0	72	2	0
28	b	51	0	72	3	0
28	c	102	0	144	1	0
28	j	51	0	72	3	0
28	z	37	0	44	2	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	B	49	0	74	3	0
31	D	98	0	148	11	0
31	E	42	0	57	0	0
31	L	49	0	74	2	0
31	a	49	0	74	8	0
31	b	49	0	74	4	0
31	d	49	0	74	1	0
31	e	42	0	57	4	0
31	l	49	0	74	4	0
32	C	186	0	246	8	0
32	D	62	0	82	1	0
32	H	62	0	82	5	0
32	c	186	0	246	8	0
32	d	62	0	82	2	0
32	h	62	0	82	3	0
33	E	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	V	43	0	30	4	0
33	e	43	0	30	3	0
33	v	43	0	30	1	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	49966	0	51358	1169	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 12.

All (1169) 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)
25:b:620:BCR:C19	25:b:620:BCR:C20	1.74	1.66
25:b:622:BCR:C19	25:b:622:BCR:C20	1.75	1.64
25:c:516:BCR:C20	25:c:516:BCR:C19	1.74	1.64
25:T:101:BCR:C16	25:T:101:BCR:C17	1.75	1.64
25:k:101:BCR:C19	25:k:101:BCR:C20	1.75	1.64
25:K:101:BCR:C37	25:K:101:BCR:C22	1.75	1.63
25:A:609:BCR:C19	25:A:609:BCR:C20	1.74	1.63
25:t:101:BCR:C20	25:t:101:BCR:C19	1.75	1.63
25:B:618:BCR:C20	25:B:618:BCR:C19	1.76	1.62
25:B:620:BCR:C19	25:B:620:BCR:C20	1.74	1.62
25:C:514:BCR:C20	25:C:514:BCR:C19	1.75	1.62
25:f:101:BCR:C20	25:f:101:BCR:C19	1.74	1.62
25:t:101:BCR:C37	25:t:101:BCR:C22	1.74	1.62
25:F:101:BCR:C20	25:F:101:BCR:C21	1.77	1.61
25:f:101:BCR:C37	25:f:101:BCR:C22	1.74	1.61
25:h:101:BCR:C18	25:h:101:BCR:C36	1.77	1.61
25:A:609:BCR:C22	25:A:609:BCR:C37	1.75	1.61
25:B:619:BCR:C22	25:B:619:BCR:C37	1.76	1.61
25:C:514:BCR:C20	25:C:514:BCR:C21	1.78	1.61
25:c:516:BCR:C37	25:c:516:BCR:C22	1.75	1.61
25:b:622:BCR:C20	25:b:622:BCR:C21	1.79	1.60
25:c:516:BCR:C20	25:c:516:BCR:C21	1.78	1.60
25:K:101:BCR:C20	25:K:101:BCR:C19	1.75	1.60
25:b:620:BCR:C20	25:b:620:BCR:C21	1.78	1.60
25:C:521:BCR:C20	25:C:521:BCR:C21	1.77	1.60
25:T:101:BCR:C19	25:T:101:BCR:C20	1.75	1.60
25:f:101:BCR:C20	25:f:101:BCR:C21	1.79	1.60
25:C:515:BCR:C20	25:C:515:BCR:C21	1.77	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:609:BCR:C20	25:A:609:BCR:C21	1.79	1.59
25:B:620:BCR:C20	25:B:620:BCR:C21	1.79	1.59
25:K:101:BCR:C20	25:K:101:BCR:C21	1.80	1.59
25:b:622:BCR:C37	25:b:622:BCR:C22	1.76	1.59
25:b:622:BCR:C36	25:b:622:BCR:C18	1.79	1.59
25:t:101:BCR:C20	25:t:101:BCR:C21	1.79	1.59
25:k:101:BCR:C20	25:k:101:BCR:C21	1.79	1.59
25:B:620:BCR:C37	25:B:620:BCR:C22	1.75	1.59
25:C:515:BCR:C22	25:C:515:BCR:C37	1.74	1.59
25:K:101:BCR:C18	25:K:101:BCR:C36	1.77	1.59
25:A:609:BCR:C36	25:A:609:BCR:C18	1.79	1.58
25:T:101:BCR:C18	25:T:101:BCR:C36	1.77	1.58
25:k:101:BCR:C37	25:k:101:BCR:C22	1.75	1.58
25:a:608:BCR:C18	25:a:608:BCR:C36	1.79	1.58
25:a:608:BCR:C37	25:a:608:BCR:C22	1.74	1.58
25:C:521:BCR:C36	25:C:521:BCR:C18	1.79	1.58
25:k:101:BCR:C18	25:k:101:BCR:C36	1.79	1.58
25:B:618:BCR:C18	25:B:618:BCR:C36	1.78	1.58
25:b:621:BCR:C18	25:b:621:BCR:C36	1.77	1.58
25:h:101:BCR:C20	25:h:101:BCR:C21	1.78	1.58
25:c:522:BCR:C18	25:c:522:BCR:C36	1.79	1.57
25:h:101:BCR:C37	25:h:101:BCR:C22	1.75	1.57
25:C:514:BCR:C18	25:C:514:BCR:C36	1.80	1.57
25:T:101:BCR:C22	25:T:101:BCR:C37	1.76	1.57
25:a:608:BCR:C20	25:a:608:BCR:C19	1.74	1.57
25:B:618:BCR:C37	25:B:618:BCR:C22	1.77	1.57
25:b:621:BCR:C20	25:b:621:BCR:C21	1.79	1.57
25:c:515:BCR:C20	25:c:515:BCR:C21	1.78	1.57
25:c:522:BCR:C20	25:c:522:BCR:C21	1.78	1.57
25:c:516:BCR:C18	25:c:516:BCR:C36	1.79	1.56
25:t:101:BCR:C18	25:t:101:BCR:C36	1.79	1.56
25:H:101:BCR:C20	25:H:101:BCR:C21	1.77	1.56
25:B:618:BCR:C20	25:B:618:BCR:C21	1.79	1.56
25:b:620:BCR:C36	25:b:620:BCR:C18	1.78	1.56
25:f:101:BCR:C18	25:f:101:BCR:C36	1.79	1.56
25:B:619:BCR:C20	25:B:619:BCR:C21	1.77	1.56
25:B:620:BCR:C18	25:B:620:BCR:C36	1.78	1.55
25:c:515:BCR:C18	25:c:515:BCR:C36	1.78	1.55
25:c:515:BCR:C22	25:c:515:BCR:C37	1.75	1.55
25:C:515:BCR:C36	25:C:515:BCR:C18	1.79	1.55
25:b:621:BCR:C20	25:b:621:BCR:C19	1.74	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:F:101:BCR:C18	25:F:101:BCR:C36	1.77	1.54
25:b:620:BCR:C22	25:b:620:BCR:C37	1.74	1.54
25:H:101:BCR:C18	25:H:101:BCR:C36	1.80	1.54
25:b:621:BCR:C37	25:b:621:BCR:C22	1.76	1.54
25:T:101:BCR:C20	25:T:101:BCR:C21	1.80	1.53
25:B:619:BCR:C18	25:B:619:BCR:C36	1.81	1.53
25:a:608:BCR:C20	25:a:608:BCR:C21	1.79	1.51
25:T:101:BCR:H17C	25:b:621:BCR:H17C	1.31	1.11
25:T:101:BCR:H17C	25:b:621:BCR:C17	1.94	0.98
27:b:602:SQD:H121	23:b:617:CLA:H43	1.44	0.95
25:F:101:BCR:C20	25:F:101:BCR:C22	2.42	0.95
25:C:521:BCR:C20	25:C:521:BCR:C22	2.44	0.95
25:C:515:BCR:C21	25:C:515:BCR:C37	2.41	0.94
25:T:101:BCR:C37	25:T:101:BCR:C21	2.43	0.94
3:c:165:LEU:HD21	23:c:507:CLA:HAB	1.50	0.94
25:B:620:BCR:C21	25:B:620:BCR:C37	2.42	0.94
25:c:522:BCR:C20	25:c:522:BCR:C22	2.44	0.94
25:f:101:BCR:C37	25:f:101:BCR:C21	2.45	0.93
25:B:618:BCR:C37	25:B:618:BCR:C21	2.42	0.92
25:B:619:BCR:C37	25:B:619:BCR:C21	2.44	0.92
25:t:101:BCR:C37	25:t:101:BCR:C21	2.45	0.92
25:b:620:BCR:C19	25:b:620:BCR:H20C	2.01	0.91
25:T:101:BCR:C17	25:b:621:BCR:H17C	2.00	0.90
25:A:609:BCR:C19	25:A:609:BCR:H20C	2.02	0.90
25:b:621:BCR:C19	25:b:621:BCR:H20C	2.01	0.89
25:h:101:BCR:C21	25:h:101:BCR:C37	2.45	0.89
25:k:101:BCR:C21	25:k:101:BCR:C37	2.44	0.89
25:B:618:BCR:C20	25:B:618:BCR:C22	2.45	0.89
23:B:615:CLA:H43	27:B:623:SQD:H121	1.54	0.89
25:b:621:BCR:C21	25:b:621:BCR:C37	2.46	0.89
25:A:609:BCR:C37	25:A:609:BCR:C21	2.45	0.88
3:c:213[B]:LEU:HD21	25:c:516:BCR:H20C	1.53	0.88
3:C:165:LEU:HD21	23:C:506:CLA:HAB	1.55	0.88
25:H:101:BCR:C20	25:H:101:BCR:C22	2.46	0.88
25:C:514:BCR:C19	25:C:514:BCR:H20C	2.01	0.88
25:b:622:BCR:C21	25:b:622:BCR:C37	2.48	0.88
25:c:516:BCR:C21	25:c:516:BCR:H20C	2.03	0.88
25:C:515:BCR:C20	25:C:515:BCR:C22	2.47	0.88
25:a:608:BCR:C22	25:a:608:BCR:C20	2.49	0.88
25:B:619:BCR:C22	25:B:619:BCR:C20	2.47	0.87
25:T:101:BCR:C17	25:T:101:BCR:H16C	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:101:BCR:C20	25:T:101:BCR:C18	2.51	0.87
25:b:620:BCR:C21	25:b:620:BCR:C37	2.45	0.87
25:c:515:BCR:C20	25:c:515:BCR:C22	2.46	0.87
25:B:620:BCR:C19	25:B:620:BCR:H20C	2.01	0.87
25:b:622:BCR:C19	25:b:622:BCR:H20C	2.03	0.87
25:t:101:BCR:C19	25:t:101:BCR:H20C	2.02	0.86
25:c:515:BCR:C21	25:c:515:BCR:C37	2.46	0.86
25:a:608:BCR:C19	25:a:608:BCR:H20C	2.02	0.85
25:c:516:BCR:C19	25:c:516:BCR:H20C	2.00	0.85
25:T:101:BCR:C19	25:T:101:BCR:H20C	2.05	0.85
25:f:101:BCR:C19	25:f:101:BCR:H20C	2.02	0.85
25:A:609:BCR:C21	25:A:609:BCR:H20C	2.06	0.85
25:c:515:BCR:C21	25:c:515:BCR:H20C	2.03	0.85
25:C:515:BCR:C21	25:C:515:BCR:H20C	2.04	0.85
25:K:101:BCR:C19	25:K:101:BCR:H20C	2.04	0.85
25:b:621:BCR:C21	25:b:621:BCR:H20C	2.05	0.84
25:c:522:BCR:C21	25:c:522:BCR:H20C	2.05	0.84
23:B:617:CLA:H3A	25:B:620:BCR:H17C	1.60	0.84
25:b:620:BCR:C21	25:b:620:BCR:H20C	2.04	0.84
25:H:101:BCR:C21	25:H:101:BCR:H20C	2.04	0.84
25:h:101:BCR:C21	25:h:101:BCR:H20C	2.05	0.84
25:F:101:BCR:C21	25:F:101:BCR:H20C	2.06	0.84
25:b:622:BCR:C21	25:b:622:BCR:H20C	2.07	0.84
25:t:101:BCR:C21	25:t:101:BCR:H20C	2.06	0.83
25:k:101:BCR:C19	25:k:101:BCR:H20C	2.05	0.83
25:C:514:BCR:C20	25:C:514:BCR:C22	2.48	0.83
25:K:101:BCR:C19	25:K:101:BCR:C36	2.53	0.83
25:C:521:BCR:H15C	25:K:101:BCR:H342	1.60	0.83
25:B:618:BCR:C19	25:B:618:BCR:H20C	2.05	0.83
25:C:521:BCR:C21	25:C:521:BCR:H20C	2.03	0.83
25:b:620:BCR:C19	25:b:620:BCR:C36	2.55	0.83
25:f:101:BCR:C20	25:f:101:BCR:C18	2.54	0.82
25:C:514:BCR:C21	25:C:514:BCR:H20C	2.04	0.82
25:B:620:BCR:C19	25:B:620:BCR:C36	2.55	0.82
25:c:516:BCR:C37	25:c:516:BCR:C21	2.48	0.82
25:K:101:BCR:C21	25:K:101:BCR:H20C	2.08	0.82
25:B:620:BCR:C21	25:B:620:BCR:H20C	2.04	0.81
7:H:38:PHE:HB2	25:H:101:BCR:H10C	1.61	0.81
25:T:101:BCR:C20	25:T:101:BCR:C22	2.51	0.81
25:f:101:BCR:C21	25:f:101:BCR:H20C	2.06	0.81
25:B:618:BCR:H12C	25:B:619:BCR:H10C	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:408:LHG:H382	31:D:408:LHG:H112	1.62	0.81
25:b:620:BCR:C20	25:b:620:BCR:C22	2.51	0.81
25:a:608:BCR:C21	25:a:608:BCR:H20C	2.06	0.81
25:c:516:BCR:C19	25:c:516:BCR:C36	2.56	0.81
25:a:608:BCR:C37	25:a:608:BCR:C21	2.50	0.81
25:K:101:BCR:C37	25:K:101:BCR:C21	2.48	0.80
2:b:432:PHE:O	13:o:178:LYS:NZ	2.15	0.80
1:A:50:ILE:HG22	25:A:609:BCR:H271	1.63	0.79
25:B:619:BCR:C36	25:B:619:BCR:C19	2.56	0.79
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.45	0.79
25:b:621:BCR:C36	25:b:621:BCR:C19	2.55	0.79
25:t:101:BCR:C19	25:t:101:BCR:C36	2.56	0.79
10:K:17:ILE:H	10:K:17:ILE:HD13	1.48	0.79
25:b:621:BCR:C18	25:b:621:BCR:C20	2.54	0.79
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.65	0.78
25:b:622:BCR:C20	25:b:622:BCR:C22	2.49	0.78
25:h:101:BCR:C20	25:h:101:BCR:C22	2.50	0.78
25:T:101:BCR:C21	25:T:101:BCR:H20C	2.10	0.78
25:k:101:BCR:C21	25:k:101:BCR:H20C	2.08	0.78
25:B:620:BCR:C20	25:B:620:BCR:C18	2.53	0.78
25:b:622:BCR:C20	25:b:622:BCR:C18	2.56	0.77
23:c:507:CLA:H162	25:c:516:BCR:H15C	1.67	0.77
25:c:522:BCR:C36	25:c:522:BCR:C19	2.57	0.77
1:a:50:ILE:HG22	25:a:608:BCR:H271	1.65	0.77
25:c:522:BCR:H15C	25:k:101:BCR:H342	1.66	0.77
25:c:516:BCR:C20	25:c:516:BCR:C18	2.55	0.77
3:c:124:VAL:HG11	25:c:515:BCR:H17C	1.65	0.77
3:c:24:THR:OG1	3:c:138:GLU:OE1	2.03	0.76
25:B:618:BCR:C21	25:B:618:BCR:H20C	2.09	0.76
25:c:516:BCR:C20	25:c:516:BCR:C22	2.51	0.76
25:t:101:BCR:C20	25:t:101:BCR:C22	2.52	0.76
25:A:609:BCR:C20	25:A:609:BCR:C18	2.55	0.76
25:T:101:BCR:C19	25:T:101:BCR:C36	2.55	0.76
5:e:56:TYR:O	16:v:1:ALA:N	2.15	0.76
25:C:514:BCR:C20	25:C:514:BCR:C18	2.56	0.76
3:c:210:PHE:HA	3:c:213[B]:LEU:HD13	1.68	0.76
25:h:101:BCR:C36	25:h:101:BCR:C19	2.55	0.76
23:C:507:CLA:H142	25:C:515:BCR:H362	1.68	0.76
31:D:408:LHG:H151	31:D:408:LHG:H352	1.67	0.75
25:B:620:BCR:C20	25:B:620:BCR:C22	2.51	0.75
25:C:515:BCR:C36	25:C:515:BCR:C19	2.55	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:614:LHG:H352	31:a:614:LHG:H151	1.66	0.75
23:b:617:CLA:HAB	25:b:620:BCR:H19C	1.66	0.75
25:b:621:BCR:C20	25:b:621:BCR:C22	2.53	0.75
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.67	0.75
27:A:611:SQD:O7	3:C:28:GLN:NE2	2.16	0.75
25:F:101:BCR:C36	25:F:101:BCR:C19	2.58	0.74
25:B:618:BCR:C20	25:B:618:BCR:C18	2.59	0.74
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.68	0.74
25:B:619:BCR:C21	25:B:619:BCR:H20C	2.13	0.73
25:B:619:BCR:H17C	25:t:101:BCR:C17	2.18	0.73
25:k:101:BCR:H10C	17:y:28:ILE:HG23	1.69	0.73
32:D:406:DGD:HA72	25:F:101:BCR:HC22	1.70	0.72
25:A:609:BCR:C19	25:A:609:BCR:C36	2.57	0.72
20:a:601:OEX:O2	3:c:357:ARG:NH2	2.22	0.72
14:T:15:ALA:HA	25:T:101:BCR:H12C	1.70	0.72
25:c:515:BCR:C36	25:c:515:BCR:C19	2.58	0.72
25:A:609:BCR:C20	25:A:609:BCR:C22	2.54	0.72
25:C:521:BCR:C36	25:C:521:BCR:C19	2.57	0.72
25:k:101:BCR:C20	25:k:101:BCR:C22	2.55	0.72
18:x:24:THR:HA	27:x:101:SQD:H331	1.72	0.71
18:x:35:ASP:OD1	27:x:101:SQD:H5	1.90	0.71
25:c:522:BCR:H20C	25:c:522:BCR:H372	1.70	0.71
4:d:24:ARG:HD3	18:x:37:VAL:HG22	1.72	0.71
25:a:608:BCR:C18	25:a:608:BCR:C20	2.57	0.71
25:K:101:BCR:H17C	17:Y:33:PRO:HD3	1.72	0.71
3:C:124:VAL:HG11	25:C:514:BCR:H17C	1.72	0.70
25:T:101:BCR:HC41	27:b:601:SQD:H132	1.74	0.70
1:a:310:LYS:NZ	5:e:58:GLN:O	2.21	0.70
16:v:93:PRO:HG2	33:v:201:HEM:HMC3	1.73	0.70
25:a:608:BCR:C36	25:a:608:BCR:C19	2.60	0.70
25:F:101:BCR:C36	25:F:101:BCR:C17	2.63	0.69
25:K:101:BCR:C17	17:Y:33:PRO:HD3	2.21	0.69
25:K:101:BCR:HC8	19:Z:20:VAL:HG21	1.73	0.69
1:A:40:THR:HG23	23:A:608:CLA:HBB1	1.74	0.69
25:k:101:BCR:C20	25:k:101:BCR:C18	2.58	0.69
3:C:213[B]:LEU:HD21	25:C:515:BCR:H20C	1.74	0.69
25:T:101:BCR:H17C	25:T:101:BCR:H20C	1.75	0.69
25:c:522:BCR:H20C	25:c:522:BCR:C37	2.21	0.69
25:f:101:BCR:C19	25:f:101:BCR:C36	2.59	0.69
23:A:606:CLA:H152	26:A:610:PL9:H262	1.74	0.69
32:d:405:DGD:HA72	25:f:101:BCR:HC22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:464:GLU:OE2	4:D:245:SER:OG	2.11	0.68
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.74	0.68
23:B:615:CLA:H18	28:B:621:LMG:H421	1.75	0.67
4:d:279:LEU:HD22	24:d:401:PHO:HBC3	1.77	0.67
23:b:617:CLA:H101	25:b:620:BCR:H362	1.76	0.67
4:d:49:LEU:HD13	25:f:101:BCR:H16C	1.75	0.67
25:T:101:BCR:C20	25:T:101:BCR:C37	2.72	0.67
25:k:101:BCR:C19	25:k:101:BCR:C36	2.59	0.67
2:b:33:TRP:N	25:b:621:BCR:H15C	2.10	0.67
25:B:618:BCR:C20	25:B:618:BCR:C37	2.73	0.66
25:K:101:BCR:H17C	17:Y:33:PRO:HG3	1.75	0.66
25:T:101:BCR:H341	25:b:621:BCR:H381	1.78	0.66
2:b:18:ARG:NH2	27:b:602:SQD:O9	2.28	0.66
27:a:612:SQD:H132	25:t:101:BCR:HC41	1.77	0.66
10:k:34:ALA:HB1	25:k:101:BCR:C20	2.26	0.66
25:c:522:BCR:C36	25:c:522:BCR:C17	2.70	0.66
10:K:34:ALA:HB1	25:K:101:BCR:C20	2.26	0.66
25:f:101:BCR:C20	25:f:101:BCR:C22	2.56	0.65
2:B:106:LEU:HB3	25:B:620:BCR:H15C	1.78	0.65
23:C:501:CLA:C1D	23:C:503:CLA:H2	2.27	0.65
3:c:25:ASN:HD21	3:c:45:LEU:HD11	1.61	0.65
6:f:41:GLN:OE1	9:j:31:GLY:HA3	1.97	0.65
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.30	0.65
1:A:214:MET:HG2	26:A:610:PL9:H102	1.79	0.65
31:a:614:LHG:H112	31:a:614:LHG:H382	1.79	0.65
23:A:606:CLA:H122	26:A:610:PL9:H23	1.79	0.65
27:b:602:SQD:H1	27:b:602:SQD:H462	1.79	0.65
25:C:514:BCR:C19	25:C:514:BCR:C36	2.60	0.65
5:e:69:ARG:NH2	7:h:50:ASN:O	2.30	0.64
25:C:515:BCR:C20	25:C:515:BCR:C37	2.75	0.64
25:f:101:BCR:C36	25:f:101:BCR:C17	2.70	0.64
14:t:15:ALA:HA	25:t:101:BCR:H12C	1.79	0.64
3:C:123:ALA:HB2	25:C:521:BCR:H12C	1.78	0.64
23:C:501:CLA:C1C	23:C:503:CLA:H71	2.26	0.64
25:K:101:BCR:C20	25:K:101:BCR:C18	2.59	0.64
4:D:279:LEU:HD22	24:D:401:PHO:HBC3	1.79	0.64
25:C:521:BCR:C36	25:C:521:BCR:C17	2.70	0.64
25:b:620:BCR:C20	25:b:620:BCR:C18	2.61	0.64
27:B:623:SQD:H462	27:B:623:SQD:H1	1.79	0.63
6:f:29:PRO:HB3	25:f:101:BCR:H12C	1.80	0.63
25:B:618:BCR:H15C	25:B:619:BCR:C13	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K:101:BCR:H17C	17:Y:33:PRO:CG	2.28	0.63
23:C:501:CLA:C2D	23:C:503:CLA:H2	2.29	0.63
2:B:432:PHE:O	13:O:178:LYS:NZ	2.24	0.63
25:B:618:BCR:C37	25:B:618:BCR:H20C	2.29	0.63
23:C:506:CLA:HMB3	23:C:506:CLA:HBB1	1.78	0.63
3:C:123:ALA:HB2	25:C:521:BCR:C12	2.29	0.62
27:b:602:SQD:H62	11:l:7:ARG:HH21	1.64	0.62
23:c:511:CLA:H192	23:c:511:CLA:HBC3	1.81	0.62
25:K:101:BCR:HC21	19:Z:13:VAL:HG13	1.81	0.62
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.80	0.62
3:C:429:SER:HB3	32:C:517:DGD:HBT2	1.82	0.62
1:a:200:LEU:HG	32:c:519:DGD:HAT2	1.80	0.62
23:B:608:CLA:HMC2	25:B:619:BCR:HC8	1.82	0.61
3:c:123:ALA:HB2	25:c:522:BCR:C12	2.29	0.61
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.81	0.61
27:b:602:SQD:H62	11:l:7:ARG:NH2	2.15	0.61
3:c:72:LEU:HD23	10:k:11:LEU:HD23	1.83	0.61
23:a:605:CLA:HBB1	23:a:605:CLA:HMB1	1.81	0.61
25:B:619:BCR:H17C	25:t:101:BCR:H17C	1.82	0.61
16:V:93:PRO:HG2	33:V:202:HEM:HMC3	1.82	0.61
1:a:326:LEU:HD22	16:v:134:LYS:HB2	1.83	0.61
18:x:31:ILE:HG23	27:x:101:SQD:H462	1.83	0.61
23:C:508:CLA:H92	31:D:408:LHG:H371	1.81	0.61
2:B:467:ILE:HG13	4:D:126:MET:HE1	1.83	0.61
6:f:30:THR:HG23	25:f:101:BCR:C19	2.31	0.61
3:C:124:VAL:HG11	25:C:514:BCR:C17	2.30	0.61
23:C:512:CLA:HBB1	23:C:512:CLA:HMB1	1.82	0.61
23:c:502:CLA:C1C	23:c:504:CLA:H71	2.31	0.61
2:b:383:PHE:O	13:o:166:SER:HA	2.00	0.61
25:f:101:BCR:H17C	28:j:101:LMG:H352	1.83	0.61
5:e:8:ARG:NH2	9:j:3:SER:O	2.34	0.60
2:B:471:ALA:HB1	4:D:140:PRO:HG2	1.83	0.60
2:b:393:GLU:HB3	15:u:18:GLY:CA	2.31	0.60
1:A:310:LYS:NZ	5:E:58:GLN:O	2.26	0.60
25:K:101:BCR:H17C	17:Y:33:PRO:CD	2.31	0.60
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.82	0.60
2:B:201:HIS:CE1	23:B:604:CLA:HMB2	2.37	0.60
4:d:315:TYR:CZ	4:d:319:LEU:HD11	2.36	0.60
1:a:74:GLY:O	4:d:301:GLN:NE2	2.34	0.60
33:E:102:HEM:HBC2	33:E:102:HEM:HMC2	1.82	0.60
26:a:609:PL9:H221	24:d:401:PHO:HMA2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:40:ILE:HG12	13:o:243:ILE:HD13	1.83	0.60
23:B:606:CLA:HBB2	25:B:620:BCR:H342	1.84	0.60
3:c:339:LYS:NZ	15:u:99:ASN:O	2.35	0.60
1:A:235:TYR:OH	11:L:11:GLU:OE1	2.13	0.60
25:a:608:BCR:H24C	25:a:608:BCR:H371	1.82	0.60
18:x:3:ILE:HG23	18:x:7:LEU:HD23	1.83	0.59
25:B:619:BCR:C17	25:t:101:BCR:H17C	2.32	0.59
1:a:214:MET:HG2	26:a:609:PL9:H102	1.82	0.59
3:c:406:SER:HA	3:c:420:VAL:HG23	1.84	0.59
1:a:323:ARG:HB3	4:d:329:MET:HA	1.83	0.59
1:A:84:PRO:HA	1:A:112:TYR:CG	2.37	0.59
5:E:56:TYR:O	16:V:1:ALA:N	2.21	0.59
25:b:621:BCR:C37	25:b:621:BCR:H24C	2.32	0.59
31:a:614:LHG:H371	23:c:509:CLA:H92	1.83	0.59
25:f:101:BCR:H383	28:j:101:LMG:H172	1.85	0.59
33:e:102:HEM:HMB1	33:e:102:HEM:HBB2	1.85	0.59
31:b:624:LHG:O4	4:d:141:TYR:OH	2.15	0.59
25:B:618:BCR:H402	27:B:623:SQD:H82	1.83	0.59
25:H:101:BCR:C36	25:H:101:BCR:C19	2.63	0.59
23:C:505:CLA:H141	8:I:16:VAL:HG13	1.84	0.58
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.86	0.58
3:c:347:GLY:HA3	13:o:17:ASN:HB2	1.86	0.58
2:B:33:TRP:N	25:B:619:BCR:H15C	2.18	0.58
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.85	0.58
27:b:601:SQD:H272	25:b:622:BCR:H19C	1.86	0.58
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.34	0.58
3:C:38:GLY:HA3	23:C:511:CLA:HMD2	1.85	0.58
23:C:501:CLA:C3D	23:C:503:CLA:H2	2.34	0.58
23:C:505:CLA:HBB1	23:C:505:CLA:HMB3	1.85	0.58
4:d:186:GLN:HB2	23:d:402:CLA:HBC1	1.85	0.58
2:B:450:TRP:CD1	23:B:608:CLA:HBA1	2.39	0.58
1:a:215:HIS:ND1	26:a:609:PL9:O1	2.34	0.58
23:b:607:CLA:HMB1	23:b:607:CLA:HBB1	1.86	0.58
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	1.83	0.58
23:C:501:CLA:H192	23:C:506:CLA:C1B	2.34	0.58
25:T:101:BCR:C17	25:T:101:BCR:H20C	2.34	0.58
3:c:429:SER:HB3	32:c:518:DGD:HBT2	1.86	0.58
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.86	0.58
2:b:12:LEU:HB2	23:b:615:CLA:HMC2	1.86	0.58
25:t:101:BCR:C20	25:t:101:BCR:C18	2.62	0.58
25:B:618:BCR:C19	25:B:618:BCR:C36	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:57:LYS:O	13:O:58:ASN:HB2	2.03	0.57
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.19	0.57
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.39	0.57
23:a:604:CLA:HBD	23:a:613:CLA:HAC2	1.86	0.57
23:c:502:CLA:C2D	23:c:504:CLA:H2	2.34	0.57
23:a:605:CLA:H152	26:a:609:PL9:H262	1.84	0.57
31:b:624:LHG:HC82	31:b:624:LHG:H371	1.86	0.57
25:B:618:BCR:H353	25:t:101:BCR:H372	1.86	0.57
2:b:461:LEU:HD22	31:b:624:LHG:H301	1.85	0.57
4:d:123:ILE:HD11	32:h:102:DGD:HAE1	1.87	0.57
6:f:25:THR:O	6:f:29:PRO:HG2	2.04	0.57
3:C:213[B]:LEU:HD11	25:C:515:BCR:C21	2.34	0.57
23:a:605:CLA:H122	26:a:609:PL9:H23	1.86	0.57
2:b:28:ALA:HB1	27:b:602:SQD:H221	1.86	0.57
6:F:34:LEU:HD21	25:F:101:BCR:H373	1.87	0.57
2:b:341:LYS:HA	2:b:405[A]:GLU:HG2	1.87	0.57
23:D:404:CLA:H2	18:X:14:LEU:HA	1.85	0.57
23:c:502:CLA:C1D	23:c:504:CLA:H2	2.34	0.57
3:C:170:ILE:HD13	23:C:512:CLA:H111	1.87	0.57
3:c:72:LEU:HD11	3:c:108:THR:HB	1.87	0.56
3:C:165:LEU:HD21	23:C:506:CLA:CAB	2.32	0.56
31:a:614:LHG:H223	32:c:519:DGD:HBH2	1.86	0.56
2:b:475:PHE:CD2	4:d:140:PRO:HG3	2.40	0.56
25:k:101:BCR:H17C	17:y:33:PRO:HD3	1.88	0.56
2:B:32:GLY:HA3	25:B:619:BCR:H19C	1.85	0.56
5:e:23:HIS:NE2	33:e:102:HEM:ND	2.53	0.56
2:B:12:LEU:HB2	23:B:613:CLA:HMC2	1.88	0.56
7:H:65:LEU:HD12	7:H:66:GLY:H	1.70	0.56
25:A:609:BCR:C36	25:A:609:BCR:C17	2.73	0.56
3:c:262:ARG:HG2	8:i:38:GLU:HG2	1.88	0.56
23:C:501:CLA:C4D	23:C:503:CLA:H2	2.35	0.56
3:c:213[B]:LEU:HD11	25:c:516:BCR:C22	2.36	0.56
31:l:101:LHG:H272	12:m:22:LEU:HD21	1.87	0.56
23:A:608:CLA:C1B	8:I:12:VAL:HG22	2.35	0.56
2:B:383:PHE:O	13:O:166:SER:HA	2.05	0.56
25:B:619:BCR:H381	25:t:101:BCR:H341	1.87	0.56
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.87	0.56
25:b:622:BCR:C19	25:b:622:BCR:C36	2.63	0.56
2:B:29:LEU:CD2	25:B:618:BCR:H17C	2.35	0.56
2:b:115:TRP:HB2	25:b:620:BCR:H292	1.88	0.56
3:c:124:VAL:HG11	25:c:515:BCR:C17	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:522:BCR:C15	25:k:101:BCR:H342	2.34	0.56
23:A:605:CLA:HBB1	23:A:605:CLA:HMB3	1.88	0.55
23:C:507:CLA:H91	25:C:515:BCR:C17	2.36	0.55
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.88	0.55
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.39	0.55
1:a:64:ARG:NH1	13:o:105:PRO:O	2.37	0.55
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.88	0.55
25:b:620:BCR:C37	25:b:620:BCR:C23	2.78	0.55
5:e:35:TRP:HA	6:f:39:ALA:HB2	1.87	0.55
2:B:461:LEU:HD22	31:B:622:LHG:H301	1.89	0.55
23:B:614:CLA:H193	25:B:619:BCR:C5	2.37	0.55
33:E:102:HEM:HBB2	33:E:102:HEM:HMB2	1.87	0.55
3:C:347:GLY:HA3	13:O:17:ASN:HB2	1.87	0.55
26:A:610:PL9:H403	6:F:22:ALA:HB2	1.89	0.55
18:X:27:VAL:HG21	27:X:101:SQD:H321	1.88	0.55
2:b:101:ILE:HG23	25:b:621:BCR:C21	2.37	0.55
23:b:613:CLA:H152	23:b:613:CLA:OBD	2.05	0.55
1:A:330:VAL:HG21	4:D:328:TRP:CE2	2.41	0.55
23:A:605:CLA:HBD	23:D:402:CLA:HAC2	1.88	0.55
25:k:101:BCR:C17	17:y:33:PRO:HD3	2.37	0.55
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.40	0.55
25:k:101:BCR:HC21	19:z:13:VAL:HG13	1.89	0.55
25:C:521:BCR:H391	10:K:36:ALA:HB2	1.87	0.55
23:c:509:CLA:HBC3	23:c:511:CLA:H71	1.89	0.55
23:b:606:CLA:C4D	23:b:608:CLA:H43	2.37	0.54
4:d:201:VAL:HG13	23:d:402:CLA:HBB1	1.89	0.54
11:l:26:VAL:HG21	31:l:101:LHG:H192	1.88	0.54
26:A:610:PL9:H221	24:D:401:PHO:HMA2	1.88	0.54
31:e:101:LHG:H152	6:f:22:ALA:HB1	1.89	0.54
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.89	0.54
2:b:57:ARG:HH22	2:b:334:ASP:CG	2.15	0.54
3:c:178:LYS:HB2	23:c:503:CLA:H141	1.88	0.54
31:l:101:LHG:H271	12:m:22:LEU:HD11	1.88	0.54
14:t:8:PHE:CD1	25:t:101:BCR:H373	2.43	0.54
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.89	0.54
3:C:406:SER:HA	3:C:420:VAL:HG23	1.88	0.54
2:b:384:ARG:HD3	15:u:102:LEU:HG	1.90	0.54
3:c:170:ILE:HD13	23:c:513:CLA:H111	1.89	0.54
2:B:29:LEU:HD21	25:B:618:BCR:H17C	1.90	0.54
2:B:61:PHE:CZ	23:B:608:CLA:HBB1	2.42	0.54
23:B:611:CLA:H152	23:B:611:CLA:OBD	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:f:101:BCR:C37	25:f:101:BCR:C23	2.76	0.54
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.37	0.54
25:K:101:BCR:C37	25:K:101:BCR:C23	2.79	0.54
3:c:397:THR:HG21	16:v:40:CYS:SG	2.48	0.54
25:B:618:BCR:H341	25:t:101:BCR:H24C	1.89	0.54
3:C:223:TRP:CG	3:C:224:ILE:H	2.26	0.54
1:a:129:ARG:NH2	4:d:255:GLN:O	2.41	0.54
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.43	0.54
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.90	0.54
13:o:57:LYS:O	13:o:58:ASN:HB2	2.08	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.42	0.54
1:a:308:ASP:HB2	5:e:52:PRO:O	2.08	0.54
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.89	0.54
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.89	0.54
6:f:34:LEU:HG	25:f:101:BCR:H19C	1.89	0.54
25:t:101:BCR:C20	25:t:101:BCR:C37	2.86	0.54
3:C:339:LYS:NZ	15:U:99:ASN:O	2.27	0.54
14:T:8:PHE:CE1	23:b:617:CLA:H171	2.43	0.54
2:B:325:PHE:CG	11:L:34:TYR:HB3	2.43	0.53
4:D:123:ILE:HD11	32:H:102:DGD:HAE1	1.90	0.53
3:C:178:LYS:HB2	23:C:502:CLA:H141	1.90	0.53
2:b:422:ARG:HH21	13:o:169:ASP:CG	2.16	0.53
2:B:28:ALA:HB1	27:B:623:SQD:H221	1.90	0.53
25:C:515:BCR:C37	25:C:515:BCR:C23	2.81	0.53
5:E:20:TRP:HZ2	9:J:13:VAL:HG13	1.72	0.53
1:a:245:THR:OG1	4:d:265:ARG:NE	2.35	0.53
3:c:464:GLU:OE2	4:d:245:SER:OG	2.16	0.53
25:C:521:BCR:C15	25:K:101:BCR:H342	2.35	0.53
1:a:136:ARG:HH12	8:i:27:ASP:CG	2.16	0.53
2:b:29:LEU:HD21	25:b:620:BCR:H17C	1.89	0.53
23:b:604:CLA:H152	25:h:101:BCR:H17C	1.91	0.53
4:d:24:ARG:NH2	18:x:35:ASP:OD2	2.42	0.53
2:B:422:ARG:HH21	13:O:169:ASP:CG	2.17	0.53
23:B:605:CLA:H12	23:B:606:CLA:ND	2.24	0.53
4:D:303:ILE:HG21	12:M:2:GLU:HG3	1.90	0.53
25:f:101:BCR:C37	25:f:101:BCR:C24	2.87	0.53
1:A:308:ASP:HB2	5:E:52:PRO:O	2.07	0.53
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.44	0.53
25:C:515:BCR:C37	25:C:515:BCR:H20C	2.39	0.53
1:a:191:ASN:HB2	3:c:411:ALA:HB1	1.91	0.53
25:a:608:BCR:C36	25:a:608:BCR:C17	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:393:GLU:HB3	15:u:18:GLY:N	2.22	0.53
23:B:602:CLA:HAC1	25:H:101:BCR:H23C	1.91	0.53
23:C:513:CLA:HBB1	23:C:513:CLA:HMB3	1.90	0.53
25:K:101:BCR:H16C	17:Y:33:PRO:HD3	1.91	0.53
23:b:604:CLA:H202	25:h:101:BCR:H12C	1.90	0.53
23:b:604:CLA:CMC	25:h:101:BCR:H19C	2.39	0.53
25:t:101:BCR:C36	25:t:101:BCR:C17	2.75	0.53
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.90	0.53
10:K:31:LEU:HB3	25:K:101:BCR:C15	2.38	0.53
1:a:249:VAL:HG12	2:b:491:VAL:HG21	1.91	0.53
1:a:330:VAL:HG21	4:d:328:TRP:CE2	2.44	0.53
23:b:617:CLA:H18	28:b:623:LMG:H421	1.90	0.53
25:b:621:BCR:HC31	28:b:623:LMG:H131	1.91	0.53
1:A:74:GLY:O	4:D:301:GLN:NE2	2.41	0.52
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.44	0.52
3:c:223:TRP:CG	3:c:224:ILE:H	2.26	0.52
2:B:365:SER:OG	4:D:326:ARG:NH2	2.38	0.52
3:C:324:LEU:HB3	15:U:32:ILE:HD13	1.89	0.52
9:J:9:PRO:HD2	9:J:12:ILE:HD12	1.91	0.52
2:b:24:LEU:HD21	23:b:619:CLA:CAB	2.39	0.52
25:k:101:BCR:HC8	25:k:101:BCR:H311	1.90	0.52
2:B:106:LEU:HB3	25:B:620:BCR:C15	2.38	0.52
23:D:404:CLA:C2	18:X:14:LEU:HA	2.39	0.52
1:a:221[B]:SER:HA	4:d:139:ARG:HB2	1.91	0.52
1:A:133:LEU:HD23	4:D:256:ILE:HG12	1.91	0.52
25:C:521:BCR:C36	25:C:521:BCR:C16	2.88	0.52
1:a:39:PRO:HA	25:a:608:BCR:H12C	1.90	0.52
2:b:433:ASP:OD1	2:b:436:THR:OG1	2.21	0.52
1:A:121[A]:LEU:HG	28:A:612:LMG:H182	1.90	0.52
23:A:606:CLA:HMB1	23:A:606:CLA:HBB1	1.92	0.52
23:C:510:CLA:HBC3	23:C:510:CLA:H192	1.92	0.52
25:c:522:BCR:C22	25:c:522:BCR:H20C	2.27	0.52
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.45	0.52
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.39	0.52
25:C:521:BCR:C20	25:C:521:BCR:C37	2.87	0.52
4:D:49:LEU:HD13	25:F:101:BCR:H16C	1.92	0.52
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.92	0.52
25:b:622:BCR:H24C	25:b:622:BCR:H371	1.92	0.52
25:c:522:BCR:C36	25:c:522:BCR:C16	2.88	0.52
2:B:472:ARG:HA	2:B:479:PHE:CE1	2.44	0.52
3:C:213[B]:LEU:HD21	25:C:515:BCR:C20	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:393:ALA:HB1	16:V:48:THR:HG21	1.92	0.52
2:b:385:ARG:HG2	13:o:165:ALA:O	2.10	0.52
3:c:296:VAL:HG11	23:c:502:CLA:HMA2	1.91	0.52
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.92	0.52
23:A:608:CLA:HAC2	25:A:609:BCR:H362	1.90	0.52
4:D:129:GLN:NE2	24:D:401:PHO:OBD	2.43	0.52
23:B:604:CLA:C4D	23:B:606:CLA:H43	2.39	0.51
23:B:613:CLA:H91	23:B:614:CLA:HBB1	1.92	0.51
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.91	0.51
5:e:8:ARG:HB3	5:e:13:ILE:HD11	1.92	0.51
3:C:206:PRO:HG3	3:C:239:TRP:HZ2	1.74	0.51
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.45	0.51
23:d:403:CLA:C2	18:x:14:LEU:HA	2.40	0.51
13:o:58:ASN:HA	13:o:60:ARG:NH2	2.25	0.51
25:b:621:BCR:C37	25:b:621:BCR:C23	2.81	0.51
23:c:507:CLA:H121	25:c:516:BCR:H12C	1.92	0.51
1:A:64:ARG:NH1	13:O:105:PRO:O	2.41	0.51
1:a:247:ASN:HB3	2:b:482:ILE:HD11	1.91	0.51
25:b:621:BCR:H24C	25:b:621:BCR:H371	1.92	0.51
6:f:20:TRP:CE2	6:f:24:HIS:CE1	2.98	0.51
2:b:127:ARG:HH11	2:b:127:ARG:HG3	1.76	0.51
2:b:382:PRO:HG2	2:b:385:ARG:HD2	1.92	0.51
27:b:602:SQD:H121	23:b:617:CLA:C4	2.29	0.51
25:b:620:BCR:H12C	25:b:621:BCR:H10C	1.91	0.51
4:d:56:THR:HB	5:e:49:THR:HG23	1.92	0.51
10:k:17:ILE:HD13	10:k:17:ILE:H	1.75	0.51
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.45	0.51
27:b:602:SQD:H462	27:b:602:SQD:C1	2.41	0.51
25:b:620:BCR:H383	25:b:620:BCR:H23C	1.93	0.51
1:A:217:SER:HB2	4:D:142:ASN:HA	1.93	0.51
1:A:232:SER:HB2	2:B:4:PRO:HG3	1.92	0.51
3:c:213[B]:LEU:HD11	25:c:516:BCR:C21	2.41	0.51
25:c:522:BCR:HC42	10:k:15:TYR:CE1	2.46	0.51
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.46	0.51
4:D:53:THR:HA	4:D:67:TYR:CD2	2.46	0.51
4:D:186:GLN:HB2	23:D:403:CLA:HBC1	1.93	0.51
5:e:53:ASP:HB2	16:v:2:GLU:HG2	1.91	0.51
10:k:21:LEU:HD21	25:k:101:BCR:HC31	1.93	0.51
23:B:604:CLA:C1C	23:B:606:CLA:H71	2.40	0.51
23:b:616:CLA:H193	25:b:621:BCR:C5	2.41	0.51
23:d:403:CLA:H2	18:x:14:LEU:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:102:HEM:HMC1	6:f:31:ILE:HG13	1.93	0.51
2:B:18:ARG:NH2	27:B:623:SQD:O9	2.41	0.50
25:B:618:BCR:C37	25:B:618:BCR:C23	2.82	0.50
25:F:101:BCR:C20	25:F:101:BCR:C37	2.89	0.50
6:f:29:PRO:HB3	25:f:101:BCR:C12	2.40	0.50
1:A:323:ARG:HB3	4:D:329:MET:HA	1.92	0.50
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.46	0.50
23:B:617:CLA:H11	25:B:620:BCR:H362	1.93	0.50
23:a:607:CLA:C1B	8:i:12:VAL:HG22	2.41	0.50
2:b:442:ILE:HG12	13:o:173:ALA:O	2.11	0.50
3:c:286:ALA:HB2	23:c:503:CLA:HMD2	1.93	0.50
19:z:15:LEU:HD22	19:z:46:LEU:HD23	1.93	0.50
32:c:519:DGD:HA42	4:d:74:LEU:HG	1.93	0.50
1:A:215:HIS:ND1	26:A:610:PL9:O1	2.39	0.50
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.47	0.50
2:B:63:LEU:HA	2:B:66:MET:HE3	1.94	0.50
2:B:393:GLU:HB3	15:U:18:GLY:CA	2.41	0.50
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.94	0.50
2:b:224:ARG:NH1	4:d:16:ASP:OD2	2.41	0.50
25:b:620:BCR:HC32	28:b:623:LMG:H311	1.94	0.50
23:B:617:CLA:H3A	25:B:620:BCR:C17	2.39	0.50
24:A:607:PHO:HMB3	24:A:607:PHO:HBB1	1.94	0.50
25:H:101:BCR:C36	25:H:101:BCR:C17	2.77	0.50
1:a:68:SER:N	4:d:312:GLU:O	2.40	0.50
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.47	0.50
23:B:605:CLA:H2	23:B:606:CLA:C4C	2.41	0.50
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.94	0.50
3:C:213[B]:LEU:HD11	25:C:515:BCR:C22	2.41	0.50
2:b:325:PHE:CG	11:l:34:TYR:HB3	2.47	0.50
3:c:168:LEU:HD21	23:c:510:CLA:H61	1.94	0.50
2:B:113:TRP:HB2	25:B:620:BCR:C21	2.42	0.49
14:T:19:PHE:CD2	27:b:602:SQD:H302	2.46	0.49
3:c:158:THR:O	3:c:251:HIS:HB3	2.12	0.49
2:B:181:VAL:HG11	2:B:195:PRO:HB2	1.94	0.49
27:B:623:SQD:H462	27:B:623:SQD:C1	2.41	0.49
2:b:18:ARG:NH1	27:b:602:SQD:O8	2.39	0.49
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.94	0.49
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.95	0.49
23:b:606:CLA:C1C	23:b:608:CLA:H71	2.42	0.49
23:c:508:CLA:H142	25:c:516:BCR:H362	1.95	0.49
23:B:617:CLA:C3A	25:B:620:BCR:H17C	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:172:MET:HE1	23:a:613:CLA:CHC	2.43	0.49
4:d:161:PRO:HB3	4:d:170:ALA:HB2	1.95	0.49
1:A:132:GLU:O	1:A:136:ARG:HG2	2.12	0.49
25:T:101:BCR:C17	25:T:101:BCR:C36	2.76	0.49
1:A:191:ASN:HB2	3:C:411:ALA:HB1	1.94	0.49
3:C:55:ALA:HB1	25:C:521:BCR:H373	1.93	0.49
25:b:621:BCR:C37	25:b:621:BCR:C24	2.90	0.49
3:c:25:ASN:O	3:c:31:SER:HB3	2.13	0.49
20:A:601:OEX:O2	3:C:357:ARG:NH2	2.46	0.49
31:B:622:LHG:HC11	4:D:269:PHE:CD2	2.48	0.49
13:o:49[A]:THR:OG1	13:o:236:GLN:HB2	2.12	0.49
13:O:127:ALA:HA	13:O:144:GLY:HA3	1.95	0.49
4:d:193:LEU:O	11:l:34:TYR:OH	2.22	0.49
13:O:58:ASN:HA	13:O:60:ARG:NH2	2.28	0.49
23:b:607:CLA:H12	23:b:608:CLA:ND	2.28	0.49
3:C:158:THR:O	3:C:251:HIS:HB3	2.13	0.48
26:D:405:PL9:H453	26:D:405:PL9:H421	1.68	0.48
25:B:619:BCR:C37	25:B:619:BCR:C23	2.81	0.48
18:X:24:THR:HA	27:X:101:SQD:H331	1.95	0.48
1:a:202:VAL:HG11	23:a:605:CLA:C3D	2.43	0.48
2:b:63:LEU:HA	2:b:66:MET:HE3	1.94	0.48
2:b:394:GLN:HG2	15:u:22:GLY:HA3	1.95	0.48
25:b:620:BCR:C36	25:b:620:BCR:C17	2.77	0.48
25:b:620:BCR:H12C	25:b:621:BCR:C10	2.43	0.48
3:C:203:THR:O	3:C:235:GLY:HA3	2.13	0.48
25:C:521:BCR:H15C	25:K:101:BCR:C34	2.39	0.48
4:D:209:LEU:HD22	26:D:405:PL9:H161	1.94	0.48
8:I:1[C]:MET:HE3	8:I:4:LEU:HB2	1.95	0.48
2:b:58:GLN:C	2:b:329:PRO:HB3	2.39	0.48
25:c:515:BCR:HC31	10:k:15:TYR:OH	2.11	0.48
1:a:37:MET:HG3	1:a:122:GLY:O	2.13	0.48
4:d:129:GLN:NE2	24:d:401:PHO:OBD	2.46	0.48
25:h:101:BCR:C36	25:h:101:BCR:C17	2.75	0.48
2:b:422:ARG:O	2:b:425:ILE:HG12	2.14	0.48
3:c:223:TRP:CE3	3:c:224:ILE:HG12	2.48	0.48
9:j:9:PRO:HD2	9:j:12:ILE:HD12	1.95	0.48
2:B:440:ASP:OD1	4:D:299:ILE:HD13	2.14	0.48
23:B:606:CLA:H162	23:B:610:CLA:HBB2	1.96	0.48
25:B:618:BCR:C36	25:B:618:BCR:C17	2.75	0.48
1:a:58:VAL:HB	1:a:83:VAL:HB	1.95	0.48
2:b:204:ALA:CB	23:b:605:CLA:HAB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:506:CLA:H141	8:i:16:VAL:HG13	1.95	0.48
23:C:506:CLA:CBB	23:C:507:CLA:HMA3	2.43	0.48
2:b:29:LEU:CD2	25:b:620:BCR:H17C	2.44	0.48
8:i:1[C]:MET:HE3	8:i:4:LEU:HB2	1.94	0.48
1:A:334:ARG:HG3	13:O:157:LEU:HB2	1.96	0.48
2:B:149:LEU:HD22	23:B:605:CLA:H152	1.96	0.48
25:B:618:BCR:C20	25:B:618:BCR:H372	2.43	0.48
1:a:132:GLU:O	1:a:136:ARG:HG2	2.14	0.48
1:a:133:LEU:HD23	4:d:256:ILE:HG12	1.94	0.48
1:a:296:ASN:HB2	3:c:400:PRO:O	2.14	0.48
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.75	0.48
2:B:33:TRP:CD1	25:t:101:BCR:H381	2.49	0.48
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.48	0.48
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.48	0.48
23:b:609[B]:CLA:H61	23:b:609[B]:CLA:H102	1.62	0.48
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.96	0.48
1:A:306:VAL:HG12	1:A:314:ILE:HB	1.95	0.48
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.48	0.48
1:a:232:SER:HB2	2:b:4:PRO:HG3	1.96	0.48
23:a:604:CLA:HMB1	23:a:604:CLA:HBB1	1.95	0.48
2:b:450:TRP:CD1	23:b:610:CLA:HBA1	2.48	0.48
5:e:9:PRO:HA	31:e:101:LHG:O3	2.13	0.48
14:t:22:PHE:CE2	25:t:101:BCR:H333	2.49	0.48
2:B:101:ILE:HG23	25:B:619:BCR:C21	2.44	0.47
23:B:616:CLA:H51	25:B:620:BCR:H11C	1.96	0.47
25:B:618:BCR:H15C	25:B:619:BCR:C35	2.43	0.47
1:A:215:HIS:HA	26:A:610:PL9:O1	2.14	0.47
2:B:29:LEU:HD21	27:B:623:SQD:H191	1.97	0.47
1:a:215:HIS:HA	26:a:609:PL9:O1	2.13	0.47
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.47	0.47
1:A:217:SER:HA	4:D:272:LEU:HD12	1.96	0.47
23:B:613:CLA:CMB	23:B:615:CLA:HBB1	2.44	0.47
32:C:517:DGD:HB22	28:C:519:LMG:H302	1.96	0.47
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.78	0.47
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.97	0.47
2:b:193:TYR:OH	32:h:102:DGD:HE1	2.15	0.47
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.97	0.47
1:A:131:TRP:CH2	23:C:505:CLA:HAA2	2.49	0.47
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.97	0.47
5:E:34:GLY:HA3	6:F:32:PHE:O	2.14	0.47
2:b:103:LEU:HD21	23:b:608:CLA:HMC3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.97	0.47
1:A:340:PRO:HD3	15:U:103:TYR:CZ	2.50	0.47
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.97	0.47
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.50	0.47
2:B:126:PRO:HB3	7:H:12[B]:ARG:NH1	2.30	0.47
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.50	0.47
3:C:29:GLU:CD	3:C:29:GLU:H	2.23	0.47
3:C:323:LYS:O	15:U:47:LYS:HD2	2.15	0.47
4:D:283:ALA:O	4:D:287:VAL:HG23	2.14	0.47
23:D:402:CLA:H41	26:D:405:PL9:H202	1.96	0.47
31:a:614:LHG:H382	31:a:614:LHG:C11	2.44	0.47
2:b:112:CYS:HA	25:b:620:BCR:H281	1.97	0.47
25:b:620:BCR:H333	12:m:13:LEU:HD12	1.97	0.47
3:c:203:THR:O	3:c:235:GLY:HA3	2.15	0.47
3:c:324:LEU:HB3	15:u:32:ILE:HD13	1.97	0.47
32:d:405:DGD:HA42	32:d:405:DGD:HB22	1.96	0.47
1:A:32:TRP:CD2	8:I:22:GLY:HA3	2.50	0.47
1:A:49:VAL:HG13	26:D:405:PL9:H503	1.97	0.47
2:B:422:ARG:O	2:B:425:ILE:HG12	2.14	0.47
3:C:233:VAL:O	3:C:237:HIS:ND1	2.41	0.47
3:C:286:ALA:HB2	23:C:502:CLA:HMD2	1.97	0.47
3:C:416[A]:SER:HB2	16:V:42:VAL:HG23	1.96	0.47
2:b:471:ALA:HB1	4:d:140:PRO:HG2	1.96	0.47
4:d:84:SER:O	5:e:69:ARG:HB2	2.14	0.47
2:B:139:PHE:HE2	2:B:216:HIS:CE1	2.33	0.47
23:B:616:CLA:H2	23:B:617:CLA:HBB2	1.96	0.47
18:X:31:ILE:HG23	27:X:101:SQD:H462	1.97	0.47
1:a:331:MET:SD	4:d:347:PRO:HB2	2.55	0.47
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.96	0.47
13:o:193:THR:HG21	13:o:220:LEU:HD12	1.96	0.47
17:y:27:MET:O	17:y:30:ILE:HG22	2.15	0.47
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.97	0.47
23:B:602:CLA:HHC	23:B:602:CLA:HBB1	1.97	0.47
25:B:619:BCR:HC31	28:B:621:LMG:H131	1.96	0.47
2:B:464:PHE:HD2	23:B:612:CLA:HAC2	1.80	0.46
3:C:344:SER:O	13:O:75:THR:HG22	2.15	0.46
25:b:620:BCR:C20	25:b:620:BCR:C37	2.93	0.46
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.96	0.46
19:z:5:PHE:HB2	19:z:57:LEU:HB3	1.97	0.46
1:A:340:PRO:HB3	15:U:103:TYR:CG	2.49	0.46
26:A:610:PL9:H252	26:A:610:PL9:H272	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.97	0.46
23:C:509:CLA:H141	23:C:512:CLA:HMD3	1.97	0.46
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.96	0.46
26:A:610:PL9:H203	26:A:610:PL9:H172	1.74	0.46
3:c:25:ASN:ND2	3:c:45:LEU:HD11	2.28	0.46
23:b:604:CLA:HMC1	25:h:101:BCR:H19C	1.97	0.46
6:f:37:ILE:O	6:f:40:MET:HB2	2.14	0.46
13:o:154:ALA:HB1	13:o:165:ALA:HB2	1.98	0.46
23:B:607[B]:CLA:H61	23:B:607[B]:CLA:H102	1.62	0.46
3:C:168:LEU:HD21	23:C:509:CLA:H61	1.98	0.46
3:C:418:ASN:HB2	32:C:518:DGD:O4E	2.15	0.46
3:C:397:THR:HG21	16:V:40:CYS:SG	2.55	0.46
13:O:137:THR:C	13:O:139:SER:H	2.24	0.46
4:d:149:PRO:HA	23:d:402:CLA:H41	1.97	0.46
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.31	0.46
25:B:620:BCR:H383	27:a:612:SQD:H241	1.98	0.46
4:D:113:PHE:CE1	25:F:101:BCR:H332	2.51	0.46
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.04	0.46
25:T:101:BCR:C17	25:T:101:BCR:C20	2.92	0.46
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.51	0.46
28:c:520:LMG:H171	10:k:27:VAL:HG11	1.97	0.46
1:A:105:TRP:HZ3	25:A:609:BCR:H24C	1.80	0.46
1:A:141:PRO:HG3	3:C:446:GLY:C	2.41	0.46
1:A:288:LEU:HD22	3:C:432:VAL:HA	1.98	0.46
2:B:150:CYS:HB2	23:B:604:CLA:CMC	2.46	0.46
2:b:57:ARG:NH2	2:b:334:ASP:OD2	2.39	0.46
4:d:342:PRO:O	4:d:345:VAL:HG22	2.16	0.46
2:B:454:ALA:HB2	28:B:621:LMG:H172	1.98	0.46
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.98	0.46
3:c:429:SER:HA	32:c:518:DGD:HBE1	1.97	0.46
23:c:506:CLA:H3A	23:c:506:CLA:HBA2	1.65	0.46
25:B:619:BCR:C37	25:B:619:BCR:H24C	2.46	0.45
3:C:344:SER:OG	3:C:348:GLU:OE2	2.32	0.45
23:C:508:CLA:HMB3	23:C:508:CLA:HBB1	1.99	0.45
4:D:154:VAL:HG21	32:H:102:DGD:HAN1	1.97	0.45
23:c:502:CLA:H193	23:c:508:CLA:HBB1	1.98	0.45
6:f:28:VAL:N	6:f:29:PRO:CD	2.79	0.45
2:B:450:TRP:NE1	23:B:608:CLA:HBA1	2.31	0.45
23:C:506:CLA:H162	25:C:515:BCR:H15C	1.99	0.45
32:C:518:DGD:HBH2	31:D:408:LHG:H223	1.97	0.45
5:E:82:GLN:C	5:E:84:LYS:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:202:HEM:HBB2	33:V:202:HEM:HMB2	1.98	0.45
1:a:131:TRP:CH2	23:c:506:CLA:HAA2	2.51	0.45
3:c:24:THR:O	3:c:25:ASN:OD1	2.35	0.45
1:A:202:VAL:HG11	23:A:606:CLA:C3D	2.47	0.45
25:B:619:BCR:C36	25:B:619:BCR:C17	2.77	0.45
1:a:161:TYR:HB3	1:a:162:PRO:HD3	1.97	0.45
2:b:419:SER:HA	2:b:422:ARG:NH1	2.31	0.45
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.99	0.45
2:B:460:LEU:O	2:B:463:PHE:HB3	2.16	0.45
3:C:171:GLY:O	3:C:174:LEU:HB2	2.16	0.45
5:E:17:VAL:HG23	9:J:7:ARG:HB2	1.97	0.45
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.17	0.45
16:V:76:MET:HG2	33:V:202:HEM:HMB3	1.98	0.45
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.51	0.45
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.99	0.45
4:d:53:THR:HG22	6:f:40:MET:HE1	1.97	0.45
6:f:37:ILE:HG22	6:f:41:GLN:HE21	1.81	0.45
10:k:20:PRO:HB3	17:y:21:GLN:HG3	1.99	0.45
18:x:27:VAL:HG21	27:x:101:SQD:H321	1.98	0.45
2:B:155:ALA:O	2:B:159:THR:OG1	2.29	0.45
4:D:53:THR:HA	4:D:67:TYR:HD2	1.81	0.45
2:b:226:TYR:OH	7:h:19:GLY:HA2	2.17	0.45
13:o:58:ASN:HA	13:o:60:ARG:HH21	1.81	0.45
3:C:41:ARG:NH2	10:K:46:ARG:O	2.42	0.45
3:C:223:TRP:HE3	32:C:516:DGD:HB21	1.82	0.45
32:C:518:DGD:HE4	9:J:40:LEU:HD21	1.99	0.45
23:c:509:CLA:H52	23:c:511:CLA:HED3	1.98	0.45
25:c:515:BCR:C37	25:c:515:BCR:C23	2.81	0.45
25:t:101:BCR:C37	25:t:101:BCR:C23	2.82	0.45
25:B:618:BCR:H342	25:t:101:BCR:H402	1.99	0.45
3:C:343:ARG:NH1	3:C:347:GLY:O	2.50	0.45
5:E:30:LEU:HD12	33:E:102:HEM:HMC1	1.99	0.45
3:c:206:PRO:HG3	3:c:239:TRP:HZ2	1.82	0.45
28:z:101:LMG:O2	28:z:101:LMG:HC71	2.17	0.45
23:B:607[B]:CLA:H192	23:B:607[B]:CLA:H161	1.68	0.45
14:T:15:ALA:HB2	25:T:101:BCR:H14C	1.99	0.45
26:a:609:PL9:C22	24:d:401:PHO:HMA2	2.46	0.45
1:A:249:VAL:HG12	2:B:491:VAL:HG21	1.99	0.44
26:A:610:PL9:H152	26:A:610:PL9:H122	1.79	0.44
3:C:334:PRO:HA	13:O:153:THR:OG1	2.17	0.44
31:D:408:LHG:H382	31:D:408:LHG:C11	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:267:ASN:HB3	1:a:270[B]:SER:OG	2.17	0.44
23:b:604:CLA:H202	25:h:101:BCR:C12	2.47	0.44
2:B:24:LEU:HD21	23:B:617:CLA:CAB	2.46	0.44
2:B:193:TYR:OH	32:H:102:DGD:HE1	2.17	0.44
2:B:386:ALA:HB1	15:U:100:ASN:ND2	2.33	0.44
4:D:125:PHE:CE2	24:D:401:PHO:HBA1	2.52	0.44
31:D:408:LHG:H372	31:D:408:LHG:H132	1.99	0.44
3:c:182:PHE:CG	23:c:503:CLA:H191	2.53	0.44
3:c:390:ARG:HD3	16:v:100:ILE:HD12	1.98	0.44
23:c:506:CLA:HMD3	23:c:508:CLA:HAB	1.98	0.44
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.17	0.44
25:B:620:BCR:H24C	25:B:620:BCR:H371	1.99	0.44
24:D:401:PHO:HMB3	24:D:401:PHO:HBB1	1.99	0.44
2:b:115:TRP:CE3	25:b:620:BCR:H401	2.52	0.44
23:b:615:CLA:HBB1	23:b:617:CLA:HMB2	2.00	0.44
3:c:443:TRP:CE2	23:c:509:CLA:HMD2	2.52	0.44
25:c:515:BCR:C36	25:c:515:BCR:C17	2.77	0.44
5:e:70:PHE:HZ	7:h:51:SER:HB3	1.83	0.44
13:o:85:LEU:HD22	13:o:243:ILE:HD12	2.00	0.44
26:A:610:PL9:H503	18:X:24:THR:OG1	2.17	0.44
25:B:619:BCR:C37	25:B:619:BCR:C24	2.95	0.44
7:H:65:LEU:CD1	7:H:66:GLY:H	2.31	0.44
16:V:12:LEU:O	16:V:70:GLU:HG2	2.17	0.44
2:b:150:CYS:HB2	23:b:606:CLA:CMC	2.47	0.44
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.99	0.44
1:A:176:ILE:O	1:A:179:THR:HB	2.18	0.44
1:A:316:THR:HG22	4:D:64:ALA:HB3	1.99	0.44
23:A:608:CLA:HAB	8:I:15:PHE:CD1	2.52	0.44
3:C:78:GLU:OE2	16:V:106:ASN:ND2	2.50	0.44
23:C:506:CLA:H162	23:C:506:CLA:H122	1.72	0.44
4:D:342:PRO:O	4:D:345:VAL:HG22	2.17	0.44
7:H:35:MET:CG	25:H:101:BCR:HC42	2.48	0.44
23:B:606:CLA:H62	23:B:606:CLA:H41	1.77	0.44
25:B:618:BCR:H12C	25:B:619:BCR:C10	2.41	0.44
23:C:505:CLA:HMD3	23:C:507:CLA:HAB	2.00	0.44
25:F:101:BCR:H381	28:J:101:LMG:H231	2.00	0.44
3:c:119:LEU:HG	25:c:522:BCR:H10C	1.99	0.44
7:h:38:PHE:HB2	25:h:101:BCR:H10C	1.99	0.44
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.98	0.44
3:C:338:GLY:HA3	3:C:341:LEU:O	2.18	0.44
4:D:201:VAL:HG13	23:D:403:CLA:HBB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:136:ARG:NH1	8:i:27:ASP:OD2	2.46	0.44
23:c:507:CLA:HBB1	23:c:507:CLA:HMB1	2.00	0.44
1:A:214:MET:HG2	26:A:610:PL9:C10	2.47	0.44
1:A:326:LEU:HD11	16:V:137:TYR:HB2	1.98	0.44
2:B:103:LEU:HD21	23:B:606:CLA:HMC3	1.99	0.44
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.53	0.44
3:C:269:GLU:OE2	3:C:447:ARG:HD3	2.17	0.44
26:D:405:PL9:H102	26:D:405:PL9:HC72	1.63	0.44
3:c:179:ALA:O	3:c:184:GLY:HA2	2.18	0.44
23:c:505:CLA:C1D	32:c:518:DGD:HB21	2.47	0.44
25:c:516:BCR:C36	25:c:516:BCR:C17	2.79	0.44
5:e:82:GLN:C	5:e:84:LYS:H	2.26	0.44
23:B:602:CLA:CMC	25:H:101:BCR:H19C	2.47	0.44
2:b:348:ASN:HB3	2:b:354:LEU:HD11	2.00	0.44
23:b:606:CLA:HMB1	23:b:606:CLA:HBB1	2.00	0.44
6:f:33:PHE:HB3	25:f:101:BCR:H363	1.99	0.44
2:B:458:PHE:HB3	23:B:605:CLA:HBC2	2.00	0.43
23:A:608:CLA:H192	23:C:505:CLA:H142	2.00	0.43
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.53	0.43
23:B:607[B]:CLA:H111	23:B:607[B]:CLA:H142	1.76	0.43
3:C:330:SER:O	13:O:123:LYS:NZ	2.42	0.43
23:C:511:CLA:H111	19:Z:24:PRO:HB3	2.00	0.43
9:J:19:MET:HG3	25:K:101:BCR:H372	2.00	0.43
23:b:610:CLA:HMC3	25:b:621:BCR:HC8	2.01	0.43
24:d:401:PHO:H61	23:d:402:CLA:H111	2.00	0.43
23:C:513:CLA:H172	25:C:514:BCR:H19C	2.00	0.43
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.90	0.43
6:F:21:VAL:O	6:F:25:THR:HG23	2.18	0.43
23:b:613:CLA:H162	23:b:618:CLA:CAD	2.48	0.43
31:b:624:LHG:HC11	4:d:269:PHE:CD2	2.53	0.43
3:c:437:PHE:HA	23:c:509:CLA:HMC2	1.99	0.43
31:B:622:LHG:O9	31:L:101:LHG:HC81	2.18	0.43
26:D:405:PL9:H43	26:D:405:PL9:H471	1.80	0.43
2:b:383:PHE:CE1	13:o:167:GLY:HA2	2.53	0.43
4:d:125:PHE:CE1	24:d:401:PHO:HBD	2.52	0.43
6:f:21:VAL:O	6:f:25:THR:HG23	2.18	0.43
1:a:329:GLU:O	1:a:332:HIS:ND1	2.47	0.43
3:c:205:ASP:HA	3:c:206:PRO:HD3	1.90	0.43
5:e:20:TRP:HZ2	9:j:13:VAL:HG13	1.82	0.43
25:f:101:BCR:H381	28:j:101:LMG:H231	1.99	0.43
2:B:33:TRP:HD1	25:t:101:BCR:H381	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:VAL:O	3:C:134:ILE:HG12	2.18	0.43
3:C:206:PRO:HG3	3:C:239:TRP:CZ2	2.52	0.43
31:L:101:LHG:H272	12:M:22:LEU:HD21	2.00	0.43
2:b:460:LEU:O	2:b:463:PHE:HB3	2.19	0.43
23:c:512:CLA:C4A	25:c:522:BCR:H271	2.48	0.43
27:A:611:SQD:H132	31:D:408:LHG:H142	2.00	0.43
23:B:604:CLA:H3A	23:B:604:CLA:CGA	2.49	0.43
3:C:416[B]:SER:HB3	16:V:42:VAL:HG23	2.01	0.43
28:Z:101:LMG:O2	28:Z:101:LMG:HC71	2.19	0.43
2:b:347[B]:ARG:HG2	2:b:353:GLU:HA	2.01	0.43
4:d:214:HIS:ND1	26:d:404:PL9:O2	2.33	0.43
5:e:51:ARG:N	5:e:54[B]:SER:OG	2.51	0.43
25:F:101:BCR:H17C	28:J:101:LMG:H352	2.01	0.43
11:L:14:ARG:HB3	14:T:25[A]:GLU:HG2	2.01	0.43
3:c:327:ASN:HB3	13:o:99:ASP:OD2	2.17	0.43
15:u:76:ARG:HA	15:u:79:LEU:HG	2.00	0.43
28:z:101:LMG:H111	28:z:101:LMG:HC8	1.94	0.43
1:A:136:ARG:NH2	8:I:30:ARG:HB2	2.34	0.43
23:C:505:CLA:CMD	23:C:507:CLA:HAB	2.49	0.43
23:a:607:CLA:H192	23:c:506:CLA:H142	2.00	0.43
2:b:440:ASP:O	13:o:174:LEU:HD22	2.18	0.43
1:A:58:VAL:HB	1:A:83:VAL:HB	2.01	0.43
2:b:139:PHE:HE2	2:b:216:HIS:CE1	2.37	0.43
2:b:201:HIS:HB2	23:b:605:CLA:C4A	2.49	0.43
3:c:175:LEU:HD23	3:c:237:HIS:CD2	2.54	0.43
23:c:502:CLA:H192	23:c:507:CLA:C1B	2.48	0.43
1:A:225:ARG:HA	2:B:480:SER:O	2.19	0.42
2:B:33:TRP:HD1	25:B:619:BCR:H12C	1.84	0.42
3:C:205:ASP:HA	3:C:206:PRO:HD3	1.85	0.42
4:D:125:PHE:CE1	24:D:401:PHO:HBD	2.54	0.42
31:D:408:LHG:H332	31:D:408:LHG:H302	1.96	0.42
26:a:609:PL9:H252	26:a:609:PL9:H272	1.66	0.42
2:b:113:TRP:HB2	25:b:622:BCR:C21	2.48	0.42
2:b:498:LYS:HA	4:d:24:ARG:HA	2.00	0.42
23:b:613:CLA:HHC	23:b:613:CLA:HBB1	2.00	0.42
25:c:522:BCR:H391	10:k:36:ALA:HB2	2.01	0.42
5:e:23:HIS:HA	5:e:26:THR:OG1	2.18	0.42
1:A:28:LEU:HD21	4:D:258:GLY:HA2	2.00	0.42
23:A:608:CLA:HMA2	28:A:612:LMG:H132	2.01	0.42
2:B:33:TRP:CD1	23:B:614:CLA:HBC1	2.54	0.42
2:B:208:VAL:HG21	23:B:603:CLA:HMC1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:LYS:HD3	2:B:406:LEU:HD11	2.02	0.42
27:B:623:SQD:O8	11:L:7:ARG:HD2	2.19	0.42
1:a:328:MET:HE1	4:d:183:LEU:HD22	2.00	0.42
2:b:386:ALA:HB1	15:u:100:ASN:HD22	1.85	0.42
25:b:620:BCR:H15C	25:b:621:BCR:C13	2.50	0.42
23:c:510:CLA:HMB1	23:c:510:CLA:HBB1	2.00	0.42
16:v:41:HIS:HA	16:v:45:ILE:O	2.18	0.42
1:A:183:MET:HB3	23:A:605:CLA:HBC2	2.00	0.42
27:A:611:SQD:O10	31:D:408:LHG:H122	2.19	0.42
10:K:40:GLN:HB3	10:K:45:PHE:CD1	2.54	0.42
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.54	0.42
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.01	0.42
1:A:237:TYR:CE1	1:A:241:GLN:HG2	2.54	0.42
2:B:32:GLY:CA	25:B:619:BCR:H19C	2.50	0.42
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.54	0.42
3:C:335:THR:O	13:O:152:ARG:NH2	2.50	0.42
23:a:613:CLA:HED2	4:d:198:MET:SD	2.59	0.42
2:b:65:PHE:HE1	23:b:607:CLA:HED2	1.83	0.42
2:b:418:LYS:HZ1	15:u:14:ASP:HB3	1.84	0.42
23:b:607:CLA:H2	23:b:608:CLA:C4C	2.49	0.42
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.00	0.42
2:B:256:MET:HA	2:B:263:THR:HG21	2.00	0.42
3:C:303:GLY:O	3:C:423:ARG:NE	2.38	0.42
4:D:17:ILE:HD12	18:X:36:LYS:HE3	2.01	0.42
6:F:30:THR:HA	25:F:101:BCR:C16	2.49	0.42
23:a:607:CLA:H162	23:a:607:CLA:H122	1.76	0.42
26:a:609:PL9:H102	26:a:609:PL9:HC72	1.77	0.42
2:b:149:LEU:HD22	23:b:607:CLA:H152	2.02	0.42
4:d:56:THR:HG21	5:e:50:PRO:HD3	2.02	0.42
5:e:67:THR:OG1	5:e:75:GLN:NE2	2.41	0.42
1:A:97:TRP:CZ2	8:I:9:TYR:HE2	2.37	0.42
2:B:25:MET:HE3	25:B:618:BCR:C25	2.49	0.42
23:B:609:CLA:HBB1	23:B:609:CLA:HMB3	2.01	0.42
1:A:153:SER:HB3	23:A:605:CLA:HED1	2.02	0.42
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.02	0.42
25:A:609:BCR:C37	25:A:609:BCR:C23	2.83	0.42
2:B:383:PHE:CE1	13:O:167:GLY:HA2	2.54	0.42
3:C:453:ALA:O	8:I:33:LYS:HB3	2.19	0.42
5:E:51:ARG:N	5:E:54[B]:SER:OG	2.53	0.42
10:K:34:ALA:HB3	25:K:101:BCR:H19C	2.01	0.42
15:U:76:ARG:HA	15:U:79:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:131:TRP:O	1:a:134:SER:OG	2.30	0.42
1:a:262:TYR:CE2	31:e:101:LHG:HC31	2.55	0.42
3:c:318:LEU:HD21	3:c:380:ILE:CG2	2.49	0.42
4:d:53:THR:HA	4:d:67:TYR:CD2	2.53	0.42
31:d:406:LHG:H141	11:l:22:LEU:HD21	2.01	0.42
1:A:310:LYS:HE3	16:V:7:VAL:HG21	2.02	0.42
2:B:102:VAL:HA	25:B:619:BCR:C40	2.50	0.42
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.54	0.42
2:B:377:VAL:HG11	4:D:342:PRO:HG3	2.02	0.42
3:C:338:GLY:HA2	13:O:103:PHE:HZ	1.85	0.42
23:C:502:CLA:H51	23:C:503:CLA:NC	2.35	0.42
23:C:505:CLA:H3A	23:C:505:CLA:HBA2	1.63	0.42
23:b:609[A]:CLA:H91	23:b:609[A]:CLA:H112	1.88	0.42
23:b:609[B]:CLA:H142	23:b:609[B]:CLA:H111	1.76	0.42
3:c:76:ILE:HA	3:c:77:PRO:HD3	1.88	0.42
10:k:32:PHE:CE2	25:k:101:BCR:H352	2.55	0.42
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.01	0.42
2:B:112:CYS:HA	25:B:618:BCR:H281	2.02	0.42
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.42
23:B:611:CLA:HHC	23:B:611:CLA:HBB1	2.00	0.42
4:D:48:TRP:CD1	24:D:401:PHO:H162	2.54	0.42
7:H:61:SER:HA	32:H:102:DGD:HE2	2.01	0.42
10:K:17:ILE:HD13	10:K:17:ILE:N	2.26	0.42
1:a:217:SER:HB2	4:d:142:ASN:HA	2.02	0.42
2:b:472:ARG:HA	2:b:479:PHE:CE1	2.55	0.42
23:c:508:CLA:OBD	23:c:510:CLA:H122	2.20	0.42
4:d:328:TRP:CZ3	16:v:135:VAL:HA	2.55	0.42
5:e:8:ARG:HG3	6:f:13:TYR:CD1	2.55	0.42
14:t:22:PHE:HE2	25:t:101:BCR:H312	1.85	0.42
2:B:149:LEU:HD23	23:B:604:CLA:HBC1	2.02	0.42
2:B:385:ARG:HG2	13:O:165:ALA:O	2.20	0.42
2:B:393:GLU:HB3	15:U:18:GLY:N	2.35	0.42
28:a:611:LMG:H151	32:c:517:DGD:HA62	2.02	0.42
23:b:608:CLA:H122	23:b:613:CLA:HMA2	2.02	0.42
3:c:210:PHE:HD2	3:c:213[B]:LEU:HD22	1.84	0.42
4:d:283:ALA:O	4:d:287:VAL:HG23	2.20	0.42
14:t:8:PHE:HD1	25:t:101:BCR:H373	1.85	0.42
26:A:610:PL9:C22	24:D:401:PHO:HMA2	2.49	0.41
23:B:612:CLA:H41	23:B:615:CLA:HAC2	2.02	0.41
23:C:504:CLA:H202	31:D:408:LHG:H172	2.02	0.41
23:C:507:CLA:H92	23:C:507:CLA:H61	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:TRP:CZ2	9:J:13:VAL:HG13	2.53	0.41
1:a:249:VAL:HG12	2:b:491:VAL:CG2	2.50	0.41
2:b:198:VAL:HG13	23:b:606:CLA:HMA3	2.02	0.41
27:b:601:SQD:H291	23:b:609[A]:CLA:H203	2.02	0.41
27:b:602:SQD:H82	25:b:620:BCR:H402	2.01	0.41
25:b:621:BCR:C36	25:b:621:BCR:C17	2.76	0.41
3:c:123:ALA:HB2	25:c:522:BCR:H12C	2.02	0.41
23:c:503:CLA:H51	23:c:504:CLA:NC	2.35	0.41
2:B:204:ALA:CB	23:B:603:CLA:HAB	2.51	0.41
2:B:325:PHE:CD2	11:L:34:TYR:HB3	2.55	0.41
23:C:501:CLA:CGA	23:C:501:CLA:H3A	2.50	0.41
23:C:507:CLA:OBD	23:C:509:CLA:H122	2.20	0.41
7:H:48:ILE:HG13	7:H:53:LEU:HD23	2.02	0.41
13:O:42:ARG:O	13:O:241:ALA:HA	2.19	0.41
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.02	0.41
26:a:609:PL9:HC2	26:a:609:PL9:H103	2.02	0.41
2:b:382:PRO:HG2	2:b:385:ARG:CD	2.50	0.41
23:b:604:CLA:H152	25:h:101:BCR:C17	2.50	0.41
3:c:447:ARG:NH2	4:d:229:ALA:HB1	2.34	0.41
1:A:35:VAL:HG22	25:A:609:BCR:HC21	2.01	0.41
25:T:101:BCR:C37	25:T:101:BCR:C23	2.84	0.41
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.55	0.41
23:b:612:CLA:HBA1	23:b:612:CLA:H3A	1.81	0.41
23:b:615:CLA:H91	23:b:616:CLA:HBB1	2.01	0.41
3:c:130:VAL:O	3:c:134:ILE:HG12	2.20	0.41
4:d:103:ARG:HE	5:e:77:GLU:HG3	1.85	0.41
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.02	0.41
1:A:24:THR:C	4:D:255:GLN:HE22	2.29	0.41
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.03	0.41
23:B:605:CLA:H43	23:B:606:CLA:H2	2.01	0.41
2:b:125:ASP:HA	2:b:126:PRO:HD3	1.90	0.41
23:b:607:CLA:H43	23:b:608:CLA:H2	2.01	0.41
6:f:34:LEU:HD22	9:j:24:ILE:HG12	2.02	0.41
1:A:200:LEU:HG	32:C:518:DGD:HAT2	2.03	0.41
1:A:217:SER:O	1:A:221[A]:SER:HB3	2.20	0.41
3:C:223:TRP:CG	3:C:224:ILE:N	2.88	0.41
1:a:112:TYR:O	1:a:116:ILE:HG12	2.21	0.41
1:a:326:LEU:CD2	16:v:134:LYS:HB2	2.49	0.41
27:a:610:SQD:O10	31:a:614:LHG:H122	2.20	0.41
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.55	0.41
2:b:157:HIS:HA	2:b:163:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:606:CLA:HAB	23:b:608:CLA:H171	2.02	0.41
4:d:53:THR:HA	4:d:67:TYR:HD2	1.84	0.41
4:d:123:ILE:HD11	32:h:102:DGD:HAH2	2.03	0.41
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.51	0.41
26:A:610:PL9:H103	26:A:610:PL9:H121	1.79	0.41
2:B:201:HIS:HE1	23:B:604:CLA:HMB2	1.84	0.41
13:O:154:ALA:HB1	13:O:165:ALA:HB2	2.01	0.41
14:T:15:ALA:CA	25:T:101:BCR:H12C	2.45	0.41
23:a:607:CLA:HAB	8:i:15:PHE:CD1	2.56	0.41
2:b:25:MET:HE3	25:b:620:BCR:C25	2.51	0.41
2:b:341:LYS:HD3	2:b:406:LEU:HD11	2.03	0.41
31:e:101:LHG:H241	31:e:101:LHG:HC61	1.81	0.41
27:B:623:SQD:H302	14:t:19:PHE:CD2	2.55	0.41
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.02	0.41
8:I:33:LYS:HB3	8:I:34:ARG:H	1.45	0.41
1:a:193:LEU:HD13	4:d:179:PHE:HB3	2.03	0.41
27:b:601:SQD:C27	25:b:622:BCR:H19C	2.51	0.41
4:d:236:ASN:O	4:d:239:GLN:HG2	2.21	0.41
26:A:610:PL9:H523	26:A:610:PL9:H531	1.87	0.41
2:B:86:ILE:H	2:B:86:ILE:HG13	1.72	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.86	0.41
6:F:37:ILE:HA	6:F:40:MET:SD	2.60	0.41
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.02	0.41
1:a:40:THR:HG23	23:a:607:CLA:HBB1	2.02	0.41
1:a:92:HIS:HE2	3:c:360:ASP:CG	2.28	0.41
1:a:176:ILE:O	1:a:179:THR:HB	2.20	0.41
1:a:235:TYR:O	1:a:238[B]:LYS:HE3	2.20	0.41
26:d:404:PL9:H33	31:l:101:LHG:H222	2.03	0.41
25:k:101:BCR:H17C	17:y:33:PRO:CD	2.50	0.41
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.85	0.41
1:A:188:ALA:HB2	1:A:328:MET:CB	2.51	0.41
1:A:206:PHE:CZ	23:D:403:CLA:HAA1	2.55	0.41
1:A:343:LEU:O	3:C:401:LEU:HD11	2.21	0.41
25:C:515:BCR:H11C	25:C:515:BCR:H341	1.83	0.41
12:M:16[C]:LEU:CD2	12:m:16[C]:LEU:HD22	2.50	0.41
1:a:330:VAL:HG21	4:d:328:TRP:NE1	2.36	0.41
2:b:172:TYR:CE1	2:b:283:GLU:HB2	2.56	0.41
3:c:206:PRO:HG3	3:c:239:TRP:CZ2	2.56	0.41
23:c:503:CLA:H51	23:c:504:CLA:C4C	2.51	0.41
23:c:514:CLA:CAB	25:c:515:BCR:H24C	2.50	0.41
25:k:101:BCR:H17C	17:y:33:PRO:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:19:CYS:SG	13:o:46:GLN:HB2	2.60	0.41
14:t:22:PHE:CE2	25:t:101:BCR:H312	2.56	0.41
23:A:608:CLA:H162	23:A:608:CLA:H122	1.76	0.41
27:A:611:SQD:H291	23:C:508:CLA:H71	2.03	0.41
23:B:608:CLA:C4A	23:B:608:CLA:HBA2	2.50	0.41
3:C:223:TRP:CE3	32:C:516:DGD:HB21	2.56	0.41
3:C:327:ASN:HB3	13:O:99:ASP:OD2	2.20	0.41
23:b:608:CLA:H162	23:b:612:CLA:HBB2	2.03	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.40
23:B:614:CLA:H121	23:B:614:CLA:H162	1.89	0.40
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.98	0.40
23:C:504:CLA:HAC2	10:K:26:PRO:O	2.21	0.40
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.03	0.40
12:M:16[C]:LEU:HD21	12:m:16[C]:LEU:HD22	2.03	0.40
31:a:614:LHG:H342	23:c:505:CLA:H201	2.02	0.40
2:b:33:TRP:CA	25:b:621:BCR:H15C	2.51	0.40
23:b:608:CLA:HBB2	25:b:622:BCR:H342	2.02	0.40
32:c:518:DGD:HAT1	32:c:519:DGD:HBH1	2.02	0.40
4:d:51:GLY:HA3	4:d:78:VAL:HG22	2.03	0.40
26:d:404:PL9:H271	26:d:404:PL9:H302	1.71	0.40
1:A:37:MET:HG3	1:A:122:GLY:O	2.21	0.40
1:A:82:VAL:HB	1:A:174:LEU:HB2	2.03	0.40
1:A:330:VAL:HG21	4:D:328:TRP:NE1	2.36	0.40
25:B:620:BCR:H15C	25:B:620:BCR:H351	1.95	0.40
3:C:59:LEU:HD13	23:C:510:CLA:HMD2	2.02	0.40
25:F:101:BCR:H20C	28:J:101:LMG:H301	2.03	0.40
16:V:40:CYS:SG	33:V:202:HEM:CAC	3.09	0.40
28:a:611:LMG:H291	3:c:214:LEU:O	2.21	0.40
31:a:614:LHG:H132	31:a:614:LHG:H372	2.03	0.40
2:b:243:ALA:HB2	2:b:466:HIS:CE1	2.56	0.40
23:c:507:CLA:CBB	23:c:508:CLA:HMA3	2.51	0.40
25:f:101:BCR:H403	9:j:25:VAL:HG21	2.04	0.40
10:k:28:ILE:HG12	17:y:28:ILE:HG21	2.03	0.40
15:u:64:ILE:HA	15:u:65:PRO:HD3	1.97	0.40
1:A:334:ARG:HB2	13:O:157:LEU:HD12	2.02	0.40
26:A:610:PL9:H102	26:A:610:PL9:HC72	1.79	0.40
2:B:200:ALA:HB3	23:B:603:CLA:HMB1	2.03	0.40
2:B:249:ALA:HA	2:B:252:VAL:HG22	2.02	0.40
2:B:457:VAL:HG11	28:B:621:LMG:H211	2.03	0.40
23:B:616:CLA:HBA1	23:B:616:CLA:H3A	1.65	0.40
3:C:179:ALA:O	3:C:184:GLY:HA2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:502:CLA:H61	23:C:512:CLA:H42	2.03	0.40
4:D:87:HIS:ND1	32:H:102:DGD:O2D	2.45	0.40
31:D:407:LHG:H141	11:L:22:LEU:HD21	2.03	0.40
1:a:237:TYR:CE1	1:a:241:GLN:HG2	2.56	0.40
23:b:617:CLA:H203	25:b:620:BCR:C10	2.52	0.40
25:t:101:BCR:C20	25:t:101:BCR:C17	2.99	0.40
23:B:610:CLA:HBA1	23:B:610:CLA:H3A	1.80	0.40
23:B:617:CLA:H3A	23:B:617:CLA:HBA1	1.90	0.40
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.57	0.40
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.56	0.40
6:F:29:PRO:C	25:F:101:BCR:H15C	2.47	0.40
25:T:101:BCR:H372	25:b:620:BCR:H353	2.03	0.40
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.84	0.40
2:b:494:GLY:HA3	5:e:4:THR:O	2.21	0.40
23:b:608:CLA:C14	23:b:613:CLA:HED2	2.52	0.40
23:b:608:CLA:H41	23:b:608:CLA:H62	1.77	0.40
23:b:617:CLA:C10	25:b:620:BCR:H362	2.48	0.40
3:c:63:TRP:CZ2	3:c:67:MET:HG2	2.57	0.40
8:i:33:LYS:HB3	8:i:34:ARG:H	1.37	0.40
1:A:322:ASN:OD1	3:C:412:THR:HA	2.22	0.40
2:B:383:PHE:CG	4:D:347:PRO:HA	2.56	0.40
25:B:618:BCR:H15C	25:B:619:BCR:H352	2.03	0.40
23:C:505:CLA:H202	8:I:12:VAL:HG11	2.04	0.40
5:E:8:ARG:HB2	6:F:13:TYR:HB3	2.02	0.40
13:O:184:ARG:HA	15:U:9:LEU:CD1	2.51	0.40
15:U:38:TYR:HB2	15:U:41:LEU:HD12	2.03	0.40
1:a:315:ASN:O	4:d:63:LEU:HA	2.21	0.40
2:b:385:ARG:HG2	13:o:165:ALA:C	2.47	0.40
23:c:503:CLA:H61	23:c:513:CLA:H42	2.03	0.40
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	36	71
1	a	336/334 (101%)	330 (98%)	5 (2%)	1 (0%)	36	71
2	B	512/504 (102%)	507 (99%)	5 (1%)	0	100	100
2	b	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
3	C	454/451 (101%)	443 (98%)	9 (2%)	2 (0%)	30	67
3	c	454/451 (101%)	441 (97%)	11 (2%)	2 (0%)	30	67
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	57 (88%)	8 (12%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (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	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (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	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	67
13	o	245/243 (101%)	235 (96%)	9 (4%)	1 (0%)	30	67
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	29 (100%)	0	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5134 (98%)	110 (2%)	8 (0%)	48	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
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	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	272 (100%)	1 (0%)	84	82
2	B	412/402 (102%)	408 (99%)	4 (1%)	68	76
2	b	412/402 (102%)	409 (99%)	3 (1%)	76	79
3	C	357/352 (101%)	352 (99%)	5 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	357/352 (101%)	353 (99%)	4 (1%)	65	74
4	D	277/277 (100%)	275 (99%)	2 (1%)	76	79
4	d	277/277 (100%)	276 (100%)	1 (0%)	84	82
5	E	74/72 (103%)	73 (99%)	1 (1%)	59	71
5	e	74/72 (103%)	74 (100%)	0	100	100
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	52
6	f	28/28 (100%)	27 (96%)	1 (4%)	31	52
7	H	56/54 (104%)	53 (95%)	3 (5%)	20	42
7	h	56/54 (104%)	54 (96%)	2 (4%)	31	52
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	37
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	37
11	L	36/35 (103%)	35 (97%)	1 (3%)	38	59
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	59
12	M	32/31 (103%)	31 (97%)	1 (3%)	35	56
12	m	32/31 (103%)	32 (100%)	0	100	100
13	O	210/206 (102%)	206 (98%)	4 (2%)	50	66
13	o	210/206 (102%)	207 (99%)	3 (1%)	59	71
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	63	73
15	u	84/84 (100%)	83 (99%)	1 (1%)	63	73
16	V	118/117 (101%)	117 (99%)	1 (1%)	73	77
16	v	118/117 (101%)	117 (99%)	1 (1%)	73	77
17	Y	22/22 (100%)	21 (96%)	1 (4%)	24	46
17	y	22/22 (100%)	22 (100%)	0	100	100
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	32 (97%)	1 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	51
All	All	4370/4302 (102%)	4318 (99%)	52 (1%)	63	73

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	86	ILE
2	B	127	ARG
2	B	467	ILE
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
3	C	142	GLU
3	C	289	PHE
3	C	315	MET
4	D	11	GLU
4	D	90	LEU
5	E	71	GLU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	65	LEU
10	K	13	GLU
10	K	17	ILE
11	L	1	MET
12	M	9	ILE
13	O	61	GLN
13	O	62	GLU
13	O	181	GLU
13	O	234	LYS
15	U	70	ARG
16	V	30	LYS
17	Y	27	MET
19	Z	4	LEU
19	Z	6	GLN
1	a	12	ASN
2	b	127	ARG
2	b	362	PHE
2	b	472	ARG
3	c	29	GLU

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Mol	Chain	Res	Type
3	c	240	ILE
3	c	289	PHE
3	c	355	THR
4	d	150	ILE
6	f	44	GLN
7	h	12[A]	ARG
7	h	12[B]	ARG
10	k	13	GLU
10	k	17	ILE
11	l	1	MET
13	o	61	GLN
13	o	194	LYS
13	o	225	MET
15	u	70	ARG
16	v	23	GLU
18	x	2	THR
19	z	4	LEU
19	z	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
3	C	44	ASN
3	C	132	HIS
12	M	5	GLN
12	M	33	GLN
19	Z	6	GLN
1	a	75	ASN
1	a	165	GLN
1	a	198	HIS
1	a	234	ASN
1	a	261	GLN
2	b	409	GLN
2	b	490	GLN
3	c	25	ASN
3	c	39	ASN
3	c	44	ASN
4	d	197	HIS
4	d	255	GLN
5	e	74	GLN

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Mol	Chain	Res	Type
10	k	40	GLN
11	l	6	ASN
12	m	5	GLN
12	m	33	GLN
15	u	78	ASN
15	u	81	HIS
17	y	21	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 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	$\# Z > 2$
33	HEM	E	102	5,6	50,50,50	2.01	10 (20%)	67,82,82	1.19	4 (5%)
25	BCR	B	618	-	41,41,41	7.66	29 (70%)	56,56,56	6.20	32 (57%)
23	CLA	C	512	-	69,73,73	3.04	34 (49%)	82,113,113	1.75	18 (21%)
28	LMG	Z	101	-	37,37,55	1.45	4 (10%)	45,45,63	1.25	3 (6%)
23	CLA	b	612	-	69,73,73	3.04	32 (46%)	82,113,113	1.67	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	L	101	-	48,48,48	1.12	3 (6%)	51,54,54	0.88	3 (5%)
23	CLA	C	509	-	69,73,73	3.05	33 (47%)	82,113,113	1.74	18 (21%)
28	LMG	C	519	-	51,51,55	1.34	4 (7%)	59,59,63	1.06	2 (3%)
28	LMG	j	101	34	51,51,55	1.33	4 (7%)	59,59,63	0.93	4 (6%)
23	CLA	C	508	-	69,73,73	3.06	33 (47%)	82,113,113	1.76	16 (19%)
23	CLA	B	613	-	69,73,73	3.09	32 (46%)	82,113,113	1.74	17 (20%)
31	LHG	d	406	-	48,48,48	1.13	3 (6%)	51,54,54	0.91	3 (5%)
23	CLA	B	603	-	69,73,73	3.03	33 (47%)	82,113,113	1.77	19 (23%)
20	OEX	a	601	1,3	0,15,15	-	-	-	-	-
25	BCR	b	621	-	41,41,41	7.71	29 (70%)	56,56,56	5.78	30 (53%)
23	CLA	B	612	-	69,73,73	3.07	33 (47%)	82,113,113	1.82	15 (18%)
23	CLA	b	605	-	69,73,73	3.06	32 (46%)	82,113,113	1.75	16 (19%)
23	CLA	b	607	-	69,73,73	3.06	33 (47%)	82,113,113	1.77	17 (20%)
31	LHG	D	408	-	48,48,48	1.12	3 (6%)	51,54,54	0.98	3 (5%)
25	BCR	c	516	-	41,41,41	7.72	30 (73%)	56,56,56	5.96	27 (48%)
23	CLA	C	501	-	69,73,73	3.04	32 (46%)	82,113,113	1.78	19 (23%)
23	CLA	C	505	-	69,73,73	3.09	31 (44%)	82,113,113	1.68	11 (13%)
23	CLA	C	506	-	69,73,73	3.04	33 (47%)	82,113,113	1.73	18 (21%)
23	CLA	C	504	-	69,73,73	3.06	33 (47%)	82,113,113	1.79	17 (20%)
23	CLA	C	510	-	69,73,73	3.07	32 (46%)	82,113,113	1.67	17 (20%)
23	CLA	B	602	-	69,73,73	3.03	33 (47%)	82,113,113	1.75	16 (19%)
23	CLA	a	607	-	69,73,73	3.08	33 (47%)	82,113,113	1.71	17 (20%)
25	BCR	T	101	-	41,41,41	7.69	30 (73%)	56,56,56	6.14	28 (50%)
23	CLA	a	613	-	69,73,73	3.07	34 (49%)	82,113,113	1.76	17 (20%)
24	PHO	d	401	-	58,69,69	2.22	10 (17%)	55,99,99	1.41	7 (12%)
25	BCR	c	515	-	41,41,41	7.59	31 (75%)	56,56,56	6.41	32 (57%)
23	CLA	b	616	-	69,73,73	3.05	33 (47%)	82,113,113	1.73	18 (21%)
25	BCR	k	101	-	41,41,41	7.73	30 (73%)	56,56,56	5.81	26 (46%)
32	DGD	C	518	-	63,63,67	1.69	16 (25%)	77,77,81	1.03	5 (6%)
27	SQD	X	101	-	41,43,54	1.16	3 (7%)	51,54,65	1.42	7 (13%)
23	CLA	d	402	-	69,73,73	3.08	32 (46%)	82,113,113	1.62	13 (15%)
22	BCT	A	604	29	3,3,3	2.87	1 (33%)	2,3,3	3.85	2 (100%)
23	CLA	A	605	-	69,73,73	3.07	32 (46%)	82,113,113	1.72	15 (18%)
23	CLA	c	506	-	69,73,73	3.08	31 (44%)	82,113,113	1.66	12 (14%)
23	CLA	c	513	-	69,73,73	3.04	33 (47%)	82,113,113	1.72	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	K	101	-	41,41,41	7.69	29 (70%)	56,56,56	6.01	27 (48%)
32	DGD	d	405	-	63,63,67	1.72	15 (23%)	77,77,81	1.04	7 (9%)
23	CLA	b	617	-	69,73,73	3.05	32 (46%)	82,113,113	1.73	17 (20%)
25	BCR	B	619	-	41,41,41	8.02	30 (73%)	56,56,56	5.44	28 (50%)
23	CLA	b	614	-	69,73,73	3.10	33 (47%)	82,113,113	1.80	16 (19%)
25	BCR	a	608	-	41,41,41	7.74	30 (73%)	56,56,56	5.81	25 (44%)
33	HEM	v	201	16	50,50,50	1.93	9 (18%)	67,82,82	1.27	6 (8%)
25	BCR	H	101	-	41,41,41	7.59	30 (73%)	56,56,56	5.98	36 (64%)
23	CLA	c	505	-	69,73,73	3.04	34 (49%)	82,113,113	1.79	17 (20%)
28	LMG	b	623	-	51,51,55	1.31	4 (7%)	59,59,63	0.95	2 (3%)
28	LMG	J	101	34	51,51,55	1.33	4 (7%)	59,59,63	0.99	4 (6%)
23	CLA	B	616	-	69,73,73	3.02	33 (47%)	82,113,113	1.75	18 (21%)
23	CLA	b	609[B]	-	69,73,73	3.06	32 (46%)	82,113,113	1.84	19 (23%)
31	LHG	e	101	-	41,41,48	1.22	3 (7%)	44,47,54	0.97	2 (4%)
23	CLA	C	502	-	69,73,73	3.05	33 (47%)	82,113,113	1.76	18 (21%)
23	CLA	b	609[A]	-	69,73,73	3.03	32 (46%)	82,113,113	1.85	18 (21%)
23	CLA	c	509	-	69,73,73	3.03	33 (47%)	82,113,113	1.81	16 (19%)
23	CLA	B	606	-	69,73,73	3.04	32 (46%)	82,113,113	1.73	17 (20%)
25	BCR	C	521	-	41,41,41	7.67	29 (70%)	56,56,56	6.02	27 (48%)
23	CLA	c	512	3	69,73,73	3.05	33 (47%)	82,113,113	1.71	14 (17%)
28	LMG	a	611	-	51,51,55	1.32	4 (7%)	59,59,63	1.00	2 (3%)
27	SQD	a	610	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)
23	CLA	B	617	-	69,73,73	3.05	33 (47%)	82,113,113	1.74	15 (18%)
32	DGD	C	517	-	63,63,67	1.66	17 (26%)	77,77,81	1.03	5 (6%)
32	DGD	c	518	-	63,63,67	1.67	16 (25%)	77,77,81	1.00	6 (7%)
23	CLA	B	604	-	69,73,73	3.08	32 (46%)	82,113,113	1.69	17 (20%)
23	CLA	B	615	-	69,73,73	3.04	32 (46%)	82,113,113	1.74	18 (21%)
23	CLA	c	507	-	69,73,73	3.06	33 (47%)	82,113,113	1.74	17 (20%)
26	PL9	D	405	-	55,55,55	4.35	21 (38%)	68,69,69	3.68	35 (51%)
23	CLA	b	610	-	69,73,73	3.06	32 (46%)	82,113,113	1.76	19 (23%)
23	CLA	C	511	3	69,73,73	3.06	33 (47%)	82,113,113	1.76	16 (19%)
28	LMG	c	520	-	51,51,55	1.34	4 (7%)	59,59,63	1.03	2 (3%)
32	DGD	h	102	-	63,63,67	1.70	15 (23%)	77,77,81	0.98	4 (5%)
31	LHG	E	101	-	41,41,48	1.22	3 (7%)	44,47,54	0.92	3 (6%)
23	CLA	A	606	-	69,73,73	3.08	32 (46%)	82,113,113	1.76	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	c	521	-	51,51,55	1.33	4 (7%)	59,59,63	1.01	3 (5%)
23	CLA	c	508	-	69,73,73	3.03	31 (44%)	82,113,113	1.88	17 (20%)
23	CLA	b	618	-	69,73,73	3.02	33 (47%)	82,113,113	1.76	19 (23%)
20	OEX	A	601	1,3	0,15,15	-	-	-	-	-
27	SQD	A	611	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)
27	SQD	b	602	-	52,54,54	1.03	3 (5%)	62,65,65	1.41	9 (14%)
23	CLA	a	604	-	69,73,73	3.07	33 (47%)	82,113,113	1.73	15 (18%)
23	CLA	b	615	-	69,73,73	3.08	33 (47%)	82,113,113	1.76	17 (20%)
23	CLA	b	611	-	69,73,73	3.03	31 (44%)	82,113,113	1.79	17 (20%)
23	CLA	B	608	-	69,73,73	3.05	33 (47%)	82,113,113	1.76	19 (23%)
23	CLA	B	605	-	69,73,73	3.06	33 (47%)	82,113,113	1.73	16 (19%)
23	CLA	B	609	-	69,73,73	3.03	31 (44%)	82,113,113	1.77	20 (24%)
23	CLA	D	403	-	69,73,73	3.08	32 (46%)	82,113,113	1.63	16 (19%)
26	PL9	a	609	-	55,55,55	4.32	22 (40%)	68,69,69	3.75	37 (54%)
27	SQD	x	101	-	41,43,54	1.15	3 (7%)	51,54,65	1.42	7 (13%)
23	CLA	B	610	-	69,73,73	3.04	32 (46%)	82,113,113	1.69	15 (18%)
23	CLA	c	510	-	69,73,73	3.05	33 (47%)	82,113,113	1.76	17 (20%)
25	BCR	A	609	-	41,41,41	7.78	30 (73%)	56,56,56	5.79	26 (46%)
23	CLA	B	607[B]	-	69,73,73	3.06	32 (46%)	82,113,113	1.84	18 (21%)
24	PHO	A	607	-	58,69,69	2.21	10 (17%)	55,99,99	1.38	5 (9%)
25	BCR	h	101	-	41,41,41	7.66	30 (73%)	56,56,56	5.99	37 (66%)
26	PL9	A	610	-	55,55,55	4.35	22 (40%)	68,69,69	3.70	38 (55%)
25	BCR	c	522	-	41,41,41	7.64	30 (73%)	56,56,56	5.98	27 (48%)
23	CLA	B	607[A]	-	69,73,73	3.05	32 (46%)	82,113,113	1.85	19 (23%)
28	LMG	C	520	-	51,51,55	1.32	4 (7%)	59,59,63	1.02	4 (6%)
33	HEM	V	202	16	50,50,50	1.87	8 (16%)	67,82,82	1.26	5 (7%)
32	DGD	D	406	-	63,63,67	1.74	14 (22%)	77,77,81	1.13	7 (9%)
23	CLA	C	513	-	69,73,73	3.03	32 (46%)	82,113,113	1.73	17 (20%)
28	LMG	z	101	-	37,37,55	1.45	4 (10%)	45,45,63	1.21	4 (8%)
31	LHG	l	101	-	48,48,48	1.14	2 (4%)	51,54,54	0.90	2 (3%)
32	DGD	C	516	-	63,63,67	1.72	16 (25%)	77,77,81	0.93	3 (3%)
23	CLA	b	619	-	69,73,73	3.07	31 (44%)	82,113,113	1.72	16 (19%)
27	SQD	a	612	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
23	CLA	B	611	-	69,73,73	3.05	34 (49%)	82,113,113	1.71	16 (19%)
23	CLA	C	507	-	69,73,73	3.00	32 (46%)	82,113,113	1.86	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	620	-	41,41,41	7.63	31 (75%)	56,56,56	6.22	31 (55%)
23	CLA	b	608	-	69,73,73	3.06	32 (46%)	82,113,113	1.75	17 (20%)
25	BCR	C	514	-	41,41,41	7.60	31 (75%)	56,56,56	6.31	31 (55%)
31	LHG	b	624	-	48,48,48	1.12	3 (6%)	51,54,54	0.97	3 (5%)
23	CLA	D	402	-	69,73,73	3.06	32 (46%)	82,113,113	1.74	18 (21%)
33	HEM	e	102	5,6	50,50,50	1.99	9 (18%)	67,82,82	1.21	3 (4%)
32	DGD	c	517	-	63,63,67	1.72	16 (25%)	77,77,81	0.93	5 (6%)
23	CLA	b	604	-	69,73,73	3.04	34 (49%)	82,113,113	1.73	17 (20%)
25	BCR	b	620	-	41,41,41	7.56	30 (73%)	56,56,56	6.01	28 (50%)
31	LHG	B	622	-	48,48,48	1.15	3 (6%)	51,54,54	0.98	5 (9%)
23	CLA	B	614	-	69,73,73	3.08	32 (46%)	82,113,113	1.69	17 (20%)
25	BCR	C	515	-	41,41,41	7.66	30 (73%)	56,56,56	6.11	29 (51%)
28	LMG	A	612	-	51,51,55	1.32	4 (7%)	59,59,63	0.98	3 (5%)
23	CLA	c	511	-	69,73,73	3.07	34 (49%)	82,113,113	1.66	16 (19%)
23	CLA	c	503	-	69,73,73	3.06	32 (46%)	82,113,113	1.79	18 (21%)
22	BCT	a	603	29	3,3,3	2.81	1 (33%)	2,3,3	3.31	2 (100%)
23	CLA	c	514	-	69,73,73	3.02	33 (47%)	82,113,113	1.73	14 (17%)
23	CLA	c	502	-	69,73,73	3.05	32 (46%)	82,113,113	1.75	16 (19%)
27	SQD	b	601	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
32	DGD	c	519	-	63,63,67	1.68	16 (25%)	77,77,81	1.07	4 (5%)
25	BCR	b	622	-	41,41,41	7.74	31 (75%)	56,56,56	5.97	31 (55%)
23	CLA	d	403	-	69,73,73	3.03	33 (47%)	82,113,113	1.77	17 (20%)
24	PHO	a	606	-	58,69,69	2.18	10 (17%)	55,99,99	1.38	6 (10%)
31	LHG	D	407	-	48,48,48	1.13	3 (6%)	51,54,54	0.91	3 (5%)
25	BCR	t	101	-	41,41,41	7.71	29 (70%)	56,56,56	5.91	28 (50%)
23	CLA	D	404	-	69,73,73	3.04	32 (46%)	82,113,113	1.80	17 (20%)
23	CLA	a	605	-	69,73,73	3.06	33 (47%)	82,113,113	1.73	17 (20%)
24	PHO	D	401	-	58,69,69	2.20	10 (17%)	55,99,99	1.41	7 (12%)
23	CLA	b	613	-	69,73,73	3.07	33 (47%)	82,113,113	1.73	16 (19%)
25	BCR	F	101	-	41,41,41	7.64	29 (70%)	56,56,56	6.19	28 (50%)
23	CLA	C	503	-	69,73,73	3.05	33 (47%)	82,113,113	1.72	17 (20%)
23	CLA	c	504	-	69,73,73	3.03	33 (47%)	82,113,113	1.67	17 (20%)
23	CLA	b	606	-	69,73,73	3.12	33 (47%)	82,113,113	1.70	16 (19%)
27	SQD	B	623	-	52,54,54	1.03	3 (5%)	62,65,65	1.41	9 (14%)
23	CLA	A	608	-	69,73,73	3.07	32 (46%)	82,113,113	1.73	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	DGD	H	102	-	63,63,67	1.71	15 (23%)	77,77,81	0.92	3 (3%)
26	PL9	d	404	-	55,55,55	4.37	21 (38%)	68,69,69	3.67	35 (51%)
25	BCR	f	101	-	41,41,41	7.72	30 (73%)	56,56,56	5.93	27 (48%)
31	LHG	a	614	-	48,48,48	1.11	2 (4%)	51,54,54	1.04	3 (5%)
28	LMG	B	621	-	51,51,55	1.29	4 (7%)	59,59,63	0.91	2 (3%)

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
33	HEM	E	102	5,6	-	4/14/54/54	-
25	BCR	B	618	-	-	24/29/63/63	0/2/2/2
23	CLA	C	512	-	1/1/15/20	9/39/115/115	-
28	LMG	Z	101	-	-	15/31/51/70	0/1/1/1
23	CLA	b	612	-	1/1/15/20	5/39/115/115	-
31	LHG	L	101	-	-	17/53/53/53	-
23	CLA	C	509	-	1/1/15/20	6/39/115/115	-
28	LMG	C	519	-	-	20/46/66/70	0/1/1/1
28	LMG	j	101	34	-	19/46/66/70	0/1/1/1
23	CLA	C	508	-	1/1/15/20	3/39/115/115	-
23	CLA	B	613	-	1/1/15/20	4/39/115/115	-
31	LHG	d	406	-	-	13/53/53/53	-
23	CLA	B	603	-	1/1/15/20	4/39/115/115	-
25	BCR	b	621	-	-	21/29/63/63	0/2/2/2
23	CLA	B	612	-	1/1/15/20	5/39/115/115	-
23	CLA	b	605	-	1/1/15/20	4/39/115/115	-
23	CLA	b	607	-	1/1/15/20	7/39/115/115	-
31	LHG	D	408	-	-	16/53/53/53	-
25	BCR	c	516	-	-	21/29/63/63	0/2/2/2
23	CLA	C	501	-	1/1/15/20	9/39/115/115	-
23	CLA	C	505	-	1/1/15/20	8/39/115/115	-
23	CLA	C	506	-	1/1/15/20	15/39/115/115	-
23	CLA	C	504	-	1/1/15/20	10/39/115/115	-
23	CLA	C	510	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	602	-	1/1/15/20	17/39/115/115	-
23	CLA	a	607	-	1/1/15/20	11/39/115/115	-
25	BCR	T	101	-	-	24/29/63/63	0/2/2/2
23	CLA	a	613	-	1/1/15/20	3/39/115/115	-
24	PHO	d	401	-	-	0/37/103/103	0/5/6/6
25	BCR	c	515	-	-	24/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/15/20	5/39/115/115	-
25	BCR	k	101	-	-	19/29/63/63	0/2/2/2
32	DGD	C	518	-	-	16/51/91/95	0/2/2/2
27	SQD	X	101	-	-	17/38/58/69	0/1/1/1
23	CLA	d	402	-	1/1/15/20	2/39/115/115	-
23	CLA	c	506	-	1/1/15/20	6/39/115/115	-
23	CLA	A	605	-	1/1/15/20	0/39/115/115	-
23	CLA	c	513	-	1/1/15/20	7/39/115/115	-
25	BCR	K	101	-	-	21/29/63/63	0/2/2/2
32	DGD	d	405	-	-	33/51/91/95	0/2/2/2
23	CLA	b	617	-	1/1/15/20	12/39/115/115	-
25	BCR	B	619	-	-	24/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/15/20	5/39/115/115	-
25	BCR	a	608	-	-	19/29/63/63	0/2/2/2
33	HEM	v	201	16	-	2/14/54/54	-
25	BCR	H	101	-	-	23/29/63/63	0/2/2/2
23	CLA	c	505	-	1/1/15/20	11/39/115/115	-
28	LMG	b	623	-	-	21/46/66/70	0/1/1/1
28	LMG	J	101	34	-	19/46/66/70	0/1/1/1
23	CLA	B	616	-	1/1/15/20	13/39/115/115	-
23	CLA	b	609[B]	-	1/1/15/20	9/39/115/115	-
31	LHG	e	101	-	-	20/46/46/53	-
23	CLA	C	502	-	1/1/15/20	8/39/115/115	-
23	CLA	b	609[A]	-	1/1/15/20	8/39/115/115	-
23	CLA	c	509	-	1/1/15/20	3/39/115/115	-
23	CLA	B	606	-	1/1/15/20	5/39/115/115	-
25	BCR	C	521	-	-	17/29/63/63	0/2/2/2
23	CLA	c	512	3	1/1/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	a	611	-	-	31/46/66/70	0/1/1/1
27	SQD	a	610	-	-	17/49/69/69	0/1/1/1
23	CLA	B	617	-	1/1/15/20	16/39/115/115	-
32	DGD	C	517	-	-	28/51/91/95	0/2/2/2
32	DGD	c	518	-	-	30/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/15/20	8/39/115/115	-
23	CLA	B	615	-	1/1/15/20	13/39/115/115	-
23	CLA	c	507	-	1/1/15/20	14/39/115/115	-
26	PL9	D	405	-	-	25/53/73/73	0/1/1/1
23	CLA	b	610	-	1/1/15/20	3/39/115/115	-
23	CLA	C	511	3	1/1/15/20	3/39/115/115	-
28	LMG	c	520	-	-	22/46/66/70	0/1/1/1
32	DGD	h	102	-	-	19/51/91/95	0/2/2/2
31	LHG	E	101	-	-	22/46/46/53	-
23	CLA	A	606	-	1/1/15/20	7/39/115/115	-
28	LMG	c	521	-	-	19/46/66/70	0/1/1/1
23	CLA	c	508	-	1/1/15/20	12/39/115/115	-
23	CLA	b	618	-	1/1/15/20	13/39/115/115	-
27	SQD	A	611	-	-	17/49/69/69	0/1/1/1
27	SQD	b	602	-	-	29/49/69/69	0/1/1/1
23	CLA	a	604	-	1/1/15/20	1/39/115/115	-
23	CLA	b	615	-	1/1/15/20	4/39/115/115	-
23	CLA	b	611	-	1/1/15/20	2/39/115/115	-
23	CLA	B	608	-	1/1/15/20	3/39/115/115	-
23	CLA	B	605	-	1/1/15/20	7/39/115/115	-
23	CLA	B	609	-	1/1/15/20	3/39/115/115	-
23	CLA	D	403	-	1/1/15/20	2/39/115/115	-
26	PL9	a	609	-	-	26/53/73/73	0/1/1/1
27	SQD	x	101	-	-	17/38/58/69	0/1/1/1
23	CLA	B	610	-	1/1/15/20	1/39/115/115	-
23	CLA	c	510	-	1/1/15/20	7/39/115/115	-
25	BCR	A	609	-	-	21/29/63/63	0/2/2/2
23	CLA	B	607[B]	-	1/1/15/20	9/39/115/115	-
24	PHO	A	607	-	-	2/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	h	101	-	-	25/29/63/63	0/2/2/2
26	PL9	A	610	-	-	25/53/73/73	0/1/1/1
25	BCR	c	522	-	-	20/29/63/63	0/2/2/2
23	CLA	B	607[A]	-	1/1/15/20	9/39/115/115	-
28	LMG	C	520	-	-	19/46/66/70	0/1/1/1
33	HEM	V	202	16	-	2/14/54/54	-
32	DGD	D	406	-	-	35/51/91/95	0/2/2/2
23	CLA	C	513	-	1/1/15/20	9/39/115/115	-
28	LMG	z	101	-	-	18/31/51/70	0/1/1/1
31	LHG	l	101	-	-	22/53/53/53	-
32	DGD	C	516	-	-	25/51/91/95	0/2/2/2
23	CLA	b	619	-	1/1/15/20	16/39/115/115	-
27	SQD	a	612	-	-	23/49/69/69	0/1/1/1
23	CLA	B	611	-	1/1/15/20	8/39/115/115	-
23	CLA	C	507	-	1/1/15/20	12/39/115/115	-
25	BCR	B	620	-	-	17/29/63/63	0/2/2/2
23	CLA	b	608	-	1/1/15/20	6/39/115/115	-
25	BCR	C	514	-	-	22/29/63/63	0/2/2/2
31	LHG	b	624	-	-	13/53/53/53	-
23	CLA	D	402	-	1/1/15/20	2/39/115/115	-
33	HEM	e	102	5,6	-	2/14/54/54	-
32	DGD	c	517	-	-	25/51/91/95	0/2/2/2
23	CLA	b	604	-	1/1/15/20	18/39/115/115	-
25	BCR	b	620	-	-	18/29/63/63	0/2/2/2
31	LHG	B	622	-	-	13/53/53/53	-
23	CLA	B	614	-	1/1/15/20	5/39/115/115	-
25	BCR	C	515	-	-	19/29/63/63	0/2/2/2
28	LMG	A	612	-	-	31/46/66/70	0/1/1/1
23	CLA	c	511	-	1/1/15/20	9/39/115/115	-
23	CLA	c	503	-	1/1/15/20	9/39/115/115	-
23	CLA	c	514	-	1/1/15/20	9/39/115/115	-
23	CLA	c	502	-	1/1/15/20	9/39/115/115	-
27	SQD	b	601	-	-	23/49/69/69	0/1/1/1
32	DGD	c	519	-	-	18/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	622	-	-	21/29/63/63	0/2/2/2
23	CLA	d	403	-	1/1/15/20	13/39/115/115	-
24	PHO	a	606	-	-	0/37/103/103	0/5/6/6
31	LHG	D	407	-	-	13/53/53/53	-
25	BCR	t	101	-	-	23/29/63/63	0/2/2/2
23	CLA	D	404	-	1/1/15/20	13/39/115/115	-
23	CLA	a	605	-	1/1/15/20	7/39/115/115	-
24	PHO	D	401	-	-	1/37/103/103	0/5/6/6
23	CLA	b	613	-	1/1/15/20	8/39/115/115	-
25	BCR	F	101	-	-	22/29/63/63	0/2/2/2
23	CLA	C	503	-	1/1/15/20	5/39/115/115	-
23	CLA	c	504	-	1/1/15/20	3/39/115/115	-
23	CLA	b	606	-	1/1/15/20	7/39/115/115	-
27	SQD	B	623	-	-	29/49/69/69	0/1/1/1
23	CLA	A	608	-	1/1/15/20	11/39/115/115	-
32	DGD	H	102	-	-	24/51/91/95	0/2/2/2
26	PL9	d	404	-	-	26/53/73/73	0/1/1/1
25	BCR	f	101	-	-	23/29/63/63	0/2/2/2
31	LHG	a	614	-	-	16/53/53/53	-
28	LMG	B	621	-	-	22/46/66/70	0/1/1/1

All (3416) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	BCR	C14-C13	15.92	1.72	1.35
25	B	618	BCR	C20-C19	15.90	1.76	1.34
25	a	608	BCR	C14-C13	15.84	1.72	1.35
25	C	521	BCR	C14-C13	15.77	1.72	1.35
25	t	101	BCR	C14-C13	15.74	1.72	1.35
25	K	101	BCR	C20-C19	15.73	1.75	1.34
25	C	514	BCR	C20-C19	15.72	1.75	1.34
25	C	515	BCR	C14-C13	15.70	1.72	1.35
25	b	622	BCR	C20-C19	15.69	1.75	1.34
25	T	101	BCR	C14-C13	15.65	1.72	1.35
25	c	522	BCR	C14-C13	15.63	1.71	1.35
25	F	101	BCR	C14-C13	15.63	1.71	1.35
25	c	516	BCR	C14-C13	15.61	1.71	1.35
25	T	101	BCR	C20-C19	15.55	1.75	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	t	101	BCR	C20-C19	15.49	1.75	1.34
25	B	619	BCR	C19-C18	-15.48	1.12	1.46
25	k	101	BCR	C20-C19	15.45	1.75	1.34
25	b	621	BCR	C20-C19	15.42	1.74	1.34
25	a	608	BCR	C20-C19	15.40	1.74	1.34
25	b	622	BCR	C14-C13	15.40	1.71	1.35
25	B	620	BCR	C20-C19	15.36	1.74	1.34
25	B	619	BCR	C36-C18	15.36	1.81	1.50
25	f	101	BCR	C20-C19	15.35	1.74	1.34
25	A	609	BCR	C20-C19	15.33	1.74	1.34
25	c	516	BCR	C20-C19	15.33	1.74	1.34
25	b	620	BCR	C20-C19	15.32	1.74	1.34
25	K	101	BCR	C14-C13	15.30	1.71	1.35
25	k	101	BCR	C14-C13	15.27	1.71	1.35
25	H	101	BCR	C14-C13	15.27	1.71	1.35
25	B	619	BCR	C5-C6	15.22	1.60	1.34
25	B	620	BCR	C14-C13	15.21	1.71	1.35
25	b	621	BCR	C5-C6	15.21	1.60	1.34
25	b	621	BCR	C14-C13	15.19	1.70	1.35
25	b	620	BCR	C14-C13	15.19	1.70	1.35
25	h	101	BCR	C14-C13	15.18	1.70	1.35
25	f	101	BCR	C14-C13	15.16	1.70	1.35
25	c	522	BCR	C20-C19	15.11	1.74	1.34
25	B	619	BCR	C21-C22	-15.09	1.00	1.35
25	C	515	BCR	C20-C19	15.08	1.74	1.34
25	c	515	BCR	C20-C19	15.08	1.74	1.34
25	C	514	BCR	C5-C6	15.04	1.59	1.34
25	B	619	BCR	C20-C19	15.03	1.73	1.34
25	B	618	BCR	C14-C13	14.99	1.70	1.35
25	t	101	BCR	C5-C6	14.95	1.59	1.34
25	c	515	BCR	C5-C6	14.94	1.59	1.34
25	B	619	BCR	C14-C13	14.94	1.70	1.35
25	F	101	BCR	C20-C19	14.93	1.73	1.34
25	h	101	BCR	C20-C19	14.93	1.73	1.34
25	C	521	BCR	C20-C19	14.83	1.73	1.34
25	H	101	BCR	C20-C19	14.82	1.73	1.34
25	b	622	BCR	C5-C6	14.79	1.59	1.34
25	C	514	BCR	C14-C13	14.72	1.69	1.35
25	c	515	BCR	C14-C13	14.69	1.69	1.35
25	k	101	BCR	C5-C6	14.60	1.59	1.34
25	K	101	BCR	C5-C6	14.51	1.58	1.34
25	B	620	BCR	C5-C6	14.50	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	H	101	BCR	C36-C18	14.48	1.80	1.50
25	C	514	BCR	C36-C18	14.44	1.80	1.50
25	b	622	BCR	C36-C18	14.38	1.79	1.50
25	C	515	BCR	C5-C6	14.27	1.58	1.34
25	c	516	BCR	C5-C6	14.25	1.58	1.34
25	k	101	BCR	C36-C18	14.18	1.79	1.50
25	T	101	BCR	C5-C6	14.17	1.58	1.34
25	c	522	BCR	C5-C6	14.13	1.58	1.34
25	a	608	BCR	C36-C18	14.13	1.79	1.50
25	C	521	BCR	C5-C6	14.13	1.58	1.34
25	c	522	BCR	C36-C18	14.12	1.79	1.50
25	A	609	BCR	C5-C6	14.11	1.58	1.34
25	C	521	BCR	C36-C18	14.10	1.79	1.50
25	a	608	BCR	C5-C6	14.09	1.58	1.34
25	C	515	BCR	C36-C18	14.06	1.79	1.50
25	f	101	BCR	C36-C18	13.95	1.79	1.50
25	c	516	BCR	C36-C18	13.93	1.79	1.50
25	f	101	BCR	C5-C6	13.93	1.57	1.34
25	A	609	BCR	C36-C18	13.91	1.79	1.50
25	F	101	BCR	C19-C18	-13.91	1.16	1.46
25	t	101	BCR	C36-C18	13.90	1.79	1.50
25	c	515	BCR	C36-C18	13.88	1.78	1.50
25	F	101	BCR	C5-C6	13.88	1.57	1.34
25	b	620	BCR	C36-C18	13.86	1.78	1.50
25	K	101	BCR	C19-C18	-13.85	1.16	1.46
25	H	101	BCR	C5-C6	13.79	1.57	1.34
25	H	101	BCR	C21-C22	-13.69	1.04	1.35
25	B	618	BCR	C5-C6	13.69	1.57	1.34
25	h	101	BCR	C5-C6	13.67	1.57	1.34
25	B	620	BCR	C36-C18	13.67	1.78	1.50
25	h	101	BCR	C19-C18	-13.64	1.16	1.46
25	b	620	BCR	C5-C6	13.57	1.57	1.34
25	B	618	BCR	C36-C18	13.56	1.78	1.50
25	C	521	BCR	C19-C18	-13.56	1.16	1.46
25	b	621	BCR	C19-C18	-13.56	1.16	1.46
25	T	101	BCR	C19-C18	-13.47	1.17	1.46
25	c	515	BCR	C19-C18	-13.44	1.17	1.46
25	k	101	BCR	C19-C18	-13.44	1.17	1.46
25	c	522	BCR	C19-C18	-13.29	1.17	1.46
25	h	101	BCR	C36-C18	13.29	1.77	1.50
25	B	618	BCR	C37-C22	13.26	1.77	1.50
25	F	101	BCR	C21-C22	-13.24	1.05	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	514	BCR	C21-C22	-13.24	1.05	1.35
25	T	101	BCR	C16-C15	13.22	1.72	1.36
25	c	516	BCR	C21-C22	-13.20	1.05	1.35
25	c	515	BCR	C21-C22	-13.17	1.05	1.35
25	f	101	BCR	C19-C18	-13.16	1.17	1.46
25	C	515	BCR	C21-C22	-13.16	1.05	1.35
25	b	621	BCR	C36-C18	13.14	1.77	1.50
25	C	521	BCR	C21-C22	-13.13	1.05	1.35
25	K	101	BCR	C36-C18	13.05	1.77	1.50
25	F	101	BCR	C36-C18	13.05	1.77	1.50
25	T	101	BCR	C36-C18	12.96	1.77	1.50
25	B	620	BCR	C21-C22	-12.88	1.06	1.35
25	C	521	BCR	C16-C15	12.87	1.71	1.36
25	B	619	BCR	C37-C22	12.84	1.76	1.50
25	b	620	BCR	C19-C18	-12.82	1.18	1.46
25	t	101	BCR	C19-C18	-12.81	1.18	1.46
25	k	101	BCR	C21-C22	-12.81	1.06	1.35
25	B	618	BCR	C21-C22	-12.79	1.06	1.35
25	B	620	BCR	C19-C18	-12.79	1.18	1.46
25	C	514	BCR	C19-C18	-12.77	1.18	1.46
25	A	609	BCR	C19-C18	-12.77	1.18	1.46
25	K	101	BCR	C16-C15	12.74	1.71	1.36
25	t	101	BCR	C16-C15	12.73	1.71	1.36
25	a	608	BCR	C19-C18	-12.69	1.18	1.46
25	h	101	BCR	C21-C22	-12.69	1.06	1.35
25	B	618	BCR	C16-C15	12.68	1.70	1.36
25	b	622	BCR	C21-C22	-12.67	1.06	1.35
25	A	609	BCR	C21-C22	-12.65	1.06	1.35
25	h	101	BCR	C16-C15	12.63	1.70	1.36
25	b	622	BCR	C37-C22	12.63	1.76	1.50
25	A	609	BCR	C16-C15	12.62	1.70	1.36
25	b	622	BCR	C19-C18	-12.58	1.19	1.46
25	b	620	BCR	C21-C22	-12.58	1.06	1.35
25	c	516	BCR	C19-C18	-12.55	1.19	1.46
25	T	101	BCR	C37-C22	12.53	1.76	1.50
25	C	515	BCR	C19-C18	-12.52	1.19	1.46
25	b	620	BCR	C16-C15	12.52	1.70	1.36
25	H	101	BCR	C19-C18	-12.51	1.19	1.46
25	a	608	BCR	C16-C15	12.47	1.70	1.36
25	f	101	BCR	C21-C22	-12.47	1.07	1.35
25	B	618	BCR	C19-C18	-12.44	1.19	1.46
25	t	101	BCR	C21-C22	-12.43	1.07	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	621	BCR	C37-C22	12.42	1.76	1.50
25	f	101	BCR	C16-C15	12.36	1.70	1.36
25	b	622	BCR	C16-C15	12.36	1.70	1.36
25	h	101	BCR	C37-C22	12.32	1.75	1.50
25	B	620	BCR	C37-C22	12.32	1.75	1.50
25	c	516	BCR	C16-C15	12.30	1.69	1.36
25	H	101	BCR	C16-C15	12.29	1.69	1.36
25	c	516	BCR	C37-C22	12.25	1.75	1.50
25	c	522	BCR	C16-C15	12.24	1.69	1.36
25	k	101	BCR	C16-C15	12.22	1.69	1.36
25	c	522	BCR	C21-C22	-12.21	1.07	1.35
25	K	101	BCR	C37-C22	12.21	1.75	1.50
25	C	515	BCR	C16-C15	12.20	1.69	1.36
25	c	515	BCR	C16-C15	12.18	1.69	1.36
25	A	609	BCR	C10-C9	12.17	1.63	1.35
25	b	622	BCR	C10-C9	12.16	1.63	1.35
25	t	101	BCR	C10-C9	12.14	1.63	1.35
25	F	101	BCR	C16-C15	12.14	1.69	1.36
25	B	620	BCR	C16-C15	12.12	1.69	1.36
25	T	101	BCR	C10-C9	12.10	1.63	1.35
25	b	621	BCR	C21-C22	-12.10	1.07	1.35
25	c	522	BCR	C10-C9	12.09	1.63	1.35
25	T	101	BCR	C20-C21	12.09	1.80	1.43
25	K	101	BCR	C21-C22	-12.07	1.07	1.35
25	B	619	BCR	C16-C15	12.06	1.69	1.36
25	a	608	BCR	C10-C9	12.05	1.63	1.35
25	k	101	BCR	C37-C22	12.04	1.75	1.50
25	c	516	BCR	C10-C9	12.03	1.63	1.35
25	h	101	BCR	C10-C9	12.02	1.63	1.35
25	k	101	BCR	C10-C9	12.02	1.63	1.35
25	c	515	BCR	C37-C22	12.00	1.75	1.50
25	K	101	BCR	C20-C21	11.99	1.80	1.43
25	A	609	BCR	C37-C22	11.96	1.75	1.50
25	C	514	BCR	C16-C15	11.95	1.68	1.36
25	b	621	BCR	C16-C15	11.94	1.68	1.36
25	b	620	BCR	C37-C22	11.89	1.74	1.50
25	B	618	BCR	C20-C21	11.85	1.79	1.43
25	a	608	BCR	C21-C22	-11.85	1.08	1.35
25	B	620	BCR	C10-C9	11.85	1.63	1.35
25	a	608	BCR	C20-C21	11.85	1.79	1.43
25	C	521	BCR	C10-C9	11.84	1.63	1.35
25	T	101	BCR	C21-C22	-11.83	1.08	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	515	BCR	C37-C22	11.83	1.74	1.50
25	a	608	BCR	C37-C22	11.83	1.74	1.50
25	t	101	BCR	C20-C21	11.82	1.79	1.43
25	C	515	BCR	C10-C9	11.81	1.63	1.35
25	t	101	BCR	C37-C22	11.80	1.74	1.50
25	b	622	BCR	C20-C21	11.80	1.79	1.43
25	c	515	BCR	C10-C9	11.77	1.63	1.35
25	f	101	BCR	C10-C9	11.74	1.62	1.35
25	f	101	BCR	C37-C22	11.73	1.74	1.50
25	K	101	BCR	C10-C9	11.73	1.62	1.35
25	H	101	BCR	C10-C9	11.73	1.62	1.35
25	F	101	BCR	C10-C9	11.71	1.62	1.35
25	b	621	BCR	C20-C21	11.69	1.79	1.43
25	f	101	BCR	C20-C21	11.68	1.79	1.43
25	A	609	BCR	C20-C21	11.63	1.79	1.43
25	c	516	BCR	C8-C7	11.62	1.67	1.33
25	k	101	BCR	C20-C21	11.61	1.79	1.43
25	C	514	BCR	C10-C9	11.58	1.62	1.35
25	A	609	BCR	C8-C7	11.57	1.67	1.33
25	B	620	BCR	C20-C21	11.56	1.79	1.43
25	h	101	BCR	C20-C21	11.53	1.78	1.43
25	f	101	BCR	C8-C7	11.51	1.67	1.33
25	b	621	BCR	C10-C9	11.51	1.62	1.35
25	a	608	BCR	C8-C7	11.47	1.67	1.33
25	B	619	BCR	C10-C9	11.47	1.62	1.35
25	C	514	BCR	C20-C21	11.45	1.78	1.43
25	F	101	BCR	C8-C7	11.44	1.67	1.33
25	c	522	BCR	C20-C21	11.40	1.78	1.43
25	b	620	BCR	C20-C21	11.39	1.78	1.43
25	B	618	BCR	C10-C9	11.38	1.62	1.35
25	t	101	BCR	C8-C7	11.37	1.66	1.33
25	C	515	BCR	C8-C7	11.36	1.66	1.33
25	c	522	BCR	C37-C22	11.35	1.73	1.50
25	C	514	BCR	C37-C22	11.33	1.73	1.50
25	b	620	BCR	C10-C9	11.32	1.62	1.35
25	K	101	BCR	C8-C7	11.31	1.66	1.33
25	k	101	BCR	C8-C7	11.30	1.66	1.33
25	B	618	BCR	C8-C7	11.28	1.66	1.33
25	C	521	BCR	C37-C22	11.26	1.73	1.50
25	c	516	BCR	C20-C21	11.26	1.78	1.43
25	b	620	BCR	C8-C7	11.26	1.66	1.33
25	c	515	BCR	C20-C21	11.23	1.78	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	515	BCR	C20-C21	11.20	1.77	1.43
25	c	522	BCR	C8-C7	11.19	1.66	1.33
25	b	621	BCR	C8-C7	11.17	1.66	1.33
25	B	619	BCR	C8-C7	11.14	1.66	1.33
25	C	521	BCR	C20-C21	11.13	1.77	1.43
25	F	101	BCR	C37-C22	11.11	1.73	1.50
26	a	609	PL9	C18-C19	11.10	1.58	1.33
25	B	619	BCR	C20-C21	11.09	1.77	1.43
25	T	101	BCR	C8-C7	11.06	1.66	1.33
25	H	101	BCR	C8-C7	11.04	1.66	1.33
26	A	610	PL9	C18-C19	11.04	1.58	1.33
26	D	405	PL9	C18-C19	11.04	1.58	1.33
25	H	101	BCR	C37-C22	11.03	1.73	1.50
26	d	404	PL9	C18-C19	11.03	1.58	1.33
25	C	521	BCR	C8-C7	11.01	1.65	1.33
25	F	101	BCR	C20-C21	10.96	1.77	1.43
25	h	101	BCR	C8-C7	10.95	1.65	1.33
25	H	101	BCR	C20-C21	10.93	1.77	1.43
25	b	622	BCR	C8-C7	10.93	1.65	1.33
25	C	514	BCR	C8-C7	10.90	1.65	1.33
25	c	515	BCR	C8-C7	10.88	1.65	1.33
25	B	620	BCR	C8-C7	10.72	1.65	1.33
23	B	611	CLA	C4B-NB	10.54	1.51	1.37
23	B	602	CLA	C4B-NB	10.53	1.51	1.37
23	b	613	CLA	C4B-NB	10.49	1.51	1.37
25	B	619	BCR	C26-C25	10.43	1.52	1.34
23	b	616	CLA	C4B-NB	10.40	1.51	1.37
23	b	604	CLA	C4B-NB	10.40	1.51	1.37
23	D	404	CLA	C4B-NB	10.34	1.51	1.37
26	D	405	PL9	C38-C39	10.33	1.56	1.33
25	T	101	BCR	C16-C17	10.33	1.75	1.43
23	d	403	CLA	C4B-NB	10.28	1.51	1.37
23	B	610	CLA	C4B-NB	10.27	1.51	1.37
26	d	404	PL9	C23-C24	10.27	1.56	1.33
23	B	607[B]	CLA	C4B-NB	10.25	1.51	1.37
23	B	612	CLA	C4B-NB	10.22	1.51	1.37
23	C	504	CLA	C4B-NB	10.21	1.51	1.37
23	b	611	CLA	C4B-NB	10.21	1.51	1.37
26	A	610	PL9	C38-C39	10.21	1.56	1.33
26	D	405	PL9	C23-C24	10.20	1.56	1.33
23	b	607	CLA	C4B-NB	10.20	1.51	1.37
23	c	505	CLA	C4B-NB	10.19	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	404	PL9	C38-C39	10.19	1.56	1.33
23	C	505	CLA	C4B-NB	10.18	1.51	1.37
23	B	614	CLA	C4B-NB	10.17	1.51	1.37
23	B	609	CLA	C4B-NB	10.17	1.51	1.37
23	c	503	CLA	C4B-NB	10.16	1.51	1.37
23	C	511	CLA	C4B-NB	10.16	1.51	1.37
23	c	508	CLA	C4B-NB	10.15	1.51	1.37
23	A	608	CLA	C4B-NB	10.14	1.51	1.37
23	c	511	CLA	C4B-NB	10.13	1.51	1.37
26	A	610	PL9	C23-C24	10.13	1.56	1.33
25	b	621	BCR	C26-C25	10.12	1.51	1.34
26	a	609	PL9	C38-C39	10.11	1.56	1.33
23	B	608	CLA	C4B-NB	10.11	1.51	1.37
23	b	612	CLA	C4B-NB	10.11	1.51	1.37
23	c	504	CLA	C4B-NB	10.11	1.51	1.37
23	b	609[A]	CLA	C4B-NB	10.11	1.51	1.37
23	b	619	CLA	C4B-NB	10.10	1.51	1.37
23	a	607	CLA	C4B-NB	10.09	1.51	1.37
23	B	617	CLA	C4B-NB	10.09	1.51	1.37
23	B	605	CLA	C4B-NB	10.08	1.51	1.37
23	c	502	CLA	C4B-NB	10.08	1.51	1.37
23	b	609[B]	CLA	C4B-NB	10.07	1.51	1.37
23	B	616	CLA	C4B-NB	10.05	1.51	1.37
23	B	615	CLA	C4B-NB	10.05	1.51	1.37
23	C	502	CLA	C4B-NB	10.04	1.51	1.37
23	B	613	CLA	C4B-NB	10.04	1.51	1.37
23	B	607[A]	CLA	C4B-NB	10.04	1.51	1.37
23	b	614	CLA	C4B-NB	10.04	1.51	1.37
23	b	618	CLA	C4B-NB	10.02	1.51	1.37
23	b	617	CLA	C4B-NB	10.01	1.51	1.37
23	C	506	CLA	C4B-NB	10.01	1.51	1.37
23	c	509	CLA	C4B-NB	9.99	1.51	1.37
23	c	513	CLA	C4B-NB	9.98	1.51	1.37
23	c	507	CLA	C4B-NB	9.97	1.51	1.37
23	C	507	CLA	C4B-NB	9.97	1.51	1.37
23	b	606	CLA	C4B-NB	9.96	1.50	1.37
23	A	605	CLA	C4B-NB	9.96	1.50	1.37
23	a	605	CLA	C4B-NB	9.96	1.50	1.37
26	a	609	PL9	C23-C24	9.95	1.56	1.33
23	C	510	CLA	C4B-NB	9.95	1.50	1.37
24	A	607	PHO	C1B-C2B	9.94	1.50	1.39
23	C	503	CLA	C4B-NB	9.94	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	521	BCR	C16-C17	9.94	1.74	1.43
23	b	615	CLA	C4B-NB	9.92	1.50	1.37
23	C	512	CLA	C4B-NB	9.92	1.50	1.37
23	c	510	CLA	C4B-NB	9.92	1.50	1.37
23	B	603	CLA	C4B-NB	9.91	1.50	1.37
23	a	613	CLA	C4B-NB	9.91	1.50	1.37
23	A	606	CLA	C4B-NB	9.91	1.50	1.37
23	c	506	CLA	C4B-NB	9.90	1.50	1.37
23	C	508	CLA	C4B-NB	9.89	1.50	1.37
23	b	605	CLA	C4B-NB	9.89	1.50	1.37
23	b	608	CLA	C4B-NB	9.89	1.50	1.37
23	C	513	CLA	C4B-NB	9.86	1.50	1.37
24	a	606	PHO	C1B-C2B	9.86	1.50	1.39
23	c	512	CLA	C4B-NB	9.86	1.50	1.37
23	C	501	CLA	C4B-NB	9.85	1.50	1.37
23	D	402	CLA	C4B-NB	9.85	1.50	1.37
23	B	606	CLA	C4B-NB	9.85	1.50	1.37
25	b	620	BCR	C16-C17	9.83	1.73	1.43
23	C	509	CLA	C4B-NB	9.82	1.50	1.37
25	f	101	BCR	C16-C17	9.81	1.73	1.43
23	b	610	CLA	C4B-NB	9.78	1.50	1.37
23	d	402	CLA	C4B-NB	9.77	1.50	1.37
23	a	604	CLA	C4B-NB	9.76	1.50	1.37
25	t	101	BCR	C16-C17	9.75	1.73	1.43
23	D	403	CLA	C4B-NB	9.75	1.50	1.37
23	B	604	CLA	C4B-NB	9.74	1.50	1.37
25	h	101	BCR	C16-C17	9.73	1.73	1.43
25	B	618	BCR	C16-C17	9.72	1.73	1.43
23	c	514	CLA	C4B-NB	9.70	1.50	1.37
25	a	608	BCR	C16-C17	9.67	1.73	1.43
25	c	522	BCR	C16-C17	9.65	1.73	1.43
24	D	401	PHO	C1B-C2B	9.62	1.50	1.39
25	F	101	BCR	C26-C25	9.59	1.50	1.34
25	b	622	BCR	C16-C17	9.53	1.72	1.43
24	d	401	PHO	C1B-C2B	9.53	1.50	1.39
25	A	609	BCR	C26-C25	9.52	1.50	1.34
25	A	609	BCR	C16-C17	9.50	1.72	1.43
25	a	608	BCR	C26-C25	9.47	1.50	1.34
25	c	516	BCR	C16-C17	9.46	1.72	1.43
25	H	101	BCR	C16-C17	9.45	1.72	1.43
25	C	515	BCR	C16-C17	9.42	1.72	1.43
25	c	515	BCR	C16-C17	9.38	1.72	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	101	BCR	C26-C25	9.37	1.50	1.34
25	K	101	BCR	C16-C17	9.31	1.72	1.43
26	D	405	PL9	C13-C14	9.31	1.54	1.33
25	B	619	BCR	C16-C17	9.30	1.72	1.43
26	d	404	PL9	C13-C14	9.28	1.54	1.33
24	d	401	PHO	C3B-C4B	9.27	1.50	1.41
25	k	101	BCR	C16-C17	9.19	1.71	1.43
24	D	401	PHO	C3B-C4B	9.15	1.50	1.41
25	B	620	BCR	C16-C17	9.15	1.71	1.43
26	A	610	PL9	C13-C14	9.14	1.54	1.33
25	F	101	BCR	C16-C17	9.11	1.71	1.43
25	C	514	BCR	C16-C17	9.09	1.71	1.43
26	D	405	PL9	C43-C44	9.05	1.53	1.33
26	d	404	PL9	C43-C44	9.04	1.53	1.33
26	a	609	PL9	C28-C29	9.03	1.53	1.33
26	d	404	PL9	C28-C29	9.02	1.53	1.33
26	a	609	PL9	C13-C14	8.95	1.53	1.33
26	A	610	PL9	C43-C44	8.94	1.53	1.33
25	H	101	BCR	C26-C25	8.91	1.49	1.34
26	A	610	PL9	C28-C29	8.89	1.53	1.33
25	b	621	BCR	C16-C17	8.89	1.70	1.43
25	h	101	BCR	C26-C25	8.86	1.49	1.34
26	D	405	PL9	C8-C9	8.84	1.53	1.33
26	d	404	PL9	C8-C9	8.84	1.53	1.33
26	a	609	PL9	C8-C9	8.82	1.53	1.33
24	A	607	PHO	C3B-C4B	8.75	1.50	1.41
26	A	610	PL9	C8-C9	8.75	1.53	1.33
26	D	405	PL9	C28-C29	8.73	1.53	1.33
26	a	609	PL9	C43-C44	8.72	1.53	1.33
26	A	610	PL9	C33-C34	8.59	1.52	1.33
24	a	606	PHO	C3B-C4B	8.54	1.50	1.41
26	a	609	PL9	C48-C49	8.47	1.57	1.32
26	a	609	PL9	C33-C34	8.47	1.52	1.33
25	b	620	BCR	C26-C25	8.42	1.48	1.34
26	D	405	PL9	C48-C49	8.40	1.57	1.32
26	d	404	PL9	C33-C34	8.40	1.52	1.33
26	D	405	PL9	C33-C34	8.35	1.52	1.33
26	d	404	PL9	C48-C49	8.32	1.57	1.32
25	c	516	BCR	C26-C25	8.24	1.48	1.34
26	A	610	PL9	C48-C49	8.17	1.56	1.32
25	k	101	BCR	C26-C25	8.12	1.48	1.34
25	C	515	BCR	C26-C25	8.09	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	BCR	C8-C9	8.07	1.63	1.46
25	c	522	BCR	C26-C25	8.04	1.48	1.34
25	b	622	BCR	C26-C25	8.03	1.48	1.34
25	a	608	BCR	C8-C9	7.99	1.63	1.46
25	C	521	BCR	C26-C25	7.98	1.47	1.34
25	B	620	BCR	C26-C25	7.94	1.47	1.34
33	v	201	HEM	C3D-C2D	7.94	1.53	1.36
23	A	605	CLA	C3A-C2A	-7.92	1.33	1.54
25	K	101	BCR	C26-C25	7.91	1.47	1.34
23	a	604	CLA	C3A-C2A	-7.87	1.33	1.54
25	c	516	BCR	C8-C9	7.84	1.62	1.46
23	a	607	CLA	C3A-C2A	-7.84	1.33	1.54
23	b	611	CLA	C3A-C2A	-7.84	1.33	1.54
25	B	618	BCR	C26-C25	7.83	1.47	1.34
25	C	514	BCR	C26-C25	7.80	1.47	1.34
23	B	609	CLA	C3A-C2A	-7.79	1.33	1.54
23	b	610	CLA	C3A-C2A	-7.77	1.33	1.54
23	B	607[A]	CLA	C3A-C2A	-7.77	1.33	1.54
23	C	510	CLA	C3A-C2A	-7.76	1.33	1.54
23	B	607[B]	CLA	C3A-C2A	-7.76	1.33	1.54
23	b	613	CLA	C3A-C2A	-7.75	1.33	1.54
23	b	615	CLA	C3A-C2A	-7.74	1.33	1.54
23	C	505	CLA	C3A-C2A	-7.74	1.33	1.54
23	D	404	CLA	C3A-C2A	-7.74	1.33	1.54
23	b	607	CLA	C3A-C2A	-7.73	1.33	1.54
25	c	522	BCR	C8-C9	7.73	1.62	1.46
23	b	605	CLA	C3A-C2A	-7.73	1.33	1.54
23	c	511	CLA	C3A-C2A	-7.72	1.33	1.54
23	d	403	CLA	C3A-C2A	-7.72	1.33	1.54
23	c	507	CLA	C3A-C2A	-7.72	1.33	1.54
25	f	101	BCR	C8-C9	7.72	1.62	1.46
33	V	202	HEM	C3D-C2D	7.71	1.53	1.36
23	B	613	CLA	C3A-C2A	-7.71	1.33	1.54
26	D	405	PL9	O1-C4	7.70	1.40	1.23
23	B	611	CLA	C3A-C2A	-7.70	1.33	1.54
33	e	102	HEM	C3D-C2D	7.70	1.53	1.36
23	A	608	CLA	C3A-C2A	-7.70	1.33	1.54
25	C	515	BCR	C8-C9	7.70	1.62	1.46
23	b	609[B]	CLA	C3A-C2A	-7.69	1.33	1.54
25	t	101	BCR	C8-C9	7.69	1.62	1.46
23	D	403	CLA	C3A-C2A	-7.69	1.33	1.54
23	B	615	CLA	C3A-C2A	-7.69	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	C3A-C2A	-7.69	1.33	1.54
23	D	402	CLA	C3A-C2A	-7.68	1.33	1.54
23	B	614	CLA	C3A-C2A	-7.68	1.33	1.54
26	d	404	PL9	O1-C4	7.67	1.40	1.23
23	C	508	CLA	C3A-C2A	-7.67	1.33	1.54
23	b	606	CLA	C3A-C2A	-7.66	1.33	1.54
23	b	612	CLA	C3A-C2A	-7.65	1.33	1.54
23	C	512	CLA	C3A-C2A	-7.64	1.33	1.54
23	b	604	CLA	C3A-C2A	-7.64	1.33	1.54
23	C	501	CLA	C3A-C2A	-7.64	1.33	1.54
23	c	513	CLA	C3A-C2A	-7.64	1.33	1.54
23	B	605	CLA	C3A-C2A	-7.64	1.33	1.54
23	b	616	CLA	C3A-C2A	-7.64	1.33	1.54
23	d	402	CLA	C3A-C2A	-7.63	1.33	1.54
23	b	619	CLA	C3A-C2A	-7.63	1.33	1.54
23	C	502	CLA	C3A-C2A	-7.63	1.33	1.54
25	T	101	BCR	C8-C9	7.63	1.62	1.46
33	E	102	HEM	C3D-C2D	7.63	1.53	1.36
23	B	603	CLA	C3A-C2A	-7.63	1.33	1.54
23	c	512	CLA	C3A-C2A	-7.62	1.33	1.54
23	c	506	CLA	C3A-C2A	-7.62	1.33	1.54
23	a	613	CLA	C3A-C2A	-7.62	1.33	1.54
23	b	609[A]	CLA	C3A-C2A	-7.62	1.33	1.54
23	b	614	CLA	C3A-C2A	-7.61	1.33	1.54
23	c	503	CLA	C3A-C2A	-7.60	1.33	1.54
23	B	606	CLA	C3A-C2A	-7.60	1.33	1.54
23	b	608	CLA	C3A-C2A	-7.60	1.33	1.54
23	a	605	CLA	C3A-C2A	-7.60	1.33	1.54
23	C	503	CLA	C3A-C2A	-7.59	1.33	1.54
23	C	511	CLA	C3A-C2A	-7.59	1.33	1.54
25	c	515	BCR	C26-C25	7.59	1.47	1.34
23	B	612	CLA	C3A-C2A	-7.58	1.34	1.54
23	c	514	CLA	C3A-C2A	-7.58	1.34	1.54
23	B	608	CLA	C3A-C2A	-7.58	1.34	1.54
23	B	604	CLA	C3A-C2A	-7.57	1.34	1.54
23	c	502	CLA	C3A-C2A	-7.57	1.34	1.54
25	K	101	BCR	C8-C9	7.57	1.62	1.46
23	b	618	CLA	C3A-C2A	-7.57	1.34	1.54
23	c	509	CLA	C3A-C2A	-7.57	1.34	1.54
23	c	510	CLA	C3A-C2A	-7.55	1.34	1.54
23	C	504	CLA	C3A-C2A	-7.54	1.34	1.54
23	C	506	CLA	C3A-C2A	-7.54	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	606	CLA	C3A-C2A	-7.54	1.34	1.54
23	B	617	CLA	C3A-C2A	-7.54	1.34	1.54
25	h	101	BCR	C8-C9	7.53	1.62	1.46
23	c	505	CLA	C3A-C2A	-7.53	1.34	1.54
23	B	610	CLA	C3A-C2A	-7.53	1.34	1.54
23	B	602	CLA	C3A-C2A	-7.53	1.34	1.54
25	k	101	BCR	C8-C9	7.52	1.62	1.46
23	C	509	CLA	C3A-C2A	-7.51	1.34	1.54
23	b	614	CLA	MG-ND	-7.50	1.90	2.05
23	c	504	CLA	C3A-C2A	-7.50	1.34	1.54
25	F	101	BCR	C8-C9	7.47	1.61	1.46
23	b	619	CLA	MG-ND	-7.46	1.91	2.05
25	H	101	BCR	C8-C9	7.46	1.61	1.46
23	C	513	CLA	C3A-C2A	-7.44	1.34	1.54
25	t	101	BCR	C26-C25	7.43	1.47	1.34
25	c	515	BCR	C34-C9	-7.42	1.35	1.50
23	B	616	CLA	C3A-C2A	-7.41	1.34	1.54
23	c	508	CLA	C3A-C2A	-7.41	1.34	1.54
23	b	615	CLA	MG-ND	-7.38	1.91	2.05
23	A	606	CLA	MG-ND	-7.38	1.91	2.05
25	C	521	BCR	C8-C9	7.38	1.61	1.46
25	T	101	BCR	C26-C25	7.36	1.46	1.34
25	B	618	BCR	C34-C9	-7.35	1.36	1.50
25	B	619	BCR	C8-C9	7.34	1.61	1.46
23	C	507	CLA	C3A-C2A	-7.33	1.34	1.54
25	B	619	BCR	C34-C9	-7.33	1.36	1.50
26	A	610	PL9	O1-C4	7.33	1.39	1.23
25	K	101	BCR	C34-C9	-7.32	1.36	1.50
25	b	621	BCR	C34-C9	-7.32	1.36	1.50
23	B	613	CLA	MG-ND	-7.31	1.91	2.05
26	a	609	PL9	O1-C4	7.29	1.39	1.23
23	a	607	CLA	MG-ND	-7.27	1.91	2.05
23	B	612	CLA	MG-ND	-7.27	1.91	2.05
23	c	506	CLA	MG-ND	-7.24	1.91	2.05
25	b	622	BCR	C8-C9	7.24	1.61	1.46
25	k	101	BCR	C34-C9	-7.23	1.36	1.50
23	a	613	CLA	MG-ND	-7.22	1.91	2.05
23	b	606	CLA	MG-ND	-7.21	1.91	2.05
25	b	621	BCR	C8-C9	7.21	1.61	1.46
23	C	510	CLA	MG-ND	-7.19	1.91	2.05
23	c	508	CLA	MG-ND	-7.19	1.91	2.05
23	C	509	CLA	MG-ND	-7.19	1.91	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	MG-ND	-7.18	1.91	2.05
25	c	516	BCR	C34-C9	-7.17	1.36	1.50
25	c	515	BCR	C8-C9	7.16	1.61	1.46
23	B	607[A]	CLA	MG-ND	-7.16	1.91	2.05
23	B	605	CLA	MG-ND	-7.15	1.91	2.05
23	B	607[B]	CLA	MG-ND	-7.15	1.91	2.05
23	c	510	CLA	MG-ND	-7.15	1.91	2.05
23	b	613	CLA	MG-ND	-7.14	1.91	2.05
23	b	609[B]	CLA	MG-ND	-7.14	1.91	2.05
25	f	101	BCR	C38-C26	7.14	1.62	1.50
23	B	616	CLA	MG-ND	-7.13	1.91	2.05
25	b	620	BCR	C8-C9	7.13	1.61	1.46
23	C	513	CLA	MG-ND	-7.13	1.91	2.05
23	b	610	CLA	MG-ND	-7.12	1.91	2.05
23	C	511	CLA	MG-ND	-7.11	1.91	2.05
23	c	511	CLA	MG-ND	-7.11	1.91	2.05
23	a	604	CLA	MG-ND	-7.11	1.91	2.05
23	C	507	CLA	MG-ND	-7.11	1.91	2.05
23	C	505	CLA	MG-ND	-7.10	1.91	2.05
25	B	618	BCR	C8-C9	7.10	1.61	1.46
25	B	620	BCR	C34-C9	-7.10	1.36	1.50
23	b	617	CLA	MG-ND	-7.09	1.91	2.05
23	D	402	CLA	MG-ND	-7.08	1.91	2.05
23	C	503	CLA	MG-ND	-7.08	1.91	2.05
23	c	503	CLA	MG-ND	-7.08	1.91	2.05
33	E	102	HEM	FE-ND	7.07	2.16	1.94
23	C	502	CLA	MG-ND	-7.07	1.91	2.05
23	a	605	CLA	MG-ND	-7.07	1.91	2.05
23	b	607	CLA	MG-ND	-7.07	1.91	2.05
25	H	101	BCR	C34-C9	-7.06	1.36	1.50
25	b	620	BCR	C34-C9	-7.06	1.36	1.50
25	C	515	BCR	C34-C9	-7.06	1.36	1.50
25	C	514	BCR	C8-C9	7.05	1.61	1.46
23	B	608	CLA	MG-ND	-7.05	1.91	2.05
23	b	608	CLA	MG-ND	-7.05	1.91	2.05
23	b	609[A]	CLA	MG-ND	-7.05	1.91	2.05
23	C	508	CLA	MG-ND	-7.05	1.91	2.05
23	b	605	CLA	MG-ND	-7.04	1.91	2.05
23	B	604	CLA	MG-ND	-7.04	1.91	2.05
23	C	506	CLA	MG-ND	-7.04	1.91	2.05
23	A	605	CLA	MG-ND	-7.04	1.91	2.05
23	D	404	CLA	MG-ND	-7.04	1.91	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	101	BCR	C34-C9	-7.04	1.36	1.50
23	c	507	CLA	MG-ND	-7.03	1.91	2.05
23	c	513	CLA	MG-ND	-7.02	1.91	2.05
25	B	620	BCR	C8-C9	7.02	1.61	1.46
25	T	101	BCR	C34-C9	-7.02	1.36	1.50
25	t	101	BCR	C34-C9	-7.02	1.36	1.50
25	C	514	BCR	C34-C9	-7.01	1.36	1.50
23	b	612	CLA	MG-ND	-7.01	1.91	2.05
25	a	608	BCR	C34-C9	-7.01	1.36	1.50
23	B	614	CLA	MG-ND	-7.01	1.91	2.05
23	B	603	CLA	MG-ND	-7.01	1.91	2.05
23	B	617	CLA	MG-ND	-7.01	1.91	2.05
23	d	402	CLA	MG-ND	-7.01	1.91	2.05
25	F	101	BCR	C38-C26	7.00	1.62	1.50
23	B	610	CLA	MG-ND	-6.99	1.91	2.05
23	c	512	CLA	MG-ND	-6.99	1.91	2.05
25	F	101	BCR	C34-C9	-6.99	1.36	1.50
23	B	615	CLA	MG-ND	-6.99	1.91	2.05
23	B	609	CLA	MG-ND	-6.98	1.91	2.05
25	A	609	BCR	C34-C9	-6.96	1.36	1.50
23	C	504	CLA	MG-ND	-6.96	1.92	2.05
25	h	101	BCR	C34-C9	-6.95	1.36	1.50
23	A	608	CLA	MG-ND	-6.95	1.92	2.05
23	b	616	CLA	MG-ND	-6.95	1.92	2.05
25	C	521	BCR	C34-C9	-6.95	1.36	1.50
23	c	505	CLA	MG-ND	-6.94	1.92	2.05
23	B	611	CLA	MG-ND	-6.94	1.92	2.05
25	b	622	BCR	C34-C9	-6.92	1.36	1.50
23	c	509	CLA	MG-ND	-6.92	1.92	2.05
23	b	611	CLA	MG-ND	-6.92	1.92	2.05
23	c	502	CLA	MG-ND	-6.91	1.92	2.05
23	b	604	CLA	MG-ND	-6.91	1.92	2.05
23	C	512	CLA	MG-ND	-6.90	1.92	2.05
23	b	618	CLA	MG-ND	-6.90	1.92	2.05
25	c	522	BCR	C34-C9	-6.89	1.36	1.50
23	C	501	CLA	MG-ND	-6.88	1.92	2.05
23	B	606	CLA	MG-ND	-6.83	1.92	2.05
23	B	602	CLA	MG-ND	-6.83	1.92	2.05
25	A	609	BCR	C38-C26	6.82	1.61	1.50
23	c	514	CLA	MG-ND	-6.81	1.92	2.05
23	c	504	CLA	MG-ND	-6.80	1.92	2.05
23	d	403	CLA	MG-ND	-6.75	1.92	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	h	101	BCR	C38-C26	6.74	1.61	1.50
25	H	101	BCR	C38-C26	6.71	1.61	1.50
25	a	608	BCR	C38-C26	6.69	1.61	1.50
25	B	619	BCR	C38-C26	6.68	1.61	1.50
26	a	609	PL9	O2-C1	6.60	1.42	1.24
25	b	621	BCR	C38-C26	6.57	1.61	1.50
26	A	610	PL9	O2-C1	6.53	1.41	1.24
23	b	607	CLA	C1B-NB	-6.50	1.29	1.37
23	b	606	CLA	C1B-NB	-6.48	1.29	1.37
23	b	610	CLA	C1B-NB	-6.48	1.29	1.37
23	d	402	CLA	C1B-NB	-6.46	1.29	1.37
23	B	612	CLA	C1B-NB	-6.46	1.29	1.37
23	D	403	CLA	C1B-NB	-6.46	1.29	1.37
23	C	508	CLA	C1B-NB	-6.45	1.29	1.37
23	c	507	CLA	C1B-NB	-6.45	1.29	1.37
23	b	614	CLA	C1B-NB	-6.44	1.29	1.37
23	B	604	CLA	C1B-NB	-6.43	1.29	1.37
26	D	405	PL9	O2-C1	6.40	1.41	1.24
23	B	605	CLA	C1B-NB	-6.39	1.29	1.37
23	C	509	CLA	C1B-NB	-6.38	1.29	1.37
25	c	522	BCR	C38-C26	6.37	1.61	1.50
23	B	613	CLA	C1B-NB	-6.37	1.29	1.37
23	b	615	CLA	C1B-NB	-6.36	1.29	1.37
23	b	605	CLA	C1B-NB	-6.35	1.29	1.37
25	C	515	BCR	C38-C26	6.34	1.61	1.50
25	c	516	BCR	C38-C26	6.30	1.61	1.50
23	C	502	CLA	C1B-NB	-6.28	1.29	1.37
23	c	509	CLA	C1B-NB	-6.26	1.29	1.37
23	c	502	CLA	C1B-NB	-6.25	1.29	1.37
26	d	404	PL9	O2-C1	6.25	1.41	1.24
25	C	521	BCR	C38-C26	6.24	1.60	1.50
23	A	606	CLA	C1B-NB	-6.23	1.29	1.37
25	B	618	BCR	C23-C22	6.21	1.59	1.46
23	C	510	CLA	C1B-NB	-6.21	1.29	1.37
25	k	101	BCR	C38-C26	6.21	1.60	1.50
25	B	620	BCR	C38-C26	6.21	1.60	1.50
23	C	512	CLA	C1B-NB	-6.19	1.29	1.37
23	B	614	CLA	C1B-NB	-6.19	1.29	1.37
23	b	609[B]	CLA	C1B-NB	-6.19	1.29	1.37
23	c	510	CLA	C1B-NB	-6.18	1.29	1.37
23	a	604	CLA	C1B-NB	-6.18	1.29	1.37
25	b	622	BCR	C38-C26	6.18	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C1B-NB	-6.18	1.29	1.37
23	B	603	CLA	C1B-NB	-6.17	1.29	1.37
23	a	605	CLA	C1B-NB	-6.17	1.29	1.37
25	b	622	BCR	C23-C22	6.16	1.59	1.46
23	c	513	CLA	C1B-NB	-6.15	1.29	1.37
23	c	506	CLA	C1D-C2D	-6.14	1.33	1.45
23	C	501	CLA	C1B-NB	-6.13	1.29	1.37
23	a	613	CLA	C1B-NB	-6.11	1.29	1.37
25	K	101	BCR	C38-C26	6.09	1.60	1.50
23	A	605	CLA	C1B-NB	-6.08	1.29	1.37
23	b	617	CLA	C1B-NB	-6.07	1.29	1.37
23	c	506	CLA	C1B-NB	-6.07	1.29	1.37
23	D	402	CLA	C1B-NB	-6.07	1.29	1.37
23	c	512	CLA	C1B-NB	-6.06	1.29	1.37
23	b	606	CLA	C1D-C2D	-6.06	1.33	1.45
23	b	608	CLA	C1B-NB	-6.05	1.29	1.37
23	B	607[A]	CLA	C1B-NB	-6.05	1.29	1.37
23	c	511	CLA	C1B-NB	-6.04	1.29	1.37
25	b	620	BCR	C38-C26	6.03	1.60	1.50
23	C	505	CLA	C1B-NB	-6.02	1.30	1.37
25	B	620	BCR	C23-C22	6.02	1.58	1.46
23	C	506	CLA	C1B-NB	-6.02	1.30	1.37
23	c	514	CLA	C1B-NB	-6.02	1.30	1.37
25	C	514	BCR	C38-C26	6.01	1.60	1.50
23	C	504	CLA	C1B-NB	-6.01	1.30	1.37
23	B	607[B]	CLA	C1B-NB	-6.00	1.30	1.37
23	C	511	CLA	C1B-NB	-6.00	1.30	1.37
23	b	616	CLA	C1B-NB	-5.99	1.30	1.37
23	b	609[A]	CLA	C1B-NB	-5.98	1.30	1.37
23	B	615	CLA	C1B-NB	-5.97	1.30	1.37
23	c	503	CLA	C1B-NB	-5.97	1.30	1.37
23	B	606	CLA	C1B-NB	-5.96	1.30	1.37
23	C	513	CLA	C1B-NB	-5.95	1.30	1.37
23	A	608	CLA	C1B-NB	-5.95	1.30	1.37
25	T	101	BCR	C38-C26	5.95	1.60	1.50
23	B	617	CLA	C1B-NB	-5.94	1.30	1.37
23	b	619	CLA	C1B-NB	-5.94	1.30	1.37
23	c	505	CLA	C1B-NB	-5.94	1.30	1.37
23	a	607	CLA	C1B-NB	-5.93	1.30	1.37
23	d	403	CLA	C1B-NB	-5.93	1.30	1.37
25	c	515	BCR	C38-C26	5.92	1.60	1.50
23	C	505	CLA	C1D-C2D	-5.92	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	618	BCR	C38-C26	5.90	1.60	1.50
23	b	618	CLA	C1B-NB	-5.90	1.30	1.37
23	b	613	CLA	C1B-NB	-5.90	1.30	1.37
25	t	101	BCR	C38-C26	5.89	1.60	1.50
23	D	404	CLA	C1B-NB	-5.89	1.30	1.37
23	c	504	CLA	C1B-NB	-5.88	1.30	1.37
33	e	102	HEM	FE-ND	5.86	2.12	1.94
23	B	604	CLA	C1D-C2D	-5.85	1.33	1.45
23	B	616	CLA	C1B-NB	-5.85	1.30	1.37
23	c	508	CLA	C1B-NB	-5.84	1.30	1.37
23	B	611	CLA	C1B-NB	-5.84	1.30	1.37
23	B	608	CLA	C1B-NB	-5.79	1.30	1.37
23	B	602	CLA	C1B-NB	-5.76	1.30	1.37
23	b	604	CLA	C1B-NB	-5.74	1.30	1.37
23	B	609	CLA	C1B-NB	-5.74	1.30	1.37
23	B	610	CLA	C1B-NB	-5.73	1.30	1.37
23	b	611	CLA	C1B-NB	-5.72	1.30	1.37
23	C	507	CLA	C1B-NB	-5.71	1.30	1.37
23	C	508	CLA	C1D-C2D	-5.71	1.34	1.45
25	T	101	BCR	C23-C22	5.70	1.58	1.46
23	a	607	CLA	C1D-C2D	-5.66	1.34	1.45
23	d	402	CLA	C1D-C2D	-5.65	1.34	1.45
26	d	404	PL9	C3-C4	-5.64	1.40	1.49
25	K	101	BCR	C23-C22	5.64	1.58	1.46
23	B	605	CLA	C1D-C2D	-5.63	1.34	1.45
23	b	619	CLA	C1D-C2D	-5.63	1.34	1.45
25	t	101	BCR	C23-C22	5.63	1.58	1.46
23	B	613	CLA	C1D-C2D	-5.62	1.34	1.45
23	b	614	CLA	C1D-C2D	-5.62	1.34	1.45
23	b	609[B]	CLA	C1D-C2D	-5.62	1.34	1.45
23	B	606	CLA	C1D-C2D	-5.61	1.34	1.45
23	b	608	CLA	C1D-C2D	-5.60	1.34	1.45
23	b	615	CLA	C1D-C2D	-5.59	1.34	1.45
25	b	621	BCR	C24-C23	5.58	1.49	1.33
23	C	511	CLA	C1D-C2D	-5.57	1.34	1.45
23	b	612	CLA	C1D-C2D	-5.57	1.34	1.45
23	C	506	CLA	C1D-C2D	-5.56	1.34	1.45
23	D	403	CLA	C1D-C2D	-5.56	1.34	1.45
23	c	507	CLA	C1D-C2D	-5.55	1.34	1.45
23	C	509	CLA	C1D-C2D	-5.54	1.34	1.45
25	C	521	BCR	C24-C23	5.54	1.49	1.33
23	C	512	CLA	C1D-C2D	-5.54	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C1D-C2D	-5.54	1.34	1.45
23	B	607[B]	CLA	C1D-C2D	-5.54	1.34	1.45
23	c	505	CLA	C1D-C2D	-5.53	1.34	1.45
25	c	522	BCR	C24-C23	5.53	1.49	1.33
25	C	514	BCR	C23-C22	5.51	1.57	1.46
25	h	101	BCR	C23-C22	5.51	1.57	1.46
25	k	101	BCR	C23-C22	5.51	1.57	1.46
23	b	607	CLA	C1D-C2D	-5.51	1.34	1.45
23	B	616	CLA	C1D-C2D	-5.51	1.34	1.45
25	c	516	BCR	C23-C22	5.50	1.57	1.46
23	b	605	CLA	C1D-C2D	-5.49	1.34	1.45
25	B	618	BCR	C24-C23	5.49	1.49	1.33
23	B	603	CLA	C1D-C2D	-5.49	1.34	1.45
23	b	617	CLA	C1D-C2D	-5.49	1.34	1.45
23	b	616	CLA	C1D-C2D	-5.48	1.34	1.45
23	b	610	CLA	C1D-C2D	-5.48	1.34	1.45
23	c	509	CLA	C1D-C2D	-5.48	1.34	1.45
25	b	621	BCR	C23-C22	5.48	1.57	1.46
23	b	618	CLA	C1D-C2D	-5.47	1.34	1.45
23	b	612	CLA	C1B-NB	-5.47	1.30	1.37
23	b	613	CLA	C1D-C2D	-5.47	1.34	1.45
23	b	609[A]	CLA	C1D-C2D	-5.47	1.34	1.45
25	F	101	BCR	C24-C23	5.47	1.49	1.33
23	C	507	CLA	C1D-C2D	-5.47	1.34	1.45
23	B	607[A]	CLA	C1D-C2D	-5.46	1.34	1.45
23	B	612	CLA	C1D-C2D	-5.45	1.34	1.45
23	B	611	CLA	C1D-C2D	-5.45	1.34	1.45
23	c	513	CLA	C1D-C2D	-5.45	1.34	1.45
23	A	606	CLA	C1D-C2D	-5.45	1.34	1.45
23	C	503	CLA	C1D-C2D	-5.44	1.34	1.45
23	c	510	CLA	C1D-C2D	-5.43	1.34	1.45
23	c	514	CLA	C1D-C2D	-5.43	1.34	1.45
23	c	508	CLA	C1D-C2D	-5.43	1.34	1.45
25	B	619	BCR	C24-C23	5.43	1.49	1.33
23	C	513	CLA	C1D-C2D	-5.43	1.34	1.45
23	a	605	CLA	C1D-C2D	-5.42	1.34	1.45
25	B	620	BCR	C24-C23	5.41	1.49	1.33
23	B	617	CLA	C1D-C2D	-5.40	1.34	1.45
23	c	503	CLA	C1D-C2D	-5.39	1.34	1.45
23	B	608	CLA	C1D-C2D	-5.39	1.34	1.45
33	V	202	HEM	FE-ND	5.38	2.11	1.94
25	c	516	BCR	C11-C12	5.38	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C1D-C2D	-5.38	1.34	1.45
23	A	605	CLA	C1D-C2D	-5.38	1.34	1.45
23	D	402	CLA	C1D-C2D	-5.38	1.34	1.45
23	b	604	CLA	C1D-C2D	-5.37	1.34	1.45
23	C	501	CLA	C1D-C2D	-5.37	1.34	1.45
23	c	502	CLA	C1D-C2D	-5.37	1.34	1.45
23	c	504	CLA	C1D-C2D	-5.37	1.34	1.45
23	a	604	CLA	C1D-C2D	-5.37	1.34	1.45
25	C	515	BCR	C23-C22	5.36	1.57	1.46
23	A	608	CLA	C1D-C2D	-5.36	1.34	1.45
25	a	608	BCR	C24-C23	5.35	1.49	1.33
25	f	101	BCR	C24-C23	5.35	1.49	1.33
23	B	610	CLA	C1D-C2D	-5.35	1.34	1.45
25	b	622	BCR	C24-C23	5.35	1.49	1.33
23	C	504	CLA	C1D-C2D	-5.34	1.34	1.45
23	d	403	CLA	C1D-C2D	-5.34	1.34	1.45
26	A	610	PL9	C3-C4	-5.33	1.41	1.49
25	t	101	BCR	C24-C23	5.33	1.48	1.33
23	a	613	CLA	CHC-C4B	-5.32	1.27	1.39
25	t	101	BCR	C11-C12	5.32	1.48	1.34
26	D	405	PL9	C3-C4	-5.32	1.41	1.49
23	D	404	CLA	C1D-C2D	-5.32	1.34	1.45
25	T	101	BCR	C11-C12	5.31	1.48	1.34
23	B	609	CLA	C1D-C2D	-5.31	1.34	1.45
25	C	521	BCR	C23-C22	5.31	1.57	1.46
23	B	615	CLA	C1D-C2D	-5.31	1.34	1.45
25	c	522	BCR	C23-C22	5.31	1.57	1.46
23	B	605	CLA	CHC-C4B	-5.31	1.27	1.39
23	c	512	CLA	C1D-C2D	-5.30	1.34	1.45
23	C	502	CLA	C1D-C2D	-5.28	1.34	1.45
23	C	510	CLA	C1D-C2D	-5.28	1.34	1.45
23	b	610	CLA	CHC-C4B	-5.27	1.27	1.39
25	h	101	BCR	C11-C12	5.26	1.48	1.34
25	f	101	BCR	C23-C22	5.26	1.57	1.46
23	B	602	CLA	C1D-C2D	-5.26	1.34	1.45
25	k	101	BCR	C24-C23	5.26	1.48	1.33
25	a	608	BCR	C11-C12	5.25	1.48	1.34
23	a	613	CLA	C1D-C2D	-5.25	1.35	1.45
23	b	614	CLA	CHC-C4B	-5.24	1.27	1.39
25	c	516	BCR	C24-C23	5.24	1.48	1.33
26	a	609	PL9	C3-C4	-5.24	1.41	1.49
25	A	609	BCR	C11-C12	5.24	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	BCR	C24-C23	5.24	1.48	1.33
25	K	101	BCR	C24-C23	5.23	1.48	1.33
25	c	515	BCR	C23-C22	5.22	1.57	1.46
25	c	522	BCR	C11-C12	5.21	1.48	1.34
23	B	617	CLA	CHC-C4B	-5.20	1.27	1.39
25	C	515	BCR	C24-C23	5.19	1.48	1.33
25	C	514	BCR	C24-C23	5.17	1.48	1.33
25	k	101	BCR	C11-C12	5.17	1.48	1.34
25	A	609	BCR	C23-C22	5.16	1.57	1.46
25	B	619	BCR	C24-C25	5.15	1.62	1.45
23	b	607	CLA	CHC-C4B	-5.15	1.27	1.39
25	C	515	BCR	C11-C12	5.14	1.48	1.34
23	c	510	CLA	CHC-C4B	-5.14	1.27	1.39
23	B	608	CLA	CHC-C4B	-5.13	1.27	1.39
23	b	606	CLA	CHC-C4B	-5.12	1.27	1.39
23	b	611	CLA	C1D-C2D	-5.12	1.35	1.45
23	c	513	CLA	CHC-C4B	-5.12	1.27	1.39
23	B	614	CLA	CHC-C4B	-5.12	1.27	1.39
25	H	101	BCR	C11-C12	5.11	1.48	1.34
23	B	612	CLA	CHC-C4B	-5.10	1.28	1.39
25	b	622	BCR	C11-C12	5.10	1.48	1.34
23	C	512	CLA	CHC-C4B	-5.10	1.28	1.39
23	C	510	CLA	CHC-C4B	-5.09	1.28	1.39
23	b	614	CLA	MG-NB	-5.09	1.95	2.05
23	b	619	CLA	CHC-C4B	-5.08	1.28	1.39
23	B	604	CLA	CHC-C4B	-5.07	1.28	1.39
23	C	504	CLA	CHC-C4B	-5.07	1.28	1.39
23	b	615	CLA	CHC-C4B	-5.07	1.28	1.39
23	C	508	CLA	CHC-C4B	-5.06	1.28	1.39
23	B	613	CLA	CHC-C4B	-5.06	1.28	1.39
25	F	101	BCR	C24-C25	5.06	1.62	1.45
23	a	613	CLA	CHD-C1D	5.05	1.48	1.38
25	a	608	BCR	C23-C22	5.04	1.56	1.46
23	C	509	CLA	CHC-C4B	-5.03	1.28	1.39
23	c	511	CLA	CHC-C4B	-5.03	1.28	1.39
23	D	402	CLA	CHC-C4B	-5.03	1.28	1.39
25	b	621	BCR	C24-C25	5.03	1.62	1.45
23	C	506	CLA	CHC-C4B	-5.03	1.28	1.39
23	D	402	CLA	CHD-C1D	5.02	1.48	1.38
25	C	521	BCR	C11-C12	5.02	1.47	1.34
23	C	507	CLA	CHC-C4B	-5.02	1.28	1.39
23	C	502	CLA	MG-NB	-5.02	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	CHC-C4B	-5.02	1.28	1.39
23	b	616	CLA	CHC-C4B	-5.01	1.28	1.39
23	B	606	CLA	CHC-C4B	-5.01	1.28	1.39
23	c	506	CLA	CHC-C4B	-5.01	1.28	1.39
23	a	605	CLA	CHC-C4B	-5.01	1.28	1.39
25	F	101	BCR	C23-C22	5.01	1.56	1.46
25	B	620	BCR	C11-C12	5.00	1.47	1.34
23	c	503	CLA	CHC-C4B	-5.00	1.28	1.39
23	B	602	CLA	CHC-C4B	-5.00	1.28	1.39
23	c	508	CLA	CHC-C4B	-5.00	1.28	1.39
23	b	604	CLA	CHC-C4B	-5.00	1.28	1.39
23	B	610	CLA	CHC-C4B	-4.99	1.28	1.39
23	c	512	CLA	CHC-C4B	-4.98	1.28	1.39
23	b	617	CLA	CHC-C4B	-4.98	1.28	1.39
23	A	606	CLA	CHC-C4B	-4.98	1.28	1.39
23	B	612	CLA	MG-NB	-4.97	1.95	2.05
23	a	604	CLA	CHC-C4B	-4.96	1.28	1.39
23	D	403	CLA	CHC-C4B	-4.96	1.28	1.39
23	c	505	CLA	CHC-C4B	-4.96	1.28	1.39
23	C	501	CLA	CHC-C4B	-4.96	1.28	1.39
23	b	607	CLA	CHD-C1D	4.96	1.48	1.38
23	B	616	CLA	CHC-C4B	-4.96	1.28	1.39
25	a	608	BCR	C24-C25	4.96	1.62	1.45
25	c	515	BCR	C24-C23	4.95	1.47	1.33
23	c	514	CLA	CHD-C1D	4.94	1.48	1.38
23	c	507	CLA	CHC-C4B	-4.94	1.28	1.39
23	C	503	CLA	CHC-C4B	-4.94	1.28	1.39
23	d	403	CLA	CHC-C4B	-4.93	1.28	1.39
25	H	101	BCR	C24-C23	4.93	1.47	1.33
23	c	504	CLA	CHC-C4B	-4.93	1.28	1.39
23	B	607[A]	CLA	CHC-C4B	-4.93	1.28	1.39
23	C	502	CLA	CHC-C4B	-4.93	1.28	1.39
23	b	609[A]	CLA	CHD-C1D	4.93	1.48	1.38
25	T	101	BCR	C24-C23	4.92	1.47	1.33
23	D	404	CLA	CHC-C4B	-4.92	1.28	1.39
23	B	609	CLA	CHC-C4B	-4.92	1.28	1.39
25	b	620	BCR	C24-C23	4.91	1.47	1.33
23	b	608	CLA	CHC-C4B	-4.91	1.28	1.39
23	b	618	CLA	CHC-C4B	-4.90	1.28	1.39
23	c	502	CLA	MG-NB	-4.90	1.96	2.05
23	C	511	CLA	CHC-C4B	-4.90	1.28	1.39
23	B	610	CLA	CHD-C1D	4.90	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	CHC-C4B	-4.90	1.28	1.39
23	C	505	CLA	CHD-C1D	4.90	1.48	1.38
25	K	101	BCR	C11-C12	4.90	1.47	1.34
23	C	513	CLA	CHD-C1D	4.90	1.48	1.38
26	d	404	PL9	C6-C1	-4.89	1.40	1.48
23	b	606	CLA	MG-NB	-4.89	1.96	2.05
23	c	502	CLA	CHD-C1D	4.89	1.48	1.38
23	B	604	CLA	CHD-C1D	4.89	1.48	1.38
23	c	509	CLA	CHC-C4B	-4.89	1.28	1.39
23	B	604	CLA	MG-NB	-4.88	1.96	2.05
23	B	615	CLA	CHC-C4B	-4.88	1.28	1.39
26	D	405	PL9	C6-C1	-4.88	1.40	1.48
23	D	403	CLA	MG-NB	-4.88	1.96	2.05
23	b	611	CLA	CHD-C1D	4.87	1.47	1.38
25	f	101	BCR	C24-C25	4.87	1.61	1.45
25	b	620	BCR	C23-C22	4.87	1.56	1.46
23	b	608	CLA	MG-NB	-4.87	1.96	2.05
23	b	609[B]	CLA	CHC-C4B	-4.87	1.28	1.39
23	b	612	CLA	CHC-C4B	-4.87	1.28	1.39
24	d	401	PHO	C1D-C2D	4.87	1.44	1.39
23	B	602	CLA	CHD-C1D	4.86	1.47	1.38
23	B	603	CLA	CHC-C4B	-4.86	1.28	1.39
23	B	612	CLA	CHD-C1D	4.86	1.47	1.38
25	B	618	BCR	C11-C12	4.86	1.47	1.34
25	c	515	BCR	C11-C12	4.86	1.47	1.34
23	B	615	CLA	CHD-C1D	4.86	1.47	1.38
23	B	608	CLA	CHD-C1D	4.86	1.47	1.38
23	B	603	CLA	CHD-C1D	4.85	1.47	1.38
23	b	605	CLA	CHC-C4B	-4.85	1.28	1.39
23	C	511	CLA	CHB-C1B	4.85	1.50	1.39
23	a	607	CLA	CHD-C4C	-4.85	1.28	1.39
23	A	608	CLA	CHD-C1D	4.85	1.47	1.38
33	e	102	HEM	FE-NA	4.85	2.11	1.95
23	c	507	CLA	CHD-C1D	4.84	1.47	1.38
25	A	609	BCR	C24-C25	4.84	1.61	1.45
23	A	606	CLA	CHD-C1D	4.84	1.47	1.38
23	c	512	CLA	CHD-C1D	4.84	1.47	1.38
23	B	613	CLA	MG-NB	-4.84	1.96	2.05
23	C	510	CLA	CHD-C1D	4.84	1.47	1.38
23	B	609	CLA	CHD-C1D	4.84	1.47	1.38
23	C	501	CLA	CHD-C1D	4.84	1.47	1.38
23	a	605	CLA	CHD-C1D	4.84	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	CHC-C4B	-4.83	1.28	1.39
23	C	503	CLA	MG-NB	-4.83	1.96	2.05
23	c	514	CLA	CHC-C4B	-4.83	1.28	1.39
23	c	512	CLA	MG-NB	-4.83	1.96	2.05
23	c	512	CLA	CHB-C1B	4.83	1.50	1.39
23	c	503	CLA	CHD-C1D	4.83	1.47	1.38
23	b	609[A]	CLA	CHC-C4B	-4.83	1.28	1.39
23	C	504	CLA	CHD-C1D	4.82	1.47	1.38
23	A	605	CLA	CHC-C4B	-4.82	1.28	1.39
23	c	506	CLA	CHB-C1B	4.82	1.50	1.39
23	C	505	CLA	CHC-C4B	-4.82	1.28	1.39
23	A	608	CLA	CHC-C4B	-4.82	1.28	1.39
23	B	611	CLA	CHD-C1D	4.81	1.47	1.38
23	b	605	CLA	CHD-C1D	4.81	1.47	1.38
23	B	607[B]	CLA	CHC-C4B	-4.81	1.28	1.39
23	C	510	CLA	MG-NB	-4.81	1.96	2.05
23	b	609[B]	CLA	CHD-C1D	4.81	1.47	1.38
23	C	509	CLA	MG-NB	-4.80	1.96	2.05
23	a	604	CLA	MG-NB	-4.80	1.96	2.05
23	B	617	CLA	CHB-C1B	4.80	1.50	1.39
23	D	404	CLA	CHD-C1D	4.79	1.47	1.38
23	B	605	CLA	CHD-C1D	4.79	1.47	1.38
23	B	607[A]	CLA	CHD-C1D	4.79	1.47	1.38
23	B	611	CLA	CHC-C4B	-4.78	1.28	1.39
25	h	101	BCR	C24-C23	4.78	1.47	1.33
23	c	510	CLA	CHB-C1B	4.78	1.50	1.39
23	d	402	CLA	MG-NB	-4.78	1.96	2.05
23	A	605	CLA	CHD-C1D	4.78	1.47	1.38
23	C	513	CLA	CHC-C4B	-4.77	1.28	1.39
25	H	101	BCR	C23-C22	4.77	1.56	1.46
25	f	101	BCR	C11-C12	4.77	1.47	1.34
23	b	611	CLA	CHC-C4B	-4.77	1.28	1.39
23	a	604	CLA	CHD-C1D	4.77	1.47	1.38
22	A	604	BCT	O1-C	4.77	1.42	1.25
23	A	608	CLA	MG-NB	-4.77	1.96	2.05
23	B	617	CLA	CHD-C1D	4.77	1.47	1.38
23	b	616	CLA	CHD-C1D	4.77	1.47	1.38
23	b	613	CLA	CHD-C1D	4.76	1.47	1.38
23	c	514	CLA	MG-NB	-4.76	1.96	2.05
23	b	605	CLA	MG-NB	-4.76	1.96	2.05
23	C	508	CLA	MG-NB	-4.76	1.96	2.05
23	c	513	CLA	CHD-C1D	4.75	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	613	CLA	MG-NB	-4.75	1.96	2.05
23	b	610	CLA	CHD-C1D	4.75	1.47	1.38
23	c	511	CLA	CHD-C1D	4.75	1.47	1.38
25	F	101	BCR	C11-C12	4.75	1.47	1.34
23	B	617	CLA	MG-NB	-4.74	1.96	2.05
23	b	615	CLA	MG-NB	-4.74	1.96	2.05
23	C	502	CLA	CHD-C1D	4.74	1.47	1.38
23	c	503	CLA	MG-NB	-4.74	1.96	2.05
23	C	506	CLA	CHD-C1D	4.74	1.47	1.38
23	D	404	CLA	CHB-C1B	4.73	1.50	1.39
23	C	501	CLA	MG-NB	-4.73	1.96	2.05
23	a	607	CLA	CHC-C4B	-4.73	1.28	1.39
23	b	604	CLA	CHB-C1B	4.72	1.50	1.39
23	b	618	CLA	C4C-C3C	-4.72	1.37	1.45
23	a	607	CLA	CHB-C1B	4.72	1.50	1.39
23	A	605	CLA	MG-NB	-4.72	1.96	2.05
23	A	606	CLA	MG-NB	-4.72	1.96	2.05
23	B	614	CLA	MG-NB	-4.72	1.96	2.05
23	d	403	CLA	CHB-C1B	4.72	1.50	1.39
33	v	201	HEM	FE-ND	4.72	2.09	1.94
23	c	509	CLA	MG-NB	-4.72	1.96	2.05
24	D	401	PHO	C1D-C2D	4.72	1.44	1.39
23	b	617	CLA	CHD-C1D	4.71	1.47	1.38
23	a	605	CLA	MG-NB	-4.71	1.96	2.05
23	b	612	CLA	CHD-C1D	4.71	1.47	1.38
23	C	507	CLA	CHD-C4C	-4.71	1.28	1.39
25	C	514	BCR	C11-C12	4.71	1.47	1.34
23	B	603	CLA	MG-NB	-4.71	1.96	2.05
23	a	607	CLA	CHC-C1C	4.70	1.47	1.38
23	B	606	CLA	CHD-C1D	4.70	1.47	1.38
23	B	606	CLA	MG-NB	-4.70	1.96	2.05
23	b	604	CLA	CHD-C1D	4.70	1.47	1.38
23	d	402	CLA	CHD-C1D	4.70	1.47	1.38
23	B	607[B]	CLA	CHD-C1D	4.69	1.47	1.38
23	c	508	CLA	CHD-C1D	4.69	1.47	1.38
23	b	609[B]	CLA	MG-NB	-4.69	1.96	2.05
23	C	504	CLA	MG-NB	-4.69	1.96	2.05
23	C	507	CLA	CHD-C1D	4.69	1.47	1.38
23	c	509	CLA	CHD-C1D	4.69	1.47	1.38
23	C	513	CLA	CHB-C1B	4.69	1.49	1.39
22	a	603	BCT	O1-C	4.68	1.41	1.25
23	c	508	CLA	CHD-C4C	-4.68	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	CHD-C1D	4.68	1.47	1.38
23	b	619	CLA	CHD-C1D	4.68	1.47	1.38
23	c	506	CLA	CHD-C1D	4.68	1.47	1.38
23	C	511	CLA	CHD-C1D	4.67	1.47	1.38
23	D	402	CLA	MG-NB	-4.67	1.96	2.05
23	b	614	CLA	CHB-C1B	4.67	1.49	1.39
23	c	507	CLA	MG-NB	-4.67	1.96	2.05
23	B	613	CLA	CHD-C1D	4.66	1.47	1.38
25	B	619	BCR	C23-C22	4.66	1.55	1.46
23	B	609	CLA	CHB-C1B	4.66	1.49	1.39
23	A	608	CLA	CHB-C1B	4.66	1.49	1.39
23	c	505	CLA	CHD-C1D	4.66	1.47	1.38
23	C	505	CLA	CHB-C1B	4.66	1.49	1.39
25	b	620	BCR	C11-C12	4.66	1.46	1.34
23	B	614	CLA	CHD-C4C	-4.66	1.28	1.39
23	B	616	CLA	CHD-C4C	-4.66	1.28	1.39
23	B	605	CLA	CHB-C1B	4.66	1.49	1.39
23	C	511	CLA	MG-NB	-4.66	1.96	2.05
23	B	614	CLA	CHD-C1D	4.65	1.47	1.38
23	B	607[A]	CLA	MG-NB	-4.65	1.96	2.05
23	A	608	CLA	CHD-C4C	-4.65	1.28	1.39
23	C	512	CLA	CHD-C1D	4.65	1.47	1.38
23	c	506	CLA	CHD-C4C	-4.65	1.28	1.39
23	C	512	CLA	MG-NB	-4.65	1.96	2.05
24	A	607	PHO	C1D-C2D	4.65	1.44	1.39
23	b	606	CLA	CHB-C1B	4.65	1.49	1.39
23	b	619	CLA	CHB-C1B	4.65	1.49	1.39
23	B	602	CLA	CHB-C1B	4.64	1.49	1.39
23	B	608	CLA	CHB-C1B	4.64	1.49	1.39
23	b	618	CLA	MG-NB	-4.64	1.96	2.05
23	b	615	CLA	CHD-C1D	4.64	1.47	1.38
23	c	514	CLA	CHB-C1B	4.64	1.49	1.39
23	b	616	CLA	CHD-C4C	-4.64	1.28	1.39
23	b	608	CLA	CHD-C4C	-4.64	1.28	1.39
23	b	614	CLA	CHD-C4C	-4.64	1.28	1.39
23	d	403	CLA	CHD-C1D	4.64	1.47	1.38
23	C	503	CLA	C4C-C3C	-4.63	1.37	1.45
23	b	618	CLA	CHD-C4C	-4.63	1.28	1.39
23	c	504	CLA	CHD-C1D	4.63	1.47	1.38
23	b	611	CLA	CHB-C1B	4.63	1.49	1.39
23	c	506	CLA	MG-NB	-4.63	1.96	2.05
31	B	622	LHG	O8-C23	4.63	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	CHD-C1D	4.62	1.47	1.38
23	b	606	CLA	CHD-C4C	-4.62	1.28	1.39
25	B	619	BCR	C11-C12	4.62	1.46	1.34
23	c	510	CLA	MG-NB	-4.62	1.96	2.05
23	c	510	CLA	CHD-C1D	4.62	1.47	1.38
23	b	613	CLA	CHB-C1B	4.62	1.49	1.39
23	B	607[B]	CLA	MG-NB	-4.62	1.96	2.05
23	a	607	CLA	MG-NB	-4.62	1.96	2.05
23	C	509	CLA	CHD-C4C	-4.62	1.28	1.39
23	C	502	CLA	CHB-C1B	4.61	1.49	1.39
23	C	503	CLA	CHB-C1B	4.61	1.49	1.39
23	b	616	CLA	CHB-C1B	4.61	1.49	1.39
23	c	504	CLA	CHB-C1B	4.61	1.49	1.39
23	c	508	CLA	CHB-C1B	4.61	1.49	1.39
23	c	508	CLA	MG-NB	-4.61	1.96	2.05
23	C	513	CLA	MG-NB	-4.61	1.96	2.05
23	B	605	CLA	MG-NB	-4.61	1.96	2.05
23	A	606	CLA	CHB-C1B	4.61	1.49	1.39
23	c	511	CLA	CHB-C1B	4.61	1.49	1.39
23	b	607	CLA	MG-NB	-4.60	1.96	2.05
23	C	505	CLA	MG-NB	-4.60	1.96	2.05
23	c	510	CLA	CHD-C4C	-4.60	1.28	1.39
23	C	509	CLA	CHD-C1D	4.60	1.47	1.38
23	C	506	CLA	MG-NB	-4.60	1.96	2.05
23	b	608	CLA	C4C-C3C	-4.59	1.37	1.45
23	B	614	CLA	CHB-C1B	4.59	1.49	1.39
23	B	613	CLA	CHD-C4C	-4.59	1.28	1.39
23	c	504	CLA	MG-NB	-4.59	1.96	2.05
23	b	612	CLA	CHD-C4C	-4.59	1.28	1.39
23	a	607	CLA	CHD-C1D	4.59	1.47	1.38
26	A	610	PL9	C6-C1	-4.59	1.40	1.48
23	D	404	CLA	CHD-C4C	-4.59	1.28	1.39
23	B	616	CLA	CHB-C1B	4.59	1.49	1.39
23	b	619	CLA	MG-NB	-4.59	1.96	2.05
23	c	513	CLA	CHB-C1B	4.59	1.49	1.39
25	c	522	BCR	C24-C25	4.59	1.60	1.45
23	b	615	CLA	CHD-C4C	-4.58	1.28	1.39
23	C	508	CLA	CHD-C4C	-4.58	1.28	1.39
23	c	513	CLA	MG-NB	-4.58	1.96	2.05
23	b	618	CLA	CHD-C1D	4.58	1.47	1.38
23	C	505	CLA	CHD-C4C	-4.58	1.28	1.39
23	b	604	CLA	CHD-C4C	-4.58	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	CHD-C4C	-4.58	1.28	1.39
23	b	610	CLA	CHD-C4C	-4.58	1.28	1.39
23	b	613	CLA	CHD-C4C	-4.58	1.28	1.39
23	D	404	CLA	MG-NB	-4.58	1.96	2.05
28	c	521	LMG	O7-C10	4.58	1.47	1.34
23	C	503	CLA	CHD-C4C	-4.57	1.28	1.39
23	b	619	CLA	CHD-C4C	-4.57	1.28	1.39
23	b	613	CLA	MG-NB	-4.57	1.96	2.05
23	B	607[B]	CLA	CHD-C4C	-4.57	1.28	1.39
23	b	608	CLA	CHD-C1D	4.57	1.47	1.38
23	B	607[A]	CLA	CHD-C4C	-4.57	1.28	1.39
23	B	610	CLA	CHB-C1B	4.57	1.49	1.39
23	C	507	CLA	MG-NB	-4.57	1.96	2.05
23	C	510	CLA	CHB-C1B	4.56	1.49	1.39
28	C	520	LMG	O7-C10	4.56	1.47	1.34
23	d	403	CLA	MG-NB	-4.56	1.96	2.05
23	C	512	CLA	CHD-C4C	-4.56	1.28	1.39
23	b	606	CLA	CHD-C1D	4.56	1.47	1.38
23	C	502	CLA	CHD-C4C	-4.56	1.28	1.39
23	c	511	CLA	CHD-C4C	-4.56	1.28	1.39
25	H	101	BCR	C24-C25	4.56	1.60	1.45
27	X	101	SQD	O48-C23	4.55	1.46	1.33
23	C	506	CLA	CHD-C4C	-4.55	1.28	1.39
23	b	609[B]	CLA	CHD-C4C	-4.55	1.28	1.39
23	C	509	CLA	CHB-C1B	4.55	1.49	1.39
23	b	609[A]	CLA	MG-NB	-4.55	1.96	2.05
23	b	617	CLA	CHD-C4C	-4.55	1.28	1.39
23	B	606	CLA	CHB-C1B	4.54	1.49	1.39
27	x	101	SQD	O48-C23	4.54	1.46	1.33
23	b	614	CLA	CHD-C1D	4.54	1.47	1.38
23	c	505	CLA	MG-NB	-4.54	1.96	2.05
23	B	611	CLA	CHD-C4C	-4.54	1.28	1.39
23	B	603	CLA	CHC-C1C	4.54	1.47	1.38
23	c	503	CLA	CHD-C4C	-4.54	1.28	1.39
23	d	403	CLA	CHD-C4C	-4.54	1.28	1.39
23	A	606	CLA	CHD-C4C	-4.54	1.28	1.39
31	l	101	LHG	O8-C23	4.54	1.46	1.33
23	b	616	CLA	MG-NB	-4.53	1.96	2.05
23	B	616	CLA	MG-NB	-4.53	1.96	2.05
23	B	614	CLA	C4C-C3C	-4.53	1.37	1.45
23	B	605	CLA	CHD-C4C	-4.53	1.28	1.39
25	k	101	BCR	C24-C25	4.53	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	CHB-C1B	4.52	1.49	1.39
26	a	609	PL9	C6-C1	-4.52	1.41	1.48
23	B	610	CLA	CHD-C4C	-4.52	1.28	1.39
23	c	503	CLA	CHB-C1B	4.52	1.49	1.39
23	b	610	CLA	MG-NB	-4.52	1.96	2.05
23	b	608	CLA	CHB-C1B	4.52	1.49	1.39
28	c	520	LMG	O7-C10	4.52	1.47	1.34
23	c	512	CLA	CHD-C4C	-4.51	1.28	1.39
23	B	606	CLA	C4C-C3C	-4.51	1.37	1.45
25	b	621	BCR	C11-C12	4.51	1.46	1.34
23	b	617	CLA	CHB-C1B	4.51	1.49	1.39
23	c	504	CLA	CHD-C4C	-4.51	1.28	1.39
23	b	611	CLA	MG-NB	-4.51	1.96	2.05
23	b	612	CLA	CHB-C1B	4.51	1.49	1.39
23	c	511	CLA	MG-NB	-4.51	1.96	2.05
23	C	501	CLA	CHD-C4C	-4.51	1.28	1.39
23	B	615	CLA	MG-NB	-4.51	1.96	2.05
23	b	606	CLA	C4C-C3C	-4.50	1.37	1.45
31	d	406	LHG	O8-C23	4.50	1.46	1.33
23	C	508	CLA	CHB-C1B	4.49	1.49	1.39
27	b	601	SQD	O48-C23	4.49	1.46	1.33
23	D	403	CLA	CHD-C4C	-4.49	1.29	1.39
23	A	605	CLA	CHB-C1B	4.49	1.49	1.39
27	a	612	SQD	O48-C23	4.49	1.46	1.33
23	b	617	CLA	MG-NB	-4.49	1.96	2.05
28	a	611	LMG	O7-C10	4.49	1.47	1.34
23	C	507	CLA	CHB-C1B	4.49	1.49	1.39
23	C	512	CLA	CHB-C1B	4.49	1.49	1.39
23	b	605	CLA	CHC-C1C	4.48	1.47	1.38
23	C	511	CLA	CHD-C4C	-4.48	1.29	1.39
25	K	101	BCR	C24-C25	4.48	1.60	1.45
23	B	616	CLA	CHD-C1D	4.48	1.47	1.38
23	b	607	CLA	CHB-C1B	4.48	1.49	1.39
23	a	604	CLA	CHB-C1B	4.48	1.49	1.39
25	B	620	BCR	C24-C25	4.48	1.60	1.45
23	B	612	CLA	CHB-C1B	4.48	1.49	1.39
23	c	513	CLA	CHD-C4C	-4.48	1.29	1.39
23	B	611	CLA	CHB-C1B	4.48	1.49	1.39
23	b	604	CLA	MG-NB	-4.47	1.96	2.05
23	B	607[B]	CLA	C4C-C3C	-4.47	1.37	1.45
27	X	101	SQD	O47-C7	4.47	1.46	1.34
23	C	504	CLA	CHB-C1B	4.47	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	MG-NB	-4.47	1.96	2.05
27	x	101	SQD	O47-C7	4.47	1.46	1.34
23	B	615	CLA	CHD-C4C	-4.47	1.29	1.39
23	B	604	CLA	CHB-C1B	4.46	1.49	1.39
23	B	608	CLA	CHD-C4C	-4.46	1.29	1.39
23	B	602	CLA	CHD-C4C	-4.46	1.29	1.39
31	e	101	LHG	O8-C23	4.46	1.46	1.33
31	D	407	LHG	O8-C23	4.46	1.46	1.33
23	b	609[A]	CLA	CHD-C4C	-4.46	1.29	1.39
23	b	605	CLA	CHD-C4C	-4.45	1.29	1.39
23	B	612	CLA	CHD-C4C	-4.45	1.29	1.39
23	B	617	CLA	CHD-C4C	-4.45	1.29	1.39
23	B	613	CLA	CHB-C1B	4.45	1.49	1.39
23	b	610	CLA	CHB-C1B	4.45	1.49	1.39
23	b	615	CLA	CHB-C1B	4.45	1.49	1.39
23	b	607	CLA	CHD-C4C	-4.45	1.29	1.39
28	z	101	LMG	O7-C10	4.45	1.46	1.34
23	c	509	CLA	CHD-C4C	-4.45	1.29	1.39
28	C	519	LMG	O7-C10	4.45	1.46	1.34
23	c	505	CLA	CHC-C1C	4.45	1.47	1.38
23	B	610	CLA	MG-NB	-4.45	1.97	2.05
23	c	502	CLA	CHB-C1B	4.45	1.49	1.39
23	C	510	CLA	CHD-C4C	-4.44	1.29	1.39
23	b	616	CLA	C4C-C3C	-4.44	1.37	1.45
23	b	609[A]	CLA	CHB-C1B	4.44	1.49	1.39
23	b	605	CLA	C4C-C3C	-4.44	1.37	1.45
23	C	513	CLA	CHD-C4C	-4.44	1.29	1.39
23	b	618	CLA	CHB-C1B	4.44	1.49	1.39
23	B	608	CLA	MG-NB	-4.44	1.97	2.05
23	d	402	CLA	CHD-C4C	-4.43	1.29	1.39
23	C	508	CLA	CHD-C1D	4.43	1.47	1.38
23	c	505	CLA	CHB-C1B	4.43	1.49	1.39
25	b	622	BCR	C24-C25	4.43	1.60	1.45
23	c	505	CLA	CHD-C4C	-4.42	1.29	1.39
27	B	623	SQD	O48-C23	4.42	1.46	1.33
27	b	602	SQD	O48-C23	4.42	1.46	1.33
23	C	504	CLA	C4C-C3C	-4.42	1.37	1.45
23	c	507	CLA	CHD-C4C	-4.42	1.29	1.39
28	A	612	LMG	O7-C10	4.42	1.46	1.34
23	D	404	CLA	CHC-C1C	4.41	1.47	1.38
23	C	506	CLA	CHB-C1B	4.41	1.49	1.39
33	E	102	HEM	FE-NA	4.41	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	CHD-C4C	-4.41	1.29	1.39
23	b	609[B]	CLA	CHB-C1B	4.41	1.49	1.39
23	c	512	CLA	C4C-C3C	-4.41	1.37	1.45
23	a	605	CLA	CHD-C4C	-4.40	1.29	1.39
23	D	403	CLA	CHC-C1C	4.40	1.47	1.38
32	D	406	DGD	O2G-C1B	4.40	1.46	1.34
27	b	602	SQD	O47-C7	4.40	1.46	1.34
25	h	101	BCR	C24-C25	4.40	1.60	1.45
23	a	604	CLA	CHC-C1C	4.40	1.47	1.38
23	c	504	CLA	C4C-C3C	-4.40	1.37	1.45
23	c	502	CLA	CHD-C4C	-4.40	1.29	1.39
23	a	604	CLA	CHD-C4C	-4.40	1.29	1.39
32	C	518	DGD	O2G-C2G	-4.40	1.36	1.46
23	a	605	CLA	CHB-C1B	4.40	1.49	1.39
23	a	613	CLA	CHB-C1B	4.39	1.49	1.39
23	B	604	CLA	CHD-C4C	-4.39	1.29	1.39
23	b	614	CLA	C4C-C3C	-4.39	1.37	1.45
31	E	101	LHG	O8-C23	4.39	1.46	1.33
27	B	623	SQD	O47-C7	4.39	1.46	1.34
23	B	603	CLA	CHD-C4C	-4.39	1.29	1.39
23	C	513	CLA	CHC-C1C	4.38	1.47	1.38
31	L	101	LHG	O8-C23	4.38	1.46	1.33
23	A	605	CLA	CHD-C4C	-4.38	1.29	1.39
23	D	402	CLA	CHB-C1B	4.38	1.49	1.39
23	D	403	CLA	CHB-C1B	4.38	1.49	1.39
25	C	521	BCR	C24-C25	4.38	1.60	1.45
28	Z	101	LMG	O7-C10	4.38	1.46	1.34
25	c	516	BCR	C24-C25	4.38	1.60	1.45
23	B	609	CLA	MG-NB	-4.38	1.97	2.05
23	A	608	CLA	C4C-C3C	-4.37	1.37	1.45
31	b	624	LHG	O8-C23	4.37	1.46	1.33
23	b	609[B]	CLA	CHC-C1C	4.37	1.47	1.38
31	a	614	LHG	O8-C23	4.37	1.46	1.33
23	B	616	CLA	C4C-C3C	-4.37	1.37	1.45
23	A	605	CLA	CHC-C1C	4.37	1.47	1.38
23	B	607[A]	CLA	C4C-C3C	-4.37	1.37	1.45
23	c	504	CLA	CHC-C1C	4.36	1.47	1.38
23	d	403	CLA	CHC-C1C	4.36	1.47	1.38
23	B	604	CLA	C4C-C3C	-4.36	1.37	1.45
23	b	617	CLA	C4C-C3C	-4.36	1.37	1.45
23	b	611	CLA	CHC-C1C	4.36	1.47	1.38
23	B	607[B]	CLA	CHC-C1C	4.36	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609[A]	CLA	CHC-C1C	4.36	1.47	1.38
23	B	615	CLA	CHC-C1C	4.36	1.47	1.38
23	C	505	CLA	CHC-C1C	4.36	1.47	1.38
23	c	514	CLA	CHC-C1C	4.35	1.47	1.38
23	B	607[B]	CLA	CHB-C1B	4.35	1.49	1.39
23	C	501	CLA	CHB-C1B	4.35	1.49	1.39
23	B	611	CLA	MG-NB	-4.35	1.97	2.05
23	c	502	CLA	C4C-C3C	-4.35	1.37	1.45
32	c	519	DGD	O2G-C2G	-4.35	1.36	1.46
23	c	511	CLA	CHC-C1C	4.35	1.47	1.38
23	c	502	CLA	CHC-C1C	4.34	1.47	1.38
23	B	609	CLA	CHD-C4C	-4.34	1.29	1.39
23	b	610	CLA	C4C-C3C	-4.34	1.37	1.45
23	d	402	CLA	CHB-C1B	4.34	1.49	1.39
23	B	615	CLA	C4C-C3C	-4.34	1.37	1.45
24	a	606	PHO	C1D-C2D	4.33	1.44	1.39
25	C	515	BCR	C24-C25	4.33	1.59	1.45
23	B	611	CLA	CHC-C1C	4.33	1.47	1.38
23	b	617	CLA	CHC-C1C	4.33	1.47	1.38
23	b	612	CLA	CHC-C1C	4.33	1.47	1.38
31	D	408	LHG	O8-C23	4.32	1.45	1.33
23	B	607[A]	CLA	CHC-C1C	4.32	1.47	1.38
23	c	514	CLA	CHD-C4C	-4.32	1.29	1.39
32	d	405	DGD	O2G-C1B	4.32	1.46	1.34
23	c	503	CLA	CHC-C1C	4.32	1.47	1.38
23	A	606	CLA	CHC-C1C	4.31	1.47	1.38
23	b	609[B]	CLA	C4C-C3C	-4.31	1.37	1.45
23	c	507	CLA	CHC-C1C	4.31	1.47	1.38
23	c	513	CLA	C4C-C3C	-4.31	1.37	1.45
23	c	509	CLA	CHC-C1C	4.31	1.47	1.38
28	b	623	LMG	O7-C10	4.31	1.46	1.34
23	D	402	CLA	CHD-C4C	-4.31	1.29	1.39
23	b	611	CLA	CHD-C4C	-4.31	1.29	1.39
23	B	607[A]	CLA	CHB-C1B	4.31	1.49	1.39
23	c	509	CLA	CHB-C1B	4.31	1.49	1.39
23	c	503	CLA	C4C-C3C	-4.30	1.37	1.45
23	B	616	CLA	CHC-C1C	4.30	1.47	1.38
23	C	508	CLA	CHC-C1C	4.29	1.47	1.38
23	C	510	CLA	C4C-C3C	-4.29	1.37	1.45
23	A	608	CLA	CHC-C1C	4.29	1.47	1.38
23	C	505	CLA	C4C-C3C	-4.29	1.37	1.45
27	b	601	SQD	O47-C7	4.29	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	605	CLA	CHC-C1C	4.29	1.47	1.38
23	C	502	CLA	CHC-C1C	4.28	1.47	1.38
23	c	509	CLA	C4C-C3C	-4.28	1.37	1.45
27	a	612	SQD	O47-C7	4.28	1.46	1.34
23	a	613	CLA	CHD-C4C	-4.28	1.29	1.39
23	b	609[A]	CLA	C4C-C3C	-4.27	1.37	1.45
32	c	518	DGD	O2G-C2G	-4.27	1.36	1.46
23	C	502	CLA	C4C-C3C	-4.27	1.37	1.45
23	c	507	CLA	C4C-C3C	-4.27	1.37	1.45
32	c	517	DGD	O2G-C2G	-4.27	1.36	1.46
23	B	613	CLA	CHC-C1C	4.27	1.47	1.38
23	b	618	CLA	CHC-C1C	4.27	1.47	1.38
23	c	512	CLA	CHC-C1C	4.27	1.47	1.38
23	C	501	CLA	CHC-C1C	4.27	1.47	1.38
23	C	503	CLA	CHC-C1C	4.27	1.47	1.38
23	d	402	CLA	CHC-C1C	4.27	1.47	1.38
23	d	402	CLA	C4C-C3C	-4.26	1.37	1.45
23	b	619	CLA	C4C-C3C	-4.26	1.37	1.45
23	D	402	CLA	CHC-C1C	4.26	1.47	1.38
23	a	613	CLA	CMA-C3A	-4.26	1.44	1.53
23	b	612	CLA	C4C-C3C	-4.26	1.37	1.45
23	b	616	CLA	MG-NB	-4.25	1.97	2.05
23	b	616	CLA	CHC-C1C	4.25	1.47	1.38
23	C	512	CLA	CHC-C1C	4.25	1.47	1.38
23	b	615	CLA	CHC-C1C	4.25	1.47	1.38
23	c	508	CLA	C4C-C3C	-4.25	1.37	1.45
23	C	511	CLA	CHC-C1C	4.25	1.47	1.38
23	B	612	CLA	C4C-C3C	-4.25	1.37	1.45
32	D	406	DGD	O1G-C1A	4.24	1.45	1.33
25	B	618	BCR	C24-C25	4.24	1.59	1.45
23	B	605	CLA	CMA-C3A	-4.24	1.44	1.53
23	b	607	CLA	CHC-C1C	4.24	1.47	1.38
23	c	511	CLA	C4C-C3C	-4.24	1.37	1.45
28	B	621	LMG	O7-C10	4.24	1.46	1.34
23	c	507	CLA	CHB-C1B	4.23	1.48	1.39
23	c	510	CLA	CHC-C1C	4.23	1.47	1.38
31	l	101	LHG	O7-C7	4.23	1.46	1.34
32	C	516	DGD	O2G-C2G	-4.23	1.36	1.46
23	c	506	CLA	CHC-C1C	4.23	1.47	1.38
28	j	101	LMG	O7-C10	4.23	1.46	1.34
23	c	514	CLA	C4C-C3C	-4.22	1.37	1.45
23	b	608	CLA	CHC-C1C	4.22	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607[B]	CLA	CMA-C3A	-4.22	1.44	1.53
23	B	613	CLA	CMA-C3A	-4.22	1.44	1.53
23	B	609	CLA	CHC-C1C	4.22	1.46	1.38
23	d	403	CLA	C4C-C3C	-4.22	1.37	1.45
23	c	513	CLA	CHC-C1C	4.22	1.46	1.38
23	C	512	CLA	C4C-C3C	-4.21	1.37	1.45
23	A	608	CLA	CMA-C3A	-4.21	1.44	1.53
28	J	101	LMG	O7-C10	4.21	1.46	1.34
23	C	507	CLA	C4C-C3C	-4.21	1.37	1.45
23	A	605	CLA	C4C-C3C	-4.21	1.37	1.45
23	c	512	CLA	CMA-C3A	-4.21	1.44	1.53
23	b	619	CLA	CHC-C1C	4.21	1.46	1.38
23	B	617	CLA	C4C-C3C	-4.20	1.37	1.45
23	C	511	CLA	CMA-C3A	-4.20	1.44	1.53
23	b	613	CLA	CHC-C1C	4.20	1.46	1.38
32	C	516	DGD	O2G-C1B	4.20	1.46	1.34
31	E	101	LHG	O7-C7	4.20	1.46	1.34
32	H	102	DGD	O2G-C2G	-4.20	1.36	1.46
23	c	505	CLA	C4C-C3C	-4.20	1.37	1.45
31	e	101	LHG	O7-C7	4.20	1.46	1.34
23	B	603	CLA	CHB-C1B	4.19	1.48	1.39
23	C	507	CLA	CHC-C1C	4.19	1.46	1.38
23	D	402	CLA	CMA-C3A	-4.19	1.44	1.53
23	c	510	CLA	C4C-C3C	-4.19	1.37	1.45
23	c	510	CLA	CMA-C3A	-4.19	1.44	1.53
23	C	513	CLA	C4C-C3C	-4.18	1.37	1.45
23	C	511	CLA	C4C-C3C	-4.17	1.38	1.45
23	C	506	CLA	CHC-C1C	4.17	1.46	1.38
23	B	607[A]	CLA	CMA-C3A	-4.17	1.44	1.53
32	h	102	DGD	O2G-C1B	4.17	1.46	1.34
23	C	509	CLA	CHC-C1C	4.17	1.46	1.38
32	c	517	DGD	O2G-C1B	4.16	1.46	1.34
23	a	607	CLA	C4C-C3C	-4.16	1.38	1.45
32	C	517	DGD	O2G-C1B	4.16	1.46	1.34
23	b	608	CLA	CMA-C3A	-4.16	1.44	1.53
23	C	501	CLA	C4C-C3C	-4.16	1.38	1.45
31	D	408	LHG	O7-C7	4.15	1.46	1.34
23	B	608	CLA	C4C-C3C	-4.15	1.38	1.45
23	C	504	CLA	CMA-C3A	-4.15	1.44	1.53
23	C	506	CLA	C4C-C3C	-4.15	1.38	1.45
23	C	510	CLA	CMA-C3A	-4.15	1.44	1.53
23	B	608	CLA	CHC-C1C	4.15	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	t	101	BCR	C24-C25	4.15	1.59	1.45
33	v	201	HEM	FE-NB	4.15	2.07	1.94
23	b	612	CLA	CMA-C3A	-4.15	1.44	1.53
23	b	606	CLA	CMA-C3A	-4.15	1.44	1.53
23	b	610	CLA	CHC-C1C	4.14	1.46	1.38
23	B	610	CLA	C4C-C3C	-4.14	1.38	1.45
23	D	404	CLA	C4C-C3C	-4.14	1.38	1.45
23	b	609[B]	CLA	CMA-C3A	-4.14	1.44	1.53
32	C	517	DGD	O2G-C2G	-4.14	1.36	1.46
23	b	615	CLA	CMA-C3A	-4.13	1.44	1.53
23	B	608	CLA	CMA-C3A	-4.13	1.44	1.53
32	c	517	DGD	O1G-C1A	4.13	1.45	1.33
23	b	604	CLA	C4C-C3C	-4.13	1.38	1.45
23	B	612	CLA	CMA-C3A	-4.13	1.44	1.53
23	c	505	CLA	CMA-C3A	-4.13	1.44	1.53
23	B	606	CLA	CHC-C1C	4.13	1.46	1.38
23	C	510	CLA	CHC-C1C	4.12	1.46	1.38
23	C	505	CLA	CMA-C3A	-4.12	1.44	1.53
23	B	613	CLA	C4C-C3C	-4.12	1.38	1.45
32	H	102	DGD	O1G-C1A	4.12	1.45	1.33
23	a	605	CLA	CMA-C3A	-4.12	1.44	1.53
23	D	403	CLA	C4C-C3C	-4.12	1.38	1.45
27	A	611	SQD	O47-C7	4.12	1.45	1.34
23	b	610	CLA	CMA-C3A	-4.11	1.44	1.53
31	d	406	LHG	O7-C7	4.11	1.45	1.34
23	B	610	CLA	CHC-C1C	4.11	1.46	1.38
32	d	405	DGD	O1G-C1A	4.11	1.45	1.33
23	a	604	CLA	C4C-C3C	-4.11	1.38	1.45
23	b	611	CLA	CMA-C3A	-4.11	1.44	1.53
23	c	506	CLA	CMA-C3A	-4.11	1.44	1.53
27	a	610	SQD	O47-C7	4.11	1.45	1.34
23	B	609	CLA	CMA-C3A	-4.11	1.44	1.53
25	c	522	BCR	C40-C30	4.11	1.61	1.53
25	c	516	BCR	C40-C30	4.10	1.61	1.53
25	C	514	BCR	C24-C25	4.10	1.59	1.45
23	c	507	CLA	CMA-C3A	-4.10	1.44	1.53
23	a	607	CLA	CMA-C3A	-4.10	1.44	1.53
23	b	604	CLA	CMA-C3A	-4.10	1.44	1.53
23	c	506	CLA	C4C-C3C	-4.10	1.38	1.45
31	L	101	LHG	O7-C7	4.09	1.45	1.34
23	b	604	CLA	CHC-C1C	4.09	1.46	1.38
32	D	406	DGD	O2G-C2G	-4.09	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	CMA-C3A	-4.09	1.44	1.53
23	B	606	CLA	CMA-C3A	-4.09	1.44	1.53
23	C	508	CLA	C4C-C3C	-4.09	1.38	1.45
32	C	516	DGD	O1G-C1A	4.09	1.45	1.33
23	B	605	CLA	CHC-C1C	4.09	1.46	1.38
23	B	614	CLA	CHC-C1C	4.08	1.46	1.38
33	v	201	HEM	FE-NC	4.08	2.08	1.95
23	c	509	CLA	CMA-C3A	-4.08	1.44	1.53
32	c	518	DGD	O1G-C1A	4.08	1.45	1.33
23	a	604	CLA	CMA-C3A	-4.08	1.44	1.53
23	b	615	CLA	C4C-C3C	-4.08	1.38	1.45
23	b	617	CLA	CMA-C3A	-4.08	1.44	1.53
23	b	609[A]	CLA	CMA-C3A	-4.08	1.44	1.53
23	A	606	CLA	CMA-C3A	-4.08	1.44	1.53
23	B	612	CLA	CHC-C1C	4.08	1.46	1.38
23	B	615	CLA	CMA-C3A	-4.08	1.44	1.53
25	b	620	BCR	C24-C25	4.08	1.59	1.45
31	B	622	LHG	O7-C7	4.07	1.45	1.34
32	c	518	DGD	O2G-C1B	4.07	1.45	1.34
23	d	403	CLA	CMA-C3A	-4.07	1.44	1.53
32	c	519	DGD	O2G-C1B	4.07	1.45	1.34
23	C	504	CLA	CHC-C1C	4.07	1.46	1.38
23	B	602	CLA	CHC-C1C	4.07	1.46	1.38
23	B	610	CLA	CMA-C3A	-4.07	1.44	1.53
32	h	102	DGD	O2G-C2G	-4.06	1.37	1.46
23	d	402	CLA	CMA-C3A	-4.06	1.44	1.53
25	C	521	BCR	C40-C30	4.06	1.61	1.53
23	C	501	CLA	CMA-C3A	-4.06	1.44	1.53
23	C	509	CLA	CMA-C3A	-4.06	1.44	1.53
23	c	514	CLA	CMA-C3A	-4.06	1.44	1.53
23	b	605	CLA	CHB-C1B	4.06	1.48	1.39
25	B	620	BCR	C40-C30	4.06	1.61	1.53
23	B	603	CLA	C4C-C3C	-4.06	1.38	1.45
31	D	407	LHG	O7-C7	4.06	1.45	1.34
23	a	605	CLA	C4C-C3C	-4.05	1.38	1.45
23	c	508	CLA	CHC-C1C	4.05	1.46	1.38
23	A	605	CLA	CMA-C3A	-4.05	1.44	1.53
23	c	503	CLA	CMA-C3A	-4.04	1.44	1.53
23	b	605	CLA	CMA-C3A	-4.04	1.44	1.53
23	a	613	CLA	CHC-C1C	4.04	1.46	1.38
23	B	614	CLA	CMA-C3A	-4.04	1.44	1.53
23	C	506	CLA	CMA-C3A	-4.04	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	405	DGD	O2G-C2G	-4.04	1.37	1.46
23	C	508	CLA	CMA-C3A	-4.04	1.44	1.53
32	C	518	DGD	O2G-C1B	4.03	1.45	1.34
23	c	511	CLA	CMA-C3A	-4.03	1.44	1.53
25	k	101	BCR	C40-C30	4.03	1.61	1.53
23	B	611	CLA	CMA-C3A	-4.03	1.44	1.53
23	b	618	CLA	CMA-C3A	-4.03	1.44	1.53
23	c	513	CLA	CMA-C3A	-4.03	1.44	1.53
23	D	404	CLA	CMA-C3A	-4.03	1.44	1.53
27	a	610	SQD	O48-C23	4.03	1.45	1.33
23	c	504	CLA	CMA-C3A	-4.03	1.44	1.53
31	a	614	LHG	O7-C7	4.03	1.45	1.34
23	b	614	CLA	CMA-C3A	-4.02	1.44	1.53
23	C	512	CLA	CMA-C3A	-4.02	1.44	1.53
25	C	515	BCR	C40-C30	4.02	1.61	1.53
23	B	605	CLA	C4C-C3C	-4.02	1.38	1.45
23	B	604	CLA	CHC-C1C	4.01	1.46	1.38
23	b	614	CLA	CHC-C1C	4.00	1.46	1.38
23	A	606	CLA	C4C-C3C	-4.00	1.38	1.45
25	c	515	BCR	C24-C25	4.00	1.58	1.45
23	b	607	CLA	CMA-C3A	-4.00	1.44	1.53
23	b	606	CLA	CHC-C1C	4.00	1.46	1.38
25	F	101	BCR	C2-C3	4.00	1.62	1.52
23	C	502	CLA	CMA-C3A	-4.00	1.44	1.53
32	H	102	DGD	O2G-C1B	3.99	1.45	1.34
27	A	611	SQD	O48-C23	3.99	1.45	1.33
25	B	618	BCR	C2-C3	3.99	1.62	1.52
23	C	509	CLA	C4C-C3C	-3.99	1.38	1.45
31	b	624	LHG	O7-C7	3.99	1.45	1.34
23	B	611	CLA	C4C-C3C	-3.98	1.38	1.45
23	b	613	CLA	CMA-C3A	-3.98	1.44	1.53
23	C	513	CLA	CMA-C3A	-3.97	1.44	1.53
23	c	502	CLA	CMA-C3A	-3.97	1.44	1.53
23	B	602	CLA	CMA-C3A	-3.97	1.44	1.53
23	B	603	CLA	CMA-C3A	-3.97	1.44	1.53
23	B	617	CLA	CHC-C1C	3.97	1.46	1.38
32	h	102	DGD	O1G-C1A	3.97	1.44	1.33
23	b	611	CLA	C4C-C3C	-3.96	1.38	1.45
23	B	602	CLA	C4C-C3C	-3.95	1.38	1.45
23	c	508	CLA	CMA-C3A	-3.94	1.44	1.53
32	C	517	DGD	O1G-C1A	3.94	1.44	1.33
25	H	101	BCR	C40-C30	3.94	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	619	CLA	CMA-C3A	-3.93	1.44	1.53
25	T	101	BCR	C24-C25	3.93	1.58	1.45
23	b	616	CLA	CMA-C3A	-3.92	1.44	1.53
25	f	101	BCR	C2-C3	3.92	1.61	1.52
23	C	507	CLA	CMA-C3A	-3.92	1.44	1.53
23	B	604	CLA	CMA-C3A	-3.92	1.44	1.53
23	B	617	CLA	CMA-C3A	-3.91	1.44	1.53
26	A	610	PL9	C36-C34	3.90	1.59	1.51
23	b	619	CLA	C3D-C4D	-3.90	1.35	1.44
33	e	102	HEM	FE-NB	3.90	2.06	1.94
23	C	503	CLA	CMA-C3A	-3.90	1.45	1.53
32	C	518	DGD	O1G-C1A	3.89	1.44	1.33
25	b	622	BCR	C40-C30	3.88	1.61	1.53
23	a	613	CLA	C4C-C3C	-3.88	1.38	1.45
23	b	610	CLA	C3D-C4D	-3.88	1.35	1.44
23	B	604	CLA	C3D-C4D	-3.88	1.35	1.44
32	H	102	DGD	O6E-C5E	3.87	1.53	1.44
23	D	402	CLA	C4C-C3C	-3.87	1.38	1.45
23	b	606	CLA	C3D-C2D	-3.87	1.28	1.39
23	A	606	CLA	C3D-C4D	-3.87	1.35	1.44
25	b	620	BCR	C2-C3	3.87	1.61	1.52
23	b	605	CLA	C3D-C4D	-3.87	1.35	1.44
25	K	101	BCR	C40-C30	3.86	1.61	1.53
23	b	613	CLA	C4C-C3C	-3.86	1.38	1.45
23	C	506	CLA	C1C-NC	-3.86	1.31	1.37
23	a	605	CLA	C1C-NC	-3.86	1.31	1.37
23	a	613	CLA	C3D-C4D	-3.85	1.35	1.44
23	a	613	CLA	C1C-NC	-3.85	1.31	1.37
23	c	511	CLA	CAA-C2A	-3.85	1.47	1.54
23	b	605	CLA	C1C-NC	-3.85	1.31	1.37
23	b	606	CLA	C1C-NC	-3.85	1.31	1.37
23	b	610	CLA	C3D-C2D	-3.85	1.28	1.39
28	C	519	LMG	O8-C28	3.84	1.44	1.33
23	B	606	CLA	C3D-C2D	-3.84	1.28	1.39
23	b	608	CLA	C3D-C2D	-3.84	1.28	1.39
23	B	616	CLA	CMA-C3A	-3.84	1.45	1.53
23	b	606	CLA	C3D-C4D	-3.83	1.35	1.44
23	a	604	CLA	C1A-CHA	-3.83	1.27	1.43
23	A	606	CLA	C1C-NC	-3.83	1.31	1.37
25	a	608	BCR	C2-C3	3.83	1.61	1.52
32	c	519	DGD	O1G-C1A	3.83	1.44	1.33
23	C	505	CLA	CAA-C2A	-3.82	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C3D-C4D	-3.82	1.35	1.44
23	d	402	CLA	C3D-C4D	-3.82	1.35	1.44
23	D	404	CLA	O2A-CGA	3.82	1.44	1.33
23	B	608	CLA	C1C-NC	-3.82	1.31	1.37
23	C	506	CLA	C3D-C4D	-3.82	1.35	1.44
23	D	402	CLA	C3D-C4D	-3.82	1.35	1.44
23	b	607	CLA	C4C-C3C	-3.81	1.38	1.45
23	a	605	CLA	C3D-C4D	-3.81	1.35	1.44
23	C	503	CLA	C3D-C2D	-3.81	1.28	1.39
32	h	102	DGD	O6E-C5E	3.80	1.53	1.44
23	B	603	CLA	C3D-C4D	-3.80	1.35	1.44
23	D	403	CLA	C3D-C4D	-3.80	1.35	1.44
23	c	507	CLA	C3D-C4D	-3.80	1.35	1.44
23	B	604	CLA	C1C-NC	-3.80	1.31	1.37
23	B	606	CLA	C3D-C4D	-3.80	1.35	1.44
23	B	613	CLA	C1A-CHA	-3.80	1.27	1.43
23	b	617	CLA	C1A-CHA	-3.80	1.27	1.43
23	B	614	CLA	C3D-C4D	-3.79	1.35	1.44
23	b	608	CLA	C1C-NC	-3.79	1.31	1.37
23	b	617	CLA	C3D-C4D	-3.79	1.35	1.44
23	c	511	CLA	C3D-C4D	-3.79	1.35	1.44
23	B	612	CLA	C1A-CHA	-3.78	1.27	1.43
25	c	522	BCR	C2-C3	3.78	1.61	1.52
23	b	618	CLA	C1C-NC	-3.78	1.31	1.37
23	B	608	CLA	CAA-C2A	-3.78	1.47	1.54
23	B	609	CLA	C3D-C4D	-3.78	1.35	1.44
23	C	510	CLA	C3D-C4D	-3.78	1.35	1.44
23	a	604	CLA	CAA-C2A	-3.78	1.47	1.54
28	z	101	LMG	O6-C1	3.77	1.51	1.41
25	h	101	BCR	C40-C30	3.77	1.60	1.53
23	B	617	CLA	C1C-NC	-3.77	1.31	1.37
28	A	612	LMG	O8-C28	3.77	1.44	1.33
23	A	605	CLA	CAA-C2A	-3.77	1.47	1.54
25	C	521	BCR	C2-C3	3.77	1.61	1.52
23	C	501	CLA	C1A-CHA	-3.77	1.27	1.43
23	b	608	CLA	C3D-C4D	-3.76	1.35	1.44
23	c	512	CLA	C1C-NC	-3.76	1.31	1.37
23	b	609[B]	CLA	C3D-C4D	-3.76	1.35	1.44
28	j	101	LMG	O6-C1	3.76	1.51	1.41
23	A	605	CLA	C1A-CHA	-3.76	1.27	1.43
23	D	402	CLA	C1C-NC	-3.76	1.32	1.37
23	A	605	CLA	C3D-C4D	-3.76	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C3D-C4D	-3.75	1.35	1.44
23	C	504	CLA	C1A-CHA	-3.75	1.27	1.43
23	B	608	CLA	C3D-C4D	-3.75	1.35	1.44
28	Z	101	LMG	O6-C1	3.75	1.51	1.41
23	a	605	CLA	C3D-C2D	-3.75	1.28	1.39
23	B	609	CLA	C1A-CHA	-3.75	1.27	1.43
23	D	403	CLA	C1A-CHA	-3.75	1.27	1.43
23	d	403	CLA	O2A-CGA	3.75	1.44	1.33
23	c	503	CLA	C1A-CHA	-3.75	1.27	1.43
23	b	611	CLA	C1A-CHA	-3.75	1.27	1.43
23	B	613	CLA	C3D-C4D	-3.75	1.35	1.44
23	b	612	CLA	CAA-C2A	-3.74	1.47	1.54
23	c	506	CLA	C3D-C4D	-3.74	1.35	1.44
25	b	621	BCR	C27-C26	3.74	1.58	1.51
23	A	606	CLA	C3D-C2D	-3.74	1.28	1.39
28	C	519	LMG	O6-C1	3.74	1.51	1.41
23	B	614	CLA	CBD-CGD	-3.74	1.41	1.52
23	C	510	CLA	C1A-CHA	-3.74	1.27	1.43
25	h	101	BCR	C2-C3	3.74	1.61	1.52
23	d	402	CLA	C1C-NC	-3.73	1.32	1.37
23	b	615	CLA	C1C-NC	-3.73	1.32	1.37
23	b	614	CLA	C3D-C4D	-3.73	1.35	1.44
23	c	506	CLA	CAA-C2A	-3.73	1.47	1.54
25	c	515	BCR	C40-C30	3.73	1.60	1.53
23	A	608	CLA	C1A-CHA	-3.73	1.27	1.43
23	C	509	CLA	C3D-C2D	-3.73	1.28	1.39
23	C	501	CLA	C1C-NC	-3.73	1.32	1.37
23	A	608	CLA	C3D-C4D	-3.73	1.35	1.44
23	a	607	CLA	C3D-C4D	-3.73	1.35	1.44
28	c	521	LMG	O8-C28	3.73	1.44	1.33
25	A	609	BCR	C2-C3	3.73	1.61	1.52
23	B	604	CLA	C1A-CHA	-3.73	1.27	1.43
23	B	615	CLA	C1A-CHA	-3.72	1.27	1.43
28	c	520	LMG	O8-C28	3.72	1.44	1.33
23	B	610	CLA	C1C-NC	-3.72	1.32	1.37
23	b	612	CLA	C3D-C4D	-3.72	1.35	1.44
23	b	617	CLA	C3D-C2D	-3.72	1.28	1.39
23	C	510	CLA	CAA-C2A	-3.72	1.47	1.54
23	B	608	CLA	C1A-CHA	-3.72	1.27	1.43
28	J	101	LMG	O6-C1	3.72	1.51	1.41
23	b	615	CLA	C3D-C2D	-3.71	1.28	1.39
23	A	608	CLA	C1C-NC	-3.71	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C3D-C4D	-3.71	1.35	1.44
23	B	609	CLA	C4C-C3C	-3.71	1.38	1.45
23	C	507	CLA	O2A-CGA	3.71	1.44	1.33
23	b	609[B]	CLA	C3D-C2D	-3.71	1.28	1.39
23	C	502	CLA	C1C-NC	-3.71	1.32	1.37
23	C	505	CLA	C3D-C4D	-3.71	1.35	1.44
32	D	406	DGD	O6E-C5E	3.71	1.53	1.44
23	b	615	CLA	C3D-C4D	-3.71	1.35	1.44
23	c	506	CLA	C3D-C2D	-3.71	1.28	1.39
23	B	616	CLA	C3D-C2D	-3.71	1.28	1.39
28	a	611	LMG	O8-C28	3.71	1.44	1.33
23	a	604	CLA	C3D-C4D	-3.71	1.35	1.44
23	B	614	CLA	C3D-C2D	-3.70	1.28	1.39
23	B	614	CLA	C1C-NC	-3.70	1.32	1.37
23	b	613	CLA	CAA-C2A	-3.70	1.47	1.54
23	B	607[B]	CLA	C3D-C4D	-3.70	1.35	1.44
32	d	405	DGD	O6E-C5E	3.70	1.53	1.44
33	V	202	HEM	FE-NC	3.70	2.07	1.95
23	b	605	CLA	C1A-CHA	-3.70	1.27	1.43
23	D	403	CLA	C1C-NC	-3.70	1.32	1.37
23	c	507	CLA	CAA-C2A	-3.70	1.47	1.54
25	B	619	BCR	C27-C26	3.70	1.57	1.51
23	d	402	CLA	C1A-CHA	-3.70	1.27	1.43
23	b	618	CLA	C3D-C2D	-3.70	1.28	1.39
23	c	502	CLA	C3D-C4D	-3.69	1.35	1.44
23	c	505	CLA	C3D-C4D	-3.69	1.35	1.44
23	C	510	CLA	C3D-C2D	-3.69	1.28	1.39
25	A	609	BCR	C27-C26	3.69	1.57	1.51
23	C	504	CLA	C1C-NC	-3.69	1.32	1.37
23	C	510	CLA	C1C-NC	-3.69	1.32	1.37
23	B	612	CLA	C3D-C4D	-3.69	1.35	1.44
23	b	605	CLA	CAA-C2A	-3.69	1.47	1.54
25	A	609	BCR	C40-C30	3.69	1.60	1.53
23	c	505	CLA	C1A-CHA	-3.69	1.27	1.43
23	D	402	CLA	C1A-CHA	-3.69	1.27	1.43
23	b	615	CLA	C1A-CHA	-3.69	1.27	1.43
23	c	503	CLA	C1C-NC	-3.68	1.32	1.37
23	C	508	CLA	C1A-CHA	-3.68	1.27	1.43
23	A	606	CLA	C1A-CHA	-3.68	1.27	1.43
25	F	101	BCR	C40-C30	3.68	1.60	1.53
25	f	101	BCR	C27-C26	3.68	1.57	1.51
23	a	607	CLA	O2A-CGA	3.68	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	CBD-CGD	-3.68	1.41	1.52
23	b	609[A]	CLA	C3D-C4D	-3.68	1.35	1.44
23	C	513	CLA	C1A-CHA	-3.68	1.28	1.43
23	c	504	CLA	C3D-C2D	-3.68	1.28	1.39
23	c	504	CLA	CBD-CGD	-3.67	1.41	1.52
23	B	613	CLA	CAA-C2A	-3.67	1.47	1.54
23	c	505	CLA	C3D-C2D	-3.67	1.29	1.39
23	b	611	CLA	C1C-NC	-3.67	1.32	1.37
23	b	609[B]	CLA	C1A-CHA	-3.67	1.28	1.43
23	c	511	CLA	C3D-C2D	-3.67	1.29	1.39
23	d	402	CLA	C3D-C2D	-3.67	1.29	1.39
23	b	608	CLA	C1A-CHA	-3.67	1.28	1.43
23	a	607	CLA	C1A-CHA	-3.67	1.28	1.43
23	b	607	CLA	O2A-CGA	3.67	1.44	1.33
23	B	604	CLA	C3D-C2D	-3.67	1.29	1.39
25	b	620	BCR	C40-C30	3.67	1.60	1.53
23	c	513	CLA	C1C-NC	-3.67	1.32	1.37
32	C	516	DGD	O6E-C5E	3.67	1.53	1.44
23	B	615	CLA	C3D-C4D	-3.67	1.35	1.44
28	c	520	LMG	O6-C1	3.67	1.51	1.41
28	b	623	LMG	O8-C28	3.66	1.44	1.33
23	B	607[A]	CLA	C3D-C4D	-3.66	1.35	1.44
23	C	501	CLA	C3D-C4D	-3.66	1.35	1.44
23	b	613	CLA	C3D-C4D	-3.66	1.35	1.44
23	b	619	CLA	C1A-CHA	-3.66	1.28	1.43
26	d	404	PL9	C36-C34	3.66	1.58	1.51
23	c	510	CLA	C3D-C2D	-3.66	1.29	1.39
23	c	504	CLA	C3D-C4D	-3.66	1.36	1.44
23	A	605	CLA	C3D-C2D	-3.66	1.29	1.39
23	b	607	CLA	C3D-C2D	-3.66	1.29	1.39
23	B	610	CLA	C3D-C4D	-3.66	1.36	1.44
23	c	506	CLA	C1D-ND	-3.65	1.33	1.37
23	B	617	CLA	C3D-C4D	-3.65	1.36	1.44
23	D	403	CLA	CBD-CGD	-3.65	1.41	1.52
23	b	615	CLA	CAA-C2A	-3.65	1.47	1.54
23	D	403	CLA	C3D-C2D	-3.65	1.29	1.39
23	c	514	CLA	C3D-C4D	-3.65	1.36	1.44
32	c	519	DGD	O6E-C5E	3.65	1.53	1.44
23	c	510	CLA	O2A-CGA	3.65	1.44	1.33
23	a	613	CLA	C1A-CHA	-3.65	1.28	1.43
23	c	503	CLA	C3D-C4D	-3.65	1.36	1.44
23	B	614	CLA	C1A-CHA	-3.65	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	607	CLA	C3D-C2D	-3.65	1.29	1.39
23	C	506	CLA	C3D-C2D	-3.65	1.29	1.39
25	C	514	BCR	C40-C30	3.64	1.60	1.53
23	a	613	CLA	C3D-C2D	-3.64	1.29	1.39
23	a	613	CLA	CBD-CGD	-3.64	1.41	1.52
23	B	602	CLA	C1A-CHA	-3.64	1.28	1.43
23	B	603	CLA	C1A-CHA	-3.64	1.28	1.43
23	b	616	CLA	CAA-C2A	-3.64	1.47	1.54
28	b	623	LMG	O6-C1	3.64	1.51	1.41
23	B	608	CLA	CBD-CGD	-3.64	1.41	1.52
25	B	618	BCR	C40-C30	3.64	1.60	1.53
23	c	506	CLA	C1C-NC	-3.64	1.32	1.37
23	B	606	CLA	C1C-NC	-3.64	1.32	1.37
23	c	508	CLA	C3D-C4D	-3.64	1.36	1.44
23	b	606	CLA	C1D-ND	-3.63	1.33	1.37
23	c	511	CLA	C1A-CHA	-3.63	1.28	1.43
23	B	615	CLA	C3D-C2D	-3.63	1.29	1.39
23	B	607[B]	CLA	C1C-NC	-3.63	1.32	1.37
28	B	621	LMG	O8-C28	3.63	1.43	1.33
23	b	613	CLA	C1A-CHA	-3.63	1.28	1.43
23	b	607	CLA	C3D-C4D	-3.63	1.36	1.44
23	B	610	CLA	CAA-C2A	-3.63	1.47	1.54
23	b	616	CLA	C3D-C2D	-3.62	1.29	1.39
23	b	612	CLA	C1C-NC	-3.62	1.32	1.37
23	b	607	CLA	C1A-CHA	-3.62	1.28	1.43
23	C	511	CLA	C3D-C2D	-3.62	1.29	1.39
23	b	614	CLA	C1A-CHA	-3.62	1.28	1.43
23	B	614	CLA	CBD-CAD	-3.62	1.40	1.56
23	B	607[A]	CLA	C1A-CHA	-3.62	1.28	1.43
23	B	614	CLA	CAA-C2A	-3.62	1.47	1.54
23	B	615	CLA	C1C-NC	-3.62	1.32	1.37
28	C	520	LMG	O8-C28	3.62	1.43	1.33
23	B	602	CLA	O2A-CGA	3.62	1.43	1.33
23	b	606	CLA	O2A-CGA	3.62	1.43	1.33
23	d	403	CLA	C1C-NC	-3.62	1.32	1.37
23	b	610	CLA	C1A-CHA	-3.62	1.28	1.43
23	B	607[A]	CLA	C1C-NC	-3.61	1.32	1.37
23	b	610	CLA	C1C-NC	-3.61	1.32	1.37
23	C	512	CLA	CAA-C2A	-3.61	1.47	1.54
23	c	503	CLA	O2A-CGA	3.61	1.43	1.33
23	c	511	CLA	CBD-CGD	-3.61	1.41	1.52
23	c	508	CLA	O2A-CGA	3.61	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	101	BCR	C2-C3	3.61	1.61	1.52
23	B	607[B]	CLA	C3D-C2D	-3.61	1.29	1.39
23	c	509	CLA	C3D-C4D	-3.61	1.36	1.44
23	C	511	CLA	C1A-CHA	-3.61	1.28	1.43
23	C	505	CLA	C3D-C2D	-3.61	1.29	1.39
23	D	402	CLA	C3D-C2D	-3.61	1.29	1.39
23	B	613	CLA	C3D-C2D	-3.61	1.29	1.39
23	B	616	CLA	C1A-CHA	-3.61	1.28	1.43
23	C	513	CLA	O2A-CGA	3.61	1.43	1.33
23	c	506	CLA	C1A-CHA	-3.61	1.28	1.43
23	b	613	CLA	CBD-CGD	-3.61	1.41	1.52
23	B	613	CLA	C1C-NC	-3.61	1.32	1.37
23	b	614	CLA	C1C-NC	-3.61	1.32	1.37
23	c	510	CLA	C3D-C4D	-3.61	1.36	1.44
23	B	617	CLA	O2A-CGA	3.61	1.43	1.33
25	c	516	BCR	C2-C3	3.61	1.61	1.52
23	b	613	CLA	C1C-NC	-3.61	1.32	1.37
23	b	609[A]	CLA	C1A-CHA	-3.61	1.28	1.43
23	a	604	CLA	C3D-C2D	-3.61	1.29	1.39
23	c	502	CLA	C1A-CHA	-3.61	1.28	1.43
23	B	611	CLA	CBD-CGD	-3.60	1.41	1.52
23	B	602	CLA	C3D-C4D	-3.60	1.36	1.44
23	C	511	CLA	C3D-C4D	-3.60	1.36	1.44
23	b	616	CLA	C3D-C4D	-3.60	1.36	1.44
23	D	403	CLA	CAA-C2A	-3.60	1.47	1.54
23	B	611	CLA	C1C-NC	-3.60	1.32	1.37
23	B	609	CLA	C3D-C2D	-3.60	1.29	1.39
23	b	618	CLA	C3D-C4D	-3.60	1.36	1.44
23	B	605	CLA	C3D-C4D	-3.60	1.36	1.44
23	C	509	CLA	C3D-C4D	-3.60	1.36	1.44
23	C	509	CLA	C1C-NC	-3.60	1.32	1.37
23	D	402	CLA	CBD-CGD	-3.60	1.41	1.52
23	B	617	CLA	C1A-CHA	-3.60	1.28	1.43
23	C	511	CLA	C1C-NC	-3.60	1.32	1.37
32	c	517	DGD	O6E-C5E	3.60	1.53	1.44
23	B	605	CLA	C3D-C2D	-3.60	1.29	1.39
23	C	502	CLA	C1A-CHA	-3.60	1.28	1.43
25	f	101	BCR	C40-C30	3.60	1.60	1.53
23	c	509	CLA	CAA-C2A	-3.59	1.47	1.54
23	c	513	CLA	C3D-C4D	-3.59	1.36	1.44
23	C	501	CLA	CBD-CGD	-3.59	1.41	1.52
23	B	610	CLA	C1A-CHA	-3.59	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	CBD-CGD	-3.59	1.41	1.52
23	B	611	CLA	C3D-C4D	-3.59	1.36	1.44
23	B	616	CLA	C3D-C4D	-3.59	1.36	1.44
23	C	504	CLA	CBD-CGD	-3.59	1.41	1.52
23	C	503	CLA	C3D-C4D	-3.59	1.36	1.44
23	b	617	CLA	C1C-NC	-3.59	1.32	1.37
23	A	606	CLA	O2A-CGA	3.59	1.43	1.33
23	b	611	CLA	C3D-C4D	-3.59	1.36	1.44
23	A	608	CLA	O2A-CGA	3.59	1.43	1.33
23	B	607[B]	CLA	C1A-CHA	-3.59	1.28	1.43
23	D	404	CLA	C1A-CHA	-3.59	1.28	1.43
32	C	518	DGD	O6E-C5E	3.59	1.53	1.44
23	b	605	CLA	C3D-C2D	-3.59	1.29	1.39
23	B	616	CLA	O2A-CGA	3.58	1.43	1.33
23	C	505	CLA	C1A-CHA	-3.58	1.28	1.43
23	c	507	CLA	C3D-C2D	-3.58	1.29	1.39
25	K	101	BCR	C1-C6	-3.58	1.49	1.53
23	C	508	CLA	C3D-C2D	-3.58	1.29	1.39
25	B	619	BCR	C2-C3	3.58	1.61	1.52
23	c	513	CLA	O2A-CGA	3.58	1.43	1.33
23	C	505	CLA	C1C-NC	-3.58	1.32	1.37
23	C	509	CLA	O2A-CGA	3.58	1.43	1.33
25	H	101	BCR	C2-C3	3.58	1.61	1.52
23	B	604	CLA	C1D-ND	-3.58	1.33	1.37
23	c	509	CLA	C1A-CHA	-3.58	1.28	1.43
28	c	521	LMG	O6-C1	3.58	1.51	1.41
23	B	602	CLA	CBD-CGD	-3.58	1.41	1.52
23	a	605	CLA	C1A-CHA	-3.58	1.28	1.43
23	b	604	CLA	C3D-C4D	-3.58	1.36	1.44
23	c	513	CLA	C1A-CHA	-3.58	1.28	1.43
23	b	612	CLA	C1A-CHA	-3.57	1.28	1.43
23	C	507	CLA	C3D-C4D	-3.57	1.36	1.44
25	C	515	BCR	C2-C3	3.57	1.61	1.52
23	D	403	CLA	CBD-CAD	-3.57	1.40	1.56
23	c	512	CLA	C3D-C2D	-3.57	1.29	1.39
23	c	513	CLA	C3D-C2D	-3.57	1.29	1.39
25	F	101	BCR	C27-C26	3.57	1.57	1.51
23	B	607[B]	CLA	CAA-C2A	-3.57	1.47	1.54
23	C	512	CLA	C1A-CHA	-3.57	1.28	1.43
23	C	503	CLA	C1C-NC	-3.57	1.32	1.37
23	b	604	CLA	O2A-CGA	3.57	1.43	1.33
23	B	602	CLA	C3D-C2D	-3.57	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	C1C-NC	-3.57	1.32	1.37
23	c	509	CLA	C1C-NC	-3.57	1.32	1.37
23	d	403	CLA	C1A-CHA	-3.57	1.28	1.43
23	c	514	CLA	C1C-NC	-3.57	1.32	1.37
23	B	603	CLA	C3D-C2D	-3.57	1.29	1.39
23	b	614	CLA	C3D-C2D	-3.56	1.29	1.39
23	b	619	CLA	C1C-NC	-3.56	1.32	1.37
23	d	402	CLA	C1D-ND	-3.56	1.33	1.37
23	C	512	CLA	CBD-CGD	-3.56	1.41	1.52
23	C	508	CLA	CAA-C2A	-3.56	1.47	1.54
23	B	617	CLA	C3D-C2D	-3.56	1.29	1.39
23	B	609	CLA	C1C-NC	-3.56	1.32	1.37
23	C	512	CLA	C1C-NC	-3.56	1.32	1.37
23	c	507	CLA	C1A-CHA	-3.56	1.28	1.43
23	b	614	CLA	C1D-ND	-3.56	1.33	1.37
23	B	606	CLA	C1A-CHA	-3.56	1.28	1.43
23	B	608	CLA	C3D-C2D	-3.56	1.29	1.39
23	b	618	CLA	O2A-CGA	3.56	1.43	1.33
23	c	512	CLA	O2A-CGA	3.56	1.43	1.33
23	B	616	CLA	C1C-NC	-3.55	1.32	1.37
23	c	508	CLA	C1C-NC	-3.55	1.32	1.37
23	D	404	CLA	C3D-C2D	-3.55	1.29	1.39
23	b	604	CLA	C3D-C2D	-3.55	1.29	1.39
23	d	402	CLA	CBD-CAD	-3.55	1.40	1.56
23	A	606	CLA	CBD-CGD	-3.55	1.41	1.52
23	C	513	CLA	C3D-C2D	-3.55	1.29	1.39
23	C	510	CLA	CBD-CGD	-3.55	1.41	1.52
23	b	610	CLA	CBD-CGD	-3.55	1.41	1.52
23	C	507	CLA	C1C-NC	-3.55	1.32	1.37
23	C	502	CLA	O2A-CGA	3.55	1.43	1.33
23	c	507	CLA	C1C-NC	-3.55	1.32	1.37
25	a	608	BCR	C40-C30	3.55	1.60	1.53
28	B	621	LMG	O6-C1	3.55	1.51	1.41
23	B	603	CLA	C1C-NC	-3.55	1.32	1.37
23	B	602	CLA	C1C-NC	-3.54	1.32	1.37
25	f	101	BCR	C4-C5	3.54	1.57	1.51
32	c	518	DGD	O6E-C5E	3.54	1.53	1.44
23	C	512	CLA	C3D-C4D	-3.54	1.36	1.44
23	b	604	CLA	C1A-CHA	-3.54	1.28	1.43
23	b	619	CLA	C3D-C2D	-3.54	1.29	1.39
23	c	504	CLA	C1A-CHA	-3.54	1.28	1.43
23	A	608	CLA	CBD-CGD	-3.54	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	j	101	LMG	O8-C28	3.54	1.43	1.33
23	a	604	CLA	C1C-NC	-3.54	1.32	1.37
23	B	617	CLA	CAA-C2A	-3.54	1.47	1.54
23	a	604	CLA	CBD-CGD	-3.54	1.41	1.52
23	B	607[A]	CLA	C3D-C2D	-3.54	1.29	1.39
23	b	609[B]	CLA	CAA-C2A	-3.54	1.47	1.54
23	c	508	CLA	C1A-CHA	-3.54	1.28	1.43
23	c	509	CLA	C3D-C2D	-3.54	1.29	1.39
23	C	504	CLA	C3D-C2D	-3.53	1.29	1.39
25	B	620	BCR	C2-C3	3.53	1.61	1.52
28	J	101	LMG	O8-C28	3.53	1.43	1.33
23	C	506	CLA	C1A-CHA	-3.52	1.28	1.43
23	c	512	CLA	CBD-CGD	-3.52	1.41	1.52
25	b	621	BCR	C4-C5	3.52	1.57	1.51
23	B	605	CLA	C1C-NC	-3.52	1.32	1.37
23	C	503	CLA	CAA-C2A	-3.52	1.47	1.54
23	B	616	CLA	CBD-CGD	-3.52	1.41	1.52
23	c	510	CLA	C1A-CHA	-3.52	1.28	1.43
23	c	512	CLA	C1A-CHA	-3.52	1.28	1.43
23	c	505	CLA	CBD-CGD	-3.52	1.41	1.52
23	C	511	CLA	O2A-CGA	3.52	1.43	1.33
25	T	101	BCR	C40-C30	3.52	1.60	1.53
23	b	611	CLA	C3D-C2D	-3.52	1.29	1.39
23	c	512	CLA	C3D-C4D	-3.51	1.36	1.44
23	C	507	CLA	C3D-C2D	-3.51	1.29	1.39
25	b	620	BCR	C1-C6	-3.51	1.49	1.53
23	c	504	CLA	CBD-CAD	-3.51	1.41	1.56
23	B	605	CLA	C1A-CHA	-3.51	1.28	1.43
23	b	619	CLA	O2A-CGA	3.51	1.43	1.33
23	b	613	CLA	O2A-CGA	3.51	1.43	1.33
23	b	614	CLA	O2A-CGA	3.51	1.43	1.33
23	C	509	CLA	C1A-CHA	-3.51	1.28	1.43
28	C	520	LMG	O6-C1	3.51	1.50	1.41
25	B	619	BCR	C4-C5	3.51	1.57	1.51
23	c	513	CLA	CBD-CGD	-3.51	1.41	1.52
23	c	514	CLA	C1A-CHA	-3.50	1.28	1.43
23	C	502	CLA	C3D-C4D	-3.50	1.36	1.44
23	c	502	CLA	CAA-C2A	-3.50	1.47	1.54
23	b	607	CLA	C1C-NC	-3.50	1.32	1.37
23	b	616	CLA	CBD-CAD	-3.50	1.41	1.56
23	B	612	CLA	C1C-NC	-3.50	1.32	1.37
23	b	618	CLA	C1A-CHA	-3.50	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C1A-CHA	-3.50	1.28	1.43
23	A	605	CLA	C1C-NC	-3.50	1.32	1.37
23	a	605	CLA	CBD-CGD	-3.50	1.41	1.52
23	b	615	CLA	C1D-ND	-3.50	1.33	1.37
23	b	619	CLA	CAA-C2A	-3.50	1.47	1.54
23	B	605	CLA	O2A-CGA	3.50	1.43	1.33
23	b	613	CLA	C3D-C2D	-3.50	1.29	1.39
23	B	611	CLA	C1A-CHA	-3.50	1.28	1.43
23	B	612	CLA	O2A-CGA	3.50	1.43	1.33
23	C	503	CLA	CBD-CGD	-3.50	1.41	1.52
25	k	101	BCR	C4-C5	3.49	1.57	1.51
23	a	607	CLA	C1D-ND	-3.49	1.33	1.37
23	b	609[B]	CLA	O2A-CGA	3.49	1.43	1.33
23	C	506	CLA	CAA-C2A	-3.49	1.47	1.54
23	b	609[A]	CLA	CBD-CGD	-3.49	1.41	1.52
23	B	615	CLA	CBD-CGD	-3.49	1.41	1.52
23	b	609[A]	CLA	C3D-C2D	-3.49	1.29	1.39
23	B	604	CLA	CBD-CAD	-3.49	1.41	1.56
23	c	502	CLA	C1C-NC	-3.49	1.32	1.37
23	D	404	CLA	CBD-CGD	-3.48	1.41	1.52
23	c	514	CLA	C3D-C2D	-3.48	1.29	1.39
23	c	503	CLA	C3D-C2D	-3.48	1.29	1.39
23	b	609[A]	CLA	O2A-CGA	3.48	1.43	1.33
23	D	404	CLA	C3D-C4D	-3.48	1.36	1.44
23	b	609[B]	CLA	C1C-NC	-3.48	1.32	1.37
23	C	502	CLA	CAA-C2A	-3.48	1.47	1.54
23	B	604	CLA	O2A-CGA	3.48	1.43	1.33
23	C	501	CLA	CBD-CAD	-3.48	1.41	1.56
23	b	610	CLA	CBD-CAD	-3.48	1.41	1.56
23	A	608	CLA	C3D-C2D	-3.48	1.29	1.39
28	A	612	LMG	O6-C1	3.48	1.50	1.41
23	B	612	CLA	C3D-C2D	-3.48	1.29	1.39
23	B	604	CLA	CBD-CGD	-3.48	1.41	1.52
23	a	613	CLA	CBD-CAD	-3.48	1.41	1.56
25	b	622	BCR	C2-C3	3.48	1.60	1.52
23	C	511	CLA	CAA-C2A	-3.48	1.47	1.54
23	B	611	CLA	CAA-C2A	-3.47	1.47	1.54
25	b	621	BCR	C2-C3	3.47	1.60	1.52
23	B	613	CLA	C1D-ND	-3.47	1.33	1.37
23	B	612	CLA	CBD-CGD	-3.47	1.42	1.52
23	c	508	CLA	C3D-C2D	-3.47	1.29	1.39
23	b	616	CLA	C1A-CHA	-3.47	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	CAA-C2A	-3.47	1.47	1.54
23	C	513	CLA	C1C-NC	-3.47	1.32	1.37
23	b	618	CLA	CBD-CGD	-3.47	1.42	1.52
23	C	508	CLA	C1C-NC	-3.47	1.32	1.37
23	c	502	CLA	C3D-C2D	-3.46	1.29	1.39
23	b	614	CLA	CBD-CAD	-3.46	1.41	1.56
23	C	508	CLA	C1D-ND	-3.46	1.33	1.37
23	b	606	CLA	CBD-CAD	-3.46	1.41	1.56
25	K	101	BCR	C31-C1	-3.46	1.47	1.53
23	c	502	CLA	O2A-CGA	3.46	1.43	1.33
23	B	611	CLA	CBD-CAD	-3.46	1.41	1.56
23	d	402	CLA	O2A-CGA	3.46	1.43	1.33
23	C	504	CLA	CBD-CAD	-3.46	1.41	1.56
28	a	611	LMG	O6-C1	3.46	1.50	1.41
23	C	504	CLA	O2A-CGA	3.46	1.43	1.33
23	b	608	CLA	CAA-C2A	-3.45	1.47	1.54
23	B	611	CLA	O2A-CGA	3.45	1.43	1.33
23	B	615	CLA	O2A-CGA	3.45	1.43	1.33
23	B	607[A]	CLA	CBD-CGD	-3.45	1.42	1.52
23	c	505	CLA	C1C-NC	-3.45	1.32	1.37
23	B	615	CLA	CBD-CAD	-3.45	1.41	1.56
23	b	609[B]	CLA	CBD-CGD	-3.45	1.42	1.52
23	c	502	CLA	CBD-CAD	-3.45	1.41	1.56
23	C	503	CLA	C1A-CHA	-3.45	1.28	1.43
23	B	603	CLA	CAA-C2A	-3.45	1.47	1.54
23	b	606	CLA	CAA-C2A	-3.45	1.47	1.54
32	C	518	DGD	C3D-C2D	-3.45	1.43	1.52
26	D	405	PL9	C36-C34	3.44	1.58	1.51
23	C	511	CLA	CBD-CGD	-3.44	1.42	1.52
23	C	501	CLA	O2A-CGA	3.44	1.43	1.33
23	C	512	CLA	C3D-C2D	-3.44	1.29	1.39
23	c	511	CLA	CBD-CAD	-3.44	1.41	1.56
32	C	517	DGD	O6E-C5E	3.44	1.52	1.44
23	D	402	CLA	CBD-CAD	-3.44	1.41	1.56
23	c	512	CLA	CAA-C2A	-3.44	1.47	1.54
23	b	608	CLA	O2A-CGA	3.44	1.43	1.33
23	B	607[A]	CLA	O2A-CGA	3.44	1.43	1.33
23	D	404	CLA	C1C-NC	-3.44	1.32	1.37
23	A	606	CLA	C1D-ND	-3.44	1.33	1.37
23	C	512	CLA	O2A-CGA	3.43	1.43	1.33
23	b	605	CLA	CBD-CAD	-3.43	1.41	1.56
25	t	101	BCR	C40-C30	3.43	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	CAA-C2A	-3.43	1.47	1.54
23	B	617	CLA	CBD-CGD	-3.43	1.42	1.52
23	C	507	CLA	C1A-CHA	-3.43	1.29	1.43
23	c	504	CLA	C1C-NC	-3.43	1.32	1.37
23	C	509	CLA	CBD-CAD	-3.43	1.41	1.56
23	B	607[A]	CLA	CAA-C2A	-3.43	1.47	1.54
23	c	503	CLA	CBD-CGD	-3.43	1.42	1.52
23	A	605	CLA	CBD-CGD	-3.43	1.42	1.52
23	b	613	CLA	CBD-CAD	-3.43	1.41	1.56
23	B	610	CLA	C3D-C2D	-3.43	1.29	1.39
23	b	614	CLA	CAA-C2A	-3.43	1.47	1.54
23	c	507	CLA	CBD-CAD	-3.43	1.41	1.56
32	c	519	DGD	C3D-C2D	-3.43	1.43	1.52
23	C	508	CLA	O2A-CGA	3.43	1.43	1.33
23	B	617	CLA	CBD-CAD	-3.43	1.41	1.56
23	B	605	CLA	CBD-CAD	-3.42	1.41	1.56
23	C	508	CLA	CBD-CGD	-3.42	1.42	1.52
23	C	501	CLA	CAA-C2A	-3.42	1.47	1.54
23	b	606	CLA	CBD-CGD	-3.42	1.42	1.52
23	a	607	CLA	C1C-NC	-3.42	1.32	1.37
23	c	505	CLA	CAA-C2A	-3.42	1.47	1.54
25	c	516	BCR	C12-C13	3.42	1.53	1.46
23	a	605	CLA	CBD-CAD	-3.42	1.41	1.56
23	b	608	CLA	CBD-CGD	-3.42	1.42	1.52
23	c	510	CLA	C1C-NC	-3.42	1.32	1.37
23	c	508	CLA	CBD-CAD	-3.42	1.41	1.56
23	c	505	CLA	O2A-CGA	3.42	1.43	1.33
23	c	505	CLA	CBD-CAD	-3.42	1.41	1.56
26	a	609	PL9	C36-C34	3.41	1.58	1.51
23	b	612	CLA	C1D-ND	-3.41	1.33	1.37
23	a	605	CLA	O2A-CGA	3.41	1.43	1.33
23	c	504	CLA	O2A-CGA	3.41	1.43	1.33
23	b	608	CLA	CBD-CAD	-3.41	1.41	1.56
23	b	605	CLA	CBD-CGD	-3.41	1.42	1.52
23	B	613	CLA	CBD-CGD	-3.41	1.42	1.52
25	a	608	BCR	C27-C26	3.41	1.57	1.51
23	C	505	CLA	CBD-CAD	-3.41	1.41	1.56
23	C	502	CLA	CBD-CGD	-3.41	1.42	1.52
23	B	608	CLA	CBD-CAD	-3.41	1.41	1.56
23	d	403	CLA	C3D-C4D	-3.41	1.36	1.44
23	C	501	CLA	C3D-C2D	-3.41	1.29	1.39
23	b	609[A]	CLA	CAA-C2A	-3.41	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CBD-CAD	-3.41	1.41	1.56
23	B	606	CLA	O2A-CGA	3.41	1.43	1.33
23	A	605	CLA	CBD-CAD	-3.41	1.41	1.56
23	B	615	CLA	CAA-C2A	-3.40	1.47	1.54
23	C	508	CLA	CBD-CAD	-3.40	1.41	1.56
23	B	611	CLA	C3D-C2D	-3.40	1.29	1.39
23	C	502	CLA	C3D-C2D	-3.40	1.29	1.39
23	b	615	CLA	O2A-CGA	3.40	1.43	1.33
23	D	403	CLA	C1D-ND	-3.40	1.33	1.37
23	a	613	CLA	O2A-CGA	3.40	1.43	1.33
23	b	616	CLA	C1C-NC	-3.40	1.32	1.37
23	b	609[B]	CLA	CBD-CAD	-3.40	1.41	1.56
23	b	619	CLA	CBD-CAD	-3.39	1.41	1.56
23	B	607[B]	CLA	O2A-CGA	3.39	1.43	1.33
23	c	513	CLA	CBD-CAD	-3.39	1.41	1.56
23	A	605	CLA	O2A-CGA	3.39	1.43	1.33
23	b	609[A]	CLA	CBD-CAD	-3.39	1.41	1.56
23	C	510	CLA	CBD-CAD	-3.39	1.41	1.56
23	c	511	CLA	C1C-NC	-3.39	1.32	1.37
24	A	607	PHO	C4D-CHA	3.39	1.44	1.39
23	c	506	CLA	CBD-CAD	-3.39	1.41	1.56
23	c	510	CLA	CBD-CAD	-3.39	1.41	1.56
23	b	607	CLA	CBD-CAD	-3.39	1.41	1.56
23	C	509	CLA	C1D-ND	-3.39	1.33	1.37
23	C	511	CLA	CBD-CAD	-3.39	1.41	1.56
23	b	616	CLA	CBD-CGD	-3.39	1.42	1.52
23	B	602	CLA	CBD-CAD	-3.39	1.41	1.56
23	d	403	CLA	C3D-C2D	-3.39	1.29	1.39
23	A	606	CLA	CBD-CAD	-3.39	1.41	1.56
23	c	504	CLA	CAA-C2A	-3.39	1.47	1.54
23	B	606	CLA	CBD-CGD	-3.38	1.42	1.52
23	b	617	CLA	CBD-CAD	-3.38	1.41	1.56
23	c	514	CLA	CAA-C2A	-3.38	1.47	1.54
23	b	605	CLA	O2A-CGA	3.38	1.43	1.33
23	B	606	CLA	CBD-CAD	-3.38	1.41	1.56
23	d	403	CLA	CBD-CGD	-3.38	1.42	1.52
23	B	605	CLA	CBD-CGD	-3.38	1.42	1.52
25	B	618	BCR	C1-C6	-3.38	1.49	1.53
23	C	503	CLA	CBD-CAD	-3.38	1.41	1.56
23	b	612	CLA	C3D-C2D	-3.38	1.29	1.39
23	A	608	CLA	CBD-CAD	-3.38	1.41	1.56
23	a	605	CLA	CAA-C2A	-3.38	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	O2A-CGA	3.37	1.43	1.33
23	C	512	CLA	CBD-CAD	-3.37	1.41	1.56
25	C	514	BCR	C2-C3	3.37	1.60	1.52
28	J	101	LMG	O7-C8	-3.37	1.38	1.46
32	D	406	DGD	O6D-C5D	3.37	1.52	1.44
23	D	402	CLA	CAA-C2A	-3.37	1.48	1.54
23	B	612	CLA	CBD-CAD	-3.37	1.41	1.56
23	b	612	CLA	CBD-CAD	-3.37	1.41	1.56
23	B	613	CLA	CBD-CAD	-3.37	1.41	1.56
23	b	609[A]	CLA	C1C-NC	-3.37	1.32	1.37
23	C	506	CLA	O2A-CGA	3.36	1.43	1.33
25	k	101	BCR	C1-C6	-3.36	1.49	1.53
23	B	607[B]	CLA	CBD-CGD	-3.36	1.42	1.52
23	B	613	CLA	O2A-CGA	3.36	1.43	1.33
23	a	604	CLA	CBD-CAD	-3.36	1.41	1.56
23	b	604	CLA	CBD-CGD	-3.36	1.42	1.52
23	A	606	CLA	CAA-C2A	-3.36	1.48	1.54
23	c	514	CLA	O2A-CGA	3.36	1.43	1.33
23	B	607[A]	CLA	CBD-CAD	-3.36	1.41	1.56
25	k	101	BCR	C27-C26	3.36	1.57	1.51
23	B	607[B]	CLA	CBD-CAD	-3.35	1.41	1.56
23	C	506	CLA	CBD-CAD	-3.35	1.41	1.56
23	c	508	CLA	CBD-CGD	-3.35	1.42	1.52
23	D	403	CLA	O2A-CGA	3.35	1.43	1.33
23	a	613	CLA	CAA-C2A	-3.35	1.48	1.54
25	C	515	BCR	C1-C6	-3.35	1.49	1.53
23	C	509	CLA	CBD-CGD	-3.35	1.42	1.52
23	c	502	CLA	CBD-CGD	-3.35	1.42	1.52
23	B	603	CLA	O2A-CGA	3.35	1.43	1.33
32	C	518	DGD	O6D-C5D	3.35	1.52	1.44
23	A	608	CLA	C1D-ND	-3.35	1.33	1.37
25	K	101	BCR	C4-C5	3.35	1.57	1.51
23	b	617	CLA	CBD-CGD	-3.35	1.42	1.52
23	B	609	CLA	CBD-CGD	-3.34	1.42	1.52
23	C	505	CLA	C1D-ND	-3.34	1.33	1.37
23	c	514	CLA	CBD-CAD	-3.34	1.41	1.56
23	b	615	CLA	CBD-CAD	-3.34	1.41	1.56
23	B	609	CLA	CBD-CAD	-3.34	1.41	1.56
28	b	623	LMG	O7-C8	-3.34	1.38	1.46
23	b	618	CLA	CBD-CAD	-3.33	1.41	1.56
24	a	606	PHO	C4D-CHA	3.33	1.44	1.39
25	t	101	BCR	C27-C26	3.33	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	CBD-CAD	-3.33	1.41	1.56
23	b	611	CLA	O2A-CGA	3.33	1.43	1.33
23	B	609	CLA	CAA-C2A	-3.33	1.48	1.54
23	C	513	CLA	CBD-CAD	-3.33	1.41	1.56
25	c	522	BCR	C12-C13	3.33	1.53	1.46
23	c	503	CLA	CBD-CAD	-3.33	1.41	1.56
23	B	604	CLA	CAA-C2A	-3.33	1.48	1.54
25	T	101	BCR	C27-C26	3.33	1.57	1.51
23	c	510	CLA	CAA-C2A	-3.33	1.48	1.54
25	F	101	BCR	C4-C5	3.33	1.57	1.51
23	b	612	CLA	O2A-CGA	3.32	1.43	1.33
23	b	607	CLA	CBD-CGD	-3.32	1.42	1.52
25	A	609	BCR	C4-C5	3.32	1.57	1.51
23	B	614	CLA	O2A-CGA	3.32	1.43	1.33
23	C	507	CLA	CBD-CAD	-3.32	1.41	1.56
23	D	402	CLA	O2A-CGA	3.32	1.43	1.33
25	b	622	BCR	C27-C26	3.32	1.57	1.51
23	b	617	CLA	CAA-C2A	-3.31	1.48	1.54
32	C	516	DGD	O6D-C5D	3.31	1.52	1.44
23	D	404	CLA	CBD-CAD	-3.31	1.41	1.56
25	K	101	BCR	C2-C3	3.31	1.60	1.52
23	C	503	CLA	O2A-CGA	3.30	1.43	1.33
23	B	616	CLA	CBD-CAD	-3.30	1.42	1.56
23	a	604	CLA	O2A-CGA	3.30	1.43	1.33
32	d	405	DGD	O6D-C5D	3.30	1.52	1.44
23	b	608	CLA	C1D-ND	-3.30	1.33	1.37
23	c	507	CLA	CBD-CGD	-3.30	1.42	1.52
23	b	604	CLA	CBD-CAD	-3.30	1.42	1.56
23	b	618	CLA	CAA-C2A	-3.30	1.48	1.54
23	b	611	CLA	CAA-C2A	-3.29	1.48	1.54
23	C	505	CLA	CBD-CGD	-3.29	1.42	1.52
23	a	607	CLA	CBD-CAD	-3.29	1.42	1.56
23	c	509	CLA	CBD-CAD	-3.29	1.42	1.56
25	k	101	BCR	C31-C1	-3.28	1.47	1.53
23	C	505	CLA	O2A-CGA	3.28	1.42	1.33
23	B	603	CLA	CBD-CAD	-3.28	1.42	1.56
23	a	607	CLA	CBD-CGD	-3.28	1.42	1.52
23	b	611	CLA	CBD-CAD	-3.28	1.42	1.56
25	b	621	BCR	C40-C30	3.27	1.59	1.53
23	C	513	CLA	CAA-C2A	-3.27	1.48	1.54
23	B	610	CLA	O2A-CGA	3.27	1.42	1.33
23	b	610	CLA	O2A-CGA	3.27	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	515	BCR	C2-C3	3.27	1.60	1.52
25	a	608	BCR	C4-C5	3.27	1.57	1.51
23	C	506	CLA	C1D-ND	-3.27	1.33	1.37
23	c	514	CLA	CBD-CGD	-3.26	1.42	1.52
23	b	610	CLA	CAA-C2A	-3.26	1.48	1.54
23	c	511	CLA	O2A-CGA	3.26	1.42	1.33
23	c	502	CLA	C1D-ND	-3.26	1.33	1.37
23	B	602	CLA	CAA-C2A	-3.26	1.48	1.54
25	C	514	BCR	C27-C26	3.26	1.57	1.51
23	C	502	CLA	CBD-CAD	-3.26	1.42	1.56
23	B	608	CLA	O2A-CGA	3.26	1.42	1.33
23	c	503	CLA	CAA-C2A	-3.26	1.48	1.54
23	B	605	CLA	CAA-C2A	-3.25	1.48	1.54
25	c	516	BCR	C4-C5	3.25	1.57	1.51
23	C	504	CLA	CAA-C2A	-3.25	1.48	1.54
25	B	620	BCR	C27-C26	3.25	1.57	1.51
23	b	611	CLA	CBD-CGD	-3.25	1.42	1.52
23	b	619	CLA	CBD-CGD	-3.25	1.42	1.52
25	f	101	BCR	C1-C6	-3.25	1.49	1.53
25	c	515	BCR	C27-C26	3.25	1.57	1.51
32	c	517	DGD	C3D-C2D	-3.24	1.43	1.52
23	b	605	CLA	CHB-C4A	-3.24	1.29	1.37
23	B	612	CLA	CAA-C2A	-3.24	1.48	1.54
23	C	507	CLA	CBD-CGD	-3.24	1.42	1.52
32	h	102	DGD	O6D-C5D	3.23	1.52	1.44
23	c	510	CLA	CBD-CGD	-3.23	1.42	1.52
23	a	605	CLA	C1D-ND	-3.23	1.33	1.37
23	b	617	CLA	O2A-CGA	3.23	1.42	1.33
33	v	201	HEM	CAB-C3B	3.23	1.56	1.47
23	C	501	CLA	C1D-ND	-3.23	1.33	1.37
23	B	609	CLA	O2A-CGA	3.23	1.42	1.33
23	C	513	CLA	C1D-ND	-3.23	1.33	1.37
23	d	403	CLA	CBD-CAD	-3.23	1.42	1.56
32	H	102	DGD	C3D-C2D	-3.22	1.44	1.52
33	V	202	HEM	FE-NB	3.22	2.04	1.94
25	B	620	BCR	C1-C6	-3.22	1.49	1.53
23	C	509	CLA	CAA-C2A	-3.22	1.48	1.54
23	B	603	CLA	CBD-CGD	-3.22	1.42	1.52
23	c	509	CLA	O2A-CGA	3.22	1.42	1.33
23	C	510	CLA	O2A-CGA	3.22	1.42	1.33
23	b	619	CLA	C1D-ND	-3.21	1.33	1.37
24	d	401	PHO	C4D-CHA	3.21	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C3B-C4B	-3.21	1.33	1.42
25	C	514	BCR	C4-C5	3.21	1.57	1.51
23	b	612	CLA	CBD-CGD	-3.21	1.42	1.52
23	c	507	CLA	CHB-C4A	-3.21	1.29	1.37
25	k	101	BCR	C2-C3	3.21	1.60	1.52
25	h	101	BCR	C27-C26	3.21	1.57	1.51
23	b	607	CLA	CAA-C2A	-3.21	1.48	1.54
25	b	622	BCR	C4-C5	3.20	1.57	1.51
25	K	101	BCR	C27-C26	3.20	1.57	1.51
33	E	102	HEM	CAC-C3C	3.20	1.55	1.47
23	b	612	CLA	O2D-CGD	3.19	1.41	1.33
23	C	506	CLA	CBD-CGD	-3.19	1.42	1.52
23	B	610	CLA	CBD-CGD	-3.19	1.42	1.52
28	j	101	LMG	O7-C8	-3.19	1.39	1.46
23	C	513	CLA	CBD-CGD	-3.19	1.42	1.52
25	H	101	BCR	C27-C26	3.19	1.56	1.51
23	c	505	CLA	C1D-ND	-3.18	1.33	1.37
25	B	620	BCR	C4-C5	3.18	1.56	1.51
25	C	521	BCR	C4-C5	3.18	1.56	1.51
23	b	611	CLA	C1D-ND	-3.18	1.33	1.37
26	a	609	PL9	C7-C3	3.18	1.55	1.51
23	b	604	CLA	CAA-C2A	-3.18	1.48	1.54
23	B	607[A]	CLA	C1D-ND	-3.18	1.33	1.37
23	c	510	CLA	C1D-ND	-3.18	1.33	1.37
23	b	615	CLA	CBD-CGD	-3.18	1.42	1.52
28	B	621	LMG	O7-C8	-3.17	1.39	1.46
23	B	607[B]	CLA	C1D-ND	-3.17	1.33	1.37
23	c	513	CLA	CAA-C2A	-3.17	1.48	1.54
23	B	603	CLA	CHB-C4A	-3.17	1.29	1.37
23	b	616	CLA	O2A-CGA	3.17	1.42	1.33
25	B	619	BCR	C40-C30	3.17	1.59	1.53
23	C	513	CLA	O2D-CGD	3.17	1.41	1.33
32	c	517	DGD	O6D-C5D	3.17	1.52	1.44
26	A	610	PL9	C21-C19	3.16	1.57	1.51
23	C	506	CLA	CHB-C4A	-3.16	1.29	1.37
32	D	406	DGD	C3D-C2D	-3.16	1.44	1.52
23	c	509	CLA	CBD-CGD	-3.16	1.42	1.52
26	A	610	PL9	C7-C3	3.15	1.55	1.51
23	B	609	CLA	C1D-ND	-3.15	1.33	1.37
26	a	609	PL9	C21-C19	3.15	1.57	1.51
25	h	101	BCR	C35-C13	-3.15	1.44	1.50
25	k	101	BCR	C35-C13	-3.15	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	101	BCR	C12-C13	3.15	1.52	1.46
25	h	101	BCR	C12-C13	3.14	1.52	1.46
23	b	616	CLA	C1D-ND	-3.14	1.33	1.37
23	c	511	CLA	C1D-ND	-3.14	1.33	1.37
32	H	102	DGD	O6D-C5D	3.14	1.52	1.44
23	C	509	CLA	O2D-CGD	3.14	1.41	1.33
23	c	503	CLA	C1D-ND	-3.14	1.33	1.37
23	b	613	CLA	C1D-ND	-3.14	1.33	1.37
23	d	402	CLA	CHB-C4A	-3.14	1.29	1.37
23	c	506	CLA	CBD-CGD	-3.14	1.43	1.52
23	C	507	CLA	CAA-C2A	-3.14	1.48	1.54
33	E	102	HEM	CAB-C3B	3.13	1.55	1.47
25	B	619	BCR	C31-C1	-3.13	1.47	1.53
28	C	519	LMG	O7-C8	-3.13	1.39	1.46
32	c	519	DGD	O6D-C5D	3.13	1.52	1.44
23	C	506	CLA	O2D-CGD	3.13	1.40	1.33
23	c	508	CLA	CAA-C2A	-3.13	1.48	1.54
23	D	402	CLA	C1D-ND	-3.13	1.33	1.37
23	C	510	CLA	C1D-ND	-3.13	1.33	1.37
33	V	202	HEM	CAB-C3B	3.12	1.55	1.47
23	b	609[B]	CLA	C1D-ND	-3.12	1.33	1.37
23	c	509	CLA	CHB-C4A	-3.12	1.29	1.37
28	c	520	LMG	O7-C8	-3.12	1.39	1.46
23	B	607[A]	CLA	CHB-C4A	-3.12	1.29	1.37
23	B	615	CLA	C1D-ND	-3.12	1.33	1.37
23	b	617	CLA	C1D-ND	-3.12	1.33	1.37
32	h	102	DGD	C3D-C2D	-3.11	1.44	1.52
32	C	516	DGD	C3D-C2D	-3.11	1.44	1.52
23	B	606	CLA	C1D-ND	-3.11	1.33	1.37
23	B	612	CLA	C1D-ND	-3.11	1.33	1.37
33	e	102	HEM	CAB-C3B	3.10	1.55	1.47
23	B	616	CLA	CAA-C2A	-3.10	1.48	1.54
25	C	521	BCR	C27-C26	3.10	1.56	1.51
25	b	621	BCR	C31-C1	-3.10	1.47	1.53
25	B	618	BCR	C35-C13	-3.10	1.44	1.50
23	c	506	CLA	C3B-C4B	-3.10	1.33	1.42
23	a	604	CLA	CHB-C4A	-3.10	1.29	1.37
23	a	607	CLA	CAA-C2A	-3.10	1.48	1.54
28	Z	101	LMG	O7-C8	-3.10	1.39	1.46
23	D	402	CLA	CHB-C4A	-3.09	1.30	1.37
23	a	605	CLA	CHB-C4A	-3.09	1.30	1.37
28	z	101	LMG	O7-C8	-3.09	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C1D-ND	-3.09	1.33	1.37
23	c	510	CLA	O2D-CGD	3.09	1.40	1.33
25	c	522	BCR	C4-C5	3.09	1.56	1.51
23	B	612	CLA	CHB-C4A	-3.09	1.30	1.37
23	b	610	CLA	C1D-ND	-3.09	1.33	1.37
23	A	605	CLA	C1D-ND	-3.08	1.33	1.37
32	d	405	DGD	C3D-C2D	-3.08	1.44	1.52
25	C	515	BCR	C4-C5	3.08	1.56	1.51
23	c	506	CLA	O2A-CGA	3.07	1.42	1.33
28	A	612	LMG	O7-C8	-3.07	1.39	1.46
26	d	404	PL9	C21-C19	3.07	1.57	1.51
23	B	617	CLA	C1D-ND	-3.06	1.33	1.37
25	c	515	BCR	C4-C5	3.06	1.56	1.51
23	A	605	CLA	CHB-C4A	-3.06	1.30	1.37
23	b	611	CLA	CHB-C4A	-3.06	1.30	1.37
33	v	201	HEM	CAC-C3C	3.06	1.55	1.47
23	B	607[B]	CLA	CHB-C4A	-3.06	1.30	1.37
25	b	620	BCR	C4-C5	3.06	1.56	1.51
26	D	405	PL9	C21-C19	3.06	1.57	1.51
23	b	605	CLA	C1D-ND	-3.06	1.33	1.37
23	c	514	CLA	O2D-CGD	3.06	1.40	1.33
25	c	516	BCR	C27-C26	3.06	1.56	1.51
25	t	101	BCR	C12-C13	3.06	1.52	1.46
25	C	515	BCR	C27-C26	3.05	1.56	1.51
23	c	507	CLA	C1D-ND	-3.05	1.33	1.37
23	c	513	CLA	C1D-ND	-3.05	1.33	1.37
23	c	508	CLA	C3B-C4B	-3.05	1.34	1.42
25	h	101	BCR	C4-C5	3.04	1.56	1.51
23	D	403	CLA	CHB-C4A	-3.04	1.30	1.37
23	C	511	CLA	C1D-ND	-3.04	1.33	1.37
25	t	101	BCR	C31-C1	-3.04	1.48	1.53
28	c	521	LMG	O7-C8	-3.04	1.39	1.46
23	C	508	CLA	CHB-C4A	-3.03	1.30	1.37
25	A	609	BCR	C12-C13	3.03	1.52	1.46
23	c	514	CLA	CHB-C4A	-3.03	1.30	1.37
23	b	614	CLA	CHB-C4A	-3.03	1.30	1.37
23	c	509	CLA	C1D-ND	-3.03	1.33	1.37
25	C	515	BCR	C12-C13	3.03	1.52	1.46
28	a	611	LMG	O7-C8	-3.02	1.39	1.46
33	e	102	HEM	CAC-C3C	3.02	1.55	1.47
23	C	501	CLA	CHB-C4A	-3.02	1.30	1.37
25	b	622	BCR	C35-C13	-3.02	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	613	CLA	CHB-C4A	-3.02	1.30	1.37
23	C	512	CLA	C1D-ND	-3.02	1.33	1.37
33	V	202	HEM	CAC-C3C	3.02	1.55	1.47
25	B	618	BCR	C27-C26	3.02	1.56	1.51
23	B	610	CLA	O2D-CGD	3.02	1.40	1.33
23	B	617	CLA	C3B-C4B	-3.02	1.34	1.42
25	C	515	BCR	C35-C13	-3.02	1.44	1.50
23	D	404	CLA	C1D-ND	-3.02	1.33	1.37
25	f	101	BCR	C35-C13	-3.02	1.44	1.50
23	b	609[A]	CLA	CHB-C4A	-3.01	1.30	1.37
25	B	619	BCR	C35-C13	-3.01	1.44	1.50
23	b	619	CLA	O2D-CGD	3.01	1.40	1.33
23	B	609	CLA	CHB-C4A	-3.00	1.30	1.37
25	t	101	BCR	C4-C5	3.00	1.56	1.51
23	c	511	CLA	C3B-C4B	-3.00	1.34	1.42
23	B	611	CLA	CHB-C4A	-3.00	1.30	1.37
23	A	605	CLA	O2D-CED	-3.00	1.38	1.45
32	c	518	DGD	C3D-C2D	-3.00	1.44	1.52
23	a	604	CLA	O2D-CED	-3.00	1.38	1.45
25	C	515	BCR	C17-C18	3.00	1.42	1.35
23	c	510	CLA	MG-NA	-3.00	1.99	2.06
25	T	101	BCR	C4-C5	3.00	1.56	1.51
23	b	619	CLA	C3B-C4B	-3.00	1.34	1.42
23	C	504	CLA	C1D-ND	-3.00	1.33	1.37
23	b	613	CLA	CHB-C4A	-3.00	1.30	1.37
23	a	607	CLA	O2D-CGD	3.00	1.40	1.33
23	c	508	CLA	C1D-ND	-3.00	1.33	1.37
23	b	607	CLA	C3B-C4B	-3.00	1.34	1.42
23	B	610	CLA	C1D-ND	-2.99	1.33	1.37
23	B	604	CLA	C3B-C4B	-2.99	1.34	1.42
25	a	608	BCR	C35-C13	-2.99	1.44	1.50
25	B	619	BCR	C1-C6	-2.99	1.50	1.53
23	A	605	CLA	MG-NA	-2.99	1.99	2.06
23	a	604	CLA	MG-NA	-2.99	1.99	2.06
23	b	605	CLA	O2D-CGD	2.99	1.40	1.33
33	E	102	HEM	FE-NC	2.98	2.05	1.95
23	b	608	CLA	CHB-C4A	-2.98	1.30	1.37
23	b	609[B]	CLA	CHB-C4A	-2.98	1.30	1.37
23	c	505	CLA	CHB-C4A	-2.98	1.30	1.37
23	B	613	CLA	MG-NA	-2.98	1.99	2.06
23	c	506	CLA	O2D-CGD	2.98	1.40	1.33
28	C	520	LMG	O7-C8	-2.97	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	CHB-C4A	-2.97	1.30	1.37
23	D	402	CLA	MG-NA	-2.97	1.99	2.06
25	B	618	BCR	C4-C5	2.97	1.56	1.51
23	A	608	CLA	O2D-CGD	2.97	1.40	1.33
23	B	605	CLA	O2D-CGD	2.97	1.40	1.33
25	c	522	BCR	C27-C26	2.97	1.56	1.51
25	F	101	BCR	C1-C6	-2.97	1.50	1.53
23	d	403	CLA	C1D-ND	-2.97	1.34	1.37
23	b	616	CLA	C3B-C4B	-2.96	1.34	1.42
23	b	604	CLA	C1D-ND	-2.96	1.34	1.37
23	B	611	CLA	O2D-CED	-2.96	1.38	1.45
23	B	606	CLA	O2D-CGD	2.96	1.40	1.33
23	b	615	CLA	CHB-C4A	-2.96	1.30	1.37
23	a	604	CLA	C1D-ND	-2.96	1.34	1.37
23	b	607	CLA	C1D-ND	-2.96	1.34	1.37
23	B	616	CLA	C1D-ND	-2.96	1.34	1.37
23	b	606	CLA	C3B-C4B	-2.95	1.34	1.42
23	c	502	CLA	CHB-C4A	-2.95	1.30	1.37
23	C	507	CLA	C3B-C4B	-2.95	1.34	1.42
23	B	612	CLA	O2D-CGD	2.95	1.40	1.33
23	C	511	CLA	O2D-CGD	2.95	1.40	1.33
23	C	504	CLA	CHB-C4A	-2.95	1.30	1.37
23	a	613	CLA	C1D-ND	-2.95	1.34	1.37
23	b	612	CLA	CHB-C4A	-2.95	1.30	1.37
23	c	503	CLA	CHB-C4A	-2.95	1.30	1.37
23	B	603	CLA	C1D-ND	-2.95	1.34	1.37
25	c	516	BCR	C1-C6	-2.95	1.50	1.53
23	C	512	CLA	CHB-C4A	-2.95	1.30	1.37
23	c	504	CLA	O2D-CED	-2.94	1.38	1.45
23	C	510	CLA	CHB-C4A	-2.94	1.30	1.37
23	C	505	CLA	CHB-C4A	-2.94	1.30	1.37
25	t	101	BCR	C2-C3	2.94	1.59	1.52
25	H	101	BCR	C4-C5	2.94	1.56	1.51
23	b	617	CLA	C3B-C4B	-2.94	1.34	1.42
23	B	605	CLA	C1D-ND	-2.94	1.34	1.37
23	b	614	CLA	MG-NA	-2.94	1.99	2.06
23	B	609	CLA	O2D-CGD	2.94	1.40	1.33
23	B	606	CLA	C3B-C4B	-2.94	1.34	1.42
23	c	510	CLA	C3B-C4B	-2.93	1.34	1.42
23	C	502	CLA	C1D-ND	-2.93	1.34	1.37
25	T	101	BCR	C35-C13	-2.93	1.44	1.50
23	b	606	CLA	O2D-CGD	2.93	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	619	BCR	C17-C18	2.93	1.42	1.35
23	d	403	CLA	CHB-C4A	-2.93	1.30	1.37
23	C	503	CLA	C1D-ND	-2.93	1.34	1.37
23	A	608	CLA	C3B-C4B	-2.93	1.34	1.42
23	C	509	CLA	C3B-C4B	-2.93	1.34	1.42
23	b	609[A]	CLA	C1D-ND	-2.93	1.34	1.37
25	b	621	BCR	C35-C13	-2.93	1.44	1.50
23	A	608	CLA	CAA-C2A	-2.93	1.48	1.54
23	b	619	CLA	MG-NA	-2.93	1.99	2.06
23	c	513	CLA	C3B-C4B	-2.92	1.34	1.42
23	b	612	CLA	MG-NA	-2.92	1.99	2.06
23	b	615	CLA	C3B-C4B	-2.92	1.34	1.42
23	a	613	CLA	MG-NA	-2.92	1.99	2.06
23	a	613	CLA	C3B-C4B	-2.92	1.34	1.42
23	c	507	CLA	O2D-CGD	2.92	1.40	1.33
32	C	517	DGD	O6D-C5D	2.92	1.51	1.44
23	B	614	CLA	C3B-C4B	-2.92	1.34	1.42
23	B	610	CLA	CHB-C4A	-2.91	1.30	1.37
23	C	507	CLA	C1D-ND	-2.91	1.34	1.37
23	d	402	CLA	MG-NA	-2.91	1.99	2.06
23	B	602	CLA	CHB-C4A	-2.91	1.30	1.37
23	B	604	CLA	CHB-C4A	-2.91	1.30	1.37
23	c	511	CLA	CHB-C4A	-2.91	1.30	1.37
23	B	614	CLA	CHB-C4A	-2.91	1.30	1.37
23	C	503	CLA	CHB-C4A	-2.91	1.30	1.37
23	b	606	CLA	CHB-C4A	-2.91	1.30	1.37
23	B	607[A]	CLA	C3B-C4B	-2.91	1.34	1.42
23	b	607	CLA	O2D-CGD	2.91	1.40	1.33
25	B	620	BCR	C35-C13	-2.90	1.45	1.50
23	A	606	CLA	MG-NA	-2.90	1.99	2.06
23	b	613	CLA	O2D-CED	-2.90	1.38	1.45
23	C	502	CLA	CHB-C4A	-2.90	1.30	1.37
23	C	505	CLA	C3B-C4B	-2.90	1.34	1.42
23	B	615	CLA	CHB-C4A	-2.90	1.30	1.37
23	C	510	CLA	C3B-C4B	-2.90	1.34	1.42
23	b	615	CLA	O2D-CGD	2.90	1.40	1.33
23	C	512	CLA	C3B-C4B	-2.90	1.34	1.42
23	D	403	CLA	MG-NA	-2.90	1.99	2.06
23	a	605	CLA	O2D-CGD	2.90	1.40	1.33
23	C	509	CLA	CHB-C4A	-2.90	1.30	1.37
23	b	606	CLA	MG-NA	-2.89	1.99	2.06
23	a	604	CLA	C3B-C4B	-2.89	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	O2D-CED	-2.89	1.38	1.45
23	b	608	CLA	O2D-CGD	2.89	1.40	1.33
23	c	502	CLA	O2D-CGD	2.89	1.40	1.33
25	c	515	BCR	C31-C1	-2.89	1.48	1.53
23	b	607	CLA	CHB-C4A	-2.89	1.30	1.37
23	a	607	CLA	MG-NA	-2.89	1.99	2.06
25	a	608	BCR	C12-C13	2.89	1.52	1.46
23	B	613	CLA	C3B-C4B	-2.89	1.34	1.42
23	C	508	CLA	C3B-C4B	-2.88	1.34	1.42
23	b	617	CLA	CHB-C4A	-2.88	1.30	1.37
23	b	610	CLA	C3B-C4B	-2.88	1.34	1.42
23	B	603	CLA	O2D-CGD	2.88	1.40	1.33
23	B	613	CLA	O2D-CGD	2.88	1.40	1.33
23	c	505	CLA	MG-NA	-2.88	1.99	2.06
23	c	513	CLA	CHB-C4A	-2.88	1.30	1.37
23	C	504	CLA	C3B-C4B	-2.88	1.34	1.42
25	h	101	BCR	C1-C6	-2.88	1.50	1.53
25	c	516	BCR	C35-C13	-2.88	1.45	1.50
23	A	606	CLA	CHB-C4A	-2.87	1.30	1.37
23	b	605	CLA	MG-NA	-2.87	1.99	2.06
23	B	617	CLA	MG-NA	-2.87	1.99	2.06
23	B	607[B]	CLA	O2D-CGD	2.87	1.40	1.33
23	d	402	CLA	C3B-C4B	-2.87	1.34	1.42
23	b	604	CLA	CHB-C4A	-2.87	1.30	1.37
25	C	514	BCR	C35-C13	-2.87	1.45	1.50
23	B	611	CLA	C1D-ND	-2.87	1.34	1.37
25	B	620	BCR	C31-C1	-2.87	1.48	1.53
23	c	508	CLA	O2D-CGD	2.87	1.40	1.33
23	C	504	CLA	MG-NA	-2.87	1.99	2.06
23	C	505	CLA	O2D-CGD	2.87	1.40	1.33
23	B	608	CLA	C3B-C4B	-2.87	1.34	1.42
23	d	403	CLA	CAA-C2A	-2.87	1.48	1.54
32	C	517	DGD	C3D-C2D	-2.87	1.44	1.52
23	C	506	CLA	C3B-C4B	-2.86	1.34	1.42
23	D	404	CLA	O2D-CGD	2.86	1.40	1.33
23	c	504	CLA	CHB-C4A	-2.86	1.30	1.37
23	b	611	CLA	O2D-CGD	2.86	1.40	1.33
23	B	608	CLA	CHB-C4A	-2.86	1.30	1.37
23	c	504	CLA	C1D-ND	-2.86	1.34	1.37
23	b	615	CLA	MG-NA	-2.86	1.99	2.06
23	A	606	CLA	C3B-C4B	-2.86	1.34	1.42
23	b	604	CLA	O2D-CGD	2.86	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C3B-C4B	-2.86	1.34	1.42
23	b	618	CLA	CHB-C4A	-2.86	1.30	1.37
23	C	502	CLA	C3B-C4B	-2.85	1.34	1.42
23	C	513	CLA	MG-NA	-2.85	1.99	2.06
23	c	511	CLA	O2D-CED	-2.85	1.38	1.45
23	b	617	CLA	MG-NA	-2.85	1.99	2.06
23	b	608	CLA	C3B-C4B	-2.85	1.34	1.42
23	b	617	CLA	O2D-CGD	2.85	1.40	1.33
23	C	513	CLA	CHB-C4A	-2.85	1.30	1.37
23	c	514	CLA	MG-NA	-2.85	1.99	2.06
25	A	609	BCR	C35-C13	-2.85	1.45	1.50
23	B	602	CLA	O2D-CGD	2.85	1.40	1.33
23	A	608	CLA	CHB-C4A	-2.85	1.30	1.37
23	c	512	CLA	C3B-C4B	-2.85	1.34	1.42
23	C	507	CLA	CHB-C4A	-2.85	1.30	1.37
23	B	615	CLA	O2D-CGD	2.85	1.40	1.33
23	c	514	CLA	C3B-C4B	-2.84	1.34	1.42
23	B	617	CLA	O2D-CGD	2.84	1.40	1.33
23	b	609[A]	CLA	C3B-C4B	-2.84	1.34	1.42
23	b	609[B]	CLA	C3B-C4B	-2.84	1.34	1.42
32	C	517	DGD	C6E-C5E	-2.84	1.42	1.51
25	c	522	BCR	C35-C13	-2.84	1.45	1.50
23	b	614	CLA	C3B-C4B	-2.84	1.34	1.42
23	c	514	CLA	C1D-ND	-2.84	1.34	1.37
23	B	615	CLA	C3B-C4B	-2.84	1.34	1.42
23	A	605	CLA	C3B-C4B	-2.84	1.34	1.42
23	C	513	CLA	C3B-C4B	-2.84	1.34	1.42
23	B	608	CLA	O2D-CED	-2.83	1.39	1.45
23	c	507	CLA	C3B-C4B	-2.83	1.34	1.42
23	D	403	CLA	C3B-C4B	-2.83	1.34	1.42
25	A	609	BCR	C1-C6	-2.83	1.50	1.53
23	B	603	CLA	MG-NA	-2.83	1.99	2.06
25	C	521	BCR	C12-C13	2.83	1.52	1.46
23	B	607[A]	CLA	O2D-CGD	2.83	1.40	1.33
24	A	607	PHO	C3D-C4D	2.83	1.45	1.41
23	B	606	CLA	CHB-C4A	-2.83	1.30	1.37
23	c	503	CLA	C3B-C4B	-2.83	1.34	1.42
23	b	611	CLA	C3B-C4B	-2.83	1.34	1.42
23	c	512	CLA	C1D-ND	-2.83	1.34	1.37
23	D	404	CLA	CAA-C2A	-2.83	1.48	1.54
23	c	506	CLA	MG-NA	-2.83	1.99	2.06
23	C	507	CLA	O2D-CGD	2.83	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	O2D-CGD	2.83	1.40	1.33
25	b	620	BCR	C31-C1	-2.83	1.48	1.53
23	D	403	CLA	O2D-CED	-2.83	1.39	1.45
23	C	511	CLA	MG-NA	-2.82	1.99	2.06
23	d	403	CLA	O2D-CGD	2.82	1.40	1.33
23	c	502	CLA	C3B-C4B	-2.82	1.34	1.42
23	c	509	CLA	MG-NA	-2.82	1.99	2.06
23	C	503	CLA	O2D-CED	-2.82	1.39	1.45
23	d	402	CLA	O2D-CED	-2.82	1.39	1.45
23	a	605	CLA	C3B-C4B	-2.82	1.34	1.42
23	C	503	CLA	C3B-C4B	-2.82	1.34	1.42
25	b	622	BCR	C31-C1	-2.82	1.48	1.53
23	c	508	CLA	CHB-C4A	-2.82	1.30	1.37
32	C	518	DGD	C6E-C5E	-2.82	1.42	1.51
23	a	605	CLA	MG-NA	-2.82	1.99	2.06
23	b	616	CLA	O2D-CGD	2.81	1.40	1.33
25	k	101	BCR	C12-C13	2.81	1.52	1.46
23	C	509	CLA	MG-NA	-2.81	1.99	2.06
23	B	605	CLA	MG-NA	-2.81	1.99	2.06
23	C	503	CLA	MG-NA	-2.81	1.99	2.06
25	c	515	BCR	C35-C13	-2.81	1.45	1.50
32	c	518	DGD	O6D-C5D	2.81	1.51	1.44
23	b	610	CLA	O2D-CGD	2.81	1.40	1.33
24	d	401	PHO	C3D-C4D	2.81	1.45	1.41
23	D	404	CLA	C3B-C4B	-2.81	1.34	1.42
23	b	616	CLA	CHB-C4A	-2.81	1.30	1.37
23	b	609[A]	CLA	O2D-CGD	2.81	1.40	1.33
23	b	609[B]	CLA	O2D-CGD	2.81	1.40	1.33
23	C	512	CLA	O2D-CGD	2.81	1.40	1.33
32	c	519	DGD	C6E-C5E	-2.80	1.42	1.51
23	B	607[B]	CLA	C3B-C4B	-2.80	1.34	1.42
23	B	604	CLA	MG-NA	-2.80	1.99	2.06
32	c	517	DGD	C6E-C5E	-2.80	1.42	1.51
32	D	406	DGD	O5D-C1E	2.80	1.44	1.40
32	H	102	DGD	C6E-C5E	-2.80	1.42	1.51
32	c	518	DGD	C6E-C5E	-2.80	1.42	1.51
23	B	609	CLA	C3B-C4B	-2.80	1.34	1.42
23	c	503	CLA	O2D-CGD	2.80	1.40	1.33
23	B	612	CLA	C3B-C4B	-2.80	1.34	1.42
25	b	620	BCR	C35-C13	-2.79	1.45	1.50
23	a	613	CLA	O2D-CED	-2.79	1.39	1.45
25	b	620	BCR	C27-C26	2.79	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	h	102	DGD	C6E-C5E	-2.79	1.42	1.51
23	d	403	CLA	C3B-C4B	-2.78	1.34	1.42
32	C	516	DGD	C6E-C5E	-2.78	1.42	1.51
23	B	617	CLA	CHB-C4A	-2.78	1.30	1.37
23	B	610	CLA	MG-NA	-2.78	1.99	2.06
25	t	101	BCR	C35-C13	-2.78	1.45	1.50
23	B	604	CLA	O2D-CGD	2.78	1.40	1.33
23	C	505	CLA	MG-NA	-2.78	1.99	2.06
23	B	608	CLA	C1D-ND	-2.78	1.34	1.37
23	b	612	CLA	C3B-C4B	-2.77	1.34	1.42
25	H	101	BCR	C12-C13	2.77	1.51	1.46
23	B	611	CLA	O2D-CGD	2.77	1.40	1.33
25	f	101	BCR	C12-C13	2.77	1.51	1.46
23	C	504	CLA	O2D-CED	-2.77	1.39	1.45
25	C	514	BCR	C31-C1	-2.77	1.48	1.53
23	b	618	CLA	C1D-ND	-2.77	1.34	1.37
23	b	618	CLA	O2D-CGD	2.76	1.40	1.33
32	d	405	DGD	C6E-C5E	-2.76	1.42	1.51
23	c	509	CLA	C3B-C4B	-2.76	1.34	1.42
23	c	504	CLA	C3B-C4B	-2.76	1.34	1.42
25	b	622	BCR	C1-C6	-2.76	1.50	1.53
23	B	616	CLA	C3B-C4B	-2.76	1.34	1.42
25	F	101	BCR	C35-C13	-2.76	1.45	1.50
23	B	614	CLA	O2D-CED	-2.76	1.39	1.45
23	b	614	CLA	O2D-CGD	2.75	1.40	1.33
23	D	404	CLA	CHB-C4A	-2.75	1.30	1.37
23	a	607	CLA	CHB-C4A	-2.75	1.30	1.37
23	c	505	CLA	O2D-CGD	2.75	1.40	1.33
23	b	604	CLA	C3B-C4B	-2.75	1.34	1.42
23	B	603	CLA	C3B-C4B	-2.75	1.34	1.42
23	D	402	CLA	C3B-C4B	-2.75	1.34	1.42
23	b	613	CLA	O2D-CGD	2.75	1.40	1.33
23	C	508	CLA	O2D-CGD	2.75	1.40	1.33
23	b	619	CLA	CHB-C4A	-2.74	1.30	1.37
23	B	610	CLA	C3B-C4B	-2.74	1.34	1.42
23	b	618	CLA	C3B-C4B	-2.74	1.34	1.42
23	B	608	CLA	O2D-CGD	2.74	1.40	1.33
23	c	506	CLA	CHB-C4A	-2.74	1.30	1.37
25	C	521	BCR	C31-C1	-2.74	1.48	1.53
23	B	605	CLA	CHB-C4A	-2.74	1.30	1.37
32	H	102	DGD	O6E-C1E	2.73	1.48	1.41
23	C	501	CLA	C3B-C4B	-2.73	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	607	CLA	C3B-C4B	-2.73	1.34	1.42
23	c	505	CLA	O2D-CED	-2.73	1.39	1.45
23	A	608	CLA	MG-NA	-2.73	1.99	2.06
23	B	602	CLA	C1D-ND	-2.73	1.34	1.37
23	C	502	CLA	O2D-CGD	2.73	1.39	1.33
23	b	610	CLA	CHB-C4A	-2.73	1.30	1.37
24	D	401	PHO	C4D-CHA	2.73	1.43	1.39
23	C	506	CLA	MG-NA	-2.72	1.99	2.06
25	b	620	BCR	C17-C18	2.72	1.42	1.35
23	C	510	CLA	O2D-CED	-2.72	1.39	1.45
25	C	521	BCR	C1-C6	-2.72	1.50	1.53
32	D	406	DGD	O6E-C1E	2.72	1.48	1.41
23	A	606	CLA	O2D-CGD	2.72	1.39	1.33
23	D	404	CLA	O2D-CED	-2.72	1.39	1.45
23	B	612	CLA	MG-NA	-2.72	1.99	2.06
23	B	604	CLA	OBD-CAD	-2.72	1.17	1.22
32	D	406	DGD	C6E-C5E	-2.72	1.42	1.51
23	c	510	CLA	CHB-C4A	-2.71	1.30	1.37
23	b	612	CLA	C3D-CAD	2.71	1.54	1.45
23	c	505	CLA	C3B-C4B	-2.71	1.35	1.42
23	B	616	CLA	CHB-C4A	-2.71	1.30	1.37
23	c	512	CLA	O2D-CGD	2.71	1.39	1.33
23	c	502	CLA	MG-NA	-2.71	1.99	2.06
25	a	608	BCR	C17-C18	2.71	1.42	1.35
23	c	513	CLA	O2D-CGD	2.71	1.39	1.33
23	B	616	CLA	O2D-CED	-2.71	1.39	1.45
23	b	608	CLA	MG-NA	-2.70	1.99	2.06
23	A	605	CLA	O2D-CGD	2.70	1.39	1.33
23	C	503	CLA	O2D-CGD	2.70	1.39	1.33
23	D	402	CLA	O2D-CED	-2.70	1.39	1.45
23	B	610	CLA	O2D-CED	-2.70	1.39	1.45
23	B	615	CLA	MG-NA	-2.70	1.99	2.06
23	d	403	CLA	C3D-CAD	2.70	1.54	1.45
24	a	606	PHO	C3D-C4D	2.70	1.44	1.41
23	b	609[B]	CLA	MG-NA	-2.70	1.99	2.06
23	c	512	CLA	CHB-C4A	-2.69	1.31	1.37
23	B	606	CLA	MG-NA	-2.69	1.99	2.06
23	C	508	CLA	MG-NA	-2.69	1.99	2.06
23	b	610	CLA	O2D-CED	-2.69	1.39	1.45
23	b	604	CLA	O2D-CED	-2.69	1.39	1.45
25	H	101	BCR	C17-C18	2.69	1.42	1.35
23	c	503	CLA	MG-NA	-2.68	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	622	BCR	C12-C13	2.68	1.51	1.46
23	C	502	CLA	O2D-CED	-2.68	1.39	1.45
23	C	502	CLA	MG-NA	-2.68	1.99	2.06
23	C	501	CLA	O2D-CGD	2.68	1.39	1.33
23	C	511	CLA	CHB-C4A	-2.68	1.31	1.37
24	D	401	PHO	C4D-ND	-2.68	1.34	1.38
23	A	606	CLA	O2D-CED	-2.68	1.39	1.45
23	b	617	CLA	O2D-CED	-2.68	1.39	1.45
23	b	616	CLA	O2D-CED	-2.67	1.39	1.45
23	b	618	CLA	O2D-CED	-2.67	1.39	1.45
23	d	403	CLA	O2D-CED	-2.67	1.39	1.45
25	K	101	BCR	C12-C13	2.67	1.51	1.46
23	C	504	CLA	O2D-CGD	2.67	1.39	1.33
23	b	615	CLA	O2D-CED	-2.67	1.39	1.45
25	B	618	BCR	C31-C1	-2.67	1.48	1.53
23	c	512	CLA	MG-NA	-2.67	1.99	2.06
25	b	621	BCR	C1-C6	-2.67	1.50	1.53
32	H	102	DGD	O5D-C1E	2.67	1.44	1.40
23	C	501	CLA	O2D-CED	-2.67	1.39	1.45
23	B	606	CLA	O2D-CED	-2.66	1.39	1.45
25	b	621	BCR	C7-C6	2.66	1.54	1.45
25	c	516	BCR	C31-C1	-2.66	1.48	1.53
23	c	513	CLA	O2D-CED	-2.65	1.39	1.45
23	B	616	CLA	O2D-CGD	2.65	1.39	1.33
23	C	510	CLA	MG-NA	-2.65	2.00	2.06
23	C	502	CLA	C3D-CAD	2.65	1.54	1.45
25	H	101	BCR	C35-C13	-2.65	1.45	1.50
23	B	604	CLA	O2D-CED	-2.65	1.39	1.45
23	B	613	CLA	O2D-CED	-2.65	1.39	1.45
23	d	403	CLA	MG-NA	-2.65	2.00	2.06
32	C	517	DGD	O2D-C2D	2.65	1.49	1.43
25	c	522	BCR	C31-C1	-2.65	1.48	1.53
23	C	501	CLA	MG-NA	-2.65	2.00	2.06
23	b	611	CLA	MG-NA	-2.65	2.00	2.06
23	b	610	CLA	MG-NA	-2.65	2.00	2.06
25	C	521	BCR	C35-C13	-2.64	1.45	1.50
23	B	607[A]	CLA	MG-NA	-2.64	2.00	2.06
23	B	607[A]	CLA	O2D-CED	-2.64	1.39	1.45
23	b	605	CLA	C3B-C4B	-2.64	1.35	1.42
23	c	503	CLA	C3D-CAD	2.64	1.54	1.45
23	B	607[B]	CLA	O2D-CED	-2.64	1.39	1.45
23	C	512	CLA	O2D-CED	-2.64	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	O2D-CED	-2.64	1.39	1.45
23	c	509	CLA	C3D-CAD	2.63	1.54	1.45
23	a	604	CLA	C3D-CAD	2.63	1.54	1.45
23	c	503	CLA	O2D-CED	-2.63	1.39	1.45
23	C	512	CLA	MG-NA	-2.63	2.00	2.06
23	b	612	CLA	O2D-CED	-2.63	1.39	1.45
23	b	611	CLA	C3D-CAD	2.63	1.54	1.45
23	B	614	CLA	MG-NA	-2.63	2.00	2.06
23	b	609[B]	CLA	O2D-CED	-2.63	1.39	1.45
23	c	502	CLA	O2D-CED	-2.63	1.39	1.45
25	f	101	BCR	C31-C1	-2.63	1.48	1.53
23	B	615	CLA	O2D-CED	-2.62	1.39	1.45
25	h	101	BCR	C31-C1	-2.62	1.48	1.53
23	b	606	CLA	O2D-CED	-2.62	1.39	1.45
32	d	405	DGD	O5D-C1E	2.62	1.44	1.40
23	C	505	CLA	O2D-CED	-2.62	1.39	1.45
23	B	614	CLA	OBD-CAD	-2.62	1.18	1.22
32	h	102	DGD	O5D-C1E	2.62	1.44	1.40
24	D	401	PHO	C3D-C4D	2.61	1.44	1.41
23	b	604	CLA	MG-NA	-2.61	2.00	2.06
23	B	602	CLA	O2D-CED	-2.61	1.39	1.45
23	a	604	CLA	C2A-C1A	-2.61	1.46	1.52
23	c	504	CLA	MG-NA	-2.61	2.00	2.06
23	C	501	CLA	C3D-CAD	2.61	1.54	1.45
23	B	608	CLA	MG-NA	-2.61	2.00	2.06
23	B	609	CLA	C3D-CAD	2.61	1.54	1.45
23	B	617	CLA	O2D-CED	-2.61	1.39	1.45
23	B	610	CLA	C3D-CAD	2.61	1.54	1.45
23	A	608	CLA	C3D-CAD	2.61	1.54	1.45
23	C	508	CLA	C3D-CAD	2.61	1.54	1.45
23	D	402	CLA	O2D-CGD	2.61	1.39	1.33
33	e	102	HEM	FE-NC	2.61	2.03	1.95
23	b	616	CLA	MG-NA	-2.61	2.00	2.06
23	B	603	CLA	C3D-CAD	2.61	1.54	1.45
23	C	512	CLA	C3D-CAD	2.61	1.54	1.45
32	C	516	DGD	C3E-C2E	-2.60	1.45	1.52
25	A	609	BCR	C31-C1	-2.60	1.48	1.53
23	c	507	CLA	O2D-CED	-2.60	1.39	1.45
23	B	616	CLA	MG-NA	-2.60	2.00	2.06
24	d	401	PHO	CMC-C2C	-2.60	1.46	1.50
23	b	613	CLA	MG-NA	-2.60	2.00	2.06
23	b	609[A]	CLA	O2D-CED	-2.60	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609[A]	CLA	MG-NA	-2.60	2.00	2.06
23	c	511	CLA	MG-NA	-2.60	2.00	2.06
23	B	611	CLA	C3D-CAD	2.60	1.54	1.45
23	c	513	CLA	MG-NA	-2.59	2.00	2.06
23	D	404	CLA	C3D-CAD	2.59	1.54	1.45
23	a	607	CLA	O2D-CED	-2.59	1.39	1.45
23	B	607[B]	CLA	MG-NA	-2.59	2.00	2.06
23	B	611	CLA	MG-NA	-2.59	2.00	2.06
32	c	517	DGD	C3E-C2E	-2.59	1.45	1.52
32	d	405	DGD	O6E-C1E	2.59	1.48	1.41
23	D	403	CLA	O2D-CGD	2.58	1.39	1.33
32	c	518	DGD	O2D-C2D	2.58	1.49	1.43
23	c	507	CLA	MG-NA	-2.58	2.00	2.06
23	B	612	CLA	C3D-CAD	2.58	1.54	1.45
23	c	509	CLA	O2D-CED	-2.58	1.39	1.45
23	b	611	CLA	O2D-CED	-2.58	1.39	1.45
23	b	618	CLA	MG-NA	-2.58	2.00	2.06
23	B	614	CLA	O2D-CGD	2.58	1.39	1.33
25	C	515	BCR	C31-C1	-2.58	1.48	1.53
23	D	403	CLA	OBD-CAD	-2.58	1.18	1.22
23	B	602	CLA	C3B-C4B	-2.58	1.35	1.42
25	H	101	BCR	C1-C6	-2.58	1.50	1.53
23	b	606	CLA	OBD-CAD	-2.57	1.18	1.22
26	d	404	PL9	C41-C39	2.57	1.56	1.51
23	b	607	CLA	MG-NA	-2.57	2.00	2.06
23	b	614	CLA	O2D-CED	-2.57	1.39	1.45
23	B	609	CLA	O2D-CED	-2.57	1.39	1.45
23	B	602	CLA	C3D-CAD	2.57	1.54	1.45
26	D	405	PL9	C41-C39	2.57	1.56	1.51
23	C	506	CLA	C3D-CAD	2.57	1.54	1.45
23	b	604	CLA	C3D-CAD	2.57	1.54	1.45
24	a	606	PHO	CMC-C2C	-2.57	1.46	1.50
32	C	516	DGD	O2D-C2D	2.57	1.49	1.43
23	b	608	CLA	O2D-CED	-2.57	1.39	1.45
23	C	507	CLA	MG-NA	-2.57	2.00	2.06
25	F	101	BCR	C12-C13	2.56	1.51	1.46
23	C	510	CLA	O2D-CGD	2.56	1.39	1.33
23	d	402	CLA	O2D-CGD	2.56	1.39	1.33
32	h	102	DGD	O6E-C1E	2.56	1.48	1.41
23	c	505	CLA	C3D-CAD	2.56	1.53	1.45
23	C	507	CLA	C3D-CAD	2.56	1.53	1.45
23	A	605	CLA	C2A-C1A	-2.56	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	605	CLA	O2D-CED	-2.56	1.39	1.45
23	a	613	CLA	O2D-CGD	2.56	1.39	1.33
23	c	506	CLA	O2D-CED	-2.56	1.39	1.45
25	C	514	BCR	C17-C18	2.55	1.41	1.35
23	C	506	CLA	O2D-CED	-2.55	1.39	1.45
23	B	608	CLA	C2A-C1A	-2.55	1.46	1.52
23	B	613	CLA	C3D-CAD	2.55	1.53	1.45
23	A	608	CLA	O2D-CED	-2.55	1.39	1.45
23	B	611	CLA	C3B-C4B	-2.55	1.35	1.42
25	a	608	BCR	C31-C1	-2.55	1.48	1.53
23	b	613	CLA	C3B-C4B	-2.55	1.35	1.42
25	t	101	BCR	C7-C6	2.55	1.53	1.45
24	a	606	PHO	CAC-C3C	-2.54	1.47	1.51
23	a	604	CLA	O2D-CGD	2.54	1.39	1.33
23	c	511	CLA	O2D-CGD	2.54	1.39	1.33
32	C	518	DGD	O2D-C2D	2.54	1.49	1.43
25	c	516	BCR	C17-C18	2.54	1.41	1.35
23	c	504	CLA	O2D-CGD	2.54	1.39	1.33
23	B	603	CLA	O2D-CED	-2.54	1.39	1.45
23	C	510	CLA	OBD-CAD	-2.54	1.18	1.22
23	B	602	CLA	MG-NA	-2.54	2.00	2.06
25	K	101	BCR	C35-C13	-2.54	1.45	1.50
25	B	619	BCR	C7-C6	2.53	1.53	1.45
23	C	504	CLA	C3D-CAD	2.53	1.53	1.45
23	B	607[B]	CLA	C3D-CAD	2.53	1.53	1.45
25	k	101	BCR	C7-C6	2.53	1.53	1.45
32	c	519	DGD	O2D-C2D	2.53	1.49	1.43
23	C	508	CLA	O2D-CED	-2.53	1.39	1.45
23	B	612	CLA	O2D-CED	-2.53	1.39	1.45
23	A	605	CLA	C3D-CAD	2.53	1.53	1.45
25	c	522	BCR	C17-C18	2.53	1.41	1.35
23	b	619	CLA	O2D-CED	-2.53	1.39	1.45
25	C	514	BCR	C7-C6	2.52	1.53	1.45
23	D	404	CLA	MG-NA	-2.52	2.00	2.06
32	d	405	DGD	O2D-C2D	2.52	1.49	1.43
23	D	402	CLA	C3D-CAD	2.52	1.53	1.45
23	b	613	CLA	C3D-CAD	2.52	1.53	1.45
25	f	101	BCR	C17-C18	2.52	1.41	1.35
32	c	517	DGD	O2D-C2D	2.52	1.49	1.43
25	B	618	BCR	C12-C13	2.52	1.51	1.46
23	B	608	CLA	C3D-CAD	2.52	1.53	1.45
23	c	510	CLA	O2D-CED	-2.52	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	CAB-C3B	2.52	1.54	1.47
23	b	615	CLA	C3D-CAD	2.52	1.53	1.45
23	b	607	CLA	O2D-CED	-2.51	1.39	1.45
23	C	505	CLA	C3D-CAD	2.51	1.53	1.45
25	b	622	BCR	C7-C6	2.51	1.53	1.45
25	c	515	BCR	C12-C13	2.51	1.51	1.46
23	c	502	CLA	C3D-CAD	2.51	1.53	1.45
23	C	513	CLA	C3D-CAD	2.51	1.53	1.45
23	C	509	CLA	C3D-CAD	2.51	1.53	1.45
23	c	514	CLA	C3D-CAD	2.51	1.53	1.45
32	H	102	DGD	O2D-C2D	2.51	1.49	1.43
23	c	507	CLA	C3D-CAD	2.51	1.53	1.45
24	A	607	PHO	CMC-C2C	-2.50	1.46	1.50
23	b	619	CLA	OBD-CAD	-2.50	1.18	1.22
23	c	506	CLA	C3D-CAD	2.50	1.53	1.45
25	A	609	BCR	C7-C6	2.50	1.53	1.45
23	B	607[A]	CLA	C3D-CAD	2.50	1.53	1.45
25	a	608	BCR	C1-C6	-2.50	1.50	1.53
23	B	605	CLA	O2D-CED	-2.50	1.39	1.45
32	h	102	DGD	O2D-C2D	2.50	1.49	1.43
23	a	605	CLA	C3D-CAD	2.50	1.53	1.45
23	c	514	CLA	O2D-CED	-2.50	1.39	1.45
25	H	101	BCR	C31-C1	-2.49	1.49	1.53
23	C	513	CLA	O2D-CED	-2.49	1.39	1.45
25	B	620	BCR	C12-C13	2.49	1.51	1.46
23	b	609[A]	CLA	C3D-CAD	2.49	1.53	1.45
23	c	511	CLA	C3D-CAD	2.49	1.53	1.45
23	C	507	CLA	O2D-CED	-2.48	1.39	1.45
23	a	607	CLA	C3D-CAD	2.48	1.53	1.45
23	b	609[B]	CLA	C3D-CAD	2.48	1.53	1.45
23	c	508	CLA	O2D-CED	-2.48	1.39	1.45
23	b	608	CLA	C2A-C1A	-2.48	1.46	1.52
23	c	508	CLA	C3D-CAD	2.48	1.53	1.45
24	D	401	PHO	CMC-C2C	-2.48	1.46	1.50
23	B	615	CLA	C3D-CAD	2.47	1.53	1.45
23	b	617	CLA	C2A-C1A	-2.47	1.46	1.52
23	C	505	CLA	C2A-C1A	-2.47	1.46	1.52
23	d	402	CLA	OBD-CAD	-2.47	1.18	1.22
23	C	511	CLA	C3D-CAD	2.47	1.53	1.45
23	b	619	CLA	C3D-CAD	2.47	1.53	1.45
23	b	613	CLA	OBD-CAD	-2.47	1.18	1.22
23	C	509	CLA	O2D-CED	-2.47	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	406	DGD	O2D-C2D	2.47	1.49	1.43
23	b	605	CLA	C3D-CAD	2.47	1.53	1.45
23	d	402	CLA	C3D-CAD	2.47	1.53	1.45
23	B	617	CLA	C3D-CAD	2.47	1.53	1.45
23	D	403	CLA	C2A-C1A	-2.46	1.46	1.52
23	b	606	CLA	CAB-C3B	2.46	1.53	1.47
32	C	516	DGD	O6E-C1E	2.46	1.48	1.41
23	c	507	CLA	OBD-CAD	-2.46	1.18	1.22
23	B	609	CLA	MG-NA	-2.45	2.00	2.06
23	c	506	CLA	C2A-C1A	-2.45	1.46	1.52
25	F	101	BCR	C31-C1	-2.45	1.49	1.53
23	b	614	CLA	C3D-CAD	2.45	1.53	1.45
23	D	403	CLA	C3D-CAD	2.45	1.53	1.45
23	C	510	CLA	CAB-C3B	2.45	1.53	1.47
23	c	513	CLA	C3D-CAD	2.45	1.53	1.45
23	c	504	CLA	C3D-CAD	2.45	1.53	1.45
25	c	516	BCR	C7-C6	2.45	1.53	1.45
32	d	405	DGD	O3G-C1D	2.44	1.44	1.40
32	d	405	DGD	O6D-C1D	2.44	1.48	1.41
23	A	606	CLA	CAB-C3B	2.44	1.53	1.47
23	c	508	CLA	MG-NA	-2.44	2.00	2.06
23	b	607	CLA	C3D-CAD	2.44	1.53	1.45
32	h	102	DGD	C3E-C2E	-2.44	1.46	1.52
32	C	518	DGD	C3E-C2E	-2.44	1.46	1.52
25	B	620	BCR	C7-C6	2.43	1.53	1.45
23	B	617	CLA	OBD-CAD	-2.43	1.18	1.22
25	c	515	BCR	C17-C18	2.43	1.41	1.35
23	b	605	CLA	C2A-C1A	-2.43	1.46	1.52
25	a	608	BCR	C7-C6	2.43	1.53	1.45
23	A	606	CLA	C3D-CAD	2.43	1.53	1.45
23	b	605	CLA	O2D-CED	-2.43	1.39	1.45
32	D	406	DGD	O3G-C1D	2.43	1.44	1.40
23	B	606	CLA	OBD-CAD	-2.43	1.18	1.22
23	B	604	CLA	CAB-C3B	2.43	1.53	1.47
23	C	508	CLA	C2A-C1A	-2.43	1.46	1.52
23	b	617	CLA	C3D-CAD	2.42	1.53	1.45
24	A	607	PHO	CMD-C2D	-2.42	1.46	1.51
23	b	616	CLA	C3D-CAD	2.42	1.53	1.45
23	a	613	CLA	OBD-CAD	-2.42	1.18	1.22
26	D	405	PL9	C7-C3	2.42	1.54	1.51
23	a	613	CLA	C3D-CAD	2.42	1.53	1.45
23	A	605	CLA	OBD-CAD	-2.42	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C3D-CAD	2.41	1.53	1.45
23	C	510	CLA	C3D-CAD	2.41	1.53	1.45
32	c	517	DGD	O6D-C1D	2.41	1.48	1.41
32	C	518	DGD	O6E-C1E	2.41	1.48	1.41
23	B	606	CLA	C2A-C1A	-2.41	1.46	1.52
23	d	402	CLA	C2A-C1A	-2.41	1.46	1.52
32	D	406	DGD	O6D-C1D	2.41	1.48	1.41
23	b	611	CLA	CAB-C3B	2.40	1.53	1.47
23	c	512	CLA	C3D-CAD	2.40	1.53	1.45
23	B	609	CLA	C2A-C1A	-2.40	1.46	1.52
23	B	616	CLA	C3D-CAD	2.40	1.53	1.45
24	a	606	PHO	CMD-C2D	-2.40	1.46	1.51
23	C	504	CLA	C2A-C1A	-2.40	1.46	1.52
24	a	606	PHO	CMB-C2B	-2.39	1.46	1.51
23	b	611	CLA	C2A-C1A	-2.39	1.46	1.52
23	b	618	CLA	C3D-CAD	2.39	1.53	1.45
23	B	611	CLA	OBD-CAD	-2.39	1.18	1.22
23	D	402	CLA	CAB-C3B	2.39	1.53	1.47
23	B	605	CLA	C3D-CAD	2.39	1.53	1.45
23	D	402	CLA	OBD-CAD	-2.39	1.18	1.22
32	C	516	DGD	O6D-C1D	2.38	1.48	1.41
23	C	504	CLA	OBD-CAD	-2.38	1.18	1.22
23	b	616	CLA	OBD-CAD	-2.38	1.18	1.22
32	H	102	DGD	C3E-C2E	-2.38	1.46	1.52
23	a	605	CLA	OBD-CAD	-2.38	1.18	1.22
23	b	610	CLA	OBD-CAD	-2.38	1.18	1.22
25	b	622	BCR	C17-C18	2.38	1.41	1.35
23	c	514	CLA	C2A-C1A	-2.37	1.46	1.52
23	b	614	CLA	OBD-CAD	-2.37	1.18	1.22
23	a	605	CLA	CAB-C3B	2.37	1.53	1.47
23	d	403	CLA	MG-NC	-2.37	2.00	2.06
32	c	517	DGD	C6D-C5D	-2.37	1.44	1.51
25	f	101	BCR	C7-C6	2.37	1.53	1.45
23	c	505	CLA	MG-NC	-2.36	2.00	2.06
23	B	612	CLA	CAB-C3B	2.36	1.53	1.47
26	d	404	PL9	C7-C3	2.36	1.54	1.51
32	c	519	DGD	C6D-C5D	-2.36	1.44	1.51
23	a	607	CLA	CAB-C3B	2.36	1.53	1.47
23	b	608	CLA	C3D-CAD	2.36	1.53	1.45
23	C	510	CLA	C2A-C1A	-2.36	1.46	1.52
23	B	604	CLA	C3D-CAD	2.36	1.53	1.45
23	B	615	CLA	C2A-C1A	-2.36	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	h	102	DGD	O6D-C1D	2.36	1.47	1.41
25	T	101	BCR	C31-C1	-2.36	1.49	1.53
25	A	609	BCR	C17-C18	2.35	1.41	1.35
33	v	201	HEM	FE-NA	2.35	2.02	1.95
23	c	504	CLA	OBD-CAD	-2.35	1.18	1.22
32	c	517	DGD	O6E-C1E	2.35	1.47	1.41
23	b	618	CLA	OBD-CAD	-2.35	1.18	1.22
32	C	517	DGD	O3D-C3D	2.35	1.48	1.43
23	c	511	CLA	OBD-CAD	-2.35	1.18	1.22
23	C	503	CLA	CAB-C3B	2.34	1.53	1.47
23	B	614	CLA	C3D-CAD	2.34	1.53	1.45
23	c	508	CLA	OBD-CAD	-2.34	1.18	1.22
32	C	518	DGD	C6D-C5D	-2.34	1.44	1.51
23	C	505	CLA	CAB-C3B	2.34	1.53	1.47
32	c	518	DGD	C6D-C5D	-2.34	1.44	1.51
23	C	513	CLA	C2A-C1A	-2.34	1.47	1.52
24	D	401	PHO	CMD-C2D	-2.34	1.46	1.51
32	c	519	DGD	C3E-C2E	-2.34	1.46	1.52
32	c	518	DGD	C3E-C2E	-2.34	1.46	1.52
23	C	501	CLA	OBD-CAD	-2.33	1.18	1.22
23	A	605	CLA	CAB-C3B	2.33	1.53	1.47
23	A	606	CLA	OBD-CAD	-2.33	1.18	1.22
23	B	617	CLA	C2A-C1A	-2.33	1.47	1.52
23	B	604	CLA	C2A-C1A	-2.33	1.47	1.52
23	B	610	CLA	C2A-C1A	-2.33	1.47	1.52
32	D	406	DGD	O3D-C3D	2.33	1.48	1.43
23	C	509	CLA	CAB-C3B	2.33	1.53	1.47
23	B	603	CLA	C2A-C1A	-2.33	1.47	1.52
28	z	101	LMG	O8-C28	2.33	1.44	1.33
24	d	401	PHO	CMD-C2D	-2.33	1.47	1.51
23	B	613	CLA	C2A-C1A	-2.33	1.47	1.52
32	C	516	DGD	O3D-C3D	2.32	1.48	1.43
23	b	605	CLA	OBD-CAD	-2.32	1.18	1.22
23	B	615	CLA	OBD-CAD	-2.32	1.18	1.22
23	D	402	CLA	MG-NC	-2.32	2.00	2.06
25	c	515	BCR	C7-C6	2.32	1.53	1.45
28	Z	101	LMG	O8-C28	2.32	1.44	1.33
23	C	504	CLA	MG-NC	-2.32	2.00	2.06
32	c	519	DGD	O5D-C1E	2.32	1.44	1.40
25	b	620	BCR	C12-C13	2.32	1.50	1.46
23	b	615	CLA	C2A-C1A	-2.32	1.47	1.52
23	b	612	CLA	C2A-C1A	-2.32	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	h	101	BCR	C17-C18	2.32	1.41	1.35
23	C	503	CLA	C3D-CAD	2.32	1.53	1.45
23	c	504	CLA	CAB-C3B	2.31	1.53	1.47
23	B	602	CLA	CAB-C3B	2.31	1.53	1.47
32	c	519	DGD	O6E-C1E	2.31	1.47	1.41
25	h	101	BCR	C7-C6	2.31	1.53	1.45
23	c	513	CLA	CAB-C3B	2.31	1.53	1.47
23	C	503	CLA	OBD-CAD	-2.31	1.18	1.22
23	b	610	CLA	C2A-C1A	-2.31	1.47	1.52
25	B	620	BCR	C17-C18	2.31	1.41	1.35
23	C	501	CLA	MG-NC	-2.31	2.00	2.06
23	B	606	CLA	C3D-CAD	2.31	1.53	1.45
23	a	613	CLA	MG-NC	-2.31	2.00	2.06
23	c	509	CLA	CAB-C3B	2.31	1.53	1.47
24	A	607	PHO	CMB-C2B	-2.31	1.47	1.51
23	C	512	CLA	CAB-C3B	2.31	1.53	1.47
32	C	516	DGD	O5D-C1E	2.31	1.44	1.40
23	c	511	CLA	C2A-C1A	-2.31	1.47	1.52
23	b	607	CLA	OBD-CAD	-2.31	1.18	1.22
23	b	607	CLA	CAB-C3B	2.31	1.53	1.47
32	d	405	DGD	O3D-C3D	2.30	1.48	1.43
23	b	617	CLA	OBD-CAD	-2.30	1.18	1.22
32	C	517	DGD	C3E-C2E	-2.30	1.46	1.52
23	C	505	CLA	OBD-CAD	-2.30	1.18	1.22
24	d	401	PHO	C4D-ND	-2.30	1.35	1.38
23	B	609	CLA	CAB-C3B	2.30	1.53	1.47
23	C	501	CLA	CAB-C3B	2.30	1.53	1.47
25	F	101	BCR	C7-C6	2.30	1.52	1.45
25	K	101	BCR	C7-C6	2.30	1.52	1.45
24	d	401	PHO	CAC-C3C	-2.30	1.47	1.51
23	C	508	CLA	OBD-CAD	-2.30	1.18	1.22
23	c	505	CLA	C2A-C1A	-2.30	1.47	1.52
32	c	518	DGD	O3D-C3D	2.30	1.48	1.43
23	c	507	CLA	C2A-C1A	-2.30	1.47	1.52
23	D	403	CLA	CAB-C3B	2.29	1.53	1.47
32	C	516	DGD	C6D-C5D	-2.29	1.44	1.51
32	C	518	DGD	C1D-C2D	-2.29	1.45	1.52
32	H	102	DGD	O3D-C3D	2.29	1.48	1.43
23	c	502	CLA	OBD-CAD	-2.29	1.18	1.22
23	D	402	CLA	C2A-C1A	-2.29	1.47	1.52
23	d	403	CLA	C4D-CHA	2.29	1.46	1.38
23	c	512	CLA	OBD-CAD	-2.29	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	C3D-CAD	2.29	1.53	1.45
25	T	101	BCR	C17-C18	2.28	1.41	1.35
32	H	102	DGD	O6D-C1D	2.28	1.47	1.41
25	c	522	BCR	C7-C6	2.28	1.52	1.45
23	C	508	CLA	CAB-C3B	2.28	1.53	1.47
23	a	605	CLA	MG-NC	-2.28	2.00	2.06
23	A	606	CLA	MG-NC	-2.28	2.00	2.06
23	C	506	CLA	MG-NC	-2.28	2.00	2.06
32	c	517	DGD	O3D-C3D	2.28	1.48	1.43
23	c	512	CLA	CAB-C3B	2.28	1.53	1.47
23	c	514	CLA	OBD-CAD	-2.28	1.18	1.22
23	C	511	CLA	OBD-CAD	-2.28	1.18	1.22
24	D	401	PHO	CMB-C2B	-2.28	1.47	1.51
24	A	607	PHO	CAC-C3C	-2.28	1.47	1.51
26	A	610	PL9	C37-C38	2.28	1.57	1.50
25	k	101	BCR	C17-C18	2.27	1.41	1.35
23	B	603	CLA	OBD-CAD	-2.27	1.18	1.22
23	d	402	CLA	CAB-C3B	2.27	1.53	1.47
32	H	102	DGD	C6D-C5D	-2.27	1.44	1.51
23	c	506	CLA	OBD-CAD	-2.27	1.18	1.22
23	c	502	CLA	MG-NC	-2.27	2.00	2.06
23	b	611	CLA	OBD-CAD	-2.27	1.18	1.22
25	c	522	BCR	C1-C6	-2.27	1.50	1.53
25	T	101	BCR	C7-C6	2.27	1.52	1.45
23	B	613	CLA	CAB-C3B	2.27	1.53	1.47
23	b	617	CLA	MG-NC	-2.27	2.00	2.06
23	B	616	CLA	OBD-CAD	-2.26	1.18	1.22
32	C	517	DGD	O5D-C1E	2.26	1.44	1.40
23	B	614	CLA	C2A-C1A	-2.26	1.47	1.52
23	b	606	CLA	C3D-CAD	2.26	1.52	1.45
32	C	517	DGD	O6E-C1E	2.26	1.47	1.41
23	C	513	CLA	OBD-CAD	-2.26	1.18	1.22
23	c	503	CLA	MG-NC	-2.26	2.00	2.06
26	d	404	PL9	C22-C23	2.26	1.57	1.50
32	c	519	DGD	C1D-C2D	-2.26	1.45	1.52
23	c	513	CLA	OBD-CAD	-2.26	1.18	1.22
23	C	502	CLA	MG-NC	-2.26	2.00	2.06
23	c	502	CLA	CAB-C3B	2.26	1.53	1.47
23	c	512	CLA	MG-NC	-2.26	2.00	2.06
23	B	610	CLA	CAB-C3B	2.26	1.53	1.47
32	d	405	DGD	C6D-C5D	-2.26	1.44	1.51
26	d	404	PL9	C37-C38	2.26	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	516	DGD	C1D-C2D	-2.26	1.45	1.52
23	b	609[B]	CLA	C2A-C1A	-2.25	1.47	1.52
32	C	518	DGD	O3D-C3D	2.25	1.48	1.43
23	C	513	CLA	MG-NC	-2.25	2.00	2.06
23	d	403	CLA	CAB-C3B	2.25	1.53	1.47
23	c	509	CLA	C2A-C1A	-2.25	1.47	1.52
23	B	608	CLA	MG-NC	-2.25	2.00	2.06
23	c	506	CLA	CAB-C3B	2.25	1.53	1.47
23	c	509	CLA	OBD-CAD	-2.25	1.18	1.22
23	B	614	CLA	CAB-C3B	2.25	1.53	1.47
23	b	616	CLA	CAB-C3B	2.24	1.53	1.47
25	b	620	BCR	C7-C6	2.24	1.52	1.45
23	C	509	CLA	MG-NC	-2.24	2.00	2.06
23	B	612	CLA	OBD-CAD	-2.24	1.18	1.22
23	c	505	CLA	OBD-CAD	-2.24	1.18	1.22
23	C	511	CLA	C2A-C1A	-2.24	1.47	1.52
23	a	613	CLA	CAB-C3B	2.24	1.53	1.47
32	c	519	DGD	O3D-C3D	2.24	1.48	1.43
23	a	604	CLA	MG-NC	-2.24	2.00	2.06
23	a	604	CLA	CAB-C3B	2.24	1.53	1.47
26	D	405	PL9	C37-C38	2.24	1.57	1.50
25	H	101	BCR	C7-C6	2.24	1.52	1.45
32	c	517	DGD	O5D-C1E	2.24	1.43	1.40
23	B	610	CLA	OBD-CAD	-2.23	1.18	1.22
23	A	608	CLA	C2A-C1A	-2.23	1.47	1.52
23	C	510	CLA	MG-NC	-2.23	2.01	2.06
23	B	605	CLA	OBD-CAD	-2.23	1.18	1.22
23	A	608	CLA	OBD-CAD	-2.23	1.18	1.22
23	B	602	CLA	C2A-C1A	-2.23	1.47	1.52
23	b	619	CLA	C2A-C1A	-2.23	1.47	1.52
23	A	606	CLA	C2A-C1A	-2.23	1.47	1.52
23	c	514	CLA	CAB-C3B	2.23	1.53	1.47
24	d	401	PHO	CMB-C2B	-2.23	1.47	1.51
23	D	404	CLA	CAB-C3B	2.22	1.53	1.47
25	C	514	BCR	C1-C6	-2.22	1.50	1.53
23	b	604	CLA	CAB-C3B	2.22	1.53	1.47
23	A	605	CLA	MG-NC	-2.22	2.01	2.06
23	b	608	CLA	OBD-CAD	-2.22	1.18	1.22
33	E	102	HEM	FE-NB	2.22	2.01	1.94
23	B	613	CLA	OBD-CAD	-2.22	1.18	1.22
23	C	507	CLA	C4D-CHA	2.22	1.46	1.38
26	A	610	PL9	C22-C23	2.22	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C4D-CHA	2.21	1.46	1.38
23	b	615	CLA	OBD-CAD	-2.21	1.18	1.22
26	a	609	PL9	C17-C18	2.21	1.57	1.50
23	a	607	CLA	MG-NC	-2.21	2.01	2.06
23	a	607	CLA	OBD-CAD	-2.21	1.18	1.22
26	A	610	PL9	C5-C4	-2.21	1.39	1.47
32	D	406	DGD	C6D-C5D	-2.21	1.44	1.51
23	c	502	CLA	C2A-C1A	-2.21	1.47	1.52
23	C	502	CLA	C2A-C1A	-2.21	1.47	1.52
32	c	518	DGD	O5D-C1E	2.21	1.43	1.40
23	a	613	CLA	C2A-C1A	-2.21	1.47	1.52
26	A	610	PL9	C41-C39	2.20	1.55	1.51
23	C	502	CLA	OBD-CAD	-2.20	1.18	1.22
23	B	610	CLA	MG-NC	-2.20	2.01	2.06
23	b	609[A]	CLA	OBD-CAD	-2.20	1.18	1.22
23	C	504	CLA	CAB-C3B	2.20	1.53	1.47
33	V	202	HEM	CMC-C2C	2.20	1.55	1.50
23	B	603	CLA	MG-NC	-2.20	2.01	2.06
25	C	515	BCR	C7-C6	2.20	1.52	1.45
23	c	503	CLA	OBD-CAD	-2.20	1.18	1.22
23	C	512	CLA	MG-NC	-2.20	2.01	2.06
23	b	605	CLA	MG-NC	-2.20	2.01	2.06
32	c	518	DGD	C1E-C2E	-2.20	1.46	1.52
23	b	618	CLA	C2A-C1A	-2.20	1.47	1.52
23	C	511	CLA	CAB-C3B	2.20	1.53	1.47
23	c	514	CLA	MG-NC	-2.20	2.01	2.06
23	c	510	CLA	C4D-CHA	2.20	1.45	1.38
23	c	509	CLA	MG-NC	-2.20	2.01	2.06
23	c	511	CLA	CAB-C3B	2.19	1.53	1.47
23	b	613	CLA	C2A-C1A	-2.19	1.47	1.52
23	b	606	CLA	MG-NC	-2.19	2.01	2.06
32	c	518	DGD	O6E-C1E	2.19	1.47	1.41
23	b	615	CLA	CAB-C3B	2.19	1.53	1.47
26	D	405	PL9	C22-C23	2.19	1.57	1.50
23	C	506	CLA	OBD-CAD	-2.19	1.18	1.22
23	B	608	CLA	CAB-C3B	2.19	1.53	1.47
23	b	606	CLA	C2A-C1A	-2.19	1.47	1.52
23	C	512	CLA	OBD-CAD	-2.19	1.18	1.22
23	a	605	CLA	C2A-C1A	-2.19	1.47	1.52
23	C	508	CLA	MG-NC	-2.19	2.01	2.06
23	C	507	CLA	MG-NC	-2.19	2.01	2.06
24	a	606	PHO	C4D-ND	-2.19	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	MG-NC	-2.19	2.01	2.06
23	B	612	CLA	C2A-C1A	-2.19	1.47	1.52
23	c	503	CLA	C2A-C1A	-2.19	1.47	1.52
23	C	511	CLA	MG-NC	-2.19	2.01	2.06
23	b	613	CLA	CAB-C3B	2.19	1.53	1.47
23	c	504	CLA	C2A-C1A	-2.18	1.47	1.52
23	B	607[A]	CLA	OBD-CAD	-2.18	1.18	1.22
23	C	513	CLA	CAB-C3B	2.18	1.53	1.47
23	b	608	CLA	MG-NC	-2.18	2.01	2.06
23	B	605	CLA	CAB-C3B	2.18	1.53	1.47
31	e	101	LHG	C8-C7	2.18	1.57	1.50
23	d	402	CLA	MG-NC	-2.18	2.01	2.06
23	b	612	CLA	OBD-CAD	-2.18	1.18	1.22
24	D	401	PHO	CAC-C3C	-2.18	1.47	1.51
32	C	517	DGD	C6D-C5D	-2.18	1.45	1.51
32	c	519	DGD	O6D-C1D	2.18	1.47	1.41
25	C	521	BCR	C7-C6	2.18	1.52	1.45
27	b	602	SQD	O6-C1	2.18	1.43	1.40
23	B	615	CLA	CAB-C3B	2.17	1.53	1.47
23	b	610	CLA	CAB-C3B	2.17	1.53	1.47
23	B	612	CLA	MG-NC	-2.17	2.01	2.06
32	C	517	DGD	O6D-C1D	2.17	1.47	1.41
31	D	408	LHG	C8-C7	2.17	1.57	1.50
24	A	607	PHO	C4D-ND	-2.17	1.35	1.38
32	h	102	DGD	C1D-C2D	-2.17	1.46	1.52
23	B	609	CLA	OBD-CAD	-2.17	1.18	1.22
32	h	102	DGD	C6D-C5D	-2.17	1.45	1.51
23	B	608	CLA	OBD-CAD	-2.16	1.18	1.22
23	D	403	CLA	MG-NC	-2.16	2.01	2.06
23	b	609[A]	CLA	C2A-C1A	-2.16	1.47	1.52
25	C	514	BCR	C33-C5	2.16	1.54	1.50
23	c	508	CLA	C4D-CHA	2.16	1.45	1.38
32	C	518	DGD	O6D-C1D	2.16	1.47	1.41
23	C	507	CLA	OBD-CAD	-2.16	1.18	1.22
32	C	516	DGD	C1E-C2E	-2.16	1.46	1.52
31	E	101	LHG	C8-C7	2.16	1.57	1.50
23	a	604	CLA	OBD-CAD	-2.16	1.18	1.22
23	B	607[B]	CLA	C2A-C1A	-2.16	1.47	1.52
26	a	609	PL9	C41-C39	2.16	1.55	1.51
23	C	509	CLA	OBD-CAD	-2.16	1.18	1.22
26	a	609	PL9	C5-C4	-2.16	1.39	1.47
23	c	510	CLA	CAB-C3B	2.16	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	518	DGD	O6D-C1D	2.16	1.47	1.41
26	a	609	PL9	C2-C3	2.16	1.40	1.34
26	A	610	PL9	C17-C18	2.15	1.57	1.50
23	D	404	CLA	MG-NC	-2.15	2.01	2.06
23	b	617	CLA	CAB-C3B	2.15	1.53	1.47
23	B	603	CLA	C4D-CHA	2.15	1.45	1.38
33	E	102	HEM	CMB-C2B	2.15	1.55	1.50
23	C	507	CLA	CMC-C2C	2.15	1.55	1.50
26	a	609	PL9	C22-C23	2.15	1.57	1.50
23	C	503	CLA	C4D-CHA	2.15	1.45	1.38
23	B	607[A]	CLA	MG-NC	-2.15	2.01	2.06
32	h	102	DGD	O3D-C3D	2.14	1.48	1.43
23	b	604	CLA	OBD-CAD	-2.14	1.18	1.22
32	c	517	DGD	C1E-C2E	-2.14	1.46	1.52
25	B	619	BCR	C12-C13	2.14	1.50	1.46
32	C	517	DGD	O3G-C1D	2.14	1.43	1.40
27	B	623	SQD	O6-C1	2.14	1.43	1.40
23	c	512	CLA	C4D-CHA	2.14	1.45	1.38
31	B	622	LHG	C8-C7	2.14	1.56	1.50
25	C	514	BCR	C12-C13	2.14	1.50	1.46
23	B	611	CLA	CAB-C3B	2.14	1.53	1.47
23	C	512	CLA	C2A-C1A	-2.13	1.47	1.52
25	t	101	BCR	C17-C18	2.13	1.40	1.35
23	c	505	CLA	CAB-C3B	2.13	1.53	1.47
23	B	605	CLA	C4D-CHA	2.13	1.45	1.38
23	c	512	CLA	C2A-C1A	-2.13	1.47	1.52
23	c	514	CLA	C4D-CHA	2.13	1.45	1.38
23	b	614	CLA	C2A-C1A	-2.13	1.47	1.52
32	H	102	DGD	C1D-C2D	-2.13	1.46	1.52
25	c	515	BCR	C1-C6	-2.13	1.51	1.53
23	B	602	CLA	OBD-CAD	-2.13	1.18	1.22
32	C	518	DGD	C1E-C2E	-2.13	1.46	1.52
23	c	504	CLA	MG-NC	-2.13	2.01	2.06
23	B	616	CLA	C2A-C1A	-2.12	1.47	1.52
25	B	618	BCR	C7-C6	2.12	1.52	1.45
23	b	607	CLA	C4D-CHA	2.12	1.45	1.38
26	a	609	PL9	C37-C38	2.12	1.56	1.50
23	A	608	CLA	CAB-C3B	2.12	1.53	1.47
23	D	404	CLA	C4D-CHA	2.12	1.45	1.38
23	c	510	CLA	C2A-C1A	-2.12	1.47	1.52
26	A	610	PL9	C2-C3	2.12	1.40	1.34
33	V	202	HEM	C2A-C3A	-2.12	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	OBD-CAD	-2.12	1.18	1.22
23	b	615	CLA	MG-NC	-2.11	2.01	2.06
23	C	501	CLA	C2A-C1A	-2.11	1.47	1.52
23	b	616	CLA	MG-NC	-2.11	2.01	2.06
32	d	405	DGD	C3E-C2E	-2.11	1.46	1.52
23	B	607[A]	CLA	C2A-C1A	-2.11	1.47	1.52
23	B	611	CLA	C4D-CHA	2.11	1.45	1.38
23	C	502	CLA	C4D-CHA	2.11	1.45	1.38
32	C	517	DGD	C1E-C2E	-2.11	1.46	1.52
32	c	518	DGD	O3G-C1D	2.11	1.43	1.40
23	c	508	CLA	MG-NC	-2.10	2.01	2.06
25	b	622	BCR	C33-C5	2.10	1.54	1.50
23	b	609[A]	CLA	MG-NC	-2.10	2.01	2.06
23	b	610	CLA	MG-NC	-2.10	2.01	2.06
33	e	102	HEM	CMB-C2B	2.10	1.55	1.50
23	b	612	CLA	MG-NC	-2.10	2.01	2.06
23	B	617	CLA	C4D-CHA	2.10	1.45	1.38
23	B	607[B]	CLA	MG-NC	-2.10	2.01	2.06
32	c	517	DGD	C1D-C2D	-2.10	1.46	1.52
33	E	102	HEM	CMC-C2C	2.10	1.55	1.50
23	b	609[B]	CLA	OBD-CAD	-2.10	1.18	1.22
25	c	515	BCR	C33-C5	2.09	1.54	1.50
33	E	102	HEM	CMA-C3A	2.09	1.55	1.50
26	D	405	PL9	C5-C4	-2.09	1.40	1.47
23	B	606	CLA	MG-NC	-2.09	2.01	2.06
23	c	507	CLA	CAB-C3B	2.09	1.53	1.47
23	b	604	CLA	CMC-C2C	2.09	1.55	1.50
26	d	404	PL9	C17-C18	2.09	1.56	1.50
23	A	608	CLA	MG-NC	-2.09	2.01	2.06
23	a	607	CLA	C4D-CHA	2.09	1.45	1.38
23	b	618	CLA	CAB-C3B	2.09	1.53	1.47
23	C	506	CLA	CAB-C3B	2.09	1.53	1.47
23	C	506	CLA	C2A-C1A	-2.09	1.47	1.52
23	B	611	CLA	MG-NC	-2.09	2.01	2.06
32	c	519	DGD	C1E-C2E	-2.09	1.46	1.52
23	b	613	CLA	MG-NC	-2.08	2.01	2.06
26	d	404	PL9	C5-C4	-2.08	1.40	1.47
23	b	604	CLA	C4D-CHA	2.08	1.45	1.38
23	C	502	CLA	CAB-C3B	2.08	1.52	1.47
23	C	512	CLA	C4D-CHA	2.08	1.45	1.38
23	c	511	CLA	MG-NC	-2.08	2.01	2.06
23	B	616	CLA	MG-NC	-2.08	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	MG-NC	-2.08	2.01	2.06
33	v	201	HEM	CMC-C2C	2.08	1.55	1.50
23	b	604	CLA	C2A-C1A	-2.08	1.47	1.52
32	C	518	DGD	O5D-C1E	2.08	1.43	1.40
23	a	607	CLA	C2A-C1A	-2.08	1.47	1.52
23	B	616	CLA	C4D-CHA	2.07	1.45	1.38
23	b	605	CLA	CAB-C3B	2.07	1.52	1.47
23	b	607	CLA	C2A-C1A	-2.07	1.47	1.52
23	b	609[A]	CLA	C4D-CHA	2.07	1.45	1.38
23	c	503	CLA	CAB-C3B	2.07	1.52	1.47
23	b	612	CLA	CAB-C3B	2.07	1.52	1.47
23	b	609[B]	CLA	MG-NC	-2.07	2.01	2.06
26	D	405	PL9	C17-C18	2.06	1.56	1.50
23	b	604	CLA	MG-NC	-2.06	2.01	2.06
23	B	607[B]	CLA	C4D-CHA	2.06	1.45	1.38
23	B	607[A]	CLA	C4D-CHA	2.06	1.45	1.38
23	b	616	CLA	C2A-C1A	-2.06	1.47	1.52
33	v	201	HEM	CMD-C2D	2.06	1.55	1.50
23	B	606	CLA	CAB-C3B	2.06	1.52	1.47
23	B	614	CLA	MG-NC	-2.06	2.01	2.06
23	b	618	CLA	MG-NC	-2.06	2.01	2.06
23	B	607[B]	CLA	OBD-CAD	-2.06	1.18	1.22
23	b	618	CLA	C4D-CHA	2.06	1.45	1.38
23	B	617	CLA	MG-NC	-2.06	2.01	2.06
23	B	605	CLA	C2A-C1A	-2.06	1.47	1.52
23	B	612	CLA	C4D-CHA	2.06	1.45	1.38
23	D	404	CLA	CBA-CGA	2.06	1.56	1.50
23	B	603	CLA	CAB-C3B	2.06	1.52	1.47
23	C	503	CLA	MG-NC	-2.05	2.01	2.06
23	c	513	CLA	C2A-C1A	-2.05	1.47	1.52
23	c	507	CLA	MG-NC	-2.05	2.01	2.06
23	b	608	CLA	CAB-C3B	2.05	1.52	1.47
25	B	620	BCR	C33-C5	2.05	1.54	1.50
23	B	616	CLA	CAB-C3B	2.05	1.52	1.47
23	B	617	CLA	CAB-C3B	2.05	1.52	1.47
23	c	504	CLA	C4D-CHA	2.05	1.45	1.38
23	C	503	CLA	C2A-C1A	-2.05	1.47	1.52
23	b	614	CLA	MG-NC	-2.05	2.01	2.06
31	D	407	LHG	C8-C7	2.05	1.56	1.50
23	b	613	CLA	C4D-CHA	2.05	1.45	1.38
23	C	508	CLA	C4D-CHA	2.05	1.45	1.38
23	d	403	CLA	C2A-C1A	-2.05	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	406	LHG	C8-C7	2.04	1.56	1.50
31	b	624	LHG	C8-C7	2.04	1.56	1.50
23	b	614	CLA	C4D-CHA	2.04	1.45	1.38
23	b	619	CLA	C4D-CHA	2.04	1.45	1.38
23	c	511	CLA	CMC-C2C	2.04	1.55	1.50
32	C	517	DGD	C1D-C2D	-2.04	1.46	1.52
33	e	102	HEM	CMA-C3A	2.04	1.54	1.50
27	x	101	SQD	O6-C1	2.04	1.43	1.40
23	B	611	CLA	C2A-C1A	-2.04	1.47	1.52
23	B	615	CLA	MG-NC	-2.04	2.01	2.06
23	b	607	CLA	MG-NC	-2.03	2.01	2.06
23	c	513	CLA	C4D-CHA	2.03	1.45	1.38
25	T	101	BCR	C1-C6	-2.03	1.51	1.53
23	b	606	CLA	C4D-CHA	2.03	1.45	1.38
27	X	101	SQD	O6-C1	2.03	1.43	1.40
23	B	602	CLA	MG-NC	-2.03	2.01	2.06
23	c	509	CLA	C4D-CHA	2.03	1.45	1.38
23	C	512	CLA	CMC-C2C	2.03	1.54	1.50
23	B	605	CLA	MG-NC	-2.03	2.01	2.06
23	B	611	CLA	CMC-C2C	2.03	1.54	1.50
23	c	513	CLA	MG-NC	-2.03	2.01	2.06
23	c	507	CLA	C4D-CHA	2.03	1.45	1.38
23	a	604	CLA	CMC-C2C	2.02	1.54	1.50
23	a	605	CLA	C4D-CHA	2.02	1.45	1.38
23	C	509	CLA	CMC-C2C	2.02	1.54	1.50
23	B	608	CLA	C4D-CHA	2.02	1.45	1.38
23	a	613	CLA	C4D-CHA	2.02	1.45	1.38
23	C	511	CLA	C4D-CHA	2.02	1.45	1.38
31	L	101	LHG	C8-C7	2.02	1.56	1.50
23	b	609[B]	CLA	C4D-CHA	2.02	1.45	1.38
23	c	511	CLA	C4D-CHA	2.02	1.45	1.38
23	C	506	CLA	C4D-CHA	2.02	1.45	1.38
23	b	616	CLA	C4D-CHA	2.01	1.45	1.38
23	d	403	CLA	CMC-C2C	2.01	1.54	1.50
23	c	505	CLA	CMC-C2C	2.01	1.54	1.50
23	a	613	CLA	CMC-C2C	2.01	1.54	1.50
23	c	505	CLA	C4D-CHA	2.01	1.45	1.38
23	C	504	CLA	C4D-CHA	2.01	1.45	1.38
25	b	621	BCR	C12-C13	2.01	1.50	1.46
23	c	510	CLA	MG-NC	-2.00	2.01	2.06
23	B	602	CLA	CMC-C2C	2.00	1.54	1.50
23	b	615	CLA	C4D-CHA	2.00	1.45	1.38

All (2223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	621	BCR	C15-C16-C17	26.28	177.29	123.52
25	c	515	BCR	C15-C16-C17	25.42	175.54	123.52
25	T	101	BCR	C15-C16-C17	25.33	175.34	123.52
25	A	609	BCR	C15-C16-C17	25.25	175.18	123.52
25	a	608	BCR	C15-C16-C17	25.24	175.17	123.52
25	C	515	BCR	C15-C16-C17	25.13	174.94	123.52
25	F	101	BCR	C15-C16-C17	24.94	174.55	123.52
25	K	101	BCR	C15-C16-C17	24.93	174.52	123.52
25	t	101	BCR	C15-C16-C17	24.93	174.52	123.52
25	c	516	BCR	C15-C16-C17	24.66	173.98	123.52
25	B	619	BCR	C15-C16-C17	24.60	173.84	123.52
25	c	522	BCR	C15-C16-C17	24.55	173.74	123.52
25	b	622	BCR	C15-C16-C17	24.52	173.69	123.52
25	C	514	BCR	C15-C16-C17	24.48	173.62	123.52
25	B	620	BCR	C15-C16-C17	24.48	173.61	123.52
25	f	101	BCR	C15-C16-C17	24.48	173.60	123.52
25	k	101	BCR	C15-C16-C17	24.30	173.24	123.52
25	B	618	BCR	C15-C16-C17	23.96	172.54	123.52
25	C	521	BCR	C15-C16-C17	23.95	172.53	123.52
25	h	101	BCR	C15-C16-C17	23.60	171.81	123.52
25	H	101	BCR	C15-C16-C17	23.39	171.38	123.52
25	b	620	BCR	C15-C16-C17	22.01	168.55	123.52
25	c	516	BCR	C21-C20-C19	19.47	179.63	123.20
25	c	515	BCR	C21-C20-C19	19.20	178.82	123.20
25	C	514	BCR	C21-C20-C19	19.17	178.74	123.20
25	B	620	BCR	C21-C20-C19	19.13	178.62	123.20
25	b	620	BCR	C21-C20-C19	19.05	178.41	123.20
25	C	521	BCR	C21-C20-C19	19.00	178.26	123.20
25	h	101	BCR	C21-C20-C19	18.93	178.05	123.20
25	C	515	BCR	C21-C20-C19	18.88	177.89	123.20
25	b	621	BCR	C21-C20-C19	18.84	177.78	123.20
25	a	608	BCR	C21-C20-C19	18.68	177.34	123.20
25	t	101	BCR	C21-C20-C19	18.67	177.28	123.20
25	A	609	BCR	C21-C20-C19	18.49	176.77	123.20
25	H	101	BCR	C21-C20-C19	18.37	176.44	123.20
25	c	522	BCR	C21-C20-C19	18.37	176.43	123.20
25	f	101	BCR	C21-C20-C19	18.26	176.11	123.20
25	b	622	BCR	C21-C20-C19	18.20	175.94	123.20
25	K	101	BCR	C21-C20-C19	17.93	175.16	123.20
25	F	101	BCR	C21-C20-C19	17.68	174.43	123.20
25	B	618	BCR	C21-C20-C19	17.44	173.72	123.20
25	T	101	BCR	C21-C20-C19	17.26	173.22	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	101	BCR	C21-C20-C19	17.23	173.12	123.20
25	b	622	BCR	C38-C26-C25	-15.14	107.96	124.48
25	T	101	BCR	C33-C5-C6	-15.03	108.08	124.48
25	B	620	BCR	C38-C26-C25	-14.86	108.27	124.48
25	B	619	BCR	C21-C20-C19	14.52	165.28	123.20
25	c	515	BCR	C38-C26-C25	-14.50	108.66	124.48
25	C	514	BCR	C38-C26-C25	-14.11	109.09	124.48
25	F	101	BCR	C33-C5-C6	-14.04	109.17	124.48
25	T	101	BCR	C38-C26-C25	-13.96	109.26	124.48
25	t	101	BCR	C38-C26-C25	-13.94	109.27	124.48
25	b	620	BCR	C33-C5-C6	-13.86	109.36	124.48
25	B	618	BCR	C38-C26-C25	-13.75	109.48	124.48
25	K	101	BCR	C38-C26-C25	-13.69	109.55	124.48
25	B	618	BCR	C33-C5-C6	-13.68	109.56	124.48
25	C	521	BCR	C33-C5-C6	-13.66	109.58	124.48
25	k	101	BCR	C38-C26-C25	-13.63	109.62	124.48
25	f	101	BCR	C33-C5-C6	-13.47	109.79	124.48
25	h	101	BCR	C33-C5-C6	-13.47	109.79	124.48
25	b	620	BCR	C15-C14-C13	-13.42	108.45	127.28
25	A	609	BCR	C33-C5-C6	-13.40	109.86	124.48
25	c	522	BCR	C33-C5-C6	-13.26	110.02	124.48
25	k	101	BCR	C33-C5-C6	-13.21	110.07	124.48
25	a	608	BCR	C33-C5-C6	-13.09	110.21	124.48
25	C	521	BCR	C38-C26-C25	-13.07	110.22	124.48
25	C	514	BCR	C16-C17-C18	-12.99	109.06	127.28
25	K	101	BCR	C33-C5-C6	-12.99	110.31	124.48
25	H	101	BCR	C33-C5-C6	-12.68	110.64	124.48
25	c	516	BCR	C33-C5-C6	-12.64	110.69	124.48
25	c	515	BCR	C16-C17-C18	-12.53	109.71	127.28
25	T	101	BCR	C24-C23-C22	-12.51	107.72	126.23
25	F	101	BCR	C16-C17-C18	-12.48	109.77	127.28
25	c	522	BCR	C38-C26-C25	-12.47	110.87	124.48
25	H	101	BCR	C16-C17-C18	-12.36	109.95	127.28
25	c	516	BCR	C38-C26-C25	-12.27	111.09	124.48
25	C	515	BCR	C38-C26-C25	-12.11	111.27	124.48
25	C	514	BCR	C24-C23-C22	-11.86	108.68	126.23
25	B	618	BCR	C11-C10-C9	-11.65	110.94	127.28
25	b	620	BCR	C11-C10-C9	-11.58	111.03	127.28
25	B	620	BCR	C16-C17-C18	-11.48	111.18	127.28
25	h	101	BCR	C38-C26-C25	-11.20	112.26	124.48
25	h	101	BCR	C16-C17-C18	-11.12	111.69	127.28
25	B	619	BCR	C16-C17-C18	-11.08	111.74	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	620	BCR	C33-C5-C6	-11.01	112.47	124.48
25	c	515	BCR	C33-C5-C6	-10.98	112.50	124.48
25	t	101	BCR	C33-C5-C6	-10.98	112.50	124.48
25	c	515	BCR	C24-C23-C22	-10.95	110.03	126.23
25	C	515	BCR	C33-C5-C6	-10.93	112.56	124.48
25	B	618	BCR	C15-C14-C13	-10.87	112.04	127.28
25	b	620	BCR	C38-C26-C25	-10.81	112.69	124.48
25	H	101	BCR	C38-C26-C25	-10.79	112.72	124.48
25	C	515	BCR	C24-C23-C22	-10.75	110.33	126.23
25	b	622	BCR	C33-C5-C6	-10.74	112.77	124.48
25	C	514	BCR	C33-C5-C6	-10.69	112.82	124.48
25	F	101	BCR	C24-C23-C22	-10.66	110.46	126.23
25	b	621	BCR	C33-C5-C6	-10.65	112.86	124.48
25	A	609	BCR	C38-C26-C25	-10.61	112.90	124.48
25	a	608	BCR	C38-C26-C25	-10.47	113.06	124.48
25	B	619	BCR	C11-C10-C9	-10.46	112.61	127.28
25	k	101	BCR	C16-C17-C18	-10.28	112.86	127.28
25	t	101	BCR	C24-C23-C22	-10.17	111.18	126.23
25	B	620	BCR	C15-C14-C13	-10.14	113.06	127.28
25	C	521	BCR	C16-C17-C18	-10.08	113.14	127.28
25	c	516	BCR	C24-C23-C22	-9.94	111.53	126.23
25	f	101	BCR	C30-C25-C26	-9.89	109.12	122.64
25	A	609	BCR	C16-C17-C18	-9.79	113.55	127.28
25	b	622	BCR	C24-C23-C22	-9.77	111.78	126.23
25	B	619	BCR	C33-C5-C6	-9.75	113.85	124.48
25	C	515	BCR	C4-C5-C6	-9.71	109.58	122.70
25	b	622	BCR	C15-C14-C13	-9.67	113.72	127.28
26	d	404	PL9	C7-C8-C9	-9.54	110.39	126.83
25	B	620	BCR	C8-C7-C6	-9.53	101.53	127.00
25	b	621	BCR	C24-C23-C22	-9.50	112.19	126.23
25	B	619	BCR	C24-C23-C22	-9.46	112.24	126.23
26	D	405	PL9	C7-C8-C9	-9.43	110.59	126.83
25	C	515	BCR	C7-C8-C9	-9.43	112.29	126.23
25	f	101	BCR	C11-C10-C9	-9.34	114.18	127.28
25	F	101	BCR	C30-C25-C26	-9.30	109.92	122.64
25	b	621	BCR	C16-C17-C18	-9.28	114.26	127.28
25	c	522	BCR	C24-C23-C22	-9.28	112.51	126.23
25	F	101	BCR	C7-C8-C9	-9.26	112.54	126.23
25	K	101	BCR	C11-C10-C9	-9.21	114.36	127.28
25	c	522	BCR	C16-C17-C18	-9.17	114.42	127.28
25	H	101	BCR	C15-C14-C13	-9.13	114.48	127.28
25	K	101	BCR	C16-C17-C18	-9.03	114.62	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	521	BCR	C24-C23-C22	-9.02	112.89	126.23
25	C	515	BCR	C11-C10-C9	-8.98	114.69	127.28
25	C	514	BCR	C8-C7-C6	-8.96	103.07	127.00
25	b	621	BCR	C15-C14-C13	-8.88	114.83	127.28
25	c	516	BCR	C16-C17-C18	-8.87	114.84	127.28
25	C	515	BCR	C27-C26-C25	-8.86	110.73	122.70
25	h	101	BCR	C24-C23-C22	-8.69	113.37	126.23
25	b	621	BCR	C11-C10-C9	-8.66	115.13	127.28
25	c	522	BCR	C20-C21-C22	-8.63	115.18	127.28
25	a	608	BCR	C16-C17-C18	-8.61	115.21	127.28
25	c	516	BCR	C4-C5-C6	-8.57	111.12	122.70
25	b	621	BCR	C38-C26-C25	-8.57	115.14	124.48
25	c	516	BCR	C27-C26-C25	-8.56	111.14	122.70
25	f	101	BCR	C16-C17-C18	-8.55	115.28	127.28
25	b	620	BCR	C4-C5-C6	-8.54	111.17	122.70
25	K	101	BCR	C30-C25-C26	-8.46	111.07	122.64
25	f	101	BCR	C24-C23-C22	-8.46	113.72	126.23
25	f	101	BCR	C7-C8-C9	-8.43	113.76	126.23
25	b	622	BCR	C8-C7-C6	-8.40	104.55	127.00
25	B	618	BCR	C7-C8-C9	-8.39	113.82	126.23
25	K	101	BCR	C27-C26-C25	-8.34	111.43	122.70
25	F	101	BCR	C38-C26-C25	-8.34	115.39	124.48
25	c	515	BCR	C15-C14-C13	-8.34	115.58	127.28
25	t	101	BCR	C30-C25-C26	-8.33	111.25	122.64
25	T	101	BCR	C27-C26-C25	-8.30	111.49	122.70
25	T	101	BCR	C7-C6-C5	-8.30	102.44	121.56
25	b	620	BCR	C7-C8-C9	-8.27	114.00	126.23
25	a	608	BCR	C4-C5-C6	-8.24	111.58	122.70
25	B	618	BCR	C4-C5-C6	-8.21	111.61	122.70
25	B	620	BCR	C24-C23-C22	-8.21	114.09	126.23
25	B	618	BCR	C20-C21-C22	-8.21	115.77	127.28
25	C	514	BCR	C15-C14-C13	-8.20	115.78	127.28
25	T	101	BCR	C30-C25-C26	-8.06	111.63	122.64
25	h	101	BCR	C15-C14-C13	-8.05	115.99	127.28
25	h	101	BCR	C4-C5-C6	-8.05	111.83	122.70
25	a	608	BCR	C11-C10-C9	-8.03	116.01	127.28
25	F	101	BCR	C11-C10-C9	-8.03	116.01	127.28
26	A	610	PL9	C37-C38-C39	-7.95	109.42	127.62
25	B	619	BCR	C15-C14-C13	-7.91	116.18	127.28
25	a	608	BCR	C1-C6-C5	-7.91	111.83	122.64
25	a	608	BCR	C24-C23-C22	-7.90	114.54	126.23
25	H	101	BCR	C4-C5-C6	-7.89	112.04	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	f	101	BCR	C15-C14-C13	-7.88	116.23	127.28
25	B	619	BCR	C7-C8-C9	-7.87	114.59	126.23
25	k	101	BCR	C30-C25-C26	-7.85	111.92	122.64
25	t	101	BCR	C11-C10-C9	-7.84	116.28	127.28
25	t	101	BCR	C27-C26-C25	-7.81	112.15	122.70
25	f	101	BCR	C38-C26-C25	-7.81	115.96	124.48
25	B	620	BCR	C8-C9-C10	-7.77	106.79	119.01
25	A	609	BCR	C4-C5-C6	-7.77	112.21	122.70
26	a	609	PL9	C37-C38-C39	-7.74	109.91	127.62
25	b	620	BCR	C1-C6-C5	-7.72	112.09	122.64
25	C	515	BCR	C1-C6-C5	-7.67	112.16	122.64
25	F	101	BCR	C20-C21-C22	-7.65	116.55	127.28
25	c	515	BCR	C30-C25-C26	-7.61	112.23	122.64
25	f	101	BCR	C27-C26-C25	-7.56	112.49	122.70
25	B	620	BCR	C30-C25-C26	-7.52	112.36	122.64
25	c	515	BCR	C11-C10-C9	-7.50	116.76	127.28
26	d	404	PL9	C32-C33-C34	-7.45	110.58	127.62
25	A	609	BCR	C1-C6-C5	-7.41	112.51	122.64
25	c	515	BCR	C27-C26-C25	-7.41	112.69	122.70
25	k	101	BCR	C27-C26-C25	-7.38	112.72	122.70
25	c	516	BCR	C1-C6-C5	-7.35	112.59	122.64
26	d	404	PL9	C12-C13-C14	-7.33	110.84	127.62
25	B	618	BCR	C1-C6-C5	-7.32	112.64	122.64
26	A	610	PL9	C27-C28-C29	-7.28	110.95	127.62
25	F	101	BCR	C4-C5-C6	-7.28	112.87	122.70
25	C	515	BCR	C16-C17-C18	-7.26	117.10	127.28
25	A	609	BCR	C24-C23-C22	-7.25	115.51	126.23
26	d	404	PL9	C27-C28-C29	-7.21	111.11	127.62
25	A	609	BCR	C11-C10-C9	-7.21	117.17	127.28
25	c	522	BCR	C30-C25-C26	-7.20	112.80	122.64
25	H	101	BCR	C24-C23-C22	-7.19	115.60	126.23
25	C	521	BCR	C30-C25-C26	-7.18	112.83	122.64
26	D	405	PL9	C27-C28-C29	-7.13	111.30	127.62
25	f	101	BCR	C4-C5-C6	-7.09	113.13	122.70
25	K	101	BCR	C15-C14-C13	-7.08	117.34	127.28
26	a	609	PL9	C7-C8-C9	-7.08	114.63	126.83
26	A	610	PL9	C42-C43-C44	-7.06	111.46	127.62
26	a	609	PL9	C27-C28-C29	-7.05	111.49	127.62
26	a	609	PL9	C42-C43-C44	-7.04	111.51	127.62
25	c	515	BCR	C8-C7-C6	-7.04	108.20	127.00
25	f	101	BCR	C1-C6-C5	-7.01	113.05	122.64
25	B	620	BCR	C4-C5-C6	-6.93	113.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	522	BCR	C27-C26-C25	-6.93	113.34	122.70
25	t	101	BCR	C15-C14-C13	-6.92	117.58	127.28
26	a	609	PL9	C22-C23-C24	-6.92	111.79	127.62
25	A	609	BCR	C15-C14-C13	-6.90	117.60	127.28
25	C	521	BCR	C20-C21-C22	-6.88	117.63	127.28
26	D	405	PL9	C32-C33-C34	-6.88	111.88	127.62
25	F	101	BCR	C27-C26-C25	-6.87	113.42	122.70
26	A	610	PL9	C17-C18-C19	-6.85	111.93	127.62
26	a	609	PL9	C17-C18-C19	-6.84	111.98	127.62
26	D	405	PL9	C12-C13-C14	-6.83	111.99	127.62
25	C	514	BCR	C30-C25-C26	-6.81	113.33	122.64
25	F	101	BCR	C1-C6-C5	-6.80	113.34	122.64
23	A	605	CLA	C4A-NA-C1A	-6.79	103.58	106.68
25	k	101	BCR	C15-C14-C13	-6.78	117.77	127.28
25	C	514	BCR	C8-C9-C10	-6.76	108.38	119.01
25	c	515	BCR	C7-C8-C9	-6.76	116.24	126.23
25	B	618	BCR	C30-C25-C26	-6.74	113.43	122.64
26	A	610	PL9	C22-C23-C24	-6.73	112.22	127.62
25	C	521	BCR	C4-C5-C6	-6.71	113.63	122.70
25	c	522	BCR	C4-C5-C6	-6.68	113.68	122.70
25	b	620	BCR	C23-C24-C25	-6.66	109.22	127.00
26	A	610	PL9	C7-C8-C9	-6.65	115.37	126.83
25	C	521	BCR	C27-C26-C25	-6.65	113.72	122.70
25	b	622	BCR	C30-C25-C26	-6.63	113.58	122.64
25	B	618	BCR	C27-C26-C25	-6.62	113.76	122.70
25	C	521	BCR	C8-C7-C6	-6.61	109.34	127.00
23	a	604	CLA	C4A-NA-C1A	-6.60	103.67	106.68
25	C	521	BCR	C15-C14-C13	-6.58	118.04	127.28
25	C	514	BCR	C27-C26-C25	-6.58	113.81	122.70
23	C	505	CLA	C3A-C2A-C1A	6.58	111.19	101.34
25	H	101	BCR	C1-C6-C5	-6.56	113.67	122.64
26	d	404	PL9	C17-C18-C19	-6.49	112.78	127.62
25	C	521	BCR	C11-C10-C9	-6.48	118.18	127.28
25	B	620	BCR	C27-C26-C25	-6.48	113.95	122.70
25	c	516	BCR	C11-C10-C9	-6.46	118.21	127.28
25	K	101	BCR	C24-C23-C22	-6.46	116.67	126.23
25	T	101	BCR	C11-C10-C9	-6.45	118.23	127.28
25	c	516	BCR	C30-C25-C26	-6.44	113.84	122.64
26	D	405	PL9	C17-C18-C19	-6.41	112.95	127.62
25	a	608	BCR	C20-C21-C22	-6.41	118.29	127.28
25	h	101	BCR	C1-C6-C5	-6.39	113.90	122.64
25	C	515	BCR	C30-C25-C26	-6.38	113.92	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	522	BCR	C8-C7-C6	-6.37	109.98	127.00
23	c	508	CLA	O2D-CGD-CBD	6.37	122.37	111.23
23	c	506	CLA	C3A-C2A-C1A	6.37	110.88	101.34
26	d	404	PL9	C22-C23-C24	-6.33	113.14	127.62
25	b	622	BCR	C16-C17-C18	-6.32	118.42	127.28
25	c	516	BCR	C7-C8-C9	-6.31	116.89	126.23
26	a	609	PL9	C12-C13-C14	-6.31	113.18	127.62
25	b	622	BCR	C4-C5-C6	-6.31	114.18	122.70
25	b	622	BCR	C8-C9-C10	-6.29	109.11	119.01
25	k	101	BCR	C1-C6-C5	-6.27	114.06	122.64
26	D	405	PL9	C22-C23-C24	-6.27	113.28	127.62
25	B	618	BCR	C24-C23-C22	-6.25	116.99	126.23
23	C	507	CLA	O2D-CGD-CBD	6.23	122.12	111.23
25	H	101	BCR	C7-C8-C9	-6.22	117.04	126.23
26	a	609	PL9	C32-C33-C34	-6.19	113.46	127.62
26	D	405	PL9	C37-C38-C39	-6.18	113.48	127.62
25	K	101	BCR	C8-C7-C6	-6.17	110.53	127.00
25	k	101	BCR	C8-C7-C6	-6.16	110.53	127.00
25	t	101	BCR	C8-C7-C6	-6.16	110.54	127.00
25	t	101	BCR	C16-C17-C18	-6.14	118.66	127.28
26	d	404	PL9	C42-C43-C44	-6.11	113.64	127.62
25	T	101	BCR	C20-C21-C22	-6.11	118.72	127.28
25	c	515	BCR	C20-C21-C22	-6.10	118.72	127.28
25	c	522	BCR	C11-C10-C9	-6.10	118.73	127.28
25	F	101	BCR	C36-C18-C17	-6.09	112.95	122.82
26	A	610	PL9	C16-C14-C13	-6.08	107.51	121.17
26	d	404	PL9	C37-C38-C39	-6.06	113.75	127.62
25	c	515	BCR	C4-C5-C6	-6.06	114.52	122.70
26	a	609	PL9	C45-C44-C43	-6.04	108.10	123.63
26	a	609	PL9	C16-C14-C13	-6.04	107.60	121.17
26	A	610	PL9	C12-C13-C14	-6.03	113.82	127.62
26	A	610	PL9	C45-C44-C43	-6.02	108.17	123.63
25	c	522	BCR	C7-C6-C5	-6.02	107.70	121.56
23	b	612	CLA	C3A-C2A-C1A	6.01	110.34	101.34
23	c	512	CLA	C3A-C2A-C1A	6.01	110.34	101.34
25	T	101	BCR	C7-C8-C9	-6.01	117.35	126.23
23	C	511	CLA	C3A-C2A-C1A	6.00	110.33	101.34
25	b	620	BCR	C27-C26-C25	-6.00	114.60	122.70
25	C	521	BCR	C7-C6-C5	-5.96	107.82	121.56
25	b	622	BCR	C27-C26-C25	-5.95	114.66	122.70
25	H	101	BCR	C27-C26-C25	-5.94	114.68	122.70
25	B	619	BCR	C38-C26-C25	-5.94	118.01	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	522	BCR	C1-C6-C5	-5.93	114.53	122.64
26	D	405	PL9	C16-C14-C13	-5.93	107.86	121.17
25	C	514	BCR	C16-C15-C14	-5.92	111.40	123.52
23	c	504	CLA	C3A-C2A-C1A	5.92	110.21	101.34
25	k	101	BCR	C11-C10-C9	-5.92	118.97	127.28
23	c	502	CLA	C3A-C2A-C1A	5.89	110.17	101.34
26	a	609	PL9	C40-C39-C38	-5.88	108.52	123.63
23	B	605	CLA	C3A-C2A-C1A	5.88	110.14	101.34
25	c	515	BCR	C24-C25-C26	-5.86	108.05	121.56
25	k	101	BCR	C24-C23-C22	-5.86	117.57	126.23
26	D	405	PL9	C42-C43-C44	-5.86	114.22	127.62
25	A	609	BCR	C30-C25-C26	-5.85	114.65	122.64
23	B	607[B]	CLA	C3A-C2A-C1A	5.85	110.09	101.34
25	T	101	BCR	C4-C5-C6	-5.82	114.84	122.70
23	B	614	CLA	C3A-C2A-C1A	5.81	110.05	101.34
26	A	610	PL9	C10-C9-C8	-5.81	108.71	123.63
26	D	405	PL9	C30-C29-C28	-5.79	108.75	123.63
23	C	512	CLA	C3A-C2A-C1A	5.78	110.00	101.34
25	H	101	BCR	C11-C10-C9	-5.78	119.17	127.28
23	B	610	CLA	C3A-C2A-C1A	5.78	110.00	101.34
25	c	515	BCR	C7-C6-C5	-5.75	108.31	121.56
23	c	509	CLA	C3A-C2A-C1A	5.75	109.94	101.34
23	C	503	CLA	C3A-C2A-C1A	5.74	109.94	101.34
23	b	616	CLA	C3A-C2A-C1A	5.74	109.93	101.34
23	C	506	CLA	C3A-C2A-C1A	5.73	109.92	101.34
23	c	507	CLA	C3A-C2A-C1A	5.71	109.90	101.34
26	d	404	PL9	C16-C14-C13	-5.71	108.34	121.17
25	h	101	BCR	C8-C7-C6	-5.70	111.76	127.00
23	B	607[A]	CLA	C3A-C2A-C1A	5.70	109.87	101.34
25	a	608	BCR	C30-C25-C26	-5.69	114.86	122.64
25	h	101	BCR	C27-C26-C25	-5.69	115.02	122.70
23	b	605	CLA	O2D-CGD-CBD	5.69	121.17	111.23
25	H	101	BCR	C7-C6-C5	-5.69	108.46	121.56
26	a	609	PL9	C25-C24-C23	-5.68	109.04	123.63
23	B	608	CLA	C2A-C3A-C4A	5.68	111.04	101.87
23	b	614	CLA	C3A-C2A-C1A	5.67	109.83	101.34
23	C	501	CLA	C3A-C2A-C1A	5.67	109.83	101.34
23	B	616	CLA	C2A-C3A-C4A	5.66	111.02	101.87
25	h	101	BCR	C23-C24-C25	-5.66	111.87	127.00
23	b	618	CLA	C2A-C3A-C4A	5.65	111.00	101.87
23	C	507	CLA	C2A-C3A-C4A	5.65	110.99	101.87
25	b	622	BCR	C20-C21-C22	-5.63	119.38	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	101	BCR	C4-C5-C6	-5.63	115.09	122.70
23	B	602	CLA	C3A-C2A-C1A	5.63	109.77	101.34
23	C	505	CLA	O2D-CGD-CBD	5.63	121.06	111.23
25	K	101	BCR	C7-C8-C9	-5.63	117.91	126.23
23	b	609[B]	CLA	C3A-C2A-C1A	5.62	109.76	101.34
26	a	609	PL9	C10-C9-C8	-5.62	109.18	123.63
25	H	101	BCR	C29-C30-C25	5.61	118.58	110.44
25	C	521	BCR	C1-C6-C5	-5.60	114.98	122.64
23	B	615	CLA	C3A-C2A-C1A	5.59	109.72	101.34
24	a	606	PHO	C4D-CHA-CBD	-5.59	105.77	108.45
23	B	606	CLA	C2A-C3A-C4A	5.59	110.89	101.87
23	C	508	CLA	C3A-C2A-C1A	5.58	109.70	101.34
23	C	513	CLA	C3A-C2A-C1A	5.58	109.70	101.34
23	b	608	CLA	C2A-C3A-C4A	5.58	110.88	101.87
25	F	101	BCR	C15-C14-C13	-5.58	119.45	127.28
23	b	609[A]	CLA	C3A-C2A-C1A	5.58	109.69	101.34
25	C	514	BCR	C11-C10-C9	-5.58	119.46	127.28
26	A	610	PL9	C40-C39-C38	-5.57	109.32	123.63
23	b	617	CLA	C3A-C2A-C1A	5.56	109.67	101.34
23	B	603	CLA	O2D-CGD-CBD	5.56	120.95	111.23
23	C	502	CLA	C3A-C2A-C1A	5.56	109.67	101.34
23	b	619	CLA	C3A-C2A-C1A	5.56	109.67	101.34
25	b	620	BCR	C38-C26-C27	-5.55	101.75	113.60
25	t	101	BCR	C7-C6-C5	-5.55	108.78	121.56
23	c	511	CLA	C3A-C2A-C1A	5.55	109.65	101.34
26	a	609	PL9	C15-C14-C13	-5.55	109.38	123.63
23	b	615	CLA	O2D-CGD-CBD	5.54	120.92	111.23
25	H	101	BCR	C23-C24-C25	-5.54	112.20	127.00
23	b	611	CLA	C3A-C2A-C1A	5.54	109.64	101.34
23	c	508	CLA	C2A-C3A-C4A	5.54	110.82	101.87
26	d	404	PL9	C10-C9-C8	-5.54	109.41	123.63
25	C	515	BCR	C20-C21-C22	-5.53	119.52	127.28
26	d	404	PL9	C30-C29-C28	-5.53	109.42	123.63
23	b	618	CLA	C3A-C2A-C1A	5.53	109.62	101.34
23	c	513	CLA	C3A-C2A-C1A	5.53	109.62	101.34
23	B	617	CLA	C3A-C2A-C1A	5.52	109.61	101.34
24	A	607	PHO	C4D-CHA-CBD	-5.51	105.81	108.45
23	b	610	CLA	C2A-C3A-C4A	5.51	110.77	101.87
23	c	507	CLA	C2A-C3A-C4A	5.50	110.76	101.87
25	c	522	BCR	C15-C14-C13	-5.50	119.56	127.28
23	b	609[B]	CLA	C2A-C3A-C4A	5.50	110.76	101.87
26	a	609	PL9	C11-C9-C8	-5.49	108.83	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C3A-C2A-C1A	5.49	109.56	101.34
23	c	506	CLA	O2D-CGD-CBD	5.49	120.82	111.23
23	c	514	CLA	C3A-C2A-C1A	5.48	109.54	101.34
26	D	405	PL9	C11-C9-C8	-5.47	108.89	121.17
23	b	604	CLA	C3A-C2A-C1A	5.47	109.53	101.34
25	C	521	BCR	C7-C8-C9	-5.46	118.16	126.23
23	b	606	CLA	C3A-C2A-C1A	5.46	109.51	101.34
23	b	615	CLA	C3A-C2A-C1A	5.45	109.51	101.34
23	c	510	CLA	C3A-C2A-C1A	5.45	109.50	101.34
25	K	101	BCR	C34-C9-C10	-5.45	113.99	122.82
25	C	514	BCR	C24-C25-C26	-5.44	109.01	121.56
23	B	606	CLA	C3A-C2A-C1A	5.44	109.48	101.34
23	b	613	CLA	C3A-C2A-C1A	5.44	109.48	101.34
23	b	618	CLA	O2D-CGD-CBD	5.43	120.73	111.23
25	c	516	BCR	C15-C14-C13	-5.43	119.66	127.28
25	k	101	BCR	C34-C9-C10	-5.43	114.02	122.82
23	a	607	CLA	C3A-C2A-C1A	5.42	109.46	101.34
23	B	612	CLA	C3A-C2A-C1A	5.41	109.45	101.34
23	C	504	CLA	C2A-C3A-C4A	5.39	110.58	101.87
26	A	610	PL9	C11-C9-C8	-5.39	109.06	121.17
26	d	404	PL9	C15-C14-C13	-5.39	109.78	123.63
23	A	608	CLA	C3A-C2A-C1A	5.39	109.41	101.34
25	K	101	BCR	C1-C6-C5	-5.38	115.28	122.64
25	T	101	BCR	C15-C14-C13	-5.38	119.73	127.28
25	a	608	BCR	C15-C14-C13	-5.38	119.73	127.28
23	c	503	CLA	C3A-C2A-C1A	5.38	109.39	101.34
25	b	621	BCR	C12-C13-C14	-5.38	110.55	119.01
25	b	621	BCR	C1-C6-C5	-5.37	115.30	122.64
25	B	619	BCR	C38-C26-C27	-5.37	102.15	113.60
23	b	610	CLA	C3A-C2A-C1A	5.37	109.38	101.34
25	K	101	BCR	C4-C5-C6	-5.36	115.46	122.70
23	B	609	CLA	C3A-C2A-C1A	5.36	109.36	101.34
23	b	608	CLA	C3A-C2A-C1A	5.35	109.35	101.34
25	T	101	BCR	C23-C24-C25	-5.35	112.71	127.00
25	b	620	BCR	C11-C12-C13	-5.34	111.71	126.36
25	B	619	BCR	C1-C6-C5	-5.34	115.34	122.64
23	a	613	CLA	C3A-C2A-C1A	5.34	109.34	101.34
25	C	514	BCR	C20-C21-C22	-5.34	119.79	127.28
25	h	101	BCR	C7-C6-C5	-5.33	109.27	121.56
23	b	607	CLA	C3A-C2A-C1A	5.33	109.33	101.34
26	D	405	PL9	C45-C44-C43	-5.33	109.93	123.63
23	B	607[B]	CLA	C2A-C3A-C4A	5.33	110.47	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	C3A-C2A-C1A	5.33	109.32	101.34
23	C	508	CLA	C2A-C3A-C4A	5.33	110.47	101.87
23	B	610	CLA	C2A-C3A-C4A	5.32	110.47	101.87
23	B	616	CLA	O2D-CGD-CBD	5.32	120.53	111.23
23	b	611	CLA	C4A-NA-C1A	-5.32	104.25	106.68
23	A	606	CLA	C2A-C3A-C4A	5.31	110.45	101.87
23	B	604	CLA	C2A-C3A-C4A	5.31	110.44	101.87
23	B	613	CLA	C2A-C3A-C4A	5.31	110.44	101.87
26	A	610	PL9	C32-C33-C34	-5.31	115.48	127.62
23	c	505	CLA	C2A-C3A-C4A	5.29	110.42	101.87
23	C	510	CLA	C3A-C2A-C1A	5.29	109.26	101.34
23	B	616	CLA	C3A-C2A-C1A	5.29	109.26	101.34
26	d	404	PL9	C46-C44-C43	-5.29	109.30	121.17
23	b	606	CLA	C2A-C3A-C4A	5.27	110.38	101.87
23	B	607[A]	CLA	C2A-C3A-C4A	5.27	110.38	101.87
23	b	612	CLA	C2A-C3A-C4A	5.27	110.38	101.87
25	b	622	BCR	C7-C6-C5	-5.27	109.42	121.56
23	C	509	CLA	C2A-C3A-C4A	5.26	110.37	101.87
25	B	618	BCR	C8-C7-C6	-5.26	112.95	127.00
23	B	612	CLA	C2A-C3A-C4A	5.26	110.36	101.87
26	d	404	PL9	C11-C9-C8	-5.26	109.37	121.17
26	A	610	PL9	C25-C24-C23	-5.25	110.13	123.63
23	b	609[A]	CLA	C2A-C3A-C4A	5.25	110.36	101.87
23	C	501	CLA	O2D-CGD-CBD	5.25	120.41	111.23
25	C	514	BCR	C4-C5-C6	-5.25	115.61	122.70
23	c	503	CLA	C2A-C3A-C4A	5.24	110.34	101.87
23	D	404	CLA	C3A-C2A-C1A	5.24	109.19	101.34
23	b	614	CLA	O2D-CGD-CBD	5.24	120.39	111.23
23	b	606	CLA	C2A-C1A-CHA	5.23	132.95	123.87
25	h	101	BCR	C29-C30-C25	5.23	118.03	110.44
23	C	501	CLA	C2A-C3A-C4A	5.23	110.31	101.87
23	B	611	CLA	C3A-C2A-C1A	5.23	109.17	101.34
23	D	403	CLA	C3A-C2A-C1A	5.23	109.17	101.34
23	c	514	CLA	C4A-NA-C1A	-5.23	104.30	106.68
23	B	605	CLA	C2A-C3A-C4A	5.22	110.30	101.87
23	b	604	CLA	C2A-C3A-C4A	5.22	110.30	101.87
25	b	621	BCR	C7-C8-C9	-5.22	118.51	126.23
26	A	610	PL9	C30-C29-C28	-5.22	110.22	123.63
23	a	605	CLA	C3A-C2A-C1A	5.22	109.16	101.34
26	A	610	PL9	C15-C14-C13	-5.22	110.23	123.63
25	C	515	BCR	C15-C14-C13	-5.21	119.97	127.28
23	B	602	CLA	C2A-C3A-C4A	5.21	110.28	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	O2D-CGD-CBD	5.21	120.33	111.23
25	C	514	BCR	C7-C6-C5	-5.21	109.56	121.56
26	a	609	PL9	C26-C24-C23	-5.21	109.48	121.17
25	K	101	BCR	C7-C6-C5	-5.20	109.57	121.56
23	B	613	CLA	C3A-C2A-C1A	5.20	109.12	101.34
26	D	405	PL9	C15-C14-C13	-5.20	110.28	123.63
26	d	404	PL9	C21-C19-C18	-5.19	109.51	121.17
26	D	405	PL9	C10-C9-C8	-5.18	110.33	123.63
23	c	508	CLA	C3A-C2A-C1A	5.17	109.08	101.34
23	a	607	CLA	O2D-CGD-CBD	5.16	120.26	111.23
23	b	615	CLA	C2A-C3A-C4A	5.16	110.20	101.87
23	D	404	CLA	C4A-NA-C1A	-5.15	104.33	106.68
23	b	619	CLA	O2D-CGD-CBD	5.14	120.21	111.23
25	B	620	BCR	C7-C6-C5	-5.14	109.73	121.56
23	D	404	CLA	C2A-C3A-C4A	5.13	110.15	101.87
23	C	507	CLA	C3A-C2A-C1A	5.12	109.02	101.34
26	D	405	PL9	C21-C19-C18	-5.12	109.67	121.17
23	c	509	CLA	C2A-C3A-C4A	5.12	110.14	101.87
25	C	514	BCR	C23-C24-C25	-5.12	113.33	127.00
26	a	609	PL9	C35-C34-C33	-5.12	110.49	123.63
23	B	608	CLA	C3A-C2A-C1A	5.11	109.00	101.34
23	a	605	CLA	C2A-C3A-C4A	5.11	110.12	101.87
23	c	510	CLA	C2A-C3A-C4A	5.10	110.11	101.87
23	D	402	CLA	C2A-C3A-C4A	5.10	110.11	101.87
23	c	505	CLA	C3A-C2A-C1A	5.10	108.98	101.34
26	d	404	PL9	C45-C44-C43	-5.10	110.53	123.63
23	B	617	CLA	O2D-CGD-CBD	5.10	120.14	111.23
23	b	607	CLA	C2A-C3A-C4A	5.09	110.09	101.87
23	A	606	CLA	O2D-CGD-CBD	5.08	120.10	111.23
23	d	402	CLA	C3A-C2A-C1A	5.08	108.94	101.34
23	c	504	CLA	C2A-C3A-C4A	5.07	110.06	101.87
23	c	509	CLA	O2D-CGD-CBD	5.07	120.09	111.23
25	k	101	BCR	C7-C6-C5	-5.07	109.88	121.56
26	a	609	PL9	C46-C44-C43	-5.07	109.79	121.17
25	f	101	BCR	C36-C18-C17	-5.07	114.61	122.82
23	C	502	CLA	C4A-NA-C1A	-5.07	104.37	106.68
25	t	101	BCR	C24-C25-C26	-5.06	109.91	121.56
25	B	618	BCR	C23-C24-C25	-5.05	113.50	127.00
26	A	610	PL9	C26-C24-C23	-5.05	109.84	121.17
23	C	513	CLA	C2A-C3A-C4A	5.04	110.01	101.87
23	C	502	CLA	C2A-C3A-C4A	5.03	109.99	101.87
25	a	608	BCR	C7-C8-C9	-5.02	118.80	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C8-C7-C6	-5.02	113.58	127.00
23	A	606	CLA	C2A-C1A-CHA	5.02	132.58	123.87
23	a	613	CLA	C2A-C1A-CHA	5.02	132.58	123.87
23	d	403	CLA	C3A-C2A-C1A	5.02	108.86	101.34
25	B	618	BCR	C7-C6-C5	-5.02	109.99	121.56
26	D	405	PL9	C25-C24-C23	-5.01	110.76	123.63
25	K	101	BCR	C23-C22-C21	-5.00	111.14	119.01
23	b	614	CLA	C2A-C3A-C4A	5.00	109.94	101.87
23	A	606	CLA	C3A-C2A-C1A	5.00	108.82	101.34
23	B	612	CLA	O2D-CGD-CBD	4.99	119.96	111.23
23	b	607	CLA	C4A-NA-C1A	-4.99	104.40	106.68
23	D	402	CLA	C3A-C2A-C1A	4.98	108.81	101.34
25	c	522	BCR	C36-C18-C17	-4.98	114.75	122.82
23	D	404	CLA	C2A-C1A-CHA	4.98	132.50	123.87
23	B	609	CLA	O2D-CGD-CBD	4.97	119.92	111.23
25	k	101	BCR	C4-C5-C6	-4.97	115.99	122.70
23	B	614	CLA	C2A-C3A-C4A	4.96	109.88	101.87
23	b	619	CLA	C2A-C3A-C4A	4.96	109.88	101.87
23	b	617	CLA	C2A-C3A-C4A	4.95	109.87	101.87
23	c	506	CLA	C2A-C3A-C4A	4.95	109.87	101.87
23	a	605	CLA	O2D-CGD-CBD	4.94	119.87	111.23
23	B	615	CLA	C2A-C3A-C4A	4.94	109.85	101.87
25	b	620	BCR	C30-C25-C26	-4.93	115.89	122.64
26	a	609	PL9	C20-C19-C18	-4.93	110.96	123.63
26	d	404	PL9	C40-C39-C38	-4.93	110.97	123.63
23	c	502	CLA	C2A-C3A-C4A	4.93	109.83	101.87
23	B	604	CLA	C3A-C2A-C1A	4.92	108.72	101.34
23	c	510	CLA	O2D-CGD-CBD	4.92	119.83	111.23
23	b	613	CLA	C4A-NA-C1A	-4.92	104.44	106.68
23	B	617	CLA	C2A-C3A-C4A	4.92	109.81	101.87
23	A	608	CLA	C2A-C3A-C4A	4.90	109.79	101.87
23	A	608	CLA	O2D-CGD-CBD	4.90	119.80	111.23
23	c	513	CLA	C2A-C3A-C4A	4.90	109.78	101.87
23	D	402	CLA	C2A-C1A-CHA	4.90	132.37	123.87
23	C	506	CLA	C2A-C1A-CHA	4.90	132.36	123.87
26	D	405	PL9	C20-C19-C18	-4.88	111.10	123.63
25	c	515	BCR	C23-C24-C25	-4.87	113.98	127.00
23	c	502	CLA	O2D-CGD-CBD	4.86	119.72	111.23
23	c	503	CLA	O2D-CGD-CBD	4.85	119.71	111.23
23	B	603	CLA	C2A-C1A-CHA	4.85	132.28	123.87
26	A	610	PL9	C20-C19-C18	-4.85	111.18	123.63
23	a	613	CLA	C2A-C3A-C4A	4.85	109.70	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C2A-C3A-C4A	4.85	109.70	101.87
23	C	506	CLA	C2A-C3A-C4A	4.84	109.69	101.87
26	A	610	PL9	C35-C34-C33	-4.83	111.22	123.63
23	D	403	CLA	C2A-C3A-C4A	4.83	109.67	101.87
23	B	604	CLA	C2A-C1A-CHA	4.83	132.25	123.87
27	a	610	SQD	O6-C1-C2	4.83	115.61	108.27
23	c	512	CLA	C4A-NA-C1A	-4.83	104.48	106.68
23	C	504	CLA	C3A-C2A-C1A	4.83	108.57	101.34
23	b	611	CLA	O2D-CGD-CBD	4.83	119.67	111.23
26	a	609	PL9	C30-C29-C28	-4.83	111.23	123.63
23	B	607[B]	CLA	O2D-CGD-CBD	4.83	119.67	111.23
23	b	616	CLA	C2A-C3A-C4A	4.82	109.65	101.87
23	b	616	CLA	O2D-CGD-CBD	4.81	119.65	111.23
26	D	405	PL9	C46-C44-C43	-4.81	110.36	121.17
23	A	605	CLA	C2A-C1A-CHA	4.81	132.22	123.87
23	C	512	CLA	O2D-CGD-CBD	4.81	119.64	111.23
27	A	611	SQD	O6-C1-C2	4.81	115.58	108.27
26	D	405	PL9	C35-C34-C33	-4.81	111.28	123.63
23	B	611	CLA	C2A-C1A-CHA	4.80	132.20	123.87
23	C	506	CLA	O2D-CGD-CBD	4.78	119.59	111.23
23	B	613	CLA	O2D-CGD-CBD	4.78	119.58	111.23
26	d	404	PL9	C25-C24-C23	-4.78	111.36	123.63
23	B	610	CLA	O2D-CGD-CBD	4.77	119.58	111.23
25	t	101	BCR	C23-C24-C25	-4.77	114.25	127.00
23	C	512	CLA	C2A-C3A-C4A	4.77	109.57	101.87
25	c	515	BCR	C2-C1-C6	4.77	117.36	110.44
23	C	510	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	c	512	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	d	403	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	B	611	CLA	C2A-C3A-C4A	4.76	109.56	101.87
23	C	511	CLA	C4A-NA-C1A	-4.76	104.51	106.68
23	B	603	CLA	C3A-C2A-C1A	4.76	108.46	101.34
23	c	514	CLA	C2A-C3A-C4A	4.76	109.55	101.87
25	a	608	BCR	C8-C7-C6	-4.75	114.30	127.00
25	F	101	BCR	C12-C13-C14	-4.75	111.53	119.01
23	B	603	CLA	C2A-C3A-C4A	4.75	109.55	101.87
23	c	514	CLA	O2D-CGD-CBD	4.75	119.54	111.23
23	B	607[A]	CLA	C2A-C1A-CHA	4.74	132.09	123.87
23	B	604	CLA	O2D-CGD-CBD	4.73	119.50	111.23
23	a	613	CLA	O2D-CGD-CBD	4.73	119.50	111.23
23	C	507	CLA	C2A-C1A-CHA	4.73	132.08	123.87
23	c	507	CLA	C2A-C1A-CHA	4.73	132.07	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C2A-C3A-C4A	4.72	109.50	101.87
25	b	620	BCR	C7-C6-C5	-4.72	110.69	121.56
23	B	607[A]	CLA	O2D-CGD-CBD	4.71	119.47	111.23
25	b	620	BCR	C8-C7-C6	-4.71	114.43	127.00
23	c	508	CLA	C2A-C1A-CHA	4.70	132.03	123.87
23	C	503	CLA	C2A-C3A-C4A	4.70	109.46	101.87
23	C	504	CLA	C2A-C1A-CHA	4.70	132.02	123.87
23	a	607	CLA	C2A-C3A-C4A	4.69	109.45	101.87
23	C	508	CLA	O2D-CGD-CBD	4.69	119.43	111.23
23	C	503	CLA	C4A-NA-C1A	-4.69	104.54	106.68
33	e	102	HEM	C4D-ND-C1D	4.69	110.76	105.21
33	v	201	HEM	C4D-ND-C1D	4.69	110.76	105.21
23	C	509	CLA	O2D-CGD-CBD	4.69	119.42	111.23
25	B	620	BCR	C31-C1-C6	-4.69	102.89	110.24
23	B	614	CLA	C2A-C1A-CHA	4.68	131.99	123.87
23	C	513	CLA	O2D-CGD-CBD	4.68	119.41	111.23
23	d	402	CLA	C2A-C3A-C4A	4.68	109.43	101.87
25	A	609	BCR	C7-C6-C5	-4.68	110.78	121.56
26	d	404	PL9	C47-C48-C49	-4.67	112.07	127.64
25	F	101	BCR	C7-C6-C5	-4.67	110.80	121.56
23	b	609[A]	CLA	O2D-CGD-CBD	4.67	119.39	111.23
23	b	609[A]	CLA	C2A-C1A-CHA	4.67	131.96	123.87
23	c	503	CLA	C4A-NA-C1A	-4.66	104.55	106.68
23	d	403	CLA	C4A-NA-C1A	-4.66	104.55	106.68
23	c	507	CLA	O2D-CGD-CBD	4.66	119.38	111.23
25	B	619	BCR	C4-C5-C6	-4.66	116.40	122.70
25	t	101	BCR	C2-C1-C6	4.66	117.21	110.44
23	a	605	CLA	C2A-C1A-CHA	4.66	131.96	123.87
23	C	501	CLA	C2A-C1A-CHA	4.66	131.95	123.87
23	b	613	CLA	C2A-C1A-CHA	4.66	131.95	123.87
23	b	609[B]	CLA	C2A-C1A-CHA	4.65	131.94	123.87
23	C	504	CLA	O2D-CGD-CBD	4.65	119.37	111.23
25	B	619	BCR	C30-C25-C26	-4.65	116.28	122.64
25	b	621	BCR	C38-C26-C27	-4.64	103.69	113.60
25	C	521	BCR	C36-C18-C17	-4.64	115.30	122.82
25	T	101	BCR	C24-C25-C26	-4.64	110.87	121.56
23	b	609[B]	CLA	O2D-CGD-CBD	4.63	119.32	111.23
23	c	505	CLA	C2A-C1A-CHA	4.63	131.89	123.87
23	c	510	CLA	C4A-NA-C1A	-4.62	104.57	106.68
23	d	403	CLA	O2D-CGD-CBD	4.61	119.29	111.23
23	c	505	CLA	C4A-NA-C1A	-4.61	104.58	106.68
23	B	614	CLA	O2D-CGD-CBD	4.60	119.28	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607[B]	CLA	C2A-C1A-CHA	4.59	131.84	123.87
25	a	608	BCR	C7-C6-C5	-4.59	110.97	121.56
23	b	613	CLA	C2A-C3A-C4A	4.59	109.29	101.87
23	C	511	CLA	C2A-C3A-C4A	4.59	109.28	101.87
25	h	101	BCR	C24-C25-C26	-4.59	110.99	121.56
23	b	605	CLA	C2A-C3A-C4A	4.59	109.28	101.87
23	B	608	CLA	C2A-C1A-CHA	4.58	131.82	123.87
26	D	405	PL9	C47-C48-C49	-4.58	112.37	127.64
25	H	101	BCR	C20-C21-C22	-4.58	120.86	127.28
23	b	607	CLA	C2A-C1A-CHA	4.57	131.80	123.87
23	d	403	CLA	C2A-C1A-CHA	4.57	131.79	123.87
23	c	511	CLA	C2A-C3A-C4A	4.56	109.23	101.87
23	c	509	CLA	C2A-C1A-CHA	4.56	131.78	123.87
23	C	511	CLA	O2D-CGD-CBD	4.55	119.19	111.23
23	B	605	CLA	C2A-C1A-CHA	4.55	131.77	123.87
25	B	618	BCR	C37-C22-C21	-4.55	115.44	122.82
23	B	615	CLA	O2D-CGD-CBD	4.55	119.18	111.23
23	a	604	CLA	O2D-CGD-CBD	4.55	119.18	111.23
23	C	502	CLA	O2D-CGD-CBD	4.54	119.17	111.23
23	C	503	CLA	O2D-CGD-CBD	4.54	119.17	111.23
25	C	514	BCR	C2-C1-C6	4.54	117.04	110.44
23	b	604	CLA	C2A-C1A-CHA	4.54	131.74	123.87
26	d	404	PL9	C20-C19-C18	-4.53	111.98	123.63
25	f	101	BCR	C7-C6-C5	-4.53	111.11	121.56
23	b	611	CLA	C2A-C3A-C4A	4.53	109.19	101.87
26	D	405	PL9	C40-C39-C38	-4.52	112.01	123.63
25	B	620	BCR	C23-C24-C25	-4.52	114.92	127.00
25	B	618	BCR	C11-C12-C13	-4.52	113.97	126.36
25	H	101	BCR	C24-C25-C26	-4.52	111.15	121.56
26	D	405	PL9	C31-C29-C28	-4.52	111.03	121.17
25	k	101	BCR	C23-C24-C25	-4.51	114.94	127.00
23	B	611	CLA	C4A-NA-C1A	-4.50	104.62	106.68
23	c	510	CLA	C2A-C1A-CHA	4.49	131.65	123.87
23	c	514	CLA	C2A-C1A-CHA	4.49	131.65	123.87
23	B	606	CLA	C2A-C1A-CHA	4.49	131.65	123.87
23	C	503	CLA	C2A-C1A-CHA	4.48	131.64	123.87
23	c	504	CLA	C2A-C1A-CHA	4.48	131.64	123.87
26	d	404	PL9	C41-C39-C38	-4.48	111.11	121.17
24	d	401	PHO	C4D-CHA-CBD	-4.44	106.32	108.45
25	C	521	BCR	C24-C25-C26	-4.43	111.34	121.56
26	A	610	PL9	C21-C19-C18	-4.43	111.22	121.17
26	A	610	PL9	C46-C44-C43	-4.43	111.22	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	CLA	O2D-CGD-CBD	4.43	118.97	111.23
31	a	614	LHG	O7-C7-C8	4.43	121.06	111.48
26	A	610	PL9	C50-C49-C48	-4.42	109.40	122.66
23	B	609	CLA	C2A-C1A-CHA	4.42	131.53	123.87
23	C	513	CLA	C2A-C1A-CHA	4.42	131.53	123.87
23	B	612	CLA	CHB-C1B-NB	4.41	130.66	124.05
23	b	616	CLA	C2A-C1A-CHA	4.41	131.52	123.87
25	b	622	BCR	C2-C1-C6	4.41	116.84	110.44
23	C	509	CLA	C2A-C1A-CHA	4.40	131.50	123.87
23	b	616	CLA	C4A-NA-C1A	-4.40	104.67	106.68
27	B	623	SQD	O6-C1-C2	4.39	114.94	108.27
25	A	609	BCR	C7-C8-C9	-4.38	119.75	126.23
27	b	602	SQD	O6-C1-C2	4.38	114.93	108.27
23	b	607	CLA	O2D-CGD-CBD	4.38	118.88	111.23
25	A	609	BCR	C8-C7-C6	-4.37	115.31	127.00
23	c	502	CLA	C4A-NA-C1A	-4.37	104.68	106.68
23	D	403	CLA	O2D-CGD-CBD	4.37	118.87	111.23
23	C	510	CLA	C4A-NA-C1A	-4.37	104.69	106.68
23	d	402	CLA	O2D-CGD-CBD	4.37	118.86	111.23
25	b	622	BCR	C31-C1-C6	-4.36	103.40	110.24
23	c	511	CLA	C2A-C1A-CHA	4.36	131.44	123.87
23	B	612	CLA	C2A-C1A-CHA	4.36	131.43	123.87
23	b	611	CLA	C2A-C1A-CHA	4.36	131.43	123.87
26	a	609	PL9	C41-C39-C38	-4.36	111.39	121.17
25	h	101	BCR	C20-C21-C22	-4.35	121.17	127.28
23	C	510	CLA	O2D-CGD-CBD	4.35	118.84	111.23
25	H	101	BCR	C2-C1-C6	4.35	116.76	110.44
23	A	608	CLA	C2A-C1A-CHA	4.35	131.42	123.87
26	A	610	PL9	C7-C3-C4	4.35	120.49	116.91
23	c	506	CLA	C2A-C1A-CHA	4.35	131.41	123.87
23	c	503	CLA	C2A-C1A-CHA	4.34	131.40	123.87
25	t	101	BCR	C20-C21-C22	-4.33	121.20	127.28
26	a	609	PL9	C21-C19-C18	-4.33	111.45	121.17
27	A	611	SQD	O47-C7-C8	4.33	120.84	111.48
25	c	515	BCR	C31-C1-C6	-4.32	103.47	110.24
25	T	101	BCR	C1-C6-C5	-4.32	116.73	122.64
23	c	504	CLA	O2D-CGD-CBD	4.32	118.78	111.23
25	h	101	BCR	C8-C9-C10	-4.32	112.22	119.01
27	a	610	SQD	O47-C7-C8	4.32	120.82	111.48
33	E	102	HEM	C4D-ND-C1D	4.32	110.32	105.21
23	B	606	CLA	O2D-CGD-CBD	4.31	118.76	111.23
33	V	202	HEM	C4D-ND-C1D	4.31	110.31	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C4A-NA-C1A	-4.30	104.72	106.68
25	b	620	BCR	C24-C23-C22	-4.29	119.88	126.23
23	b	614	CLA	C2A-C1A-CHA	4.29	131.31	123.87
25	B	618	BCR	C38-C26-C27	-4.29	104.46	113.60
25	b	621	BCR	C32-C1-C6	4.28	116.96	110.24
23	B	602	CLA	C2A-C1A-CHA	4.28	131.29	123.87
25	c	516	BCR	C38-C26-C27	-4.27	104.48	113.60
32	c	519	DGD	O2G-C1B-C2B	4.27	120.72	111.48
23	b	609[A]	CLA	C4A-NA-C1A	-4.27	104.73	106.68
27	X	101	SQD	O6-C1-C2	4.27	114.75	108.27
27	x	101	SQD	O6-C1-C2	4.27	114.75	108.27
23	D	402	CLA	O2D-CGD-CBD	4.25	118.67	111.23
23	b	604	CLA	O2D-CGD-CBD	4.25	118.66	111.23
23	a	604	CLA	C2A-C1A-CHA	4.25	131.24	123.87
23	c	512	CLA	C2A-C1A-CHA	4.25	131.24	123.87
23	C	511	CLA	C2A-C1A-CHA	4.24	131.23	123.87
23	b	614	CLA	CHB-C1B-NB	4.24	130.42	124.05
23	B	609	CLA	C4A-NA-C1A	-4.24	104.74	106.68
23	B	602	CLA	O2D-CGD-CBD	4.24	118.65	111.23
23	C	504	CLA	C4A-NA-C1A	-4.24	104.74	106.68
23	B	602	CLA	C4A-NA-C1A	-4.24	104.75	106.68
23	c	505	CLA	O2D-CGD-CBD	4.24	118.64	111.23
23	C	508	CLA	C2A-C1A-CHA	4.23	131.21	123.87
25	B	618	BCR	C24-C25-C26	-4.23	111.81	121.56
23	b	617	CLA	O2D-CGD-CBD	4.23	118.62	111.23
25	c	516	BCR	C7-C6-C5	-4.23	111.81	121.56
23	B	615	CLA	C4A-NA-C1A	-4.22	104.75	106.68
23	b	605	CLA	C2A-C1A-CHA	4.22	131.19	123.87
23	b	612	CLA	C2A-C1A-CHA	4.21	131.17	123.87
25	c	515	BCR	C34-C9-C10	-4.21	116.00	122.82
25	c	522	BCR	C24-C25-C26	-4.21	111.86	121.56
25	c	522	BCR	C7-C8-C9	-4.21	120.01	126.23
23	c	509	CLA	CHB-C1B-NB	4.20	130.35	124.05
23	B	607[A]	CLA	C4A-NA-C1A	-4.20	104.76	106.68
25	A	609	BCR	C39-C30-C25	4.20	116.83	110.24
23	b	617	CLA	C2A-C1A-CHA	4.20	131.16	123.87
25	h	101	BCR	C2-C1-C6	4.20	116.54	110.44
23	C	505	CLA	C2A-C1A-CHA	4.20	131.15	123.87
23	B	615	CLA	C2A-C1A-CHA	4.20	131.15	123.87
23	c	508	CLA	C4A-NA-C1A	-4.20	104.76	106.68
32	h	102	DGD	O2G-C1B-C2B	4.19	120.55	111.48
26	d	404	PL9	C26-C24-C23	-4.18	111.79	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	621	BCR	C30-C25-C26	-4.17	116.94	122.64
25	H	101	BCR	C8-C7-C6	-4.16	115.87	127.00
22	A	604	BCT	O3-C-O1	-4.16	109.03	119.68
23	C	502	CLA	C2A-C1A-CHA	4.15	131.08	123.87
23	b	612	CLA	O2D-CGD-CBD	4.15	118.49	111.23
26	D	405	PL9	C26-C24-C23	-4.15	111.85	121.17
23	B	613	CLA	C2A-C1A-CHA	4.15	131.06	123.87
25	c	515	BCR	C16-C15-C14	-4.14	115.04	123.52
26	a	609	PL9	C47-C48-C49	-4.14	113.84	127.64
23	a	604	CLA	C2A-C3A-C4A	4.14	108.55	101.87
25	T	101	BCR	C37-C22-C21	-4.13	116.13	122.82
25	B	620	BCR	C2-C1-C6	4.12	116.43	110.44
25	C	514	BCR	C31-C1-C6	-4.12	103.78	110.24
23	b	606	CLA	O2D-CGD-CBD	4.12	118.43	111.23
23	c	511	CLA	O2D-CGD-CBD	4.11	118.42	111.23
23	B	607[A]	CLA	CHB-C1B-NB	4.10	130.20	124.05
23	c	502	CLA	C2A-C1A-CHA	4.09	130.96	123.87
25	B	619	BCR	C29-C30-C25	4.08	116.37	110.44
25	B	620	BCR	C24-C25-C26	-4.08	112.16	121.56
23	b	609[A]	CLA	CHB-C1B-NB	4.08	130.17	124.05
23	B	617	CLA	C2A-C1A-CHA	4.08	130.94	123.87
25	b	621	BCR	C4-C5-C6	-4.07	117.21	122.70
23	b	608	CLA	O2D-CGD-CBD	4.06	118.33	111.23
25	c	522	BCR	C38-C26-C27	-4.06	104.93	113.60
25	b	622	BCR	C38-C26-C27	-4.06	104.94	113.60
28	a	611	LMG	O7-C10-C11	4.06	120.25	111.48
24	D	401	PHO	C4D-CHA-CBD	-4.05	106.51	108.45
28	C	519	LMG	O7-C10-C11	4.05	120.25	111.48
26	D	405	PL9	C41-C39-C38	-4.05	112.07	121.17
26	A	610	PL9	C47-C48-C49	-4.04	114.16	127.64
26	a	609	PL9	C7-C3-C4	4.04	120.23	116.91
31	b	624	LHG	O7-C7-C8	4.04	120.21	111.48
26	A	610	PL9	C51-C49-C48	-4.04	110.55	122.66
23	B	605	CLA	O2D-CGD-CBD	4.03	118.28	111.23
25	b	621	BCR	C34-C9-C10	-4.03	116.29	122.82
25	a	608	BCR	C39-C30-C25	4.02	116.55	110.24
23	C	507	CLA	C4A-NA-C1A	-4.02	104.84	106.68
23	b	615	CLA	C2A-C1A-CHA	4.01	130.83	123.87
28	Z	101	LMG	O7-C10-C11	4.01	120.16	111.48
23	a	604	CLA	C3A-C2A-C1A	4.00	107.34	101.34
23	C	510	CLA	C2A-C1A-CHA	3.99	130.79	123.87
26	a	609	PL9	C36-C34-C33	-3.99	112.22	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C4A-NA-C1A	-3.98	104.86	106.68
23	d	402	CLA	C2A-C1A-CHA	3.98	130.78	123.87
25	k	101	BCR	C38-C26-C27	-3.98	105.10	113.60
23	c	507	CLA	CHB-C1B-NB	3.98	130.02	124.05
25	F	101	BCR	C8-C7-C6	-3.98	116.37	127.00
23	A	605	CLA	O2D-CGD-CBD	3.96	118.16	111.23
23	a	607	CLA	C2A-C1A-CHA	3.96	130.75	123.87
27	B	623	SQD	O47-C7-C8	3.96	120.05	111.48
25	B	620	BCR	C38-C26-C27	-3.96	105.16	113.60
25	K	101	BCR	C23-C24-C25	-3.96	116.43	127.00
27	b	602	SQD	O47-C7-C8	3.96	120.04	111.48
23	b	608	CLA	C2A-C1A-CHA	3.95	130.73	123.87
23	C	506	CLA	CHB-C1B-NB	3.95	129.98	124.05
31	e	101	LHG	O7-C7-C8	3.95	120.03	111.48
23	B	612	CLA	C4A-NA-C1A	-3.95	104.88	106.68
23	C	508	CLA	C4A-NA-C1A	-3.95	104.88	106.68
25	C	515	BCR	C38-C26-C27	-3.94	105.19	113.60
25	b	622	BCR	C24-C25-C26	-3.94	112.48	121.56
31	B	622	LHG	O7-C7-C8	3.94	120.00	111.48
25	k	101	BCR	C24-C25-C26	-3.94	112.49	121.56
23	B	610	CLA	C2A-C1A-CHA	3.93	130.69	123.87
23	b	610	CLA	O2D-CGD-CBD	3.93	118.11	111.23
25	B	620	BCR	C20-C21-C22	-3.93	121.77	127.28
23	b	613	CLA	O2D-CGD-CBD	3.92	118.09	111.23
23	c	503	CLA	CHB-C1B-NB	3.92	129.94	124.05
23	b	614	CLA	C4A-NA-C1A	-3.92	104.89	106.68
31	D	408	LHG	O7-C7-C8	3.92	119.97	111.48
25	b	622	BCR	C23-C24-C25	-3.92	116.52	127.00
25	h	101	BCR	C31-C1-C6	-3.92	104.09	110.24
28	c	520	LMG	O7-C10-C11	3.92	119.96	111.48
31	l	101	LHG	O7-C7-C8	3.92	119.96	111.48
23	c	511	CLA	C4A-NA-C1A	-3.92	104.89	106.68
25	H	101	BCR	C38-C26-C27	-3.91	105.26	113.60
23	B	607[B]	CLA	CHB-C1B-NB	3.91	129.91	124.05
23	C	501	CLA	CHB-C1B-NB	3.90	129.90	124.05
23	b	609[B]	CLA	CHB-C1B-NB	3.90	129.90	124.05
23	C	508	CLA	CHB-C1B-NB	3.90	129.89	124.05
25	C	521	BCR	C23-C24-C25	-3.90	116.59	127.00
28	c	521	LMG	O7-C10-C11	3.89	119.91	111.48
32	c	517	DGD	O2G-C1B-C2B	3.89	119.90	111.48
25	h	101	BCR	C7-C8-C9	-3.89	120.48	126.23
23	B	611	CLA	CHB-C1B-NB	3.88	129.86	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	621	BCR	C20-C21-C22	-3.87	121.86	127.28
23	b	610	CLA	CHC-C1C-NC	3.86	130.12	124.31
23	A	605	CLA	C2A-C3A-C4A	3.85	108.09	101.87
25	H	101	BCR	C30-C25-C26	-3.85	117.38	122.64
23	B	616	CLA	C2A-C1A-CHA	3.85	130.54	123.87
26	d	404	PL9	C31-C29-C28	-3.84	112.54	121.17
23	B	602	CLA	CHB-C1B-NB	3.84	129.81	124.05
25	h	101	BCR	C35-C13-C14	-3.84	116.60	122.82
23	c	505	CLA	CHB-C1B-NB	3.83	129.80	124.05
23	b	619	CLA	C2A-C1A-CHA	3.83	130.52	123.87
23	B	606	CLA	C4-C3-C5	3.83	121.88	115.23
23	B	608	CLA	C4A-NA-C1A	-3.83	104.93	106.68
25	c	516	BCR	C8-C7-C6	-3.83	116.78	127.00
25	B	620	BCR	C11-C10-C9	-3.83	121.91	127.28
23	B	606	CLA	CHB-C1B-NB	3.82	129.79	124.05
23	A	605	CLA	CHB-C1B-NB	3.82	129.78	124.05
23	b	608	CLA	C4-C3-C5	3.81	121.85	115.23
25	f	101	BCR	C8-C7-C6	-3.81	116.81	127.00
23	a	607	CLA	CHB-C1B-NB	3.81	129.77	124.05
23	c	512	CLA	O2D-CGD-CBD	3.81	117.88	111.23
23	b	617	CLA	C4A-NA-C1A	-3.80	104.95	106.68
25	C	515	BCR	C16-C15-C14	-3.80	115.75	123.52
23	b	610	CLA	C4A-NA-C1A	-3.79	104.95	106.68
25	K	101	BCR	C38-C26-C27	-3.78	105.53	113.60
28	A	612	LMG	O7-C10-C11	3.78	119.66	111.48
25	h	101	BCR	C38-C26-C27	-3.78	105.54	113.60
25	C	514	BCR	C10-C11-C12	-3.78	112.25	123.20
26	a	609	PL9	C31-C29-C28	-3.78	112.69	121.17
23	B	613	CLA	C4A-NA-C1A	-3.77	104.96	106.68
25	b	620	BCR	C20-C21-C22	-3.77	121.99	127.28
23	b	608	CLA	CHB-C1B-NB	3.77	129.70	124.05
23	B	603	CLA	CHB-C1B-NB	3.76	129.70	124.05
27	b	602	SQD	C3-C4-C5	3.76	117.06	110.23
27	x	101	SQD	O47-C7-C8	3.76	119.61	111.48
27	X	101	SQD	O47-C7-C8	3.75	119.60	111.48
25	A	609	BCR	C36-C18-C17	-3.75	116.74	122.82
25	B	619	BCR	C20-C19-C18	-3.75	116.08	126.36
27	B	623	SQD	C3-C4-C5	3.75	117.03	110.23
23	c	509	CLA	C4A-NA-C1A	-3.75	104.97	106.68
23	C	504	CLA	CHB-C1B-NB	3.74	129.66	124.05
23	B	617	CLA	CHB-C1B-NB	3.73	129.65	124.05
23	b	613	CLA	CHB-C1B-NB	3.73	129.65	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	CHB-C1B-NB	3.73	129.65	124.05
31	d	406	LHG	O7-C7-C8	3.73	119.55	111.48
23	C	512	CLA	CHB-C1B-NB	3.72	129.63	124.05
25	k	101	BCR	C23-C22-C21	-3.71	113.17	119.01
23	a	604	CLA	CHB-C1B-NB	3.71	129.61	124.05
26	d	404	PL9	C50-C49-C48	-3.71	111.53	122.66
25	C	521	BCR	C38-C26-C27	-3.70	105.71	113.60
23	D	402	CLA	CHB-C1B-NB	3.70	129.60	124.05
26	A	610	PL9	C41-C39-C38	-3.69	112.88	121.17
23	c	511	CLA	CHB-C1B-NB	3.69	129.58	124.05
28	z	101	LMG	O7-C10-C11	3.68	119.45	111.48
23	a	613	CLA	CHB-C1B-NB	3.68	129.57	124.05
31	D	407	LHG	O7-C7-C8	3.68	119.44	111.48
25	c	515	BCR	C3-C4-C5	-3.67	107.51	114.06
23	C	502	CLA	CHB-C1B-NB	3.67	129.55	124.05
26	a	609	PL9	C40-C39-C41	-3.66	108.88	115.23
32	C	517	DGD	O2G-C1B-C2B	3.66	119.40	111.48
26	A	610	PL9	C40-C39-C41	-3.65	108.89	115.23
26	A	610	PL9	C15-C14-C16	-3.65	108.89	115.23
23	B	617	CLA	CHC-C1C-NC	3.65	129.81	124.31
25	K	101	BCR	C12-C13-C14	-3.65	113.27	119.01
32	C	518	DGD	O2G-C1B-C2B	3.65	119.37	111.48
23	b	619	CLA	CHC-C1C-NC	3.64	129.80	124.31
25	C	515	BCR	C8-C7-C6	-3.64	117.26	127.00
23	B	603	CLA	CHC-C1C-NC	3.64	129.79	124.31
31	L	101	LHG	O7-C7-C8	3.64	119.35	111.48
25	A	609	BCR	C23-C22-C21	-3.64	113.29	119.01
23	d	403	CLA	CHB-C1B-NB	3.64	129.51	124.05
25	B	620	BCR	C37-C22-C21	-3.64	116.92	122.82
26	d	404	PL9	C45-C44-C46	-3.64	108.92	115.23
23	a	613	CLA	CHC-C1C-NC	3.63	129.78	124.31
25	h	101	BCR	C11-C10-C9	-3.63	122.18	127.28
23	A	608	CLA	CHB-C1B-NB	3.63	129.50	124.05
23	c	514	CLA	CHB-C1B-NB	3.63	129.50	124.05
26	a	609	PL9	C50-C49-C48	-3.63	111.77	122.66
25	H	101	BCR	C34-C9-C10	-3.62	116.95	122.82
23	D	404	CLA	CHB-C1B-NB	3.62	129.48	124.05
32	C	516	DGD	O2G-C1B-C2B	3.62	119.31	111.48
23	c	502	CLA	CHB-C1B-NB	3.62	129.48	124.05
23	c	504	CLA	CHB-C1B-NB	3.62	129.48	124.05
25	a	608	BCR	C27-C26-C25	-3.62	117.82	122.70
23	b	615	CLA	C4A-NA-C1A	-3.61	105.03	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C2A-C1A-CHA	3.61	130.13	123.87
28	C	520	LMG	O7-C10-C11	3.61	119.28	111.48
23	A	605	CLA	C3A-C2A-C1A	3.60	106.74	101.34
28	Z	101	LMG	O1-C1-C2	3.60	113.75	108.27
25	b	622	BCR	C35-C13-C14	-3.60	116.98	122.82
23	C	513	CLA	CHB-C1B-NB	3.60	129.45	124.05
25	k	101	BCR	C35-C13-C14	-3.59	116.99	122.82
23	C	512	CLA	C2A-C1A-CHA	3.59	130.10	123.87
23	B	608	CLA	CHC-C1C-NC	3.59	129.72	124.31
23	D	404	CLA	C1-O2A-CGA	3.59	125.34	116.65
23	b	604	CLA	CHB-C1B-NB	3.58	129.42	124.05
23	B	607[B]	CLA	C4A-NA-C1A	-3.58	105.05	106.68
23	C	501	CLA	C4A-NA-C1A	-3.58	105.05	106.68
23	b	614	CLA	CHC-C1C-NC	3.58	129.70	124.31
26	A	610	PL9	C36-C34-C33	-3.57	113.14	121.17
26	a	609	PL9	C15-C14-C16	-3.57	109.03	115.23
27	a	610	SQD	O9-S-C6	3.57	112.08	106.76
25	B	620	BCR	C11-C12-C13	-3.57	116.58	126.36
23	B	613	CLA	CHB-C1B-NB	3.57	129.40	124.05
23	a	607	CLA	CHA-C1A-NA	-3.57	118.32	126.39
26	D	405	PL9	C36-C34-C33	-3.56	113.17	121.17
23	B	607[B]	CLA	CHC-C1C-NC	3.56	129.68	124.31
27	A	611	SQD	O9-S-C6	3.56	112.07	106.76
26	a	609	PL9	C45-C44-C46	-3.55	109.07	115.23
26	D	405	PL9	C45-C44-C46	-3.54	109.08	115.23
25	C	515	BCR	C37-C22-C21	-3.54	117.08	122.82
25	a	608	BCR	C11-C12-C13	-3.54	116.66	126.36
23	B	605	CLA	O1D-CGD-CBD	-3.53	117.55	124.52
23	C	510	CLA	CHB-C1B-NB	3.53	129.35	124.05
23	b	616	CLA	CHB-C1B-NB	3.53	129.35	124.05
23	b	611	CLA	CHB-C1B-NB	3.53	129.35	124.05
23	c	510	CLA	CHC-C1C-NC	3.53	129.63	124.31
23	c	513	CLA	C4A-NA-C1A	-3.53	105.07	106.68
23	b	618	CLA	C2A-C1A-CHA	3.53	129.99	123.87
32	D	406	DGD	O2G-C1B-C2B	3.53	119.12	111.48
28	b	623	LMG	O7-C10-C11	3.52	119.10	111.48
22	A	604	BCT	O2-C-O1	-3.52	110.68	119.68
26	D	405	PL9	C51-C49-C48	-3.52	112.10	122.66
23	B	616	CLA	CHC-C1C-NC	3.52	129.61	124.31
23	a	605	CLA	CHB-C1B-NB	3.52	129.32	124.05
25	H	101	BCR	C31-C1-C6	-3.52	104.73	110.24
26	D	405	PL9	C50-C49-C48	-3.52	112.11	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	PL9	C51-C49-C48	-3.51	112.11	122.66
23	b	617	CLA	CHB-C1B-NB	3.51	129.32	124.05
23	B	615	CLA	CHB-C1B-NB	3.51	129.32	124.05
24	d	401	PHO	CMB-C2B-C3B	3.51	131.70	124.68
25	B	619	BCR	C11-C12-C13	-3.51	116.73	126.36
23	b	618	CLA	CHC-C1C-NC	3.50	129.59	124.31
23	B	611	CLA	O2D-CGD-CBD	3.50	117.35	111.23
23	a	607	CLA	C4-C3-C5	3.50	121.30	115.23
23	b	618	CLA	CHB-C1B-NB	3.50	129.30	124.05
23	A	608	CLA	C1-O2A-CGA	3.50	125.12	116.65
25	c	516	BCR	C16-C15-C14	-3.50	116.36	123.52
25	b	620	BCR	C2-C3-C4	3.50	118.97	111.28
23	c	513	CLA	CHB-C1B-NB	3.49	129.29	124.05
23	b	605	CLA	CHB-C1B-NB	3.49	129.29	124.05
31	E	101	LHG	O7-C7-C8	3.48	119.02	111.48
23	C	509	CLA	C4A-NA-C1A	-3.48	105.09	106.68
23	A	608	CLA	C4-C3-C5	3.48	121.27	115.23
24	D	401	PHO	CMB-C2B-C3B	3.48	131.63	124.68
23	b	609[B]	CLA	C4A-NA-C1A	-3.48	105.09	106.68
25	C	515	BCR	C7-C6-C5	-3.47	113.55	121.56
23	B	614	CLA	CHB-C1B-NB	3.47	129.26	124.05
22	a	603	BCT	O3-C-O1	-3.47	110.79	119.68
23	b	615	CLA	CHB-C1B-NB	3.47	129.26	124.05
25	C	515	BCR	C33-C5-C4	-3.47	106.21	113.60
25	b	620	BCR	C30-C25-C24	-3.46	106.26	115.65
23	d	402	CLA	CHB-C1B-NB	3.46	129.24	124.05
26	D	405	PL9	C7-C3-C4	3.46	119.76	116.91
23	C	507	CLA	CHB-C1B-NB	3.46	129.23	124.05
23	B	605	CLA	CHC-C1C-NC	3.45	129.51	124.31
25	B	619	BCR	C32-C1-C6	3.45	115.65	110.24
28	J	101	LMG	O7-C10-C11	3.45	118.94	111.48
25	T	101	BCR	C2-C1-C6	3.45	115.44	110.44
25	K	101	BCR	C24-C25-C26	-3.45	113.62	121.56
23	B	604	CLA	CHB-C1B-NB	3.44	129.21	124.05
25	b	620	BCR	C24-C25-C26	-3.44	113.63	121.56
23	B	609	CLA	CHB-C1B-NB	3.44	129.20	124.05
28	j	101	LMG	O7-C10-C11	3.43	118.91	111.48
23	b	619	CLA	CHB-C1B-NB	3.43	129.19	124.05
32	H	102	DGD	O2G-C1B-C2B	3.43	118.89	111.48
25	c	516	BCR	C34-C9-C10	-3.43	117.27	122.82
23	A	606	CLA	CHB-C1B-NB	3.42	129.18	124.05
25	F	101	BCR	C33-C5-C4	-3.42	106.31	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	621	LMG	O7-C10-C11	3.41	118.87	111.48
23	C	503	CLA	CHB-C1B-NB	3.41	129.16	124.05
26	D	405	PL9	C10-C9-C11	-3.40	109.33	115.23
23	c	510	CLA	CHB-C1B-NB	3.40	129.15	124.05
23	c	505	CLA	CHC-C1C-NC	3.39	129.42	124.31
23	C	504	CLA	CHC-C1C-NC	3.39	129.42	124.31
25	b	622	BCR	C11-C10-C9	-3.38	122.53	127.28
26	d	404	PL9	C35-C34-C33	-3.38	114.94	123.63
23	b	608	CLA	C4A-NA-C1A	-3.38	105.14	106.68
23	d	403	CLA	C1-O2A-CGA	3.38	124.82	116.65
25	t	101	BCR	C7-C8-C9	-3.37	121.24	126.23
24	D	401	PHO	O1D-CGD-CBD	3.37	129.84	124.72
27	a	612	SQD	O47-C7-C8	3.37	118.77	111.48
23	B	610	CLA	C4D-C3D-CAD	-3.37	104.45	108.11
25	h	101	BCR	C20-C19-C18	-3.37	117.13	126.36
23	b	617	CLA	C4-C3-C5	3.36	121.06	115.23
23	b	609[B]	CLA	CHC-C1C-NC	3.36	129.37	124.31
32	D	406	DGD	C4E-C3E-C2E	3.36	116.73	110.83
23	B	615	CLA	C4-C3-C5	3.36	121.06	115.23
32	d	405	DGD	O2G-C1B-C2B	3.36	118.75	111.48
27	b	601	SQD	O47-C7-C8	3.36	118.74	111.48
23	b	607	CLA	CHB-C1B-NB	3.35	129.07	124.05
23	B	613	CLA	CHC-C1C-NC	3.35	129.35	124.31
23	a	605	CLA	CHC-C1C-NC	3.34	129.35	124.31
23	C	512	CLA	CHC-C1C-NC	3.34	129.35	124.31
23	C	509	CLA	CHB-C1B-NB	3.34	129.05	124.05
26	D	405	PL9	C30-C29-C31	-3.33	109.45	115.23
25	T	101	BCR	C20-C19-C18	-3.33	117.24	126.36
25	A	609	BCR	C27-C26-C25	-3.33	118.21	122.70
23	B	608	CLA	CHB-C1B-NB	3.33	129.04	124.05
23	D	403	CLA	CHB-C1B-NB	3.32	129.03	124.05
23	C	508	CLA	CHC-C1C-NC	3.32	129.31	124.31
23	b	605	CLA	CHC-C1C-NC	3.32	129.31	124.31
23	B	610	CLA	CHC-C1C-NC	3.32	129.31	124.31
24	D	401	PHO	O2D-CGD-O1D	-3.32	117.39	123.85
23	C	506	CLA	CHC-C1C-NC	3.31	129.30	124.31
25	H	101	BCR	C33-C5-C4	-3.31	106.54	113.60
23	C	511	CLA	CHC-C1C-NC	3.30	129.29	124.31
27	A	611	SQD	C1-C2-C3	-3.30	103.06	110.01
25	h	101	BCR	C30-C25-C26	-3.30	118.13	122.64
23	C	503	CLA	CHC-C1C-NC	3.30	129.28	124.31
23	c	509	CLA	C4D-C3D-CAD	-3.30	104.53	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	CHC-C1C-NC	3.30	129.28	124.31
27	a	610	SQD	C1-C2-C3	-3.29	103.08	110.01
23	B	612	CLA	CHC-C1C-NC	3.29	129.27	124.31
23	c	513	CLA	C2A-C1A-CHA	3.29	129.57	123.87
23	B	610	CLA	CHB-C1B-NB	3.29	128.98	124.05
23	D	402	CLA	CHC-C1C-NC	3.29	129.26	124.31
23	d	403	CLA	CHC-C1C-NC	3.28	129.26	124.31
26	a	609	PL9	C51-C49-C48	-3.28	112.80	122.66
23	B	607[A]	CLA	CHC-C1C-NC	3.28	129.25	124.31
23	b	615	CLA	CHC-C1C-NC	3.28	129.25	124.31
25	h	101	BCR	C11-C12-C13	-3.27	117.41	126.36
25	B	619	BCR	C36-C18-C17	-3.26	117.53	122.82
25	C	515	BCR	C24-C25-C26	-3.26	114.04	121.56
25	H	101	BCR	C8-C9-C10	-3.26	113.88	119.01
23	C	502	CLA	CHC-C1C-NC	3.26	129.22	124.31
23	A	606	CLA	CHC-C1C-NC	3.25	129.21	124.31
23	b	612	CLA	CHB-C1B-NB	3.25	128.92	124.05
32	c	518	DGD	O2G-C1B-C2B	3.25	118.50	111.48
25	F	101	BCR	C16-C15-C14	-3.25	116.88	123.52
23	c	512	CLA	CHC-C1C-NC	3.24	129.20	124.31
23	b	608	CLA	C1-O2A-CGA	3.24	124.50	116.65
25	F	101	BCR	C2-C3-C4	3.24	118.40	111.28
23	b	607	CLA	CHC-C1C-NC	3.24	129.19	124.31
25	B	618	BCR	C36-C18-C19	3.24	123.03	118.09
25	C	515	BCR	C1-C6-C7	-3.23	106.88	115.65
25	C	514	BCR	C12-C13-C14	-3.23	113.92	119.01
23	B	616	CLA	CHB-C1B-NB	3.23	128.90	124.05
23	C	512	CLA	C4-C3-C5	3.23	120.84	115.23
25	h	101	BCR	C33-C5-C4	-3.23	106.71	113.60
23	c	503	CLA	CHC-C1C-NC	3.23	129.17	124.31
25	K	101	BCR	C11-C12-C13	-3.23	117.51	126.36
25	B	619	BCR	C27-C26-C25	-3.22	118.35	122.70
33	e	102	HEM	CBD-CAD-C3D	-3.22	103.62	112.53
23	c	513	CLA	C4-C3-C5	3.22	120.82	115.23
23	c	509	CLA	CHC-C1C-NC	3.22	129.16	124.31
27	b	602	SQD	O7-S-C6	3.21	111.56	106.76
23	B	602	CLA	O2A-CGA-CBA	3.21	121.63	111.83
24	A	607	PHO	CMB-C2B-C3B	3.21	131.10	124.68
23	b	612	CLA	C4D-C3D-CAD	-3.21	104.62	108.11
26	A	610	PL9	C45-C44-C46	-3.20	109.67	115.23
23	c	513	CLA	CHC-C1C-NC	3.20	129.13	124.31
23	a	604	CLA	CHC-C1C-NC	3.20	129.13	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	CHC-C1C-NC	3.20	129.13	124.31
27	a	612	SQD	O6-C1-C2	3.20	113.13	108.27
23	c	507	CLA	C4D-C3D-CAD	-3.19	104.64	108.11
23	b	609[A]	CLA	CHC-C1C-NC	3.19	129.11	124.31
23	c	502	CLA	CHC-C1C-NC	3.19	129.11	124.31
25	b	622	BCR	C11-C12-C13	-3.18	117.63	126.36
23	b	606	CLA	CHC-C1C-NC	3.18	129.10	124.31
23	c	504	CLA	C4A-NA-C1A	-3.18	105.23	106.68
27	B	623	SQD	O7-S-C6	3.18	111.50	106.76
23	C	502	CLA	C4D-C3D-CAD	-3.18	104.65	108.11
23	C	510	CLA	CHC-C1C-NC	3.18	129.10	124.31
27	b	601	SQD	O6-C1-C2	3.18	113.10	108.27
23	B	613	CLA	C4-C3-C5	3.18	120.74	115.23
23	B	608	CLA	C1-C2-C3	-3.17	121.00	126.20
23	C	501	CLA	C4D-C3D-CAD	-3.17	104.66	108.11
23	b	615	CLA	C4-C3-C5	3.17	120.73	115.23
23	b	610	CLA	C1-C2-C3	-3.17	121.00	126.20
25	f	101	BCR	C37-C22-C23	-3.17	113.25	118.09
25	H	101	BCR	C11-C12-C13	-3.17	117.68	126.36
25	t	101	BCR	C11-C12-C13	-3.17	117.68	126.36
24	d	401	PHO	O1D-CGD-CBD	3.16	129.52	124.72
23	C	507	CLA	CHC-C1C-NC	3.16	129.07	124.31
25	C	514	BCR	C38-C26-C27	-3.16	106.87	113.60
25	H	101	BCR	C20-C19-C18	-3.16	117.71	126.36
25	h	101	BCR	C16-C15-C14	-3.15	117.06	123.52
23	A	606	CLA	C4A-NA-C1A	-3.15	105.24	106.68
23	B	616	CLA	C4A-NA-C1A	-3.15	105.24	106.68
23	D	402	CLA	O1D-CGD-CBD	-3.15	118.31	124.52
25	B	618	BCR	C34-C9-C10	-3.15	117.72	122.82
22	a	603	BCT	O2-C-O1	-3.14	111.64	119.68
23	A	605	CLA	CHC-C1C-NC	3.14	129.04	124.31
23	D	404	CLA	CHA-C1A-NA	-3.14	119.28	126.39
23	B	617	CLA	C4D-C3D-CAD	-3.14	104.69	108.11
25	h	101	BCR	C40-C30-C25	-3.14	105.32	110.24
23	B	612	CLA	C1-C2-C3	-3.14	121.06	126.20
24	a	606	PHO	O1D-CGD-CBD	3.14	129.48	124.72
23	C	511	CLA	CHB-C1B-NB	3.14	128.75	124.05
23	b	614	CLA	C1-C2-C3	-3.13	121.06	126.20
23	B	605	CLA	CHB-C1B-NB	3.13	128.75	124.05
23	b	612	CLA	CHC-C1C-NC	3.13	129.03	124.31
23	c	511	CLA	CHC-C1C-NC	3.13	129.02	124.31
23	b	616	CLA	CHC-C1C-NC	3.13	129.02	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	CHB-C1B-NB	3.12	128.74	124.05
23	A	608	CLA	CHA-C1A-NA	-3.12	119.32	126.39
25	B	619	BCR	C34-C9-C10	-3.11	117.77	122.82
23	D	403	CLA	C2A-C1A-CHA	3.11	129.27	123.87
23	B	603	CLA	C4-C3-C5	3.11	120.62	115.23
23	D	403	CLA	C4A-NA-C1A	-3.10	105.27	106.68
23	B	611	CLA	CHC-C1C-NC	3.10	128.97	124.31
24	A	607	PHO	O1D-CGD-CBD	3.10	129.42	124.72
23	b	606	CLA	CHB-C1B-NB	3.10	128.69	124.05
23	b	617	CLA	CHC-C1C-NC	3.10	128.97	124.31
33	E	102	HEM	CBD-CAD-C3D	-3.09	103.98	112.53
23	a	605	CLA	O1D-CGD-CBD	-3.09	118.42	124.52
23	c	507	CLA	CHC-C1C-NC	3.09	128.97	124.31
24	a	606	PHO	C2B-C1B-NB	-3.09	107.20	109.43
25	b	621	BCR	C7-C6-C5	-3.08	114.47	121.56
23	b	605	CLA	C4D-C3D-CAD	-3.08	104.76	108.11
23	C	501	CLA	CHC-C1C-NC	3.07	128.94	124.31
26	A	610	PL9	C31-C29-C28	-3.07	114.28	121.17
23	b	619	CLA	C4D-C3D-CAD	-3.07	104.77	108.11
23	b	610	CLA	CHB-C1B-NB	3.07	128.65	124.05
25	b	620	BCR	C23-C22-C21	-3.07	114.18	119.01
23	b	604	CLA	O2A-CGA-CBA	3.07	121.19	111.83
25	b	621	BCR	C10-C11-C12	-3.07	114.31	123.20
33	v	201	HEM	C3B-C2B-C1B	3.07	108.71	106.41
23	C	508	CLA	C4D-C3D-CAD	-3.06	104.78	108.11
25	B	618	BCR	C33-C5-C4	-3.06	107.06	113.60
23	d	403	CLA	CHA-C1A-NA	-3.06	119.45	126.39
23	b	605	CLA	C4-C3-C5	3.06	120.54	115.23
23	B	611	CLA	C4D-C3D-CAD	-3.06	104.78	108.11
23	a	605	CLA	C4-C3-C5	3.06	120.54	115.23
23	b	611	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
25	c	516	BCR	C20-C21-C22	-3.06	122.98	127.28
23	d	403	CLA	C4D-C3D-CAD	-3.06	104.78	108.11
23	C	506	CLA	C4-C3-C5	3.06	120.54	115.23
27	X	101	SQD	O48-C23-C24	3.06	121.16	111.83
23	b	604	CLA	CHC-C1C-NC	3.06	128.91	124.31
23	A	606	CLA	C4-C3-C5	3.05	120.53	115.23
27	a	612	SQD	O48-C23-C24	3.05	121.14	111.83
32	C	518	DGD	O3G-C3G-C2G	-3.05	103.40	110.82
26	d	404	PL9	C15-C14-C16	-3.05	109.94	115.23
23	B	605	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
25	B	620	BCR	C16-C15-C14	-3.05	117.29	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	x	101	SQD	O48-C23-C24	3.04	121.12	111.83
23	c	504	CLA	CHC-C1C-NC	3.04	128.89	124.31
23	A	606	CLA	CHA-C1A-NA	-3.04	119.51	126.39
23	B	609	CLA	CHC-C1C-NC	3.04	128.88	124.31
27	b	601	SQD	O48-C23-C24	3.03	121.09	111.83
25	c	522	BCR	C23-C24-C25	-3.03	118.89	127.00
25	B	620	BCR	C10-C11-C12	-3.03	114.41	123.20
23	c	508	CLA	C4-C3-C5	3.03	120.49	115.23
23	B	603	CLA	C4D-C3D-CAD	-3.03	104.81	108.11
23	c	507	CLA	C4-C3-C5	3.03	120.49	115.23
25	c	516	BCR	C23-C24-C25	-3.02	118.92	127.00
25	B	618	BCR	C2-C3-C4	3.02	117.92	111.28
23	d	402	CLA	CHC-C1C-NC	3.02	128.86	124.31
25	k	101	BCR	C8-C9-C10	-3.02	114.26	119.01
23	B	607[A]	CLA	C3B-C4B-NB	-3.02	107.84	110.53
23	B	602	CLA	CHC-C1C-NC	3.02	128.85	124.31
23	D	402	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
28	z	101	LMG	O1-C1-C2	3.01	112.84	108.27
26	D	405	PL9	C7-C3-C2	-3.00	119.85	123.39
25	C	514	BCR	C37-C22-C21	-3.00	117.95	122.82
23	C	507	CLA	C4-C3-C5	3.00	120.43	115.23
23	C	513	CLA	O2A-CGA-CBA	3.00	120.97	111.83
25	b	621	BCR	C8-C7-C6	-2.99	119.01	127.00
23	B	605	CLA	C4D-C3D-CAD	-2.99	104.86	108.11
23	b	613	CLA	CHC-C1C-NC	2.98	128.80	124.31
26	D	405	PL9	C15-C14-C16	-2.98	110.06	115.23
23	C	504	CLA	C4D-C3D-CAD	-2.98	104.87	108.11
23	c	506	CLA	CHB-C1B-NB	2.98	128.51	124.05
25	f	101	BCR	C2-C3-C4	2.98	117.82	111.28
23	B	604	CLA	C4-C3-C5	2.98	120.39	115.23
25	C	515	BCR	C23-C24-C25	-2.98	119.05	127.00
25	c	515	BCR	C20-C19-C18	-2.98	118.20	126.36
25	b	621	BCR	C23-C22-C21	-2.98	114.33	119.01
25	C	514	BCR	C11-C12-C13	-2.97	118.21	126.36
23	b	613	CLA	C4D-C3D-CAD	-2.97	104.88	108.11
23	c	514	CLA	CHC-C1C-NC	2.97	128.78	124.31
23	D	402	CLA	C4A-NA-C1A	-2.97	105.33	106.68
23	a	605	CLA	C4A-NA-C1A	-2.97	105.33	106.68
23	C	504	CLA	C4-C3-C5	2.97	120.38	115.23
23	b	607	CLA	C4D-C3D-CAD	-2.96	104.89	108.11
23	A	606	CLA	C4D-CHA-C1A	-2.96	117.71	121.24
25	H	101	BCR	C40-C30-C25	-2.96	105.60	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C3B-C4B-NB	-2.96	107.89	110.53
23	b	606	CLA	C4-C3-C5	2.96	120.36	115.23
23	B	608	CLA	O2D-CGD-CBD	2.95	116.39	111.23
26	d	404	PL9	C10-C9-C11	-2.95	110.10	115.23
24	d	401	PHO	C1-C2-C3	-2.95	121.36	126.20
23	B	614	CLA	C4D-C3D-CAD	-2.95	104.90	108.11
23	C	506	CLA	C4D-C3D-CAD	-2.95	104.90	108.11
25	b	620	BCR	C34-C9-C10	-2.95	118.04	122.82
24	A	607	PHO	O2D-CGD-O1D	-2.94	118.12	123.85
25	C	514	BCR	C34-C9-C10	-2.94	118.05	122.82
23	c	505	CLA	C4-C3-C5	2.94	120.34	115.23
23	b	618	CLA	C3B-C4B-NB	-2.94	107.90	110.53
23	C	512	CLA	C4D-C3D-CAD	-2.94	104.91	108.11
23	B	612	CLA	C4D-C3D-CAD	-2.94	104.91	108.11
23	c	502	CLA	C4D-C3D-CAD	-2.94	104.92	108.11
23	b	617	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
27	a	610	SQD	C45-O47-C7	-2.93	110.77	117.80
23	B	604	CLA	C4D-C3D-CAD	-2.93	104.92	108.11
27	A	611	SQD	C45-O47-C7	-2.93	110.78	117.80
23	A	608	CLA	C4A-NA-C1A	-2.93	105.34	106.68
25	B	620	BCR	C35-C13-C14	-2.93	118.07	122.82
23	C	513	CLA	CHC-C1C-NC	2.93	128.72	124.31
23	D	403	CLA	C4D-C3D-CAD	-2.93	104.93	108.11
23	B	614	CLA	CHC-C1C-NC	2.93	128.72	124.31
23	D	404	CLA	CHC-C1C-NC	2.93	128.72	124.31
23	b	609[A]	CLA	C3B-C4B-NB	-2.92	107.92	110.53
24	a	606	PHO	CMB-C2B-C3B	2.92	130.52	124.68
23	a	607	CLA	C4A-NA-C1A	-2.92	105.35	106.68
23	B	606	CLA	CHC-C1C-NC	2.92	128.71	124.31
25	b	621	BCR	C16-C15-C14	-2.92	117.55	123.52
32	D	406	DGD	C1E-C2E-C3E	2.92	116.14	110.01
23	B	608	CLA	C4D-C3D-CAD	-2.92	104.94	108.11
23	C	507	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
23	b	614	CLA	C4D-C3D-CAD	-2.90	104.95	108.11
25	a	608	BCR	C36-C18-C17	-2.90	118.11	122.82
25	c	522	BCR	C29-C28-C27	2.90	117.66	111.28
23	B	607[B]	CLA	C3B-C4B-NB	-2.90	107.94	110.53
23	c	505	CLA	C4D-C3D-CAD	-2.89	104.96	108.11
24	d	401	PHO	CMA-C3A-C4A	-2.89	108.38	114.61
23	B	607[B]	CLA	C1-C2-C3	-2.89	121.46	126.20
23	c	508	CLA	C4D-C3D-CAD	-2.89	104.97	108.11
23	b	609[B]	CLA	C1-C2-C3	-2.89	121.47	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	609	BCR	C16-C15-C14	-2.88	117.62	123.52
25	A	609	BCR	C11-C12-C13	-2.88	118.46	126.36
23	b	617	CLA	C1-O2A-CGA	2.88	123.62	116.65
25	F	101	BCR	C10-C11-C12	-2.88	114.85	123.20
23	b	611	CLA	O1D-CGD-CBD	-2.88	118.84	124.52
23	B	606	CLA	C3B-C4B-NB	-2.88	107.96	110.53
23	b	609[B]	CLA	C4-C3-C5	2.88	120.22	115.23
23	B	607[B]	CLA	C4-C3-C5	2.87	120.22	115.23
25	c	516	BCR	C24-C25-C26	-2.87	114.93	121.56
23	c	509	CLA	C1D-ND-C4D	-2.87	104.30	106.31
25	a	608	BCR	C38-C26-C27	-2.87	107.47	113.60
23	a	604	CLA	C4D-C3D-CAD	-2.87	104.99	108.11
25	F	101	BCR	C34-C9-C10	-2.87	118.16	122.82
23	c	503	CLA	C4D-C3D-CAD	-2.87	104.99	108.11
25	C	515	BCR	C20-C19-C18	-2.87	118.50	126.36
27	b	601	SQD	O9-S-C6	2.86	111.03	106.76
23	B	607[A]	CLA	C4-C3-C5	2.86	120.19	115.23
23	b	607	CLA	O2A-CGA-CBA	2.86	120.55	111.83
23	b	608	CLA	CHC-C1C-NC	2.86	128.61	124.31
23	c	506	CLA	C4D-C3D-CAD	-2.86	105.00	108.11
23	B	610	CLA	C4A-NA-C1A	-2.86	105.38	106.68
23	B	612	CLA	C1-O2A-CGA	2.86	123.56	116.65
23	A	605	CLA	C4D-C3D-CAD	-2.85	105.01	108.11
23	b	618	CLA	C4D-C3D-CAD	-2.85	105.01	108.11
32	C	517	DGD	O1G-C1A-C2A	2.85	120.53	111.83
25	c	515	BCR	C12-C13-C14	-2.85	114.53	119.01
23	b	618	CLA	C1D-ND-C4D	-2.85	104.31	106.31
23	b	606	CLA	O1D-CGD-CBD	-2.85	118.90	124.52
23	a	613	CLA	CHA-C1A-NA	-2.85	119.95	126.39
25	h	101	BCR	C10-C11-C12	-2.85	114.95	123.20
23	C	506	CLA	C4A-NA-C1A	-2.85	105.38	106.68
31	a	614	LHG	O8-C23-C24	2.84	120.50	111.83
23	C	505	CLA	CHB-C1B-NB	2.84	128.31	124.05
32	c	518	DGD	O1G-C1A-C2A	2.84	120.50	111.83
25	T	101	BCR	C34-C9-C10	-2.84	118.22	122.82
23	C	505	CLA	C4D-C3D-CAD	-2.84	105.03	108.11
23	B	616	CLA	O2A-CGA-CBA	2.83	120.48	111.83
28	C	519	LMG	O8-C28-C29	2.83	120.48	111.83
23	a	607	CLA	CHC-C1C-NC	2.83	128.58	124.31
23	c	508	CLA	O2A-CGA-CBA	2.83	120.47	111.83
27	B	623	SQD	O48-C23-C24	2.83	120.47	111.83
31	b	624	LHG	C5-O7-C7	-2.83	111.03	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
23	c	508	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
23	b	616	CLA	C4D-C3D-CAD	-2.83	105.03	108.11
23	B	615	CLA	O1D-CGD-CBD	-2.83	118.94	124.52
23	D	403	CLA	CHC-C1C-NC	2.83	128.57	124.31
23	c	509	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
27	a	612	SQD	O9-S-C6	2.83	110.97	106.76
23	b	609[A]	CLA	C4-C3-C5	2.82	120.13	115.23
23	A	608	CLA	C4D-C3D-CAD	-2.82	105.04	108.11
27	b	602	SQD	O48-C23-C24	2.82	120.44	111.83
32	c	519	DGD	O3G-C3G-C2G	-2.82	103.96	110.82
25	c	522	BCR	C33-C5-C4	-2.82	107.58	113.60
23	B	604	CLA	CHC-C1C-NC	2.82	128.56	124.31
28	J	101	LMG	O6-C5-C4	2.82	114.78	109.70
23	C	502	CLA	C3B-C4B-NB	-2.82	108.01	110.53
25	A	609	BCR	C24-C25-C26	-2.82	115.06	121.56
23	B	603	CLA	C3B-C4B-NB	-2.82	108.02	110.53
23	a	613	CLA	O2A-CGA-CBA	2.82	120.42	111.83
23	D	402	CLA	CHA-C1A-NA	-2.81	120.02	126.39
25	b	621	BCR	C27-C26-C25	-2.81	118.90	122.70
23	C	513	CLA	CHA-C1A-NA	-2.81	120.02	126.39
23	a	605	CLA	CHA-C1A-NA	-2.81	120.02	126.39
23	B	612	CLA	CHA-C1A-NA	-2.81	120.02	126.39
23	b	607	CLA	O1D-CGD-CBD	-2.81	118.97	124.52
25	C	521	BCR	C33-C5-C4	-2.81	107.60	113.60
23	b	609[A]	CLA	O1D-CGD-CBD	-2.81	118.97	124.52
23	b	605	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	D	402	CLA	C4-C3-C5	2.81	120.10	115.23
23	b	609[A]	CLA	C4D-C3D-CAD	-2.80	105.06	108.11
23	A	606	CLA	O2A-CGA-CBA	2.80	120.38	111.83
28	c	520	LMG	O8-C28-C29	2.80	120.38	111.83
23	c	513	CLA	O2A-CGA-CBA	2.80	120.38	111.83
23	a	613	CLA	C4-C3-C5	2.80	120.09	115.23
23	c	513	CLA	C1-C2-C3	-2.80	121.61	126.20
23	C	507	CLA	C4D-C3D-CAD	-2.80	105.06	108.11
23	C	513	CLA	C4A-NA-C1A	-2.80	105.40	106.68
23	b	609[B]	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	b	605	CLA	O1D-CGD-CBD	-2.79	119.01	124.52
25	c	516	BCR	C33-C5-C4	-2.79	107.64	113.60
23	C	512	CLA	C1-C2-C3	-2.79	121.62	126.20
25	A	609	BCR	C33-C5-C4	-2.79	107.65	113.60
23	B	608	CLA	C4-C3-C5	2.79	120.07	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	f	101	BCR	C16-C15-C14	-2.79	117.82	123.52
23	b	611	CLA	CHC-C1C-NC	2.79	128.51	124.31
31	B	622	LHG	O8-C23-C24	2.78	120.32	111.83
23	c	512	CLA	O1D-CGD-CBD	-2.78	119.03	124.52
25	b	622	BCR	C36-C18-C19	2.78	122.34	118.09
23	c	512	CLA	C4D-C3D-CAD	-2.78	105.09	108.11
23	C	501	CLA	CHA-C1A-NA	-2.78	120.10	126.39
23	b	613	CLA	O2A-CGA-CBA	2.78	120.30	111.83
23	B	611	CLA	O2A-CGA-CBA	2.77	120.29	111.83
23	c	502	CLA	O2A-CGA-CBA	2.77	120.28	111.83
25	F	101	BCR	C23-C22-C21	2.76	123.36	119.01
31	D	407	LHG	O8-C23-C24	2.76	120.27	111.83
23	C	511	CLA	C1-O2A-CGA	2.76	123.34	116.65
31	b	624	LHG	O8-C23-C24	2.76	120.26	111.83
23	b	618	CLA	C4A-NA-C1A	-2.76	105.42	106.68
23	b	604	CLA	C4D-C3D-CAD	-2.76	105.11	108.11
23	a	607	CLA	O2A-CGA-CBA	2.76	120.25	111.83
23	b	610	CLA	C4-C3-C5	2.76	120.02	115.23
23	d	402	CLA	O2A-CGA-CBA	2.76	120.25	111.83
23	c	505	CLA	C1D-ND-C4D	-2.75	104.38	106.31
24	D	401	PHO	C1-C2-C3	-2.75	121.69	126.20
31	B	622	LHG	C5-O7-C7	-2.75	111.22	117.80
24	d	401	PHO	O2D-CGD-O1D	-2.74	118.51	123.85
23	D	402	CLA	C4D-C3D-CAD	-2.74	105.13	108.11
23	b	610	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
23	C	507	CLA	O2A-CGA-CBA	2.74	120.19	111.83
25	C	521	BCR	C40-C30-C25	2.74	114.54	110.24
23	C	510	CLA	C4D-C3D-CAD	-2.74	105.13	108.11
23	a	613	CLA	C4D-C3D-CAD	-2.74	105.14	108.11
25	B	620	BCR	C20-C19-C18	-2.73	118.86	126.36
23	C	512	CLA	O2A-CGA-CBA	2.73	120.17	111.83
31	D	408	LHG	O8-C23-C24	2.73	120.17	111.83
25	f	101	BCR	C34-C9-C10	-2.73	118.39	122.82
23	b	615	CLA	O2A-CGA-CBA	2.73	120.16	111.83
23	C	513	CLA	C4D-CHA-C1A	-2.73	117.99	121.24
23	B	607[B]	CLA	C4D-C3D-CAD	-2.73	105.14	108.11
23	C	501	CLA	O2A-CGA-CBA	2.72	120.14	111.83
23	B	615	CLA	CHC-C1C-NC	2.72	128.41	124.31
23	B	617	CLA	O2A-CGA-CBA	2.72	120.14	111.83
32	c	519	DGD	C2G-O2G-C1B	-2.72	111.28	117.80
23	D	403	CLA	O2A-CGA-CBA	2.72	120.13	111.83
23	c	514	CLA	C3B-C4B-NB	-2.72	108.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	101	BCR	C35-C13-C14	-2.71	118.42	122.82
32	H	102	DGD	O1G-C1A-C2A	2.71	120.11	111.83
25	B	619	BCR	C16-C15-C14	-2.71	117.97	123.52
23	B	616	CLA	C4D-C3D-CAD	-2.71	105.16	108.11
23	B	603	CLA	C4A-NA-C1A	-2.71	105.44	106.68
23	b	607	CLA	C4-C3-C5	2.71	119.93	115.23
24	D	401	PHO	CMA-C3A-C4A	-2.71	108.77	114.61
23	B	614	CLA	C4A-NA-C1A	-2.71	105.44	106.68
23	C	505	CLA	CHC-C1C-NC	2.71	128.39	124.31
23	c	508	CLA	C3B-C4B-NB	-2.71	108.11	110.53
23	b	609[B]	CLA	O1D-CGD-CBD	-2.71	119.18	124.52
23	b	606	CLA	C4D-C3D-CAD	-2.71	105.17	108.11
23	b	609[A]	CLA	C1-O2A-CGA	2.70	123.20	116.65
23	d	402	CLA	C4D-C3D-CAD	-2.70	105.17	108.11
23	B	612	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
23	c	514	CLA	C4D-C3D-CAD	-2.70	105.17	108.11
25	t	101	BCR	C34-C9-C10	-2.70	118.44	122.82
23	c	508	CLA	O1D-CGD-CBD	-2.70	119.20	124.52
25	K	101	BCR	C37-C22-C23	-2.70	113.97	118.09
23	a	607	CLA	C4D-C3D-CAD	-2.70	105.18	108.11
23	b	612	CLA	C1-C2-C3	-2.69	121.78	126.20
23	c	509	CLA	C4-C3-C5	2.69	119.90	115.23
23	C	513	CLA	C4D-C3D-CAD	-2.69	105.18	108.11
23	b	619	CLA	CHA-C1A-NA	-2.69	120.29	126.39
23	B	605	CLA	O2A-CGA-CBA	2.69	120.05	111.83
23	C	509	CLA	O2A-CGA-CBA	2.69	120.04	111.83
32	D	406	DGD	C3E-C4E-C5E	2.69	115.11	110.23
25	B	620	BCR	C1-C6-C5	-2.69	118.96	122.64
23	C	511	CLA	C4D-C3D-CAD	-2.69	105.18	108.11
25	C	521	BCR	C10-C11-C12	-2.69	115.41	123.20
23	B	607[A]	CLA	C1-O2A-CGA	2.69	123.16	116.65
23	C	508	CLA	C4-C3-C5	2.69	119.90	115.23
23	C	509	CLA	C4D-C3D-CAD	-2.69	105.19	108.11
25	f	101	BCR	C11-C12-C13	-2.69	118.99	126.36
25	a	608	BCR	C33-C5-C4	-2.69	107.87	113.60
25	C	514	BCR	C34-C9-C8	2.69	122.19	118.09
23	c	506	CLA	CHC-C1C-NC	2.68	128.35	124.31
23	B	605	CLA	C4-C3-C5	2.68	119.89	115.23
23	B	607[A]	CLA	C4D-C3D-CAD	-2.68	105.19	108.11
23	b	611	CLA	C4D-C3D-CAD	-2.68	105.19	108.11
23	b	609[A]	CLA	C1-C2-C3	-2.68	121.81	126.20
26	d	404	PL9	C30-C29-C31	-2.68	110.58	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	f	101	BCR	C1-C6-C7	-2.68	108.38	115.65
23	c	509	CLA	CHB-C1B-C2B	-2.68	119.65	127.43
23	D	404	CLA	C4D-C3D-CAD	-2.68	105.20	108.11
23	B	609	CLA	O1D-CGD-CBD	-2.68	119.24	124.52
25	b	620	BCR	C33-C5-C4	-2.67	107.89	113.60
24	A	607	PHO	C2B-C1B-NB	-2.67	107.50	109.43
23	c	506	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
23	b	616	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
23	C	511	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
32	h	102	DGD	O1G-C1A-C2A	2.66	119.95	111.83
23	B	610	CLA	C1-C2-C3	-2.66	121.83	126.20
23	A	608	CLA	CHC-C1C-NC	2.66	128.32	124.31
23	A	608	CLA	O1D-CGD-CBD	-2.66	119.27	124.52
23	B	607[A]	CLA	C1-C2-C3	-2.66	121.84	126.20
23	B	613	CLA	O2A-CGA-CBA	2.66	119.94	111.83
23	B	613	CLA	C4D-C3D-CAD	-2.66	105.22	108.11
27	B	623	SQD	C4-C3-C2	2.66	115.49	110.83
23	c	510	CLA	C4D-C3D-CAD	-2.66	105.22	108.11
23	c	503	CLA	CHA-C1A-NA	-2.65	120.38	126.39
26	d	404	PL9	C7-C3-C2	-2.65	120.26	123.39
23	D	402	CLA	O2A-CGA-CBA	2.65	119.92	111.83
27	x	101	SQD	O7-S-C6	2.65	110.71	106.76
23	B	607[A]	CLA	O1D-CGD-CBD	-2.65	119.29	124.52
25	H	101	BCR	C36-C18-C17	-2.65	118.53	122.82
27	b	602	SQD	C4-C3-C2	2.65	115.47	110.83
23	B	603	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
27	X	101	SQD	O7-S-C6	2.65	110.71	106.76
25	T	101	BCR	C38-C26-C27	-2.64	107.96	113.60
23	c	513	CLA	C4D-C3D-CAD	-2.64	105.23	108.11
25	F	101	BCR	C36-C18-C19	2.64	122.13	118.09
25	c	515	BCR	C10-C11-C12	-2.64	115.54	123.20
27	A	611	SQD	O8-S-C6	2.64	111.07	105.97
24	a	606	PHO	O2D-CGD-O1D	-2.64	118.71	123.85
25	H	101	BCR	C1-C6-C7	-2.64	108.49	115.65
33	V	202	HEM	C3B-C2B-C1B	2.64	108.39	106.41
23	C	509	CLA	O1D-CGD-CBD	-2.64	119.31	124.52
23	c	504	CLA	C4-C3-C5	2.64	119.81	115.23
27	a	610	SQD	O8-S-C6	2.64	111.07	105.97
23	A	608	CLA	C3B-C4B-NB	-2.64	108.17	110.53
26	a	609	PL9	C53-C6-C1	2.64	120.68	115.28
33	v	201	HEM	CBA-CAA-C2A	-2.64	105.24	112.53
23	b	617	CLA	C4D-C3D-CAD	-2.64	105.24	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	622	BCR	C10-C11-C12	-2.64	115.56	123.20
23	C	507	CLA	C3B-C4B-NB	-2.63	108.18	110.53
23	b	619	CLA	O2A-CGA-CBA	2.63	119.85	111.83
23	C	503	CLA	C4-C3-C5	2.63	119.79	115.23
23	a	613	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
25	T	101	BCR	C16-C17-C18	-2.63	123.59	127.28
23	b	615	CLA	C4D-C3D-CAD	-2.63	105.25	108.11
23	b	611	CLA	C1D-ND-C4D	-2.62	104.47	106.31
23	c	503	CLA	C1D-ND-C4D	-2.62	104.47	106.31
26	d	404	PL9	C7-C3-C4	2.62	119.07	116.91
25	t	101	BCR	C38-C26-C27	-2.62	108.00	113.60
23	c	503	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
26	A	610	PL9	C53-C6-C1	2.62	120.65	115.28
23	b	610	CLA	CHC-C1C-C2C	-2.62	119.52	126.95
23	c	504	CLA	C1D-ND-C4D	-2.62	104.48	106.31
26	A	610	PL9	C7-C3-C2	-2.62	120.31	123.39
23	c	512	CLA	O2A-CGA-CBA	2.61	119.81	111.83
23	B	615	CLA	C4D-C3D-CAD	-2.61	105.27	108.11
23	C	504	CLA	C1D-ND-C4D	-2.61	104.48	106.31
23	D	403	CLA	C4-C3-C5	2.61	119.77	115.23
25	k	101	BCR	C33-C5-C4	-2.61	108.02	113.60
25	c	515	BCR	C11-C12-C13	-2.61	119.20	126.36
23	a	605	CLA	C4D-C3D-CAD	-2.61	105.27	108.11
25	K	101	BCR	C33-C5-C4	-2.61	108.03	113.60
23	B	607[B]	CLA	C1-O2A-CGA	2.61	122.97	116.65
23	c	506	CLA	O1D-CGD-CBD	-2.61	119.38	124.52
23	d	402	CLA	C4-C3-C5	2.61	119.75	115.23
23	d	402	CLA	C4A-NA-C1A	-2.60	105.49	106.68
23	b	609[B]	CLA	C4D-C3D-CAD	-2.60	105.28	108.11
23	a	604	CLA	O2A-CGA-CBA	2.60	119.76	111.83
23	a	613	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
23	C	511	CLA	C3B-C4B-NB	-2.60	108.21	110.53
23	B	603	CLA	C1-C2-C3	-2.60	121.94	126.20
23	c	514	CLA	O2A-CGA-CBA	2.60	119.76	111.83
23	B	617	CLA	C4A-NA-C1A	-2.60	105.49	106.68
25	c	516	BCR	C35-C13-C14	-2.60	118.61	122.82
33	V	202	HEM	C1B-NB-C4B	2.60	108.28	105.21
32	d	405	DGD	O1G-C1A-C2A	2.60	119.75	111.83
23	b	610	CLA	C4D-C3D-CAD	-2.59	105.29	108.11
23	B	609	CLA	O2A-CGA-CBA	2.59	119.74	111.83
23	B	616	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	B	618	BCR	C30-C25-C24	-2.59	108.62	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	C3B-C4B-NB	-2.59	108.22	110.53
23	b	617	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
23	b	618	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
26	A	610	PL9	C25-C24-C26	-2.59	110.73	115.23
23	b	607	CLA	CHA-C1A-NA	-2.59	120.53	126.39
25	a	608	BCR	C16-C15-C14	-2.59	118.23	123.52
23	C	504	CLA	C1-O2A-CGA	2.59	122.91	116.65
23	b	609[B]	CLA	C1-O2A-CGA	2.59	122.91	116.65
23	b	605	CLA	C1-C2-C3	-2.58	121.96	126.20
28	c	521	LMG	O8-C28-C29	2.58	119.71	111.83
25	H	101	BCR	C36-C18-C19	2.58	122.03	118.09
23	B	604	CLA	C4A-NA-C1A	-2.58	105.50	106.68
27	X	101	SQD	O9-S-C6	2.58	110.61	106.76
23	b	614	CLA	O1D-CGD-CBD	-2.58	119.43	124.52
25	T	101	BCR	C11-C12-C13	-2.58	119.29	126.36
23	b	618	CLA	O2A-CGA-CBA	2.58	119.69	111.83
23	B	602	CLA	C1D-ND-C4D	-2.58	104.50	106.31
23	C	505	CLA	O1D-CGD-CBD	-2.58	119.44	124.52
27	A	611	SQD	C44-O6-C1	-2.58	108.28	113.80
23	A	606	CLA	C4D-C3D-CAD	-2.57	105.31	108.11
23	C	501	CLA	CHB-C1B-C2B	-2.57	119.95	127.43
23	B	615	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
23	b	617	CLA	C1D-ND-C4D	-2.57	104.51	106.31
27	x	101	SQD	O9-S-C6	2.57	110.60	106.76
23	b	609[A]	CLA	CHB-C1B-C2B	-2.57	119.96	127.43
25	f	101	BCR	C35-C13-C14	-2.57	118.65	122.82
23	B	615	CLA	C1D-ND-C4D	-2.57	104.51	106.31
25	F	101	BCR	C1-C6-C7	-2.57	108.69	115.65
25	B	618	BCR	C37-C22-C23	-2.57	114.17	118.09
23	C	503	CLA	C4D-C3D-CAD	-2.57	105.32	108.11
23	B	607[A]	CLA	CHB-C1B-C2B	-2.57	119.98	127.43
32	D	406	DGD	O2G-C1B-O1B	-2.56	117.71	123.70
23	b	608	CLA	C1D-ND-C4D	-2.56	104.52	106.31
23	d	403	CLA	C1D-ND-C4D	-2.56	104.52	106.31
25	B	619	BCR	C20-C21-C22	-2.56	123.69	127.28
23	a	613	CLA	C4A-NA-C1A	-2.56	105.51	106.68
32	d	405	DGD	O2G-C1B-O1B	-2.56	117.72	123.70
32	D	406	DGD	O1G-C1A-C2A	2.56	119.64	111.83
27	A	611	SQD	C1-O5-C5	-2.56	108.72	113.72
23	c	502	CLA	C3B-C4B-NB	-2.56	108.25	110.53
25	b	621	BCR	C29-C30-C25	2.56	114.16	110.44
25	A	609	BCR	C38-C26-C27	-2.56	108.14	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	610	SQD	C44-O6-C1	-2.56	108.32	113.80
25	A	609	BCR	C20-C21-C22	-2.55	123.70	127.28
25	f	101	BCR	C33-C5-C4	-2.55	108.15	113.60
23	c	503	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
23	B	614	CLA	C1D-ND-C4D	-2.55	104.52	106.31
23	c	504	CLA	C4D-C3D-CAD	-2.55	105.34	108.11
23	c	503	CLA	C4-C3-C5	2.55	119.65	115.23
23	B	602	CLA	C4D-C3D-CAD	-2.55	105.34	108.11
23	C	511	CLA	C4-C3-C5	2.55	119.65	115.23
23	b	609[B]	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
23	c	511	CLA	C4D-C3D-CAD	-2.55	105.34	108.11
23	b	607	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
23	b	618	CLA	C4-C3-C5	2.55	119.65	115.23
23	c	512	CLA	C4-C3-C5	2.54	119.64	115.23
23	B	609	CLA	C4D-C3D-CAD	-2.54	105.34	108.11
32	C	518	DGD	C2G-O2G-C1B	-2.54	111.71	117.80
23	B	607[B]	CLA	CHB-C1B-C2B	-2.54	120.07	127.43
33	v	201	HEM	C1B-NB-C4B	2.53	108.21	105.21
23	B	604	CLA	CHA-C1A-NA	-2.53	120.66	126.39
23	B	616	CLA	C4-C3-C5	2.53	119.62	115.23
23	b	604	CLA	C1D-ND-C4D	-2.53	104.54	106.31
27	a	610	SQD	C1-O5-C5	-2.53	108.78	113.72
23	c	513	CLA	CHA-C1A-NA	-2.53	120.67	126.39
23	C	502	CLA	C4-C3-C5	2.53	119.61	115.23
23	B	609	CLA	CAC-C3C-C4C	2.52	128.07	124.79
23	C	510	CLA	O2D-CGD-O1D	-2.52	118.93	123.85
23	c	507	CLA	CHB-C1B-C2B	-2.52	120.10	127.43
23	b	616	CLA	C4-C3-C5	2.52	119.61	115.23
23	B	609	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
23	D	402	CLA	CHB-C1B-C2B	-2.52	120.11	127.43
23	B	606	CLA	C4D-C3D-CAD	-2.52	105.37	108.11
23	A	606	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
23	B	614	CLA	C4-C3-C5	2.52	119.60	115.23
25	a	608	BCR	C24-C25-C26	-2.52	115.76	121.56
31	d	406	LHG	O8-C23-C24	2.52	119.51	111.83
25	b	622	BCR	C33-C5-C4	-2.52	108.23	113.60
28	b	623	LMG	O8-C28-C29	2.51	119.50	111.83
23	B	603	CLA	CHB-C1B-C2B	-2.51	120.13	127.43
23	b	606	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
23	b	619	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
25	b	622	BCR	C1-C6-C5	-2.51	119.21	122.64
23	B	605	CLA	CHC-C1C-C2C	-2.50	119.83	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
23	d	403	CLA	O2A-CGA-CBA	2.50	119.47	111.83
31	e	101	LHG	O8-C23-C24	2.50	119.47	111.83
25	B	619	BCR	C7-C6-C5	-2.50	115.80	121.56
25	c	522	BCR	C10-C11-C12	-2.50	115.96	123.20
23	b	609[B]	CLA	CHB-C1B-C2B	-2.50	120.17	127.43
23	C	506	CLA	CHB-C1B-C2B	-2.50	120.18	127.43
23	C	503	CLA	C1D-ND-C4D	-2.50	104.56	106.31
25	T	101	BCR	C8-C9-C10	-2.50	115.08	119.01
23	b	605	CLA	O2A-CGA-CBA	2.50	119.44	111.83
25	H	101	BCR	C10-C11-C12	-2.49	115.97	123.20
23	C	507	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
23	B	612	CLA	CHB-C1B-C2B	-2.49	120.19	127.43
23	B	604	CLA	CHB-C4A-NA	-2.49	120.80	124.40
25	k	101	BCR	C37-C22-C21	-2.49	118.78	122.82
23	B	611	CLA	C4-C3-C5	2.49	119.55	115.23
23	b	614	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
25	b	620	BCR	C10-C11-C12	-2.49	115.98	123.20
23	b	619	CLA	C3B-C4B-NB	-2.49	108.31	110.53
23	D	403	CLA	CHA-C1A-NA	-2.48	120.76	126.39
23	C	502	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
23	c	510	CLA	O2A-CGA-CBA	2.48	119.38	111.83
25	t	101	BCR	C33-C5-C4	-2.47	108.33	113.60
28	C	520	LMG	C3-C4-C5	2.47	114.71	110.23
23	B	605	CLA	C4A-NA-C1A	-2.47	105.55	106.68
25	b	621	BCR	C37-C22-C21	-2.47	118.82	122.82
23	b	606	CLA	CHA-C1A-NA	-2.47	120.80	126.39
23	D	404	CLA	C1D-ND-C4D	-2.47	104.58	106.31
25	B	618	BCR	C16-C17-C18	-2.47	123.82	127.28
23	c	512	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
25	c	522	BCR	C8-C9-C10	-2.47	115.13	119.01
25	C	521	BCR	C8-C9-C10	-2.46	115.13	119.01
23	b	614	CLA	C1-O2A-CGA	2.46	122.61	116.65
23	b	613	CLA	C4-C3-C5	2.46	119.50	115.23
23	D	404	CLA	C4-C3-C5	2.46	119.50	115.23
23	c	504	CLA	C3B-C4B-NB	-2.46	108.33	110.53
23	C	509	CLA	CHA-C1A-NA	-2.46	120.83	126.39
26	a	609	PL9	C35-C34-C36	-2.46	110.96	115.23
23	B	617	CLA	CHC-C1C-C2C	-2.46	119.97	126.95
23	d	403	CLA	C4-C3-C5	2.45	119.49	115.23
23	b	615	CLA	C1D-ND-C4D	-2.45	104.59	106.31
23	b	604	CLA	CHA-C1A-NA	-2.45	120.84	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	516	BCR	C20-C19-C18	-2.45	119.64	126.36
23	c	505	CLA	CHB-C1B-C2B	-2.45	120.31	127.43
23	B	606	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
25	B	620	BCR	C1-C6-C7	-2.45	109.01	115.65
25	C	514	BCR	C30-C25-C24	-2.45	109.01	115.65
23	C	509	CLA	C1-O2A-CGA	2.45	122.58	116.65
23	B	608	CLA	CHC-C1C-C2C	-2.45	120.00	126.95
23	B	616	CLA	C1D-ND-C4D	-2.44	104.60	106.31
25	c	522	BCR	C34-C9-C10	-2.44	118.86	122.82
31	E	101	LHG	O8-C23-C24	2.44	119.26	111.83
25	c	515	BCR	C38-C26-C27	-2.43	108.41	113.60
23	b	609[A]	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
33	E	102	HEM	C1B-NB-C4B	2.43	108.09	105.21
23	C	512	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
23	C	505	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
23	b	606	CLA	O2A-CGA-CBA	2.43	119.24	111.83
23	C	510	CLA	CHA-C1A-NA	-2.43	120.89	126.39
23	B	608	CLA	CHB-C4A-NA	-2.43	120.89	124.40
23	b	610	CLA	C1-O2A-CGA	2.43	122.52	116.65
23	b	618	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
23	c	510	CLA	CHC-C1C-C2C	-2.42	120.06	126.95
23	C	506	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
23	c	510	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
23	C	512	CLA	CHB-C1B-C2B	-2.42	120.40	127.43
23	c	503	CLA	C1-O2A-CGA	2.42	122.51	116.65
23	A	605	CLA	C1D-ND-C4D	-2.42	104.61	106.31
23	B	613	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
23	B	615	CLA	O2A-CGA-CBA	2.42	119.22	111.83
32	c	518	DGD	O6D-C5D-C4D	-2.42	105.34	109.70
23	b	607	CLA	CHC-C1C-C2C	-2.42	120.07	126.95
23	b	608	CLA	C4D-C3D-CAD	-2.42	105.48	108.11
23	C	503	CLA	O2A-CGA-CBA	2.42	119.21	111.83
23	B	608	CLA	CED-O2D-CGD	2.42	121.40	115.92
23	C	502	CLA	C1D-ND-C4D	-2.42	104.62	106.31
23	c	510	CLA	C1-O2A-CGA	2.42	122.50	116.65
26	d	404	PL9	C53-C6-C1	2.42	120.23	115.28
23	A	605	CLA	O2A-CGA-CBA	2.41	119.19	111.83
23	c	511	CLA	O2A-CGA-CBA	2.41	119.19	111.83
23	d	402	CLA	C1D-ND-C4D	-2.41	104.62	106.31
23	B	614	CLA	C1-C2-C3	-2.41	122.25	126.20
23	B	615	CLA	C1-O2A-CGA	2.41	122.49	116.65
28	B	621	LMG	O8-C28-C29	2.41	119.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	101	BCR	C1-C6-C5	-2.41	119.34	122.64
23	B	603	CLA	C1-O2A-CGA	2.41	122.48	116.65
23	b	610	CLA	O2A-CGA-CBA	2.41	119.18	111.83
23	B	606	CLA	C1D-ND-C4D	-2.40	104.63	106.31
23	b	606	CLA	CHB-C4A-NA	-2.40	120.93	124.40
25	b	621	BCR	C40-C30-C25	2.40	114.01	110.24
23	b	616	CLA	C1-C2-C3	-2.40	122.27	126.20
23	A	605	CLA	CHB-C1B-C2B	-2.40	120.46	127.43
23	c	511	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
23	c	508	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
23	B	616	CLA	CHA-C1A-NA	-2.40	120.97	126.39
23	c	514	CLA	C4-C3-C5	2.40	119.39	115.23
23	C	513	CLA	C4-C3-C5	2.39	119.38	115.23
23	B	606	CLA	C1-O2A-CGA	2.39	122.44	116.65
23	B	602	CLA	C3B-C4B-NB	-2.39	108.40	110.53
23	B	611	CLA	C3B-C4B-NB	-2.39	108.40	110.53
23	C	508	CLA	CHB-C1B-C2B	-2.39	120.49	127.43
32	c	519	DGD	C3G-C2G-C1G	-2.39	106.22	111.78
23	b	605	CLA	CHB-C1B-C2B	-2.39	120.50	127.43
25	A	609	BCR	C34-C9-C10	-2.39	118.95	122.82
23	c	503	CLA	C3B-C4B-NB	-2.38	108.40	110.53
23	C	511	CLA	O2A-CGA-CBA	2.38	119.10	111.83
23	a	604	CLA	CHB-C1B-C2B	-2.38	120.51	127.43
23	b	611	CLA	CHA-C1A-NA	-2.38	121.00	126.39
26	a	609	PL9	C25-C24-C26	-2.38	111.09	115.23
32	C	516	DGD	O1G-C1A-C2A	2.38	119.10	111.83
25	T	101	BCR	C30-C25-C24	-2.38	109.19	115.65
23	B	617	CLA	C3B-C4B-NB	-2.38	108.41	110.53
28	C	520	LMG	O8-C28-C29	2.38	119.09	111.83
23	c	507	CLA	C4A-NA-C1A	-2.38	105.59	106.68
23	b	616	CLA	C1-O2A-CGA	2.38	122.41	116.65
23	B	607[A]	CLA	O2A-CGA-CBA	2.38	119.09	111.83
23	C	511	CLA	C1D-ND-C4D	-2.38	104.64	106.31
23	c	503	CLA	CHB-C1B-C2B	-2.38	120.53	127.43
28	J	101	LMG	C6-C5-C4	-2.38	107.18	113.02
32	c	518	DGD	C1E-O6E-C5E	-2.38	109.08	113.72
23	C	501	CLA	O1D-CGD-CBD	-2.37	119.83	124.52
25	h	101	BCR	C34-C9-C8	2.37	121.71	118.09
23	b	605	CLA	CHA-C1A-NA	-2.37	121.02	126.39
23	C	504	CLA	C3B-C4B-NB	-2.37	108.41	110.53
23	a	613	CLA	CHB-C1B-C2B	-2.37	120.55	127.43
23	B	604	CLA	O2A-CGA-CBA	2.37	119.05	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
23	b	616	CLA	C1D-ND-C4D	-2.36	104.65	106.31
25	B	619	BCR	C10-C11-C12	-2.36	116.35	123.20
32	D	406	DGD	O6D-C5D-C6D	2.36	111.38	106.69
23	B	613	CLA	C1D-ND-C4D	-2.36	104.65	106.31
25	f	101	BCR	C30-C25-C24	-2.36	109.25	115.65
26	a	609	PL9	C20-C19-C21	-2.36	111.13	115.23
25	C	521	BCR	C37-C22-C21	-2.36	118.99	122.82
25	B	619	BCR	C2-C3-C4	2.36	116.46	111.28
23	C	507	CLA	CHA-C1A-NA	-2.36	121.05	126.39
28	Z	101	LMG	O2-C2-C3	-2.36	104.82	110.38
23	C	506	CLA	CED-O2D-CGD	2.36	121.26	115.92
23	D	404	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
25	c	522	BCR	C40-C30-C25	2.36	113.94	110.24
25	h	101	BCR	C2-C3-C4	2.35	116.45	111.28
23	B	602	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
23	b	612	CLA	C3B-C4B-NB	-2.35	108.43	110.53
25	B	619	BCR	C8-C7-C6	-2.35	120.71	127.00
23	B	617	CLA	CHA-C1A-NA	-2.35	121.07	126.39
23	B	611	CLA	CHA-C1A-NA	-2.35	121.08	126.39
28	J	101	LMG	O8-C28-C29	2.35	118.99	111.83
23	B	611	CLA	C1D-ND-C4D	-2.35	104.67	106.31
23	B	610	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
23	b	614	CLA	CHB-C1B-C2B	-2.34	120.62	127.43
23	a	607	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
23	c	503	CLA	O2A-CGA-CBA	2.34	118.98	111.83
23	D	403	CLA	C1D-ND-C4D	-2.34	104.67	106.31
23	b	614	CLA	CHA-C1A-NA	-2.34	121.10	126.39
23	B	616	CLA	CHC-C1C-C2C	-2.34	120.30	126.95
23	B	607[B]	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
23	A	608	CLA	O2A-CGA-CBA	2.34	118.96	111.83
23	c	505	CLA	C1-O2A-CGA	2.34	122.31	116.65
23	b	607	CLA	C1-O2A-CGA	2.34	122.30	116.65
32	d	405	DGD	C4E-C3E-C2E	2.33	114.93	110.83
23	C	507	CLA	C1D-ND-C4D	-2.33	104.67	106.31
23	c	507	CLA	C3B-C4B-NB	-2.33	108.45	110.53
26	D	405	PL9	C20-C19-C21	-2.33	111.18	115.23
23	b	615	CLA	CHA-C1A-NA	-2.33	121.11	126.39
23	B	607[A]	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
23	a	605	CLA	CHB-C1B-C2B	-2.33	120.67	127.43
23	b	613	CLA	CHA-C1A-NA	-2.33	121.12	126.39
23	C	504	CLA	CHB-C1B-C2B	-2.33	120.67	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	CHA-C1A-NA	-2.33	121.12	126.39
23	C	504	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
23	b	609[B]	CLA	CHA-C1A-NA	-2.33	121.12	126.39
23	c	508	CLA	CHA-C1A-NA	-2.33	121.12	126.39
24	d	401	PHO	C2B-C1B-NB	-2.32	107.75	109.43
23	c	513	CLA	C1-O2A-CGA	2.32	122.28	116.65
23	B	603	CLA	O2A-CGA-CBA	2.32	118.92	111.83
23	C	510	CLA	C1D-ND-C4D	-2.32	104.68	106.31
23	B	611	CLA	CHB-C1B-C2B	-2.32	120.69	127.43
25	H	101	BCR	C35-C13-C12	2.32	121.63	118.09
23	B	616	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
23	b	610	CLA	C1D-ND-C4D	-2.32	104.69	106.31
23	b	608	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
23	C	509	CLA	CHC-C1C-C2C	-2.31	120.37	126.95
23	A	608	CLA	C1D-ND-C4D	-2.31	104.69	106.31
23	C	513	CLA	CHB-C1B-C2B	-2.31	120.72	127.43
23	B	610	CLA	C1D-ND-C4D	-2.31	104.69	106.31
23	c	502	CLA	C1-C2-C3	-2.31	122.41	126.20
27	A	611	SQD	O48-C23-C24	2.31	118.88	111.83
32	h	102	DGD	O6D-C5D-C6D	2.31	111.27	106.69
28	j	101	LMG	O8-C28-C29	2.31	118.87	111.83
23	B	602	CLA	CHB-C1B-C2B	-2.31	120.73	127.43
23	C	509	CLA	C1D-ND-C4D	-2.31	104.69	106.31
26	A	610	PL9	C51-C49-C50	-2.31	109.28	114.59
25	t	101	BCR	C36-C18-C17	-2.31	119.08	122.82
23	b	617	CLA	CHB-C1B-C2B	-2.31	120.73	127.43
23	B	607[A]	CLA	CHA-C1A-NA	-2.30	121.17	126.39
25	h	101	BCR	C1-C6-C7	-2.30	109.41	115.65
23	C	512	CLA	CED-O2D-CGD	2.30	121.14	115.92
25	b	622	BCR	C1-C6-C7	-2.30	109.41	115.65
23	B	609	CLA	CHB-C1B-C2B	-2.30	120.75	127.43
23	C	508	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
23	D	402	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
27	a	610	SQD	O48-C23-C24	2.30	118.84	111.83
23	b	609[A]	CLA	O2A-CGA-CBA	2.30	118.84	111.83
25	f	101	BCR	C20-C19-C18	-2.30	120.06	126.36
31	B	622	LHG	O7-C7-O9	-2.30	118.33	123.70
23	b	604	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
23	b	615	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
23	C	504	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
23	C	501	CLA	C1-C2-C3	-2.30	122.44	126.20
23	c	507	CLA	O1D-CGD-CBD	-2.30	119.99	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C3B-C4B-NB	-2.29	108.48	110.53
23	b	612	CLA	O2A-CGA-CBA	2.29	118.83	111.83
33	v	201	HEM	C2A-C1A-NA	-2.29	107.61	110.15
23	a	607	CLA	CHB-C1B-C2B	-2.29	120.77	127.43
28	j	101	LMG	O6-C5-C4	2.29	113.83	109.70
33	V	202	HEM	C1D-C2D-C3D	-2.29	104.57	106.98
23	C	507	CLA	CHB-C1B-C2B	-2.29	120.78	127.43
25	c	515	BCR	C8-C9-C10	-2.29	115.41	119.01
23	C	508	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
23	C	503	CLA	C3B-C4B-NB	-2.29	108.49	110.53
23	a	605	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
23	C	503	CLA	CHA-C1A-NA	-2.29	121.21	126.39
23	C	507	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
25	B	619	BCR	C12-C13-C14	-2.29	115.41	119.01
23	c	512	CLA	C3B-C4B-NB	-2.29	108.49	110.53
23	B	608	CLA	C1D-ND-C4D	-2.28	104.71	106.31
26	A	610	PL9	C30-C29-C31	-2.28	111.26	115.23
23	c	513	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
23	D	404	CLA	O2A-CGA-CBA	2.28	118.79	111.83
23	b	619	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
23	C	507	CLA	C1-O2A-CGA	2.28	122.16	116.65
25	H	101	BCR	C16-C15-C14	-2.28	118.86	123.52
25	h	101	BCR	C34-C9-C10	-2.27	119.13	122.82
27	b	602	SQD	O9-S-C6	2.27	110.15	106.76
23	B	607[B]	CLA	CHC-C1C-C2C	-2.27	120.50	126.95
23	B	610	CLA	CHC-C1C-C2C	-2.27	120.50	126.95
32	C	518	DGD	O1G-C1A-O1A	-2.27	117.95	123.63
23	c	504	CLA	CHB-C1B-C2B	-2.27	120.84	127.43
23	B	608	CLA	CHD-C4C-C3C	2.27	128.08	124.77
23	B	606	CLA	CHB-C1B-C2B	-2.27	120.85	127.43
23	C	502	CLA	O2A-CGA-CBA	2.27	118.75	111.83
23	A	605	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
31	D	407	LHG	C5-O7-C7	-2.26	112.38	117.80
23	B	604	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
23	b	618	CLA	CHA-C1A-NA	-2.26	121.27	126.39
25	B	619	BCR	C31-C1-C6	-2.26	106.70	110.24
23	a	613	CLA	CHD-C4C-C3C	2.26	128.07	124.77
26	d	404	PL9	C20-C19-C21	-2.26	111.31	115.23
23	C	512	CLA	CHA-C1A-NA	-2.26	121.28	126.39
23	b	611	CLA	CHB-C1B-C2B	-2.26	120.87	127.43
31	a	614	LHG	C5-O7-C7	-2.26	112.39	117.80
27	B	623	SQD	O9-S-C6	2.26	110.12	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	405	PL9	C53-C6-C1	2.26	119.90	115.28
31	d	406	LHG	C5-O7-C7	-2.26	112.40	117.80
27	a	612	SQD	C3-C4-C5	2.26	114.32	110.23
23	C	511	CLA	CHC-C1C-C2C	-2.26	120.54	126.95
23	B	613	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
23	D	404	CLA	CHB-C1B-C2B	-2.25	120.88	127.43
23	B	607[B]	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
23	a	607	CLA	C1-O2A-CGA	2.25	122.11	116.65
23	b	613	CLA	C1D-ND-C4D	-2.25	104.73	106.31
23	B	612	CLA	CHC-C1C-C2C	-2.25	120.55	126.95
23	b	609[A]	CLA	CHA-C1A-NA	-2.25	121.29	126.39
25	c	515	BCR	C1-C6-C7	-2.25	109.54	115.65
23	a	605	CLA	C4D-CHA-C1A	-2.25	118.56	121.24
23	a	605	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
25	b	621	BCR	C2-C3-C4	2.25	116.22	111.28
23	a	604	CLA	C1D-ND-C4D	-2.25	104.73	106.31
27	X	101	SQD	O48-C23-O10	-2.25	118.01	123.63
23	b	611	CLA	C4-C3-C5	2.25	119.13	115.23
23	C	505	CLA	CHA-C1A-NA	-2.25	121.30	126.39
23	b	611	CLA	O2A-CGA-CBA	2.25	118.68	111.83
23	C	509	CLA	CED-O2D-CGD	2.24	121.01	115.92
23	A	605	CLA	C4-C3-C5	2.24	119.12	115.23
23	b	615	CLA	CHC-C1C-C2C	-2.24	120.57	126.95
28	c	521	LMG	C3-C4-C5	2.24	114.30	110.23
23	B	609	CLA	C4-C3-C5	2.24	119.11	115.23
27	x	101	SQD	O48-C23-O10	-2.24	118.03	123.63
27	b	601	SQD	C3-C4-C5	2.24	114.29	110.23
25	C	515	BCR	C11-C12-C13	-2.24	120.22	126.36
25	A	609	BCR	C20-C19-C18	-2.24	120.23	126.36
23	c	513	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
23	B	605	CLA	C1-O2A-CGA	2.24	122.06	116.65
23	B	615	CLA	CHB-C1B-C2B	-2.24	120.94	127.43
23	B	612	CLA	O2A-CGA-CBA	2.23	118.65	111.83
23	B	607[B]	CLA	CHA-C1A-NA	-2.23	121.33	126.39
23	A	606	CLA	CHC-C1C-C2C	-2.23	120.60	126.95
23	C	513	CLA	C3B-C4B-NB	-2.23	108.54	110.53
23	B	603	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
33	e	102	HEM	C1B-NB-C4B	2.23	107.85	105.21
23	b	616	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
23	b	608	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
23	c	511	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
23	C	511	CLA	O2D-CGD-O1D	-2.23	119.51	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
32	d	405	DGD	C1E-C2E-C3E	2.23	114.70	110.01
23	B	607[B]	CLA	O2A-CGA-CBA	2.23	118.63	111.83
31	L	101	LHG	O8-C23-C24	2.23	118.63	111.83
28	z	101	LMG	O2-C2-C3	-2.23	105.12	110.38
23	B	614	CLA	O2A-CGA-CBA	2.23	118.63	111.83
25	b	620	BCR	C36-C18-C17	-2.23	119.21	122.82
23	b	613	CLA	CHB-C1B-C2B	-2.23	120.97	127.43
23	c	506	CLA	C1D-ND-C4D	-2.22	104.75	106.31
23	a	607	CLA	C3B-C4B-NB	-2.22	108.55	110.53
23	B	614	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
25	b	620	BCR	C37-C22-C21	-2.22	119.21	122.82
25	c	516	BCR	C30-C25-C24	-2.22	109.62	115.65
23	b	611	CLA	C11-C12-C13	-2.22	108.58	115.97
23	C	510	CLA	O2A-CGA-CBA	2.22	118.61	111.83
23	a	604	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
23	B	616	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
23	b	606	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
27	A	611	SQD	O48-C23-O10	-2.22	118.08	123.63
27	a	610	SQD	O48-C23-O10	-2.22	118.08	123.63
25	h	101	BCR	C37-C22-C21	-2.22	119.22	122.82
23	B	609	CLA	CHD-C4C-C3C	2.22	128.01	124.77
23	c	513	CLA	CHB-C1B-C2B	-2.22	120.99	127.43
23	c	504	CLA	O2A-CGA-CBA	2.22	118.59	111.83
25	c	515	BCR	C30-C25-C24	-2.21	109.64	115.65
23	c	508	CLA	C1-O2A-CGA	2.21	122.01	116.65
25	b	621	BCR	C11-C12-C13	-2.21	120.29	126.36
23	b	609[B]	CLA	O2A-CGA-CBA	2.21	118.58	111.83
25	b	621	BCR	C8-C9-C10	-2.21	115.53	119.01
23	C	508	CLA	CHA-C1A-NA	-2.21	121.38	126.39
23	b	604	CLA	C3B-C4B-NB	-2.21	108.56	110.53
25	C	515	BCR	C23-C22-C21	-2.21	115.53	119.01
23	a	604	CLA	C4-C3-C5	2.21	119.07	115.23
23	B	609	CLA	C11-C12-C13	-2.21	108.62	115.97
23	c	510	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
23	d	402	CLA	CHA-C1A-NA	-2.21	121.39	126.39
23	b	618	CLA	CHB-C1B-C2B	-2.21	121.02	127.43
23	C	502	CLA	CHA-C1A-NA	-2.21	121.39	126.39
28	a	611	LMG	O8-C28-C29	2.21	118.56	111.83
23	b	608	CLA	CHB-C1B-C2B	-2.21	121.02	127.43
25	K	101	BCR	C35-C13-C14	-2.21	119.24	122.82
25	k	101	BCR	C7-C8-C9	-2.20	122.98	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	CHA-C1A-NA	-2.20	121.40	126.39
23	C	502	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
23	C	510	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
25	k	101	BCR	C10-C11-C12	-2.20	116.82	123.20
23	C	510	CLA	CHB-C1B-C2B	-2.20	121.03	127.43
25	c	516	BCR	C1-C6-C7	-2.20	109.68	115.65
25	b	622	BCR	C20-C19-C18	-2.20	120.33	126.36
23	A	608	CLA	CED-O2D-CGD	2.20	120.90	115.92
23	b	613	CLA	CHC-C1C-C2C	-2.20	120.70	126.95
27	b	602	SQD	O47-C7-O49	-2.20	118.57	123.70
23	C	508	CLA	C1D-ND-C4D	-2.20	104.77	106.31
23	B	613	CLA	CHA-C1A-NA	-2.20	121.42	126.39
23	c	511	CLA	CHA-C1A-NA	-2.20	121.42	126.39
23	d	403	CLA	CHB-C1B-C2B	-2.20	121.05	127.43
23	b	612	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
23	a	613	CLA	C4D-CHA-C1A	-2.19	118.63	121.24
23	b	616	CLA	CHA-C1A-NA	-2.19	121.42	126.39
23	b	609[B]	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
23	c	505	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
23	c	508	CLA	CHB-C1B-C2B	-2.19	121.06	127.43
23	c	506	CLA	C4D-CHA-C1A	-2.19	118.63	121.24
23	D	402	CLA	C4D-CHA-C1A	-2.19	118.63	121.24
27	B	623	SQD	O47-C7-O49	-2.19	118.58	123.70
23	b	605	CLA	CHB-C4A-NA	-2.19	121.24	124.40
25	B	620	BCR	C34-C9-C8	2.19	121.43	118.09
23	B	604	CLA	C1D-ND-C4D	-2.19	104.78	106.31
25	b	620	BCR	C37-C22-C23	-2.19	114.74	118.09
32	c	517	DGD	O6D-C5D-C6D	2.19	111.03	106.69
23	B	613	CLA	CHC-C1C-C2C	-2.19	120.73	126.95
25	B	620	BCR	C23-C22-C21	-2.19	115.57	119.01
27	B	623	SQD	O5-C1-C2	-2.19	105.88	110.37
25	K	101	BCR	C31-C1-C6	-2.19	106.81	110.24
23	c	509	CLA	CHA-C1A-NA	-2.18	121.44	126.39
23	B	610	CLA	CHB-C1B-C2B	-2.18	121.09	127.43
25	T	101	BCR	C31-C1-C6	-2.18	106.82	110.24
25	h	101	BCR	C30-C25-C24	-2.18	109.73	115.65
31	l	101	LHG	O8-C23-C24	2.18	118.49	111.83
23	C	512	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
23	A	606	CLA	CHB-C1B-C2B	-2.18	121.10	127.43
27	b	602	SQD	O5-C1-C2	-2.18	105.89	110.37
23	c	505	CLA	CHA-C1A-NA	-2.18	121.46	126.39
26	A	610	PL9	C10-C9-C11	-2.18	111.45	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
33	v	201	HEM	C1D-C2D-C3D	-2.18	104.69	106.98
23	b	606	CLA	C1D-ND-C4D	-2.17	104.79	106.31
23	D	403	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
23	D	402	CLA	CHD-C4C-C3C	2.17	127.94	124.77
25	k	101	BCR	C11-C12-C13	-2.17	120.42	126.36
23	B	611	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
25	a	608	BCR	C34-C9-C8	2.17	121.40	118.09
25	B	618	BCR	C35-C13-C14	-2.17	119.31	122.82
23	b	616	CLA	CHC-C1C-C2C	-2.16	120.80	126.95
23	b	618	CLA	CHC-C1C-C2C	-2.16	120.80	126.95
25	F	101	BCR	C37-C22-C21	-2.16	119.31	122.82
23	B	610	CLA	C1-O2A-CGA	2.16	121.88	116.65
23	B	602	CLA	CHA-C1A-NA	-2.16	121.50	126.39
23	B	613	CLA	CHB-C1B-C2B	-2.16	121.16	127.43
23	B	609	CLA	C1D-ND-C4D	-2.16	104.80	106.31
26	a	609	PL9	C7-C3-C2	-2.16	120.84	123.39
23	C	506	CLA	CHC-C1C-C2C	-2.16	120.82	126.95
25	C	514	BCR	C33-C5-C4	-2.16	109.00	113.60
23	C	503	CLA	CHC-C1C-C2C	-2.16	120.82	126.95
23	C	513	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
25	c	522	BCR	C11-C12-C13	-2.16	120.45	126.36
28	A	612	LMG	O8-C28-C29	2.16	118.41	111.83
23	C	506	CLA	C3B-C4B-NB	-2.16	108.61	110.53
23	B	607[A]	CLA	C1D-ND-C4D	-2.15	104.80	106.31
23	b	616	CLA	CHB-C1B-C2B	-2.15	121.17	127.43
23	b	615	CLA	CHB-C1B-C2B	-2.15	121.17	127.43
25	F	101	BCR	C30-C25-C24	-2.15	109.81	115.65
23	B	608	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
23	B	603	CLA	CHA-C1A-NA	-2.15	121.52	126.39
23	C	512	CLA	C1D-ND-C4D	-2.15	104.80	106.31
23	B	603	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
23	C	512	CLA	C1-O2A-CGA	2.15	121.85	116.65
23	b	604	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
23	A	605	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
23	B	607[A]	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
23	b	610	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
23	c	503	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
23	c	502	CLA	CHB-C1B-C2B	-2.14	121.21	127.43
25	b	622	BCR	C34-C9-C8	2.14	121.36	118.09
32	C	517	DGD	C1E-O6E-C5E	-2.14	109.54	113.72
25	b	622	BCR	C19-C18-C17	-2.14	115.64	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C1D-ND-C4D	-2.14	104.81	106.31
23	b	613	CLA	CED-O2D-CGD	2.14	120.77	115.92
23	B	604	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
23	b	609[A]	CLA	CHC-C1C-C2C	-2.14	120.88	126.95
25	f	101	BCR	C28-C27-C26	-2.14	110.25	114.06
23	c	504	CLA	O1D-CGD-CBD	-2.14	120.31	124.52
23	b	607	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
25	b	622	BCR	C30-C25-C24	-2.13	109.86	115.65
25	B	618	BCR	C29-C28-C27	2.13	115.97	111.28
24	D	401	PHO	C2B-C1B-NB	-2.13	107.89	109.43
31	E	101	LHG	O7-C7-O9	-2.13	118.72	123.70
23	c	507	CLA	CED-O2D-CGD	2.13	120.75	115.92
23	b	606	CLA	C1-O2A-CGA	2.13	121.81	116.65
23	c	510	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
23	B	602	CLA	CHC-C1C-C2C	-2.13	120.91	126.95
32	c	517	DGD	C2G-O2G-C1B	-2.13	112.71	117.80
23	B	608	CLA	C1-O2A-CGA	2.13	121.80	116.65
23	b	608	CLA	CED-O2D-CGD	2.13	120.74	115.92
23	C	504	CLA	CHA-C1A-NA	-2.12	121.58	126.39
33	V	202	HEM	CBA-CAA-C2A	-2.12	106.66	112.53
23	c	505	CLA	C7-C6-C5	-2.12	107.60	113.26
23	D	402	CLA	C1D-ND-C4D	-2.12	104.82	106.31
23	b	604	CLA	C1-O2A-CGA	2.12	121.78	116.65
23	C	508	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
23	C	501	CLA	C4-C3-C5	2.12	118.91	115.23
23	c	502	CLA	C4-C3-C5	2.12	118.91	115.23
23	B	610	CLA	CHA-C1A-NA	-2.12	121.59	126.39
23	c	513	CLA	C1D-ND-C4D	-2.12	104.83	106.31
23	C	501	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
23	c	507	CLA	CHA-C1A-NA	-2.12	121.60	126.39
23	b	612	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
32	h	102	DGD	O6E-C5E-C6E	2.12	111.69	106.44
25	C	514	BCR	C20-C19-C18	-2.12	120.56	126.36
27	A	611	SQD	O5-C1-C2	-2.12	106.02	110.37
23	b	604	CLA	CHB-C1B-C2B	-2.11	121.29	127.43
23	C	504	CLA	C7-C6-C5	-2.11	107.63	113.26
23	d	403	CLA	CHC-C1C-C2C	-2.11	120.94	126.95
23	b	619	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
23	C	503	CLA	CMD-C2D-C1D	2.11	128.45	124.73
23	c	509	CLA	CHC-C1C-C2C	-2.11	120.95	126.95
23	B	606	CLA	C4A-NA-C1A	-2.11	105.72	106.68
23	b	612	CLA	C1D-ND-C4D	-2.11	104.83	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
23	b	609[B]	CLA	C1D-ND-C4D	-2.11	104.83	106.31
23	B	615	CLA	C3B-C4B-NB	-2.11	108.65	110.53
28	C	520	LMG	O6-C5-C4	2.10	113.49	109.70
23	c	507	CLA	CHB-C4A-NA	-2.10	121.36	124.40
23	C	513	CLA	CED-O2D-CGD	2.10	120.69	115.92
23	a	604	CLA	CHA-C1A-NA	-2.10	121.63	126.39
23	C	506	CLA	C1-C2-C3	-2.10	122.75	126.20
33	E	102	HEM	C3B-C2B-C1B	2.10	107.99	106.41
23	c	513	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
23	B	609	CLA	CHA-C1A-NA	-2.10	121.64	126.39
23	c	507	CLA	C1-C2-C3	-2.10	122.76	126.20
23	B	614	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
23	B	604	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
23	C	513	CLA	C1-O2A-CGA	2.10	121.73	116.65
23	c	502	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
23	c	513	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
23	b	610	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
23	c	514	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
23	b	612	CLA	CHC-C1C-C2C	-2.10	120.99	126.95
23	b	617	CLA	C1-C2-C3	-2.09	122.77	126.20
32	C	517	DGD	C4E-C3E-C2E	2.09	114.51	110.83
23	B	611	CLA	O2D-CGD-O1D	-2.09	119.77	123.85
23	a	604	CLA	O2D-CGD-O1D	-2.09	119.77	123.85
23	B	608	CLA	O2A-CGA-CBA	2.09	118.22	111.83
23	B	616	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
23	D	404	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
23	D	403	CLA	C3B-C4B-NB	-2.09	108.66	110.53
23	b	605	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
23	c	506	CLA	CHA-C1A-NA	-2.09	121.66	126.39
32	d	405	DGD	C3E-C4E-C5E	2.09	114.02	110.23
25	t	101	BCR	C16-C15-C14	-2.09	119.25	123.52
23	b	614	CLA	O2D-CGD-O1D	-2.09	119.79	123.85
23	B	615	CLA	C1-C2-C3	-2.09	122.78	126.20
23	b	608	CLA	C1-C2-C3	-2.09	122.78	126.20
23	B	617	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
27	a	610	SQD	O5-C1-C2	-2.08	106.09	110.37
23	B	606	CLA	CED-O2D-CGD	2.08	120.64	115.92
23	c	512	CLA	CHC-C1C-C2C	-2.08	121.03	126.95
23	d	403	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
23	b	610	CLA	CED-O2D-CGD	2.08	120.63	115.92
28	A	612	LMG	O1-C1-C2	2.08	111.43	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	CHB-C4A-NA	-2.08	121.40	124.40
23	B	606	CLA	C1-C2-C3	-2.08	122.80	126.20
23	c	511	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
25	c	515	BCR	C35-C13-C12	2.08	121.26	118.09
25	B	620	BCR	C33-C5-C4	-2.07	109.17	113.60
25	H	101	BCR	C30-C25-C24	-2.07	110.03	115.65
23	A	608	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
23	C	509	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
23	C	502	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
23	a	607	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
23	b	619	CLA	C4-C3-C5	2.07	118.82	115.23
23	c	504	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
23	b	614	CLA	O2A-CGA-CBA	2.07	118.15	111.83
25	b	621	BCR	C20-C19-C18	-2.07	120.69	126.36
25	t	101	BCR	C29-C30-C25	2.07	113.44	110.44
23	b	617	CLA	CHA-C1A-NA	-2.07	121.71	126.39
32	C	517	DGD	C3E-C4E-C5E	2.07	113.98	110.23
23	b	617	CLA	CHC-C1C-C2C	-2.07	121.08	126.95
23	B	609	CLA	CHC-C1C-C2C	-2.07	121.08	126.95
23	b	610	CLA	CHA-C1A-NA	-2.06	121.72	126.39
23	a	607	CLA	C4D-CHA-C1A	-2.06	118.78	121.24
25	B	618	BCR	C10-C11-C12	-2.06	117.22	123.20
23	C	506	CLA	CHA-C1A-NA	-2.06	121.72	126.39
23	C	501	CLA	CHC-C1C-C2C	-2.06	121.09	126.95
23	D	403	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
32	c	518	DGD	O6E-C5E-C6E	2.06	111.55	106.44
26	A	610	PL9	C20-C19-C21	-2.06	111.65	115.23
23	C	506	CLA	C1D-ND-C4D	-2.06	104.87	106.31
23	b	612	CLA	CHA-C1A-NA	-2.06	121.72	126.39
23	b	619	CLA	C4A-NA-C1A	-2.06	105.74	106.68
32	C	518	DGD	C3G-C2G-C1G	-2.06	106.98	111.78
23	d	403	CLA	C3B-C4B-NB	-2.06	108.69	110.53
25	T	101	BCR	C16-C15-C14	-2.06	119.31	123.52
23	a	613	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
25	H	101	BCR	C2-C3-C4	2.06	115.80	111.28
23	B	617	CLA	C4-C3-C5	2.06	118.80	115.23
23	b	616	CLA	O2A-CGA-CBA	2.06	118.11	111.83
23	c	510	CLA	C1-C2-C3	-2.06	122.83	126.20
23	c	509	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
32	c	517	DGD	O1G-C1A-C2A	2.06	118.10	111.83
23	c	509	CLA	O2A-CGA-CBA	2.06	118.10	111.83
23	C	509	CLA	C1-C2-C3	-2.06	122.83	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C4-C3-C5	2.05	118.79	115.23
25	c	515	BCR	C35-C13-C14	-2.05	119.49	122.82
23	b	612	CLA	CED-O2D-CGD	2.05	120.57	115.92
25	C	514	BCR	C3-C4-C5	-2.05	110.39	114.06
23	b	611	CLA	C11-C10-C8	-2.05	109.14	115.97
23	a	605	CLA	O2A-CGA-CBA	2.05	118.09	111.83
23	B	608	CLA	CHA-C1A-NA	-2.05	121.75	126.39
23	b	619	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
23	c	502	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
25	h	101	BCR	C36-C18-C17	-2.05	119.50	122.82
25	C	515	BCR	C12-C13-C14	-2.05	115.79	119.01
23	b	612	CLA	C4A-NA-C1A	-2.05	105.75	106.68
23	c	511	CLA	C1-C2-C3	-2.05	122.84	126.20
25	C	521	BCR	C34-C9-C10	-2.05	119.50	122.82
31	D	408	LHG	O8-C23-O10	-2.05	118.51	123.63
27	X	101	SQD	C3-C4-C5	2.04	113.94	110.23
23	C	501	CLA	C3B-C4B-NB	-2.04	108.71	110.53
23	b	618	CLA	C1D-CHD-C4C	-2.04	121.68	126.02
23	C	508	CLA	O2A-CGA-CBA	2.04	118.06	111.83
23	B	614	CLA	CHA-C1A-NA	-2.04	121.77	126.39
23	c	510	CLA	CHA-C1A-NA	-2.04	121.77	126.39
23	c	504	CLA	CHC-C1C-C2C	-2.04	121.14	126.95
23	c	510	CLA	C4-C3-C5	2.04	118.77	115.23
23	B	613	CLA	CHD-C4C-C3C	2.04	127.75	124.77
23	B	604	CLA	CHC-C1C-C2C	-2.04	121.15	126.95
23	c	504	CLA	CHA-C1A-NA	-2.04	121.77	126.39
23	a	605	CLA	C1D-ND-C4D	-2.04	104.88	106.31
25	C	515	BCR	C19-C18-C17	2.04	122.22	119.01
23	C	510	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
23	C	501	CLA	C1D-ND-C4D	-2.04	104.88	106.31
23	C	510	CLA	C4-C3-C5	2.04	118.77	115.23
28	z	101	LMG	C4-C3-C2	2.04	114.41	110.83
25	K	101	BCR	C1-C6-C7	-2.04	110.12	115.65
25	a	608	BCR	C32-C1-C6	2.04	113.44	110.24
32	H	102	DGD	O6E-C5E-C6E	2.04	111.49	106.44
25	c	516	BCR	C31-C1-C6	-2.04	107.05	110.24
23	B	602	CLA	CED-O2D-CGD	2.04	120.53	115.92
27	b	601	SQD	O5-C1-C2	-2.04	106.19	110.37
23	b	618	CLA	C11-C10-C8	-2.03	109.20	115.97
27	x	101	SQD	C3-C4-C5	2.03	113.92	110.23
23	b	615	CLA	CHD-C4C-C3C	2.03	127.74	124.77
23	C	510	CLA	C1-C2-C3	-2.03	122.87	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	CHD-C4C-C3C	2.03	127.74	124.77
23	D	404	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
23	B	609	CLA	C11-C10-C8	-2.03	109.21	115.97
25	B	618	BCR	C29-C30-C25	2.03	113.39	110.44
25	B	618	BCR	C2-C1-C6	-2.03	107.49	110.44
26	a	609	PL9	C3-C4-C5	2.03	121.10	118.57
23	B	616	CLA	C11-C10-C8	-2.03	109.23	115.97
23	A	606	CLA	CHD-C4C-C3C	2.03	127.73	124.77
23	b	607	CLA	CHD-C4C-C3C	2.03	127.73	124.77
23	C	503	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
23	b	604	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
23	C	505	CLA	C4D-CHA-C1A	-2.02	118.83	121.24
23	B	603	CLA	C1D-ND-C4D	-2.02	104.89	106.31
25	C	521	BCR	C1-C6-C7	-2.02	110.17	115.65
32	C	516	DGD	O6D-C5D-C6D	2.02	110.70	106.69
23	C	501	CLA	CHD-C4C-C3C	2.02	127.72	124.77
32	c	517	DGD	O6D-C5D-C4D	-2.02	106.06	109.70
25	C	515	BCR	C34-C9-C10	-2.02	119.55	122.82
27	a	612	SQD	O5-C1-C2	-2.02	106.22	110.37
23	C	502	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
23	c	514	CLA	C1D-ND-C4D	-2.02	104.90	106.31
23	C	502	CLA	C1-O2A-CGA	2.01	121.53	116.65
24	a	606	PHO	C1-C2-C3	-2.01	122.90	126.20
28	j	101	LMG	C6-C5-C4	-2.01	108.07	113.02
23	c	507	CLA	CBA-CAA-C2A	-2.01	107.80	113.79
23	c	502	CLA	CHA-C1A-NA	-2.01	121.83	126.39
32	c	518	DGD	O6E-C5E-C4E	-2.01	106.08	109.70
32	d	405	DGD	O6D-C5D-C6D	2.01	110.68	106.69
23	c	511	CLA	C4-C3-C5	2.01	118.71	115.23
23	A	605	CLA	C3B-C4B-NB	-2.01	108.74	110.53
23	C	507	CLA	CHB-C4A-NA	-2.00	121.51	124.40
26	d	404	PL9	C25-C24-C26	-2.00	111.75	115.23
23	B	614	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
23	B	605	CLA	CED-O2D-CGD	2.00	120.46	115.92
31	L	101	LHG	C5-O7-C7	-2.00	113.00	117.80
23	C	503	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
23	B	606	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
31	B	622	LHG	O8-C23-O10	-2.00	118.62	123.63
25	t	101	BCR	C3-C4-C5	-2.00	110.49	114.06

All (72) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	605	CLA	ND
23	A	606	CLA	ND
23	A	608	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607[A]	CLA	ND
23	B	607[B]	CLA	ND
23	B	608	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	B	617	CLA	ND
23	C	501	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	402	CLA	ND
23	D	403	CLA	ND
23	D	404	CLA	ND
23	a	604	CLA	ND
23	a	605	CLA	ND
23	a	607	CLA	ND
23	a	613	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609[A]	CLA	ND
23	b	609[B]	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	b	618	CLA	ND
23	b	619	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	c	514	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND

All (1969) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	602	CLA	CAD-CBD-CGD-O2D
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	C2B-C3B-CAB-CBB
23	B	616	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C3A-C2A-CAA-CBA
23	b	617	CLA	CAD-CBD-CGD-O1D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	b	618	CLA	C2B-C3B-CAB-CBB
23	b	618	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
25	A	609	BCR	C11-C10-C9-C8
25	A	609	BCR	C11-C12-C13-C14
25	A	609	BCR	C12-C13-C14-C15
25	A	609	BCR	C13-C14-C15-C16
25	A	609	BCR	C14-C15-C16-C17
25	A	609	BCR	C16-C17-C18-C36
25	A	609	BCR	C36-C18-C19-C20
25	A	609	BCR	C18-C19-C20-C21
25	A	609	BCR	C20-C21-C22-C37
25	A	609	BCR	C37-C22-C23-C24
25	A	609	BCR	C23-C24-C25-C30
25	B	618	BCR	C10-C11-C12-C13
25	B	618	BCR	C11-C12-C13-C14
25	B	618	BCR	C11-C12-C13-C35
25	B	618	BCR	C12-C13-C14-C15
25	B	618	BCR	C35-C13-C14-C15
25	B	618	BCR	C16-C17-C18-C19
25	B	618	BCR	C16-C17-C18-C36
25	B	618	BCR	C17-C18-C19-C20
25	B	618	BCR	C36-C18-C19-C20
25	B	618	BCR	C18-C19-C20-C21
25	B	618	BCR	C20-C21-C22-C23
25	B	618	BCR	C21-C22-C23-C24
25	B	618	BCR	C22-C23-C24-C25
25	B	619	BCR	C7-C8-C9-C34
25	B	619	BCR	C11-C10-C9-C34
25	B	619	BCR	C10-C11-C12-C13
25	B	619	BCR	C11-C12-C13-C35
25	B	619	BCR	C12-C13-C14-C15
25	B	619	BCR	C14-C15-C16-C17
25	B	619	BCR	C16-C17-C18-C19
25	B	619	BCR	C16-C17-C18-C36
25	B	619	BCR	C36-C18-C19-C20
25	B	619	BCR	C20-C21-C22-C23
25	B	619	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
25	B	620	BCR	C7-C8-C9-C10
25	B	620	BCR	C11-C10-C9-C34
25	B	620	BCR	C14-C15-C16-C17
25	B	620	BCR	C16-C17-C18-C19
25	B	620	BCR	C16-C17-C18-C36
25	B	620	BCR	C17-C18-C19-C20
25	B	620	BCR	C36-C18-C19-C20
25	B	620	BCR	C18-C19-C20-C21
25	B	620	BCR	C20-C21-C22-C23
25	B	620	BCR	C20-C21-C22-C37
25	C	514	BCR	C6-C7-C8-C9
25	C	514	BCR	C11-C10-C9-C34
25	C	514	BCR	C10-C11-C12-C13
25	C	514	BCR	C12-C13-C14-C15
25	C	514	BCR	C16-C17-C18-C19
25	C	514	BCR	C16-C17-C18-C36
25	C	514	BCR	C17-C18-C19-C20
25	C	514	BCR	C18-C19-C20-C21
25	C	514	BCR	C19-C20-C21-C22
25	C	514	BCR	C20-C21-C22-C23
25	C	514	BCR	C20-C21-C22-C37
25	C	514	BCR	C22-C23-C24-C25
25	C	514	BCR	C23-C24-C25-C26
25	C	515	BCR	C6-C7-C8-C9
25	C	515	BCR	C12-C13-C14-C15
25	C	515	BCR	C35-C13-C14-C15
25	C	515	BCR	C14-C15-C16-C17
25	C	515	BCR	C17-C18-C19-C20
25	C	515	BCR	C18-C19-C20-C21
25	C	515	BCR	C20-C21-C22-C23
25	C	515	BCR	C22-C23-C24-C25
25	C	521	BCR	C5-C6-C7-C8
25	C	521	BCR	C10-C11-C12-C13
25	C	521	BCR	C11-C12-C13-C14
25	C	521	BCR	C14-C15-C16-C17
25	C	521	BCR	C17-C18-C19-C20
25	C	521	BCR	C20-C21-C22-C37
25	C	521	BCR	C21-C22-C23-C24
25	F	101	BCR	C6-C7-C8-C9
25	F	101	BCR	C10-C11-C12-C13
25	F	101	BCR	C11-C12-C13-C35
25	F	101	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	F	101	BCR	C35-C13-C14-C15
25	F	101	BCR	C14-C15-C16-C17
25	F	101	BCR	C16-C17-C18-C36
25	F	101	BCR	C17-C18-C19-C20
25	F	101	BCR	C36-C18-C19-C20
25	F	101	BCR	C18-C19-C20-C21
25	F	101	BCR	C20-C21-C22-C23
25	F	101	BCR	C20-C21-C22-C37
25	F	101	BCR	C21-C22-C23-C24
25	F	101	BCR	C37-C22-C23-C24
25	F	101	BCR	C22-C23-C24-C25
25	F	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C6-C7-C8-C9
25	H	101	BCR	C7-C8-C9-C10
25	H	101	BCR	C11-C10-C9-C8
25	H	101	BCR	C10-C11-C12-C13
25	H	101	BCR	C14-C15-C16-C17
25	H	101	BCR	C16-C17-C18-C19
25	H	101	BCR	C16-C17-C18-C36
25	H	101	BCR	C17-C18-C19-C20
25	H	101	BCR	C36-C18-C19-C20
25	H	101	BCR	C18-C19-C20-C21
25	H	101	BCR	C20-C21-C22-C23
25	H	101	BCR	C20-C21-C22-C37
25	H	101	BCR	C21-C22-C23-C24
25	H	101	BCR	C37-C22-C23-C24
25	H	101	BCR	C22-C23-C24-C25
25	K	101	BCR	C7-C8-C9-C10
25	K	101	BCR	C7-C8-C9-C34
25	K	101	BCR	C11-C10-C9-C8
25	K	101	BCR	C10-C11-C12-C13
25	K	101	BCR	C11-C12-C13-C35
25	K	101	BCR	C12-C13-C14-C15
25	K	101	BCR	C14-C15-C16-C17
25	K	101	BCR	C16-C17-C18-C19
25	K	101	BCR	C16-C17-C18-C36
25	K	101	BCR	C20-C21-C22-C37
25	K	101	BCR	C37-C22-C23-C24
25	K	101	BCR	C22-C23-C24-C25
25	T	101	BCR	C6-C7-C8-C9
25	T	101	BCR	C7-C8-C9-C10
25	T	101	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	T	101	BCR	C11-C10-C9-C34
25	T	101	BCR	C10-C11-C12-C13
25	T	101	BCR	C12-C13-C14-C15
25	T	101	BCR	C14-C15-C16-C17
25	T	101	BCR	C15-C16-C17-C18
25	T	101	BCR	C18-C19-C20-C21
25	T	101	BCR	C19-C20-C21-C22
25	T	101	BCR	C20-C21-C22-C23
25	T	101	BCR	C37-C22-C23-C24
25	T	101	BCR	C22-C23-C24-C25
25	T	101	BCR	C23-C24-C25-C26
25	a	608	BCR	C9-C10-C11-C12
25	a	608	BCR	C10-C11-C12-C13
25	a	608	BCR	C14-C15-C16-C17
25	a	608	BCR	C36-C18-C19-C20
25	a	608	BCR	C18-C19-C20-C21
25	a	608	BCR	C20-C21-C22-C37
25	a	608	BCR	C23-C24-C25-C30
25	b	620	BCR	C9-C10-C11-C12
25	b	620	BCR	C10-C11-C12-C13
25	b	620	BCR	C11-C12-C13-C14
25	b	620	BCR	C12-C13-C14-C15
25	b	620	BCR	C35-C13-C14-C15
25	b	620	BCR	C17-C18-C19-C20
25	b	620	BCR	C18-C19-C20-C21
25	b	620	BCR	C22-C23-C24-C25
25	b	621	BCR	C1-C6-C7-C8
25	b	621	BCR	C11-C12-C13-C35
25	b	621	BCR	C12-C13-C14-C15
25	b	621	BCR	C14-C15-C16-C17
25	b	621	BCR	C16-C17-C18-C19
25	b	621	BCR	C16-C17-C18-C36
25	b	621	BCR	C17-C18-C19-C20
25	b	621	BCR	C18-C19-C20-C21
25	b	621	BCR	C20-C21-C22-C23
25	b	621	BCR	C20-C21-C22-C37
25	b	621	BCR	C21-C22-C23-C24
25	b	622	BCR	C6-C7-C8-C9
25	b	622	BCR	C11-C10-C9-C34
25	b	622	BCR	C12-C13-C14-C15
25	b	622	BCR	C35-C13-C14-C15
25	b	622	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	b	622	BCR	C16-C17-C18-C19
25	b	622	BCR	C16-C17-C18-C36
25	b	622	BCR	C17-C18-C19-C20
25	b	622	BCR	C36-C18-C19-C20
25	b	622	BCR	C18-C19-C20-C21
25	b	622	BCR	C20-C21-C22-C23
25	b	622	BCR	C20-C21-C22-C37
25	c	515	BCR	C5-C6-C7-C8
25	c	515	BCR	C7-C8-C9-C10
25	c	515	BCR	C7-C8-C9-C34
25	c	515	BCR	C11-C10-C9-C8
25	c	515	BCR	C10-C11-C12-C13
25	c	515	BCR	C12-C13-C14-C15
25	c	515	BCR	C14-C15-C16-C17
25	c	515	BCR	C15-C16-C17-C18
25	c	515	BCR	C16-C17-C18-C19
25	c	515	BCR	C16-C17-C18-C36
25	c	515	BCR	C17-C18-C19-C20
25	c	515	BCR	C36-C18-C19-C20
25	c	515	BCR	C18-C19-C20-C21
25	c	515	BCR	C19-C20-C21-C22
25	c	515	BCR	C20-C21-C22-C23
25	c	515	BCR	C20-C21-C22-C37
25	c	515	BCR	C23-C24-C25-C26
25	c	516	BCR	C7-C8-C9-C10
25	c	516	BCR	C10-C11-C12-C13
25	c	516	BCR	C11-C12-C13-C35
25	c	516	BCR	C12-C13-C14-C15
25	c	516	BCR	C35-C13-C14-C15
25	c	516	BCR	C13-C14-C15-C16
25	c	516	BCR	C14-C15-C16-C17
25	c	516	BCR	C36-C18-C19-C20
25	c	516	BCR	C18-C19-C20-C21
25	c	516	BCR	C20-C21-C22-C23
25	c	516	BCR	C21-C22-C23-C24
25	c	516	BCR	C22-C23-C24-C25
25	c	522	BCR	C5-C6-C7-C8
25	c	522	BCR	C6-C7-C8-C9
25	c	522	BCR	C7-C8-C9-C34
25	c	522	BCR	C11-C10-C9-C8
25	c	522	BCR	C10-C11-C12-C13
25	c	522	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	522	BCR	C14-C15-C16-C17
25	c	522	BCR	C17-C18-C19-C20
25	c	522	BCR	C18-C19-C20-C21
25	c	522	BCR	C20-C21-C22-C37
25	c	522	BCR	C21-C22-C23-C24
25	f	101	BCR	C6-C7-C8-C9
25	f	101	BCR	C10-C11-C12-C13
25	f	101	BCR	C11-C12-C13-C14
25	f	101	BCR	C12-C13-C14-C15
25	f	101	BCR	C35-C13-C14-C15
25	f	101	BCR	C13-C14-C15-C16
25	f	101	BCR	C14-C15-C16-C17
25	f	101	BCR	C16-C17-C18-C19
25	f	101	BCR	C16-C17-C18-C36
25	f	101	BCR	C17-C18-C19-C20
25	f	101	BCR	C20-C21-C22-C37
25	f	101	BCR	C21-C22-C23-C24
25	f	101	BCR	C22-C23-C24-C25
25	f	101	BCR	C23-C24-C25-C26
25	h	101	BCR	C6-C7-C8-C9
25	h	101	BCR	C11-C10-C9-C8
25	h	101	BCR	C10-C11-C12-C13
25	h	101	BCR	C12-C13-C14-C15
25	h	101	BCR	C14-C15-C16-C17
25	h	101	BCR	C16-C17-C18-C19
25	h	101	BCR	C16-C17-C18-C36
25	h	101	BCR	C36-C18-C19-C20
25	h	101	BCR	C19-C20-C21-C22
25	h	101	BCR	C20-C21-C22-C23
25	h	101	BCR	C20-C21-C22-C37
25	h	101	BCR	C21-C22-C23-C24
25	h	101	BCR	C22-C23-C24-C25
25	k	101	BCR	C7-C8-C9-C34
25	k	101	BCR	C11-C10-C9-C8
25	k	101	BCR	C10-C11-C12-C13
25	k	101	BCR	C11-C12-C13-C35
25	k	101	BCR	C12-C13-C14-C15
25	k	101	BCR	C15-C16-C17-C18
25	k	101	BCR	C16-C17-C18-C19
25	k	101	BCR	C16-C17-C18-C36
25	k	101	BCR	C20-C21-C22-C37
25	t	101	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	t	101	BCR	C11-C10-C9-C8
25	t	101	BCR	C10-C11-C12-C13
25	t	101	BCR	C11-C12-C13-C14
25	t	101	BCR	C12-C13-C14-C15
25	t	101	BCR	C14-C15-C16-C17
25	t	101	BCR	C15-C16-C17-C18
25	t	101	BCR	C16-C17-C18-C36
25	t	101	BCR	C36-C18-C19-C20
25	t	101	BCR	C18-C19-C20-C21
25	t	101	BCR	C37-C22-C23-C24
25	t	101	BCR	C22-C23-C24-C25
26	A	610	PL9	C7-C8-C9-C10
26	A	610	PL9	C12-C13-C14-C15
26	A	610	PL9	C17-C18-C19-C20
26	A	610	PL9	C22-C23-C24-C25
26	A	610	PL9	C32-C33-C34-C35
26	D	405	PL9	C7-C8-C9-C10
26	D	405	PL9	C17-C18-C19-C20
26	D	405	PL9	C22-C23-C24-C25
26	D	405	PL9	C27-C28-C29-C30
26	a	609	PL9	C7-C8-C9-C10
26	a	609	PL9	C32-C33-C34-C35
26	d	404	PL9	C17-C18-C19-C20
26	d	404	PL9	C22-C23-C24-C25
26	d	404	PL9	C27-C28-C29-C30
27	B	623	SQD	O5-C1-O6-C44
27	B	623	SQD	C8-C7-O47-C45
27	B	623	SQD	O5-C5-C6-S
27	a	612	SQD	O6-C44-C45-O47
27	b	601	SQD	O6-C44-C45-O47
27	b	602	SQD	O5-C1-O6-C44
27	b	602	SQD	C8-C7-O47-C45
27	b	602	SQD	O5-C5-C6-S
28	Z	101	LMG	O6-C1-O1-C7
28	Z	101	LMG	O9-C10-O7-C8
28	z	101	LMG	O6-C1-O1-C7
28	z	101	LMG	O1-C7-C8-O7
28	z	101	LMG	O9-C10-O7-C8
31	D	407	LHG	O1-C1-C2-C3
31	D	407	LHG	O2-C2-C3-O3
31	D	407	LHG	C3-O3-P-O5
31	D	407	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
31	E	101	LHG	C8-C7-O7-C5
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4
31	L	101	LHG	C4-O6-P-O5
31	d	406	LHG	O1-C1-C2-C3
31	d	406	LHG	C1-C2-C3-O3
31	d	406	LHG	O2-C2-C3-O3
31	d	406	LHG	C3-O3-P-O4
31	d	406	LHG	C3-O3-P-O5
31	d	406	LHG	C3-O3-P-O6
31	e	101	LHG	C8-C7-O7-C5
31	e	101	LHG	O10-C23-O8-C6
31	l	101	LHG	C4-O6-P-O3
31	l	101	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
32	D	406	DGD	C2B-C1B-O2G-C2G
32	d	405	DGD	C2B-C1B-O2G-C2G
28	z	101	LMG	C29-C28-O8-C9
27	X	101	SQD	O10-C23-O48-C46
27	x	101	SQD	O10-C23-O48-C46
31	E	101	LHG	O10-C23-O8-C6
27	X	101	SQD	C24-C23-O48-C46
27	x	101	SQD	C24-C23-O48-C46
31	e	101	LHG	C24-C23-O8-C6
28	Z	101	LMG	C29-C28-O8-C9
23	B	617	CLA	O1A-CGA-O2A-C1
23	b	619	CLA	O1A-CGA-O2A-C1
27	B	623	SQD	O49-C7-O47-C45
27	b	602	SQD	O49-C7-O47-C45
31	E	101	LHG	O9-C7-O7-C5
32	D	406	DGD	O1B-C1B-O2G-C2G
32	d	405	DGD	O1B-C1B-O2G-C2G
23	B	615	CLA	C3-C5-C6-C7
23	b	617	CLA	C3-C5-C6-C7
23	b	619	CLA	CBA-CGA-O2A-C1
31	E	101	LHG	C24-C23-O8-C6
28	Z	101	LMG	C11-C10-O7-C8
28	z	101	LMG	C11-C10-O7-C8
23	B	606	CLA	C4-C3-C5-C6
23	b	608	CLA	C4-C3-C5-C6
26	A	610	PL9	C12-C11-C9-C10
26	A	610	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
26	a	609	PL9	C12-C11-C9-C10
26	a	609	PL9	C25-C24-C26-C27
23	B	606	CLA	C2-C3-C5-C6
23	b	608	CLA	C2-C3-C5-C6
26	D	405	PL9	C18-C19-C21-C22
26	a	609	PL9	C18-C19-C21-C22
26	a	609	PL9	C38-C39-C41-C42
28	Z	101	LMG	O10-C28-O8-C9
28	z	101	LMG	O10-C28-O8-C9
23	B	602	CLA	C3-C5-C6-C7
23	b	604	CLA	C3-C5-C6-C7
23	B	617	CLA	CBA-CGA-O2A-C1
26	A	610	PL9	C27-C28-C29-C30
26	A	610	PL9	C37-C38-C39-C40
26	A	610	PL9	C42-C43-C44-C45
26	D	405	PL9	C12-C13-C14-C15
26	D	405	PL9	C32-C33-C34-C35
26	D	405	PL9	C37-C38-C39-C40
26	a	609	PL9	C12-C13-C14-C15
26	a	609	PL9	C22-C23-C24-C25
26	a	609	PL9	C27-C28-C29-C30
26	a	609	PL9	C37-C38-C39-C40
26	a	609	PL9	C42-C43-C44-C45
26	d	404	PL9	C7-C8-C9-C10
26	d	404	PL9	C12-C13-C14-C15
26	d	404	PL9	C32-C33-C34-C35
26	d	404	PL9	C37-C38-C39-C40
26	d	404	PL9	C42-C43-C44-C45
25	A	609	BCR	C19-C20-C21-C22
25	B	618	BCR	C19-C20-C21-C22
25	B	619	BCR	C13-C14-C15-C16
25	B	620	BCR	C19-C20-C21-C22
25	C	515	BCR	C13-C14-C15-C16
25	C	515	BCR	C15-C16-C17-C18
25	C	515	BCR	C19-C20-C21-C22
25	C	521	BCR	C13-C14-C15-C16
25	F	101	BCR	C13-C14-C15-C16
25	H	101	BCR	C15-C16-C17-C18
25	K	101	BCR	C15-C16-C17-C18
25	T	101	BCR	C13-C14-C15-C16
25	a	608	BCR	C15-C16-C17-C18
25	a	608	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	b	621	BCR	C13-C14-C15-C16
25	b	621	BCR	C15-C16-C17-C18
25	b	622	BCR	C15-C16-C17-C18
25	t	101	BCR	C19-C20-C21-C22
31	e	101	LHG	O9-C7-O7-C5
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	615	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	CBD-CGD-O2D-CED
28	j	101	LMG	O6-C5-C6-O5
25	C	514	BCR	C14-C15-C16-C17
25	k	101	BCR	C14-C15-C16-C17
26	A	610	PL9	C18-C19-C21-C22
26	A	610	PL9	C9-C11-C12-C13
26	A	610	PL9	C19-C21-C22-C23
26	A	610	PL9	C24-C26-C27-C28
26	D	405	PL9	C29-C31-C32-C33
26	D	405	PL9	C39-C41-C42-C43
26	D	405	PL9	C44-C46-C47-C48
26	a	609	PL9	C14-C16-C17-C18
26	a	609	PL9	C19-C21-C22-C23
26	a	609	PL9	C24-C26-C27-C28
26	d	404	PL9	C39-C41-C42-C43
26	d	404	PL9	C44-C46-C47-C48
32	c	519	DGD	O1A-C1A-O1G-C1G
27	X	101	SQD	O5-C1-O6-C44
27	x	101	SQD	O5-C1-O6-C44
32	D	406	DGD	O6E-C1E-O5D-C6D
32	d	405	DGD	O6E-C1E-O5D-C6D
28	J	101	LMG	O6-C5-C6-O5
23	b	608	CLA	O1D-CGD-O2D-CED
23	C	511	CLA	CBD-CGD-O2D-CED
28	C	520	LMG	O6-C5-C6-O5
26	a	609	PL9	C17-C18-C19-C20
28	c	521	LMG	O6-C5-C6-O5
26	A	610	PL9	C47-C48-C49-C50
26	D	405	PL9	C47-C48-C49-C51
26	a	609	PL9	C47-C48-C49-C50
28	c	521	LMG	C4-C5-C6-O5
25	C	521	BCR	C19-C20-C21-C22
25	F	101	BCR	C19-C20-C21-C22
25	a	608	BCR	C13-C14-C15-C16
23	C	505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	D	407	LHG	C1-C2-C3-O3
23	c	514	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C11-C10-C8-C9
23	C	501	CLA	C11-C12-C13-C14
23	C	502	CLA	C14-C13-C15-C16
23	C	504	CLA	C11-C12-C13-C14
23	C	509	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	c	502	CLA	C11-C12-C13-C14
23	c	503	CLA	C14-C13-C15-C16
23	c	505	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
28	J	101	LMG	C4-C5-C6-O5
27	X	101	SQD	C2-C1-O6-C44
27	x	101	SQD	C2-C1-O6-C44
32	D	406	DGD	C2E-C1E-O5D-C6D
32	d	405	DGD	C2E-C1E-O5D-C6D
32	d	405	DGD	C1B-C2B-C3B-C4B
32	d	405	DGD	O6E-C5E-C6E-O5E
28	C	520	LMG	C4-C5-C6-O5
25	C	514	BCR	C36-C18-C19-C20
25	C	514	BCR	C37-C22-C23-C24
25	C	515	BCR	C7-C8-C9-C34
25	C	515	BCR	C11-C12-C13-C35
25	C	521	BCR	C11-C12-C13-C35
25	K	101	BCR	C36-C18-C19-C20
25	T	101	BCR	C7-C8-C9-C34
25	a	608	BCR	C11-C12-C13-C35
25	b	621	BCR	C36-C18-C19-C20
25	b	622	BCR	C37-C22-C23-C24
25	c	515	BCR	C37-C22-C23-C24
25	c	516	BCR	C37-C22-C23-C24
25	f	101	BCR	C7-C8-C9-C34
25	h	101	BCR	C7-C8-C9-C34
25	h	101	BCR	C11-C12-C13-C35
25	h	101	BCR	C37-C22-C23-C24
25	k	101	BCR	C36-C18-C19-C20
25	B	619	BCR	C7-C8-C9-C10
25	B	619	BCR	C21-C22-C23-C24
25	C	514	BCR	C21-C22-C23-C24
25	T	101	BCR	C21-C22-C23-C24
25	a	608	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	b	621	BCR	C7-C8-C9-C10
25	c	515	BCR	C21-C22-C23-C24
25	h	101	BCR	C17-C18-C19-C20
25	k	101	BCR	C17-C18-C19-C20
25	t	101	BCR	C21-C22-C23-C24
28	A	612	LMG	C28-C29-C30-C31
26	d	404	PL9	C47-C48-C49-C51
28	Z	101	LMG	O1-C7-C8-O7
32	C	517	DGD	O6E-C5E-C6E-O5E
31	d	406	LHG	O1-C1-C2-O2
32	C	516	DGD	C2A-C3A-C4A-C5A
28	C	520	LMG	C28-C29-C30-C31
25	B	618	BCR	C9-C10-C11-C12
25	B	618	BCR	C13-C14-C15-C16
25	C	514	BCR	C13-C14-C15-C16
25	b	621	BCR	C9-C10-C11-C12
25	b	622	BCR	C19-C20-C21-C22
25	c	515	BCR	C13-C14-C15-C16
25	c	516	BCR	C19-C20-C21-C22
26	A	610	PL9	C47-C48-C49-C51
28	A	612	LMG	O9-C10-O7-C8
26	D	405	PL9	C9-C11-C12-C13
26	d	404	PL9	C9-C11-C12-C13
26	d	404	PL9	C29-C31-C32-C33
28	C	519	LMG	C28-C29-C30-C31
31	b	624	LHG	C23-C24-C25-C26
32	D	406	DGD	C1B-C2B-C3B-C4B
32	d	405	DGD	C1A-C2A-C3A-C4A
28	A	612	LMG	O10-C28-O8-C9
23	A	608	CLA	C10-C11-C12-C13
23	B	616	CLA	C5-C6-C7-C8
23	a	607	CLA	C10-C11-C12-C13
23	b	618	CLA	C5-C6-C7-C8
23	B	607[A]	CLA	C2A-CAA-CBA-CGA
23	B	607[B]	CLA	C2A-CAA-CBA-CGA
23	b	609[A]	CLA	C2A-CAA-CBA-CGA
23	b	609[B]	CLA	C2A-CAA-CBA-CGA
25	A	609	BCR	C10-C11-C12-C13
25	K	101	BCR	C18-C19-C20-C21
25	h	101	BCR	C18-C19-C20-C21
23	A	608	CLA	C13-C15-C16-C17
23	B	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C5-C6-C7-C8
23	a	607	CLA	C13-C15-C16-C17
23	b	604	CLA	C10-C11-C12-C13
23	b	617	CLA	C5-C6-C7-C8
27	a	612	SQD	C23-C24-C25-C26
27	b	601	SQD	C23-C24-C25-C26
28	a	611	LMG	C28-C29-C30-C31
28	c	521	LMG	C28-C29-C30-C31
31	B	622	LHG	C23-C24-C25-C26
32	C	517	DGD	C1B-C2B-C3B-C4B
32	c	518	DGD	C1B-C2B-C3B-C4B
32	C	518	DGD	O1A-C1A-O1G-C1G
25	c	515	BCR	C22-C23-C24-C25
32	C	516	DGD	O6D-C1D-O3G-C3G
23	B	607[A]	CLA	C13-C15-C16-C17
23	B	615	CLA	C10-C11-C12-C13
23	C	509	CLA	C8-C10-C11-C12
23	b	609[A]	CLA	C13-C15-C16-C17
23	b	617	CLA	C10-C11-C12-C13
23	c	510	CLA	C8-C10-C11-C12
32	D	406	DGD	C1A-C2A-C3A-C4A
23	C	506	CLA	C5-C6-C7-C8
32	C	517	DGD	C4E-C5E-C6E-O5E
23	B	611	CLA	O1D-CGD-O2D-CED
23	c	504	CLA	O1D-CGD-O2D-CED
23	D	404	CLA	C8-C10-C11-C12
23	c	507	CLA	C5-C6-C7-C8
23	d	403	CLA	C8-C10-C11-C12
32	D	406	DGD	O6E-C5E-C6E-O5E
28	a	611	LMG	O10-C28-O8-C9
28	j	101	LMG	C4-C5-C6-O5
27	B	623	SQD	C7-C8-C9-C10
27	b	602	SQD	C7-C8-C9-C10
28	Z	101	LMG	C10-C11-C12-C13
28	z	101	LMG	C10-C11-C12-C13
23	B	606	CLA	O1D-CGD-O2D-CED
23	A	606	CLA	C13-C15-C16-C17
23	B	607[A]	CLA	C15-C16-C17-C18
23	D	404	CLA	C10-C11-C12-C13
23	a	605	CLA	C13-C15-C16-C17
23	b	609[A]	CLA	C15-C16-C17-C18
23	d	403	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	d	405	DGD	C4E-C5E-C6E-O5E
23	b	608	CLA	CBD-CGD-O2D-CED
23	B	612	CLA	O1D-CGD-O2D-CED
32	c	517	DGD	O6D-C5D-C6D-O5D
25	B	619	BCR	C15-C16-C17-C18
25	C	521	BCR	C15-C16-C17-C18
25	H	101	BCR	C19-C20-C21-C22
25	b	620	BCR	C19-C20-C21-C22
32	c	519	DGD	C2A-C1A-O1G-C1G
23	C	509	CLA	C13-C15-C16-C17
23	c	510	CLA	C13-C15-C16-C17
32	c	517	DGD	C4D-C5D-C6D-O5D
23	A	608	CLA	C15-C16-C17-C18
23	B	612	CLA	C15-C16-C17-C18
23	a	607	CLA	C15-C16-C17-C18
23	b	614	CLA	C15-C16-C17-C18
23	B	607[B]	CLA	C10-C11-C12-C13
23	B	617	CLA	C10-C11-C12-C13
23	C	501	CLA	C15-C16-C17-C18
23	C	506	CLA	C10-C11-C12-C13
23	b	609[B]	CLA	C10-C11-C12-C13
23	b	619	CLA	C10-C11-C12-C13
23	c	502	CLA	C15-C16-C17-C18
23	c	507	CLA	C10-C11-C12-C13
28	a	611	LMG	C11-C10-O7-C8
26	D	405	PL9	C42-C43-C44-C45
28	a	611	LMG	O9-C10-O7-C8
32	D	406	DGD	C2D-C1D-O3G-C3G
32	d	405	DGD	C2D-C1D-O3G-C3G
26	A	610	PL9	C14-C16-C17-C18
26	a	609	PL9	C9-C11-C12-C13
23	A	606	CLA	C16-C17-C18-C20
23	a	605	CLA	C16-C17-C18-C20
23	B	609	CLA	C2C-C3C-CAC-CBC
23	c	506	CLA	O1A-CGA-O2A-C1
25	A	609	BCR	C35-C13-C14-C15
25	B	618	BCR	C20-C21-C22-C37
25	C	514	BCR	C35-C13-C14-C15
25	H	101	BCR	C11-C10-C9-C34
25	T	101	BCR	C35-C13-C14-C15
25	a	608	BCR	C11-C10-C9-C34
25	a	608	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
25	b	620	BCR	C20-C21-C22-C37
25	b	621	BCR	C11-C10-C9-C34
25	c	515	BCR	C11-C10-C9-C34
25	c	515	BCR	C35-C13-C14-C15
25	c	516	BCR	C20-C21-C22-C37
25	h	101	BCR	C11-C10-C9-C34
25	h	101	BCR	C35-C13-C14-C15
25	t	101	BCR	C11-C10-C9-C34
25	A	609	BCR	C7-C8-C9-C34
25	B	618	BCR	C37-C22-C23-C24
25	B	619	BCR	C37-C22-C23-C24
25	C	515	BCR	C37-C22-C23-C24
25	H	101	BCR	C7-C8-C9-C34
25	H	101	BCR	C11-C12-C13-C35
25	b	620	BCR	C11-C12-C13-C35
25	b	620	BCR	C37-C22-C23-C24
25	f	101	BCR	C11-C12-C13-C35
25	A	609	BCR	C17-C18-C19-C20
25	B	619	BCR	C17-C18-C19-C20
25	K	101	BCR	C17-C18-C19-C20
25	a	608	BCR	C17-C18-C19-C20
25	k	101	BCR	C7-C8-C9-C10
33	v	201	HEM	C2D-C3D-CAD-CBD
32	C	516	DGD	O6D-C5D-C6D-O5D
23	c	512	CLA	O1A-CGA-O2A-C1
31	D	407	LHG	C14-C15-C16-C17
31	B	622	LHG	O1-C1-C2-C3
28	c	520	LMG	C28-C29-C30-C31
25	B	619	BCR	C9-C10-C11-C12
25	h	101	BCR	C13-C14-C15-C16
23	C	506	CLA	C16-C17-C18-C19
23	c	507	CLA	C16-C17-C18-C19
25	A	609	BCR	C16-C17-C18-C19
25	C	514	BCR	C11-C10-C9-C8
25	C	515	BCR	C11-C10-C9-C8
25	F	101	BCR	C16-C17-C18-C19
25	a	608	BCR	C11-C10-C9-C8
25	a	608	BCR	C12-C13-C14-C15
25	a	608	BCR	C20-C21-C22-C23
25	b	620	BCR	C16-C17-C18-C19
25	c	516	BCR	C11-C10-C9-C8
25	c	522	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	f	101	BCR	C11-C10-C9-C8
25	k	101	BCR	C20-C21-C22-C23
28	A	612	LMG	C11-C10-O7-C8
32	C	516	DGD	C4D-C5D-C6D-O5D
23	B	614	CLA	C15-C16-C17-C18
23	b	616	CLA	C15-C16-C17-C18
32	c	517	DGD	O6E-C5E-C6E-O5E
23	D	404	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
32	H	102	DGD	C6B-C7B-C8B-C9B
31	d	406	LHG	O10-C23-O8-C6
27	A	611	SQD	C11-C12-C13-C14
27	a	610	SQD	C11-C12-C13-C14
27	a	612	SQD	C15-C16-C17-C18
28	b	623	LMG	C14-C15-C16-C17
28	j	101	LMG	C12-C13-C14-C15
32	C	517	DGD	C3A-C4A-C5A-C6A
32	c	518	DGD	CAB-CBB-CCB-CDB
27	X	101	SQD	C34-C35-C36-C37
27	x	101	SQD	C29-C30-C31-C32
27	x	101	SQD	C34-C35-C36-C37
28	a	611	LMG	C34-C35-C36-C37
28	b	623	LMG	C32-C33-C34-C35
28	c	520	LMG	C15-C16-C17-C18
31	b	624	LHG	C29-C30-C31-C32
31	b	624	LHG	C32-C33-C34-C35
32	C	517	DGD	CAA-CBA-CCA-CDA
32	c	517	DGD	C8B-C9B-CAB-CBB
32	c	518	DGD	C9A-CAA-CBA-CCA
32	c	519	DGD	C9B-CAB-CBB-CCB
27	X	101	SQD	C29-C30-C31-C32
27	b	601	SQD	C15-C16-C17-C18
28	B	621	LMG	C37-C38-C39-C40
28	C	520	LMG	C29-C30-C31-C32
28	j	101	LMG	C14-C15-C16-C17
28	j	101	LMG	C16-C17-C18-C19
31	l	101	LHG	C12-C13-C14-C15
32	D	406	DGD	C7B-C8B-C9B-CAB
32	d	405	DGD	CCB-CDB-CEB-CFB
27	A	611	SQD	C12-C13-C14-C15
27	A	611	SQD	C15-C16-C17-C18
27	X	101	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
27	a	610	SQD	C15-C16-C17-C18
27	a	610	SQD	C28-C29-C30-C31
27	x	101	SQD	C26-C27-C28-C29
28	A	612	LMG	C12-C13-C14-C15
28	A	612	LMG	C15-C16-C17-C18
28	A	612	LMG	C34-C35-C36-C37
28	B	621	LMG	C14-C15-C16-C17
28	J	101	LMG	C12-C13-C14-C15
28	J	101	LMG	C14-C15-C16-C17
28	J	101	LMG	C16-C17-C18-C19
28	c	521	LMG	C29-C30-C31-C32
28	j	101	LMG	C39-C40-C41-C42
31	B	622	LHG	C25-C26-C27-C28
31	B	622	LHG	C29-C30-C31-C32
31	e	101	LHG	C24-C25-C26-C27
32	C	516	DGD	C8B-C9B-CAB-CBB
32	c	517	DGD	C5B-C6B-C7B-C8B
32	c	519	DGD	C2A-C3A-C4A-C5A
32	d	405	DGD	C2A-C3A-C4A-C5A
31	D	407	LHG	O1-C1-C2-O2
27	A	611	SQD	C28-C29-C30-C31
27	a	610	SQD	C12-C13-C14-C15
28	C	519	LMG	C15-C16-C17-C18
23	c	511	CLA	O1D-CGD-O2D-CED
23	B	617	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C4B-C3B-CAB-CBB
32	C	517	DGD	C1A-C2A-C3A-C4A
28	c	521	LMG	C31-C32-C33-C34
31	E	101	LHG	C13-C14-C15-C16
31	E	101	LHG	C14-C15-C16-C17
32	h	102	DGD	CBA-CCA-CDA-CEA
31	E	101	LHG	C15-C16-C17-C18
23	B	617	CLA	C8-C10-C11-C12
23	b	619	CLA	C8-C10-C11-C12
31	D	408	LHG	C7-C8-C9-C10
28	B	621	LMG	C32-C33-C34-C35
28	J	101	LMG	C39-C40-C41-C42
28	a	611	LMG	C15-C16-C17-C18
28	b	623	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	E	101	LHG	C24-C25-C26-C27
31	e	101	LHG	C14-C15-C16-C17
32	c	517	DGD	C4B-C5B-C6B-C7B
32	d	405	DGD	CCA-CDA-CEA-CFA
32	C	517	DGD	C9A-CAA-CBA-CCA
32	H	102	DGD	C7A-C8A-C9A-CAA
32	c	518	DGD	C3A-C4A-C5A-C6A
28	B	621	LMG	C10-C11-C12-C13
25	B	618	BCR	C15-C16-C17-C18
23	a	613	CLA	O1D-CGD-O2D-CED
32	d	405	DGD	C7B-C8B-C9B-CAB
28	c	520	LMG	C32-C33-C34-C35
32	D	406	DGD	C8B-C9B-CAB-CBB
23	c	512	CLA	CBA-CGA-O2A-C1
27	a	612	SQD	C24-C23-O48-C46
27	b	601	SQD	C24-C23-O48-C46
27	A	611	SQD	C16-C17-C18-C19
27	a	610	SQD	C16-C17-C18-C19
27	a	612	SQD	C16-C17-C18-C19
27	b	601	SQD	C16-C17-C18-C19
28	C	520	LMG	C30-C31-C32-C33
28	C	520	LMG	C31-C32-C33-C34
28	j	101	LMG	C13-C14-C15-C16
31	L	101	LHG	C25-C26-C27-C28
31	b	624	LHG	C25-C26-C27-C28
31	e	101	LHG	C25-C26-C27-C28
32	c	517	DGD	CAB-CBB-CCB-CDB
32	c	518	DGD	CAA-CBA-CCA-CDA
32	c	518	DGD	CBB-CCB-CDB-CEB
28	b	623	LMG	C10-C11-C12-C13
31	e	101	LHG	C7-C8-C9-C10
32	c	518	DGD	C1A-C2A-C3A-C4A
23	b	612	CLA	O1D-CGD-O2D-CED
27	A	611	SQD	C9-C10-C11-C12
27	B	623	SQD	C11-C10-C9-C8
27	B	623	SQD	C24-C25-C26-C27
27	a	612	SQD	C26-C27-C28-C29
27	b	601	SQD	C26-C27-C28-C29
27	b	602	SQD	C11-C10-C9-C8
27	b	602	SQD	C24-C25-C26-C27
28	B	621	LMG	C31-C32-C33-C34
28	a	611	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	a	611	LMG	C13-C14-C15-C16
28	c	521	LMG	C30-C31-C32-C33
31	D	408	LHG	C15-C16-C17-C18
31	E	101	LHG	C25-C26-C27-C28
31	e	101	LHG	C13-C14-C15-C16
32	C	516	DGD	C6A-C7A-C8A-C9A
32	C	516	DGD	CAB-CBB-CCB-CDB
32	H	102	DGD	CBA-CCA-CDA-CEA
27	B	623	SQD	C31-C32-C33-C34
27	a	610	SQD	C9-C10-C11-C12
27	b	602	SQD	C31-C32-C33-C34
27	x	101	SQD	C31-C32-C33-C34
28	B	621	LMG	C12-C13-C14-C15
32	C	518	DGD	C2A-C3A-C4A-C5A
32	D	406	DGD	C2A-C3A-C4A-C5A
32	c	517	DGD	C4A-C5A-C6A-C7A
27	X	101	SQD	C24-C25-C26-C27
27	x	101	SQD	C24-C25-C26-C27
28	j	101	LMG	C36-C37-C38-C39
32	c	517	DGD	C6A-C7A-C8A-C9A
23	b	604	CLA	O1D-CGD-O2D-CED
27	X	101	SQD	C31-C32-C33-C34
27	b	602	SQD	C34-C35-C36-C37
28	A	612	LMG	C13-C14-C15-C16
28	j	101	LMG	C30-C31-C32-C33
31	L	101	LHG	C33-C34-C35-C36
23	C	507	CLA	C16-C17-C18-C19
23	c	508	CLA	C16-C17-C18-C19
31	E	101	LHG	C7-C8-C9-C10
25	B	618	BCR	C1-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C26
25	B	619	BCR	C1-C6-C7-C8
25	B	620	BCR	C5-C6-C7-C8
25	C	514	BCR	C5-C6-C7-C8
25	C	515	BCR	C5-C6-C7-C8
25	F	101	BCR	C5-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C26
25	K	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C23-C24-C25-C30
25	T	101	BCR	C1-C6-C7-C8
25	a	608	BCR	C1-C6-C7-C8
25	b	620	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	b	621	BCR	C23-C24-C25-C30
25	b	622	BCR	C23-C24-C25-C26
25	c	516	BCR	C23-C24-C25-C26
25	f	101	BCR	C5-C6-C7-C8
25	h	101	BCR	C5-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C26
25	k	101	BCR	C1-C6-C7-C8
25	t	101	BCR	C1-C6-C7-C8
25	t	101	BCR	C5-C6-C7-C8
27	B	623	SQD	C10-C11-C12-C13
27	B	623	SQD	C34-C35-C36-C37
27	b	602	SQD	C10-C11-C12-C13
31	L	101	LHG	C12-C13-C14-C15
27	X	101	SQD	C8-C7-O47-C45
27	x	101	SQD	C8-C7-O47-C45
28	b	623	LMG	C11-C10-O7-C8
23	c	506	CLA	CBA-CGA-O2A-C1
23	B	605	CLA	C13-C15-C16-C17
28	j	101	LMG	C15-C16-C17-C18
28	z	101	LMG	C12-C13-C14-C15
32	C	517	DGD	C6B-C7B-C8B-C9B
32	C	517	DGD	CBB-CCB-CDB-CEB
32	D	406	DGD	CCA-CDA-CEA-CFA
31	B	622	LHG	C32-C33-C34-C35
23	b	607	CLA	C13-C15-C16-C17
28	z	101	LMG	C16-C17-C18-C19
32	C	517	DGD	CAB-CBB-CCB-CDB
32	d	405	DGD	O1A-C1A-O1G-C1G
26	A	610	PL9	C4-C3-C7-C8
28	Z	101	LMG	C16-C17-C18-C19
28	b	623	LMG	C16-C17-C18-C19
31	E	101	LHG	C27-C28-C29-C30
31	L	101	LHG	C13-C14-C15-C16
32	c	518	DGD	C6B-C7B-C8B-C9B
32	h	102	DGD	C7A-C8A-C9A-CAA
23	C	509	CLA	O1D-CGD-O2D-CED
27	b	602	SQD	C11-C12-C13-C14
28	J	101	LMG	C15-C16-C17-C18
31	E	101	LHG	C18-C19-C20-C21
31	a	614	LHG	C15-C16-C17-C18
31	l	101	LHG	C11-C12-C13-C14
31	l	101	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
25	B	619	BCR	C18-C19-C20-C21
25	b	622	BCR	C10-C11-C12-C13
25	f	101	BCR	C18-C19-C20-C21
26	A	610	PL9	C38-C39-C41-C42
26	d	404	PL9	C18-C19-C21-C22
27	B	623	SQD	C11-C12-C13-C14
28	z	101	LMG	C15-C16-C17-C18
32	d	405	DGD	C9A-CAA-CBA-CCA
28	Z	101	LMG	C19-C20-C21-C22
28	z	101	LMG	C19-C20-C21-C22
32	D	406	DGD	CCB-CDB-CEB-CFB
28	B	621	LMG	C15-C16-C17-C18
25	B	620	BCR	C6-C7-C8-C9
25	C	521	BCR	C22-C23-C24-C25
25	c	515	BCR	C6-C7-C8-C9
25	k	101	BCR	C6-C7-C8-C9
32	D	406	DGD	O6D-C1D-O3G-C3G
32	c	518	DGD	O6E-C1E-O5D-C6D
32	d	405	DGD	O6D-C1D-O3G-C3G
28	A	612	LMG	C14-C15-C16-C17
28	b	623	LMG	C12-C13-C14-C15
28	b	623	LMG	C37-C38-C39-C40
32	c	518	DGD	C4A-C5A-C6A-C7A
28	c	521	LMG	C17-C18-C19-C20
31	l	101	LHG	C13-C14-C15-C16
28	A	612	LMG	C18-C19-C20-C21
28	B	621	LMG	C16-C17-C18-C19
31	e	101	LHG	C18-C19-C20-C21
32	C	517	DGD	C4A-C5A-C6A-C7A
32	d	405	DGD	C9B-CAB-CBB-CCB
28	a	611	LMG	C14-C15-C16-C17
31	l	101	LHG	C34-C35-C36-C37
23	C	505	CLA	CBA-CGA-O2A-C1
31	a	614	LHG	C29-C30-C31-C32
28	B	621	LMG	O9-C10-O7-C8
28	C	520	LMG	O9-C10-O7-C8
28	c	521	LMG	O9-C10-O7-C8
28	C	519	LMG	C16-C17-C18-C19
28	c	520	LMG	C16-C17-C18-C19
32	C	516	DGD	C5B-C6B-C7B-C8B
23	C	506	CLA	C13-C15-C16-C17
23	c	507	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	C	515	BCR	C36-C18-C19-C20
25	C	521	BCR	C36-C18-C19-C20
25	c	522	BCR	C36-C18-C19-C20
28	C	519	LMG	C10-C11-C12-C13
28	J	101	LMG	C13-C14-C15-C16
31	B	622	LHG	C24-C25-C26-C27
32	D	406	DGD	C5B-C6B-C7B-C8B
25	c	516	BCR	C17-C18-C19-C20
27	a	612	SQD	C28-C29-C30-C31
32	C	516	DGD	C4B-C5B-C6B-C7B
32	C	516	DGD	C7B-C8B-C9B-CAB
32	d	405	DGD	CBA-CCA-CDA-CEA
23	C	506	CLA	C16-C17-C18-C20
23	D	404	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C20
27	b	601	SQD	C28-C29-C30-C31
32	D	406	DGD	C9B-CAB-CBB-CCB
32	H	102	DGD	CCB-CDB-CEB-CFB
28	C	519	LMG	C32-C33-C34-C35
26	a	609	PL9	C47-C48-C49-C51
23	a	613	CLA	C2C-C3C-CAC-CBC
27	a	612	SQD	O10-C23-O48-C46
23	C	504	CLA	C13-C15-C16-C17
23	c	505	CLA	C13-C15-C16-C17
32	C	516	DGD	C4A-C5A-C6A-C7A
28	c	520	LMG	C10-C11-C12-C13
27	b	602	SQD	C29-C30-C31-C32
31	D	407	LHG	C32-C33-C34-C35
32	C	516	DGD	C6B-C7B-C8B-C9B
32	C	518	DGD	C6A-C7A-C8A-C9A
27	B	623	SQD	C29-C30-C31-C32
28	A	612	LMG	C36-C37-C38-C39
28	a	611	LMG	C38-C39-C40-C41
31	a	614	LHG	C10-C11-C12-C13
32	C	518	DGD	C9B-CAB-CBB-CCB
23	C	507	CLA	C16-C17-C18-C20
23	c	507	CLA	C16-C17-C18-C20
23	c	508	CLA	C16-C17-C18-C20
23	b	615	CLA	O1A-CGA-O2A-C1
27	b	601	SQD	O10-C23-O48-C46
27	B	623	SQD	C18-C19-C20-C21
27	b	602	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
28	c	520	LMG	C34-C35-C36-C37
32	D	406	DGD	C9A-CAA-CBA-CCA
31	e	101	LHG	C15-C16-C17-C18
32	h	102	DGD	CCB-CDB-CEB-CFB
28	J	101	LMG	C38-C39-C40-C41
28	Z	101	LMG	C12-C13-C14-C15
28	b	623	LMG	C15-C16-C17-C18
28	c	520	LMG	C38-C39-C40-C41
31	e	101	LHG	C27-C28-C29-C30
32	c	519	DGD	C6A-C7A-C8A-C9A
23	C	501	CLA	C13-C15-C16-C17
23	c	502	CLA	C13-C15-C16-C17
32	C	516	DGD	O6E-C5E-C6E-O5E
28	C	520	LMG	C17-C18-C19-C20
31	D	408	LHG	C10-C11-C12-C13
31	b	624	LHG	C24-C25-C26-C27
32	D	406	DGD	CBA-CCA-CDA-CEA
27	x	101	SQD	C30-C31-C32-C33
28	C	520	LMG	C18-C19-C20-C21
28	c	520	LMG	C29-C30-C31-C32
23	A	606	CLA	C16-C17-C18-C19
23	B	605	CLA	C16-C17-C18-C20
23	a	605	CLA	C16-C17-C18-C19
23	b	607	CLA	C16-C17-C18-C20
27	X	101	SQD	C30-C31-C32-C33
27	a	610	SQD	C30-C31-C32-C33
28	c	521	LMG	C18-C19-C20-C21
32	D	406	DGD	CAA-CBA-CCA-CDA
27	A	611	SQD	C32-C33-C34-C35
27	a	610	SQD	C32-C33-C34-C35
32	c	518	DGD	C9B-CAB-CBB-CCB
33	v	201	HEM	C4D-C3D-CAD-CBD
26	D	405	PL9	C25-C24-C26-C27
27	X	101	SQD	O49-C7-O47-C45
27	x	101	SQD	O49-C7-O47-C45
31	l	101	LHG	C1-C2-C3-O3
27	A	611	SQD	C30-C31-C32-C33
28	B	621	LMG	C17-C18-C19-C20
28	C	519	LMG	C17-C18-C19-C20
31	b	624	LHG	C33-C34-C35-C36
31	l	101	LHG	C31-C32-C33-C34
32	c	517	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
23	B	607[A]	CLA	CBD-CGD-O2D-CED
23	B	612	CLA	CBD-CGD-O2D-CED
31	a	614	LHG	C27-C28-C29-C30
23	C	507	CLA	C5-C6-C7-C8
23	c	508	CLA	C5-C6-C7-C8
23	B	605	CLA	C2C-C3C-CAC-CBC
31	D	408	LHG	C29-C30-C31-C32
28	c	521	LMG	C11-C10-O7-C8
28	C	519	LMG	C38-C39-C40-C41
23	A	608	CLA	C16-C17-C18-C19
23	a	607	CLA	C16-C17-C18-C19
28	C	520	LMG	C38-C39-C40-C41
32	c	518	DGD	C8B-C9B-CAB-CBB
28	b	623	LMG	C31-C32-C33-C34
23	C	505	CLA	C1A-C2A-CAA-CBA
32	C	517	DGD	O6E-C1E-O5D-C6D
28	a	611	LMG	C32-C33-C34-C35
27	b	602	SQD	C32-C33-C34-C35
28	c	521	LMG	C33-C34-C35-C36
31	l	101	LHG	C32-C33-C34-C35
27	B	623	SQD	C32-C33-C34-C35
28	b	623	LMG	C34-C35-C36-C37
28	c	520	LMG	C17-C18-C19-C20
28	j	101	LMG	C19-C20-C21-C22
28	b	623	LMG	C28-C29-C30-C31
28	z	101	LMG	C4-C5-C6-O5
23	B	602	CLA	C11-C10-C8-C7
23	B	617	CLA	C11-C12-C13-C15
23	C	506	CLA	C11-C12-C13-C15
23	C	508	CLA	C11-C10-C8-C7
23	D	404	CLA	C11-C10-C8-C7
23	b	604	CLA	C11-C10-C8-C7
23	b	619	CLA	C11-C12-C13-C15
23	c	507	CLA	C11-C12-C13-C15
23	c	509	CLA	C11-C10-C8-C7
23	d	403	CLA	C11-C10-C8-C7
31	L	101	LHG	C31-C32-C33-C34
28	C	520	LMG	C29-C28-O8-C9
27	A	611	SQD	C34-C35-C36-C37
28	a	611	LMG	C18-C19-C20-C21
23	B	607[B]	CLA	C15-C16-C17-C18
23	b	609[B]	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	X	101	SQD	C23-C24-C25-C26
27	x	101	SQD	C23-C24-C25-C26
27	a	610	SQD	C34-C35-C36-C37
28	C	520	LMG	C15-C16-C17-C18
31	L	101	LHG	C27-C28-C29-C30
26	d	404	PL9	C28-C29-C31-C32
23	D	404	CLA	C13-C15-C16-C17
23	d	403	CLA	C13-C15-C16-C17
23	C	501	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	D	404	CLA	C11-C10-C8-C9
23	c	502	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C14
23	d	403	CLA	C11-C10-C8-C9
32	D	406	DGD	C3A-C4A-C5A-C6A
25	C	514	BCR	C15-C16-C17-C18
25	h	101	BCR	C15-C16-C17-C18
28	a	611	LMG	C31-C32-C33-C34
32	d	405	DGD	C5B-C6B-C7B-C8B
27	b	602	SQD	C27-C28-C29-C30
27	B	623	SQD	C27-C28-C29-C30
28	J	101	LMG	C35-C36-C37-C38
28	Z	101	LMG	C15-C16-C17-C18
32	C	517	DGD	C2E-C1E-O5D-C6D
32	c	518	DGD	C2E-C1E-O5D-C6D
23	b	616	CLA	O1D-CGD-O2D-CED
27	a	612	SQD	O6-C44-C45-C46
27	b	601	SQD	O6-C44-C45-C46
28	A	612	LMG	C7-C8-C9-O8
28	a	611	LMG	C7-C8-C9-O8
28	z	101	LMG	O1-C7-C8-C9
32	D	406	DGD	O1G-C1G-C2G-C3G
32	H	102	DGD	O1G-C1G-C2G-C3G
32	h	102	DGD	O1G-C1G-C2G-C3G
28	B	621	LMG	C38-C39-C40-C41
28	C	519	LMG	C34-C35-C36-C37
28	b	623	LMG	C38-C39-C40-C41
28	c	520	LMG	C39-C40-C41-C42
32	C	518	DGD	C3B-C4B-C5B-C6B
32	d	405	DGD	C8B-C9B-CAB-CBB
31	l	101	LHG	O2-C2-C3-O3
32	h	102	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
28	c	520	LMG	C21-C22-C23-C24
26	D	405	PL9	C42-C43-C44-C46
25	A	609	BCR	C11-C10-C9-C34
25	B	620	BCR	C35-C13-C14-C15
25	K	101	BCR	C11-C10-C9-C34
25	t	101	BCR	C35-C13-C14-C15
23	C	509	CLA	C10-C11-C12-C13
23	c	510	CLA	C10-C11-C12-C13
31	L	101	LHG	C11-C12-C13-C14
32	C	517	DGD	C9B-CAB-CBB-CCB
32	c	517	DGD	C1B-C2B-C3B-C4B
31	D	407	LHG	O10-C23-O8-C6
26	D	405	PL9	C43-C44-C46-C47
25	b	620	BCR	C36-C18-C19-C20
25	f	101	BCR	C36-C18-C19-C20
26	d	404	PL9	C47-C48-C49-C50
27	B	623	SQD	C13-C14-C15-C16
27	b	602	SQD	C13-C14-C15-C16
32	C	517	DGD	C8B-C9B-CAB-CBB
32	H	102	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	CAA-CBA-CCA-CDA
25	C	515	BCR	C21-C22-C23-C24
25	T	101	BCR	C17-C18-C19-C20
25	h	101	BCR	C11-C12-C13-C14
25	t	101	BCR	C17-C18-C19-C20
32	D	406	DGD	O1A-C1A-O1G-C1G
23	A	608	CLA	C5-C6-C7-C8
23	B	613	CLA	C13-C15-C16-C17
23	b	615	CLA	C13-C15-C16-C17
32	d	405	DGD	C5A-C6A-C7A-C8A
23	a	607	CLA	C5-C6-C7-C8
27	b	601	SQD	C18-C19-C20-C21
28	B	621	LMG	C18-C19-C20-C21
23	C	512	CLA	O1A-CGA-O2A-C1
27	a	612	SQD	C18-C19-C20-C21
31	a	614	LHG	C12-C13-C14-C15
25	b	621	BCR	C10-C11-C12-C13
32	d	405	DGD	CBB-CCB-CDB-CEB
25	A	609	BCR	C9-C10-C11-C12
25	F	101	BCR	C15-C16-C17-C18
25	f	101	BCR	C19-C20-C21-C22
23	A	608	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C16-C17-C18-C19
23	a	607	CLA	C16-C17-C18-C20
23	b	607	CLA	C16-C17-C18-C19
32	C	517	DGD	C3B-C4B-C5B-C6B
32	c	519	DGD	C4A-C5A-C6A-C7A
25	T	101	BCR	C16-C17-C18-C19
25	c	522	BCR	C12-C13-C14-C15
25	f	101	BCR	C20-C21-C22-C23
28	a	611	LMG	C36-C37-C38-C39
25	c	522	BCR	C22-C23-C24-C25
32	H	102	DGD	O6E-C1E-O5D-C6D
28	c	520	LMG	C11-C12-C13-C14
31	L	101	LHG	C32-C33-C34-C35
23	C	512	CLA	CBA-CGA-O2A-C1
27	B	623	SQD	C24-C23-O48-C46
27	b	602	SQD	C24-C23-O48-C46
28	A	612	LMG	C29-C28-O8-C9
28	a	611	LMG	C29-C28-O8-C9
28	c	520	LMG	C19-C20-C21-C22
31	D	408	LHG	C27-C28-C29-C30
28	j	101	LMG	C38-C39-C40-C41
32	h	102	DGD	C6B-C7B-C8B-C9B
23	B	617	CLA	C16-C17-C18-C20
23	b	619	CLA	C16-C17-C18-C20
27	a	610	SQD	C27-C28-C29-C30
28	b	623	LMG	C18-C19-C20-C21
31	L	101	LHG	C24-C25-C26-C27
32	D	406	DGD	C4B-C5B-C6B-C7B
32	c	518	DGD	C7B-C8B-C9B-CAB
32	c	519	DGD	C8B-C9B-CAB-CBB
27	x	101	SQD	C35-C36-C37-C38
27	A	611	SQD	C27-C28-C29-C30
27	B	623	SQD	C28-C29-C30-C31
27	b	602	SQD	C28-C29-C30-C31
28	C	519	LMG	C19-C20-C21-C22
31	D	408	LHG	C12-C13-C14-C15
31	e	101	LHG	C11-C10-C9-C8
32	D	406	DGD	CBB-CCB-CDB-CEB
27	X	101	SQD	C35-C36-C37-C38
28	A	612	LMG	C30-C31-C32-C33
31	B	622	LHG	C13-C14-C15-C16
31	B	622	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
32	d	405	DGD	C3A-C4A-C5A-C6A
28	z	101	LMG	C13-C14-C15-C16
32	C	516	DGD	CAA-CBA-CCA-CDA
27	b	601	SQD	C19-C20-C21-C22
28	A	612	LMG	C31-C32-C33-C34
27	a	612	SQD	C19-C20-C21-C22
27	A	611	SQD	C35-C36-C37-C38
27	B	623	SQD	C35-C36-C37-C38
27	b	602	SQD	C35-C36-C37-C38
32	h	102	DGD	CDB-CEB-CFB-CGB
28	J	101	LMG	C19-C20-C21-C22
31	B	622	LHG	C15-C16-C17-C18
31	a	614	LHG	C30-C31-C32-C33
32	c	519	DGD	C6B-C7B-C8B-C9B
32	h	102	DGD	C9A-CAA-CBA-CCA
31	B	622	LHG	C24-C23-O8-C6
27	a	610	SQD	C35-C36-C37-C38
28	Z	101	LMG	C13-C14-C15-C16
32	C	518	DGD	C9A-CAA-CBA-CCA
28	C	520	LMG	C33-C34-C35-C36
31	E	101	LHG	C9-C10-C11-C12
32	H	102	DGD	CDB-CEB-CFB-CGB
28	c	521	LMG	C38-C39-C40-C41
25	A	609	BCR	C15-C16-C17-C18
25	B	620	BCR	C15-C16-C17-C18
25	c	516	BCR	C15-C16-C17-C18
23	B	604	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C20
32	c	519	DGD	C2B-C3B-C4B-C5B
26	a	609	PL9	C45-C44-C46-C47
27	A	611	SQD	C14-C15-C16-C17
27	a	610	SQD	C14-C15-C16-C17
32	C	517	DGD	C5A-C6A-C7A-C8A
32	c	518	DGD	C3B-C4B-C5B-C6B
32	H	102	DGD	C9B-CAB-CBB-CCB
32	c	519	DGD	CBA-CCA-CDA-CEA
32	H	102	DGD	O6E-C5E-C6E-O5E
32	c	517	DGD	C7B-C8B-C9B-CAB
28	b	623	LMG	O9-C10-O7-C8
23	B	615	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	B	617	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C11-C10-C8-C9
23	C	508	CLA	C11-C10-C8-C9
23	b	617	CLA	C11-C12-C13-C14
23	b	617	CLA	C14-C13-C15-C16
23	b	619	CLA	C11-C12-C13-C14
23	c	508	CLA	C11-C10-C8-C9
23	c	509	CLA	C11-C10-C8-C9
31	D	408	LHG	C17-C18-C19-C20
32	c	519	DGD	C9A-CAA-CBA-CCA
23	B	603	CLA	C4B-C3B-CAB-CBB
23	B	607[A]	CLA	C4B-C3B-CAB-CBB
23	B	607[B]	CLA	C4B-C3B-CAB-CBB
23	C	502	CLA	C4B-C3B-CAB-CBB
23	b	605	CLA	C4B-C3B-CAB-CBB
23	b	609[A]	CLA	C4B-C3B-CAB-CBB
23	b	609[B]	CLA	C4B-C3B-CAB-CBB
23	b	619	CLA	C4B-C3B-CAB-CBB
31	L	101	LHG	C34-C35-C36-C37
32	H	102	DGD	CAA-CBA-CCA-CDA
32	c	517	DGD	C2A-C3A-C4A-C5A
28	C	519	LMG	C20-C21-C22-C23
32	D	406	DGD	C4E-C5E-C6E-O5E
28	z	101	LMG	C2-C1-O1-C7
23	b	611	CLA	C13-C15-C16-C17
28	C	519	LMG	C13-C14-C15-C16
31	l	101	LHG	C24-C25-C26-C27
32	C	517	DGD	C7B-C8B-C9B-CAB
28	c	520	LMG	C13-C14-C15-C16
23	B	605	CLA	C4C-C3C-CAC-CBC
23	b	604	CLA	CAA-CBA-CGA-O2A
32	H	102	DGD	O2G-C1B-C2B-C3B
23	A	608	CLA	C11-C10-C8-C7
23	B	602	CLA	C6-C7-C8-C10
23	B	615	CLA	C11-C12-C13-C15
23	C	501	CLA	C11-C12-C13-C15
23	C	501	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C7
23	C	512	CLA	C11-C10-C8-C7
23	C	513	CLA	C6-C7-C8-C10
23	D	404	CLA	C6-C7-C8-C10
23	a	607	CLA	C11-C10-C8-C7
23	b	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	b	617	CLA	C11-C12-C13-C15
23	c	502	CLA	C11-C12-C13-C15
23	c	502	CLA	C12-C13-C15-C16
23	c	513	CLA	C11-C10-C8-C7
23	c	514	CLA	C6-C7-C8-C10
23	d	403	CLA	C6-C7-C8-C10
23	B	609	CLA	C13-C15-C16-C17
28	a	611	LMG	C10-C11-C12-C13
28	a	611	LMG	C22-C23-C24-C25
32	D	406	DGD	CAB-CBB-CCB-CDB
23	B	608	CLA	C3A-C2A-CAA-CBA
26	D	405	PL9	C45-C44-C46-C47
26	A	610	PL9	C28-C29-C31-C32
27	a	612	SQD	O5-C1-O6-C44
27	b	601	SQD	O5-C1-O6-C44
32	H	102	DGD	CCA-CDA-CEA-CFA
31	b	624	LHG	C31-C32-C33-C34
28	c	520	LMG	C29-C28-O8-C9
27	A	611	SQD	C19-C20-C21-C22
27	a	610	SQD	C19-C20-C21-C22
32	C	517	DGD	CDB-CEB-CFB-CGB
25	F	101	BCR	C9-C10-C11-C12
25	b	621	BCR	C19-C20-C21-C22
25	c	522	BCR	C15-C16-C17-C18
25	f	101	BCR	C15-C16-C17-C18
25	t	101	BCR	C13-C14-C15-C16
28	j	101	LMG	C20-C21-C22-C23
32	D	406	DGD	C5A-C6A-C7A-C8A
23	C	510	CLA	O1A-CGA-O2A-C1
27	b	601	SQD	C25-C26-C27-C28
32	C	518	DGD	C6B-C7B-C8B-C9B
25	T	101	BCR	C11-C12-C13-C14
27	a	612	SQD	C25-C26-C27-C28
31	l	101	LHG	C26-C27-C28-C29
28	B	621	LMG	C11-C10-O7-C8
31	e	101	LHG	C12-C13-C14-C15
31	d	406	LHG	C24-C23-O8-C6
23	B	616	CLA	C13-C15-C16-C17
23	b	618	CLA	C13-C15-C16-C17
27	B	623	SQD	C44-C45-C46-O48
27	b	602	SQD	C44-C45-C46-O48
32	d	405	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C16-C17-C18-C20
23	b	604	CLA	C16-C17-C18-C20
31	E	101	LHG	C26-C27-C28-C29
31	d	406	LHG	C34-C35-C36-C37
27	b	601	SQD	C31-C32-C33-C34
31	D	408	LHG	C18-C19-C20-C21
27	a	612	SQD	C31-C32-C33-C34
26	D	405	PL9	C13-C14-C16-C17
26	d	404	PL9	C13-C14-C16-C17
26	d	404	PL9	C43-C44-C46-C47
32	H	102	DGD	C4E-C5E-C6E-O5E
28	C	520	LMG	C40-C41-C42-C43
32	C	517	DGD	C6A-C7A-C8A-C9A
32	d	405	DGD	C4B-C5B-C6B-C7B
23	b	618	CLA	C10-C11-C12-C13
25	A	609	BCR	C1-C6-C7-C8
25	C	515	BCR	C23-C24-C25-C26
25	C	521	BCR	C23-C24-C25-C30
25	K	101	BCR	C1-C6-C7-C8
25	b	622	BCR	C5-C6-C7-C8
25	c	516	BCR	C1-C6-C7-C8
25	c	522	BCR	C23-C24-C25-C30
25	k	101	BCR	C23-C24-C25-C30
25	t	101	BCR	C23-C24-C25-C26
25	t	101	BCR	C23-C24-C25-C30
32	C	517	DGD	C8A-C9A-CAA-CBA
23	B	616	CLA	C10-C11-C12-C13
23	c	509	CLA	C5-C6-C7-C8
28	b	623	LMG	C33-C34-C35-C36
23	C	511	CLA	O1A-CGA-O2A-C1
31	e	101	LHG	C9-C10-C11-C12
23	C	508	CLA	C5-C6-C7-C8
27	a	612	SQD	C32-C33-C34-C35
27	b	601	SQD	C32-C33-C34-C35
31	e	101	LHG	C17-C18-C19-C20
25	H	101	BCR	C13-C14-C15-C16
28	A	612	LMG	C22-C23-C24-C25
28	B	621	LMG	C33-C34-C35-C36
32	C	518	DGD	C5B-C6B-C7B-C8B
23	C	501	CLA	C16-C17-C18-C19
23	C	502	CLA	C16-C17-C18-C20
23	c	502	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	c	503	CLA	C16-C17-C18-C20
27	B	623	SQD	O47-C45-C46-O48
27	b	602	SQD	O47-C45-C46-O48
28	A	612	LMG	O1-C7-C8-O7
28	A	612	LMG	O7-C8-C9-O8
32	d	405	DGD	O1G-C1G-C2G-O2G
26	a	609	PL9	C4-C3-C7-C8
26	d	404	PL9	C4-C3-C7-C8
28	A	612	LMG	C32-C33-C34-C35
27	a	612	SQD	C35-C36-C37-C38
27	b	601	SQD	C35-C36-C37-C38
26	d	404	PL9	C30-C29-C31-C32
31	B	622	LHG	C11-C10-C9-C8
31	E	101	LHG	C11-C10-C9-C8
26	D	405	PL9	C28-C29-C31-C32
28	C	519	LMG	C29-C30-C31-C32
23	B	617	CLA	C16-C17-C18-C19
23	b	619	CLA	C16-C17-C18-C19
27	B	623	SQD	O10-C23-O48-C46
27	b	602	SQD	O10-C23-O48-C46
23	B	612	CLA	C14-C13-C15-C16
23	D	404	CLA	C6-C7-C8-C9
23	b	614	CLA	C14-C13-C15-C16
23	d	403	CLA	C6-C7-C8-C9
32	H	102	DGD	C9A-CAA-CBA-CCA
25	B	618	BCR	C14-C15-C16-C17
28	J	101	LMG	C30-C31-C32-C33
28	j	101	LMG	C35-C36-C37-C38
28	c	521	LMG	C40-C41-C42-C43
23	C	513	CLA	O1D-CGD-O2D-CED
28	c	521	LMG	C15-C16-C17-C18
28	Z	101	LMG	C2-C1-O1-C7
23	b	607	CLA	C2C-C3C-CAC-CBC
31	B	622	LHG	C31-C32-C33-C34
23	C	511	CLA	CBA-CGA-O2A-C1
31	D	407	LHG	C24-C23-O8-C6
28	C	519	LMG	C39-C40-C41-C42
23	C	510	CLA	C2-C3-C5-C6
23	c	511	CLA	C2-C3-C5-C6
23	B	604	CLA	C16-C17-C18-C19
23	b	606	CLA	C16-C17-C18-C19
28	c	520	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C27-C28-C29-C30
23	B	602	CLA	C15-C16-C17-C18
23	B	607[A]	CLA	C8-C10-C11-C12
23	b	604	CLA	C15-C16-C17-C18
23	b	609[A]	CLA	C8-C10-C11-C12
32	C	518	DGD	C8B-C9B-CAB-CBB
32	c	517	DGD	CBB-CCB-CDB-CEB
32	c	519	DGD	C3B-C4B-C5B-C6B
25	B	619	BCR	C35-C13-C14-C15
25	C	521	BCR	C11-C10-C9-C34
25	c	516	BCR	C16-C17-C18-C36
25	c	522	BCR	C11-C10-C9-C34
32	C	516	DGD	O1A-C1A-O1G-C1G
23	C	506	CLA	CBA-CGA-O2A-C1
23	C	510	CLA	CBA-CGA-O2A-C1
31	a	614	LHG	C24-C23-O8-C6
31	E	101	LHG	C19-C20-C21-C22
31	L	101	LHG	O6-C4-C5-C6
31	l	101	LHG	O6-C4-C5-C6
23	B	602	CLA	C16-C17-C18-C19
23	C	501	CLA	C16-C17-C18-C20
23	b	604	CLA	C16-C17-C18-C19
23	c	502	CLA	C16-C17-C18-C20
23	C	502	CLA	C15-C16-C17-C18
23	c	503	CLA	C15-C16-C17-C18
25	T	101	BCR	C36-C18-C19-C20
23	B	612	CLA	C12-C13-C15-C16
23	B	615	CLA	C12-C13-C15-C16
23	B	616	CLA	C11-C10-C8-C7
23	B	617	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	b	614	CLA	C12-C13-C15-C16
23	b	617	CLA	C12-C13-C15-C16
23	b	618	CLA	C11-C10-C8-C7
23	b	619	CLA	C12-C13-C15-C16
23	c	505	CLA	C12-C13-C15-C16
23	c	508	CLA	C11-C10-C8-C7
28	a	611	LMG	C33-C34-C35-C36
28	a	611	LMG	C30-C31-C32-C33
25	b	620	BCR	C21-C22-C23-C24
25	c	522	BCR	C11-C12-C13-C14
31	d	406	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	O1A-CGA-O2A-C1
32	C	517	DGD	CDA-CEA-CFA-CGA
28	C	520	LMG	C8-C7-O1-C1
28	c	521	LMG	C8-C7-O1-C1
32	C	517	DGD	C2G-C3G-O3G-C1D
32	C	517	DGD	C5D-C6D-O5D-C1E
32	c	518	DGD	C2G-C3G-O3G-C1D
32	c	518	DGD	C5D-C6D-O5D-C1E
27	B	623	SQD	C16-C17-C18-C19
27	b	602	SQD	C16-C17-C18-C19
28	C	519	LMG	C14-C15-C16-C17
24	A	607	PHO	C4-C3-C5-C6
31	b	624	LHG	C13-C14-C15-C16
32	c	517	DGD	C9A-CAA-CBA-CCA
32	c	518	DGD	O6E-C5E-C6E-O5E
28	C	519	LMG	C31-C32-C33-C34
23	B	607[B]	CLA	C16-C17-C18-C19
23	b	609[B]	CLA	C16-C17-C18-C19
25	B	619	BCR	C11-C10-C9-C8
25	c	522	BCR	C20-C21-C22-C23
31	L	101	LHG	O6-C4-C5-O7
31	l	101	LHG	O6-C4-C5-O7
28	C	519	LMG	C11-C12-C13-C14
28	Z	101	LMG	O1-C7-C8-C9
28	C	520	LMG	C11-C10-O7-C8
32	d	405	DGD	C6A-C7A-C8A-C9A
28	J	101	LMG	C36-C37-C38-C39
32	c	518	DGD	C5A-C6A-C7A-C8A
23	C	510	CLA	C4-C3-C5-C6
23	c	511	CLA	C4-C3-C5-C6
26	d	404	PL9	C45-C44-C46-C47
31	a	614	LHG	C17-C18-C19-C20
31	l	101	LHG	C25-C26-C27-C28
32	H	102	DGD	C5B-C6B-C7B-C8B
28	a	611	LMG	O7-C8-C9-O8
32	D	406	DGD	O1G-C1G-C2G-O2G
32	H	102	DGD	O1G-C1G-C2G-O2G
23	B	617	CLA	C14-C13-C15-C16
23	b	619	CLA	C14-C13-C15-C16
32	c	519	DGD	C7A-C8A-C9A-CAA
28	B	621	LMG	C30-C31-C32-C33
23	B	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	c	517	DGD	O1A-C1A-O1G-C1G
28	J	101	LMG	C20-C21-C22-C23
32	c	517	DGD	CAA-CBA-CCA-CDA
23	C	503	CLA	C8-C10-C11-C12
23	c	504	CLA	C8-C10-C11-C12
27	b	601	SQD	C24-C25-C26-C27
28	A	612	LMG	C38-C39-C40-C41
27	a	612	SQD	C24-C25-C26-C27
32	c	517	DGD	CCA-CDA-CEA-CFA
32	H	102	DGD	O6D-C5D-C6D-O5D
23	c	510	CLA	C2-C1-O2A-CGA
27	a	612	SQD	C2-C1-O6-C44
27	b	601	SQD	C2-C1-O6-C44
28	A	612	LMG	C2-C1-O1-C7
28	J	101	LMG	C34-C35-C36-C37
23	B	605	CLA	C3-C5-C6-C7
32	h	102	DGD	C3B-C4B-C5B-C6B
27	X	101	SQD	C11-C10-C9-C8
27	x	101	SQD	C11-C10-C9-C8
27	a	612	SQD	C29-C30-C31-C32
27	b	601	SQD	C29-C30-C31-C32
23	B	611	CLA	C16-C17-C18-C19
23	b	613	CLA	C16-C17-C18-C19
23	B	614	CLA	C13-C15-C16-C17
23	b	616	CLA	C13-C15-C16-C17
28	B	621	LMG	C28-C29-C30-C31
23	c	504	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	C3-C5-C6-C7
27	a	612	SQD	C27-C28-C29-C30
27	b	601	SQD	C27-C28-C29-C30
31	D	408	LHG	C24-C25-C26-C27
31	D	408	LHG	C9-C10-C11-C12
23	C	506	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	c	505	CLA	C4B-C3B-CAB-CBB
23	c	506	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	C	503	CLA	O1D-CGD-O2D-CED
31	e	101	LHG	C26-C27-C28-C29
26	A	610	PL9	C15-C14-C16-C17
26	a	609	PL9	C15-C14-C16-C17
26	d	404	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
31	D	408	LHG	C30-C31-C32-C33
28	z	101	LMG	O6-C5-C6-O5
25	b	622	BCR	C7-C8-C9-C10
28	A	612	LMG	C10-C11-C12-C13
28	A	612	LMG	C29-C30-C31-C32
23	A	606	CLA	C11-C10-C8-C7
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C10
23	C	509	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C12-C13-C15
23	D	404	CLA	C12-C13-C15-C16
23	a	605	CLA	C11-C10-C8-C7
23	b	618	CLA	C12-C13-C15-C16
23	c	507	CLA	C6-C7-C8-C10
23	c	510	CLA	C6-C7-C8-C10
23	d	403	CLA	C12-C13-C15-C16
28	C	519	LMG	C12-C13-C14-C15
23	b	618	CLA	C16-C17-C18-C20
32	h	102	DGD	CCA-CDA-CEA-CFA
28	a	611	LMG	C29-C30-C31-C32
28	C	519	LMG	C21-C22-C23-C24
32	D	406	DGD	C6A-C7A-C8A-C9A
23	b	613	CLA	C8-C10-C11-C12
31	D	408	LHG	C2-C3-O3-P
23	B	616	CLA	C16-C17-C18-C20
32	H	102	DGD	CDA-CEA-CFA-CGA
27	a	612	SQD	C9-C10-C11-C12
23	a	613	CLA	C4C-C3C-CAC-CBC
23	B	615	CLA	C2A-CAA-CBA-CGA
23	A	606	CLA	C11-C10-C8-C9
23	C	504	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C10-C8-C9
23	a	605	CLA	C11-C10-C8-C9
23	c	505	CLA	C14-C13-C15-C16
23	c	513	CLA	C11-C10-C8-C9
27	b	601	SQD	C9-C10-C11-C12
23	B	611	CLA	C8-C10-C11-C12
25	B	619	BCR	C19-C20-C21-C22
32	c	517	DGD	C5A-C6A-C7A-C8A
23	c	514	CLA	C3-C5-C6-C7
28	a	611	LMG	O1-C7-C8-O7
31	E	101	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
32	h	102	DGD	O1G-C1G-C2G-O2G
27	X	101	SQD	C28-C29-C30-C31
28	A	612	LMG	O1-C7-C8-C9
28	a	611	LMG	O1-C7-C8-C9
27	x	101	SQD	C28-C29-C30-C31
28	c	520	LMG	C12-C13-C14-C15
26	a	609	PL9	C28-C29-C31-C32
23	C	513	CLA	C3-C5-C6-C7
23	C	513	CLA	CBD-CGD-O2D-CED
28	Z	101	LMG	C18-C19-C20-C21
23	B	608	CLA	CAD-CBD-CGD-O2D
23	b	606	CLA	CAD-CBD-CGD-O2D
23	b	608	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	C4C-C3C-CAC-CBC
32	c	518	DGD	CDA-CEA-CFA-CGA
31	B	622	LHG	C34-C35-C36-C37
28	A	612	LMG	C21-C22-C23-C24
32	h	102	DGD	C9B-CAB-CBB-CCB
27	B	623	SQD	C19-C20-C21-C22
23	B	602	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CAD-CBD-CGD-O1D
23	b	604	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
25	K	101	BCR	C19-C20-C21-C22
25	b	620	BCR	C13-C14-C15-C16
25	b	622	BCR	C9-C10-C11-C12
25	t	101	BCR	C9-C10-C11-C12
31	D	407	LHG	C3-O3-P-O4
31	D	407	LHG	C4-O6-P-O5
27	b	602	SQD	C19-C20-C21-C22
31	d	406	LHG	C12-C13-C14-C15
31	e	101	LHG	C19-C20-C21-C22
26	A	610	PL9	C35-C34-C36-C37
26	A	610	PL9	C45-C44-C46-C47
23	B	617	CLA	C2B-C3B-CAB-CBB
23	C	502	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	C	504	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
24	A	607	PHO	C2-C3-C5-C6
28	c	520	LMG	C30-C31-C32-C33
25	B	618	BCR	C7-C8-C9-C34
25	b	621	BCR	C7-C8-C9-C34
31	a	614	LHG	C2-C3-O3-P
32	C	516	DGD	C5A-C6A-C7A-C8A
32	h	102	DGD	C5B-C6B-C7B-C8B
31	E	101	LHG	C10-C11-C12-C13
32	D	406	DGD	CDB-CEB-CFB-CGB
28	b	623	LMG	C39-C40-C41-C42
23	B	611	CLA	C16-C17-C18-C20
31	b	624	LHG	O1-C1-C2-C3
27	B	623	SQD	C46-C45-O47-C7
27	b	602	SQD	C46-C45-O47-C7
28	j	101	LMG	C17-C18-C19-C20
28	z	101	LMG	C17-C18-C19-C20
27	a	610	SQD	C23-C24-C25-C26
32	d	405	DGD	CDB-CEB-CFB-CGB
31	D	407	LHG	C33-C34-C35-C36
32	C	516	DGD	C9A-CAA-CBA-CCA
32	c	518	DGD	CBA-CCA-CDA-CEA
23	C	512	CLA	C16-C17-C18-C19
23	b	613	CLA	C16-C17-C18-C20
23	c	513	CLA	C16-C17-C18-C19
27	A	611	SQD	C23-C24-C25-C26
23	A	608	CLA	C11-C10-C8-C9
23	B	616	CLA	C11-C10-C8-C9
23	B	617	CLA	C6-C7-C8-C9
23	C	513	CLA	C6-C7-C8-C9
23	a	607	CLA	C11-C10-C8-C9
23	b	618	CLA	C11-C10-C8-C9
23	b	619	CLA	C6-C7-C8-C9
23	c	514	CLA	C6-C7-C8-C9
32	c	517	DGD	CDA-CEA-CFA-CGA
23	B	617	CLA	C6-C7-C8-C10
23	C	506	CLA	C12-C13-C15-C16
23	b	619	CLA	C6-C7-C8-C10
23	c	507	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	d	403	CLA	C11-C12-C13-C15
32	c	519	DGD	CAB-CBB-CCB-CDB
32	C	516	DGD	O6E-C1E-O5D-C6D
23	C	502	CLA	C16-C17-C18-C19
23	c	503	CLA	C16-C17-C18-C19
32	C	516	DGD	C2E-C1E-O5D-C6D
32	h	102	DGD	O2G-C1B-C2B-C3B
23	B	616	CLA	C16-C17-C18-C19
23	b	618	CLA	C16-C17-C18-C19
27	B	623	SQD	C14-C15-C16-C17
27	b	602	SQD	C14-C15-C16-C17
31	a	614	LHG	C13-C14-C15-C16
31	d	406	LHG	C10-C11-C12-C13
32	d	405	DGD	C2A-C1A-O1G-C1G
32	c	519	DGD	C3A-C4A-C5A-C6A
32	h	102	DGD	CDA-CEA-CFA-CGA
26	d	404	PL9	C12-C11-C9-C10
32	C	518	DGD	C7A-C8A-C9A-CAA
23	c	505	CLA	O1D-CGD-O2D-CED
31	E	101	LHG	C4-C5-C6-O8
31	l	101	LHG	C11-C10-C9-C8
25	k	101	BCR	C37-C22-C23-C24
32	c	517	DGD	CBA-CCA-CDA-CEA
32	c	518	DGD	C4E-C5E-C6E-O5E
32	C	518	DGD	C2A-C1A-O1G-C1G
32	C	516	DGD	C5D-C6D-O5D-C1E
28	A	612	LMG	C11-C12-C13-C14
23	C	505	CLA	C2A-CAA-CBA-CGA
25	B	620	BCR	C9-C10-C11-C12
26	a	609	PL9	C2-C3-C7-C8
23	c	507	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	618	CLA	C14-C13-C15-C16
23	c	507	CLA	C6-C7-C8-C9
32	C	516	DGD	CBA-CCA-CDA-CEA
23	b	614	CLA	CBA-CGA-O2A-C1
28	c	521	LMG	C29-C28-O8-C9
23	B	606	CLA	O1A-CGA-O2A-C1
28	a	611	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
23	b	612	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	CBA-CGA-O2A-C1
32	c	518	DGD	C7A-C8A-C9A-CAA
23	c	511	CLA	O1A-CGA-O2A-C1
31	E	101	LHG	O6-C4-C5-O7
23	a	607	CLA	O1A-CGA-O2A-C1
32	C	517	DGD	C7A-C8A-C9A-CAA
23	A	608	CLA	C12-C13-C15-C16
23	a	607	CLA	C12-C13-C15-C16
32	C	516	DGD	C8A-C9A-CAA-CBA
28	a	611	LMG	C17-C18-C19-C20
23	C	512	CLA	C16-C17-C18-C20
23	c	513	CLA	C16-C17-C18-C20
23	D	402	CLA	C2C-C3C-CAC-CBC
28	c	520	LMG	C14-C15-C16-C17
32	h	102	DGD	CAB-CBB-CCB-CDB
23	B	616	CLA	C3A-C2A-CAA-CBA
23	b	618	CLA	C3A-C2A-CAA-CBA
31	a	614	LHG	C16-C17-C18-C19
23	B	602	CLA	C2A-CAA-CBA-CGA
23	C	510	CLA	C8-C10-C11-C12
32	c	517	DGD	C4E-C5E-C6E-O5E
25	B	618	BCR	C11-C10-C9-C34
23	c	511	CLA	C8-C10-C11-C12
23	B	617	CLA	C2-C1-O2A-CGA
25	b	622	BCR	C13-C14-C15-C16
31	b	624	LHG	C11-C10-C9-C8
32	C	516	DGD	CBB-CCB-CDB-CEB
28	A	612	LMG	C19-C20-C21-C22
28	B	621	LMG	C36-C37-C38-C39
23	b	613	CLA	C13-C15-C16-C17
23	B	611	CLA	C13-C15-C16-C17
23	B	611	CLA	C14-C13-C15-C16
23	b	613	CLA	C14-C13-C15-C16
27	b	601	SQD	C10-C11-C12-C13
28	c	521	LMG	C36-C37-C38-C39
27	a	612	SQD	C10-C11-C12-C13
28	a	611	LMG	O6-C5-C6-O5
23	b	604	CLA	CBA-CGA-O2A-C1
28	b	623	LMG	C35-C36-C37-C38
28	c	520	LMG	C22-C23-C24-C25
23	b	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	B	611	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C16-C17-C18-C19
23	c	514	CLA	C16-C17-C18-C19
32	H	102	DGD	O1B-C1B-C2B-C3B
23	A	608	CLA	C2B-C3B-CAB-CBB
23	B	607[A]	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
23	b	609[A]	CLA	C2B-C3B-CAB-CBB
23	b	609[B]	CLA	C2B-C3B-CAB-CBB
25	B	619	BCR	C23-C24-C25-C30
25	B	620	BCR	C23-C24-C25-C30
25	H	101	BCR	C5-C6-C7-C8
23	c	514	CLA	O1D-CGD-O2D-CED
28	A	612	LMG	C16-C17-C18-C19
23	b	612	CLA	O1A-CGA-O2A-C1
28	z	101	LMG	C18-C19-C20-C21
32	C	517	DGD	CBA-CCA-CDA-CEA
23	C	513	CLA	C4-C3-C5-C6
23	c	514	CLA	C4-C3-C5-C6
32	D	406	DGD	C3B-C4B-C5B-C6B
28	b	623	LMG	C30-C31-C32-C33
32	C	517	DGD	C5B-C6B-C7B-C8B
32	C	518	DGD	C4B-C5B-C6B-C7B
23	B	617	CLA	C13-C15-C16-C17
23	B	607[B]	CLA	C11-C10-C8-C7
23	B	611	CLA	C12-C13-C15-C16
23	C	502	CLA	C12-C13-C15-C16
23	C	504	CLA	C11-C10-C8-C7
23	b	609[B]	CLA	C11-C10-C8-C7
23	b	613	CLA	C12-C13-C15-C16
23	c	503	CLA	C12-C13-C15-C16
23	c	505	CLA	C11-C10-C8-C7
32	c	519	DGD	C5B-C6B-C7B-C8B
23	b	605	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	c	502	CLA	C2A-CAA-CBA-CGA
28	b	623	LMG	C36-C37-C38-C39
23	b	619	CLA	C13-C15-C16-C17
27	A	611	SQD	O6-C44-C45-O47
27	a	610	SQD	O6-C44-C45-O47
28	j	101	LMG	C32-C33-C34-C35
32	C	518	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
32	c	518	DGD	C8A-C9A-CAA-CBA
28	c	521	LMG	C39-C40-C41-C42
23	C	507	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
32	c	518	DGD	CDB-CEB-CFB-CGB
28	B	621	LMG	C35-C36-C37-C38
26	A	610	PL9	C2-C3-C7-C8
23	B	609	CLA	C4C-C3C-CAC-CBC
23	A	606	CLA	C6-C7-C8-C9
23	a	605	CLA	C6-C7-C8-C9
28	C	519	LMG	C22-C23-C24-C25
33	e	102	HEM	CAD-CBD-CGD-O1D
23	b	604	CLA	CAA-CBA-CGA-O1A
23	B	602	CLA	O1A-CGA-O2A-C1
28	j	101	LMG	C11-C12-C13-C14
32	c	518	DGD	C5B-C6B-C7B-C8B
26	D	405	PL9	C34-C36-C37-C38
28	C	519	LMG	C33-C34-C35-C36
23	C	501	CLA	C2A-CAA-CBA-CGA
23	b	613	CLA	C2A-CAA-CBA-CGA
23	b	617	CLA	C2A-CAA-CBA-CGA
26	a	609	PL9	C35-C34-C36-C37
28	a	611	LMG	C16-C17-C18-C19
23	B	602	CLA	CAA-CBA-CGA-O2A
31	a	614	LHG	C11-C10-C9-C8
23	B	614	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	b	616	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	O1A-CGA-O2A-C1
31	a	614	LHG	O10-C23-O8-C6
31	b	624	LHG	C17-C18-C19-C20
25	C	521	BCR	C16-C17-C18-C36
28	c	521	LMG	C16-C17-C18-C19
23	A	608	CLA	C4-C3-C5-C6
23	a	607	CLA	C4-C3-C5-C6
32	D	406	DGD	O2G-C2G-C3G-O3G
26	D	405	PL9	C12-C11-C9-C8
32	h	102	DGD	CAA-CBA-CCA-CDA
28	A	612	LMG	O6-C1-O1-C7
32	c	519	DGD	O6D-C5D-C6D-O5D
32	c	517	DGD	C8A-C9A-CAA-CBA
23	B	604	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C6-C7-C8-C9
27	X	101	SQD	C45-C44-O6-C1
27	x	101	SQD	C45-C44-O6-C1
28	j	101	LMG	C8-C7-O1-C1
32	c	517	DGD	C5D-C6D-O5D-C1E
28	A	612	LMG	C39-C40-C41-C42
28	c	520	LMG	C31-C32-C33-C34
23	B	604	CLA	C13-C15-C16-C17
23	b	606	CLA	C13-C15-C16-C17
23	B	604	CLA	C2A-CAA-CBA-CGA
23	b	604	CLA	C2-C1-O2A-CGA
23	b	619	CLA	C2-C1-O2A-CGA
32	C	516	DGD	CDA-CEA-CFA-CGA
32	c	518	DGD	C4B-C5B-C6B-C7B
23	b	615	CLA	CBA-CGA-O2A-C1
28	C	520	LMG	C11-C12-C13-C14
26	D	405	PL9	C30-C29-C31-C32
23	B	607[A]	CLA	C16-C17-C18-C20
23	b	609[A]	CLA	C16-C17-C18-C20
28	J	101	LMG	C11-C12-C13-C14
32	H	102	DGD	C4D-C5D-C6D-O5D
28	J	101	LMG	C7-C8-C9-O8
27	b	602	SQD	C33-C34-C35-C36
27	B	623	SQD	C33-C34-C35-C36
33	e	102	HEM	CAD-CBD-CGD-O2D
31	l	101	LHG	O10-C23-O8-C6
23	c	511	CLA	CAA-CBA-CGA-O2A
23	B	604	CLA	CBD-CGD-O2D-CED
27	B	623	SQD	C17-C18-C19-C20
23	c	511	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C24-C23-O8-C6
28	c	520	LMG	O10-C28-O8-C9
28	B	621	LMG	C39-C40-C41-C42
27	b	602	SQD	C17-C18-C19-C20
32	d	405	DGD	O2G-C2G-C3G-O3G
23	B	607[A]	CLA	C11-C12-C13-C14
23	b	609[A]	CLA	C11-C12-C13-C14
33	V	202	HEM	CAD-CBD-CGD-O2D
23	A	606	CLA	C6-C7-C8-C10
23	B	604	CLA	C6-C7-C8-C10
23	B	615	CLA	C11-C10-C8-C7
23	C	504	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C12-C13-C15-C16
23	a	605	CLA	C6-C7-C8-C10
23	b	606	CLA	C6-C7-C8-C10
23	b	617	CLA	C11-C10-C8-C7
23	c	505	CLA	C11-C12-C13-C15
23	d	402	CLA	C12-C13-C15-C16
23	B	603	CLA	C2B-C3B-CAB-CBB
23	B	607[B]	CLA	C2B-C3B-CAB-CBB
23	B	614	CLA	C2B-C3B-CAB-CBB
23	C	505	CLA	C2B-C3B-CAB-CBB
23	b	605	CLA	C2B-C3B-CAB-CBB
23	b	612	CLA	C2B-C3B-CAB-CBB
23	b	616	CLA	C2B-C3B-CAB-CBB
23	b	619	CLA	C2B-C3B-CAB-CBB
23	c	505	CLA	C2B-C3B-CAB-CBB
25	T	101	BCR	C5-C6-C7-C8
25	b	620	BCR	C23-C24-C25-C26
25	k	101	BCR	C5-C6-C7-C8
23	B	602	CLA	C2-C1-O2A-CGA
23	C	506	CLA	C2-C1-O2A-CGA
32	H	102	DGD	C7B-C8B-C9B-CAB
32	C	518	DGD	O1G-C1A-C2A-C3A
32	c	518	DGD	C6A-C7A-C8A-C9A
31	L	101	LHG	O7-C7-C8-C9
32	c	519	DGD	O1G-C1A-C2A-C3A
23	c	514	CLA	C16-C17-C18-C20
31	E	101	LHG	O7-C7-C8-C9
31	e	101	LHG	O7-C7-C8-C9
31	l	101	LHG	O7-C7-C8-C9
23	C	513	CLA	C16-C17-C18-C20
28	b	623	LMG	C13-C14-C15-C16
27	A	611	SQD	C18-C19-C20-C21
27	a	610	SQD	C18-C19-C20-C21
26	d	404	PL9	C36-C37-C38-C39
31	b	624	LHG	C15-C16-C17-C18
32	H	102	DGD	CAB-CBB-CCB-CDB
23	B	606	CLA	C13-C15-C16-C17
23	b	608	CLA	C13-C15-C16-C17
23	B	607[B]	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	b	609[B]	CLA	C11-C10-C8-C9
23	d	403	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	D	405	PL9	C14-C16-C17-C18
23	B	602	CLA	C1A-C2A-CAA-CBA
23	B	603	CLA	C1A-C2A-CAA-CBA
23	b	605	CLA	C1A-C2A-CAA-CBA
23	b	613	CLA	C1A-C2A-CAA-CBA
33	V	202	HEM	CAD-CBD-CGD-O1D
23	c	513	CLA	CAA-CBA-CGA-O2A
32	C	518	DGD	CDB-CEB-CFB-CGB
33	E	102	HEM	CAA-CBA-CGA-O1A
23	C	503	CLA	CBD-CGD-O2D-CED
28	J	101	LMG	O7-C10-C11-C12
28	B	621	LMG	C34-C35-C36-C37
24	D	401	PHO	C8-C10-C11-C12
28	B	621	LMG	C13-C14-C15-C16
31	a	614	LHG	C18-C19-C20-C21
32	D	406	DGD	O6D-C5D-C6D-O5D
33	E	102	HEM	CAD-CBD-CGD-O1D
26	A	610	PL9	C21-C22-C23-C24
23	c	507	CLA	C2-C1-O2A-CGA
23	C	510	CLA	CAA-CBA-CGA-O2A
23	C	505	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C12-C13-C15
23	c	506	CLA	C12-C13-C15-C16
23	c	508	CLA	C11-C12-C13-C15
23	D	403	CLA	O2A-C1-C2-C3
23	d	402	CLA	O2A-C1-C2-C3
27	a	612	SQD	C11-C12-C13-C14
27	b	601	SQD	C11-C12-C13-C14
28	a	611	LMG	C11-C12-C13-C14
31	b	624	LHG	C34-C35-C36-C37
23	C	512	CLA	CAA-CBA-CGA-O2A
32	h	102	DGD	C7B-C8B-C9B-CAB
23	b	611	CLA	C2A-CAA-CBA-CGA
26	d	404	PL9	C24-C26-C27-C28
26	d	404	PL9	C34-C36-C37-C38
31	D	408	LHG	O10-C23-C24-C25
23	B	614	CLA	CAA-CBA-CGA-O2A
31	D	408	LHG	O8-C23-C24-C25
32	C	518	DGD	C4A-C5A-C6A-C7A
25	C	521	BCR	C20-C21-C22-C23
27	B	623	SQD	C45-C46-O48-C23
27	b	602	SQD	C45-C46-O48-C23

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Mol	Chain	Res	Type	Atoms
31	E	101	LHG	C12-C13-C14-C15
26	a	609	PL9	C31-C32-C33-C34
31	L	101	LHG	O10-C23-O8-C6
32	c	518	DGD	O1B-C1B-C2B-C3B
23	c	506	CLA	C2A-CAA-CBA-CGA
23	C	504	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	513	CLA	C11-C12-C13-C14
23	D	404	CLA	C14-C13-C15-C16
23	c	505	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C14-C13-C15-C16
23	c	514	CLA	C11-C12-C13-C14
23	d	403	CLA	C14-C13-C15-C16
23	D	402	CLA	C4C-C3C-CAC-CBC
23	C	512	CLA	CAA-CBA-CGA-O1A
31	D	408	LHG	C13-C14-C15-C16
23	C	507	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
32	C	516	DGD	CCA-CDA-CEA-CFA
28	A	612	LMG	O10-C28-C29-C30
32	C	517	DGD	O1B-C1B-C2B-C3B
23	B	613	CLA	C8-C10-C11-C12
23	b	615	CLA	C8-C10-C11-C12
23	B	616	CLA	C15-C16-C17-C18
23	b	618	CLA	C15-C16-C17-C18
27	A	611	SQD	C45-C44-O6-C1
27	a	610	SQD	C45-C44-O6-C1
28	J	101	LMG	C8-C7-O1-C1
32	D	406	DGD	C2G-C3G-O3G-C1D
32	H	102	DGD	C2G-C3G-O3G-C1D
32	d	405	DGD	C2G-C3G-O3G-C1D
23	B	607[B]	CLA	C16-C17-C18-C20
23	b	609[B]	CLA	C16-C17-C18-C20
31	e	101	LHG	C4-C5-C6-O8
23	c	511	CLA	CAA-CBA-CGA-O1A
31	a	614	LHG	O10-C23-C24-C25
32	d	405	DGD	O1A-C1A-C2A-C3A
26	D	405	PL9	C12-C11-C9-C10
26	a	609	PL9	C21-C22-C23-C24
23	C	506	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	C15-C16-C17-C18
23	B	615	CLA	O1A-CGA-O2A-C1
28	a	611	LMG	C21-C22-C23-C24
33	E	102	HEM	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	a	604	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	B	613	CLA	CAA-CBA-CGA-O2A
28	C	520	LMG	C16-C17-C18-C19
32	h	102	DGD	O1B-C1B-C2B-C3B
32	c	517	DGD	O6E-C1E-O5D-C6D
28	a	611	LMG	O10-C28-C29-C30
23	c	510	CLA	O1D-CGD-O2D-CED
28	B	621	LMG	O8-C28-C29-C30
31	a	614	LHG	O8-C23-C24-C25
28	C	520	LMG	C36-C37-C38-C39
23	b	617	CLA	CBD-CGD-O2D-CED
28	j	101	LMG	O7-C10-C11-C12
23	B	602	CLA	C8-C10-C11-C12
23	b	604	CLA	C8-C10-C11-C12
33	E	102	HEM	CAA-CBA-CGA-O2A
23	C	505	CLA	CAA-CBA-CGA-O1A
23	B	603	CLA	CAA-CBA-CGA-O2A
23	C	510	CLA	CAA-CBA-CGA-O1A
31	l	101	LHG	O9-C7-C8-C9
32	D	406	DGD	O1A-C1A-C2A-C3A
32	c	518	DGD	O6D-C5D-C6D-O5D

There are no ring outliers.

141 monomers are involved in 751 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	E	102	HEM	3	0
25	B	618	BCR	28	0
23	C	512	CLA	4	0
28	Z	101	LMG	1	0
23	b	612	CLA	2	0
31	L	101	LHG	2	0
23	C	509	CLA	3	0
28	C	519	LMG	1	0
28	j	101	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	508	CLA	3	0
23	B	613	CLA	3	0
31	d	406	LHG	1	0
23	B	603	CLA	3	0
20	a	601	OEX	1	0
25	b	621	BCR	28	0
23	B	612	CLA	2	0
23	b	605	CLA	2	0
23	b	607	CLA	6	0
31	D	408	LHG	10	0
25	c	516	BCR	17	0
23	C	501	CLA	7	0
23	C	505	CLA	8	0
23	C	506	CLA	7	0
23	C	504	CLA	2	0
23	C	510	CLA	3	0
23	B	602	CLA	3	0
23	a	607	CLA	5	0
25	T	101	BCR	28	0
23	a	613	CLA	3	0
24	d	401	PHO	6	0
25	c	515	BCR	13	0
23	b	616	CLA	2	0
25	k	101	BCR	22	0
32	C	518	DGD	4	0
27	X	101	SQD	3	0
23	d	402	CLA	5	0
23	A	605	CLA	4	0
23	c	506	CLA	5	0
23	c	513	CLA	2	0
25	K	101	BCR	25	0
32	d	405	DGD	2	0
23	b	617	CLA	9	0
25	B	619	BCR	29	0
25	a	608	BCR	14	0
33	v	201	HEM	1	0
25	H	101	BCR	10	0
23	c	505	CLA	2	0
28	b	623	LMG	3	0
28	J	101	LMG	3	0
23	B	616	CLA	3	0
23	b	609[B]	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	e	101	LHG	4	0
23	C	502	CLA	4	0
23	b	609[A]	CLA	2	0
23	c	509	CLA	5	0
23	B	606	CLA	9	0
25	C	521	BCR	15	0
23	c	512	CLA	2	0
28	a	611	LMG	2	0
27	a	610	SQD	1	0
23	B	617	CLA	7	0
32	C	517	DGD	2	0
32	c	518	DGD	4	0
23	B	604	CLA	7	0
23	B	615	CLA	4	0
23	c	507	CLA	6	0
26	D	405	PL9	6	0
23	b	610	CLA	2	0
23	C	511	CLA	3	0
28	c	520	LMG	1	0
32	h	102	DGD	3	0
23	A	606	CLA	4	0
23	c	508	CLA	5	0
23	b	618	CLA	1	0
20	A	601	OEX	1	0
27	A	611	SQD	4	0
27	b	602	SQD	11	0
23	a	604	CLA	2	0
23	b	615	CLA	3	0
23	B	608	CLA	5	0
23	B	605	CLA	5	0
23	B	609	CLA	1	0
23	D	403	CLA	3	0
26	a	609	PL9	10	0
27	x	101	SQD	4	0
23	B	610	CLA	2	0
23	c	510	CLA	3	0
25	A	609	BCR	16	0
23	B	607[B]	CLA	3	0
24	A	607	PHO	1	0
25	h	101	BCR	15	0
26	A	610	PL9	16	0
25	c	522	BCR	18	0

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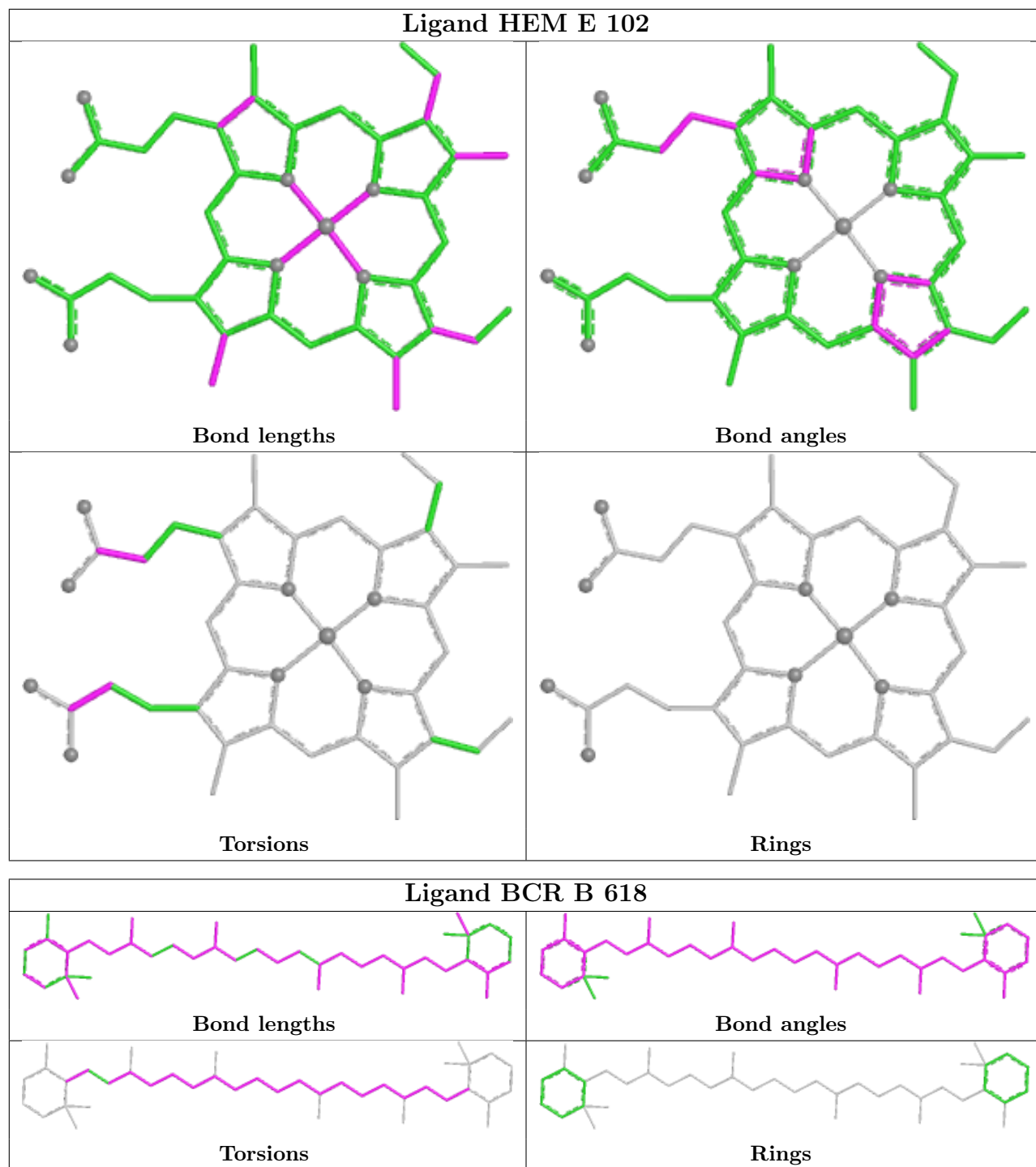
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	V	202	HEM	4	0
32	D	406	DGD	1	0
23	C	513	CLA	2	0
28	z	101	LMG	2	0
31	l	101	LHG	4	0
32	C	516	DGD	2	0
23	b	619	CLA	1	0
27	a	612	SQD	2	0
23	B	611	CLA	2	0
23	C	507	CLA	7	0
25	B	620	BCR	22	0
23	b	608	CLA	12	0
25	C	514	BCR	11	0
31	b	624	LHG	4	0
23	D	402	CLA	2	0
33	e	102	HEM	3	0
32	c	517	DGD	1	0
23	b	604	CLA	6	0
25	b	620	BCR	31	0
31	B	622	LHG	3	0
23	B	614	CLA	4	0
25	C	515	BCR	18	0
28	A	612	LMG	2	0
23	c	511	CLA	3	0
23	c	503	CLA	6	0
23	c	514	CLA	1	0
23	c	502	CLA	8	0
27	b	601	SQD	4	0
32	c	519	DGD	4	0
25	b	622	BCR	15	0
23	d	403	CLA	2	0
31	D	407	LHG	1	0
25	t	101	BCR	30	0
23	D	404	CLA	2	0
23	a	605	CLA	4	0
24	D	401	PHO	8	0
23	b	613	CLA	5	0
25	F	101	BCR	16	0
23	C	503	CLA	6	0
23	c	504	CLA	7	0
23	b	606	CLA	6	0
27	B	623	SQD	9	0

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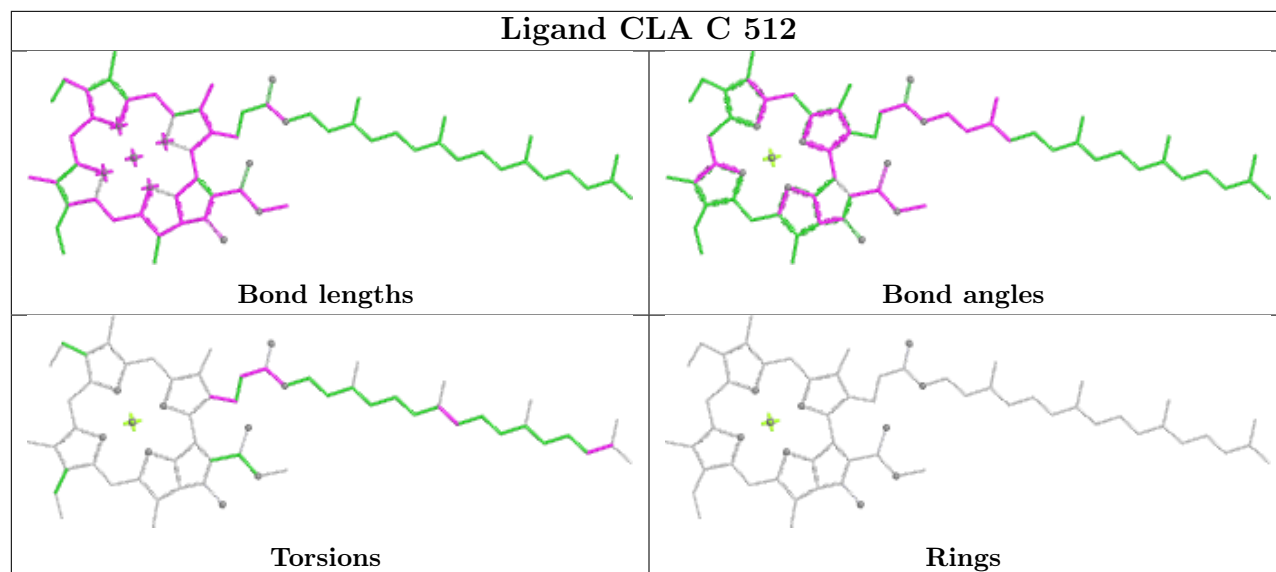
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	608	CLA	7	0
32	H	102	DGD	5	0
26	d	404	PL9	3	0
25	f	101	BCR	24	0
31	a	614	LHG	8	0
28	B	621	LMG	4	0

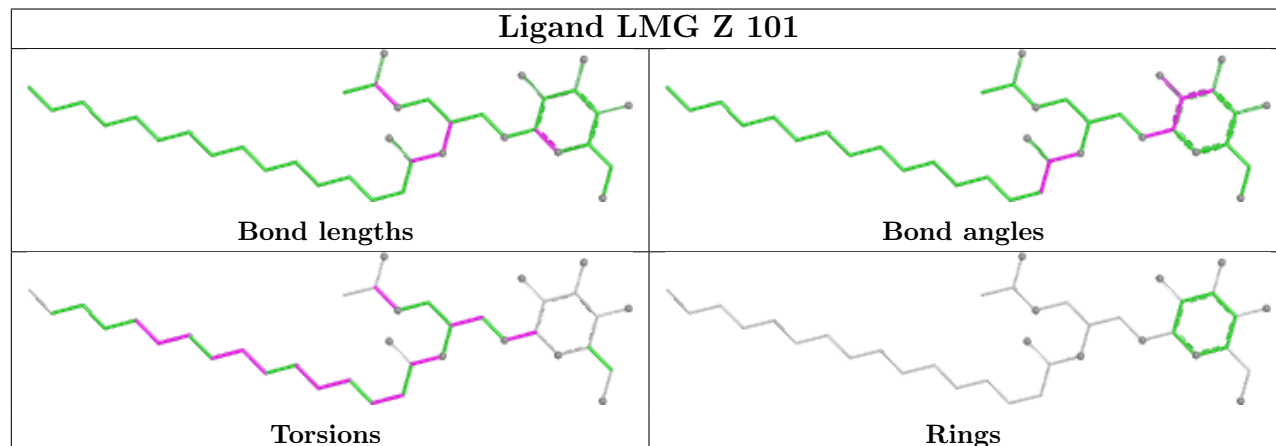
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



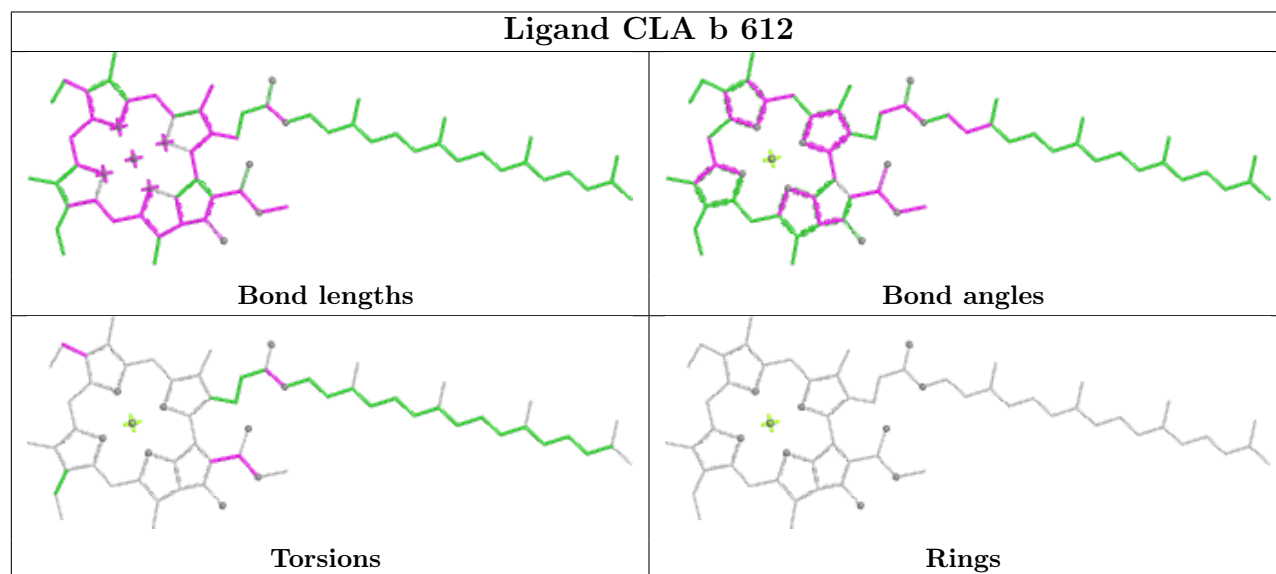
Ligand CLA C 512

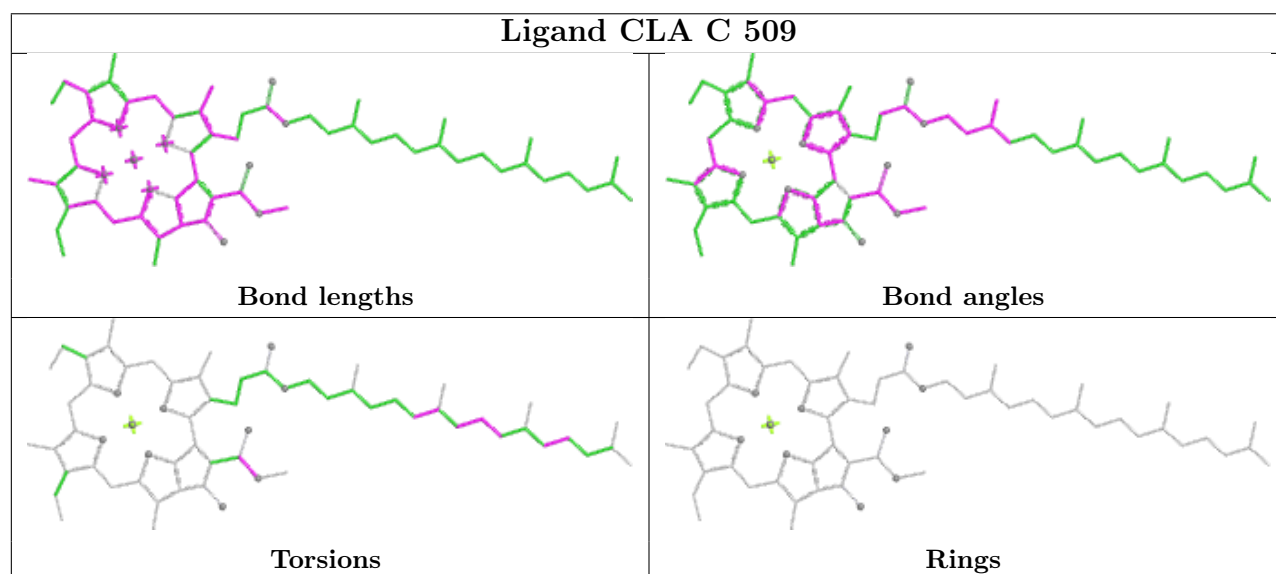
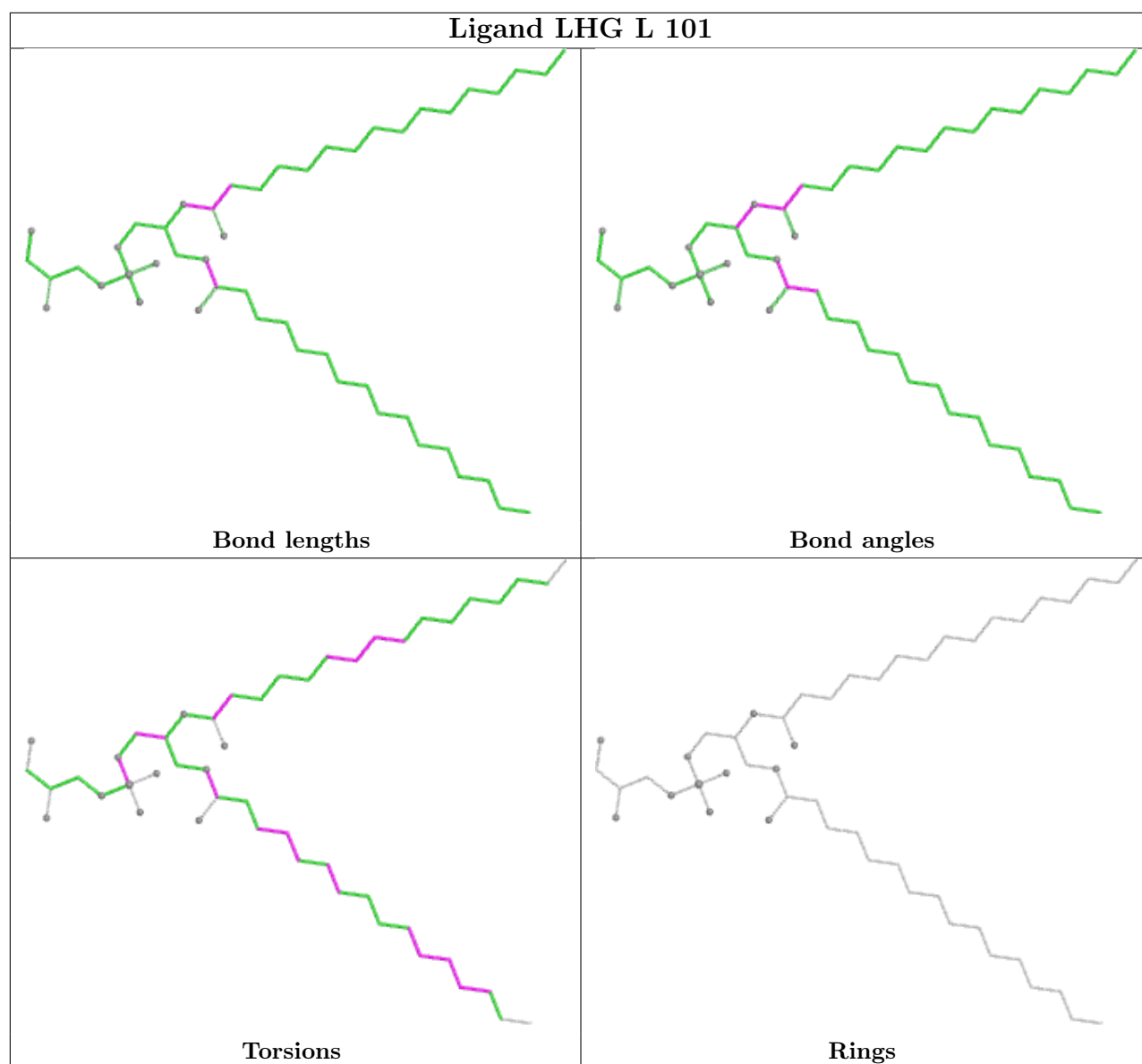


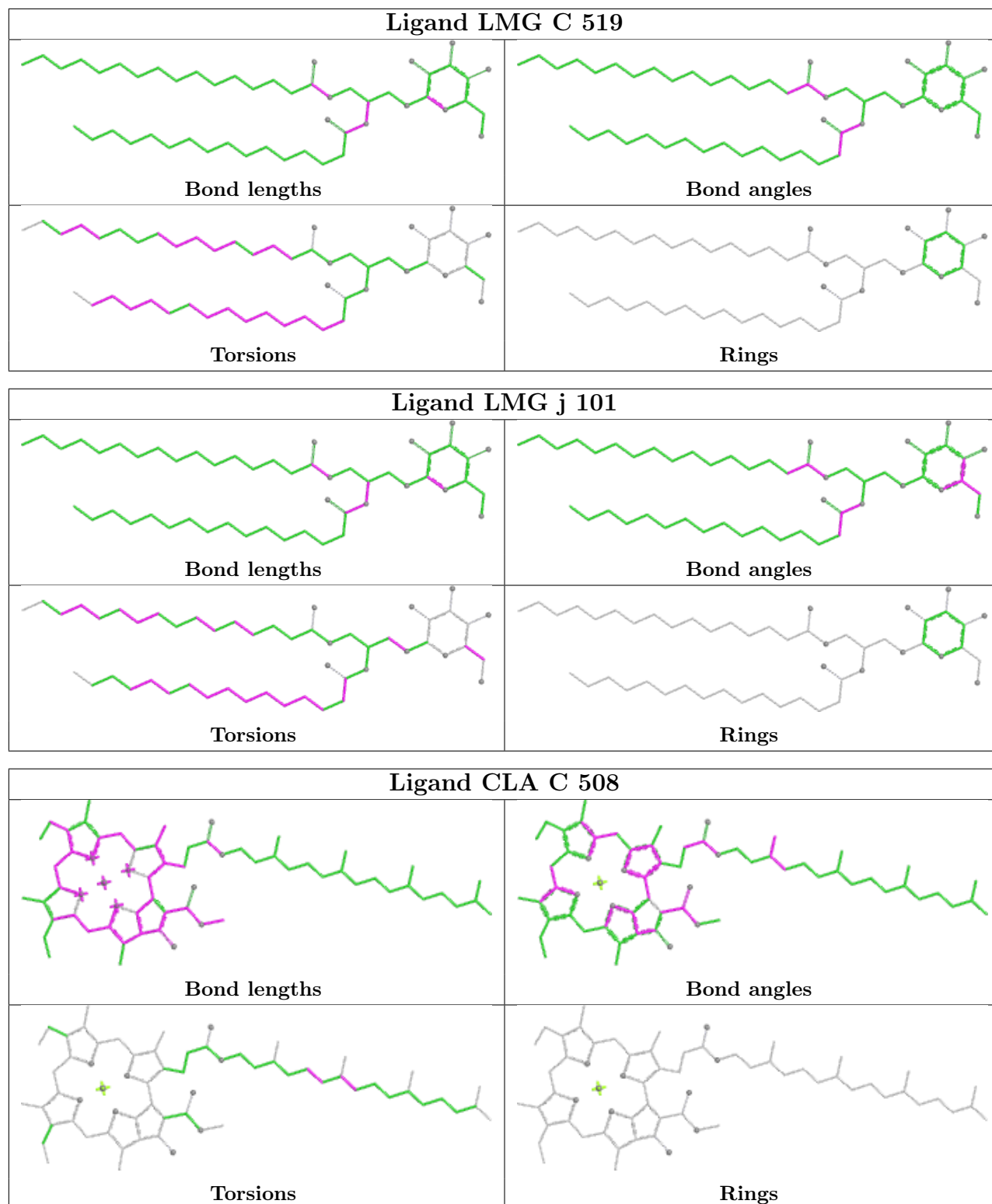
Ligand LMG Z 101

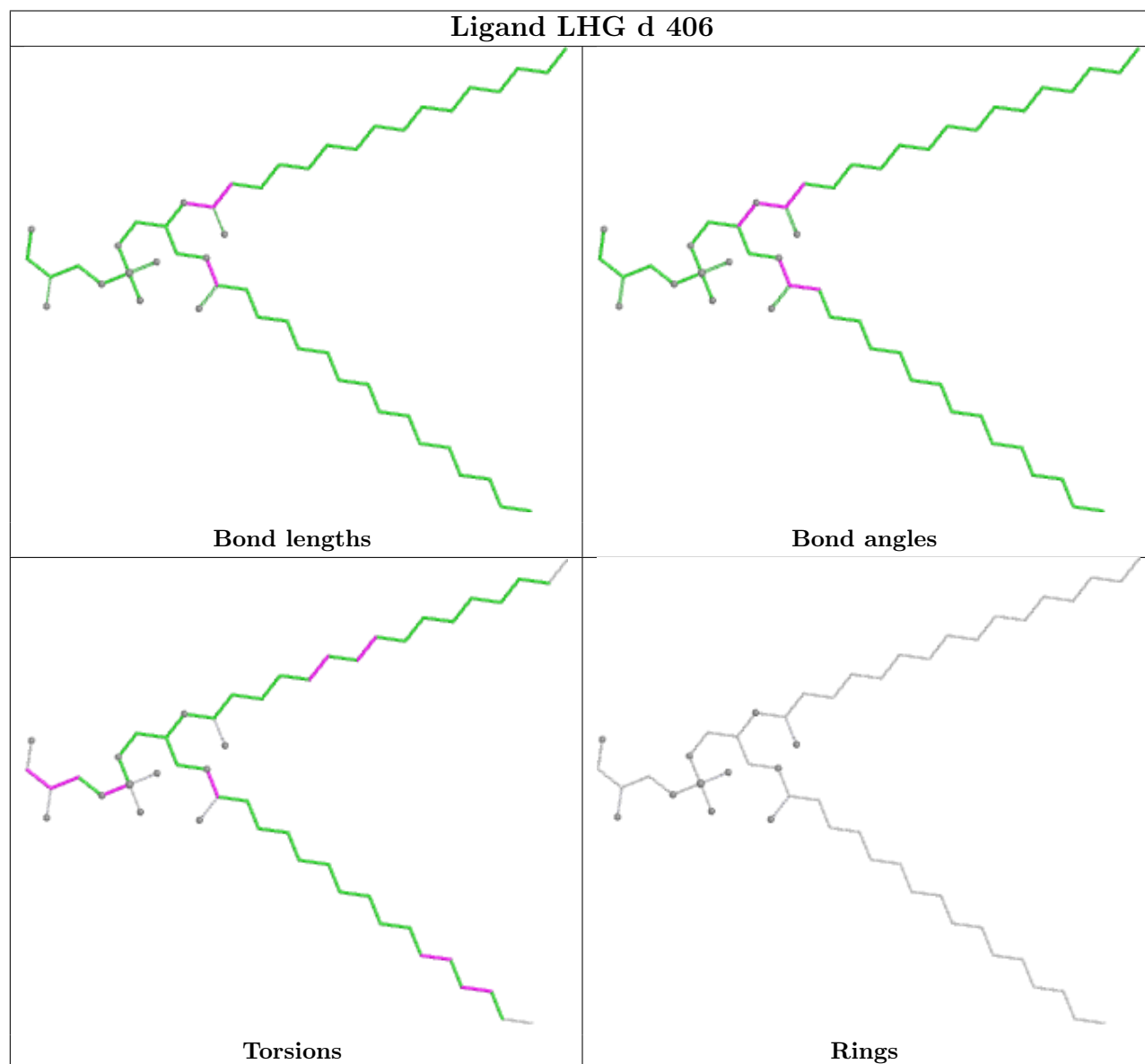
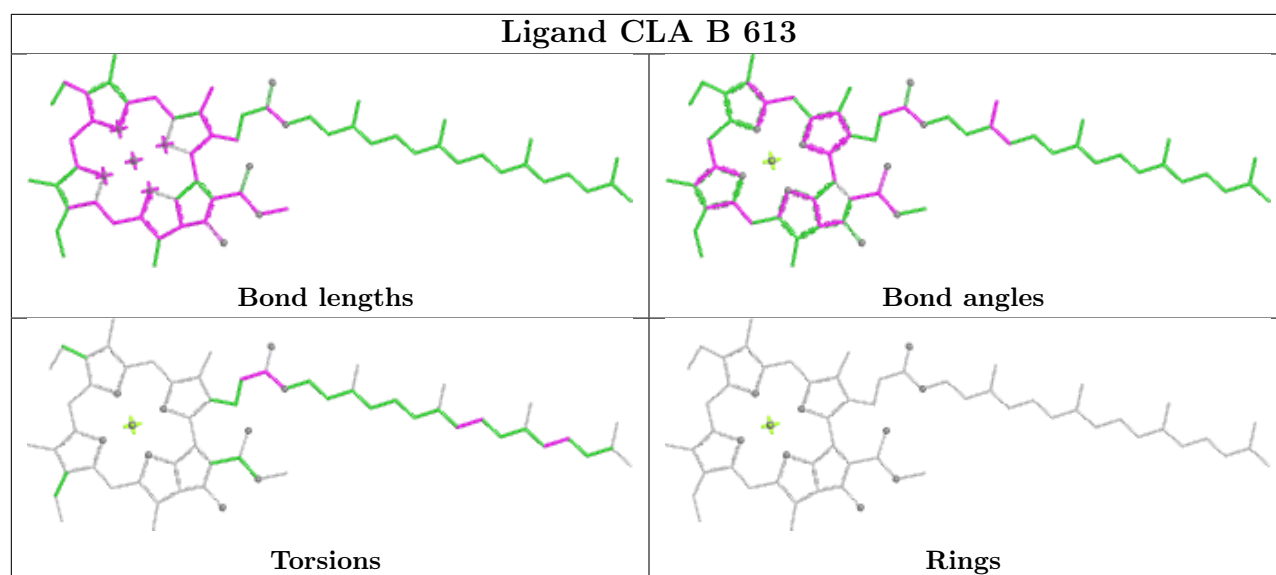


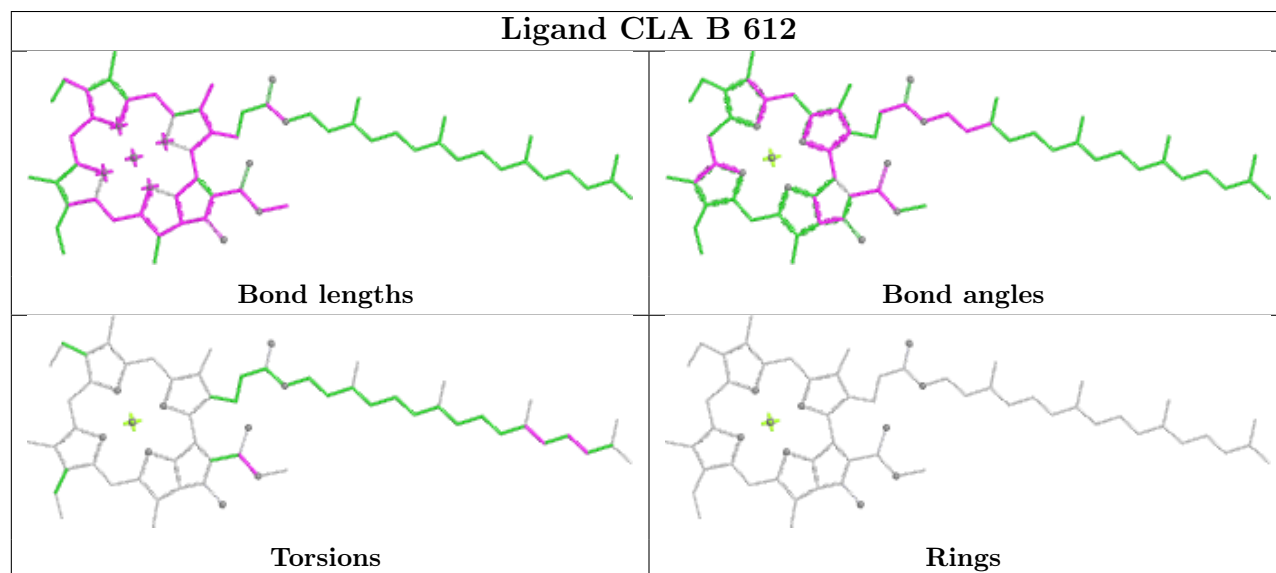
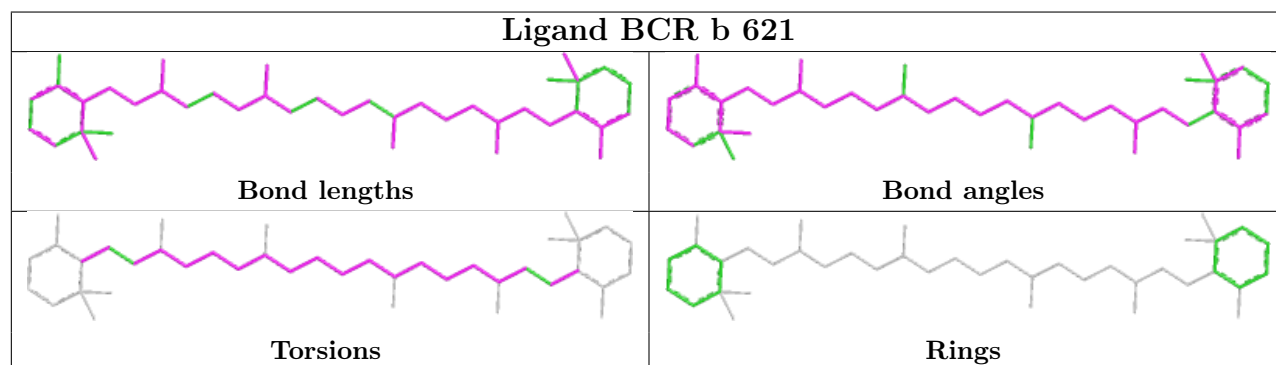
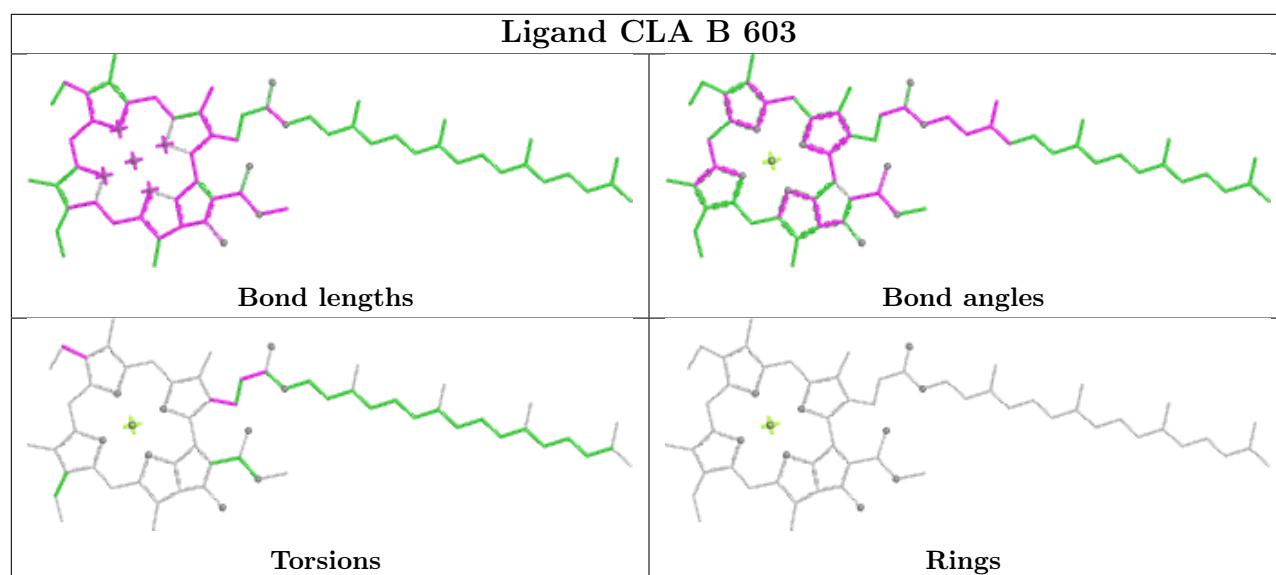
Ligand CLA b 612



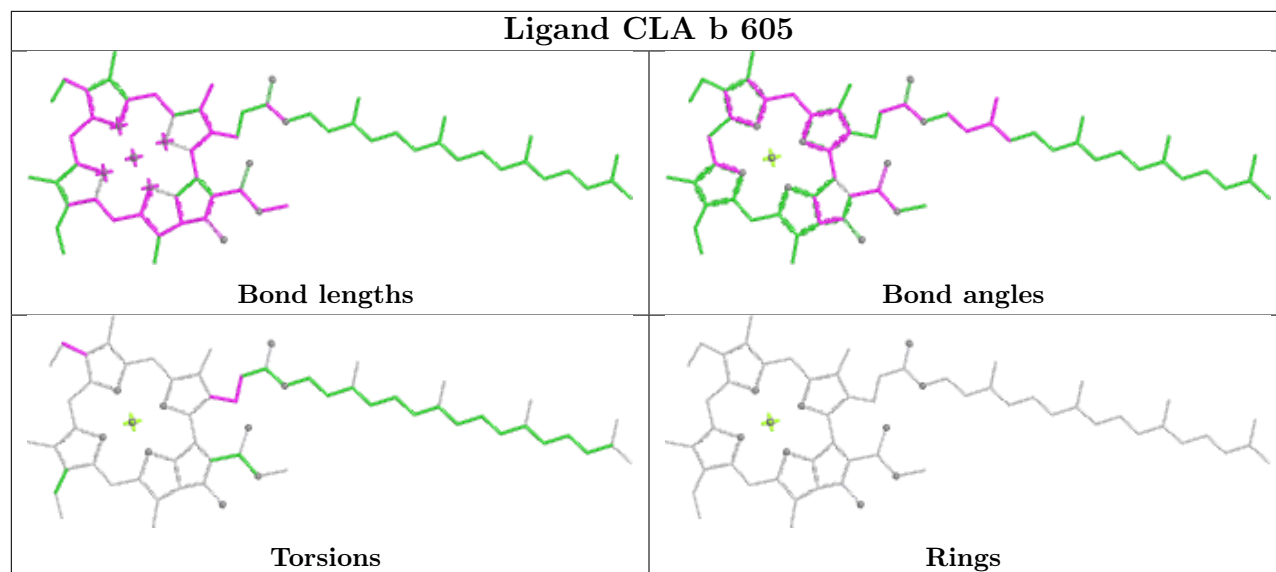




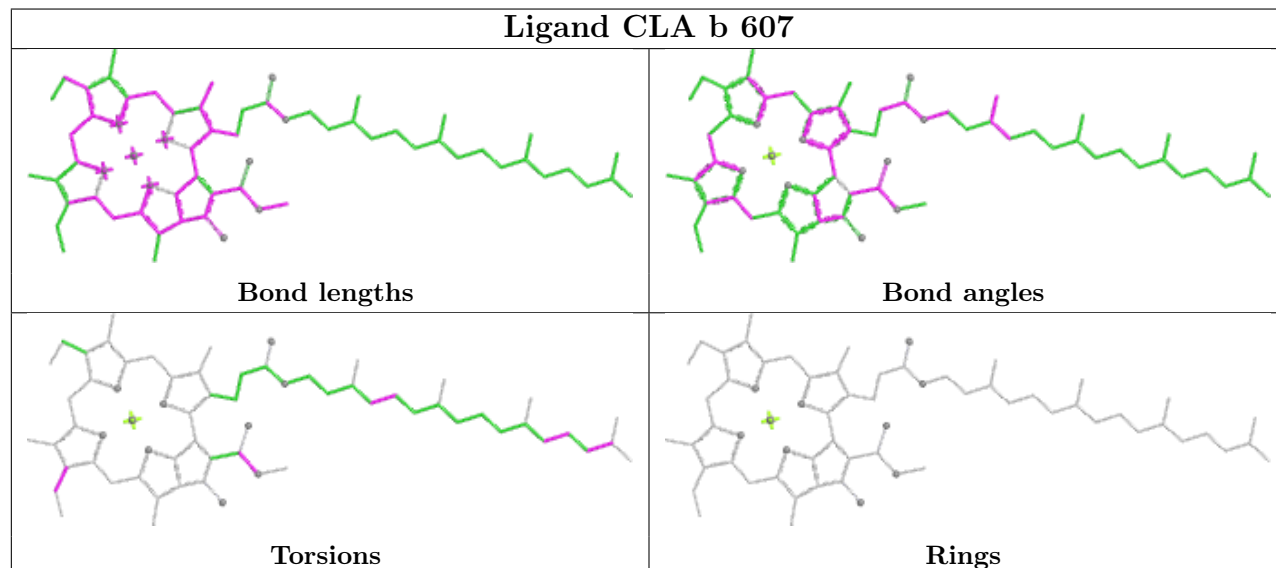


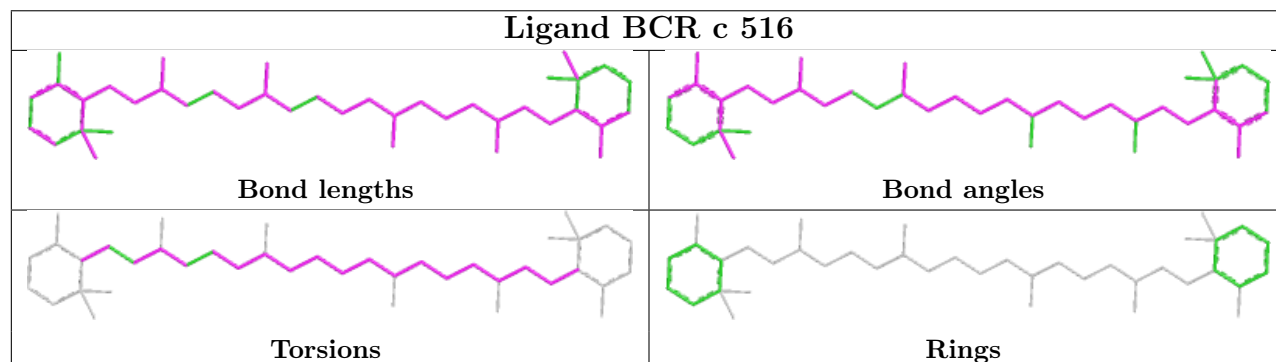
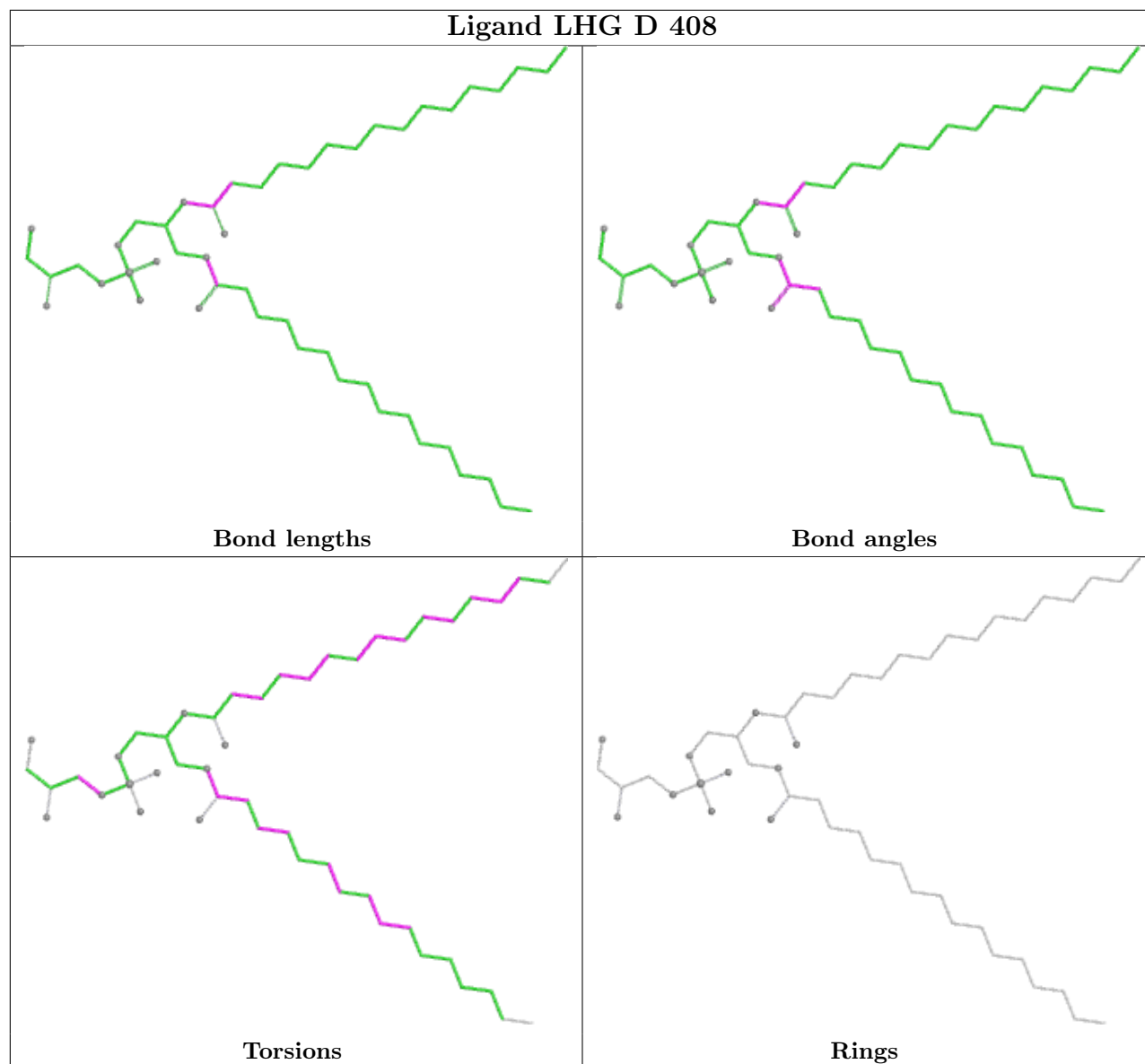


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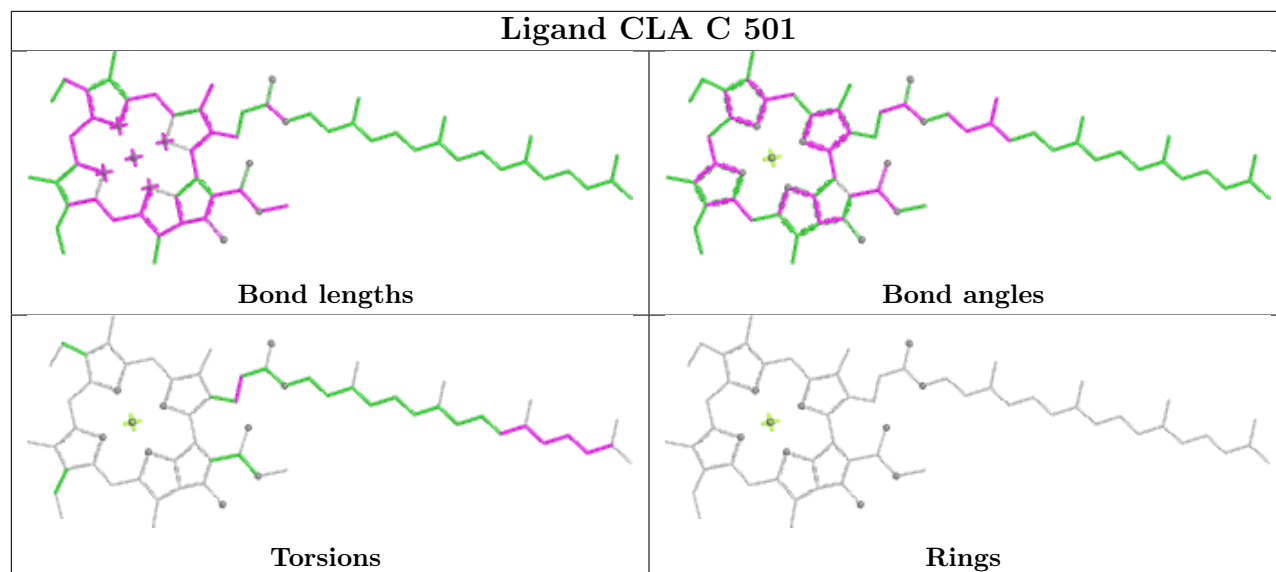


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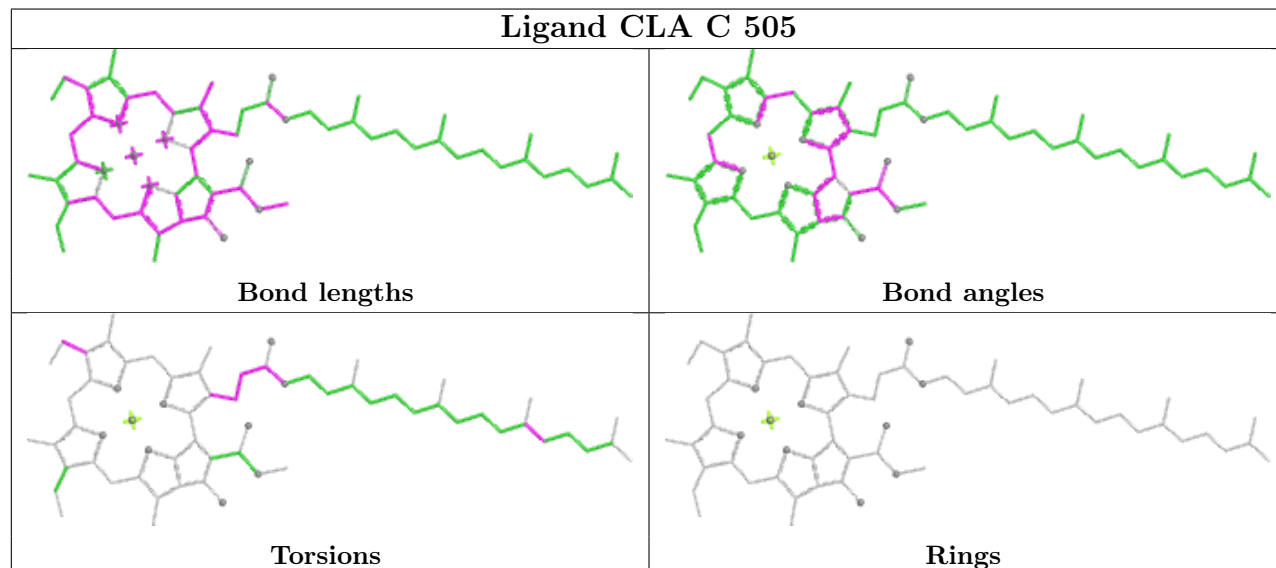




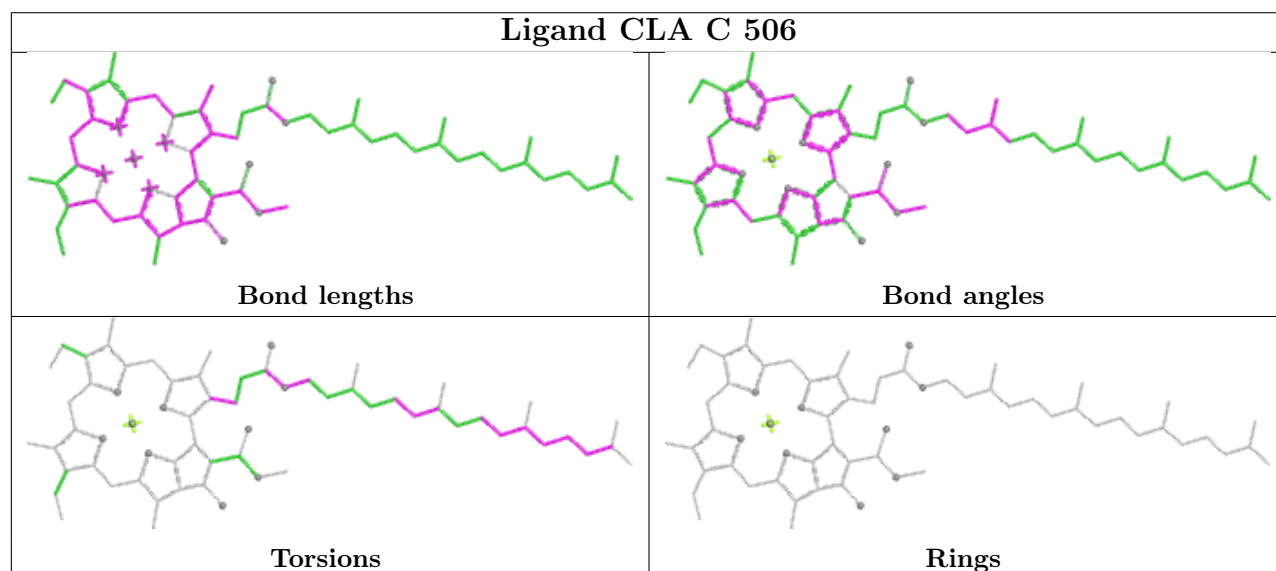
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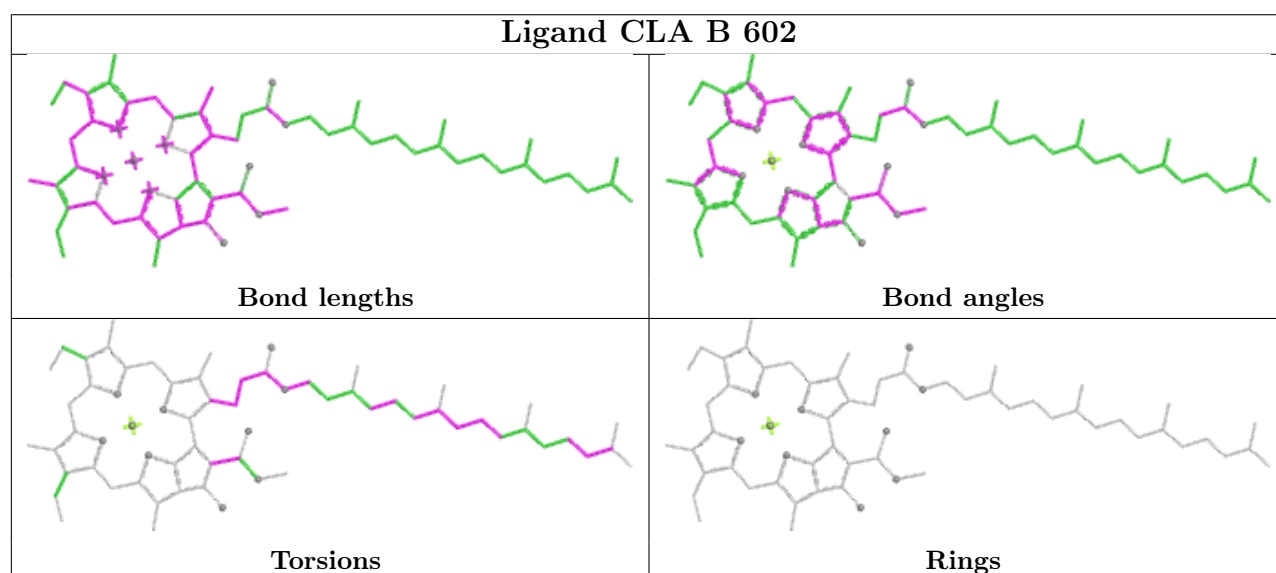
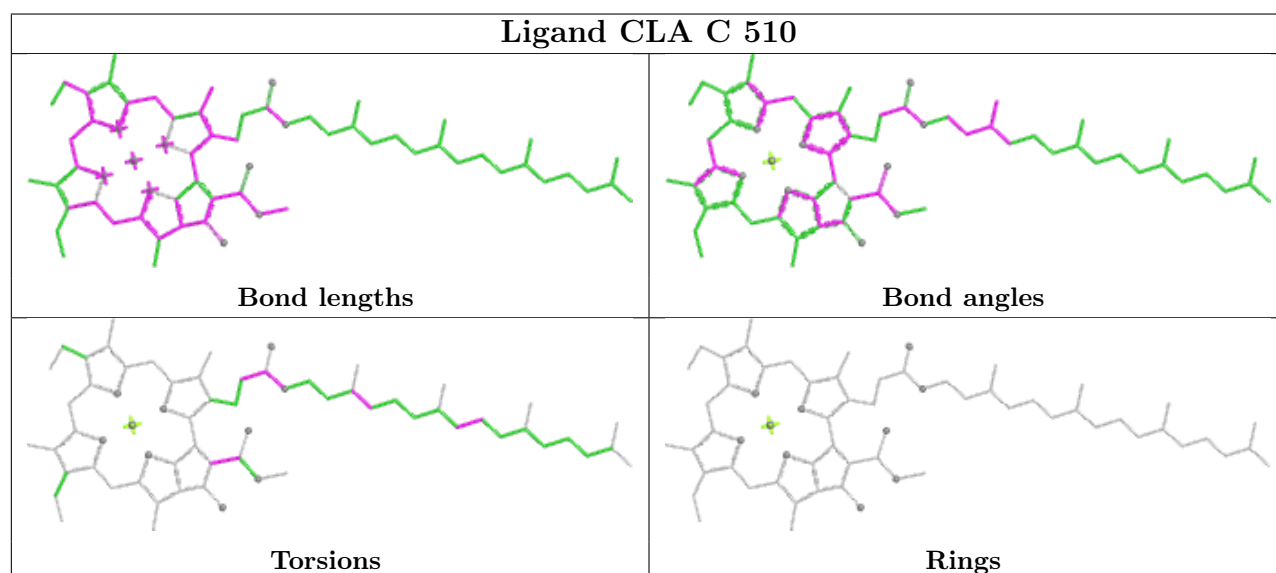
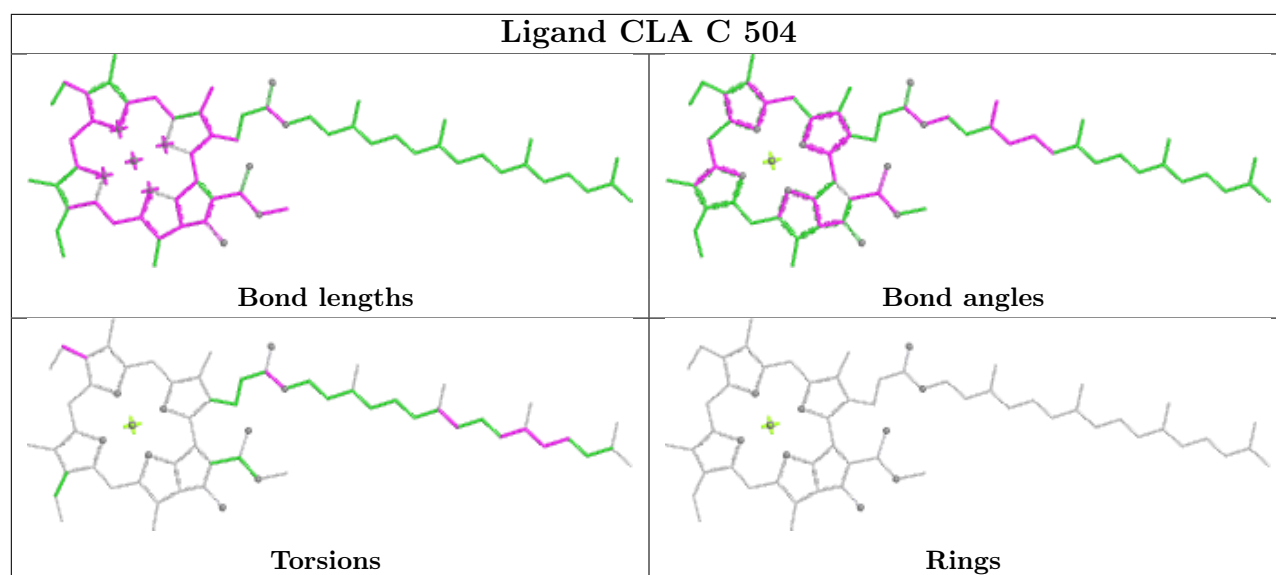


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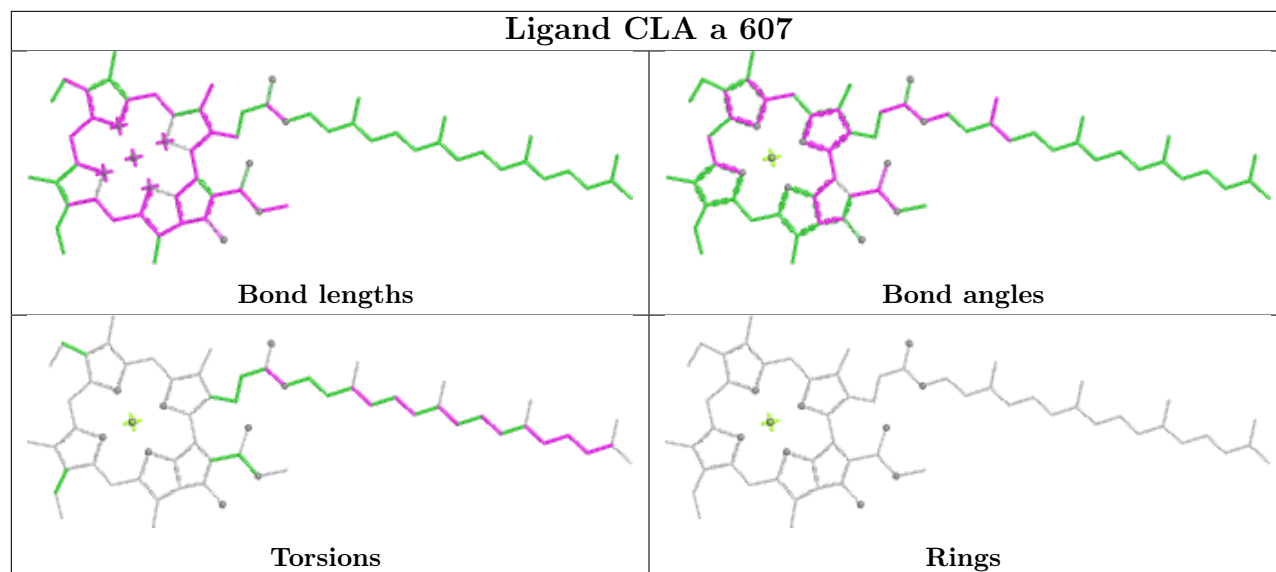


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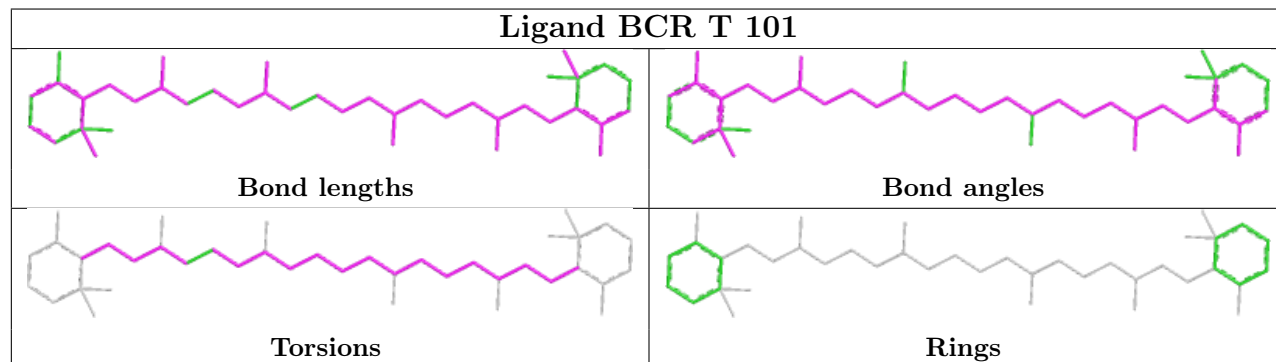




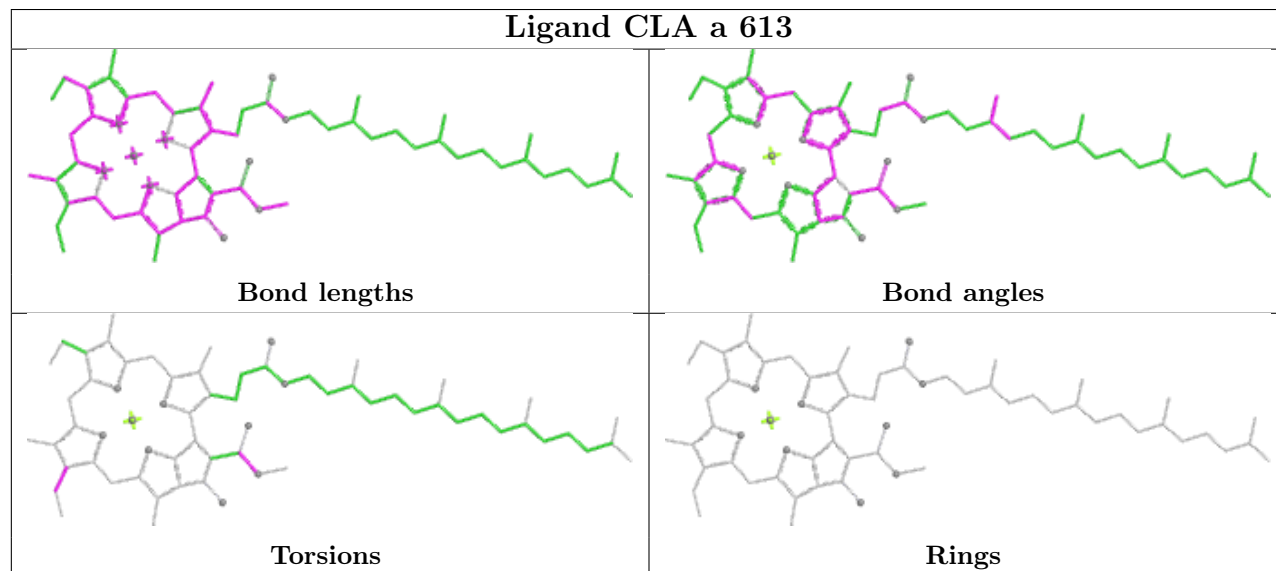
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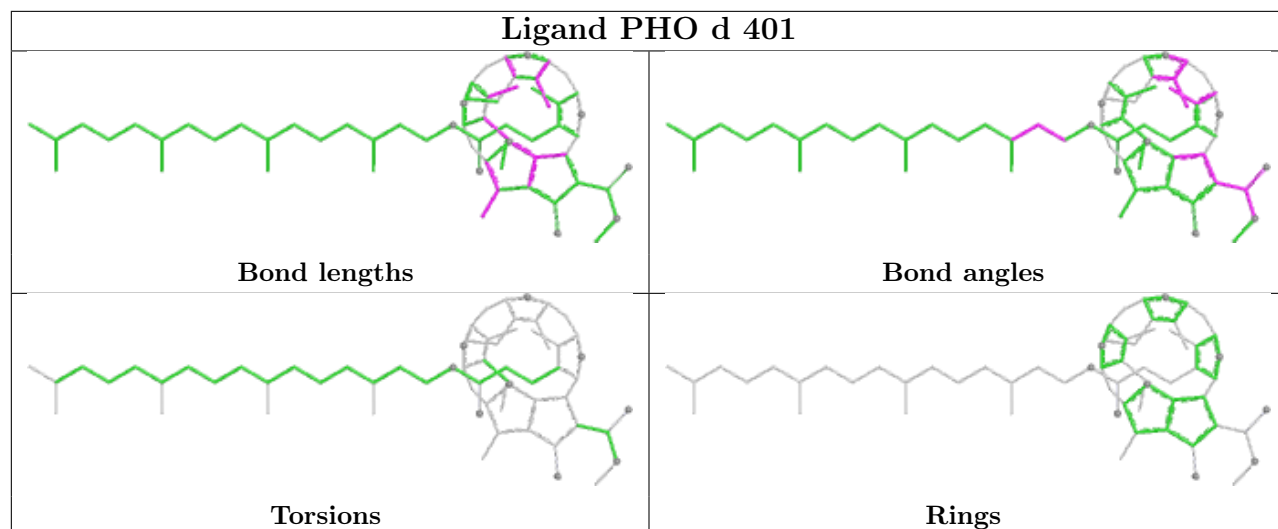
Ligand BCR T 101



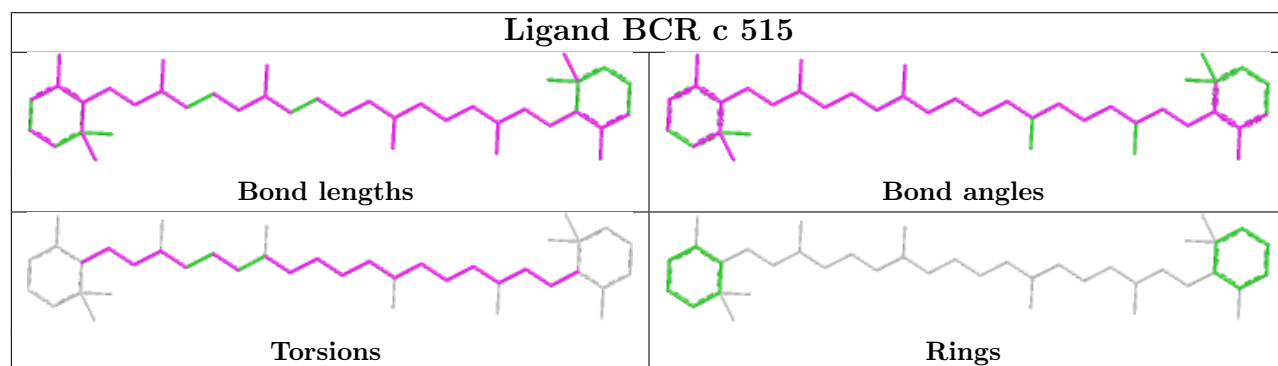
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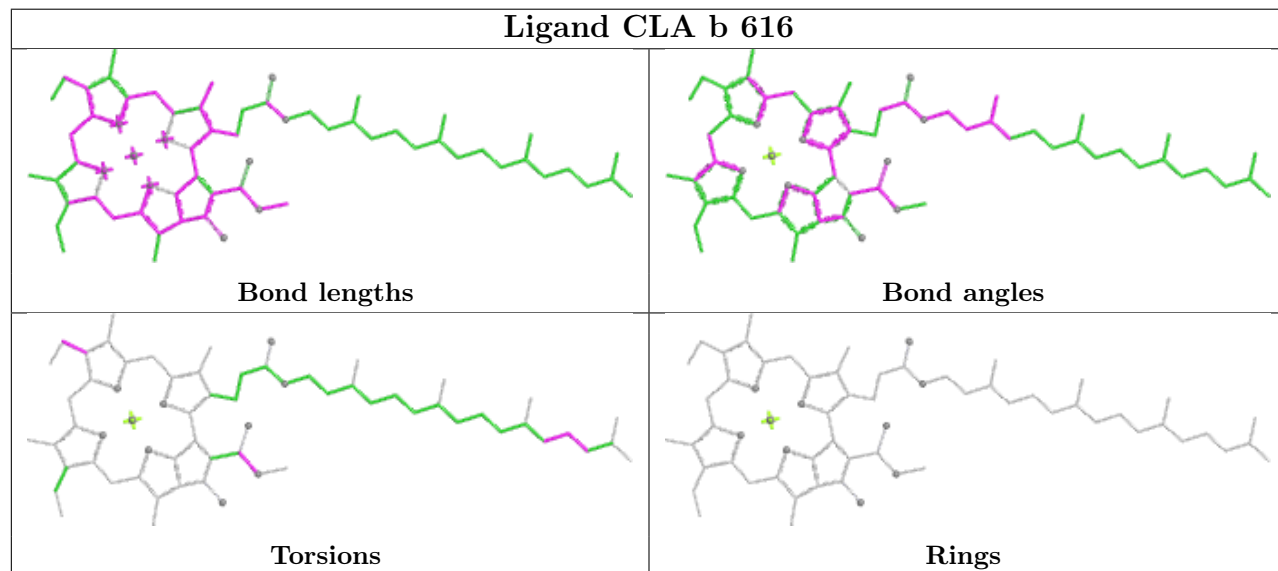
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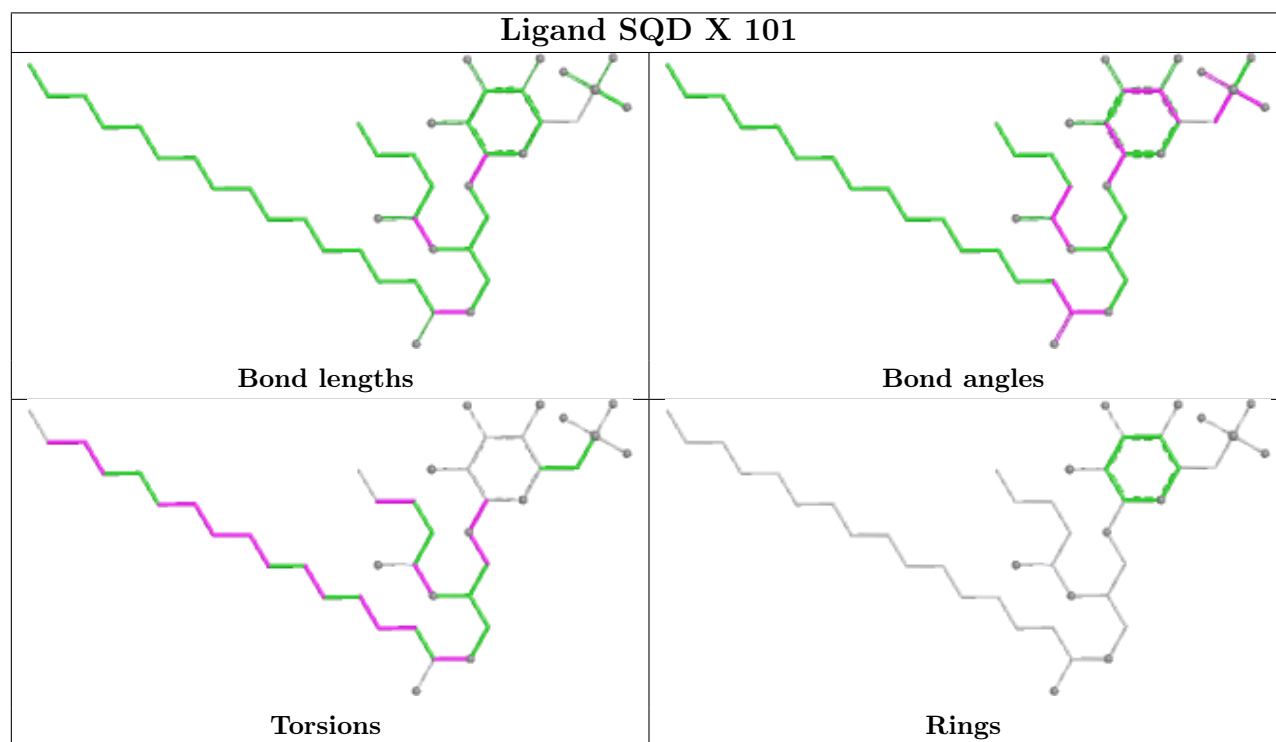
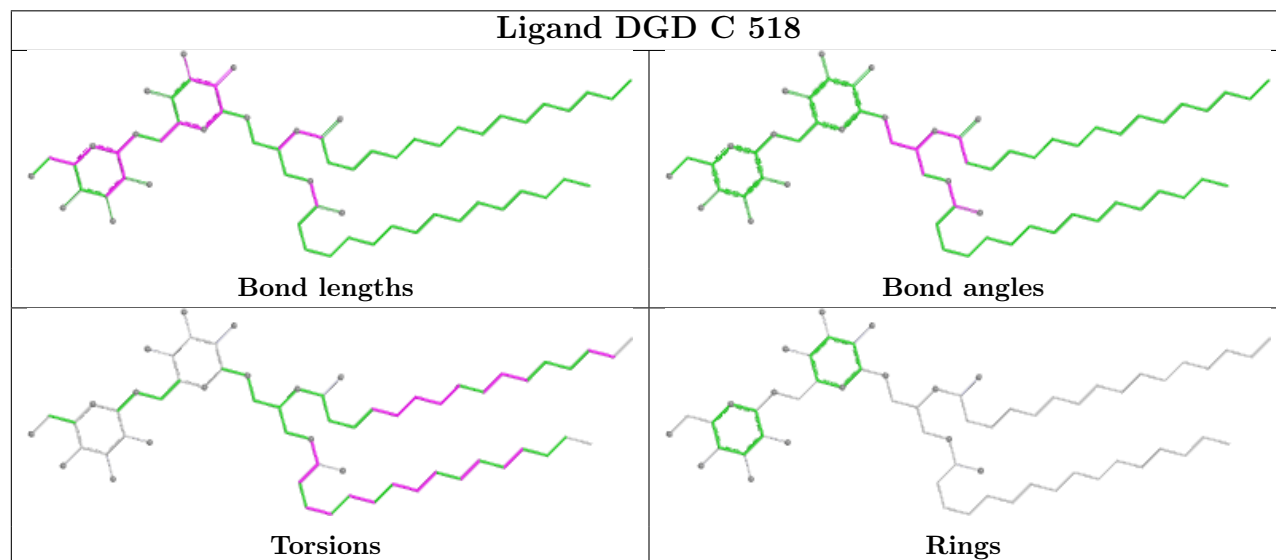
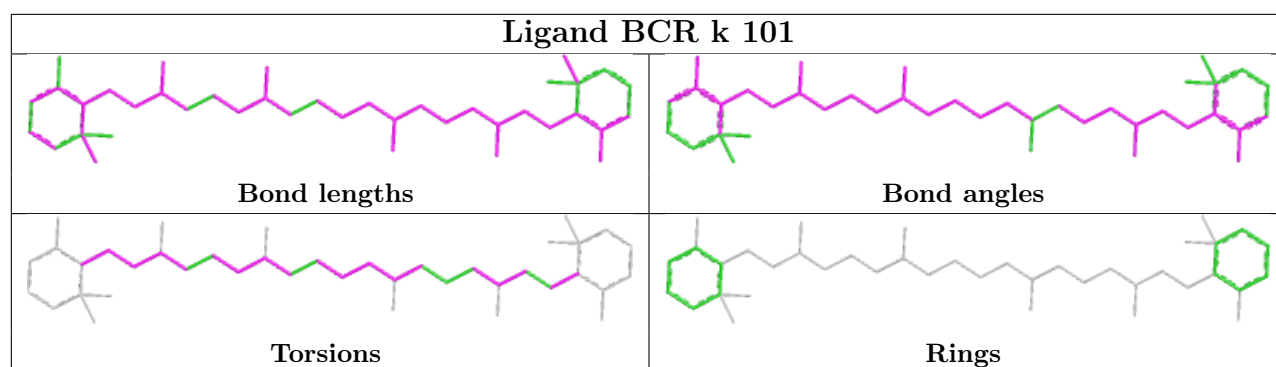


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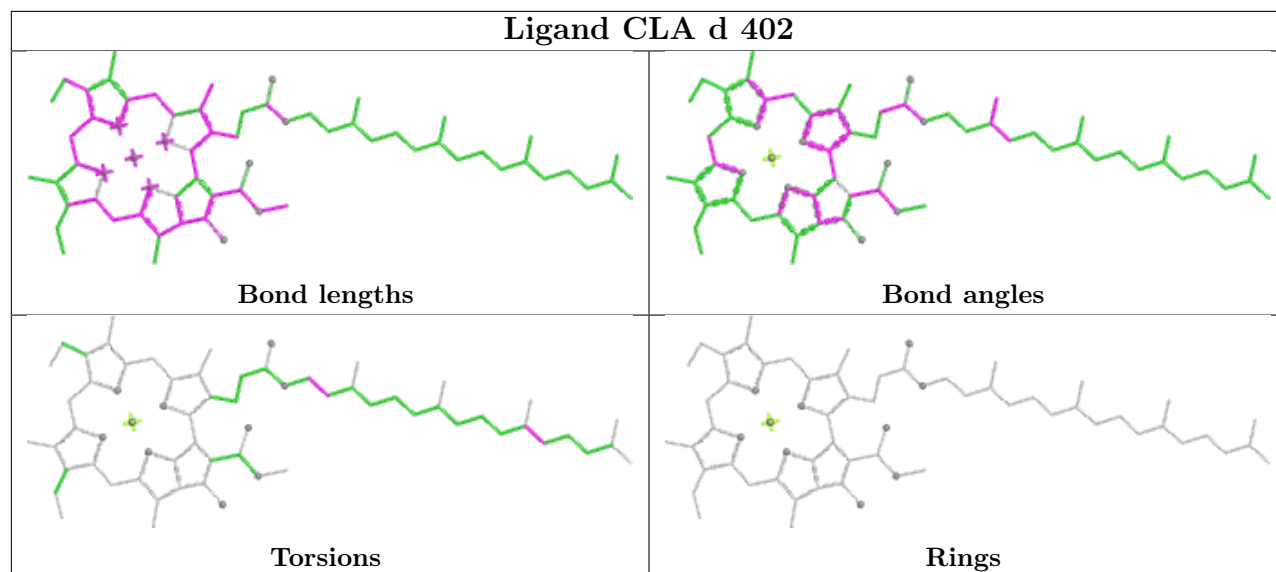


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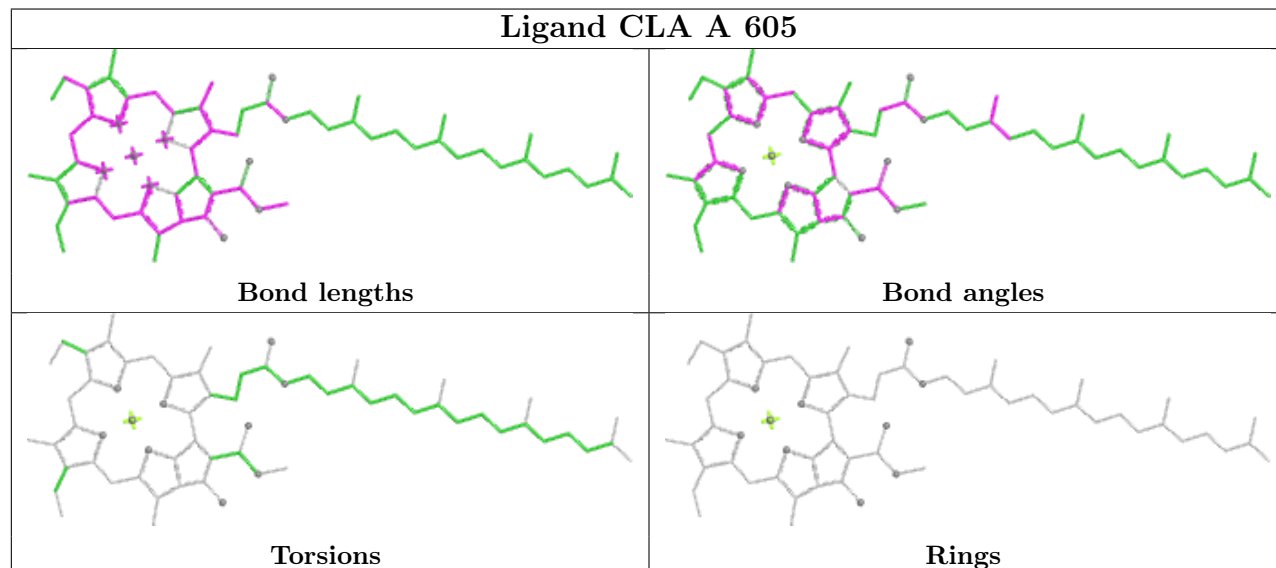




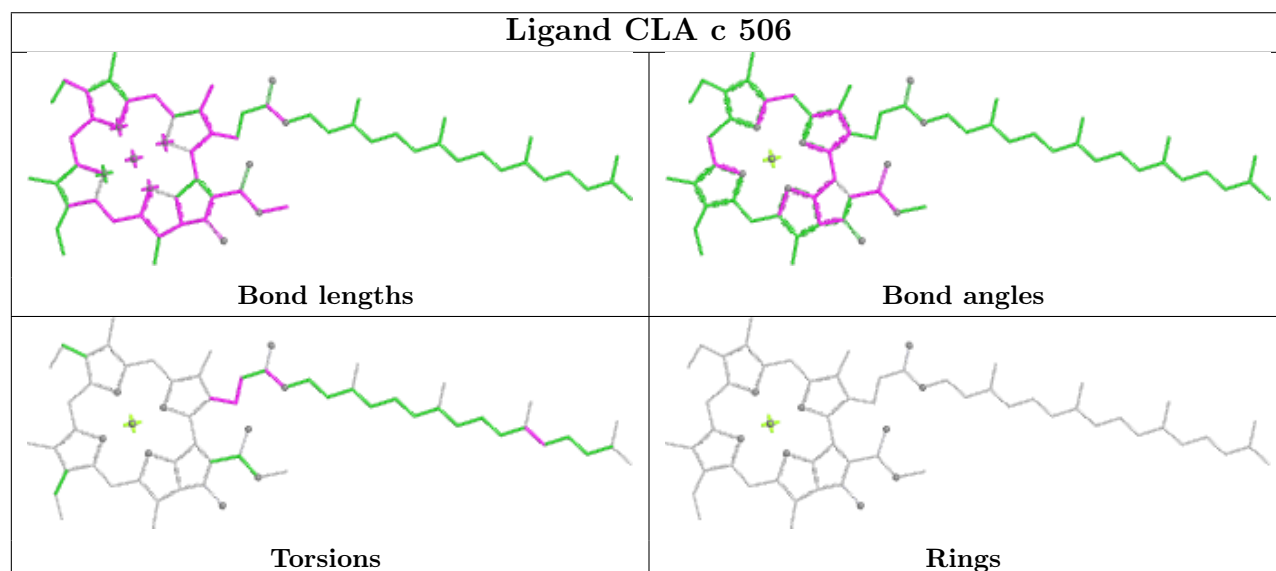
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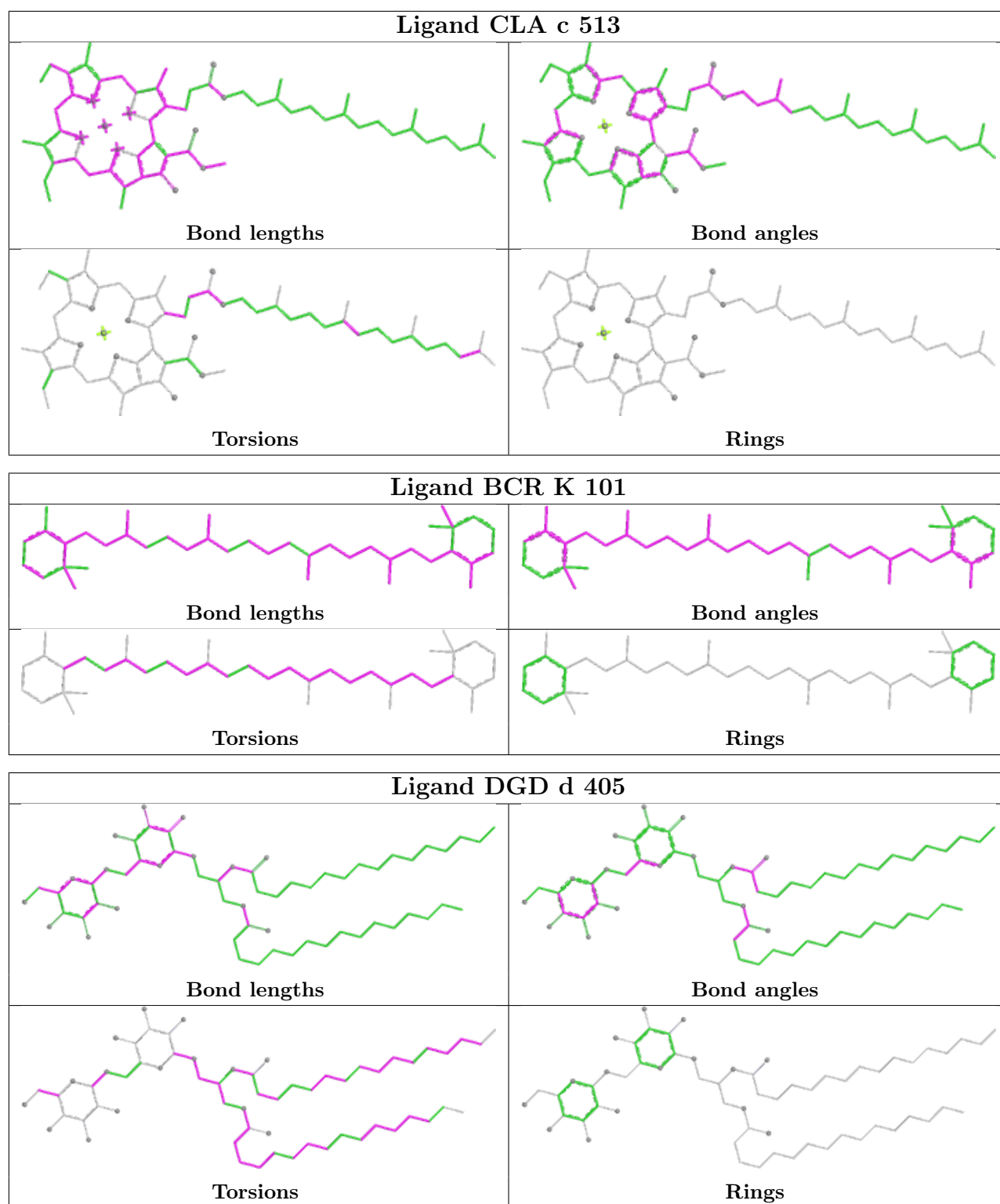


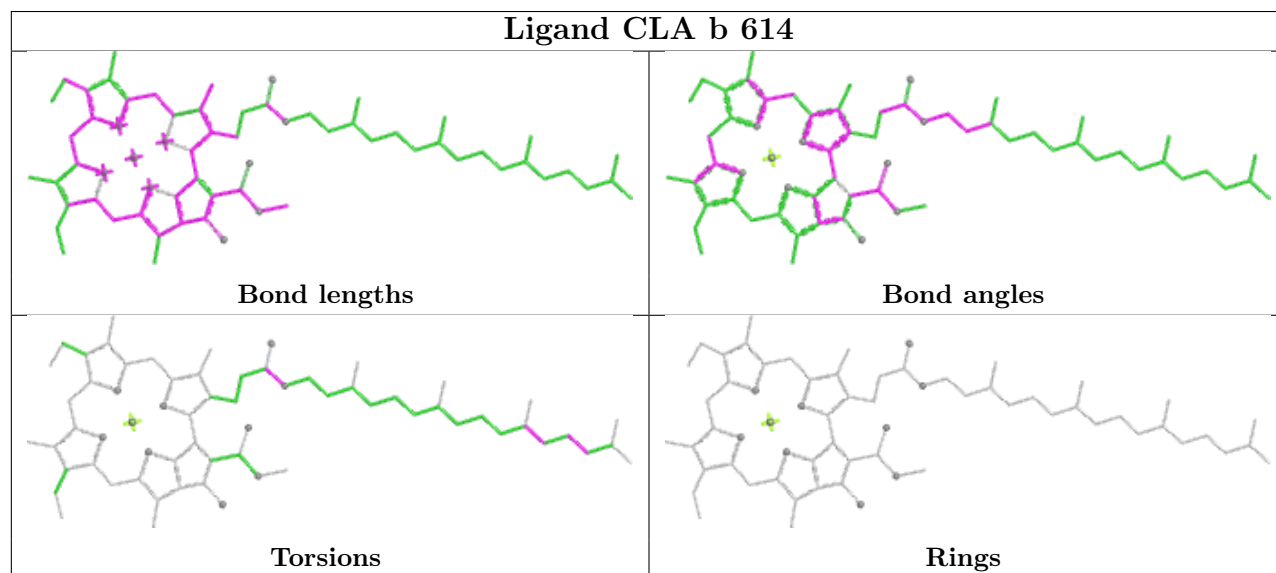
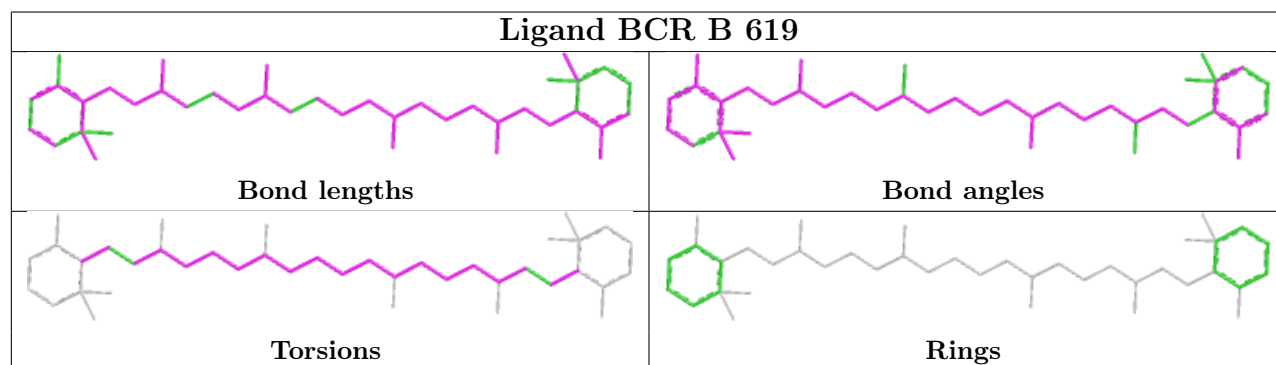
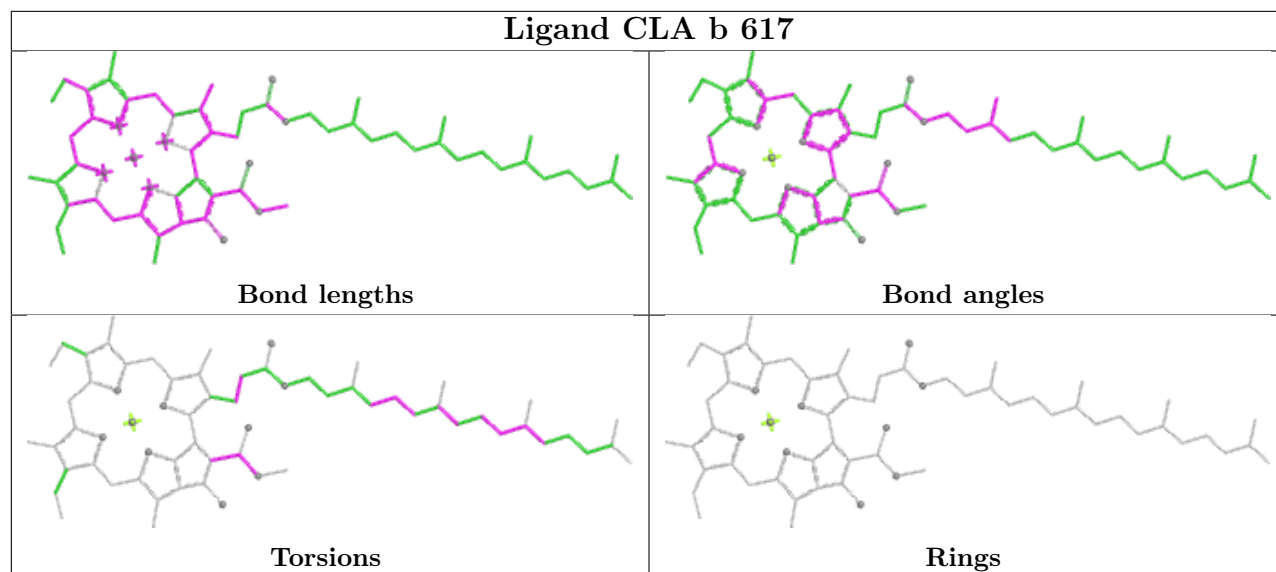
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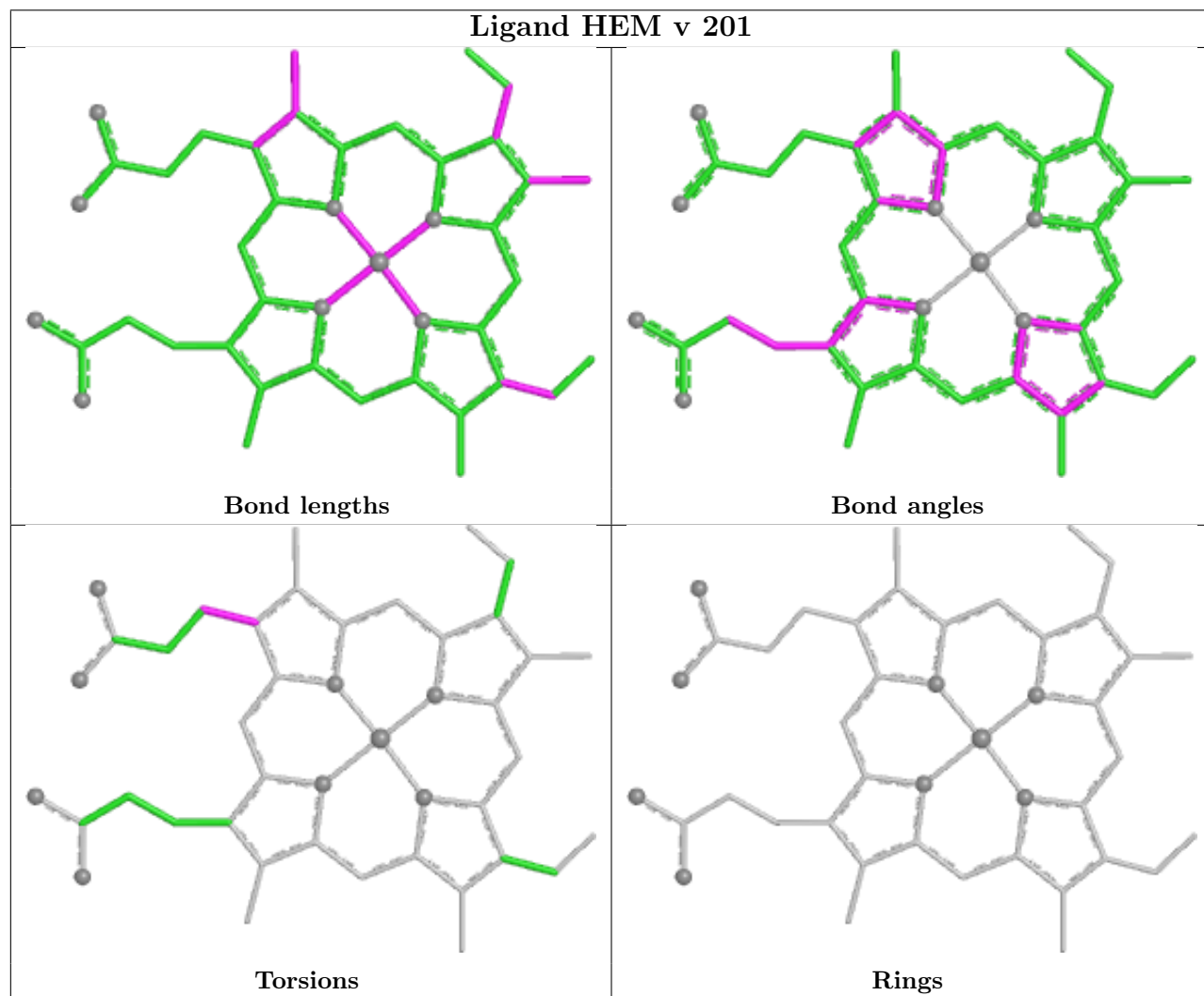
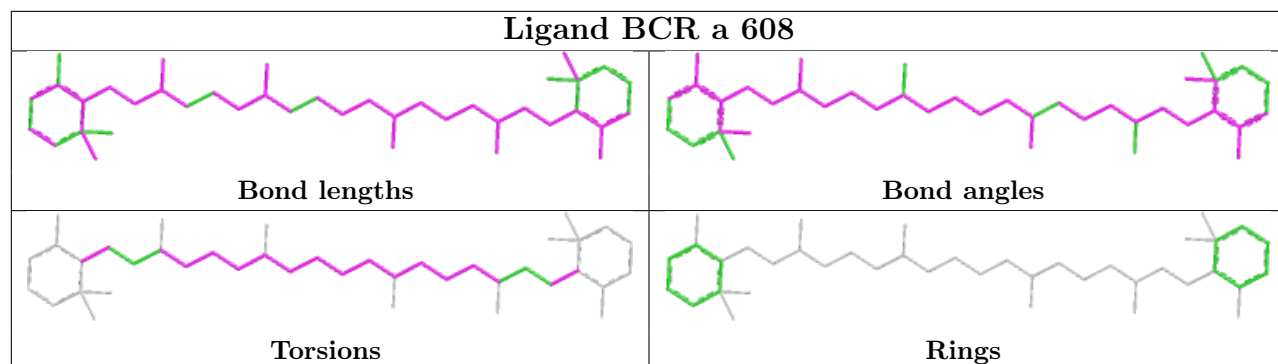


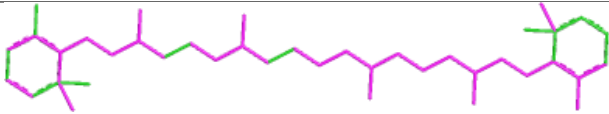
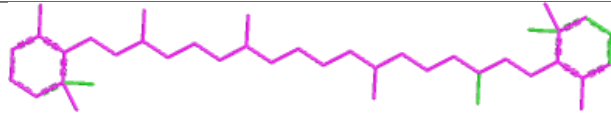
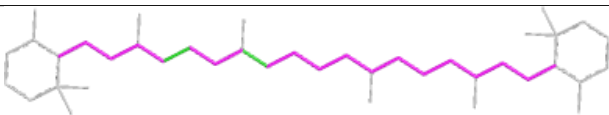
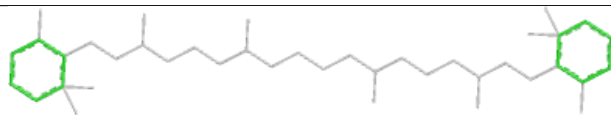
Ligand CLA c 506

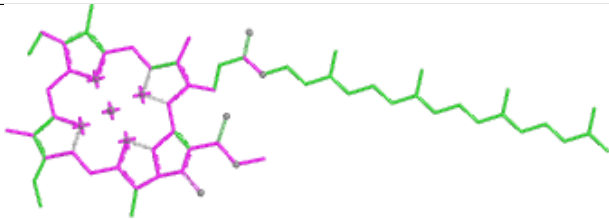
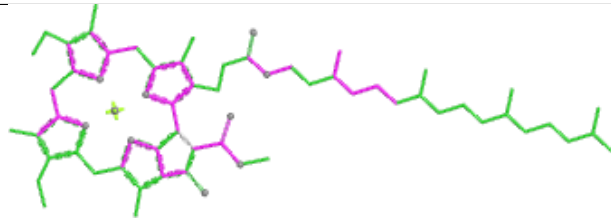
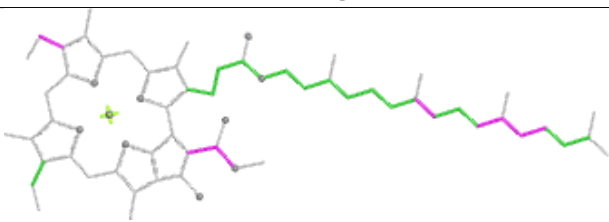
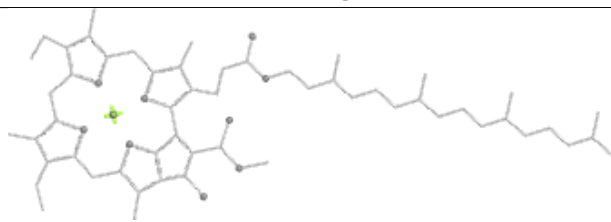


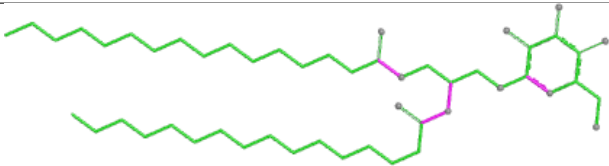
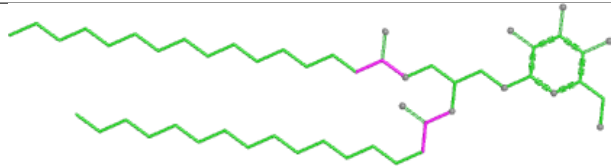
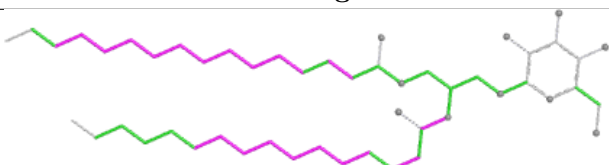
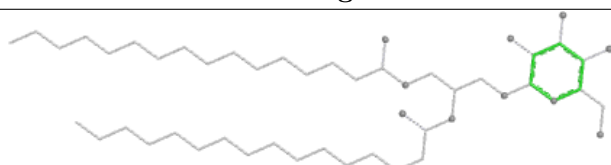


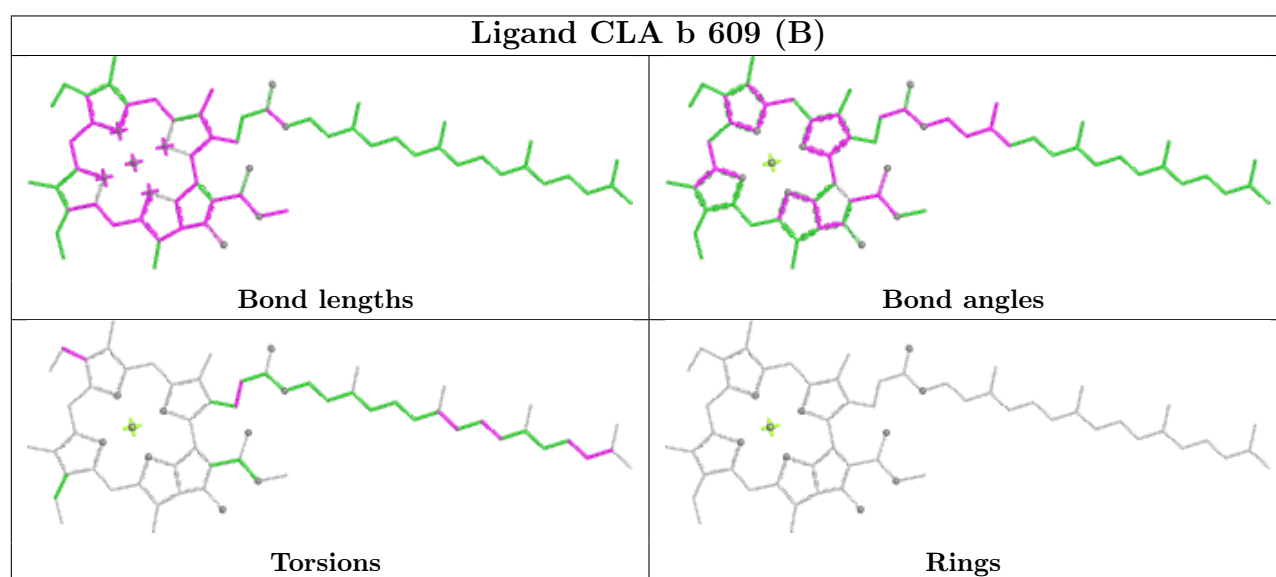
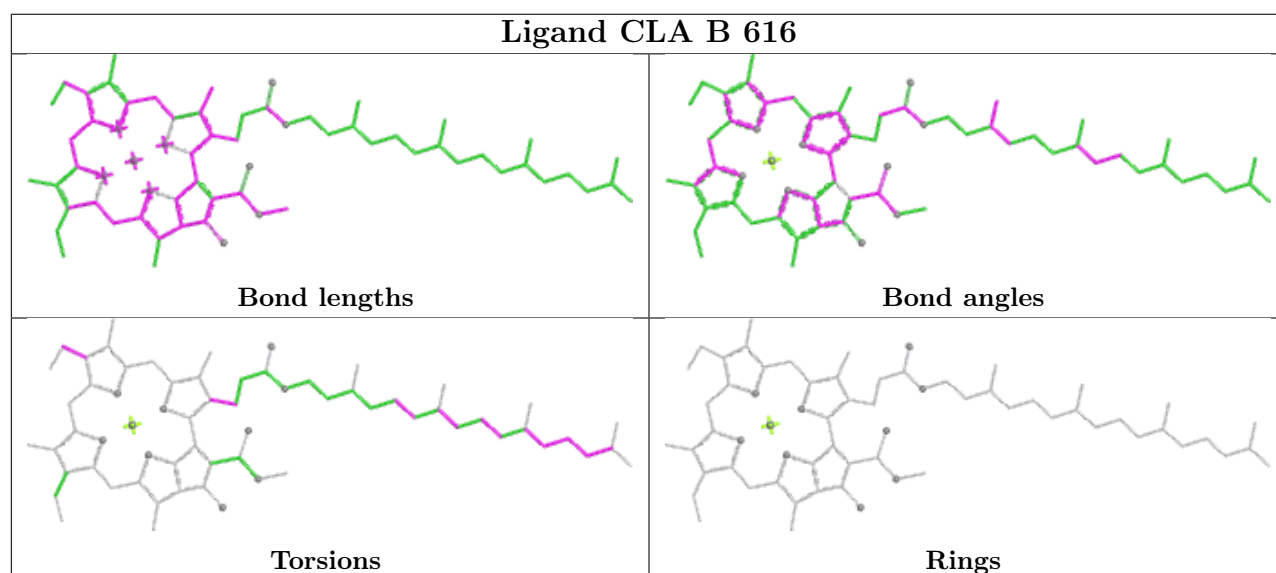
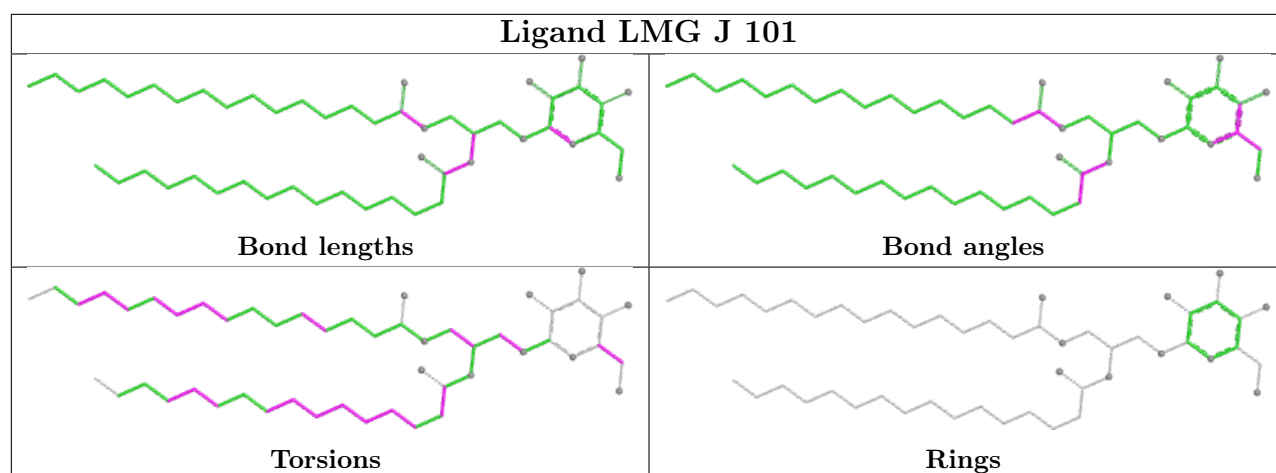




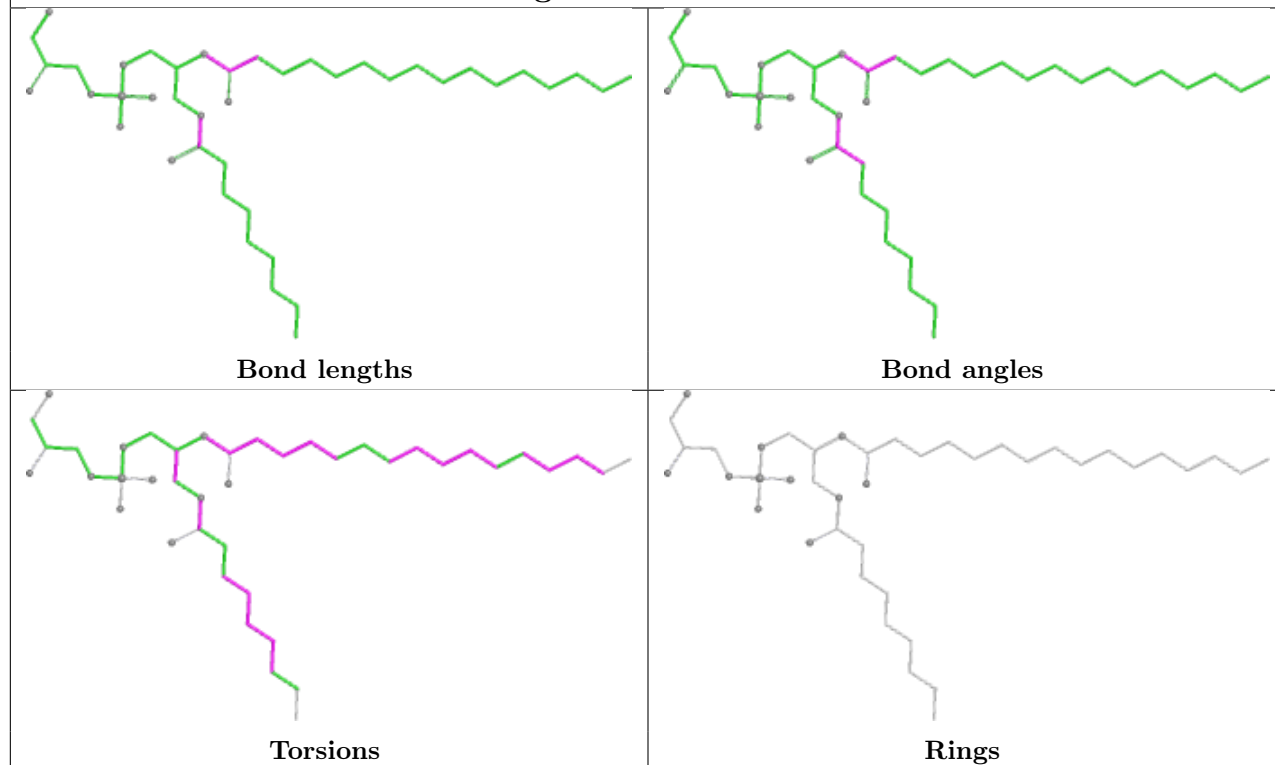
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

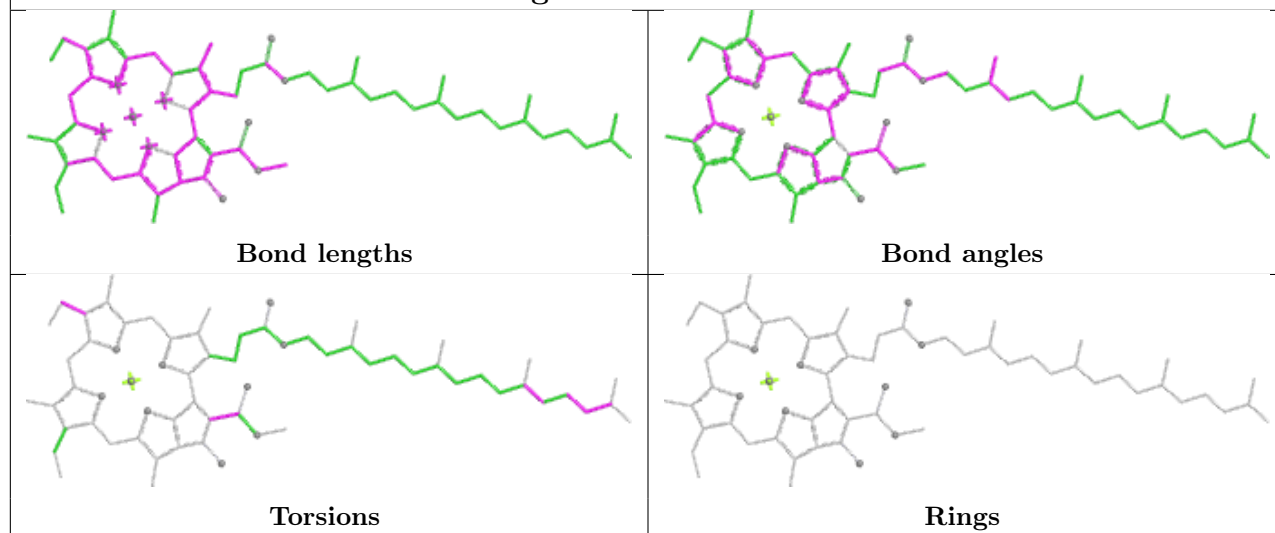
Ligand LMG b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings



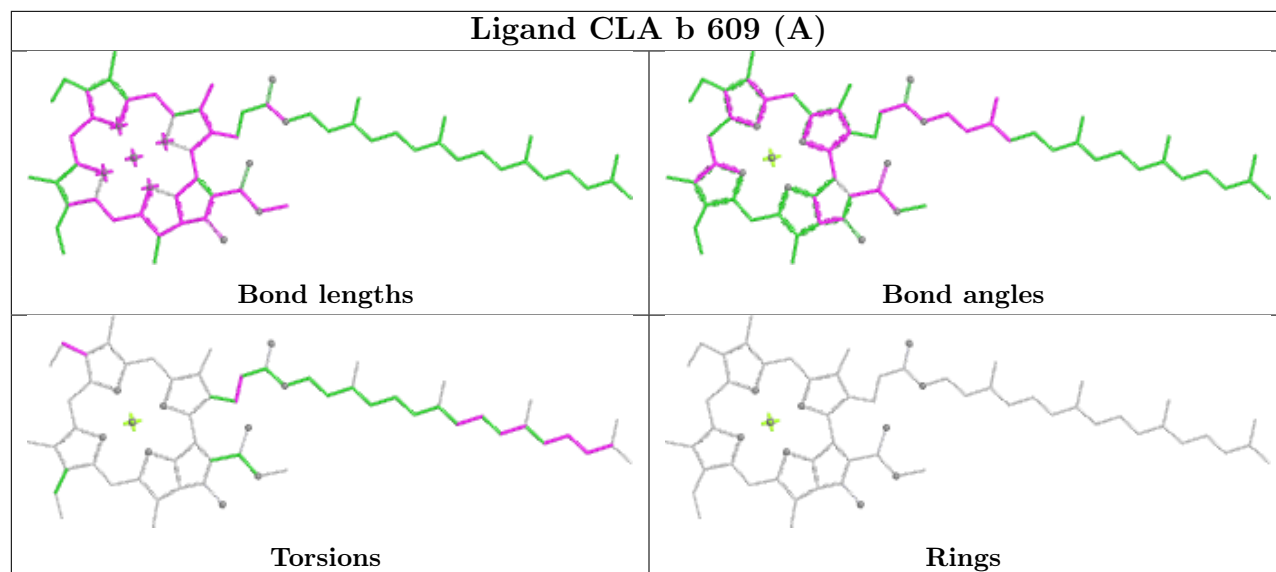
Ligand LHG e 101



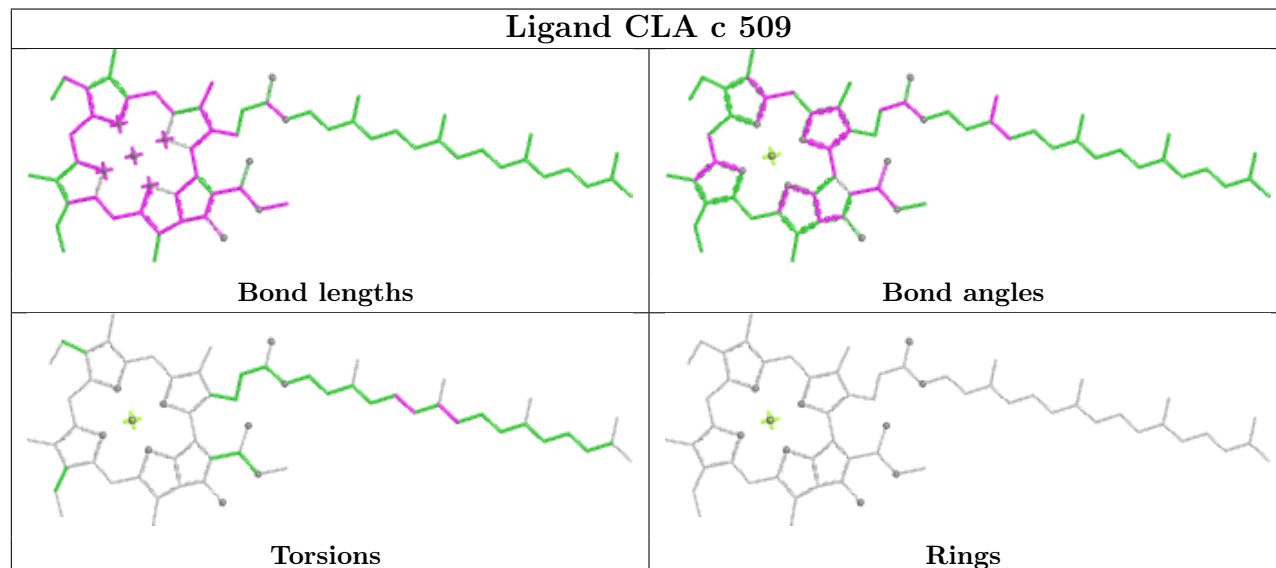
Ligand CLA C 502



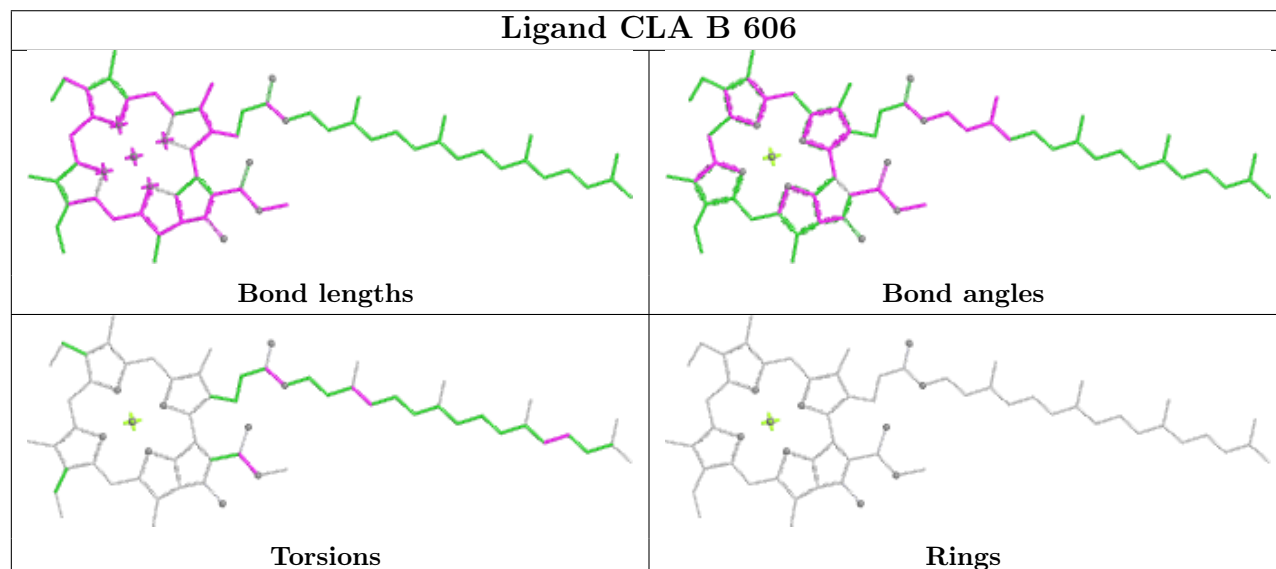
Ligand CLA b 609 (A)

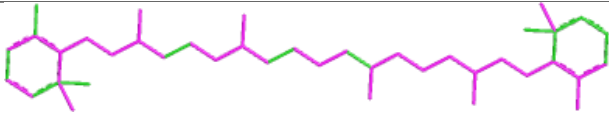
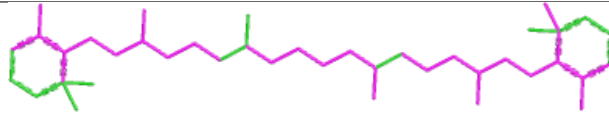
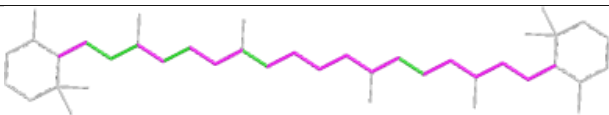
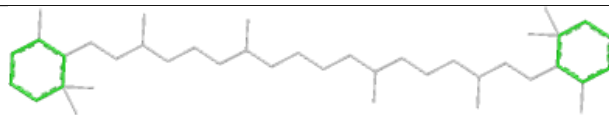


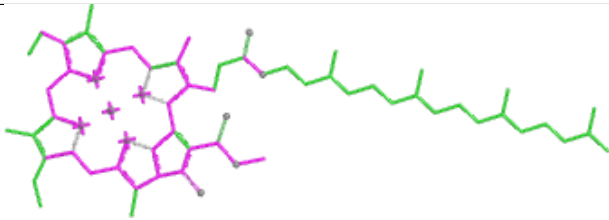
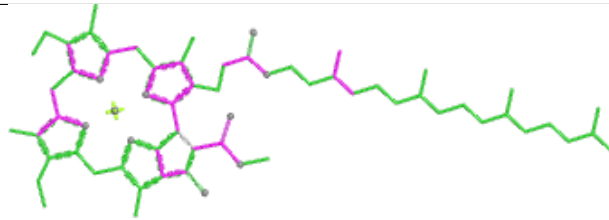
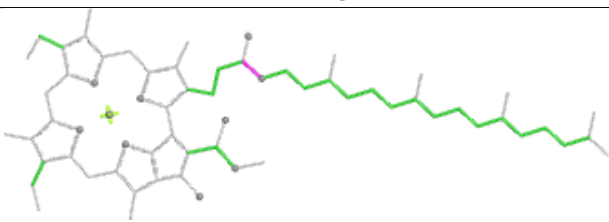
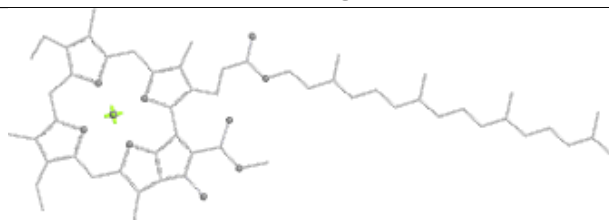
Ligand CLA c 509

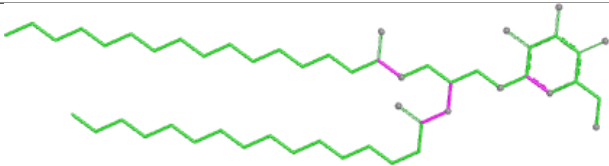
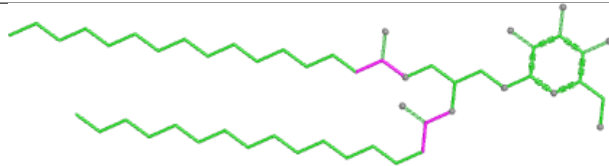
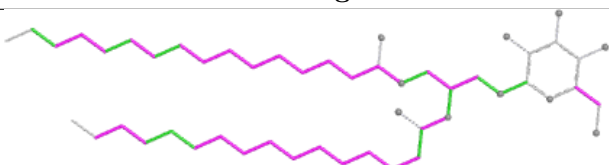
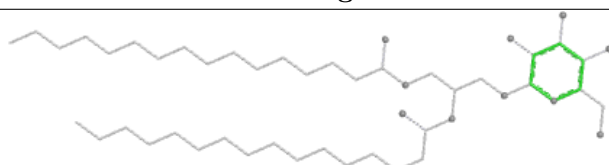


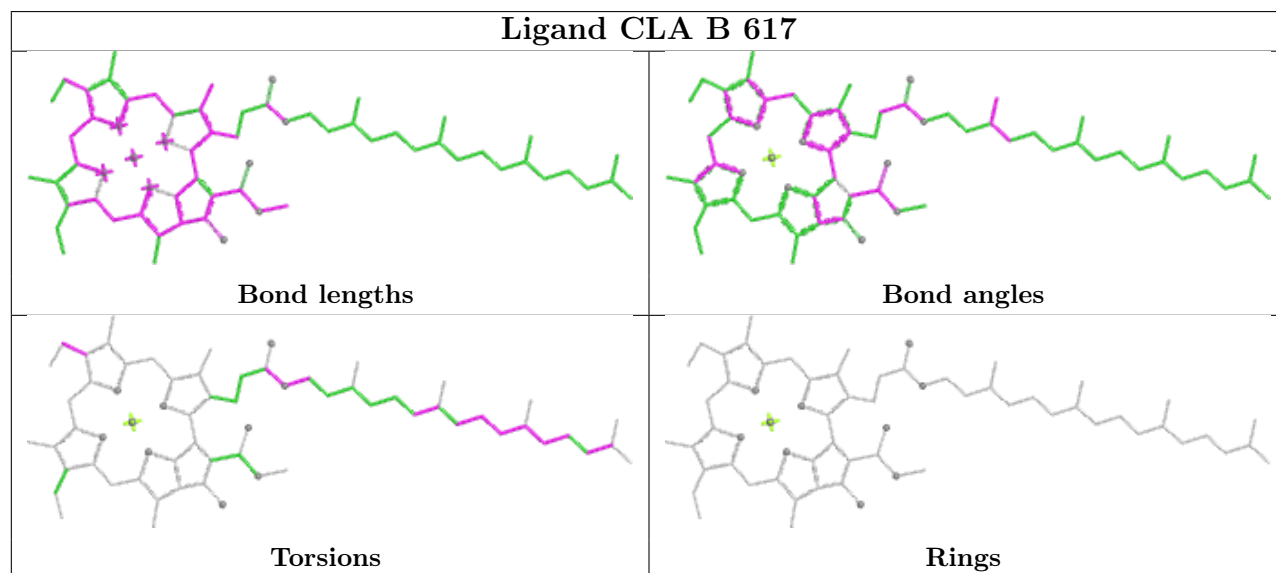
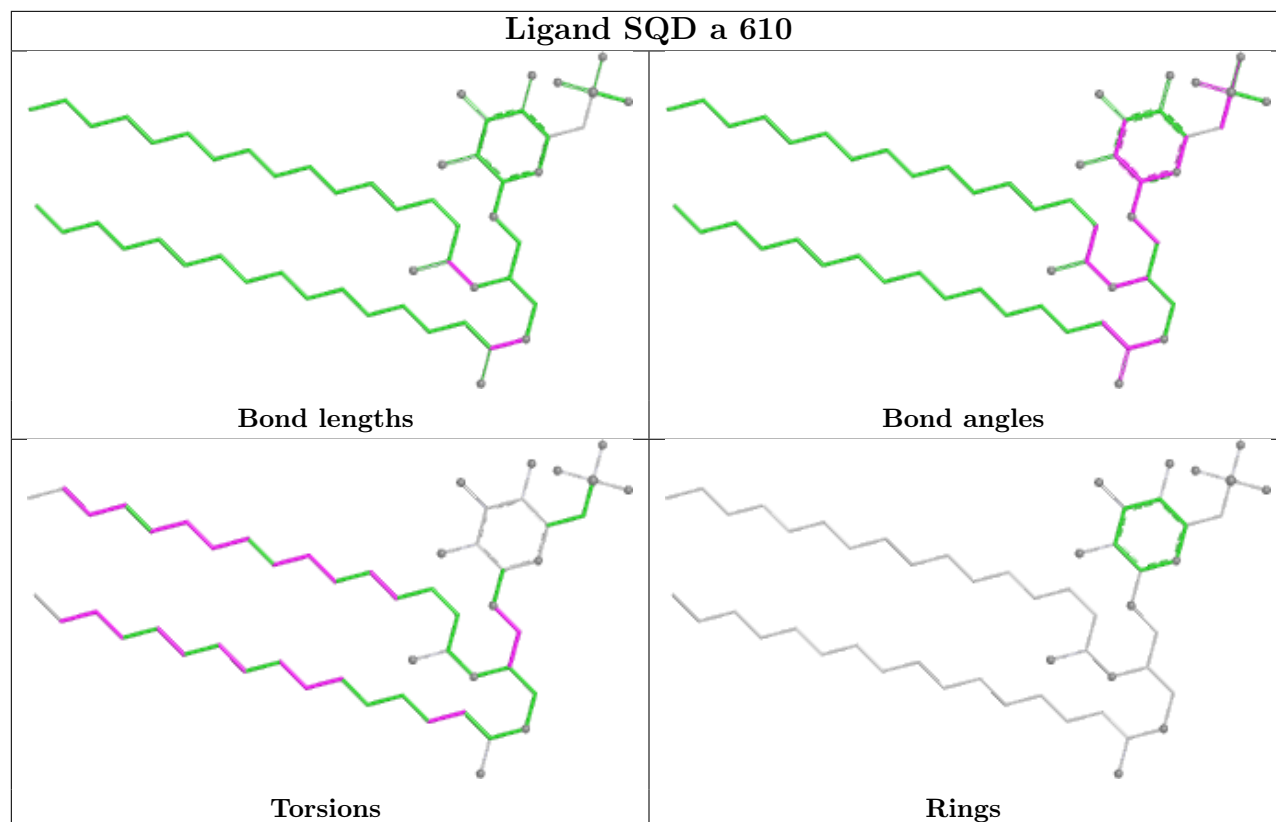
Ligand CLA B 606

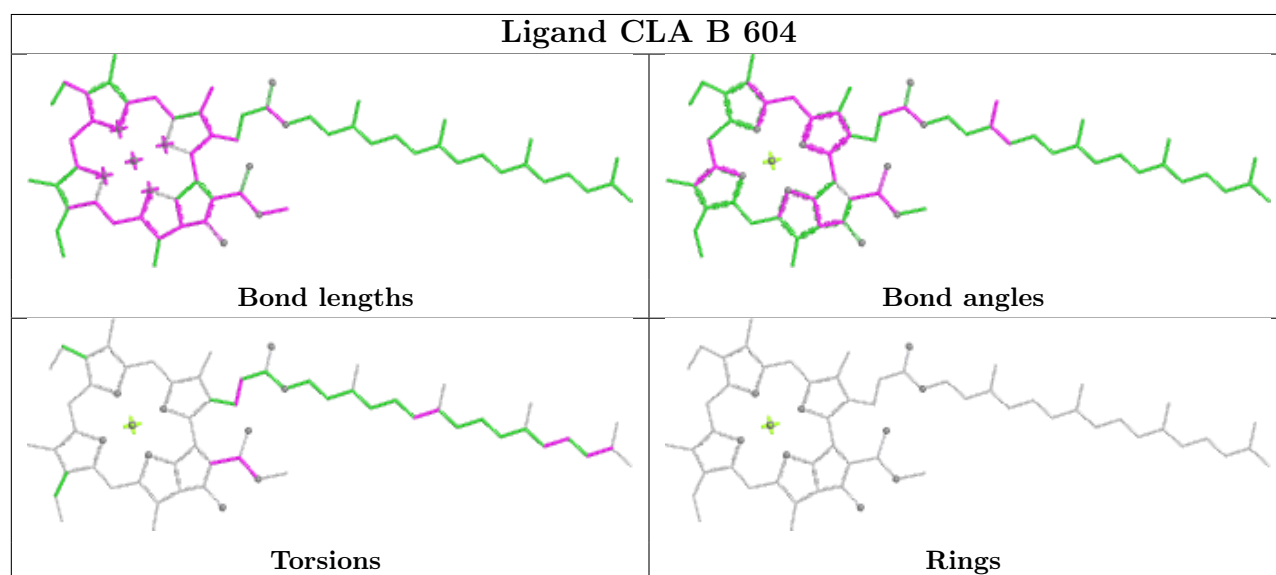
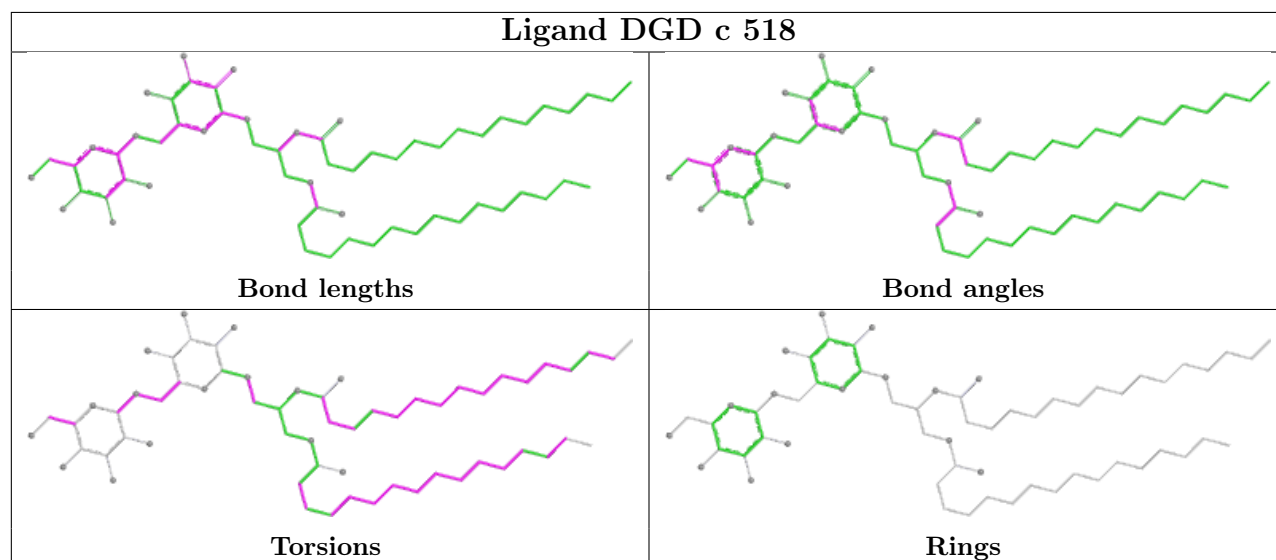
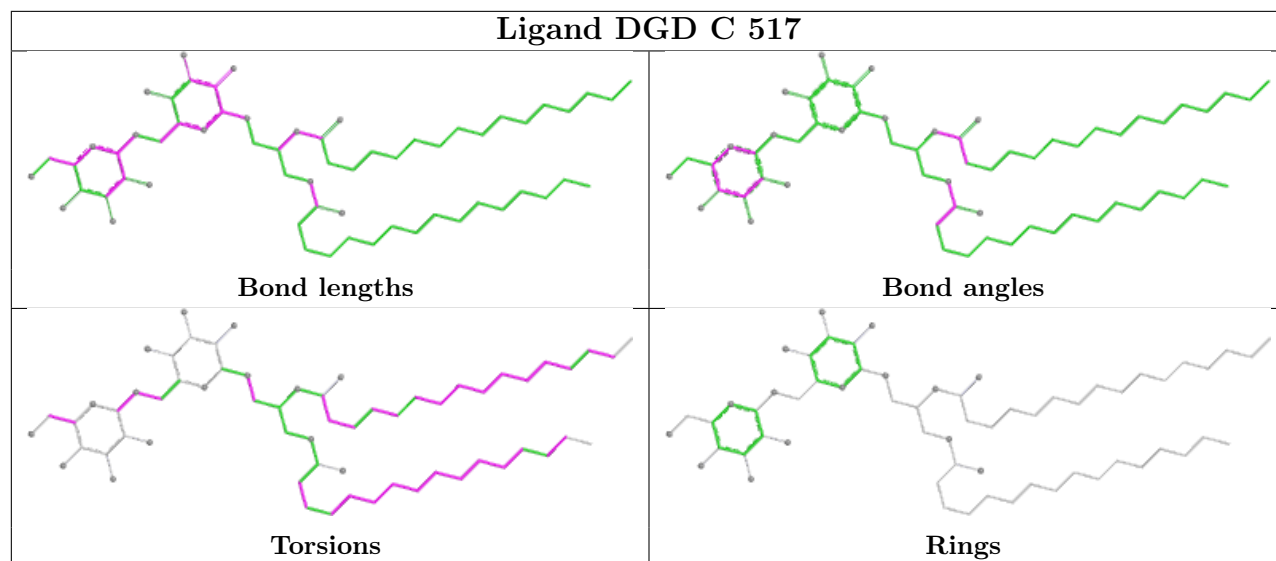


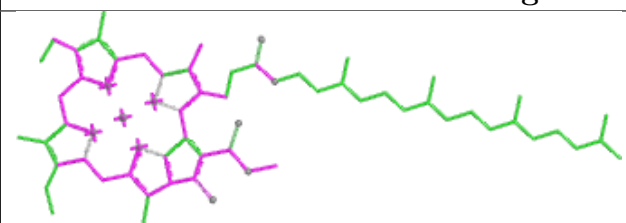
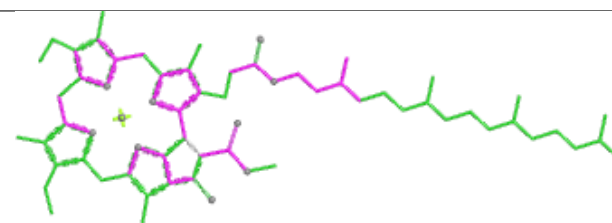
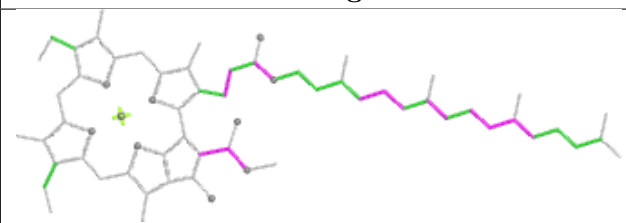
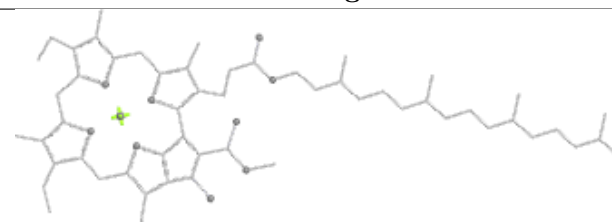
Ligand BCR C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

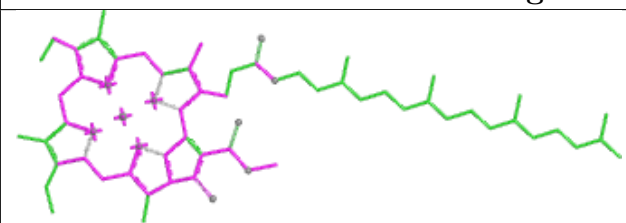
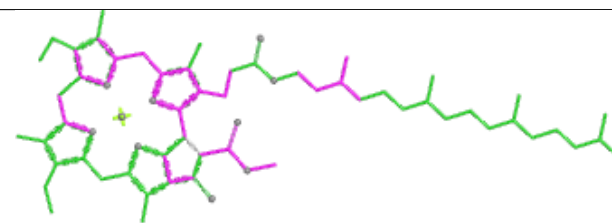
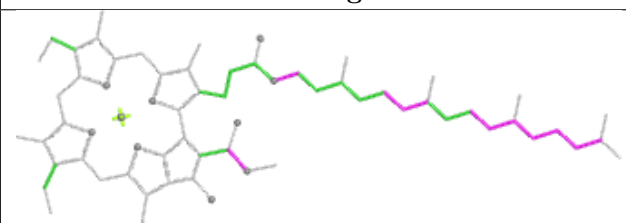
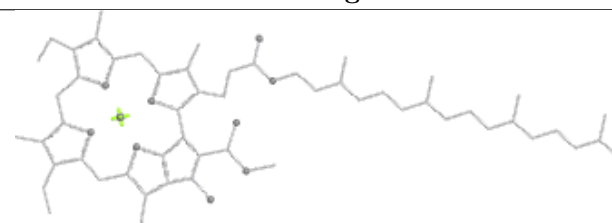
Ligand CLA c 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

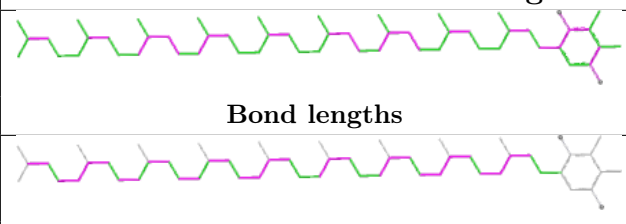
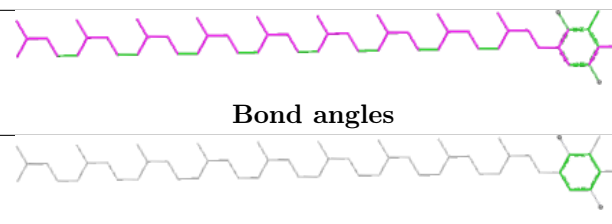
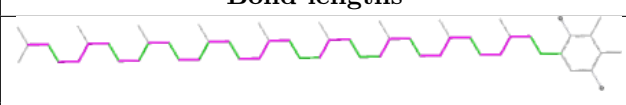
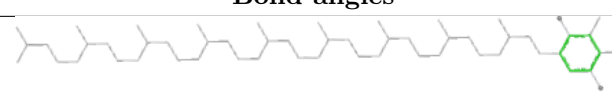
Ligand LMG a 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

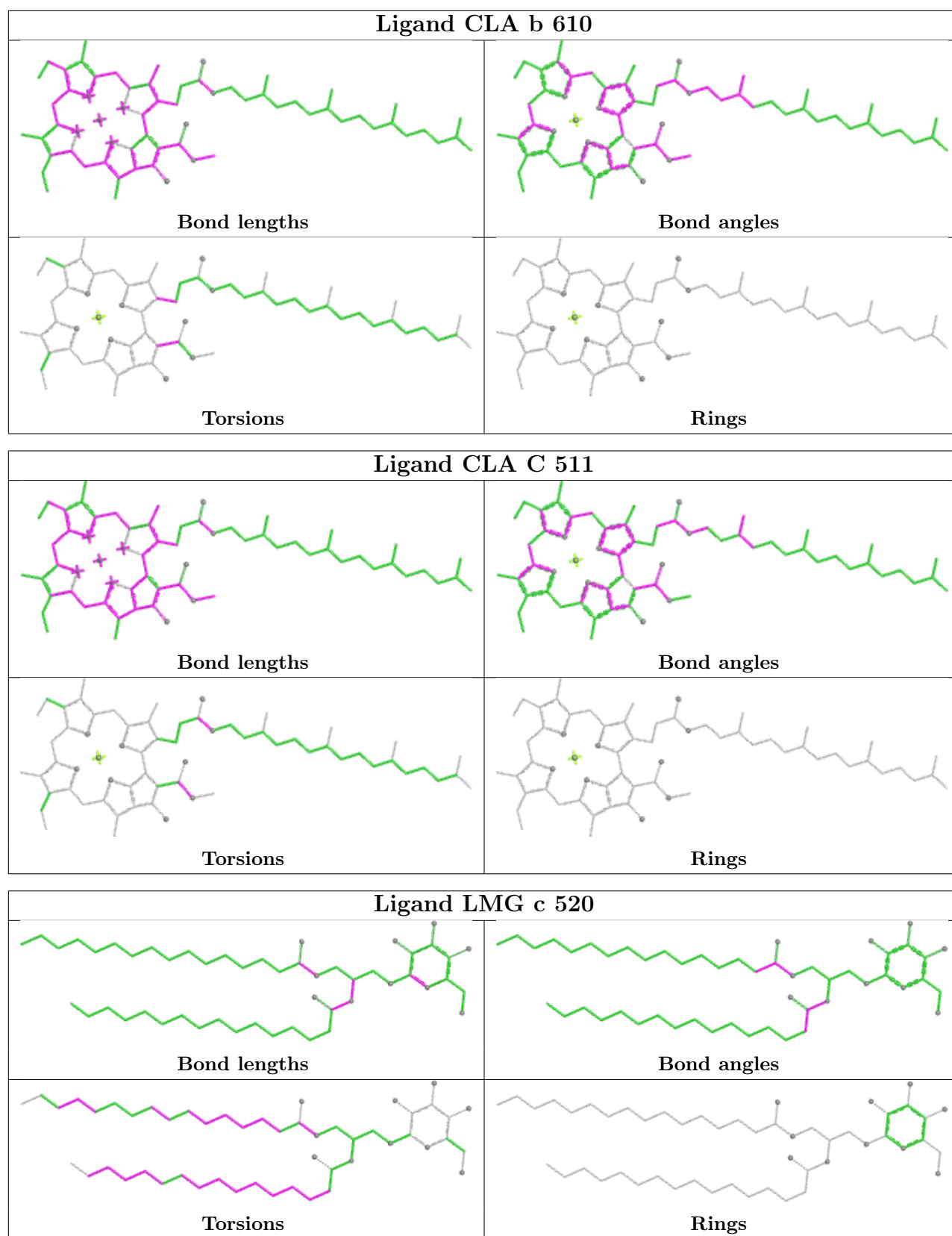


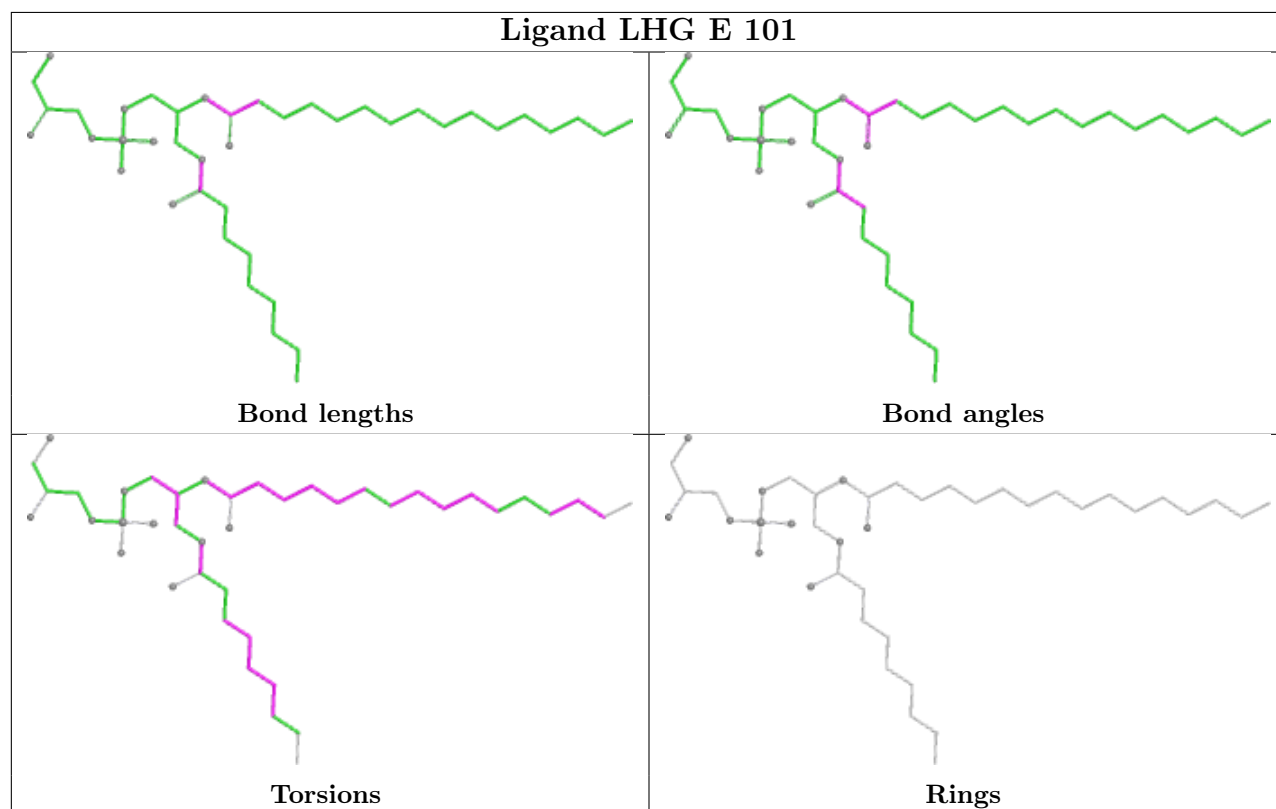
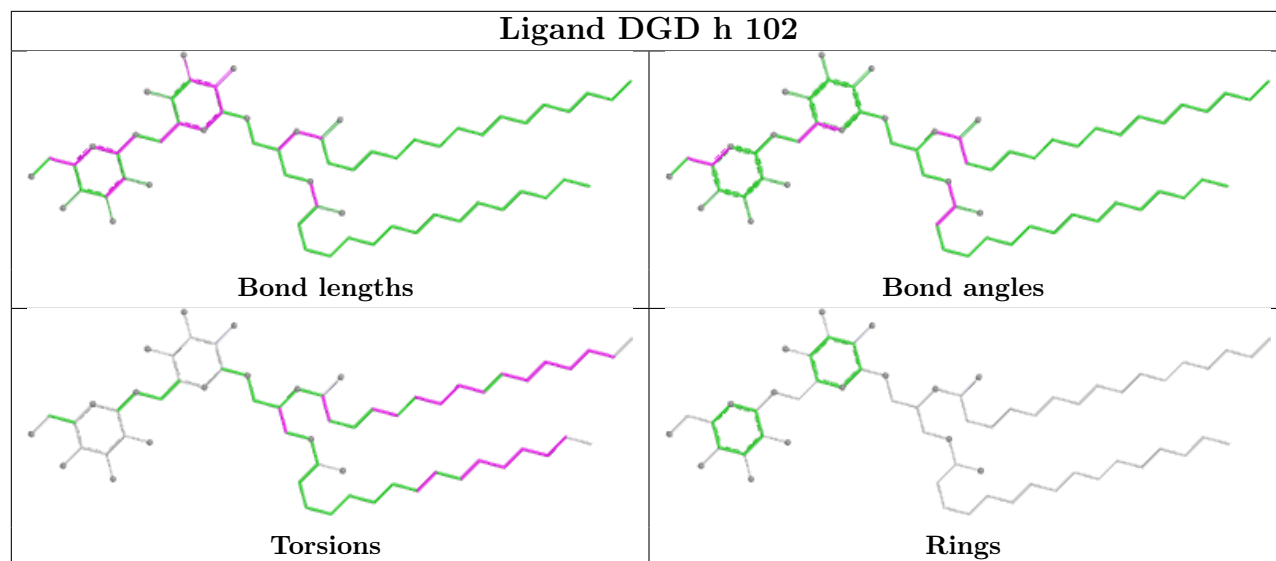


Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

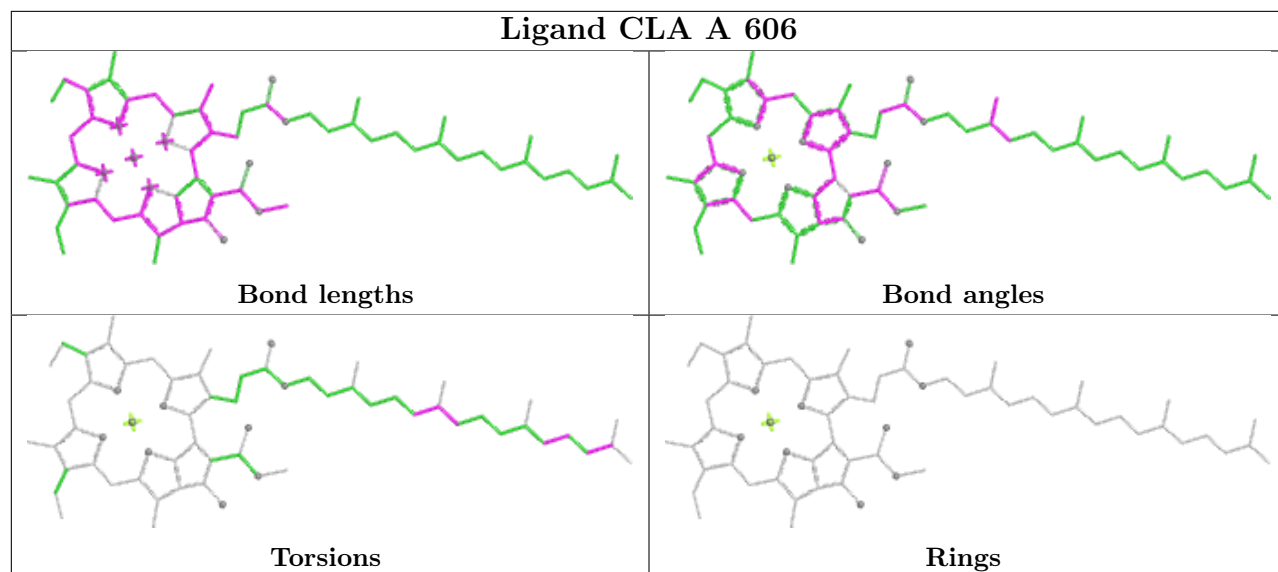
Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

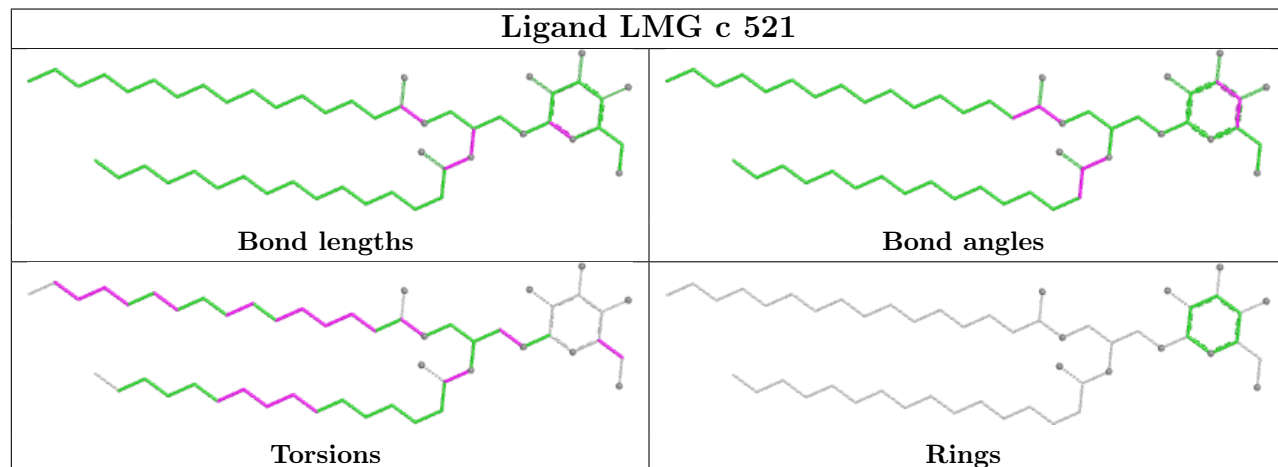




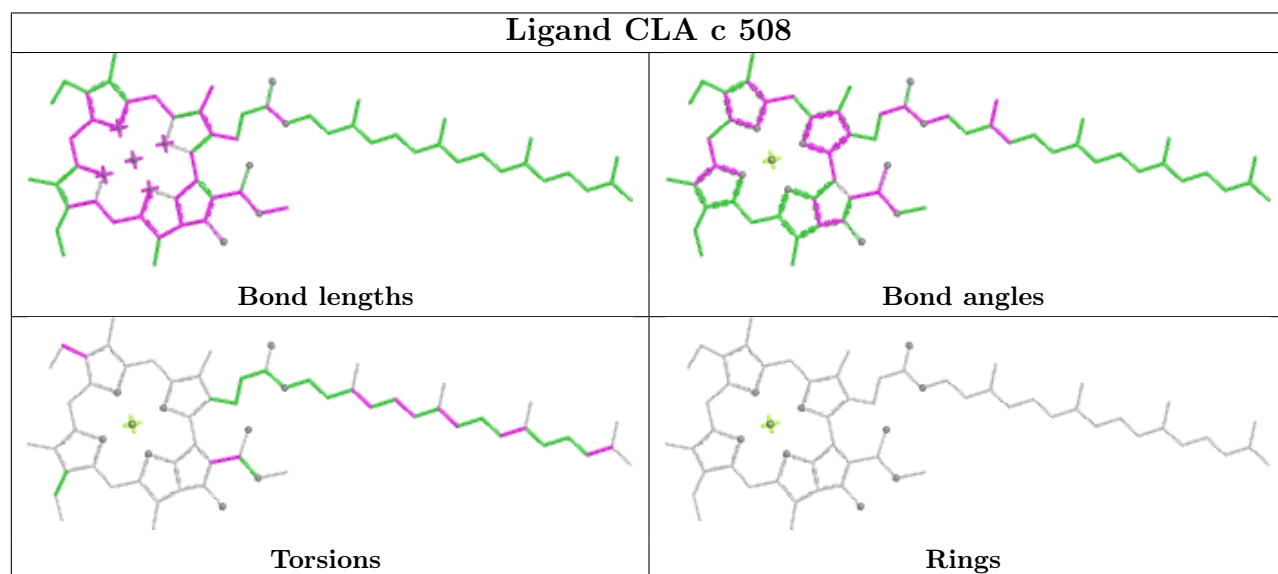
Ligand CLA A 606



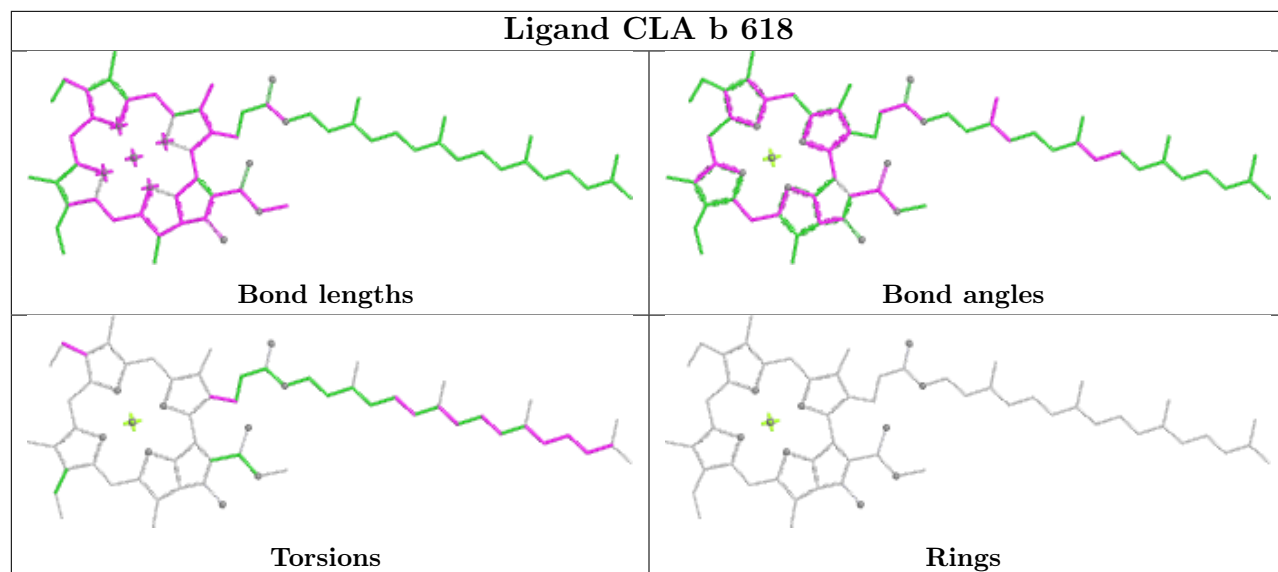
Ligand LMG c 521



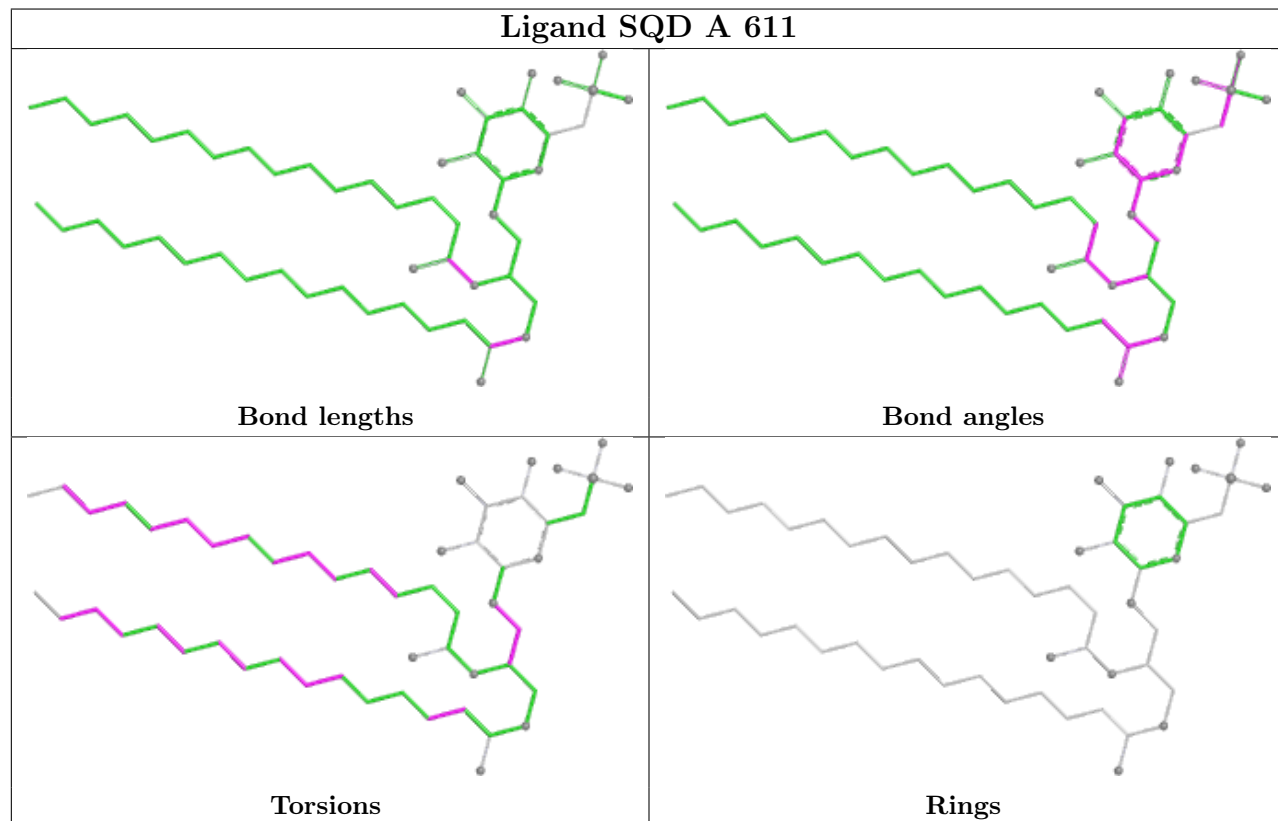
Ligand CLA c 508

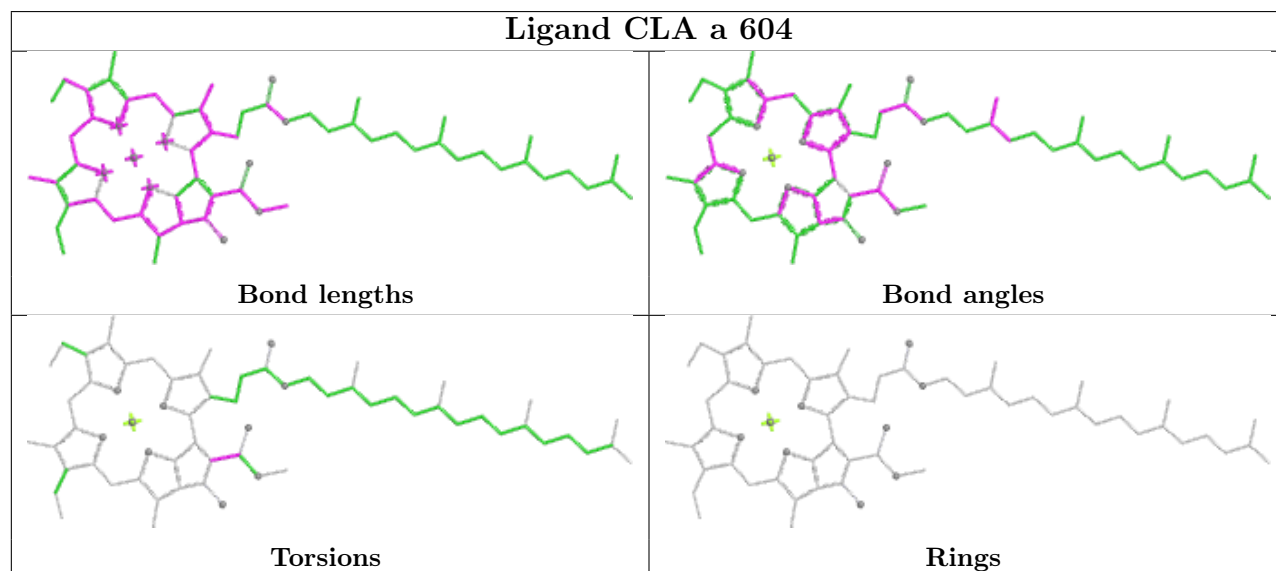
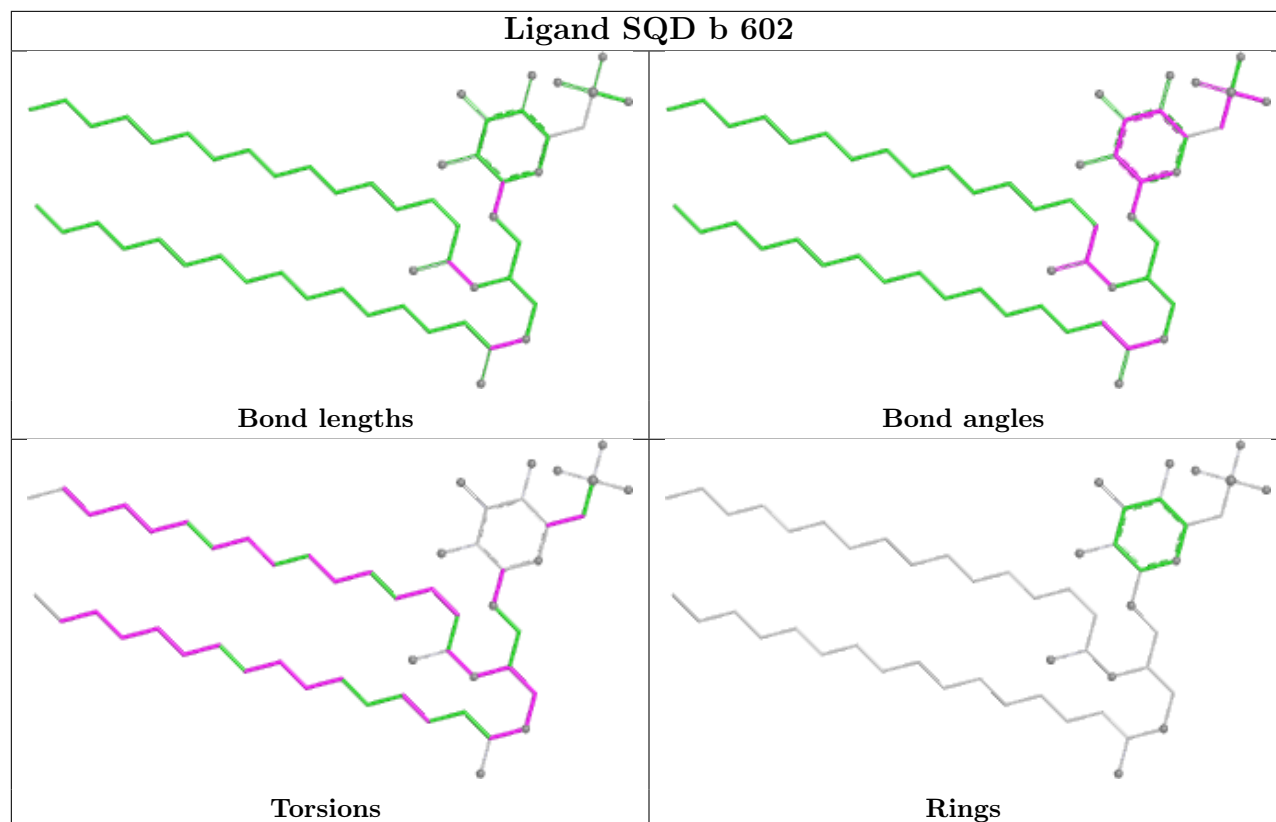


Ligand CLA b 618

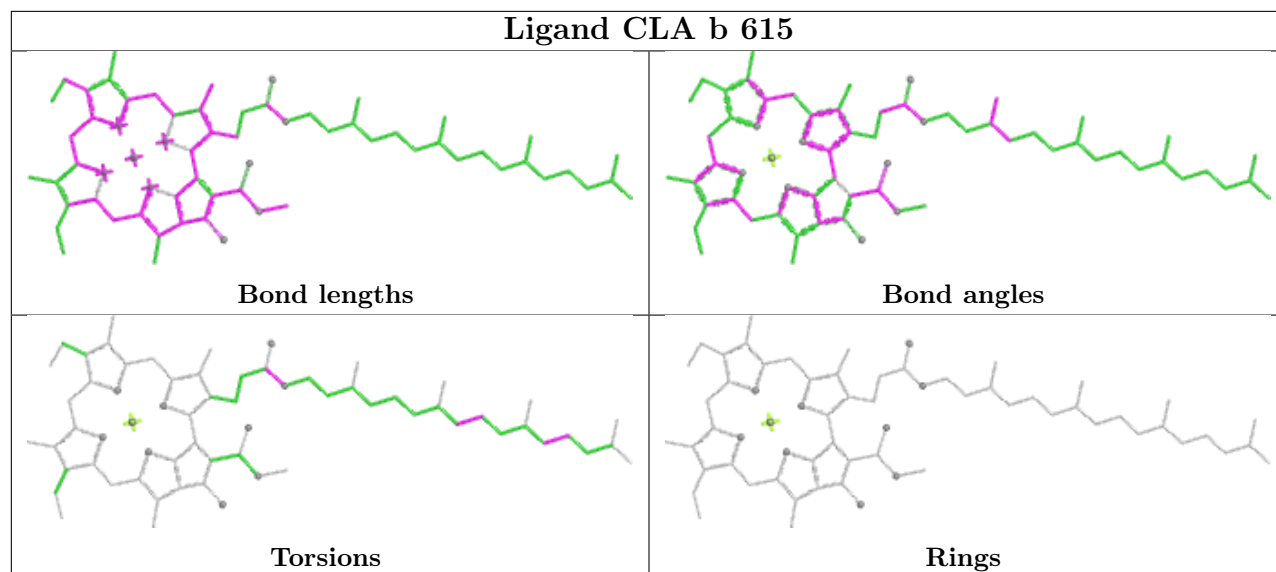


Ligand SQD A 611

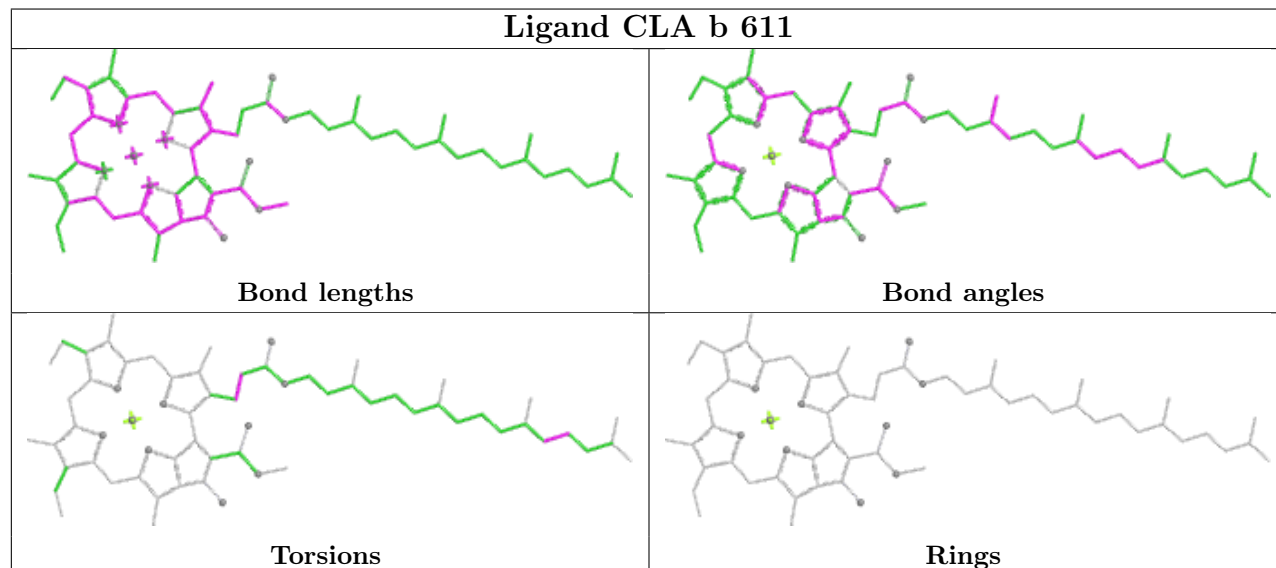




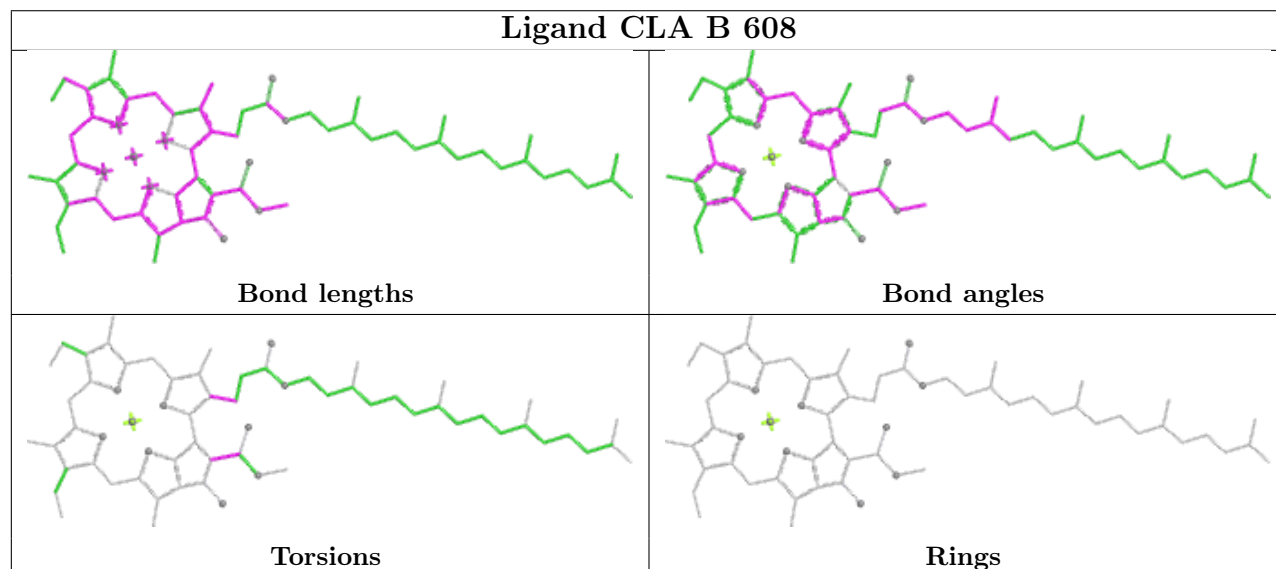
Ligand CLA b 615



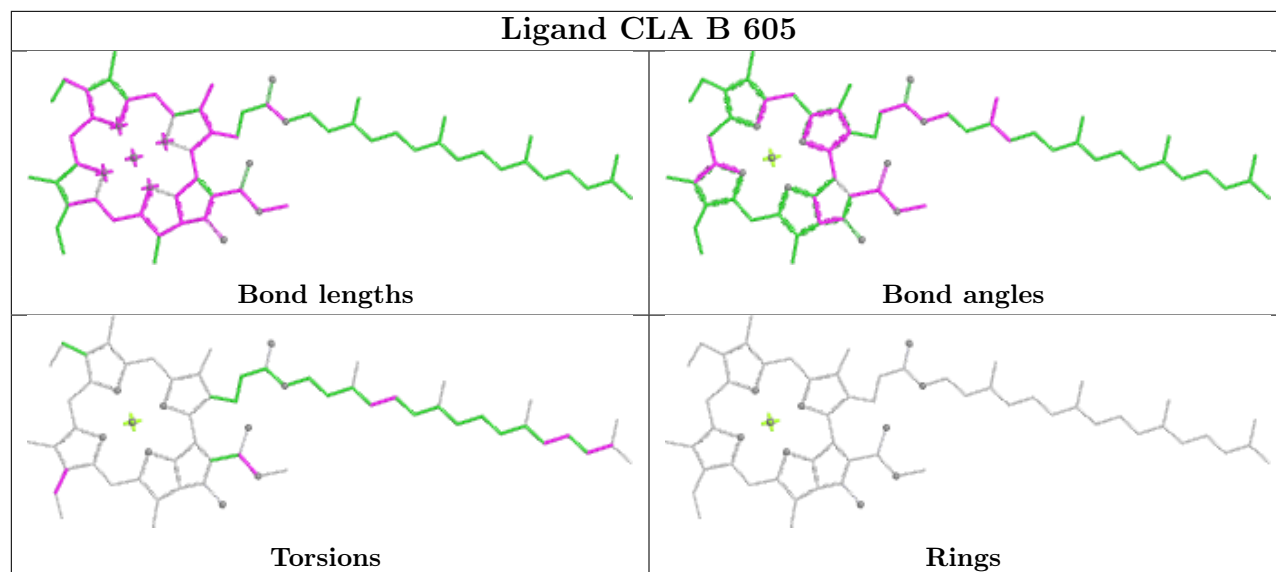
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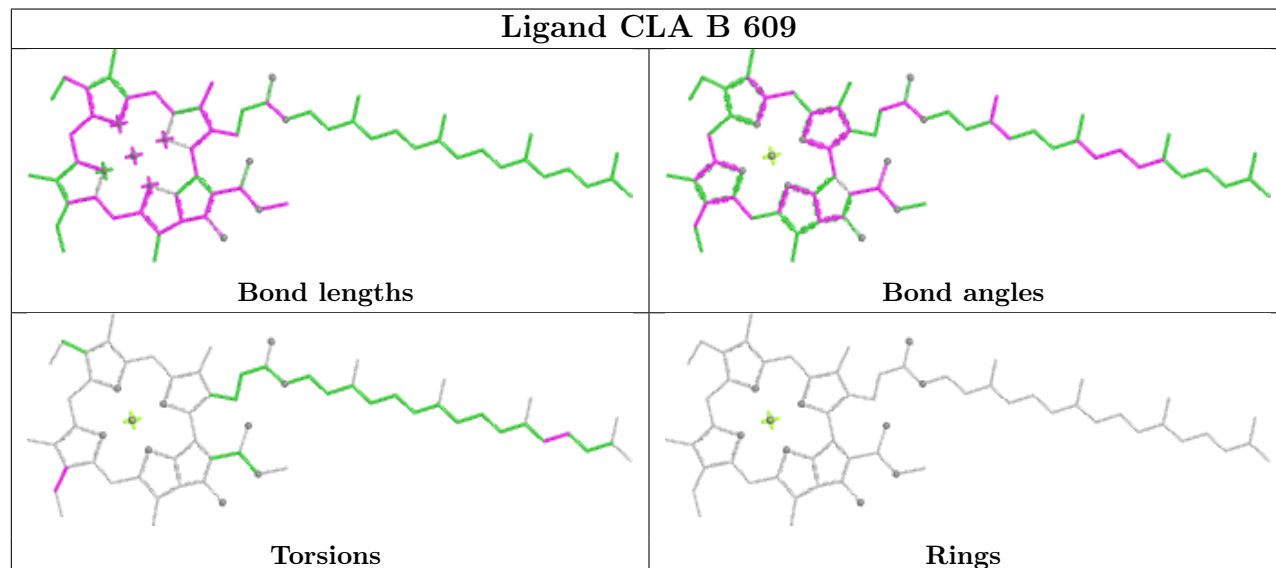
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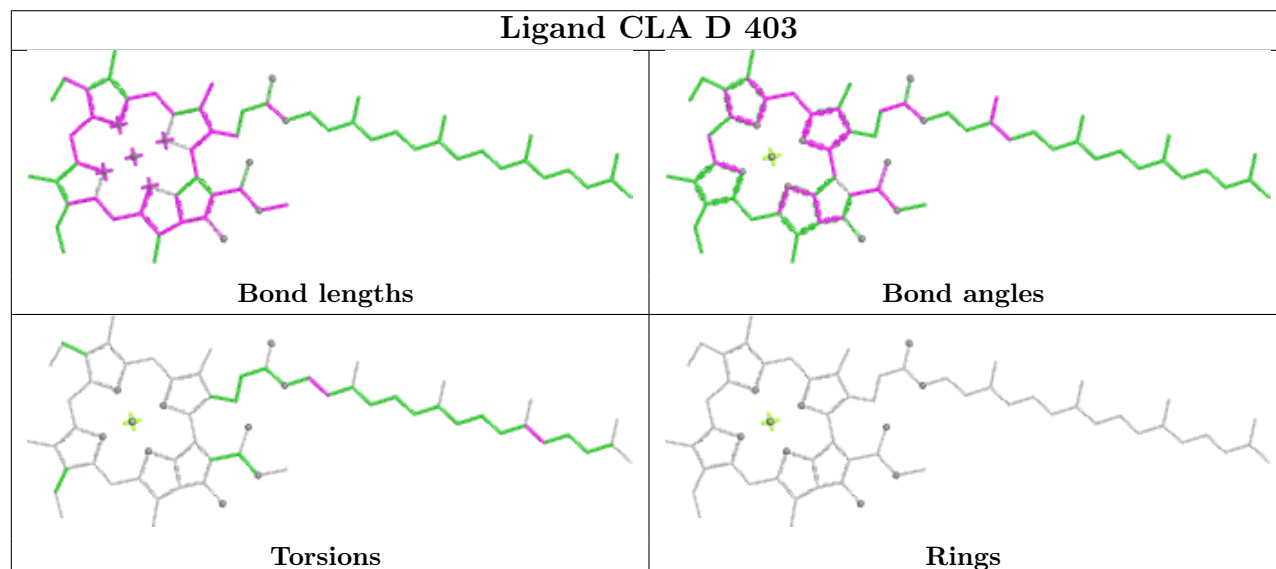
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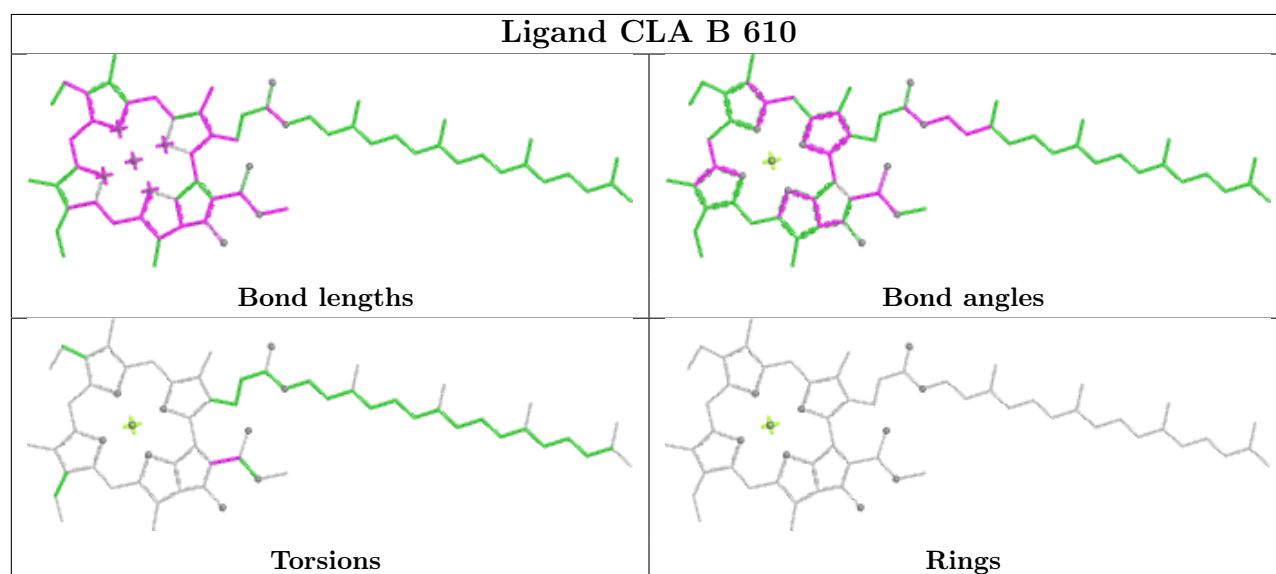
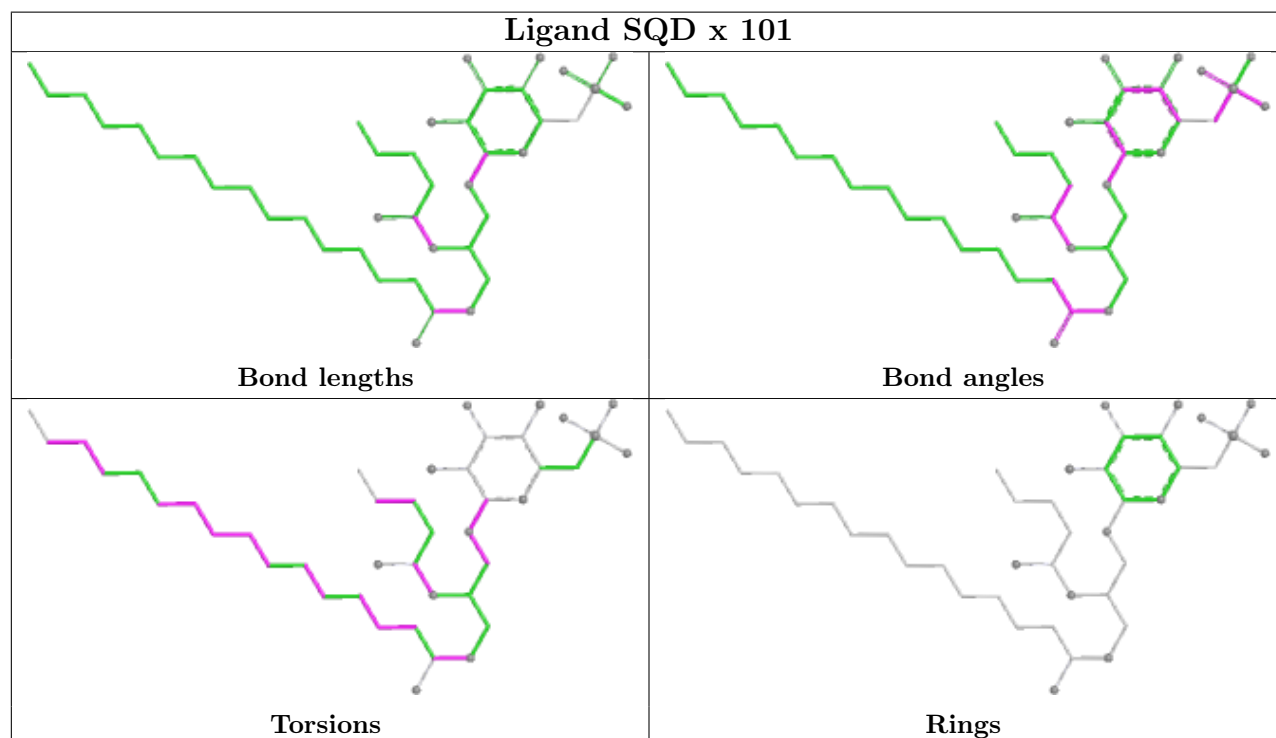
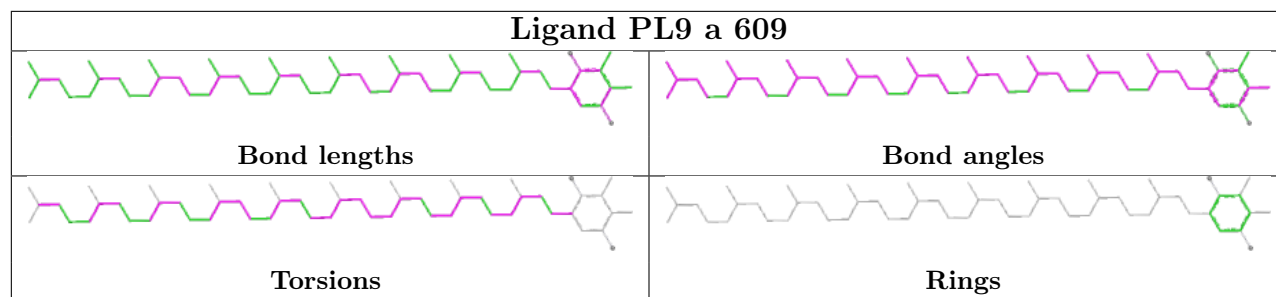


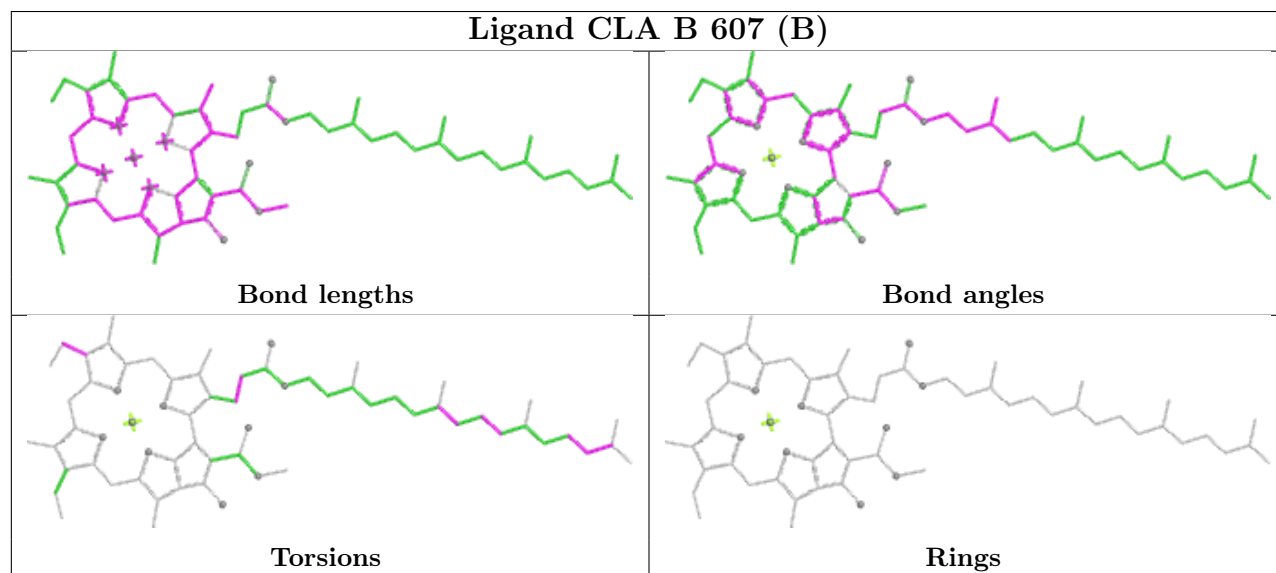
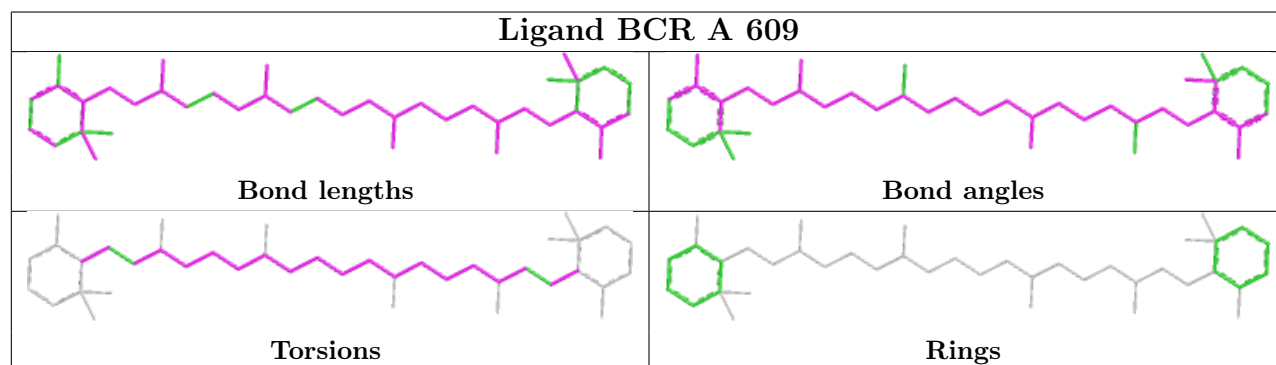
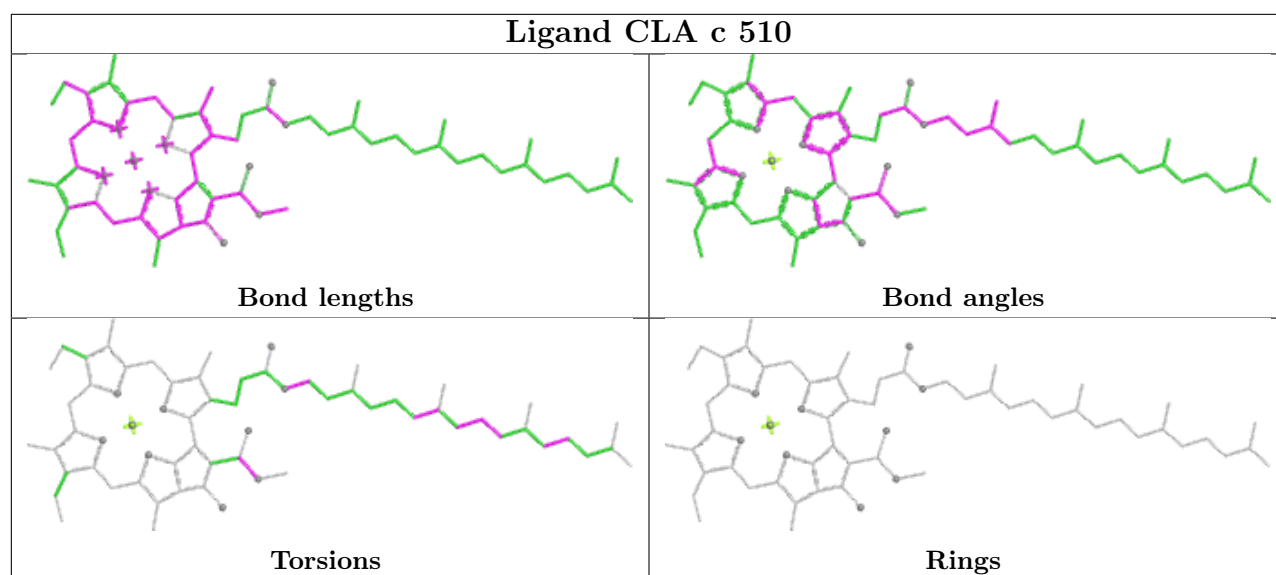
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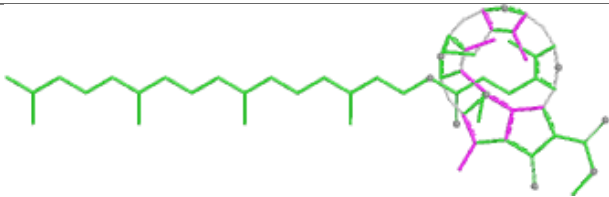
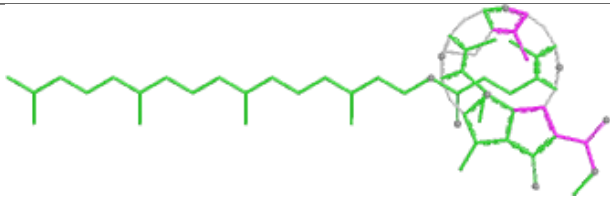
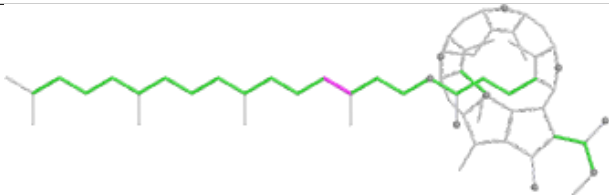
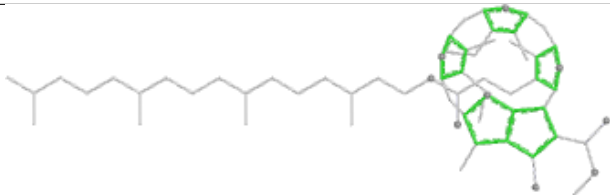


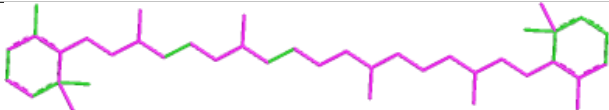
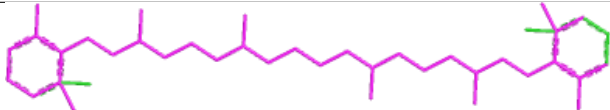
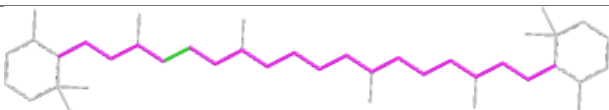
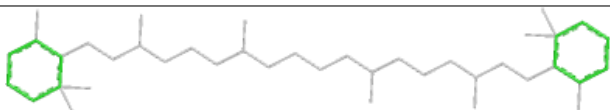
Ligand CLA D 403

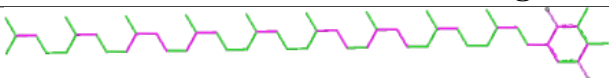
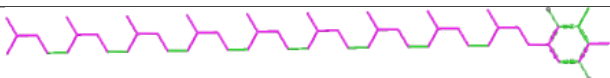
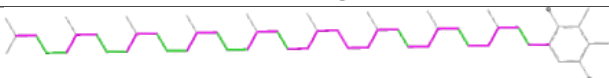
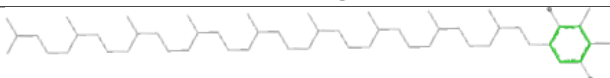


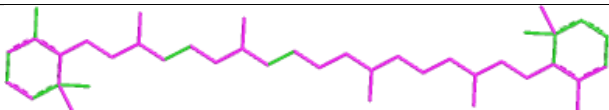
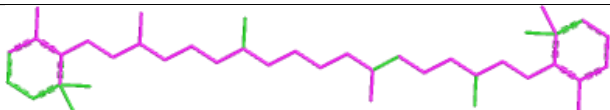
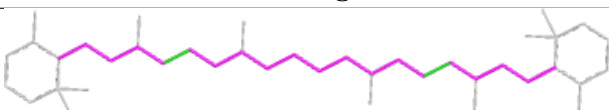
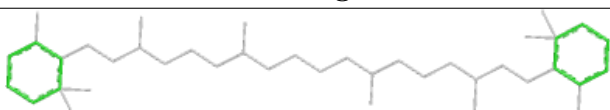


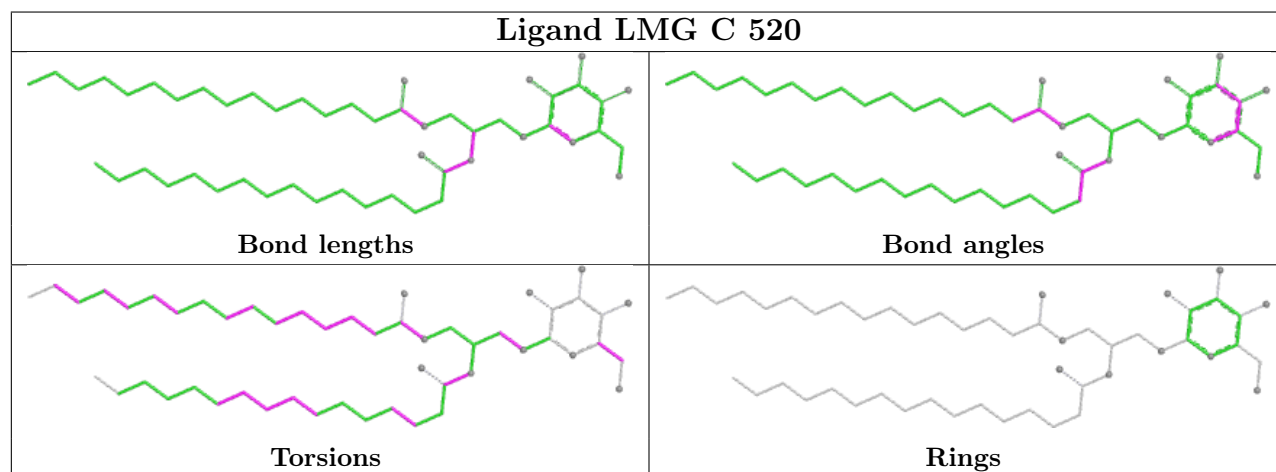
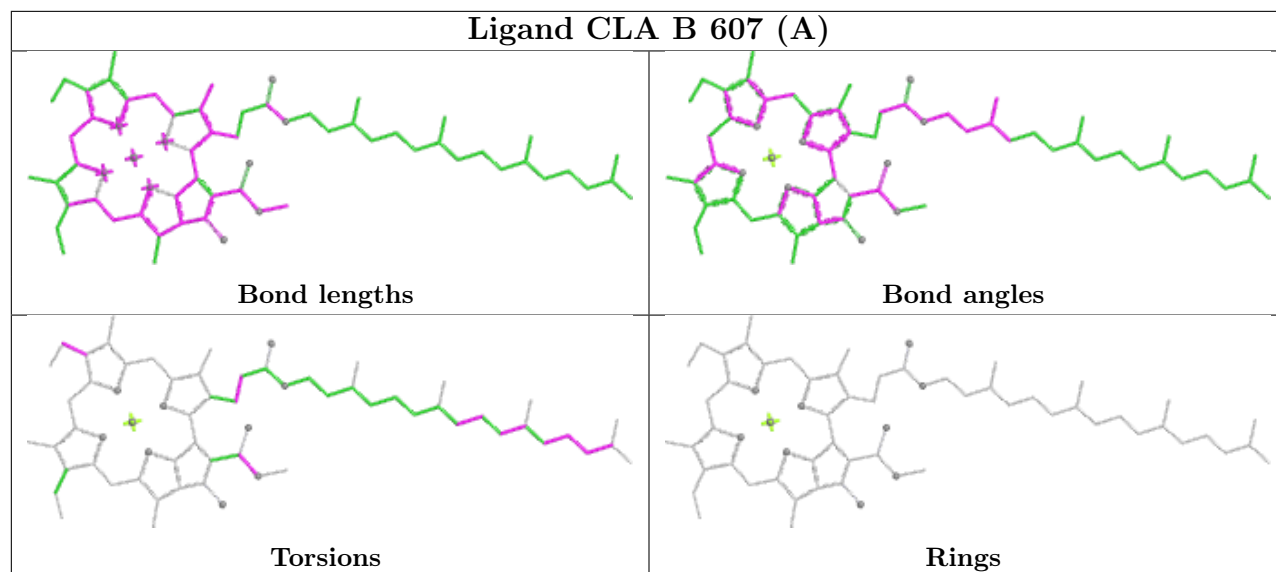


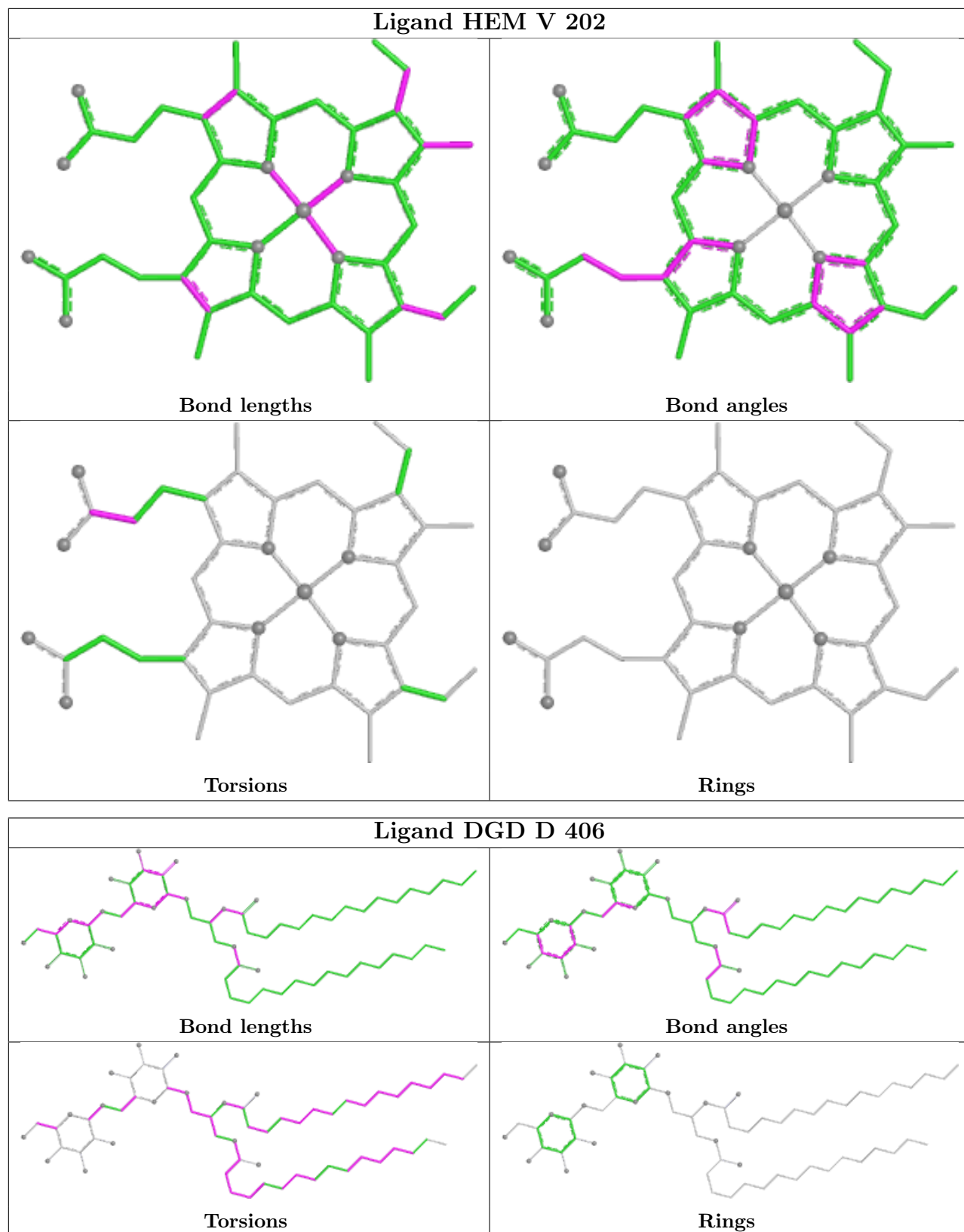
Ligand PHO A 607	
	Bond lengths
	Bond angles
	Torsions
	Rings

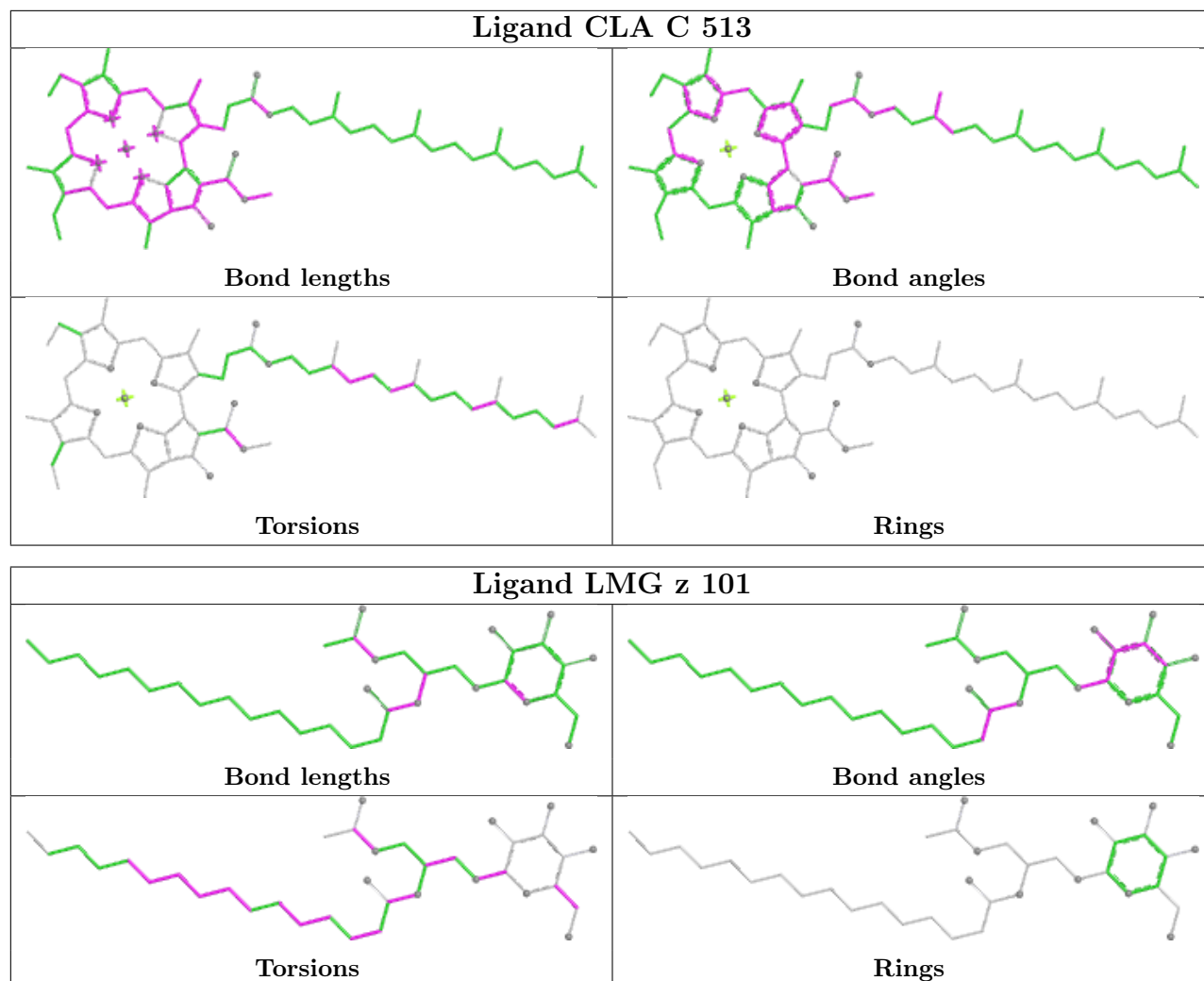
Ligand BCR h 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand PL9 A 610	
	Bond lengths
	Bond angles
	Torsions
	Rings

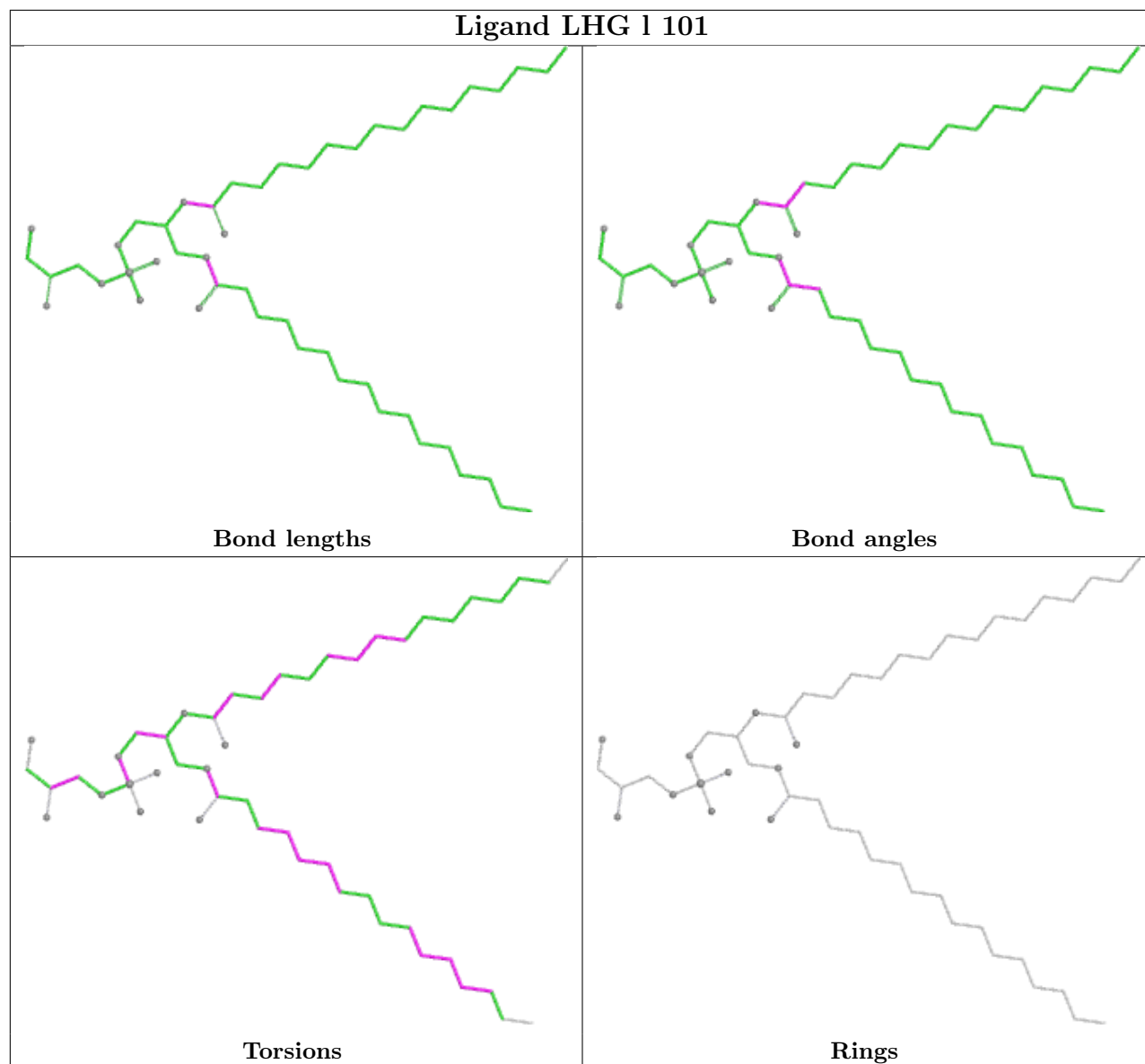
Ligand BCR c 522	
	Bond lengths
	Bond angles
	Torsions
	Rings



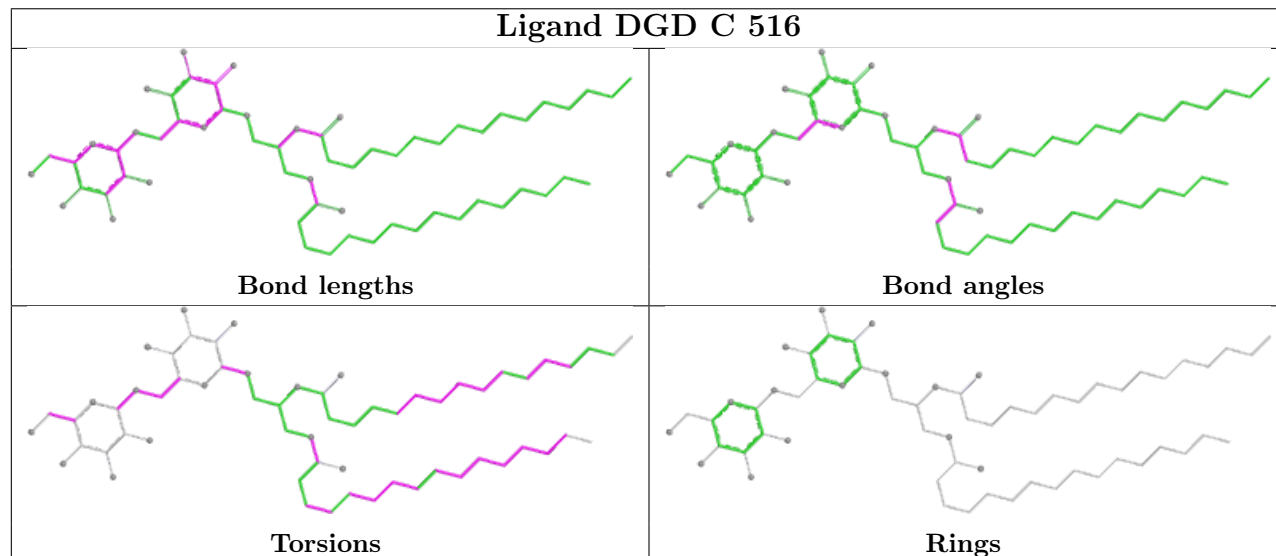


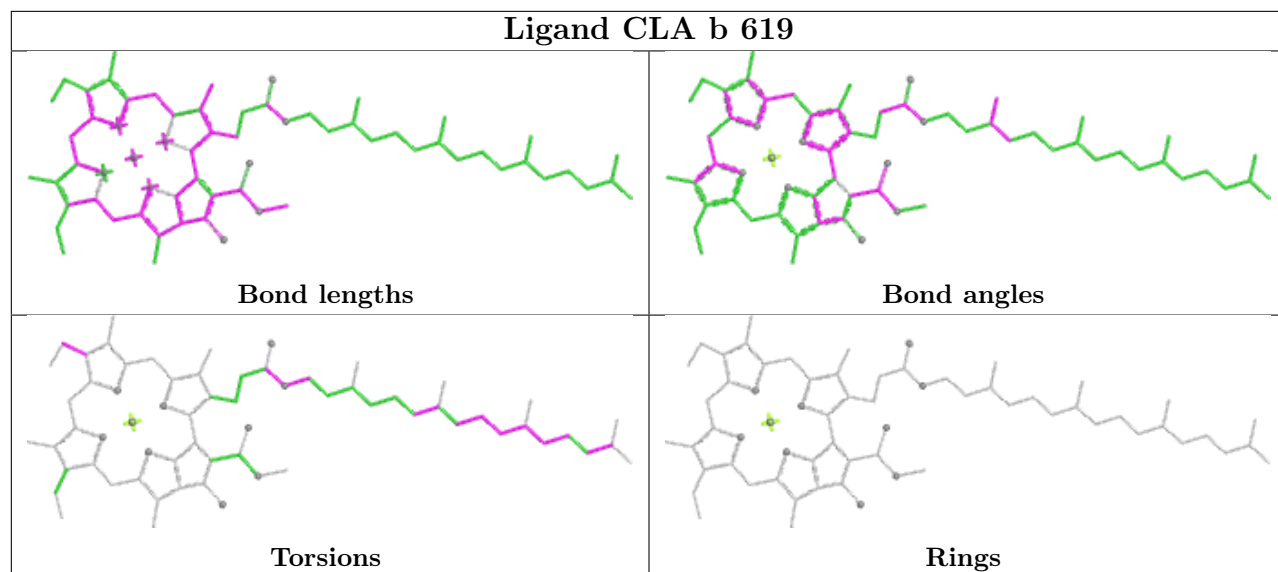
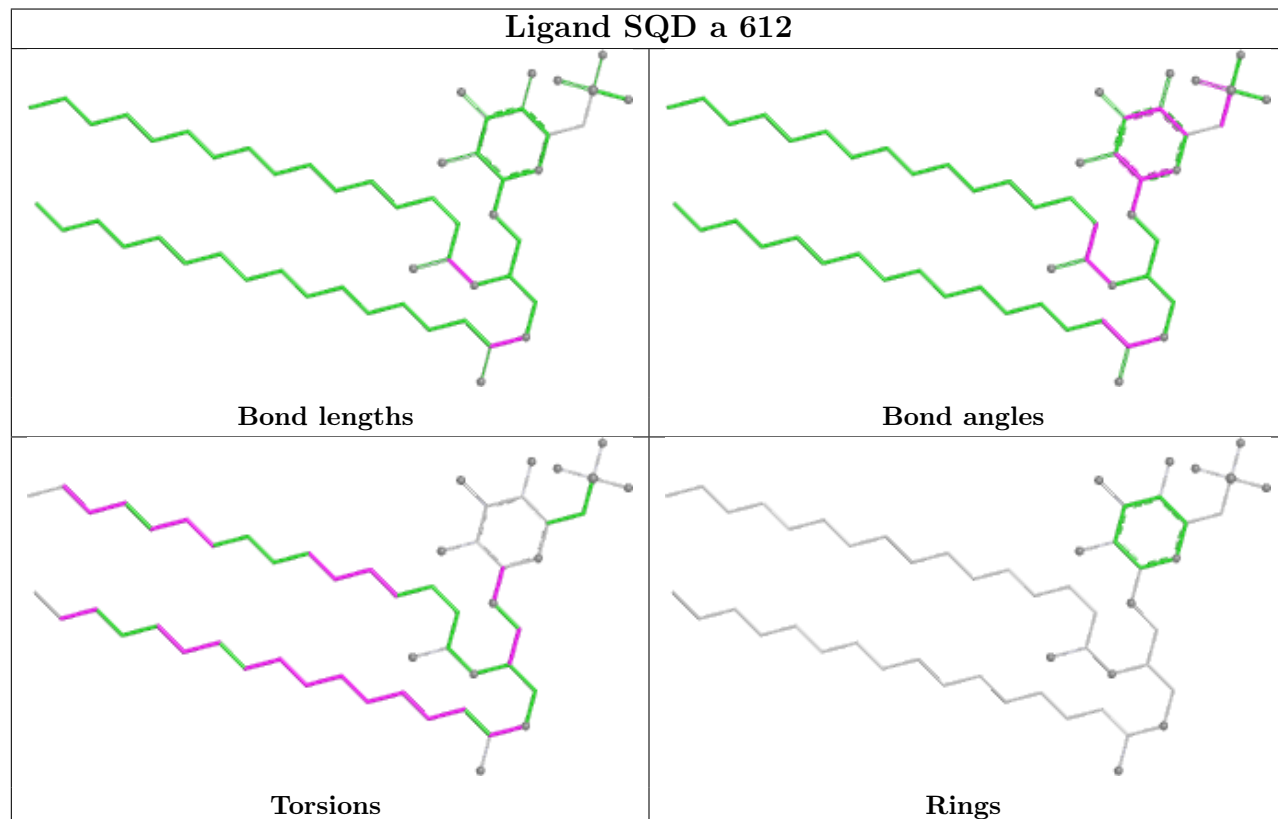


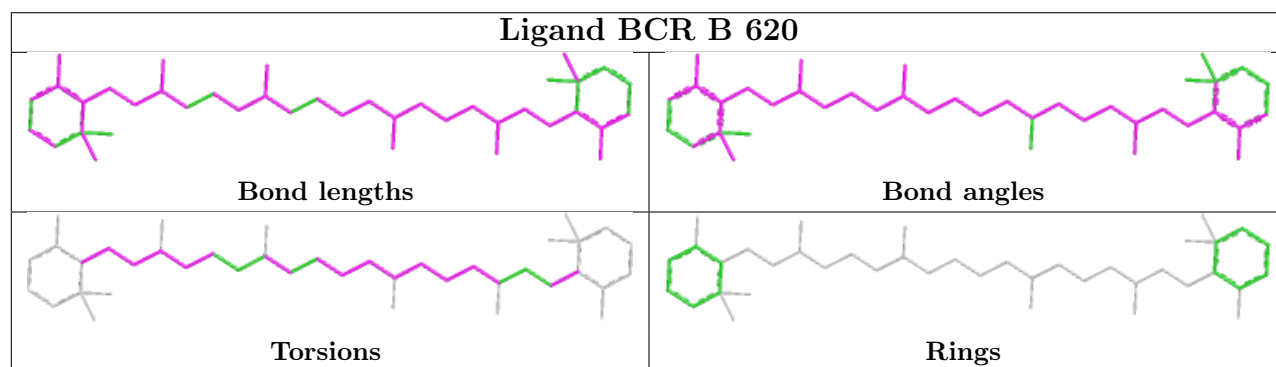
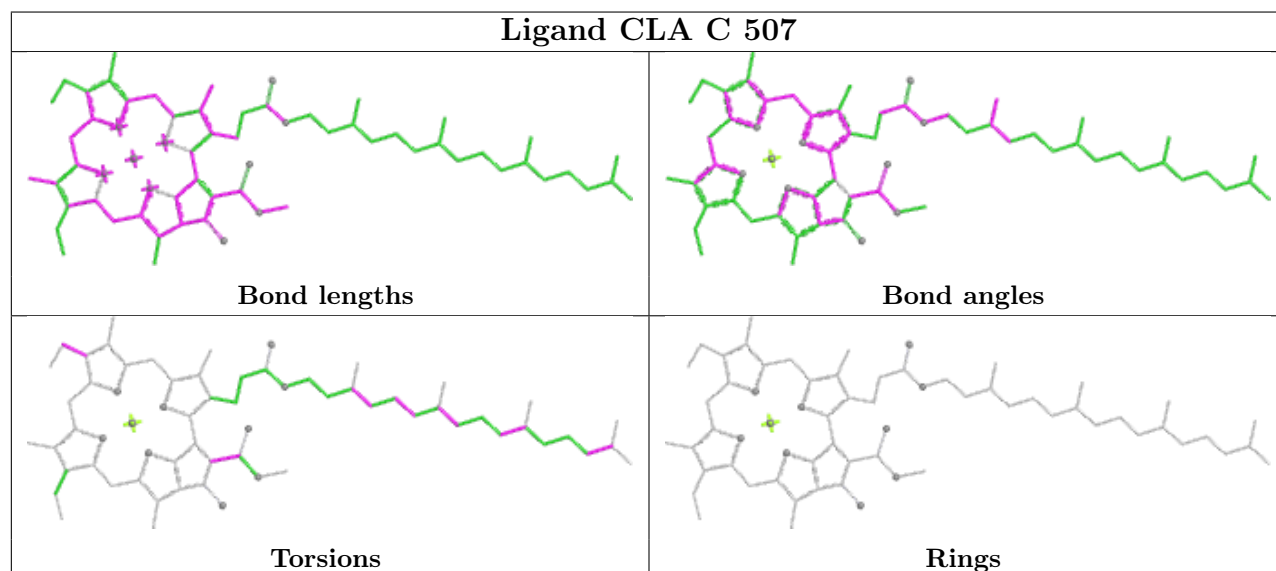
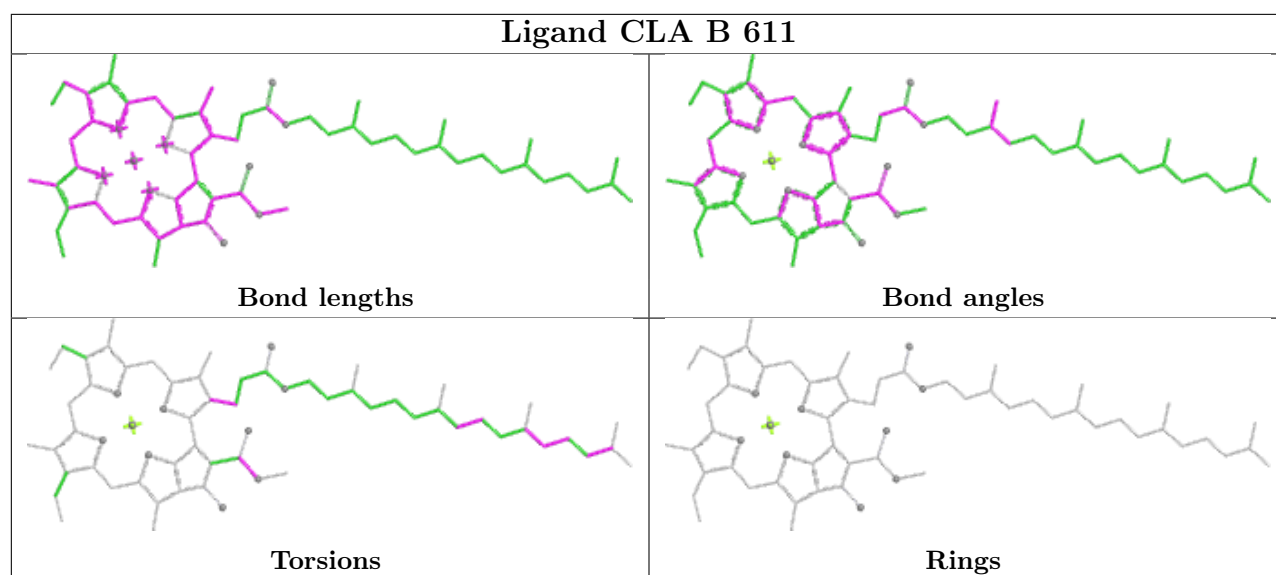
Ligand LHG 1 101

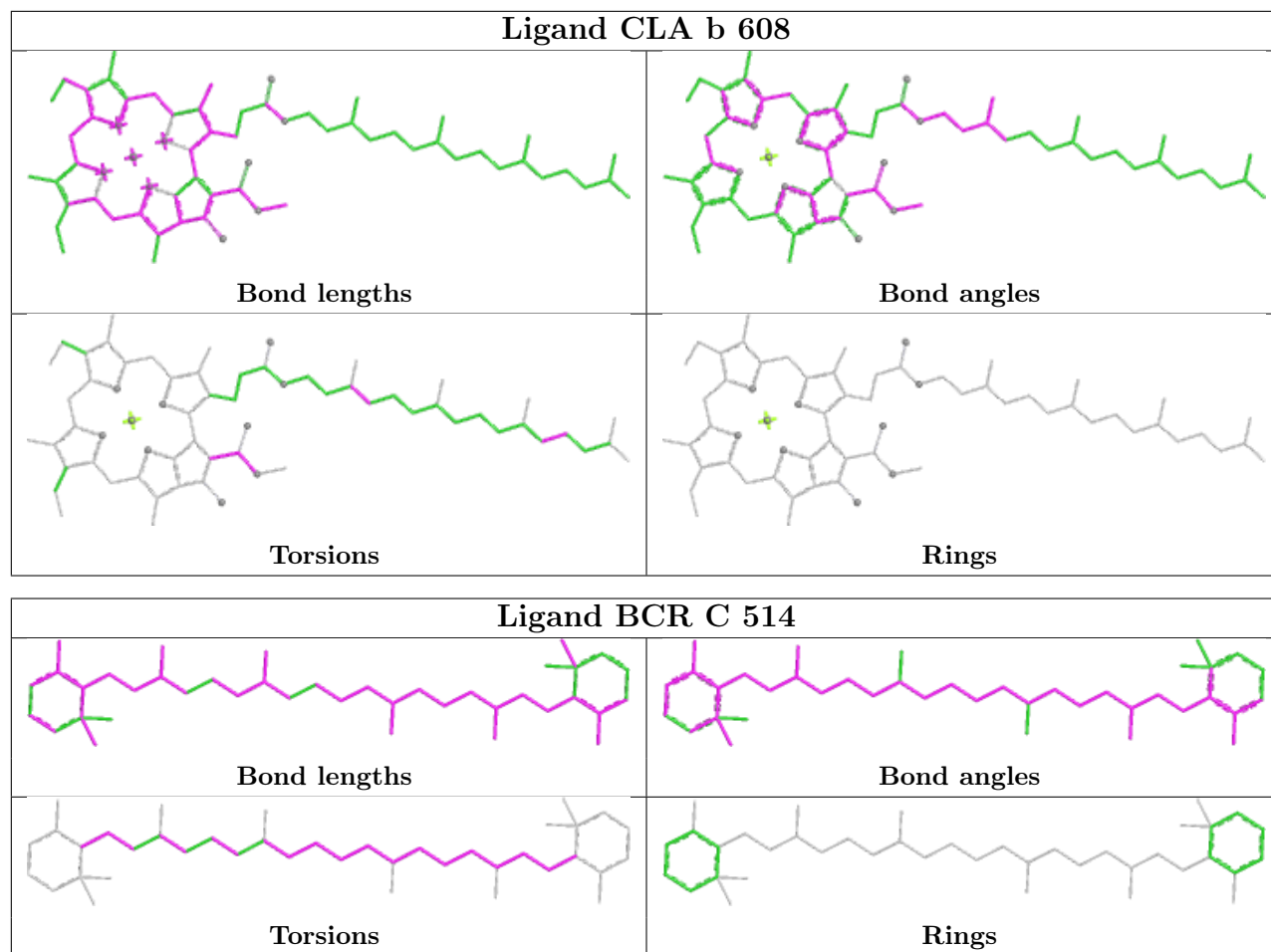


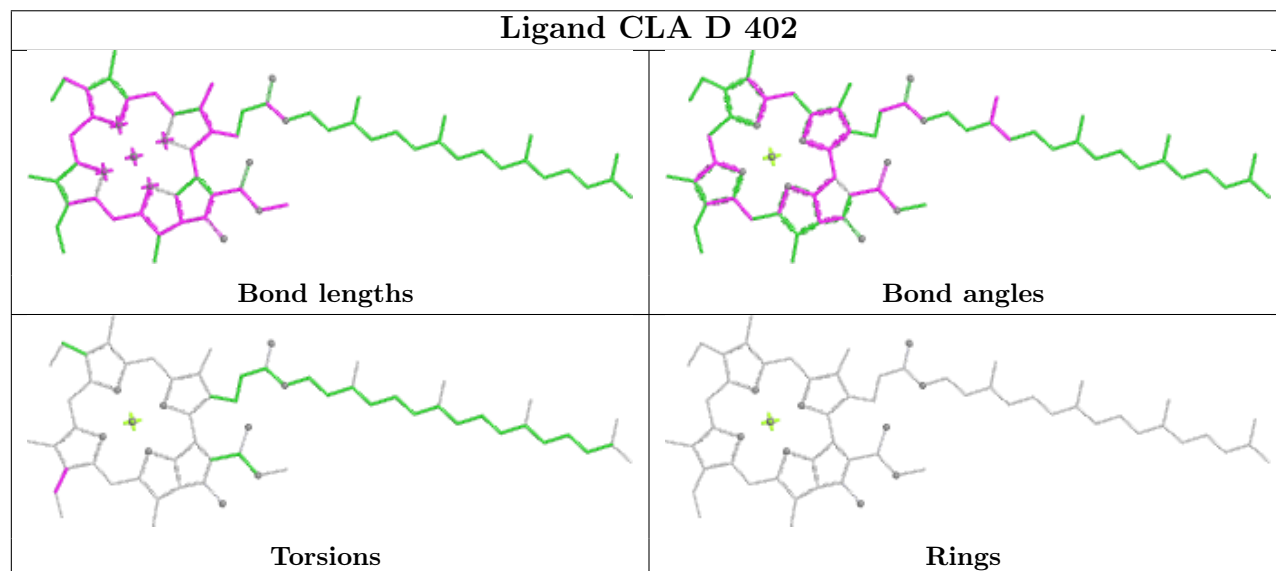
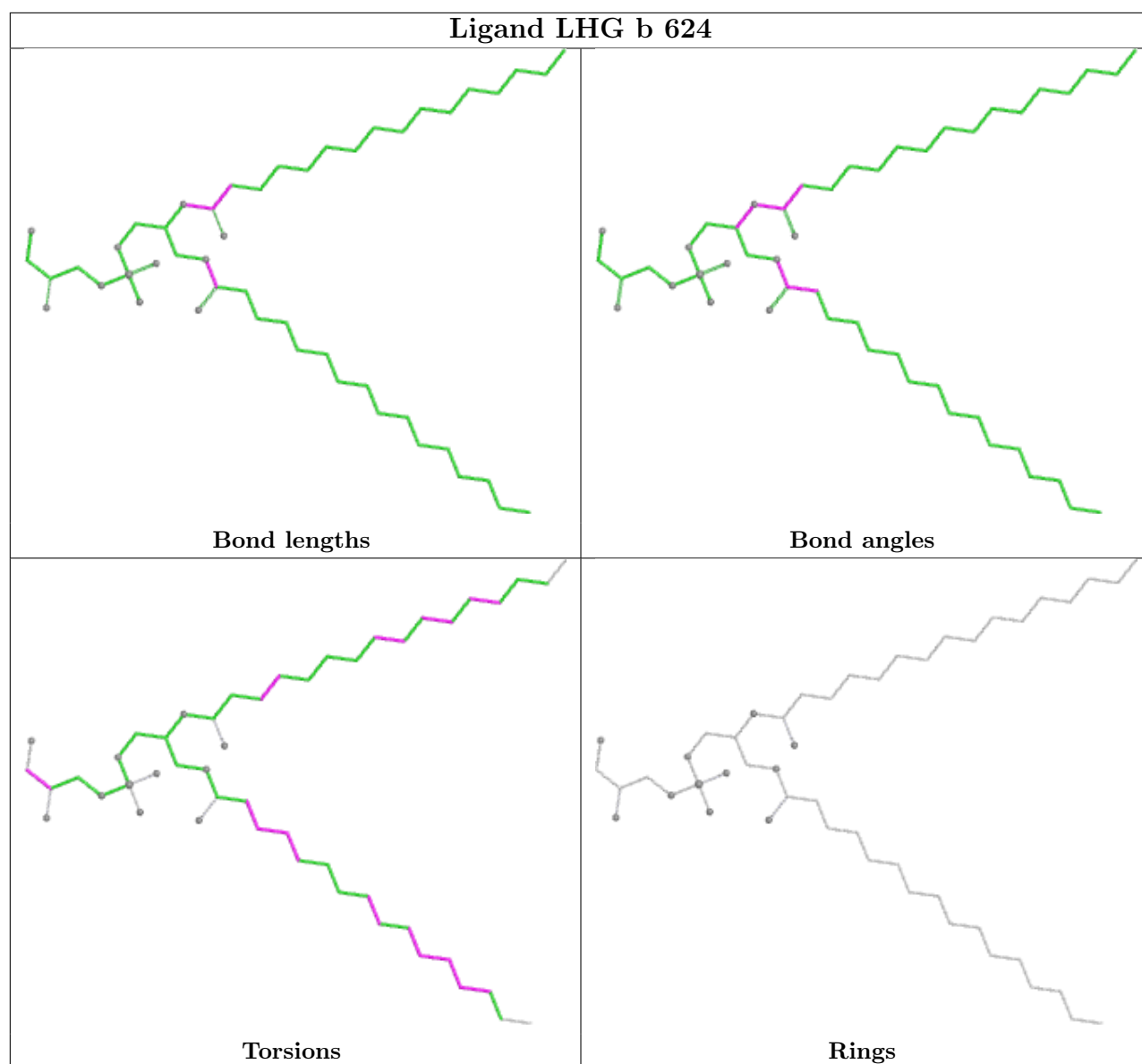
Ligand DGD C 516



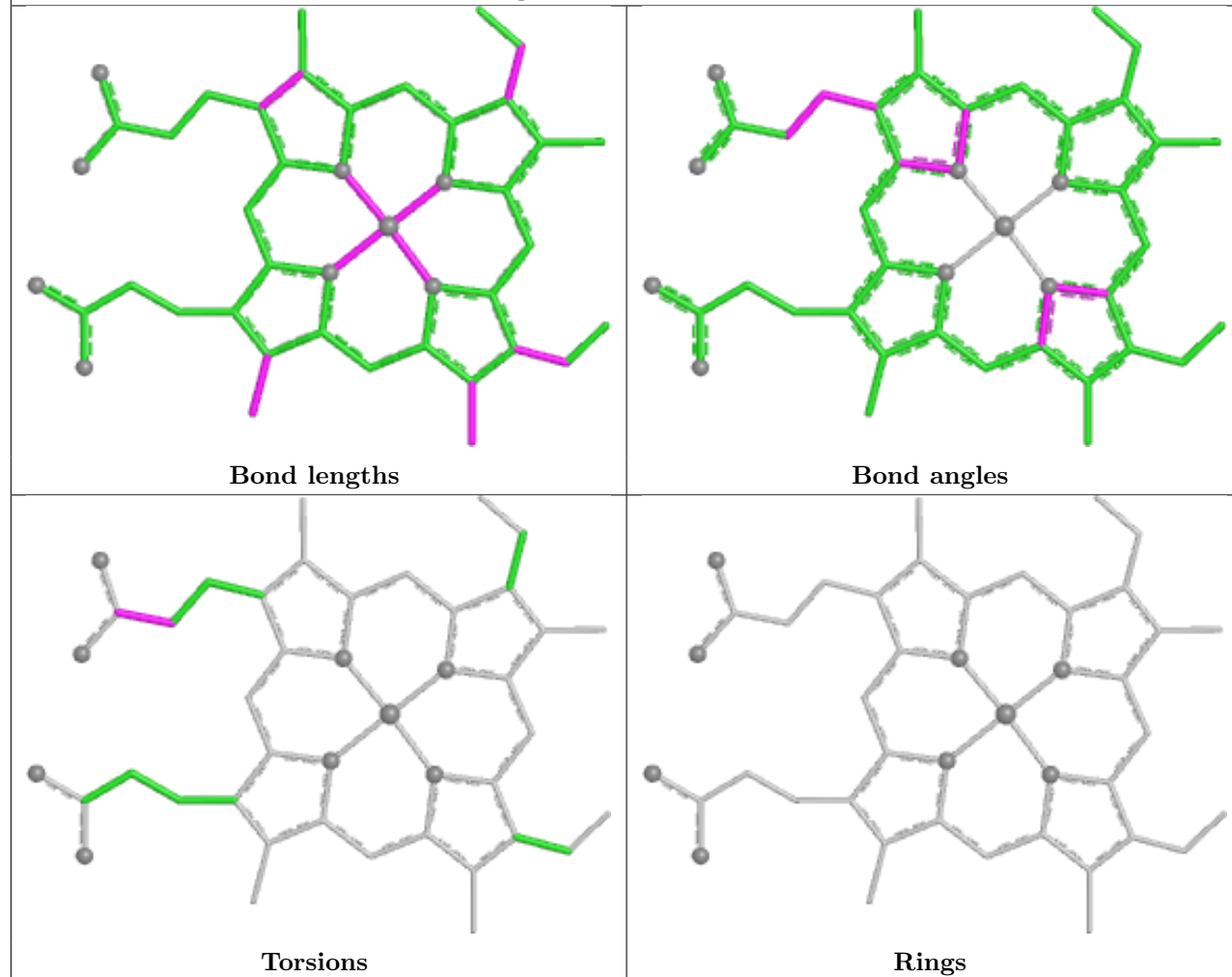
Ligand CLA b 619**Ligand SQD a 612**



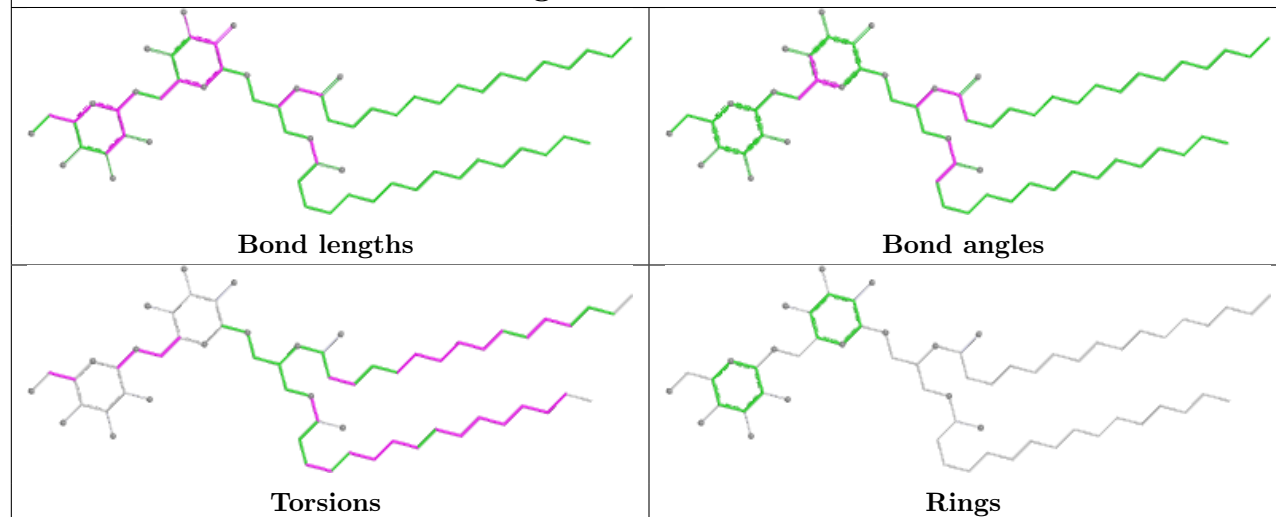


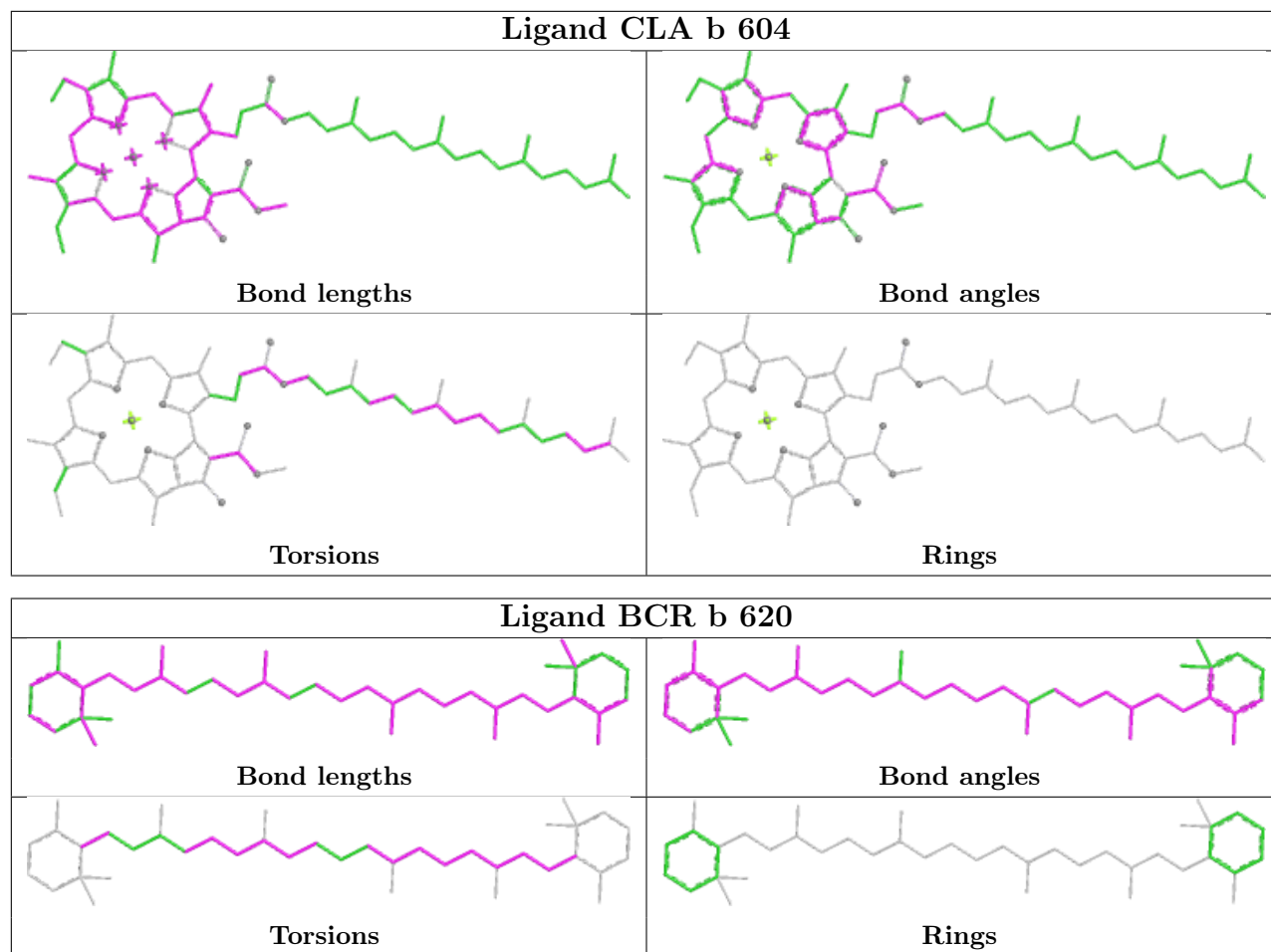


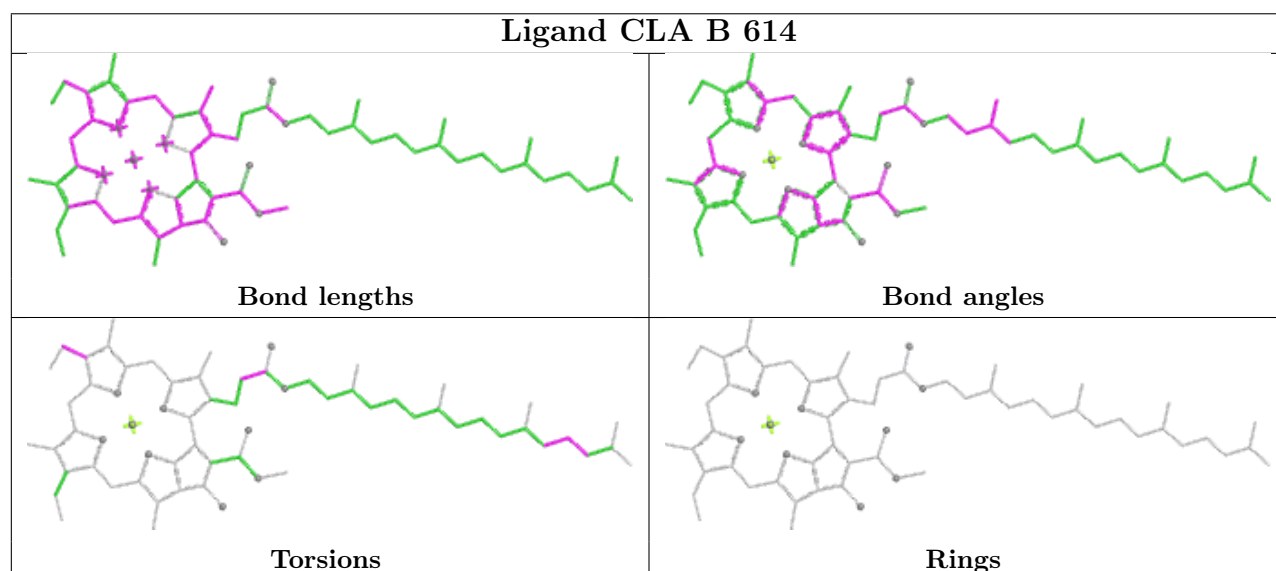
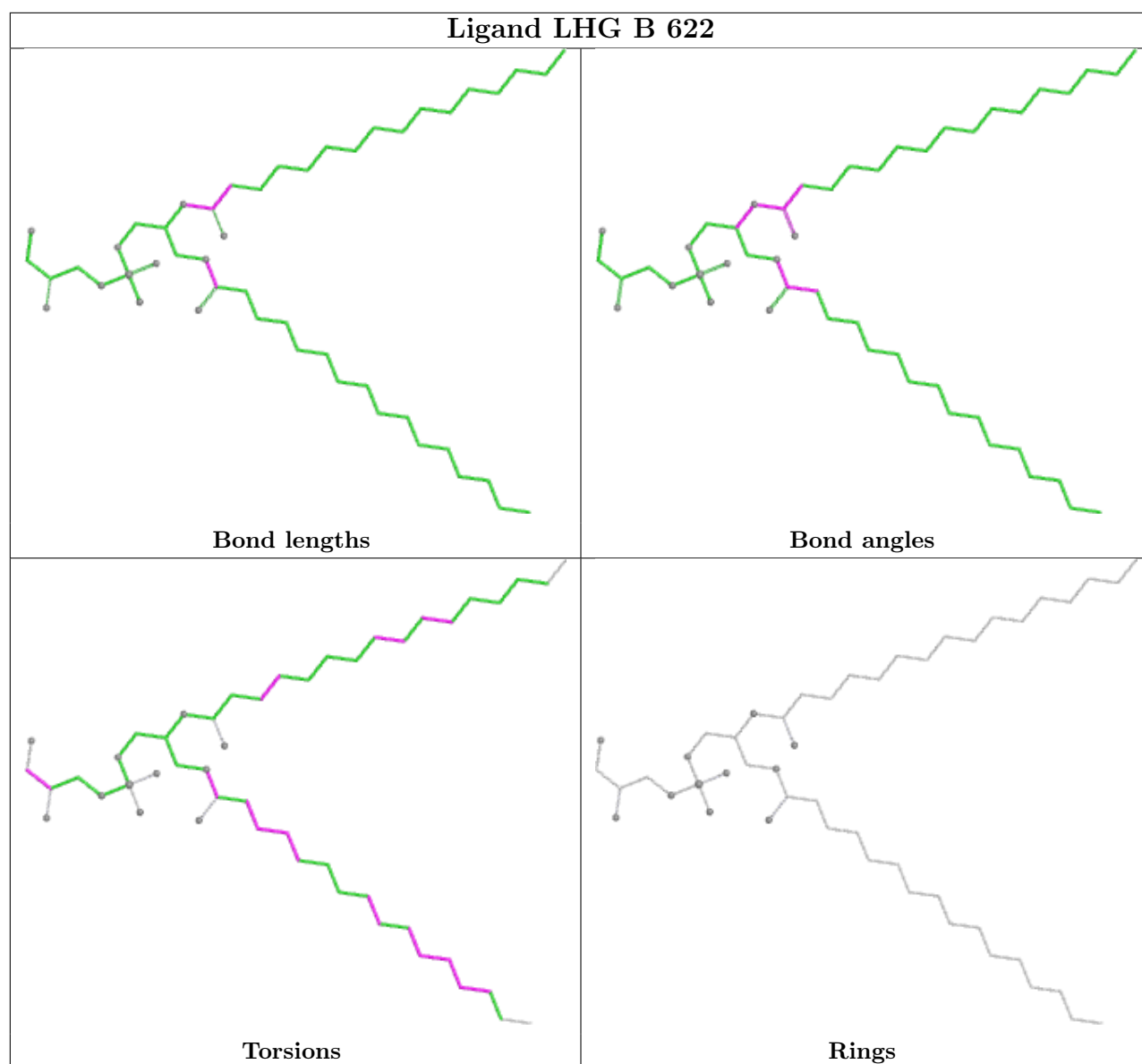
Ligand HEM e 102

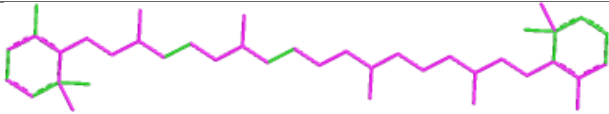
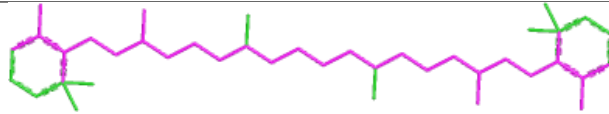
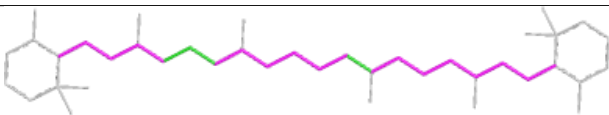
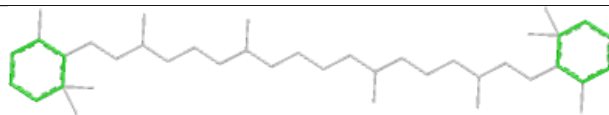


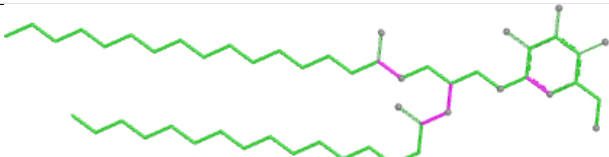
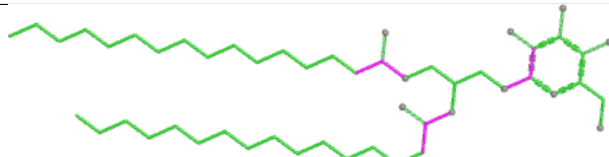
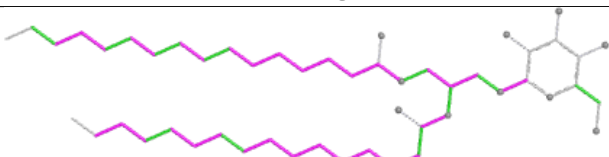
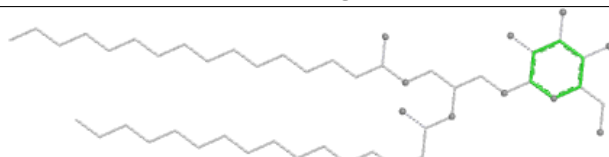
Ligand DGD c 517

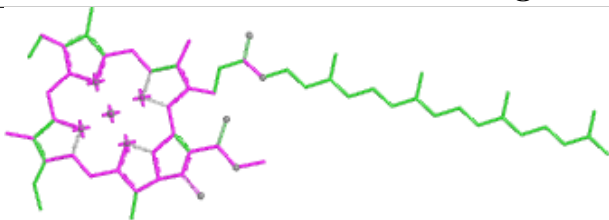
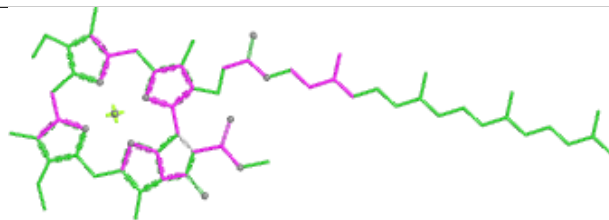
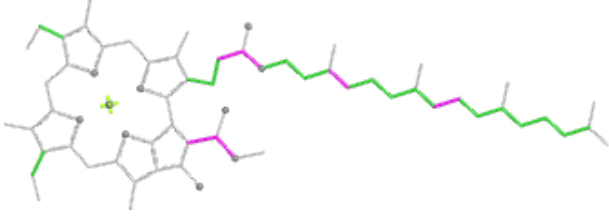
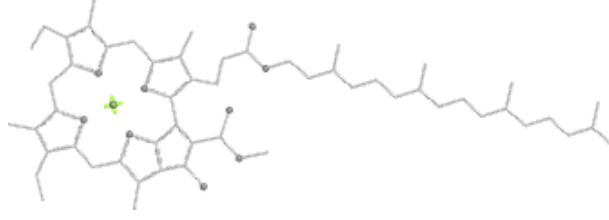




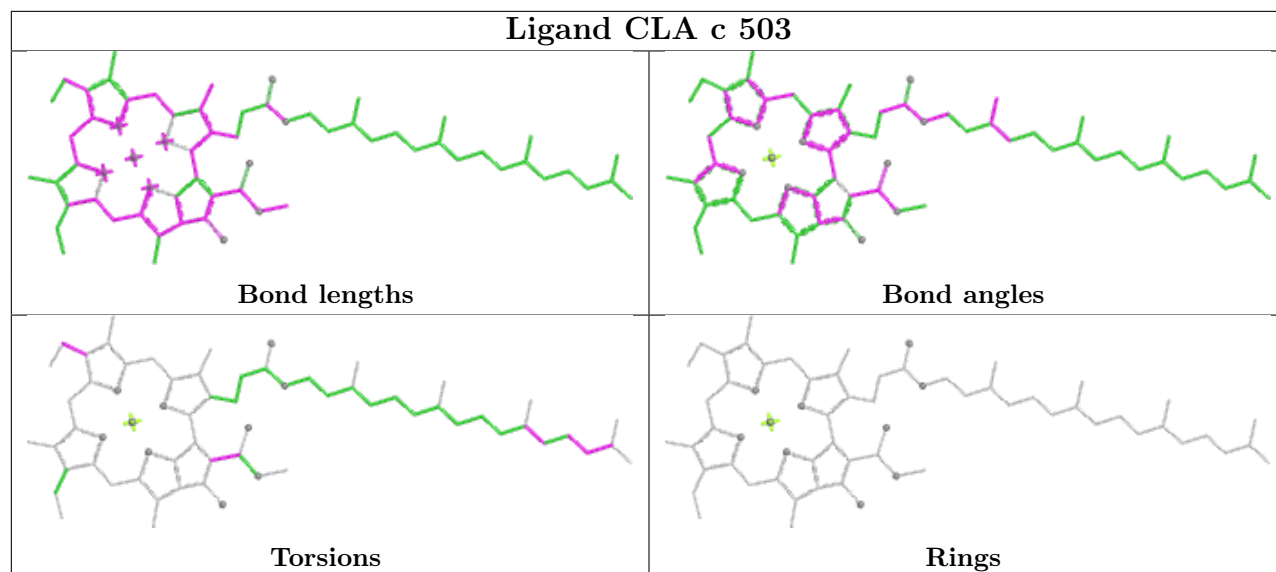


Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

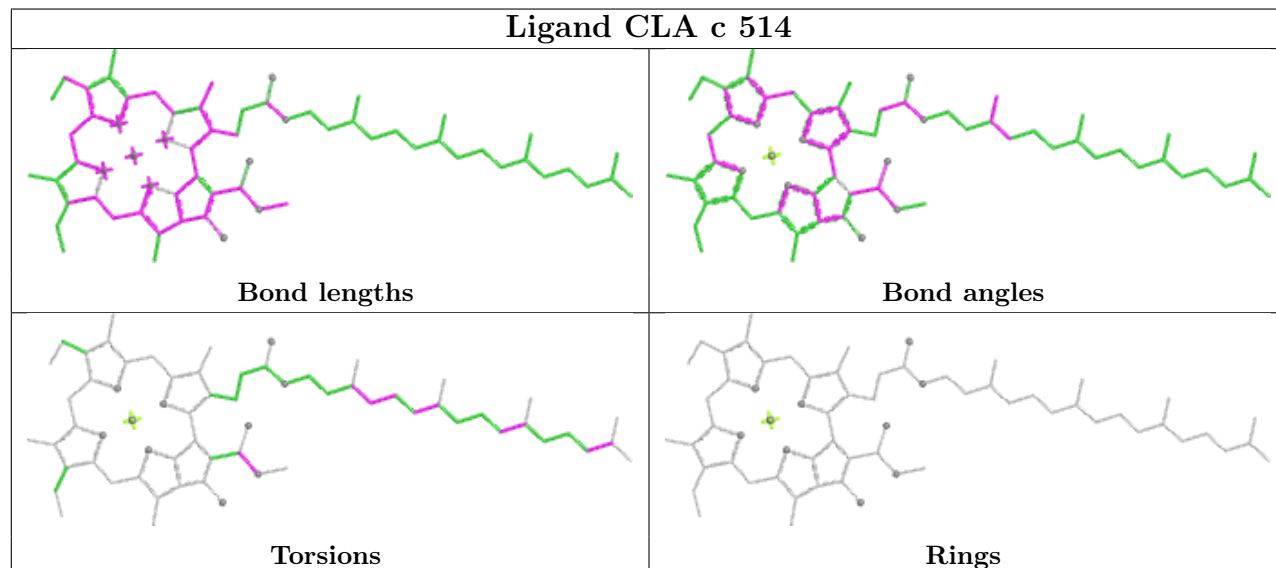
Ligand LMG A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

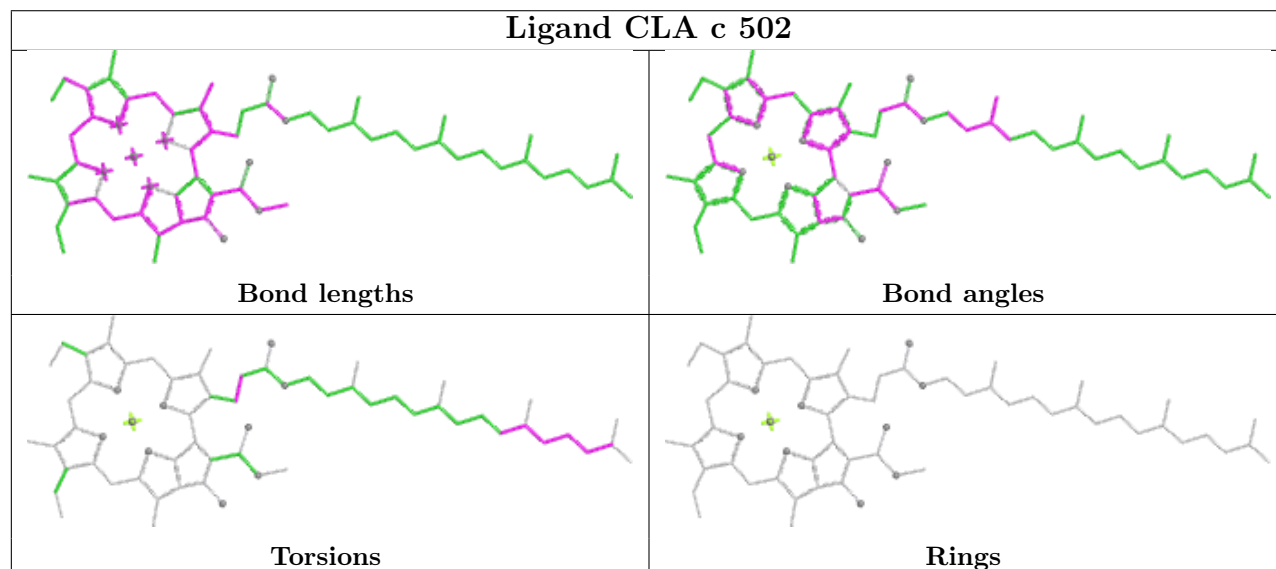
Ligand CLA c 503

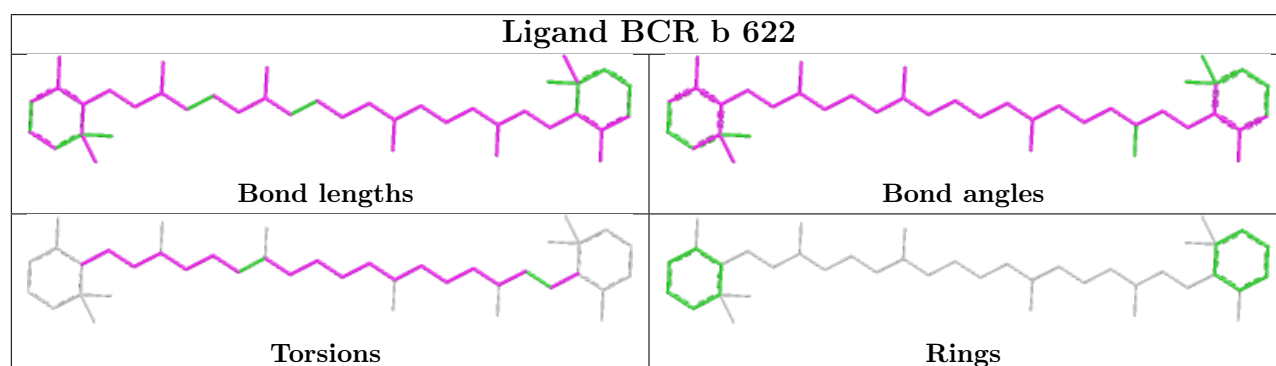
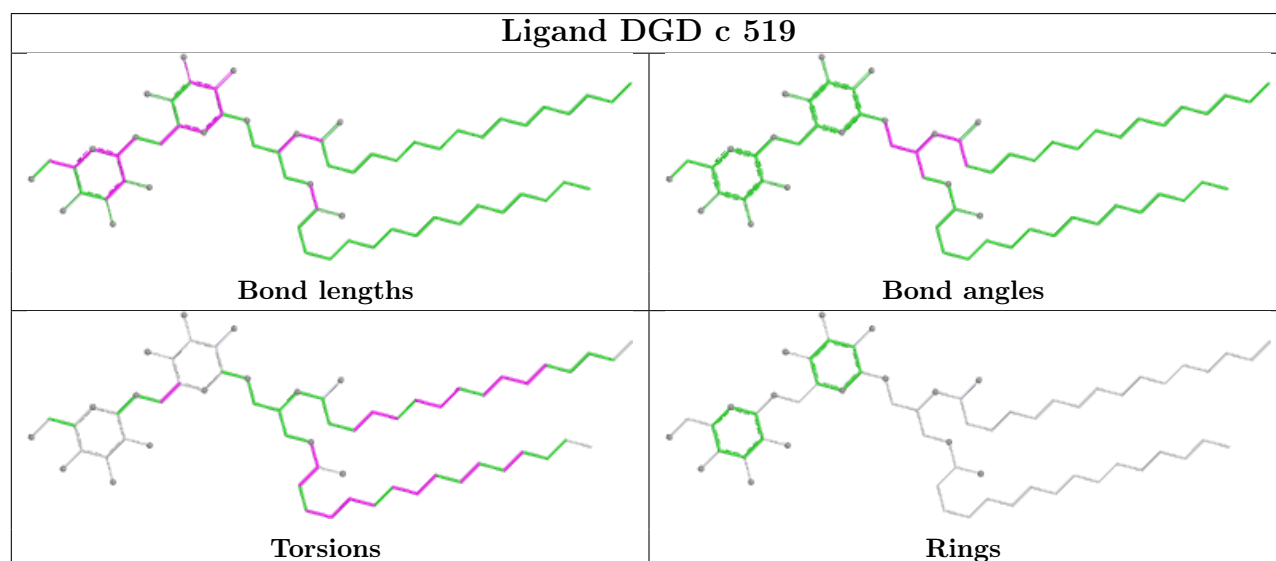
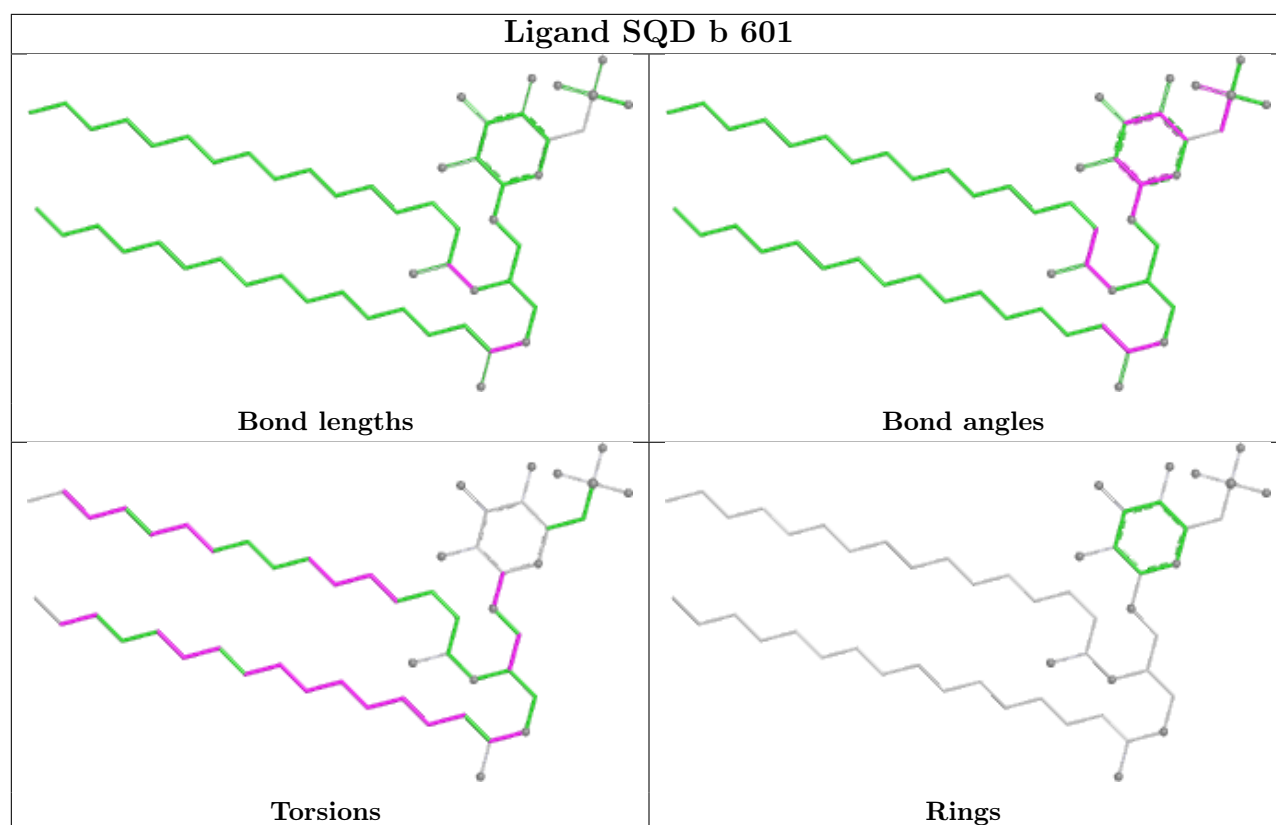


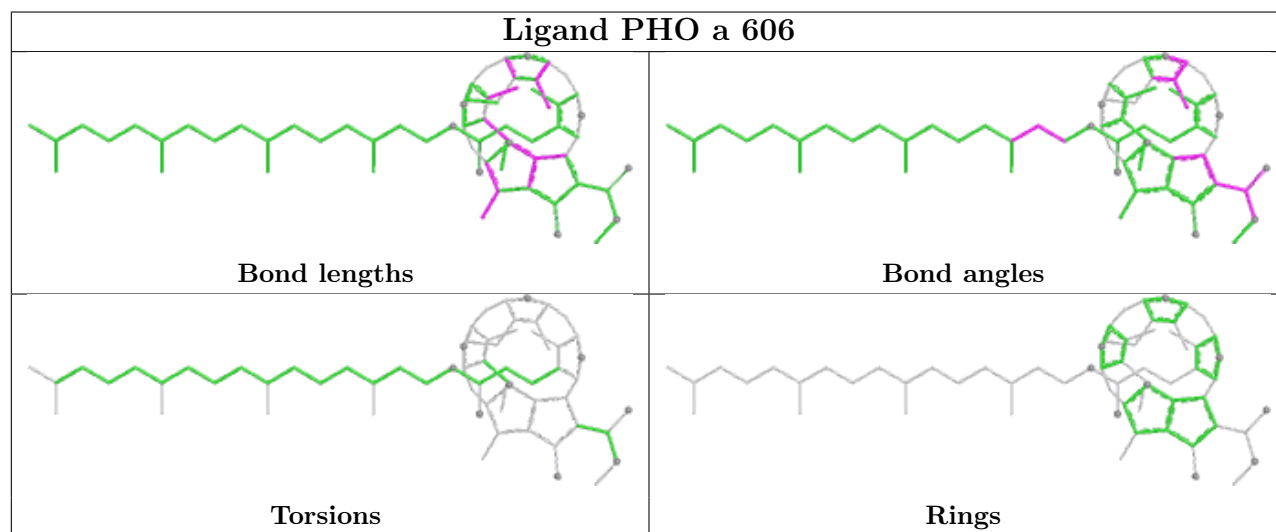
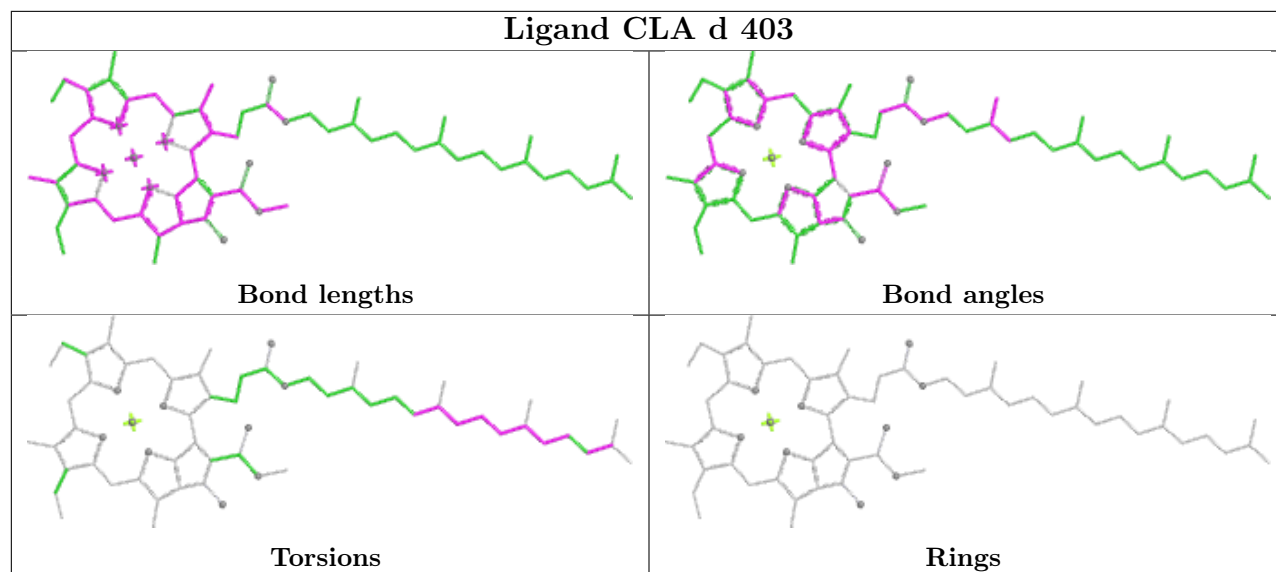
Ligand CLA c 514

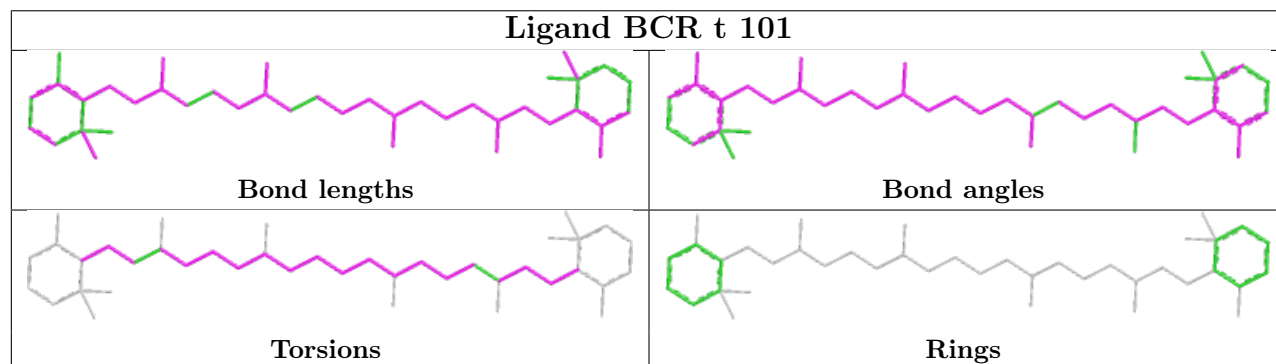
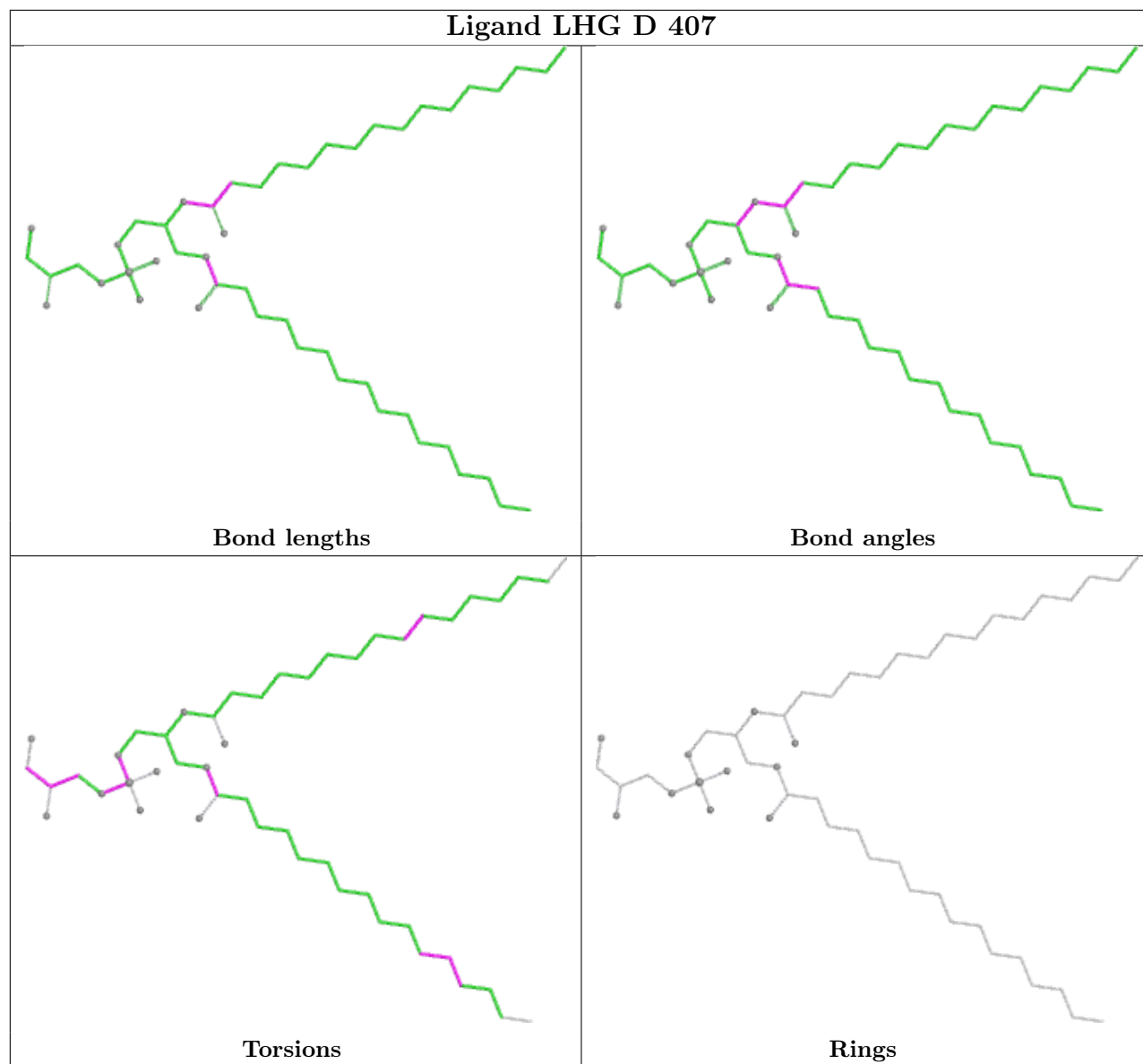


Ligand CLA c 502

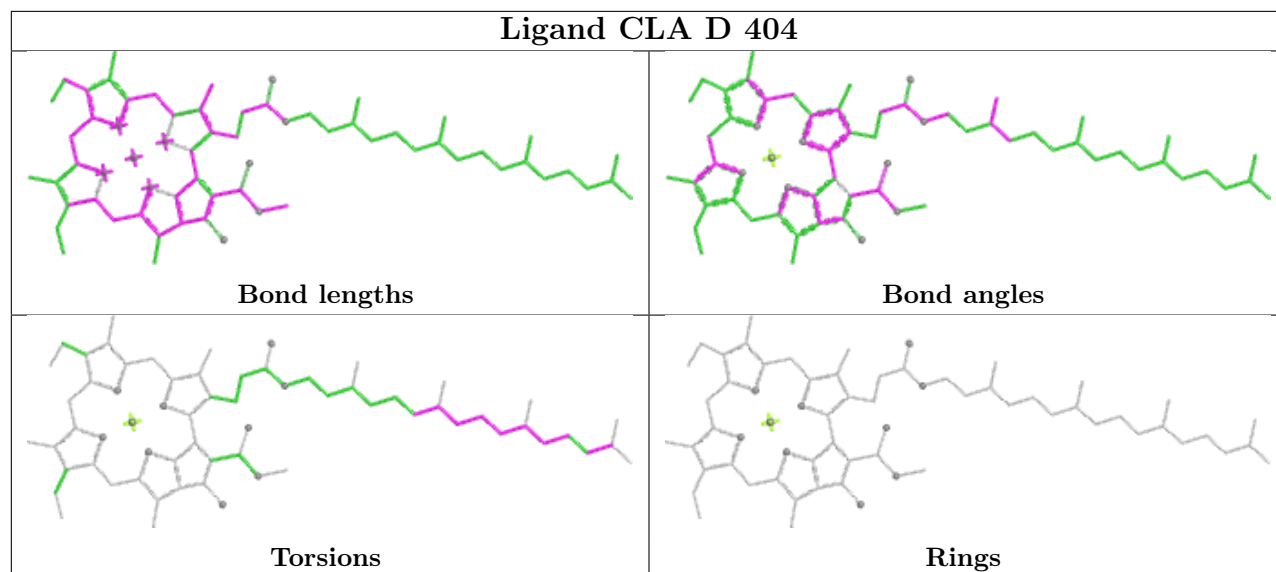




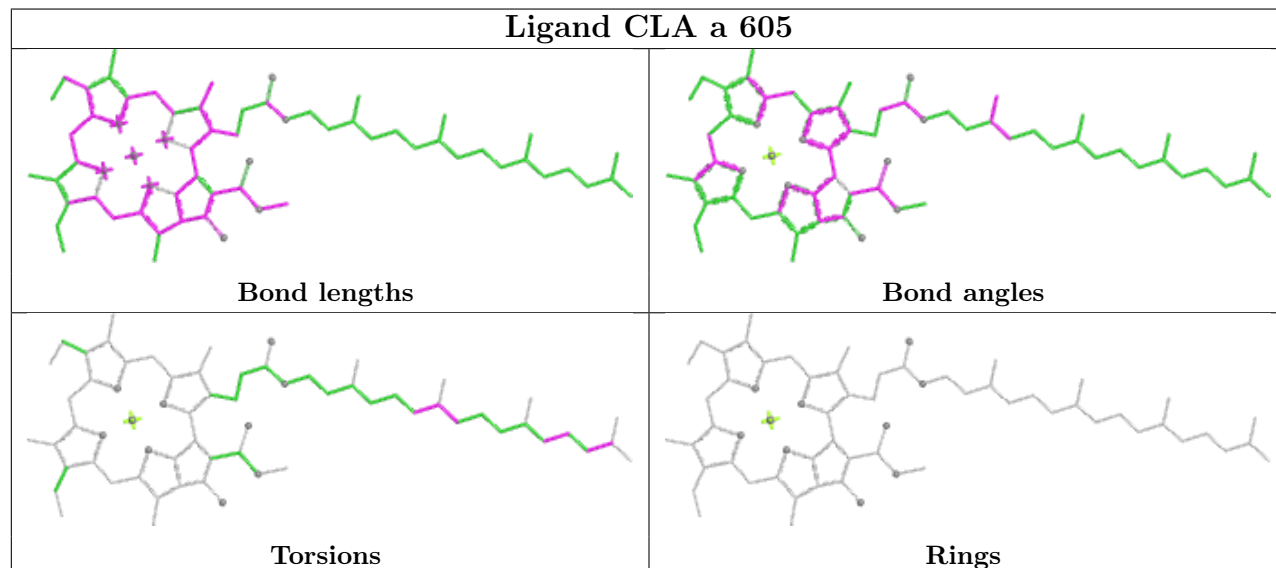




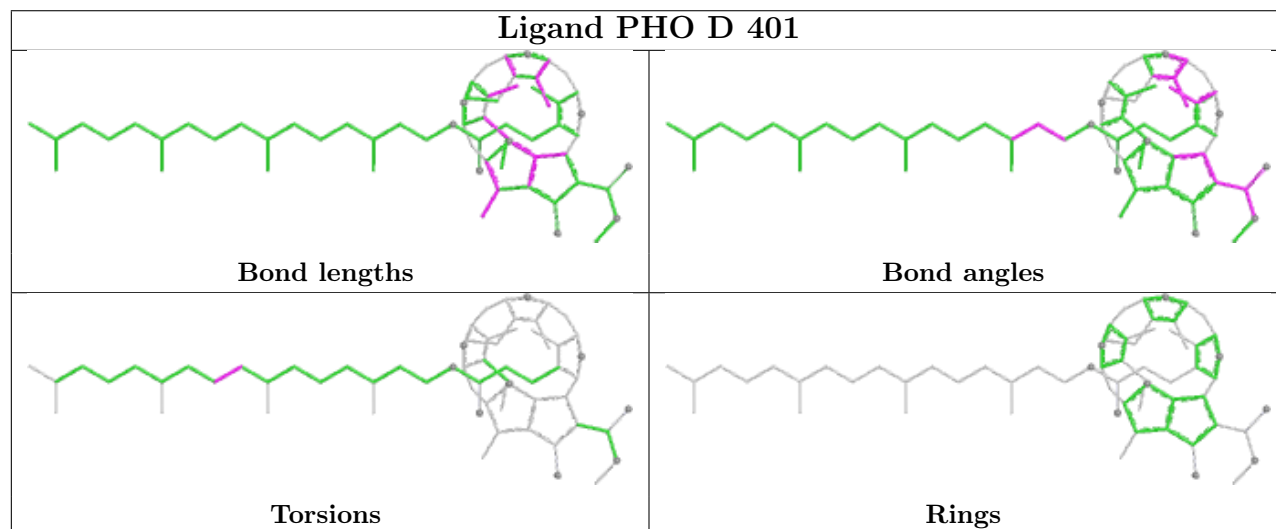
Ligand CLA D 404

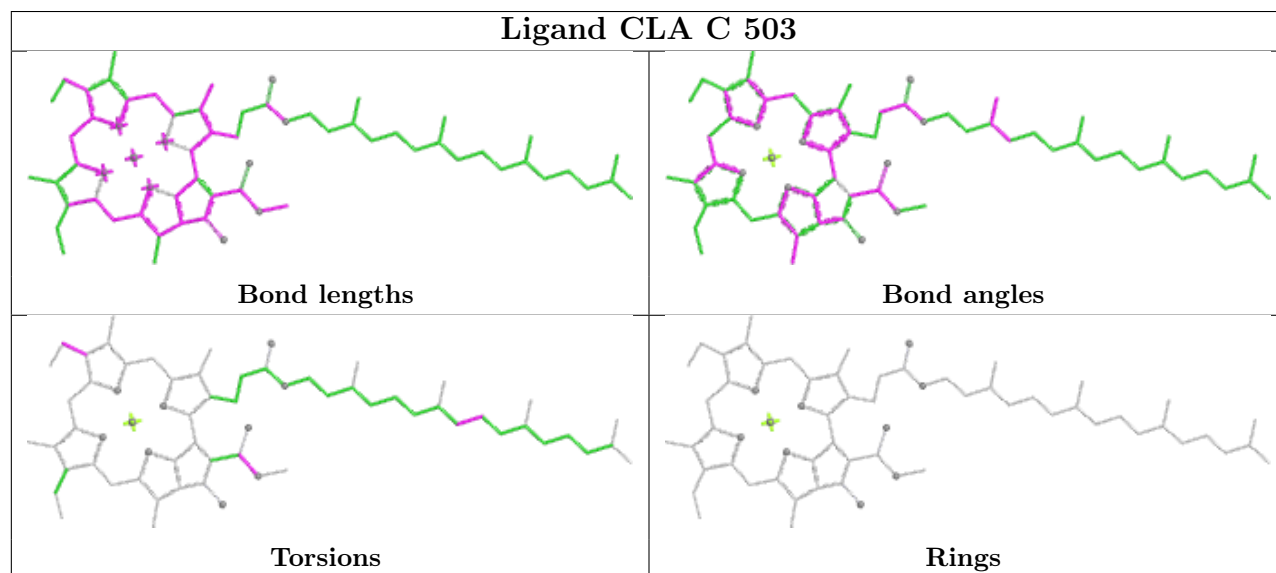
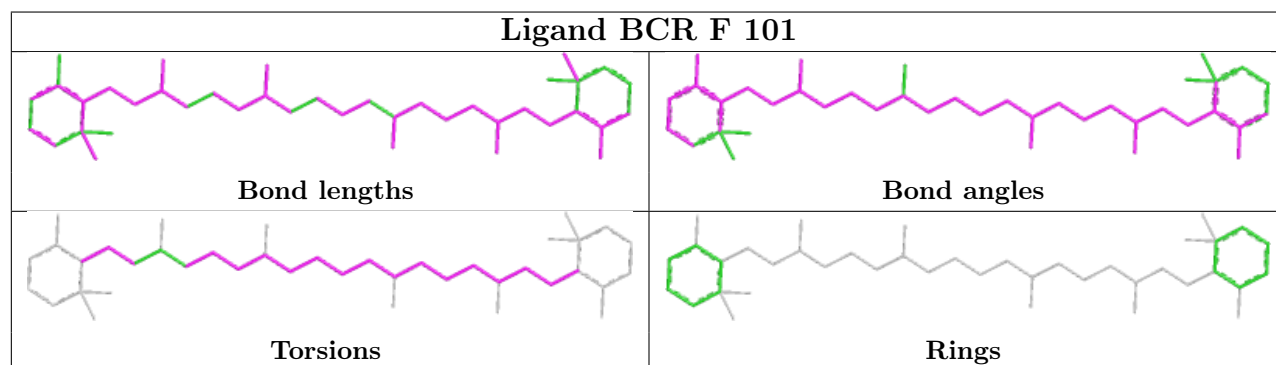
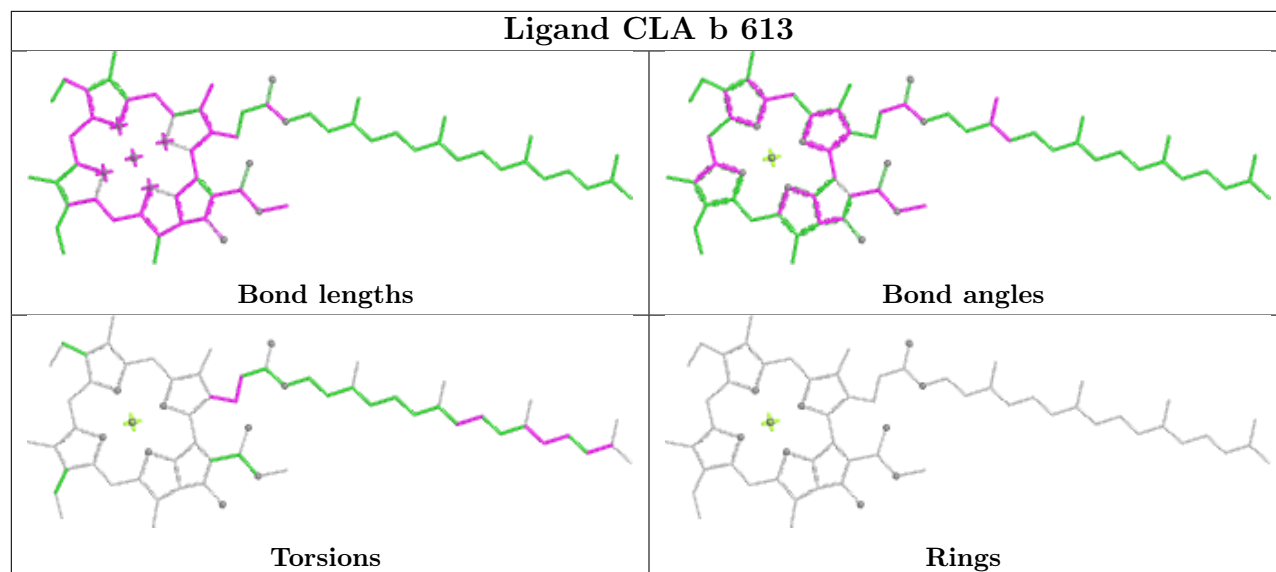


Ligand CLA a 605

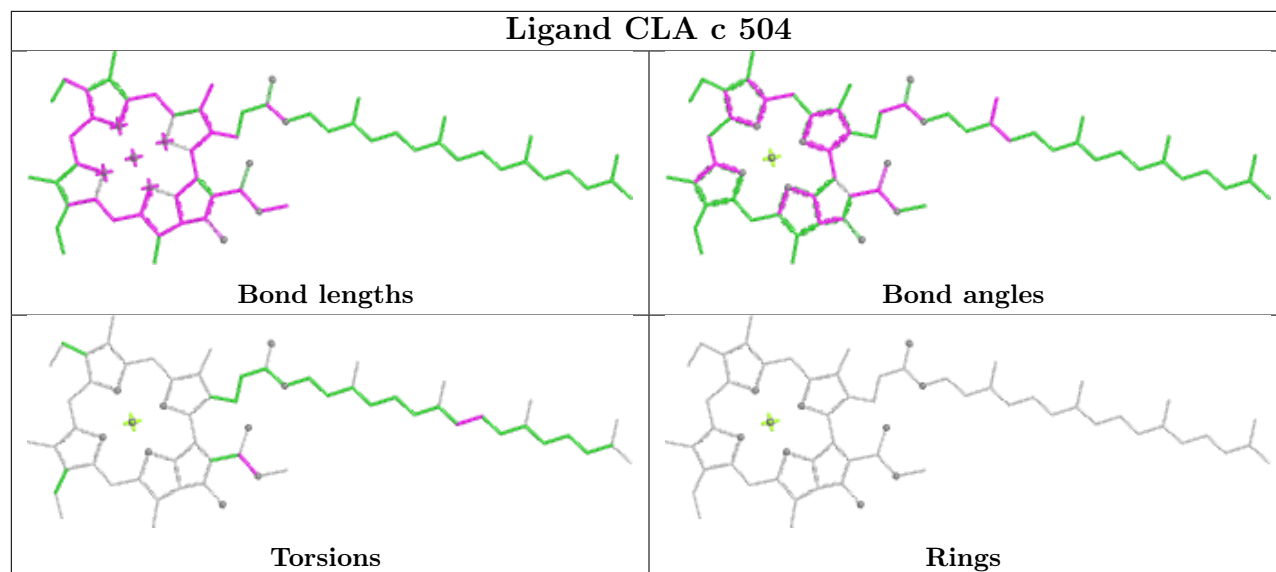


Ligand PHO D 401

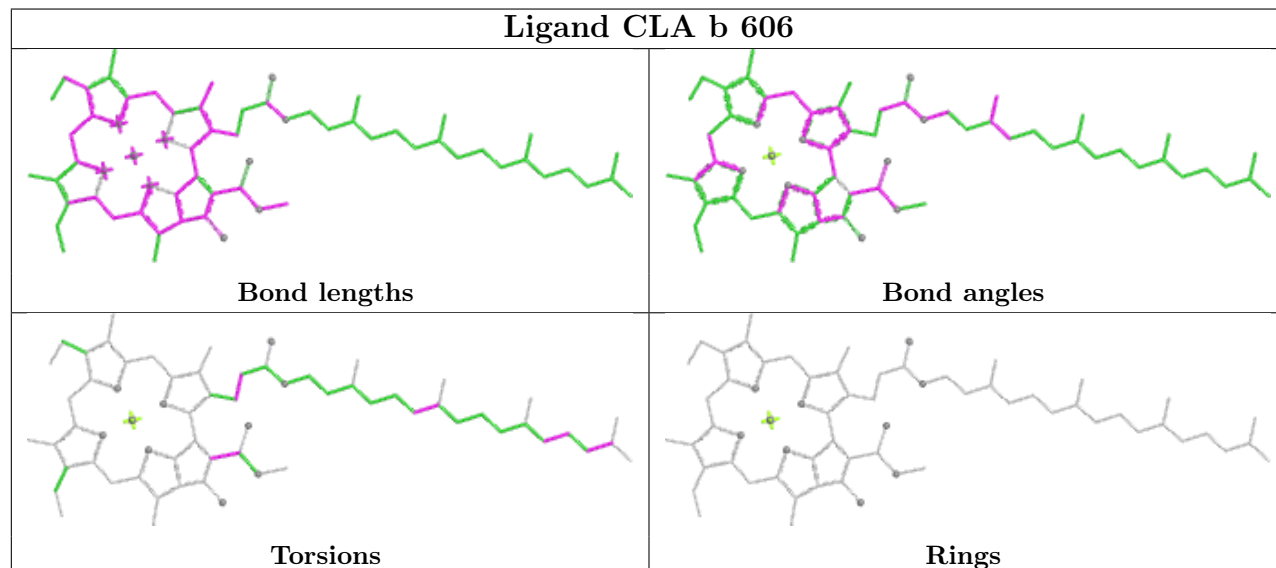


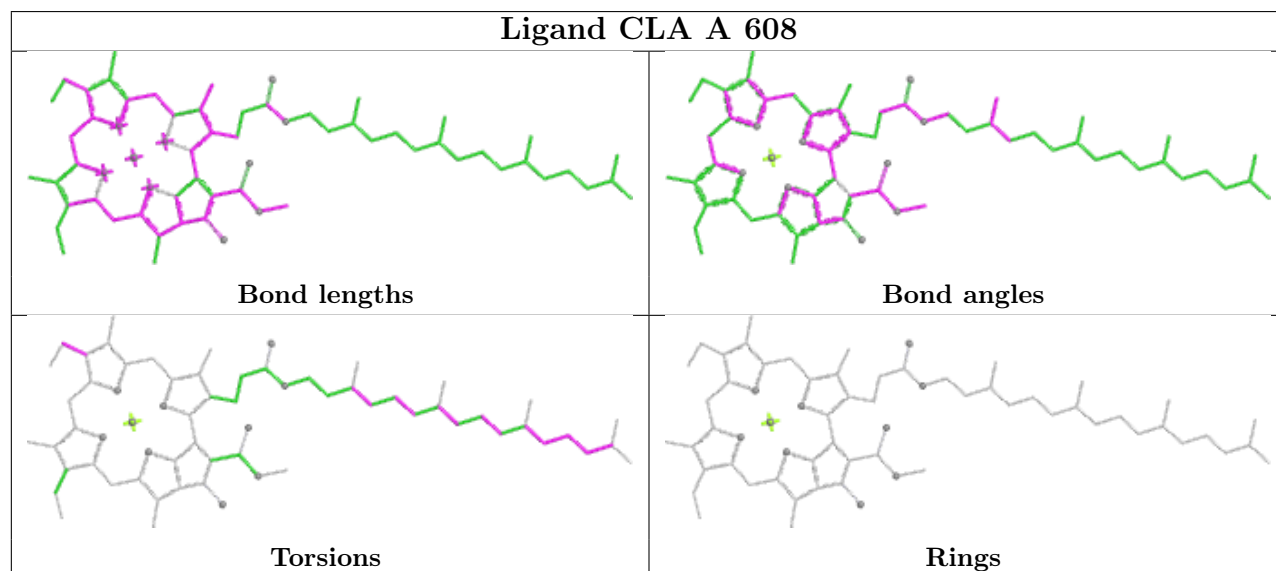
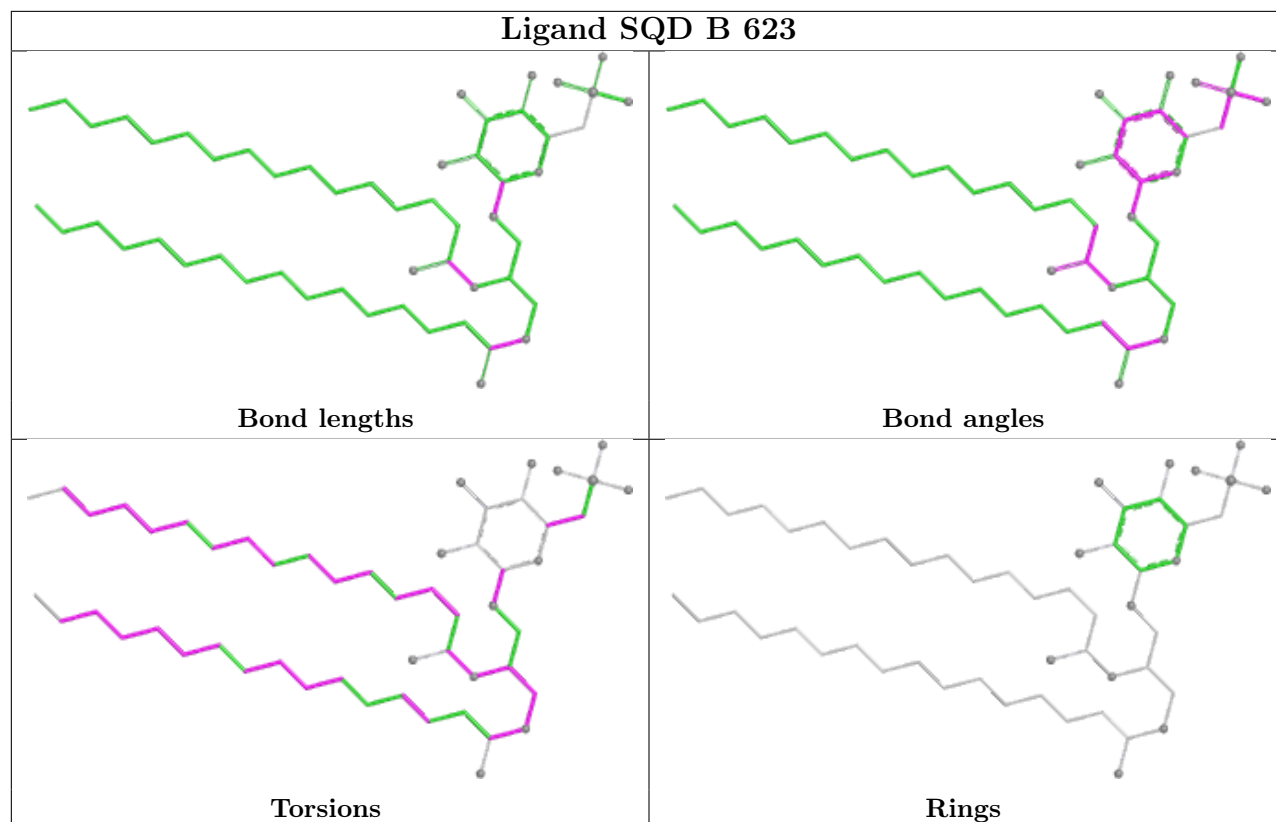


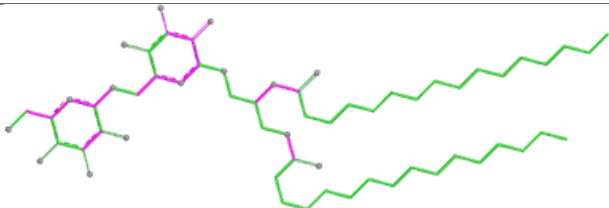
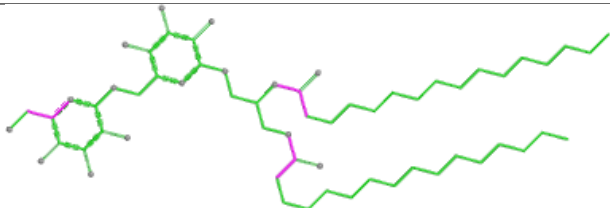
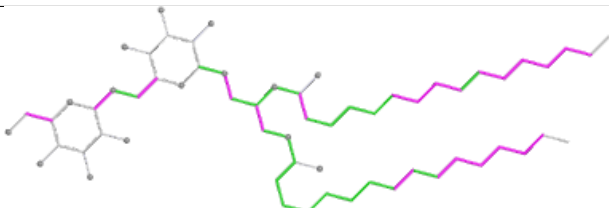
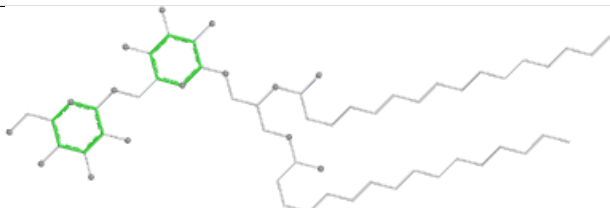
Ligand CLA c 504

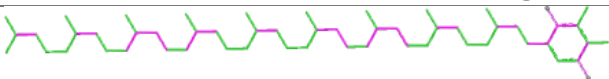
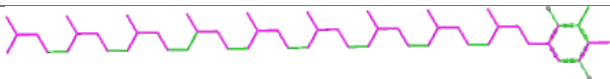
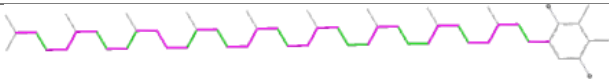
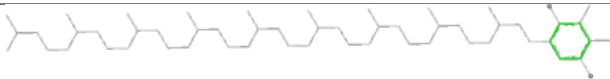


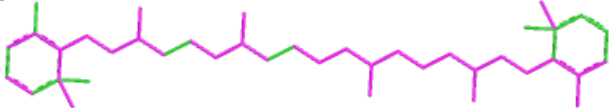
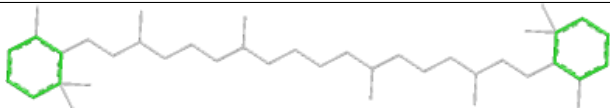
Ligand CLA b 606



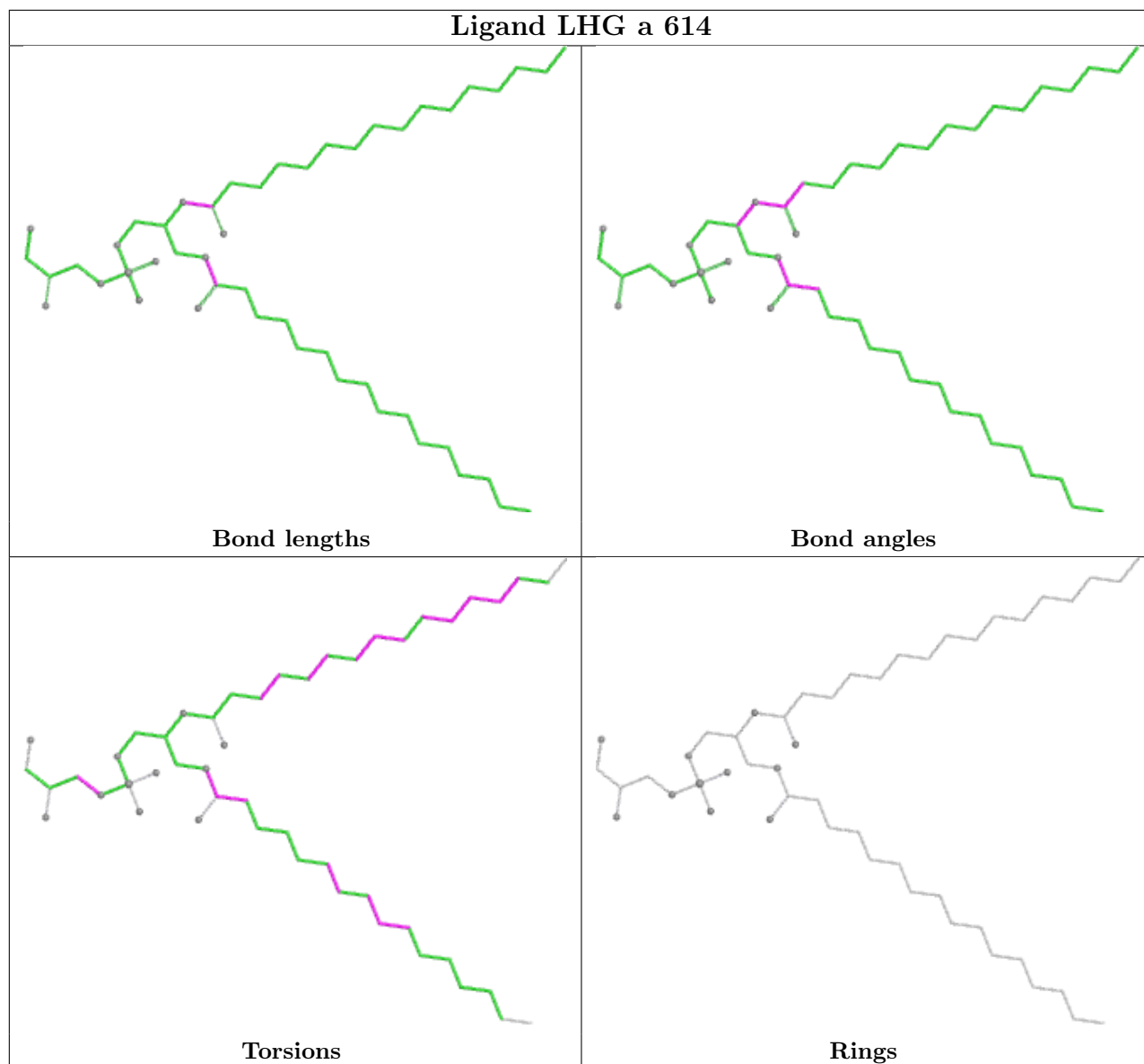


Ligand DGD H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

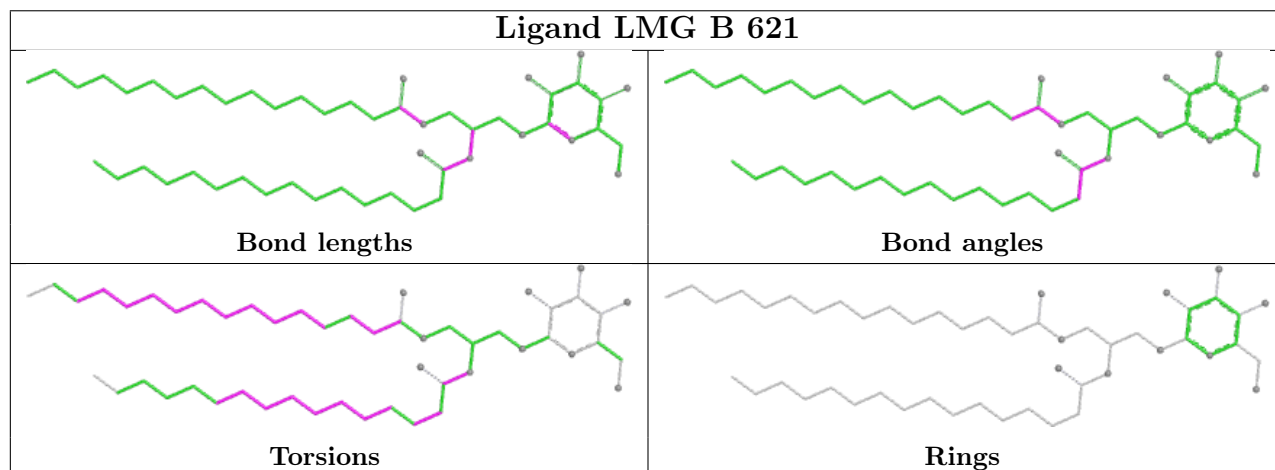
Ligand PL9 d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR f 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG a 614



Ligand LMG B 621



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%)	-0.26	1 (0%) 90 80	39, 63, 84, 93	4 (1%)
1	a	334/334 (100%)	-0.33	0 100 100	52, 84, 104, 114	4 (1%)
2	B	504/504 (100%)	-0.42	1 (0%) 91 83	41, 68, 89, 111	10 (1%)
2	b	504/504 (100%)	-0.33	4 (0%) 82 69	53, 88, 110, 131	10 (1%)
3	C	451/451 (100%)	-0.42	1 (0%) 91 83	43, 72, 84, 97	5 (1%)
3	c	451/451 (100%)	-0.43	0 100 100	57, 92, 105, 118	5 (1%)
4	D	342/342 (100%)	-0.28	3 (0%) 81 67	57, 64, 80, 102	0
4	d	342/342 (100%)	-0.18	6 (1%) 67 53	78, 85, 101, 123	0
5	E	81/81 (100%)	-0.47	0 100 100	47, 80, 98, 104	2 (2%)
5	e	81/81 (100%)	-0.42	0 100 100	61, 101, 119, 125	2 (2%)
6	F	34/34 (100%)	-0.47	0 100 100	68, 74, 99, 102	0
6	f	34/34 (100%)	-0.49	0 100 100	89, 95, 120, 122	0
7	H	65/65 (100%)	-0.40	0 100 100	43, 74, 81, 99	2 (3%)
7	h	65/65 (100%)	-0.27	0 100 100	55, 95, 101, 120	2 (3%)
8	I	38/38 (100%)	-0.40	0 100 100	36, 74, 105, 109	1 (2%)
8	i	38/38 (100%)	-0.49	0 100 100	45, 95, 126, 130	1 (2%)
9	J	38/38 (100%)	-0.69	0 100 100	66, 78, 109, 112	0
9	j	38/38 (100%)	-0.50	0 100 100	87, 99, 129, 133	0
10	K	37/37 (100%)	-0.43	0 100 100	74, 79, 86, 88	0
10	k	37/37 (100%)	-0.35	0 100 100	94, 100, 107, 108	0
11	L	37/37 (100%)	-0.41	0 100 100	37, 62, 90, 99	1 (2%)
11	l	37/37 (100%)	-0.40	0 100 100	49, 83, 111, 120	1 (2%)
12	M	34/34 (100%)	-0.40	1 (2%) 53 42	39, 64, 77, 93	1 (2%)
12	m	34/34 (100%)	-0.42	0 100 100	51, 84, 98, 114	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	-0.45	0 100 100	40, 73, 95, 111	4 (1%)
13	o	243/243 (100%)	-0.39	1 (0%) 88 77	53, 94, 116, 132	4 (1%)
14	T	30/30 (100%)	-0.47	0 100 100	32, 64, 85, 93	2 (6%)
14	t	30/30 (100%)	-0.44	0 100 100	43, 84, 105, 114	2 (6%)
15	U	97/97 (100%)	-0.45	0 100 100	64, 71, 89, 90	0
15	u	97/97 (100%)	-0.28	1 (1%) 79 64	84, 92, 110, 111	0
16	V	137/137 (100%)	-0.49	0 100 100	39, 69, 80, 88	1 (0%)
16	v	137/137 (100%)	-0.47	1 (0%) 84 71	51, 89, 101, 109	1 (0%)
17	Y	29/29 (100%)	-0.40	0 100 100	82, 89, 115, 118	0
17	y	29/29 (100%)	-0.52	0 100 100	103, 110, 136, 138	0
18	X	39/39 (100%)	-0.37	0 100 100	48, 80, 107, 108	1 (2%)
18	x	39/39 (100%)	-0.57	0 100 100	61, 101, 127, 129	1 (2%)
19	Z	62/62 (100%)	-0.39	0 100 100	80, 89, 109, 112	0
19	z	62/62 (100%)	-0.27	0 100 100	101, 110, 129, 133	0
All	All	5264/5264 (100%)	-0.37	20 (0%) 88 77	32, 83, 107, 138	68 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	d	54	PHE	3.8
2	b	63	LEU	3.7
4	D	56	THR	3.1
4	d	217	THR	3.0
2	b	268	PHE	2.9
4	D	59	TYR	2.7
2	b	64	PRO	2.6
2	b	302	TRP	2.5
4	d	264	LYS	2.3
16	v	52	LEU	2.3
13	o	25	THR	2.3
12	M	23	ILE	2.3
4	d	314	PHE	2.2
1	A	74	GLY	2.2
2	B	309	LEU	2.2
15	u	90	ALA	2.2
4	D	135	LEU	2.1
3	C	111	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	68	LEU	2.0
4	d	183	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	CL	V	201	1/1	0.18	0.11	91,91,91,91	0
30	CA	F	102	1/1	0.49	0.19	97,97,97,97	0
30	CA	b	603	1/1	0.49	0.11	137,137,137,137	0
21	CL	u	201	1/1	0.51	0.41	112,112,112,112	0
21	CL	A	602	1/1	0.64	0.16	65,65,65,65	0
30	CA	f	102	1/1	0.64	0.10	118,118,118,118	0
28	LMG	Z	101	37/55	0.66	0.12	96,124,129,129	0
28	LMG	c	521	51/55	0.68	0.15	104,137,142,143	0
28	LMG	C	520	51/55	0.68	0.13	83,117,122,123	0
27	SQD	a	610	54/54	0.69	0.11	110,119,128,128	0
30	CA	B	601	1/1	0.71	0.12	117,117,117,117	0
23	CLA	b	604	65/65	0.72	0.14	94,102,127,128	0
31	LHG	E	101	42/49	0.73	0.16	110,124,127,127	0
32	DGD	D	406	62/66	0.73	0.17	118,130,143,144	0
23	CLA	C	513	65/65	0.75	0.14	80,85,105,105	0
23	CLA	B	602	65/65	0.75	0.12	73,82,107,107	0
25	BCR	C	514	40/40	0.76	0.13	78,84,87,88	0
25	BCR	b	622	40/40	0.76	0.12	89,94,100,101	0
23	CLA	b	609[A]	65/65	0.77	0.14	85,90,102,103	65
23	CLA	b	609[B]	65/65	0.77	0.14	83,87,93,95	65
27	SQD	A	611	54/54	0.77	0.11	90,98,107,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	CA	O	301	1/1	0.77	0.08	90,90,90,90	0
31	LHG	e	101	42/49	0.78	0.12	131,145,147,148	0
27	SQD	x	101	43/54	0.78	0.15	128,136,140,140	0
25	BCR	T	101	40/40	0.79	0.12	65,78,85,86	0
32	DGD	d	405	62/66	0.79	0.16	138,151,164,165	0
28	LMG	z	101	37/55	0.80	0.10	117,145,149,150	0
25	BCR	B	620	40/40	0.80	0.10	68,74,80,80	0
32	DGD	c	519	62/66	0.81	0.10	83,93,113,117	0
27	SQD	b	602	54/54	0.81	0.15	99,107,121,121	0
34	MG	j	102	1/1	0.81	0.07	89,89,89,89	0
31	LHG	a	614	49/49	0.82	0.12	87,94,124,125	0
25	BCR	F	101	40/40	0.82	0.13	66,71,88,90	0
28	LMG	b	623	51/55	0.82	0.12	91,100,112,116	0
25	BCR	A	609	40/40	0.83	0.12	63,68,73,73	0
25	BCR	a	608	40/40	0.83	0.13	83,89,93,94	0
28	LMG	C	519	51/55	0.83	0.13	72,98,113,114	0
25	BCR	b	620	40/40	0.83	0.13	84,88,90,90	0
27	SQD	b	601	54/54	0.84	0.12	91,103,109,109	0
23	CLA	b	619	65/65	0.84	0.11	83,90,139,139	0
26	PL9	A	610	55/55	0.84	0.17	93,109,118,119	0
26	PL9	a	609	55/55	0.84	0.16	113,130,139,140	0
23	CLA	C	507	65/65	0.84	0.14	70,74,92,94	0
25	BCR	B	618	40/40	0.84	0.12	63,68,69,70	0
27	SQD	a	612	54/54	0.84	0.11	111,124,129,130	0
25	BCR	k	101	40/40	0.85	0.09	95,99,100,100	0
25	BCR	t	101	40/40	0.85	0.12	86,99,106,106	0
23	CLA	a	605	65/65	0.85	0.12	80,83,124,126	0
25	BCR	b	621	40/40	0.85	0.12	83,89,101,101	0
25	BCR	H	101	40/40	0.85	0.17	67,74,83,83	0
25	BCR	c	516	40/40	0.85	0.14	92,98,102,102	0
25	BCR	f	101	40/40	0.85	0.11	87,91,109,110	0
27	SQD	X	101	43/54	0.86	0.11	108,115,119,119	0
23	CLA	D	404	65/65	0.86	0.12	65,68,106,107	0
28	LMG	c	520	51/55	0.86	0.12	92,118,134,135	0
26	PL9	d	404	55/55	0.86	0.18	80,84,91,93	0
28	LMG	j	101	51/55	0.86	0.11	87,96,126,129	0
23	CLA	c	514	65/65	0.86	0.10	101,106,125,126	0
23	CLA	B	607[B]	65/65	0.87	0.14	63,67,72,75	65
23	CLA	B	617	65/65	0.87	0.10	63,69,118,119	0
23	CLA	B	607[A]	65/65	0.87	0.14	65,69,81,82	65
28	LMG	A	612	51/55	0.87	0.12	94,100,105,105	0
28	LMG	B	621	51/55	0.87	0.11	70,80,92,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	508	65/65	0.87	0.12	91,94,113,115	0
31	LHG	D	407	49/49	0.87	0.15	64,69,78,81	0
23	CLA	c	513	65/65	0.87	0.12	99,102,124,124	0
25	BCR	c	515	40/40	0.87	0.10	99,105,108,108	0
28	LMG	a	611	51/55	0.87	0.13	114,121,126,126	0
32	DGD	C	518	62/66	0.87	0.10	62,72,93,97	0
27	SQD	B	623	54/54	0.87	0.13	119,127,141,142	0
23	CLA	C	512	65/65	0.87	0.12	78,82,103,104	0
25	BCR	K	101	40/40	0.87	0.10	75,78,79,80	0
25	BCR	h	101	40/40	0.87	0.13	87,94,103,104	0
23	CLA	C	506	65/65	0.88	0.11	72,79,115,115	0
23	CLA	c	502	65/65	0.88	0.14	90,93,106,108	0
32	DGD	C	517	62/66	0.88	0.10	63,75,103,104	0
23	CLA	c	504	65/65	0.88	0.14	89,93,96,97	0
23	CLA	c	507	65/65	0.88	0.10	93,100,136,136	0
23	CLA	B	616	65/65	0.88	0.11	65,68,86,87	0
25	BCR	C	515	40/40	0.88	0.11	71,78,81,82	0
22	BCT	a	603	4/4	0.88	0.30	100,101,101,103	0
25	BCR	B	619	40/40	0.89	0.09	62,69,81,81	0
23	CLA	C	504	65/65	0.89	0.12	66,68,95,95	0
24	PHO	d	401	64/64	0.89	0.10	80,84,90,94	0
28	LMG	J	101	51/55	0.89	0.11	66,76,106,108	0
30	CA	o	301	1/1	0.89	0.04	110,110,110,110	0
23	CLA	b	618	65/65	0.90	0.11	86,89,107,108	0
32	DGD	c	517	62/66	0.90	0.13	84,94,122,124	0
23	CLA	B	608	65/65	0.90	0.11	58,61,73,74	0
31	LHG	D	408	49/49	0.90	0.10	67,74,103,104	0
34	MG	J	102	1/1	0.90	0.11	68,68,68,68	0
23	CLA	b	616	65/65	0.90	0.10	80,84,106,108	0
23	CLA	B	615	65/65	0.91	0.10	61,65,101,102	0
23	CLA	d	403	65/65	0.91	0.09	86,89,126,128	0
23	CLA	C	505	65/65	0.91	0.12	69,71,85,85	0
31	LHG	l	101	49/49	0.91	0.12	84,92,104,106	0
23	CLA	B	606	65/65	0.91	0.12	59,64,75,76	0
23	CLA	a	607	65/65	0.91	0.09	83,85,133,133	0
23	CLA	c	503	65/65	0.91	0.12	85,87,101,103	0
23	CLA	B	610	65/65	0.91	0.10	64,69,72,73	0
23	CLA	C	508	65/65	0.91	0.09	66,70,95,99	0
23	CLA	C	501	65/65	0.91	0.12	69,73,85,87	0
32	DGD	h	102	62/66	0.91	0.17	87,93,99,101	0
25	BCR	C	521	40/40	0.91	0.15	70,74,78,78	0
23	CLA	b	611	65/65	0.91	0.11	82,86,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	617	65/65	0.92	0.11	82,86,121,122	0
21	CL	A	603	1/1	0.92	0.15	62,62,62,62	0
31	LHG	b	624	49/49	0.92	0.14	91,96,102,102	0
31	LHG	d	406	49/49	0.92	0.15	85,89,98,102	0
23	CLA	C	511	65/65	0.92	0.12	70,75,78,79	0
23	CLA	B	603	65/65	0.92	0.12	64,67,72,73	0
32	DGD	C	516	62/66	0.92	0.11	64,73,102,103	0
23	CLA	b	605	65/65	0.92	0.13	85,88,93,94	0
23	CLA	b	608	65/65	0.92	0.12	80,84,95,97	0
23	CLA	B	605	65/65	0.92	0.12	60,63,91,91	0
32	DGD	H	102	62/66	0.92	0.13	66,72,79,81	0
23	CLA	D	403	65/65	0.92	0.12	54,59,75,76	0
32	DGD	c	518	62/66	0.92	0.08	84,96,124,124	0
23	CLA	b	610	65/65	0.92	0.12	79,82,94,95	0
23	CLA	A	608	65/65	0.92	0.10	62,65,112,113	0
23	CLA	b	612	65/65	0.92	0.10	85,90,92,93	0
24	PHO	D	401	64/64	0.92	0.10	59,63,69,73	0
23	CLA	a	604	65/65	0.92	0.12	77,80,87,95	0
23	CLA	C	509	65/65	0.93	0.14	70,72,87,88	0
23	CLA	b	606	65/65	0.93	0.14	79,84,92,96	0
23	CLA	c	506	65/65	0.93	0.10	89,92,106,106	0
23	CLA	b	614	65/65	0.93	0.10	80,83,94,96	0
25	BCR	c	522	40/40	0.93	0.13	91,95,98,99	0
22	BCT	A	604	4/4	0.93	0.10	79,80,81,82	0
31	LHG	L	101	49/49	0.93	0.12	63,72,83,85	0
23	CLA	c	510	65/65	0.93	0.12	91,93,108,108	0
23	CLA	B	614	65/65	0.94	0.08	60,63,85,87	0
23	CLA	B	609	65/65	0.94	0.09	61,65,71,72	0
23	CLA	b	613	65/65	0.94	0.12	82,86,94,98	0
21	CL	a	602	1/1	0.94	0.08	86,86,86,86	0
23	CLA	b	615	65/65	0.94	0.17	81,85,91,92	0
23	CLA	B	611	65/65	0.94	0.13	62,65,73,77	0
31	LHG	B	622	49/49	0.94	0.12	70,75,81,82	0
23	CLA	c	509	65/65	0.94	0.08	87,90,115,119	0
23	CLA	B	613	65/65	0.94	0.14	61,64,71,72	0
23	CLA	c	511	65/65	0.94	0.08	86,90,96,99	0
23	CLA	c	512	65/65	0.94	0.09	90,95,99,99	0
23	CLA	C	502	65/65	0.94	0.09	65,67,80,83	0
33	HEM	e	102	43/43	0.94	0.11	101,103,107,108	0
23	CLA	C	503	65/65	0.94	0.12	68,72,76,77	0
29	FE2	a	615	1/1	0.94	0.06	88,88,88,88	0
24	PHO	a	606	64/64	0.95	0.10	78,83,86,87	0

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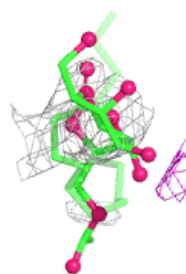
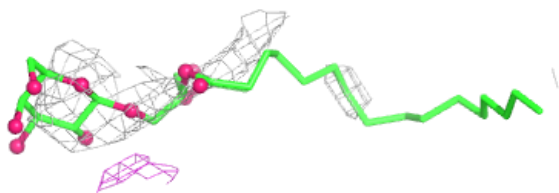
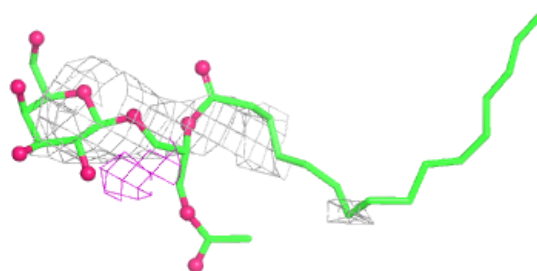
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	PL9	D	405	55/55	0.95	0.14	60,64,70,72	0
23	CLA	A	606	65/65	0.95	0.13	60,62,104,106	0
23	CLA	B	604	65/65	0.95	0.11	58,63,72,76	0
23	CLA	c	505	65/65	0.95	0.09	86,89,115,116	0
23	CLA	B	612	65/65	0.95	0.08	60,62,73,75	0
23	CLA	b	607	65/65	0.95	0.10	81,84,111,112	0
21	CL	c	501	1/1	0.95	0.08	83,83,83,83	0
20	OEX	A	601	10/10	0.95	0.15	63,64,67,67	0
20	OEX	a	601	10/10	0.96	0.15	83,84,87,88	0
23	CLA	a	613	65/65	0.96	0.13	75,79,91,96	0
23	CLA	d	402	65/65	0.96	0.12	75,80,95,96	0
23	CLA	A	605	65/65	0.96	0.12	56,59,66,75	0
33	HEM	E	102	43/43	0.96	0.08	80,82,86,87	0
24	PHO	A	607	64/64	0.96	0.07	57,62,65,67	0
33	HEM	v	201	43/43	0.96	0.15	84,86,88,90	0
23	CLA	C	510	65/65	0.96	0.09	65,69,76,78	0
23	CLA	D	402	65/65	0.96	0.11	54,59,70,76	0
29	FE2	A	613	1/1	0.97	0.08	67,67,67,67	0
33	HEM	V	202	43/43	0.97	0.10	63,65,68,69	0

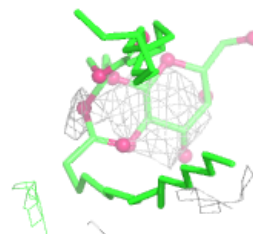
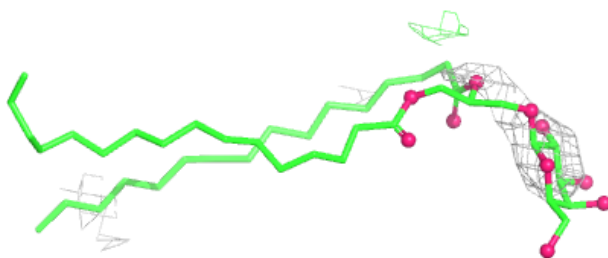
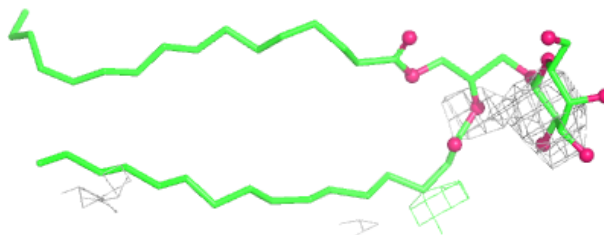
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMG Z 101:

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

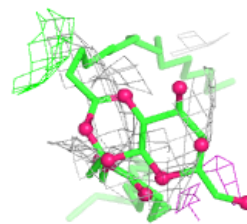
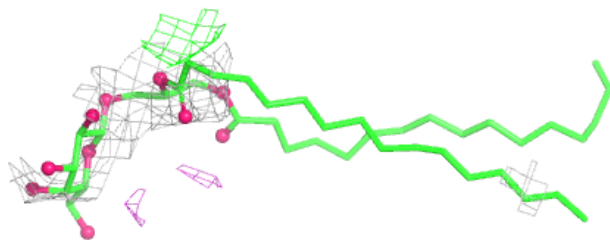
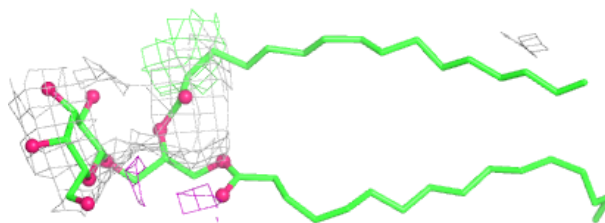
**Electron density around LMG c 521:**

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



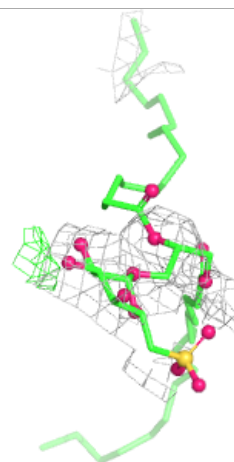
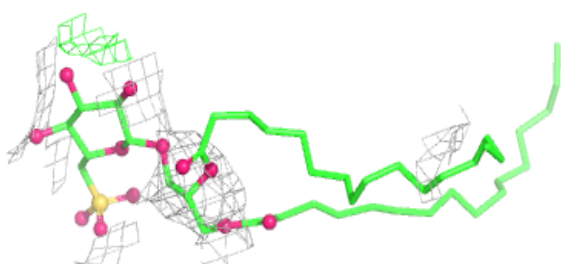
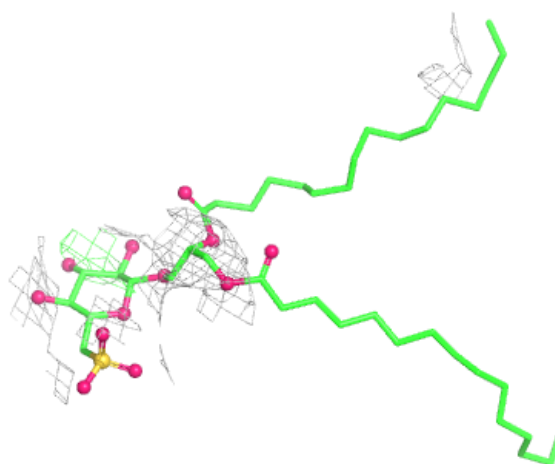
Electron density around LMG C 520:

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



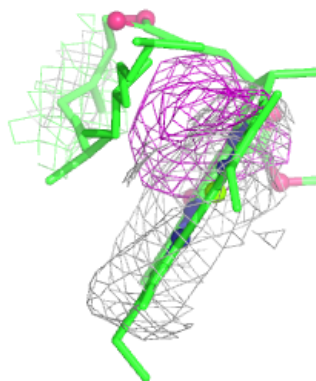
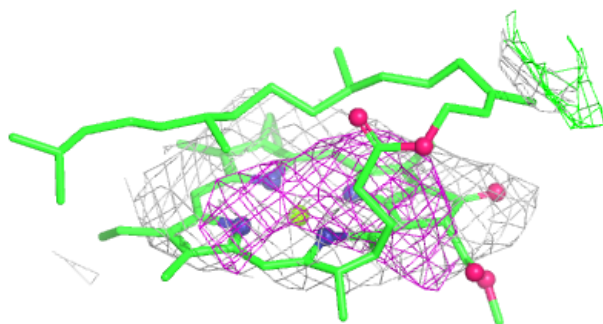
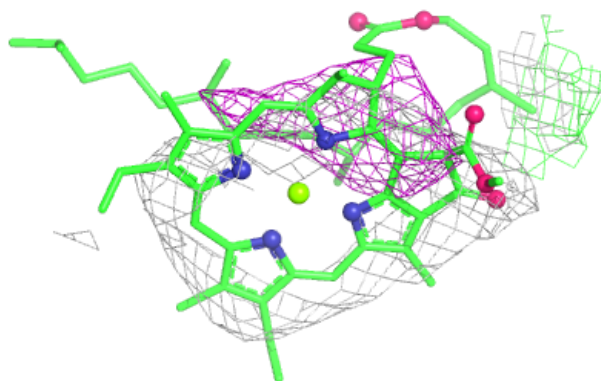
Electron density around SQD a 610:

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

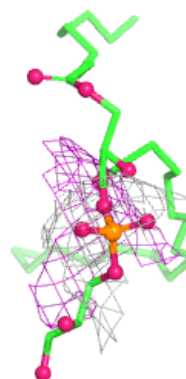
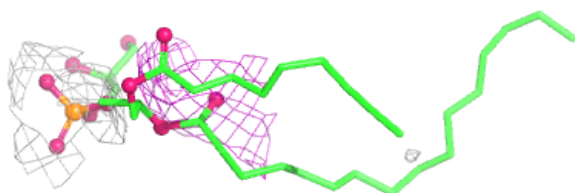
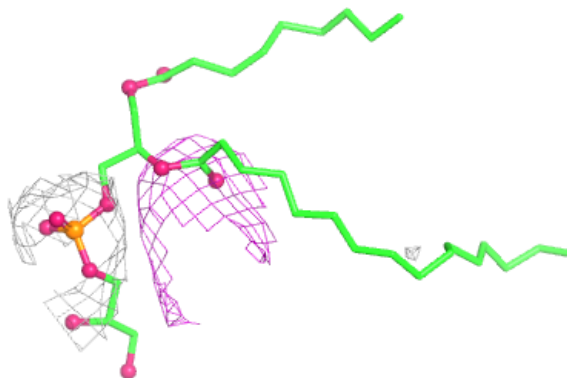


Electron density around CLA b 604:

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

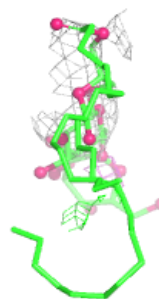
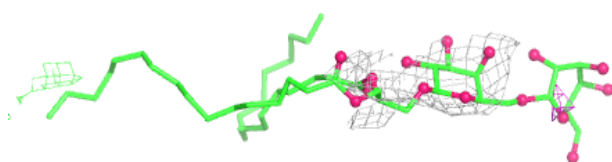
**Electron density around LHG E 101:**

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

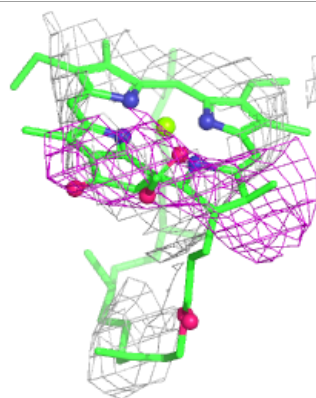
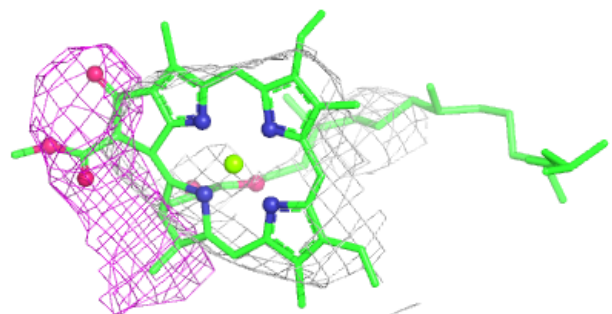
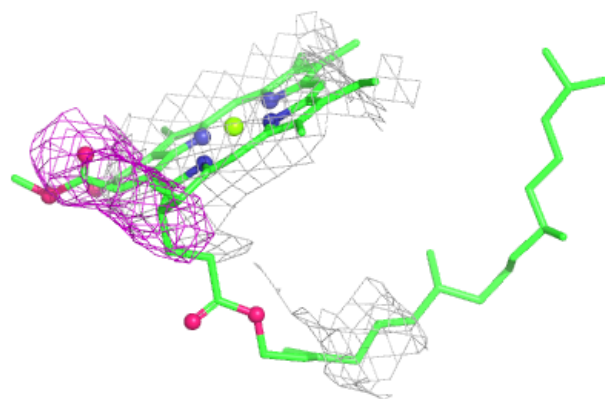


Electron density around DGD D 406:

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

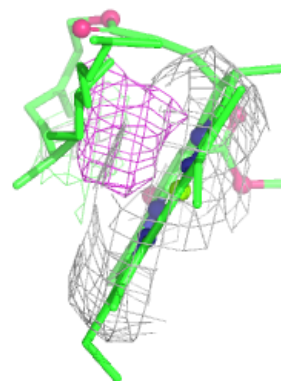
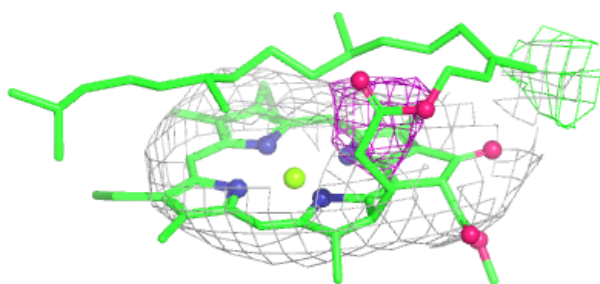
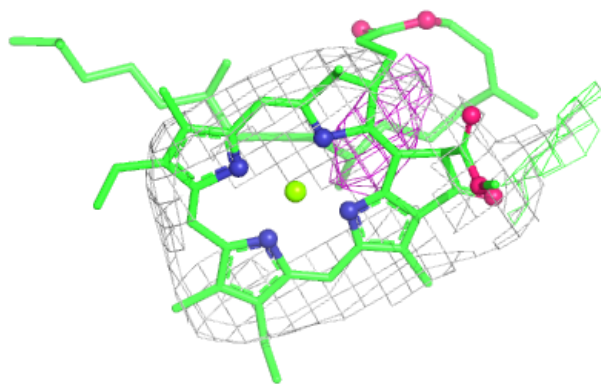
**Electron density around CLA C 513:**

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

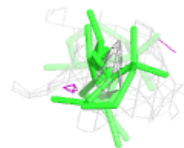
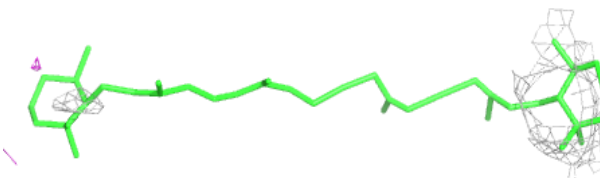
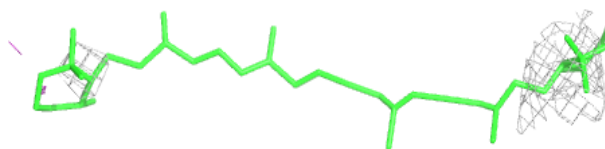


Electron density around CLA B 602:

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

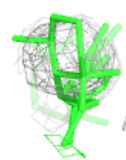
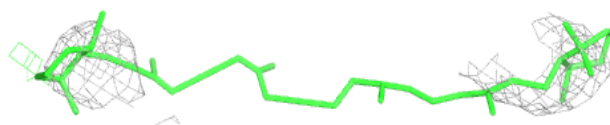
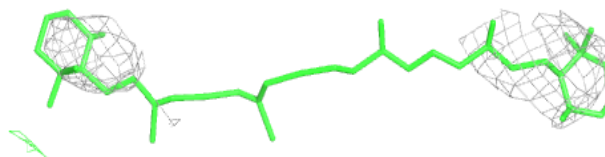
**Electron density around BCR C 514:**

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

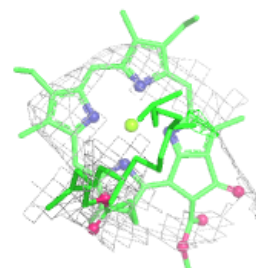
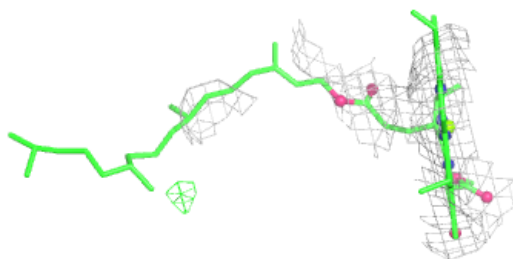
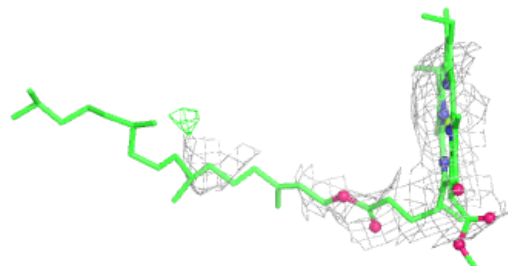


Electron density around BCR b 622:

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

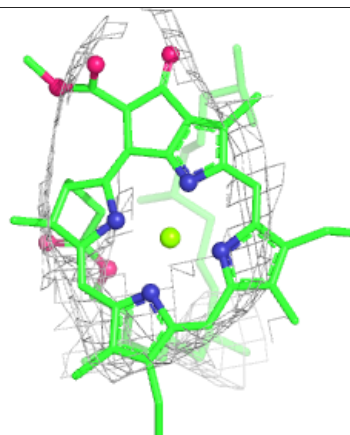
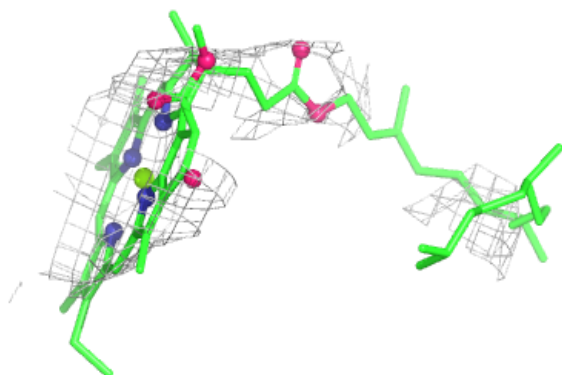
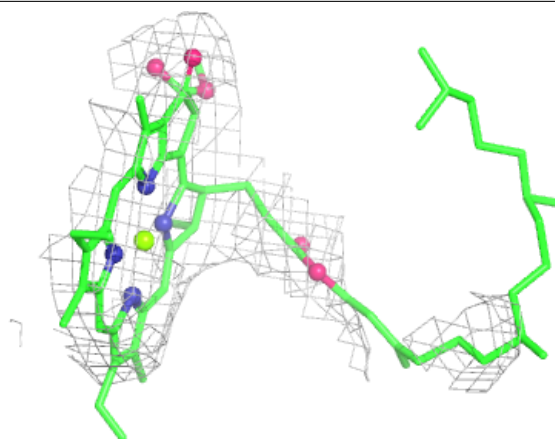
**Electron density around CLA b 609 (A):**

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



Electron density around CLA b 609 (B):

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



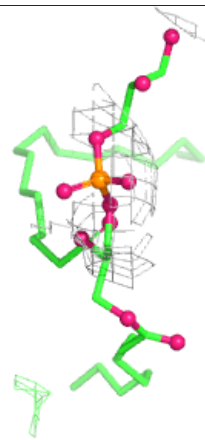
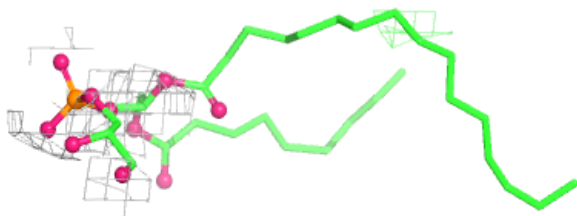
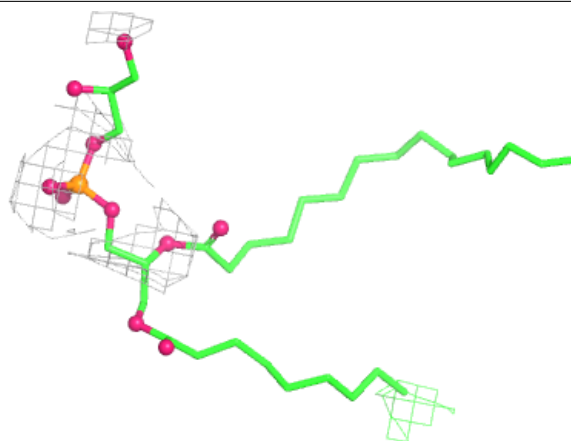
Electron density around SQD A 611:

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



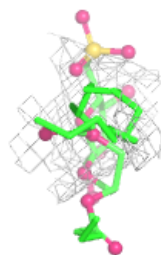
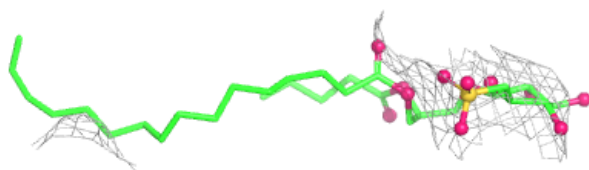
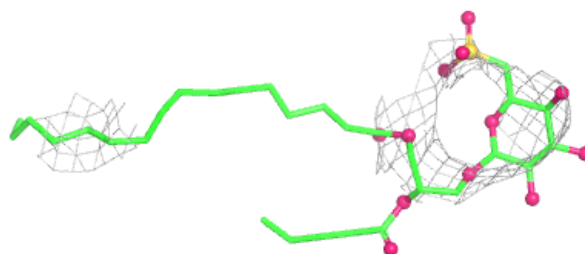
Electron density around LHG e 101:

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

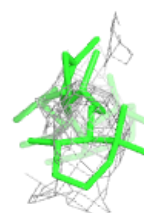
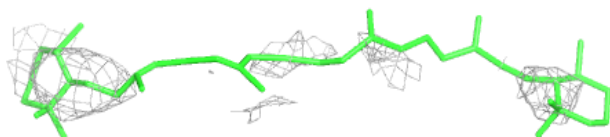
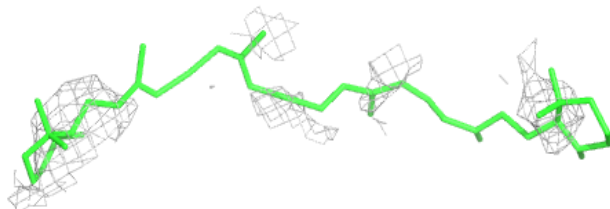


Electron density around SQD x 101:

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

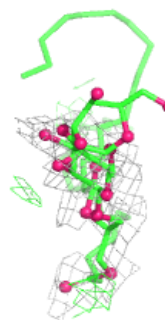
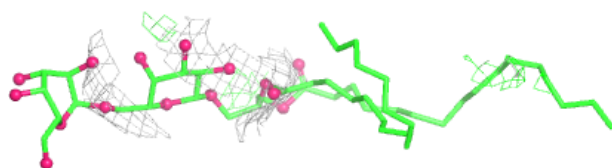
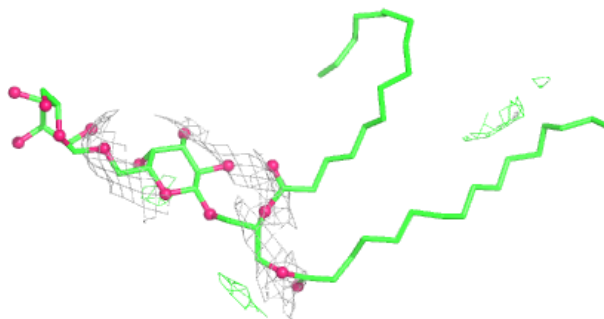
**Electron density around BCR T 101:**

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

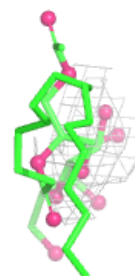
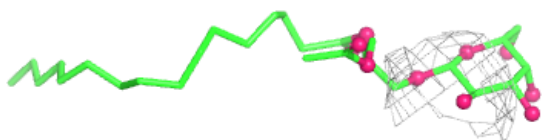
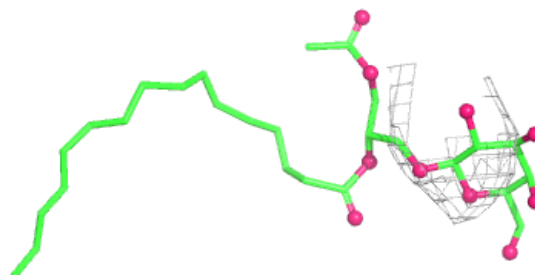


Electron density around DGD d 405:

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

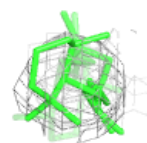
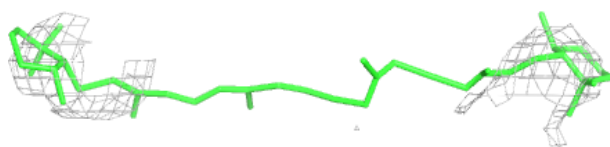
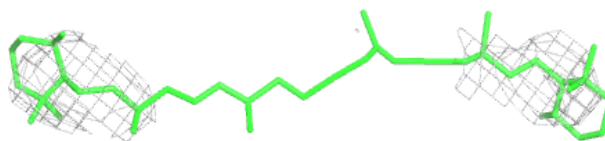
**Electron density around LMG z 101:**

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

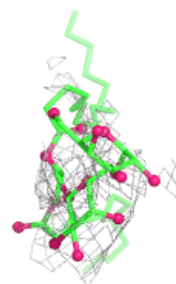
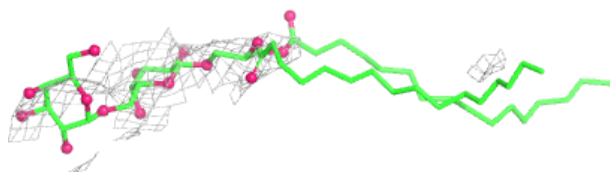
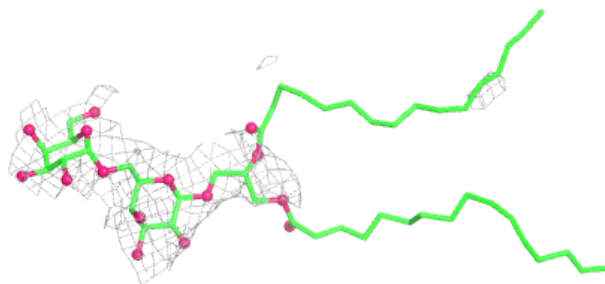


Electron density around BCR B 620:

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

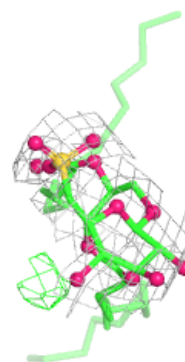
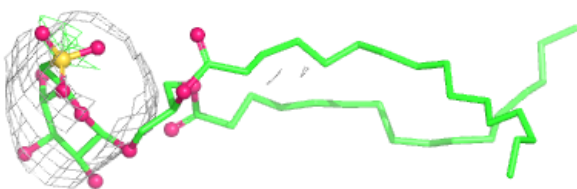
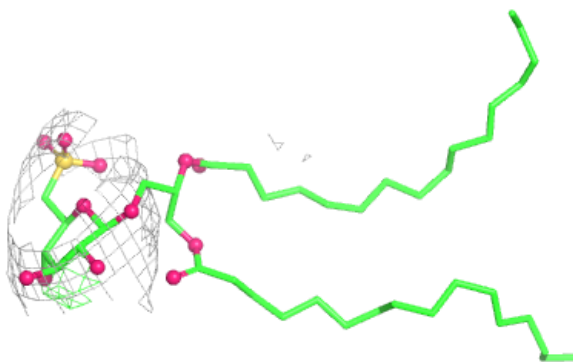
**Electron density around DGD c 519:**

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

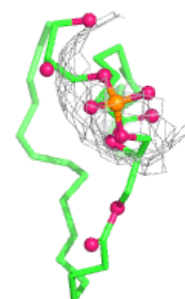


Electron density around SQD b 602:

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

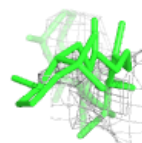
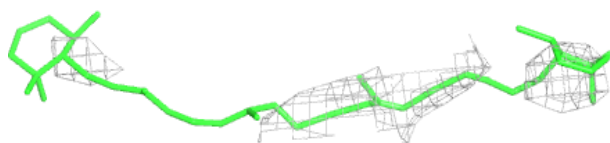
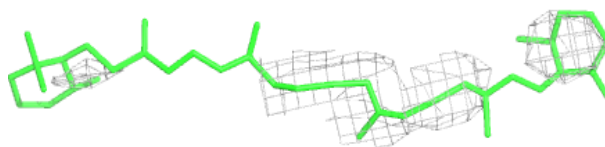
**Electron density around LHG a 614:**

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

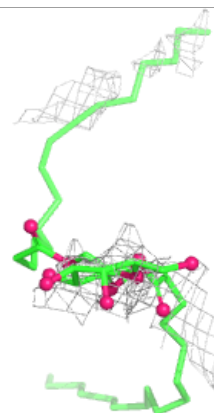
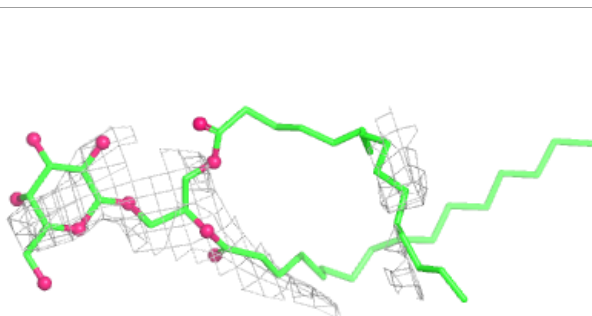
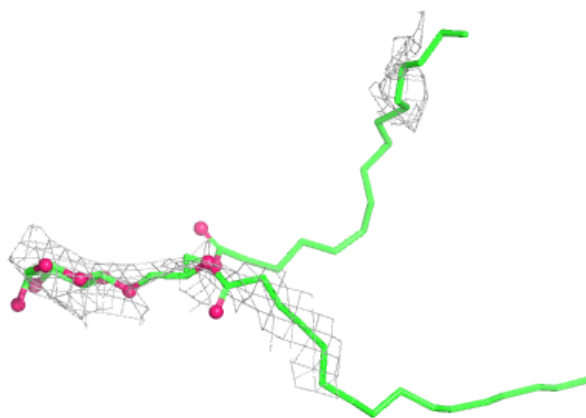


Electron density around BCR F 101:

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

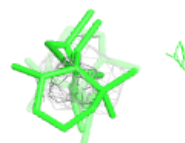
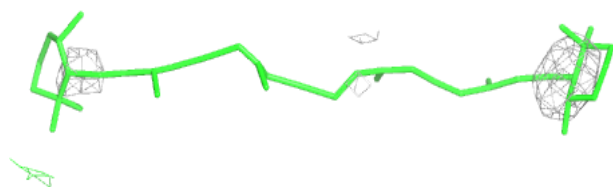
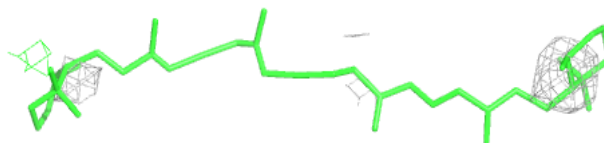
**Electron density around LMG b 623:**

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

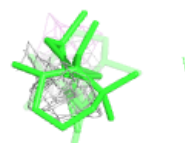
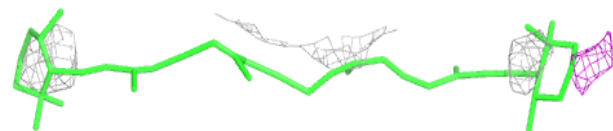
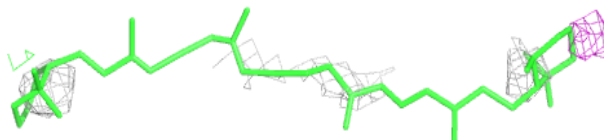


Electron density around BCR A 609:

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

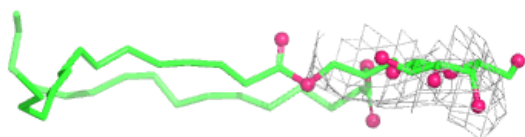
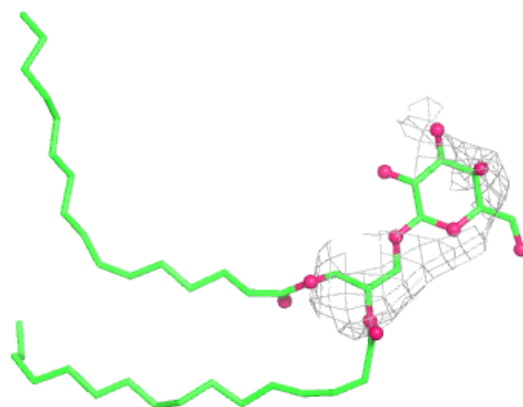
**Electron density around BCR a 608:**

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

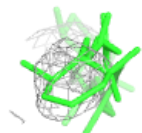
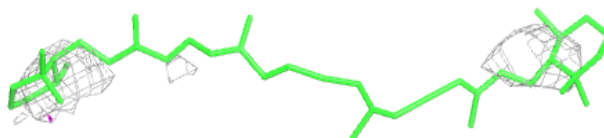


Electron density around LMG C 519:

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

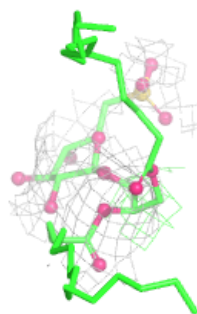
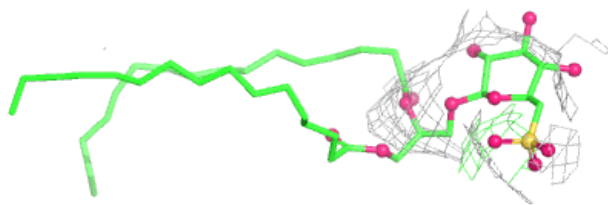
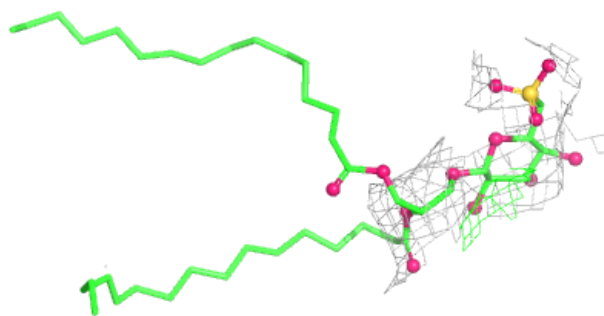
**Electron density around BCR b 620:**

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



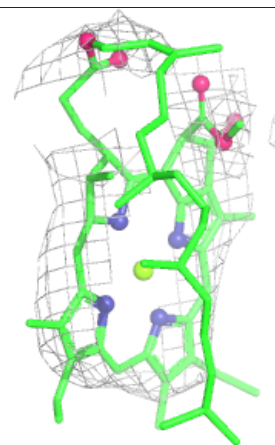
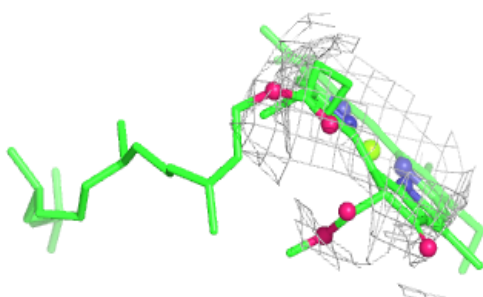
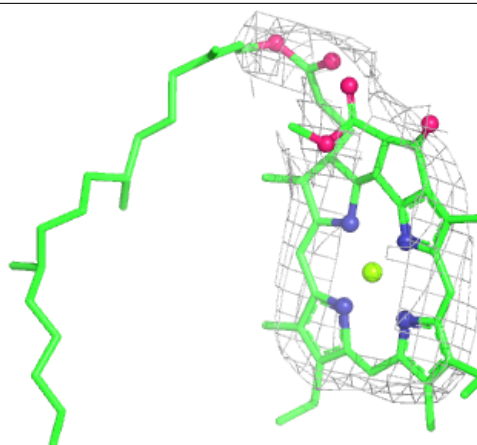
Electron density around SQD b 601:

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

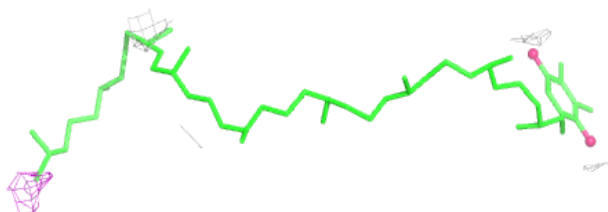


Electron density around CLA b 619:

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

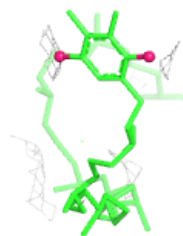
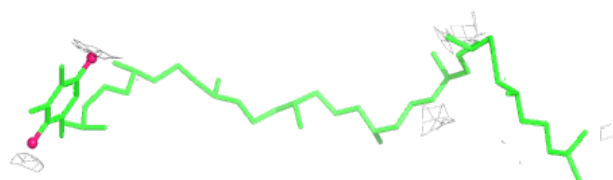
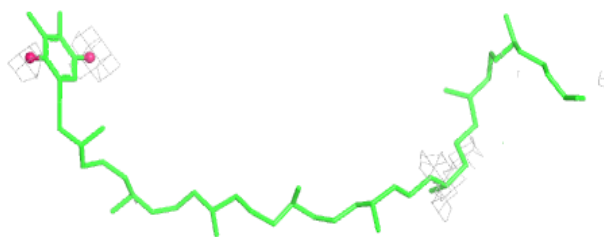
**Electron density around PL9 A 610:**

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

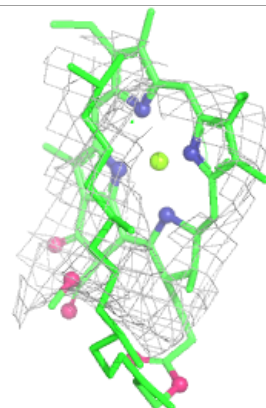
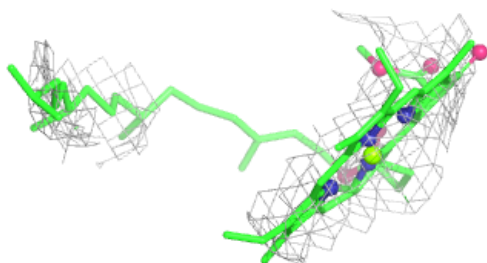
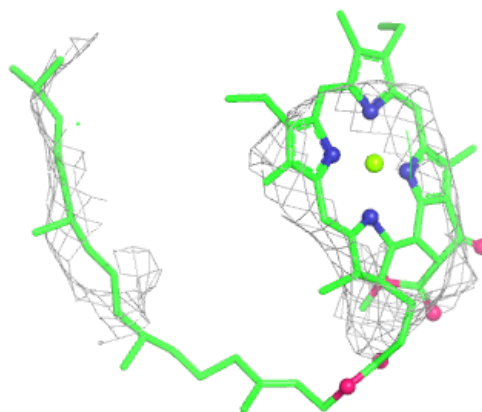


Electron density around PL9 a 609:

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

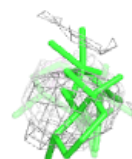
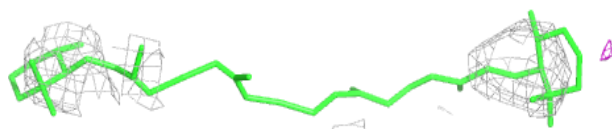
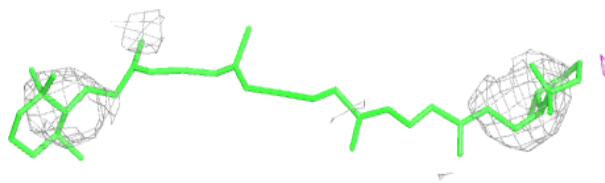
**Electron density around CLA C 507:**

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

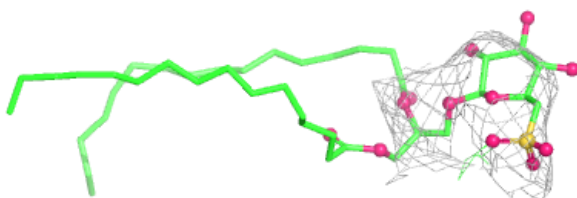
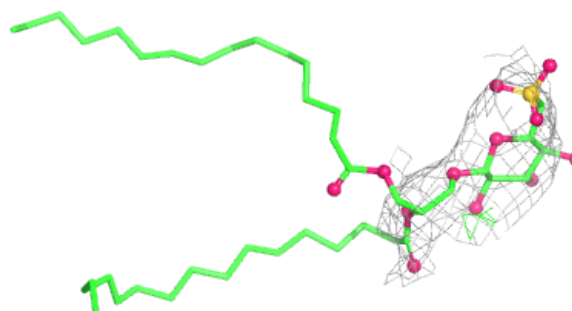


Electron density around BCR B 618:

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

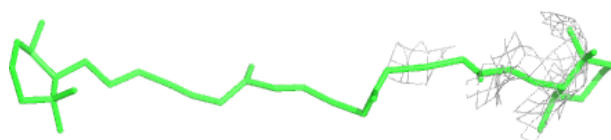
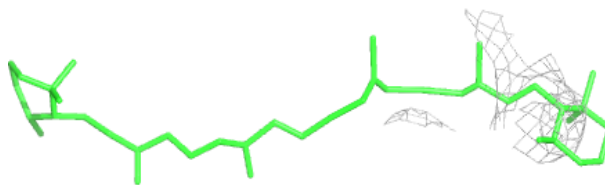
**Electron density around SQD a 612:**

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

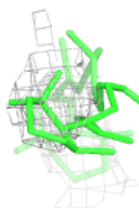
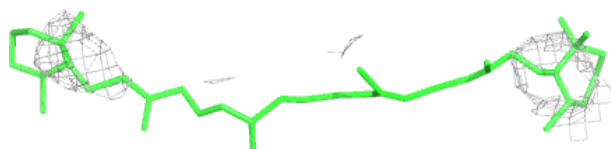
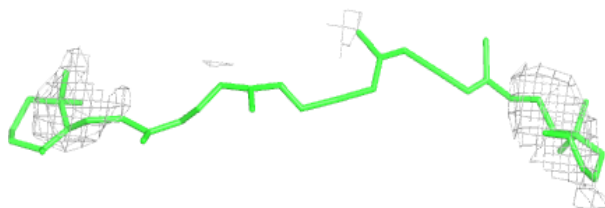


Electron density around BCR k 101:

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

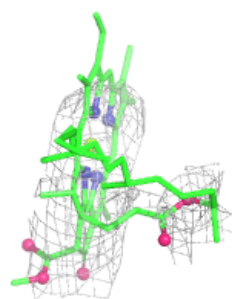
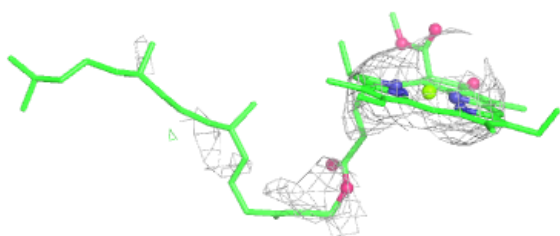
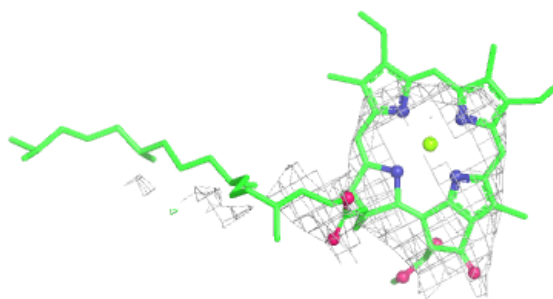
**Electron density around BCR t 101:**

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

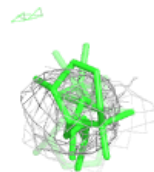
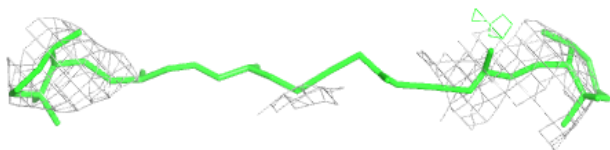
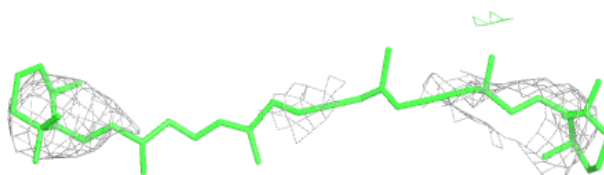


Electron density around CLA a 605:

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

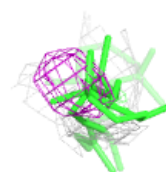
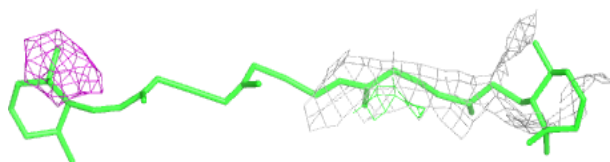
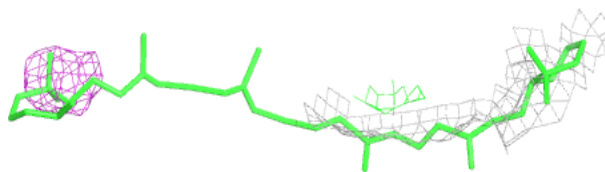
**Electron density around BCR b 621:**

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

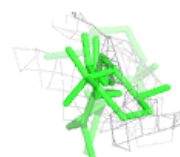
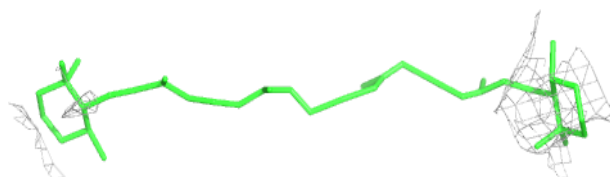
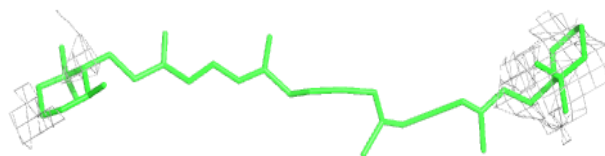


Electron density around BCR H 101:

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

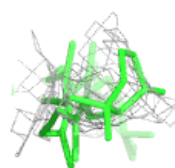
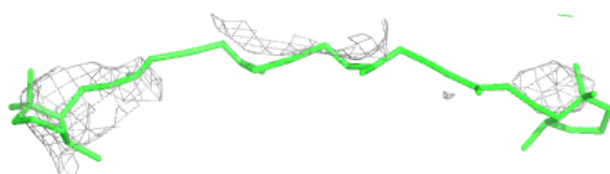
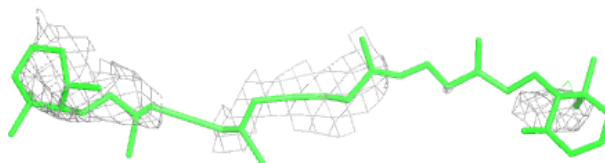
**Electron density around BCR c 516:**

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

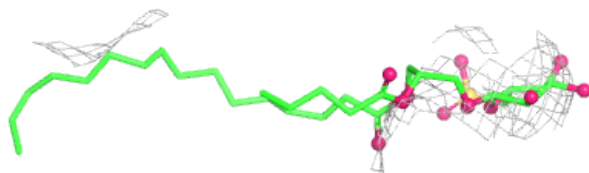
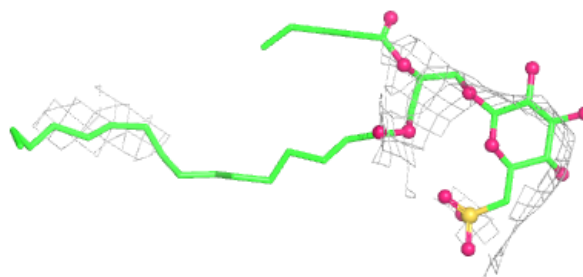


Electron density around BCR f 101:

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

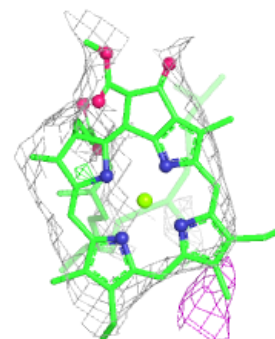
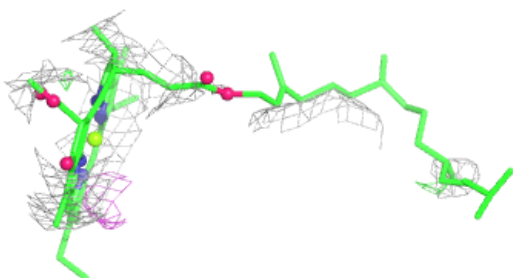
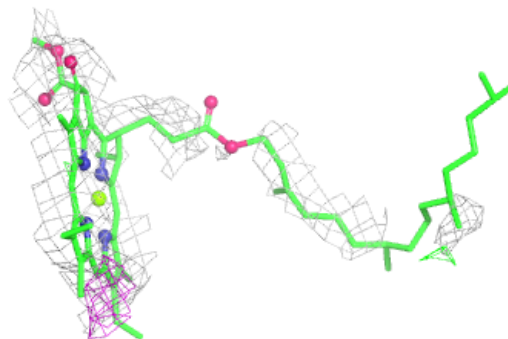
**Electron density around SQD X 101:**

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

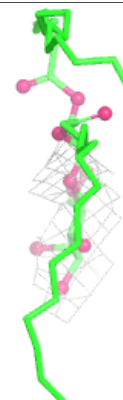
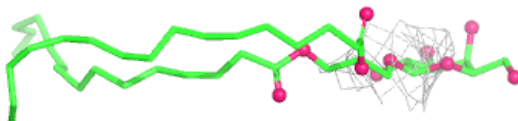
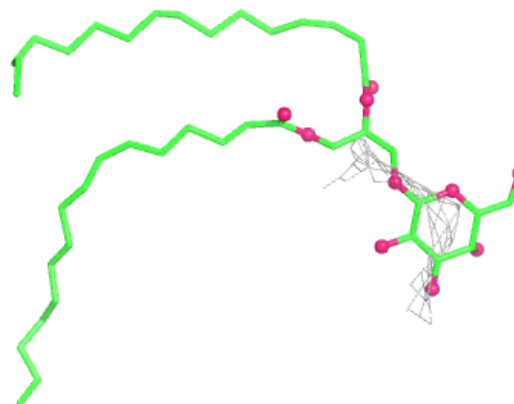


Electron density around CLA D 404:

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

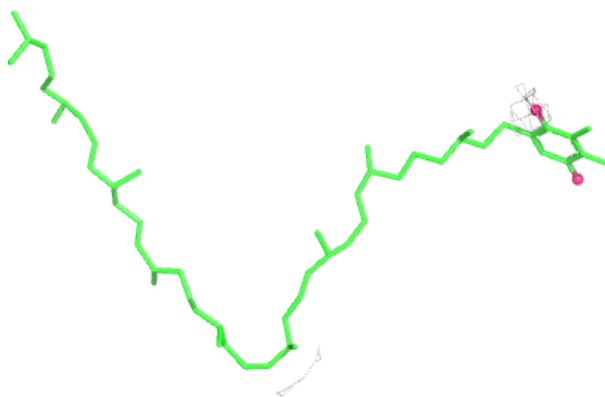
**Electron density around LMG c 520:**

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

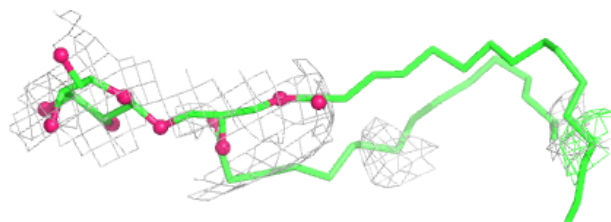
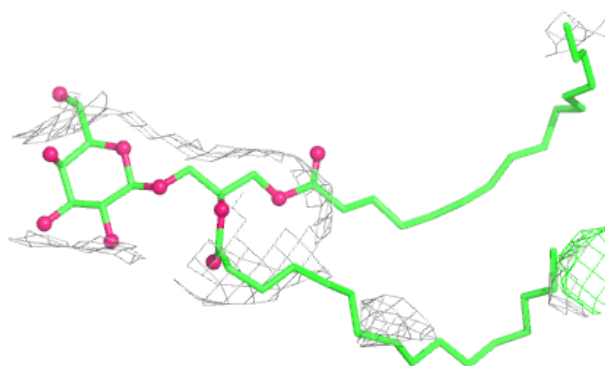


Electron density around PL9 d 404:

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

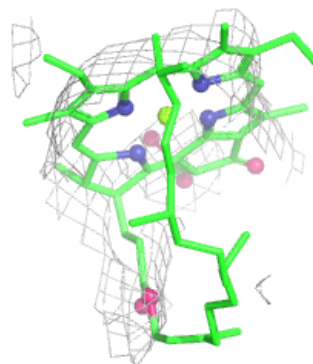
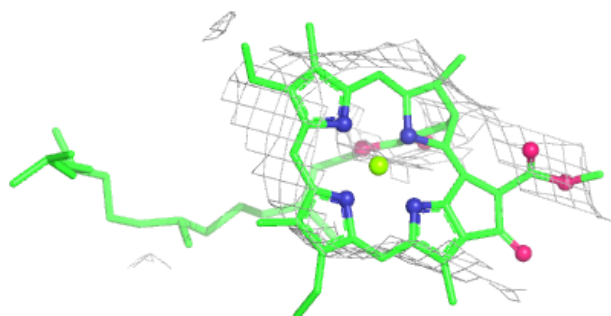
**Electron density around LMG j 101:**

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

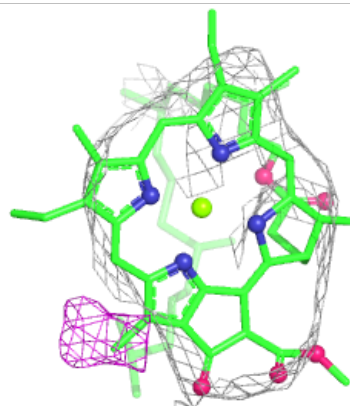
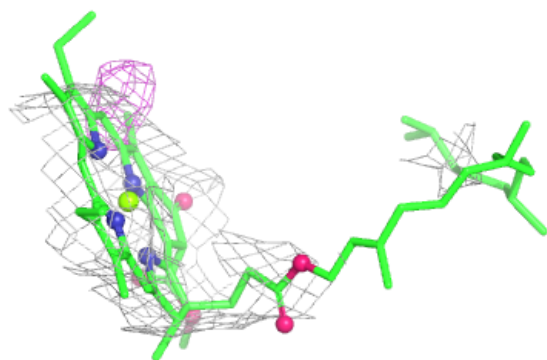
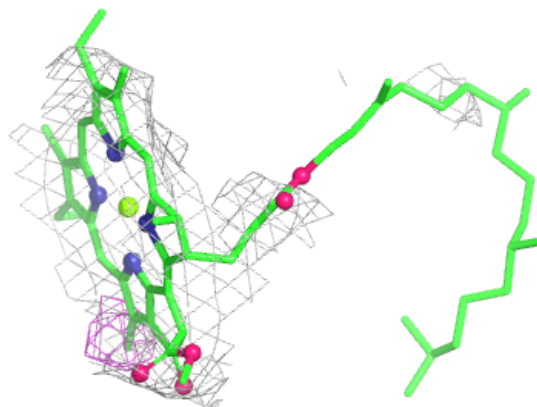


Electron density around CLA c 514:

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

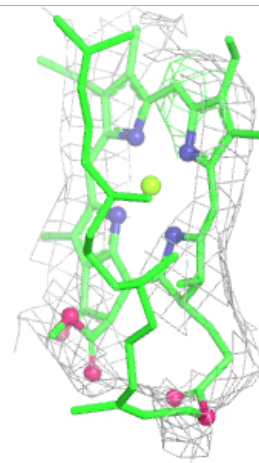
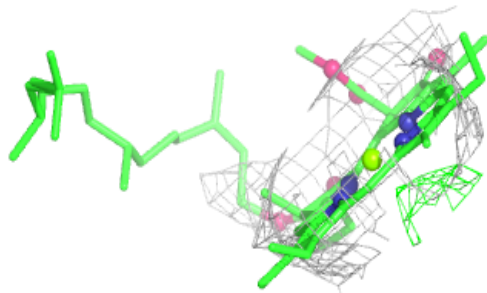
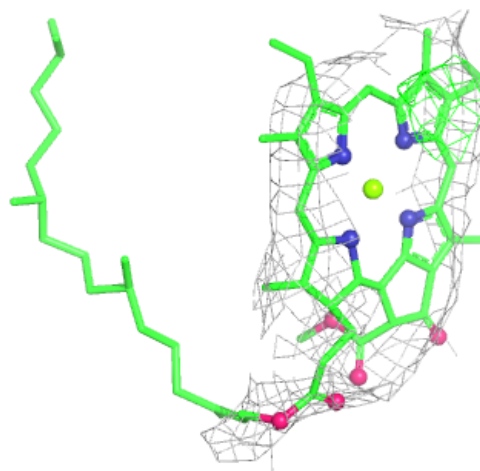
**Electron density around CLA B 607 (B):**

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



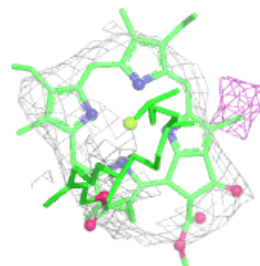
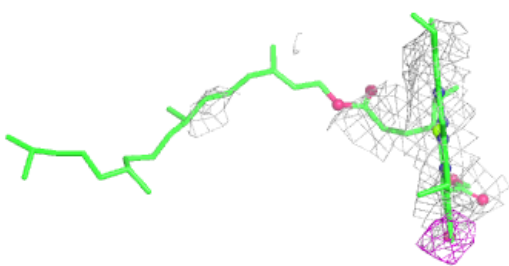
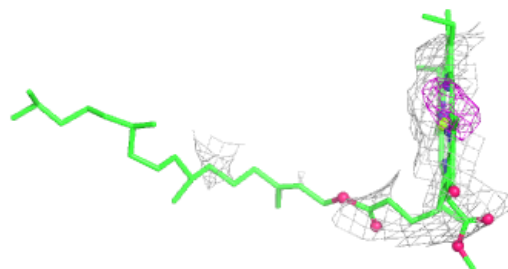
Electron density around CLA B 617:

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

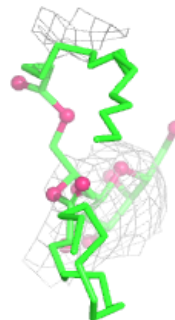
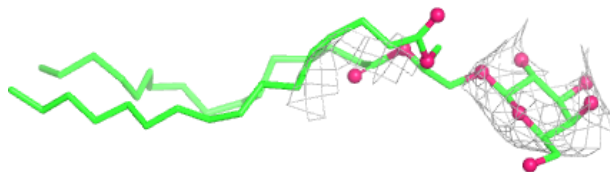


Electron density around CLA B 607 (A):

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

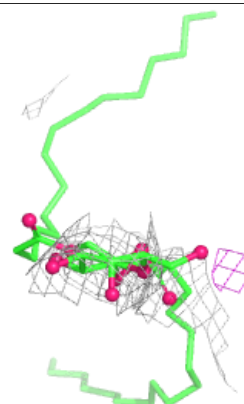
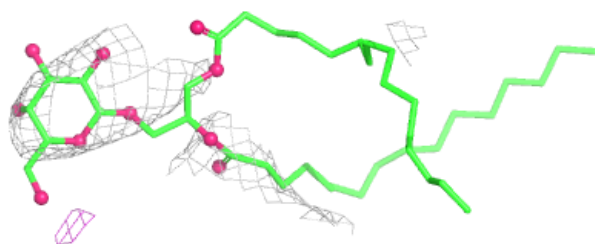
**Electron density around LMG A 612:**

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

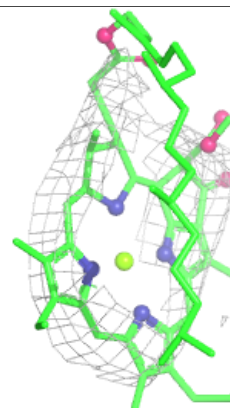
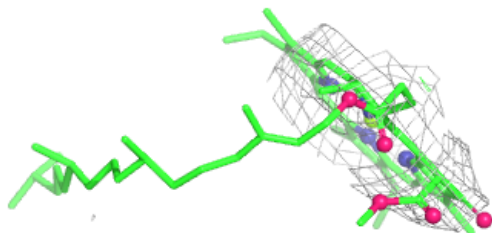
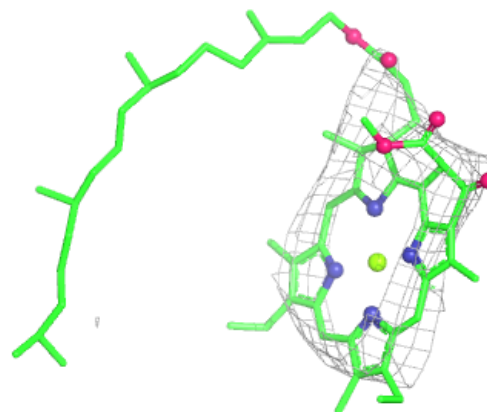


Electron density around LMG B 621:

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

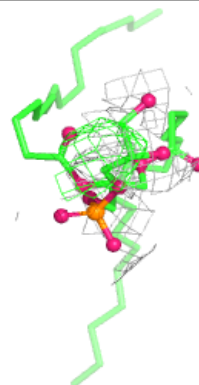
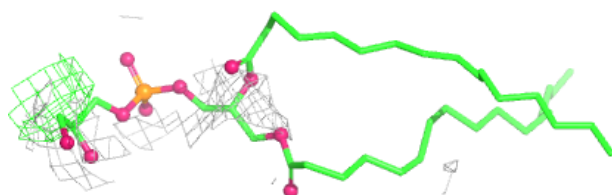
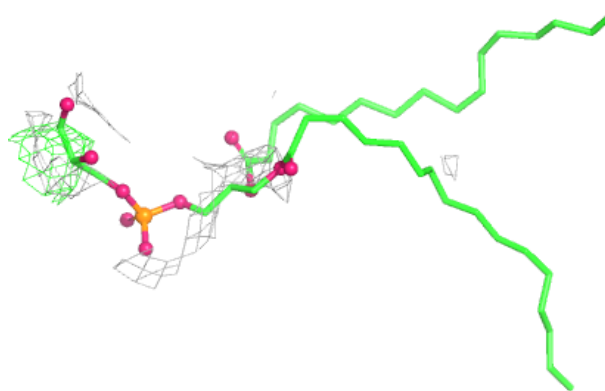
**Electron density around CLA c 508:**

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



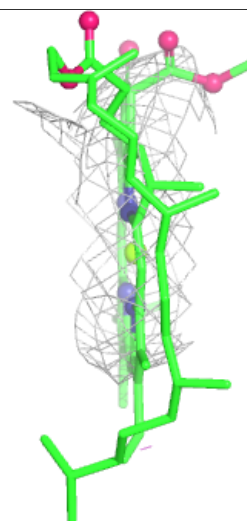
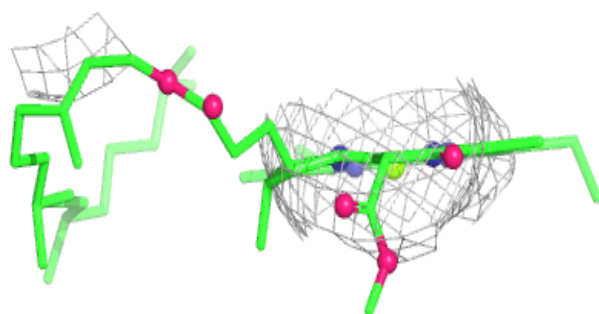
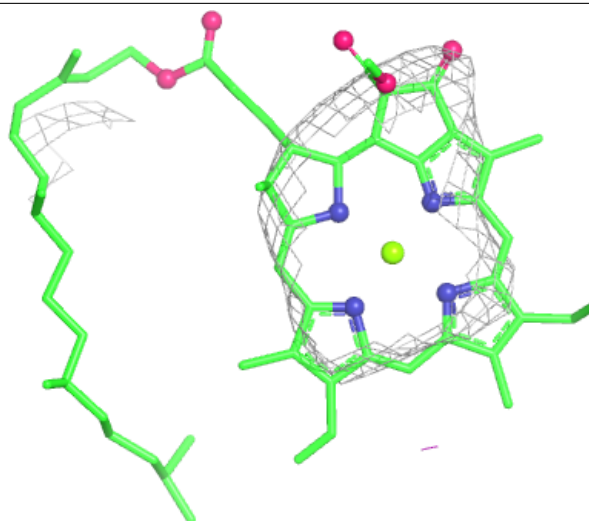
Electron density around LHG D 407:

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



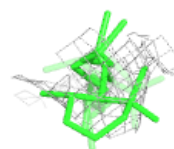
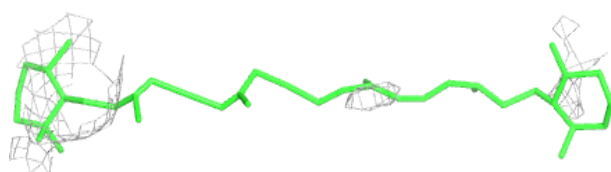
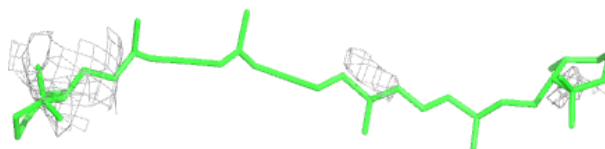
Electron density around CLA c 513:

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

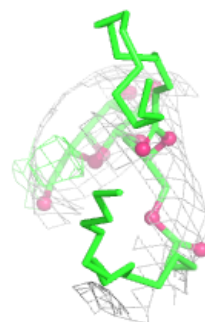
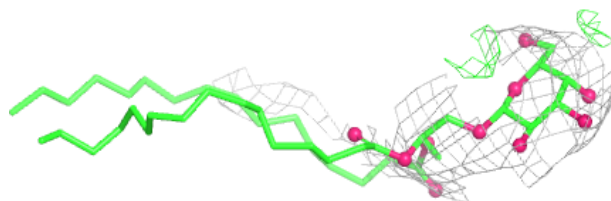
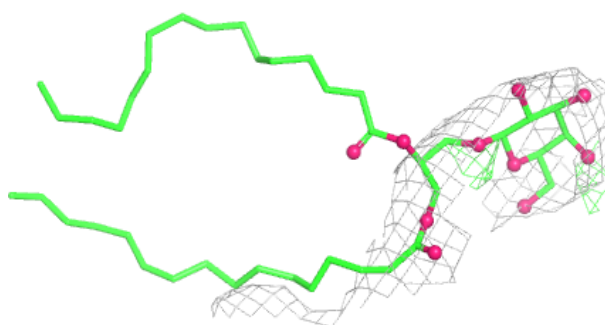


Electron density around BCR c 515:

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

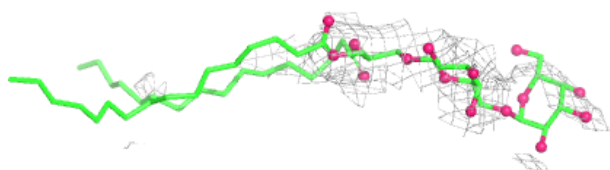
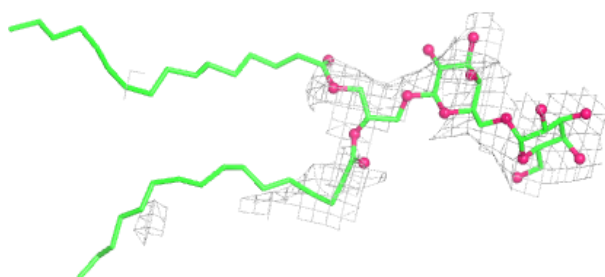
**Electron density around LMG a 611:**

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

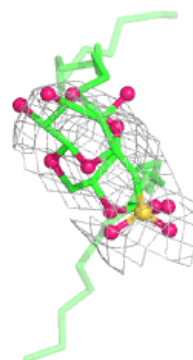
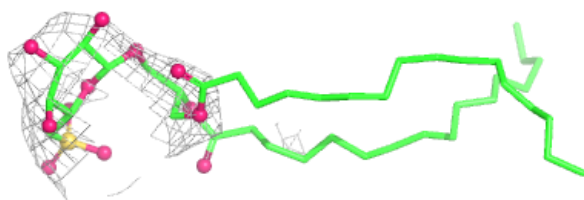
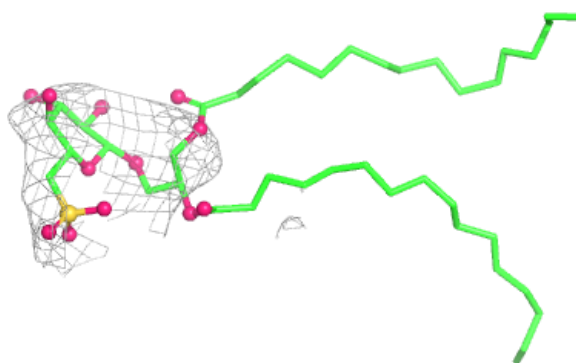


Electron density around DGD C 518:

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

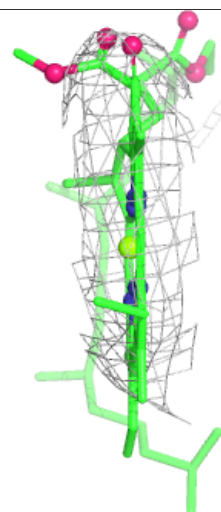
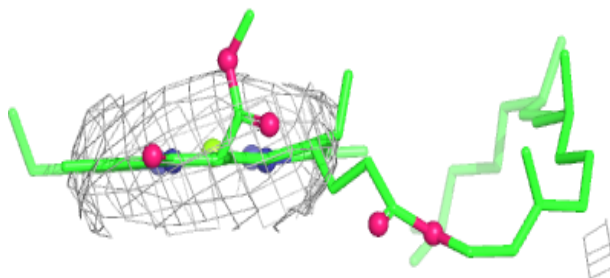
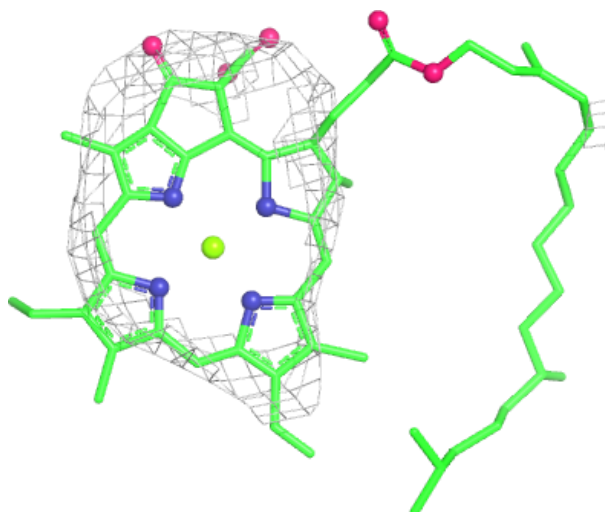
**Electron density around SQD B 623:**

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



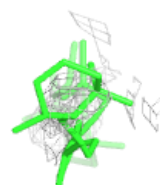
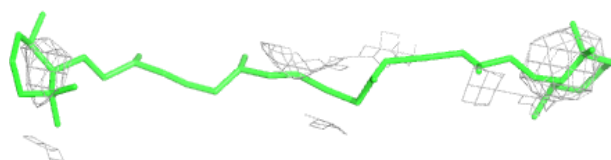
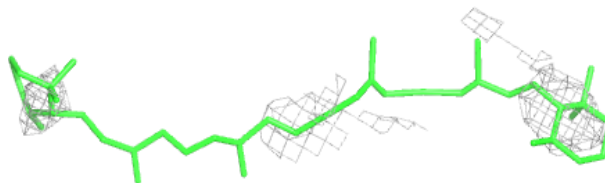
Electron density around CLA C 512:

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

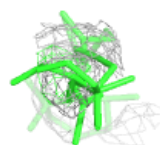
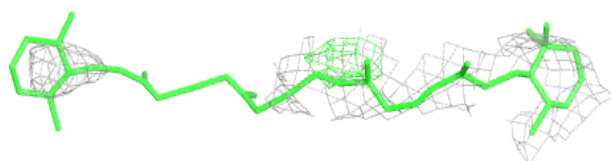
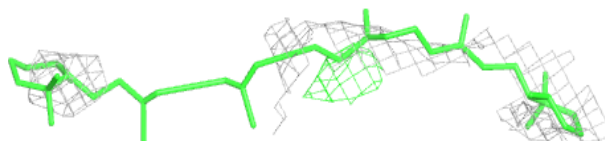


Electron density around BCR K 101:

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

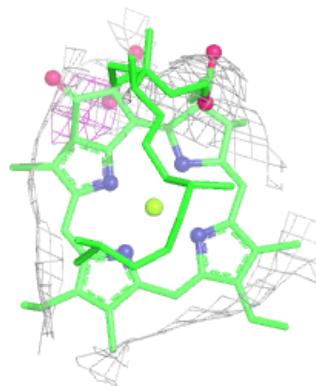
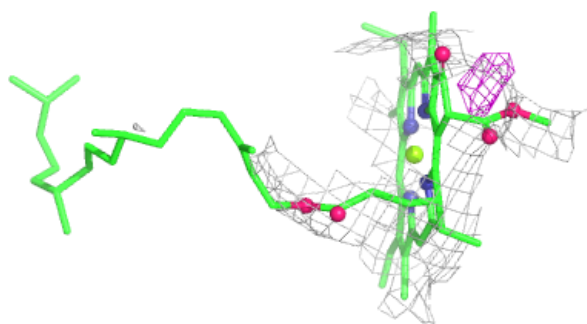
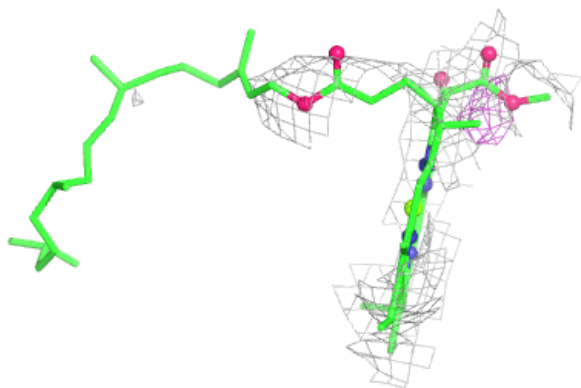
**Electron density around BCR h 101:**

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

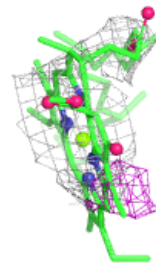
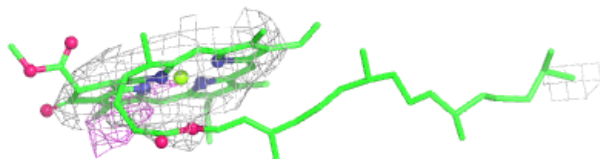
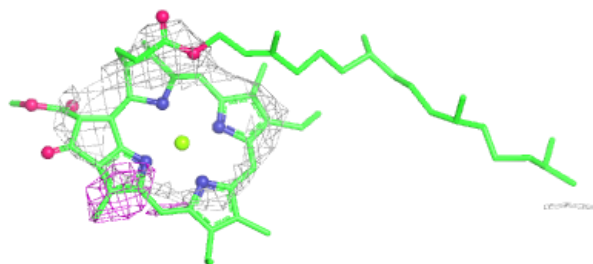


Electron density around CLA C 506:

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

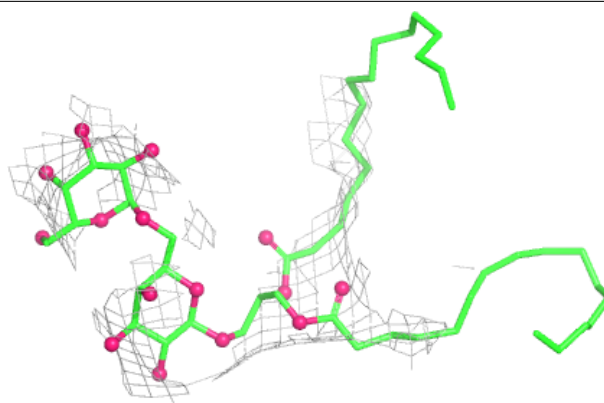
**Electron density around CLA c 502:**

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

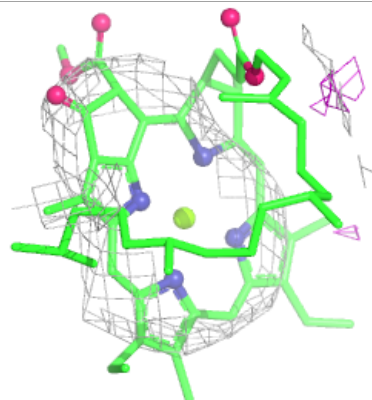
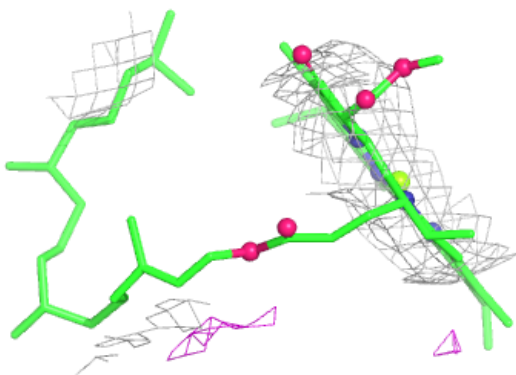
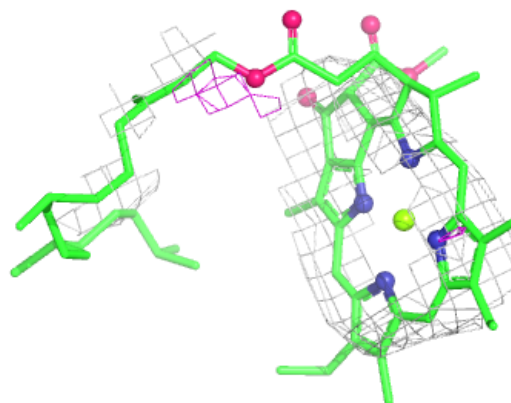


Electron density around DGD C 517:

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

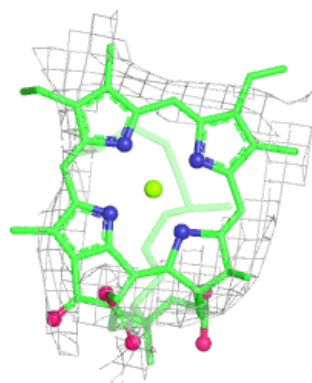
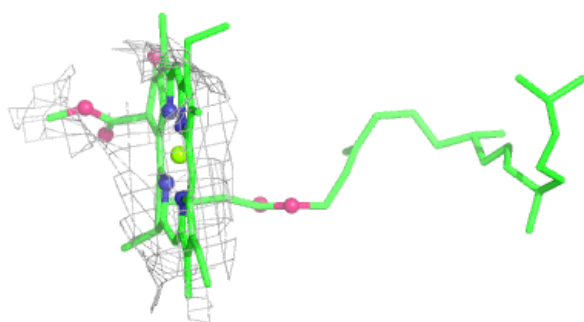
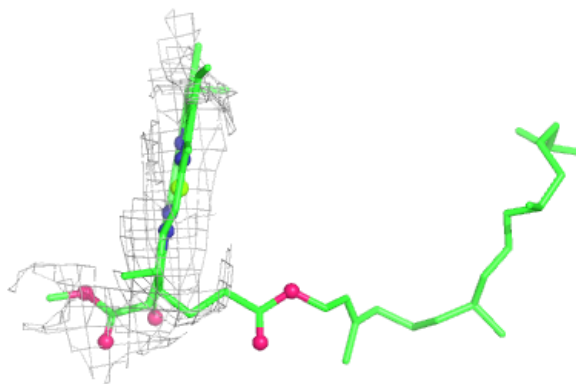
**Electron density around CLA c 504:**

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



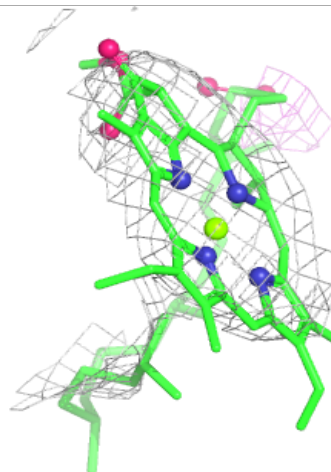
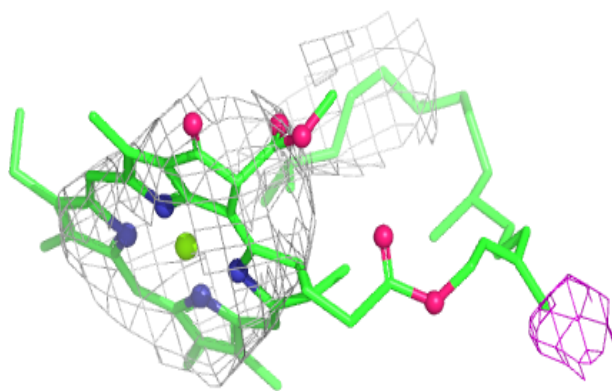
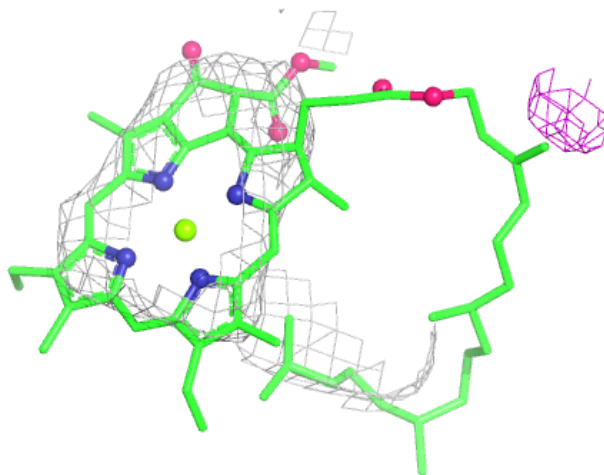
Electron density around CLA c 507:

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



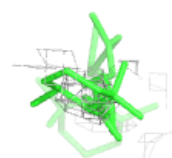
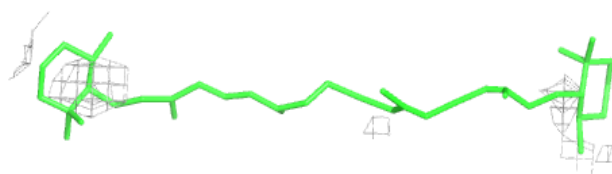
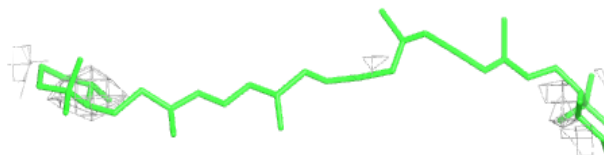
Electron density around CLA B 616:

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

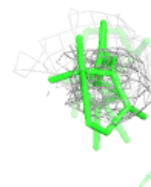
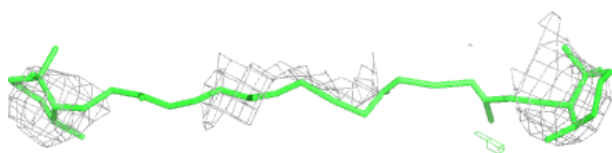
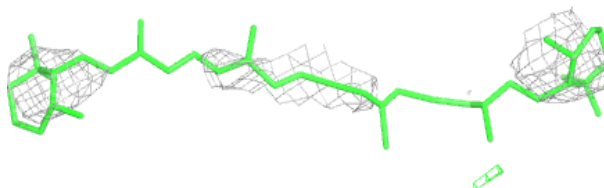


Electron density around BCR C 515:

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

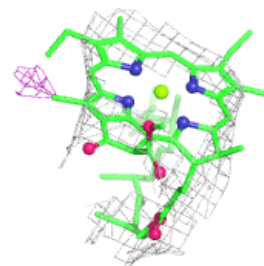
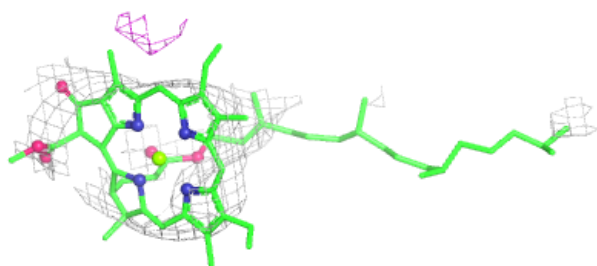
**Electron density around BCR B 619:**

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



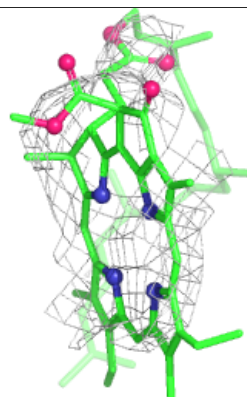
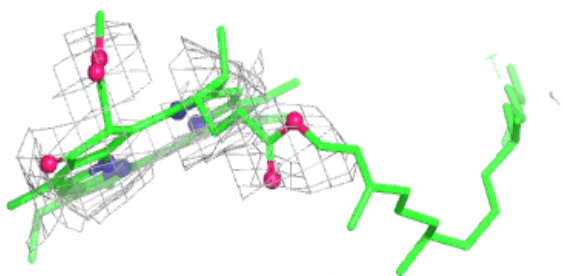
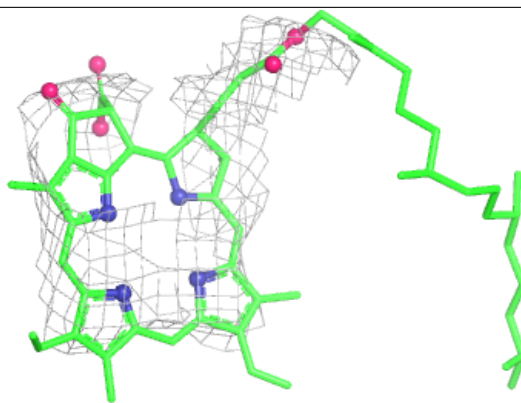
Electron density around CLA C 504:

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

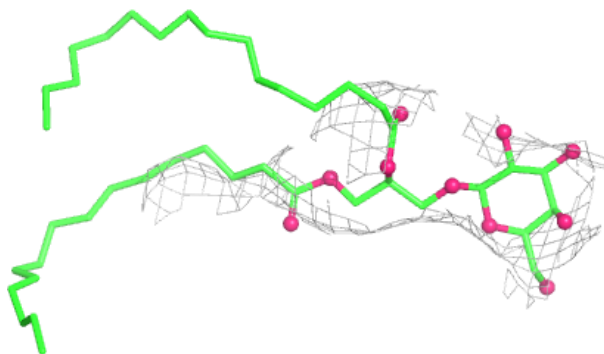


Electron density around PHO d 401:

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

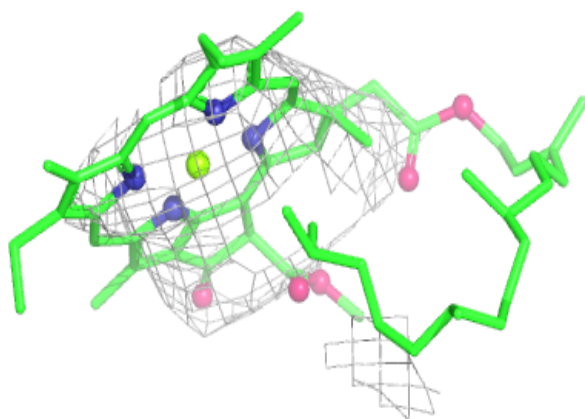
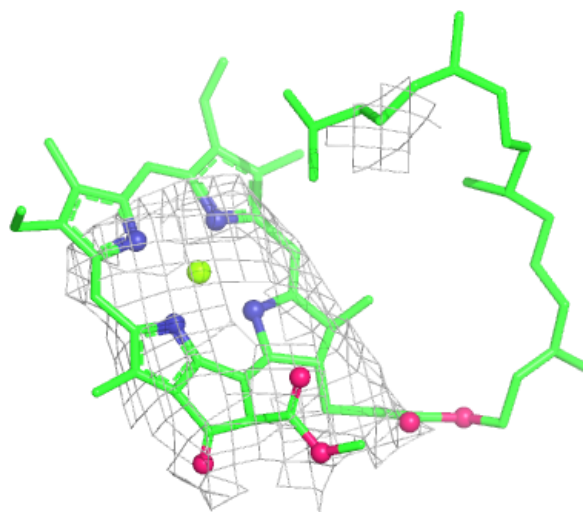
**Electron density around LMG J 101:**

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



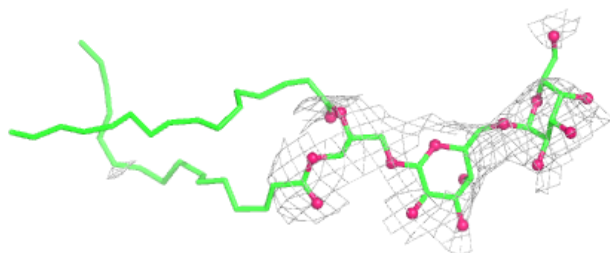
Electron density around CLA b 618:

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

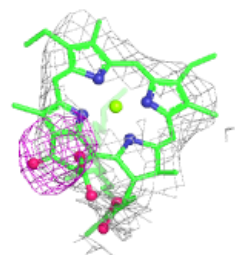
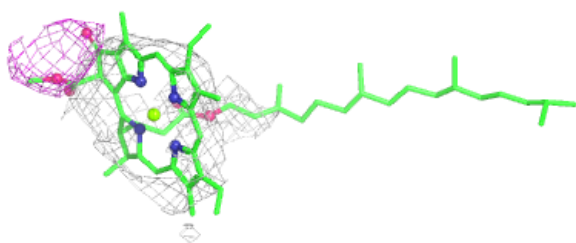
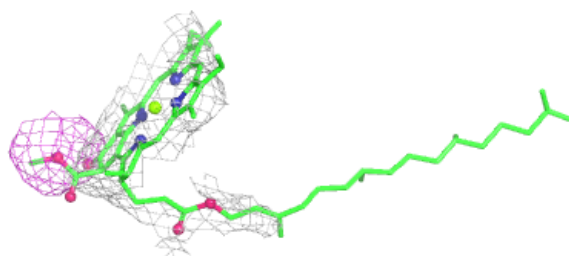


Electron density around DGD c 517:

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

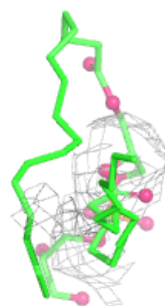
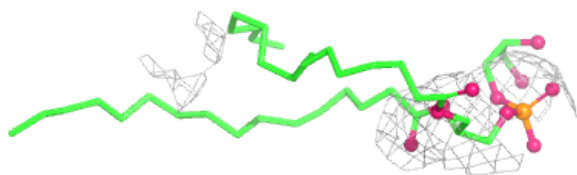
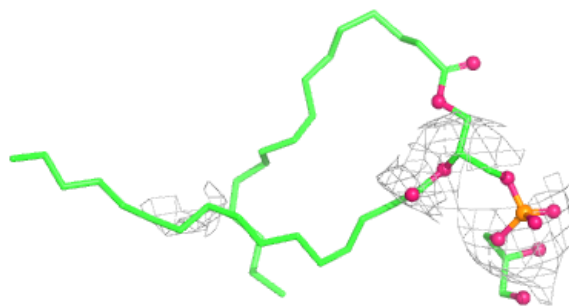
**Electron density around CLA B 608:**

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



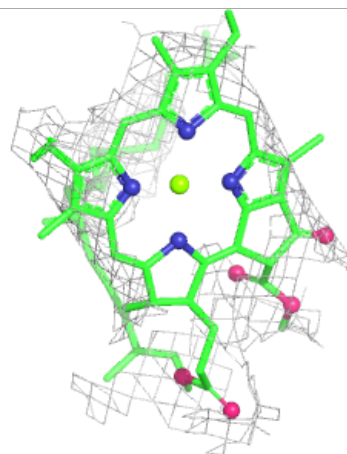
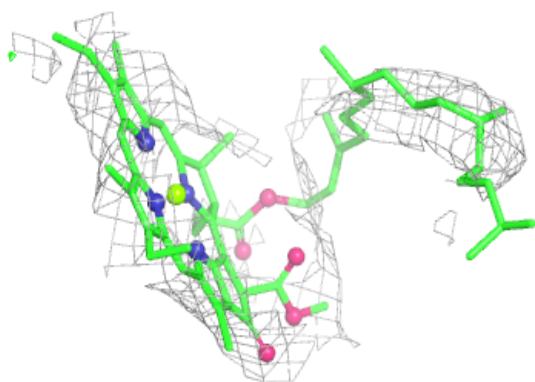
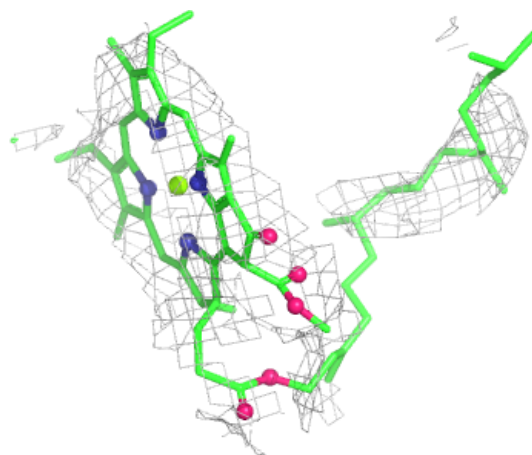
Electron density around LHG D 408:

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



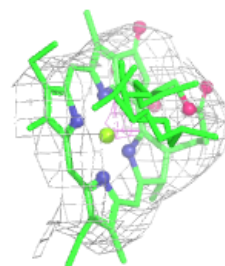
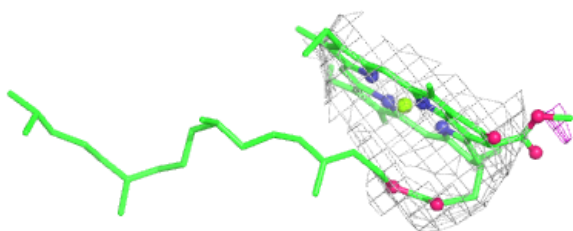
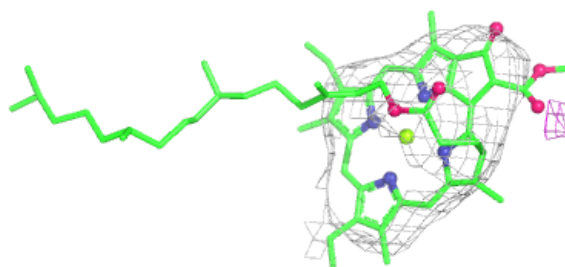
Electron density around CLA b 616:

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

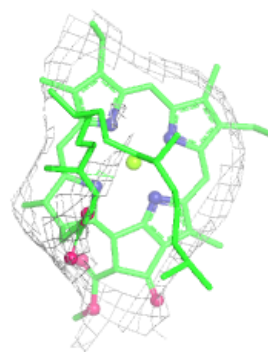
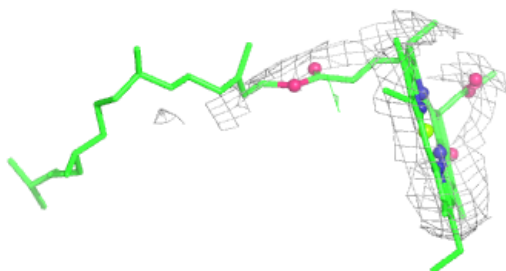
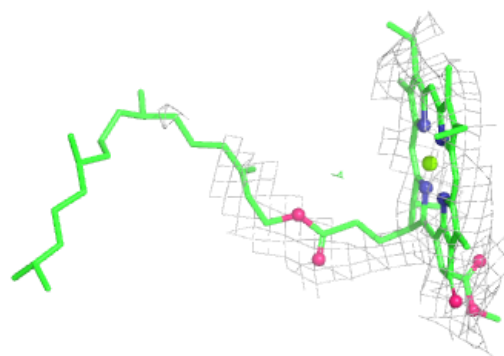


Electron density around CLA B 615:

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

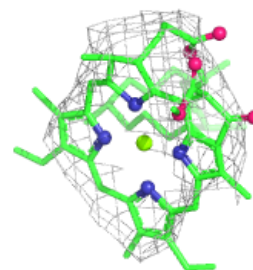
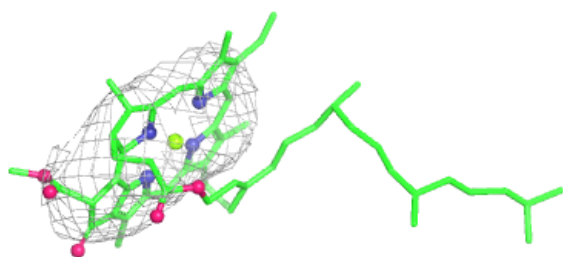
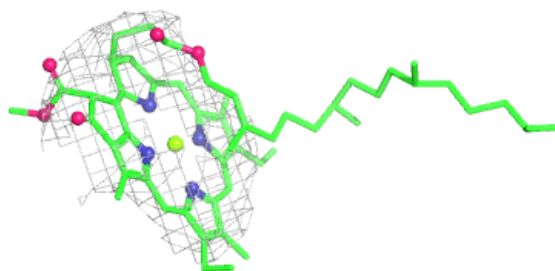
**Electron density around CLA d 403:**

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



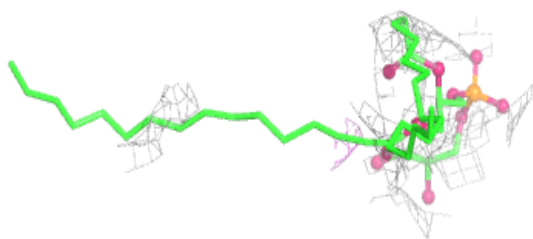
Electron density around CLA C 505:

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



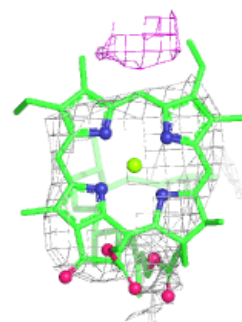
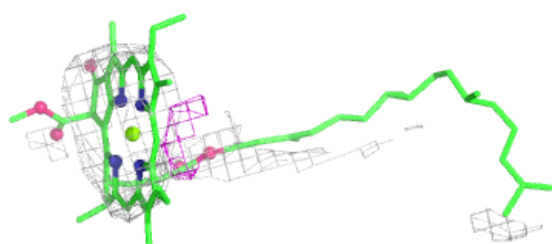
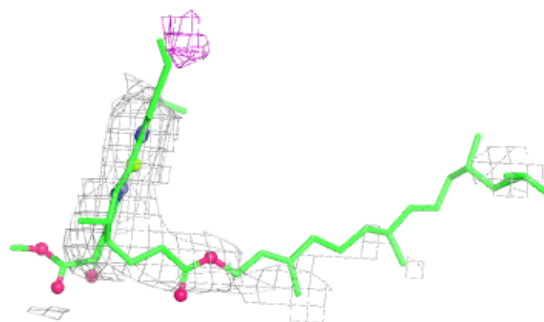
Electron density around LHG 1 101:

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

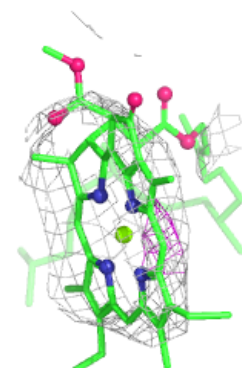
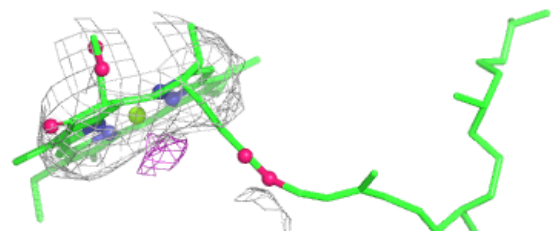


Electron density around CLA B 606:

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

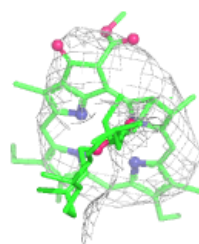
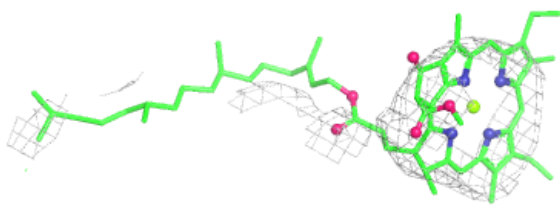
**Electron density around CLA a 607:**

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

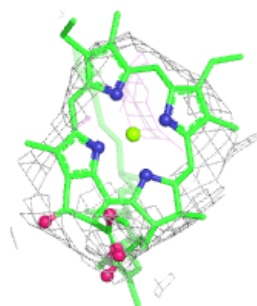
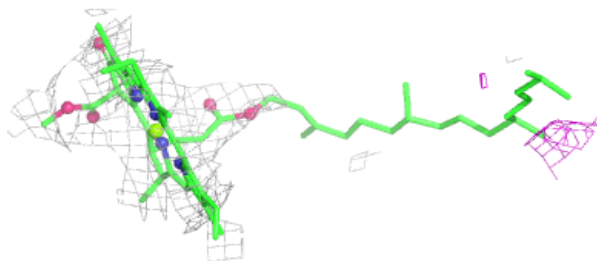
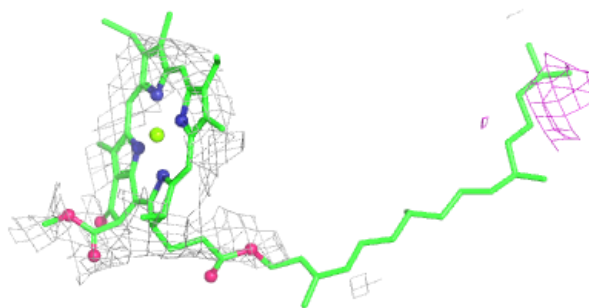


Electron density around CLA c 503:

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

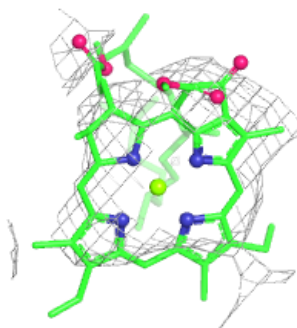
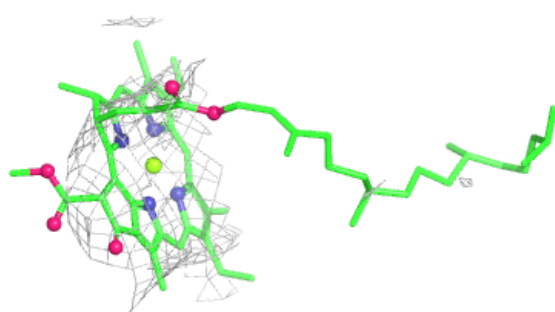
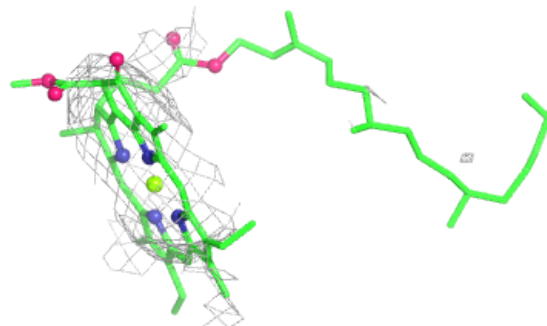
**Electron density around CLA B 610:**

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

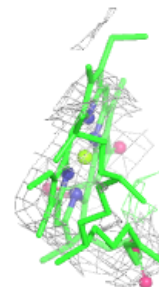
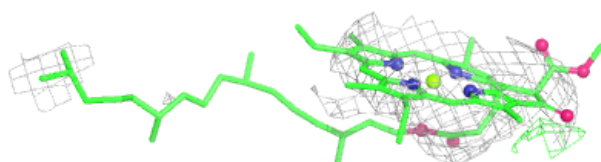
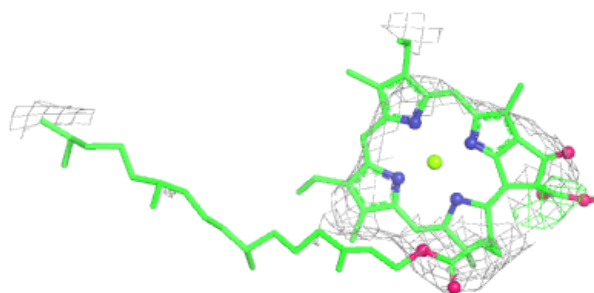


Electron density around CLA C 508:

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

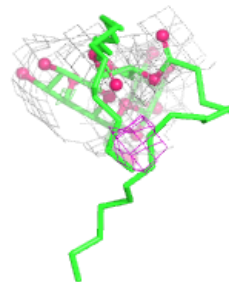
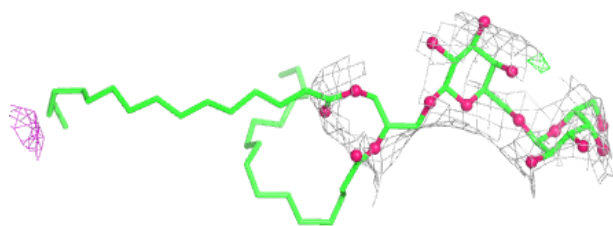
**Electron density around CLA C 501:**

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

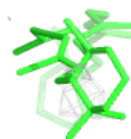
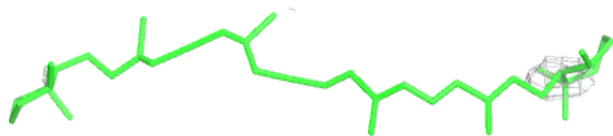
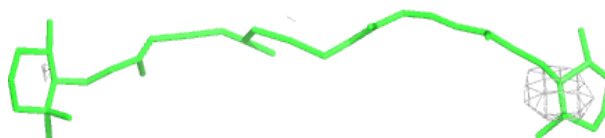


Electron density around DGD h 102:

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

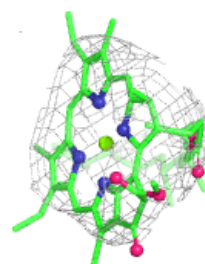
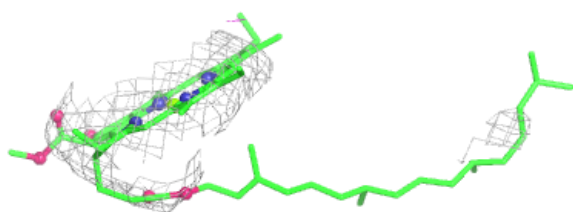
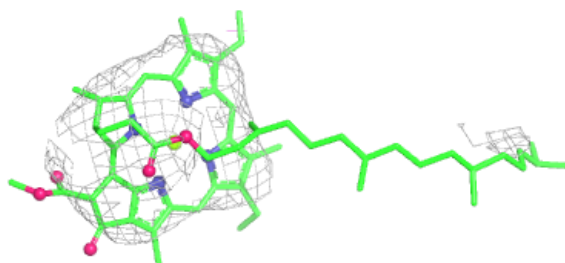
**Electron density around BCR C 521:**

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

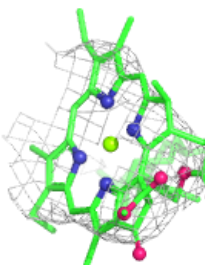
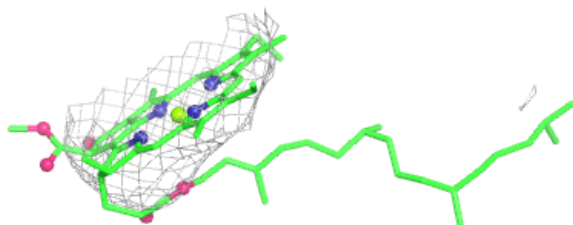
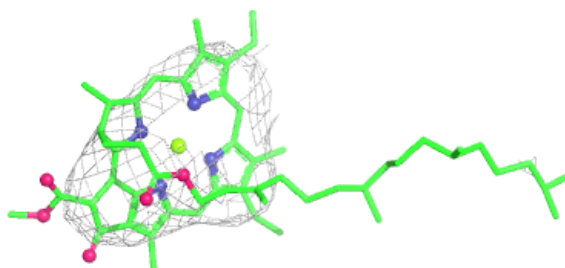


Electron density around CLA b 611:

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

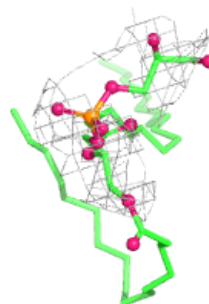
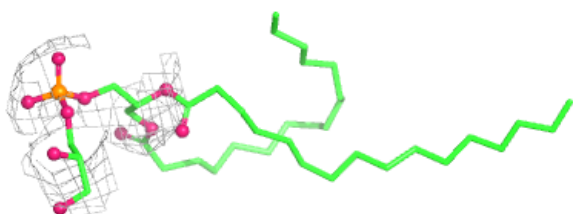
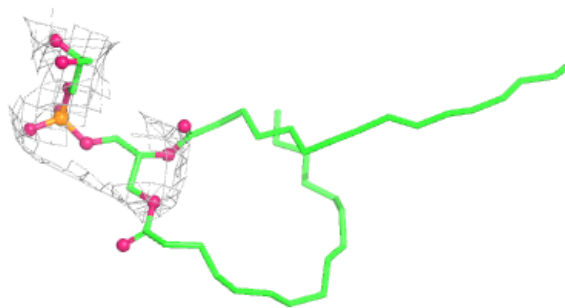
**Electron density around CLA b 617:**

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

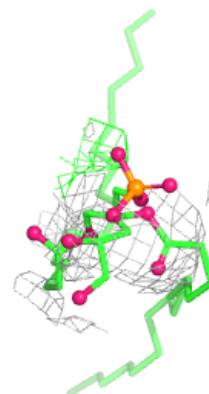
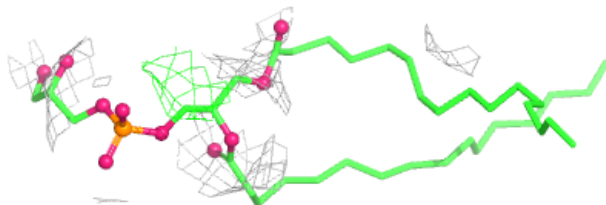
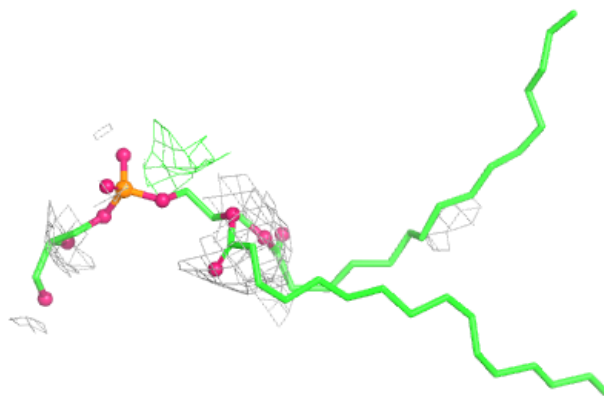


Electron density around LHG b 624:

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

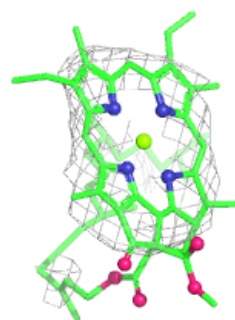
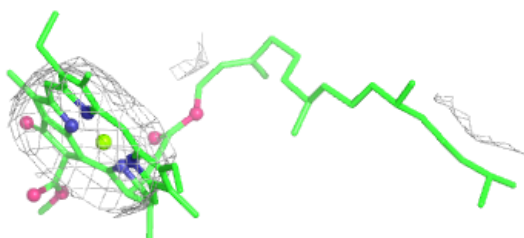
**Electron density around LHG d 406:**

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

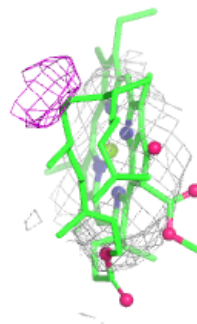
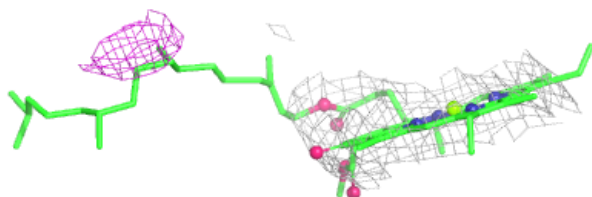
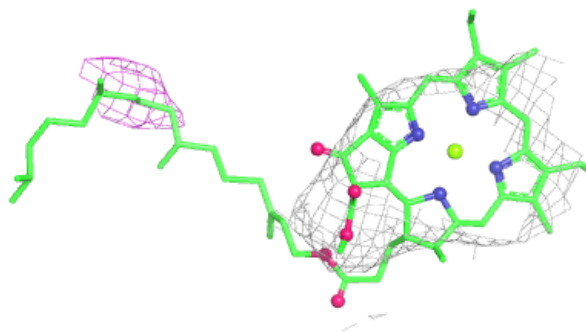


Electron density around CLA C 511:

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

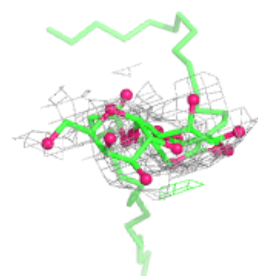
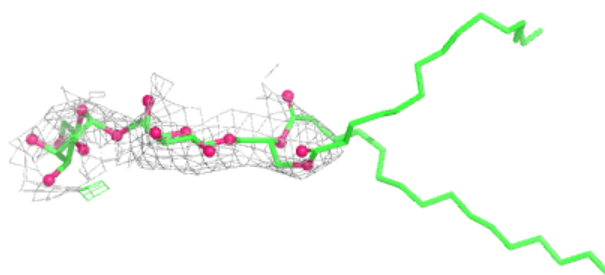
**Electron density around CLA B 603:**

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

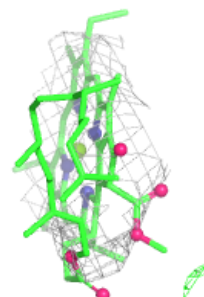
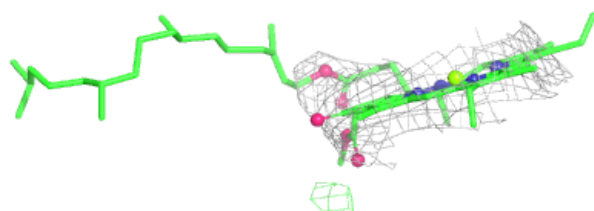
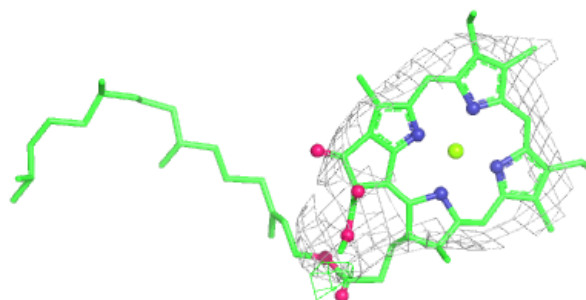


Electron density around DGD C 516:

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

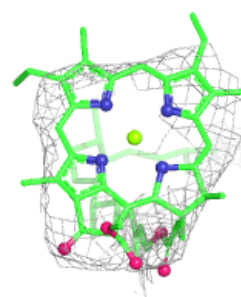
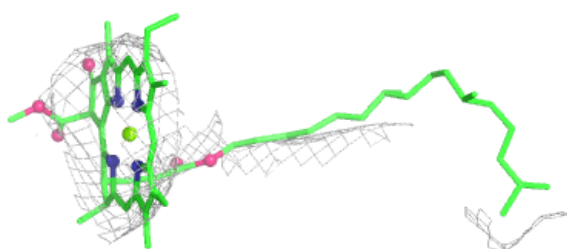
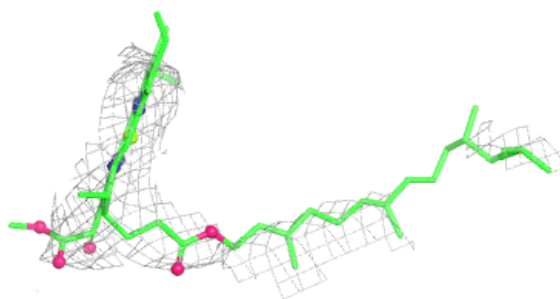
**Electron density around CLA b 605:**

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

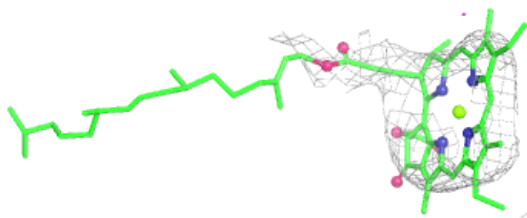
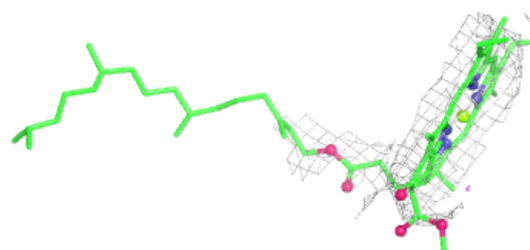


Electron density around CLA b 608:

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

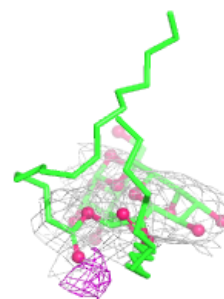
**Electron density around CLA B 605:**

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

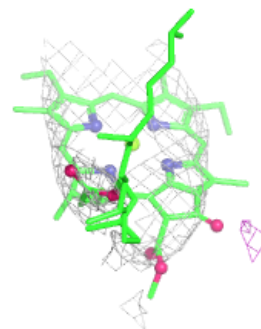
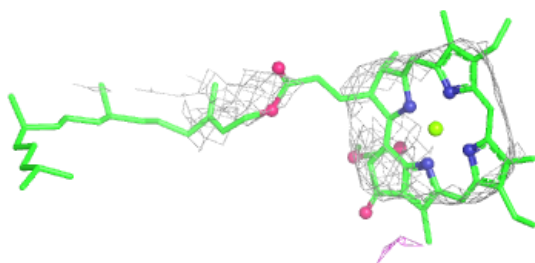
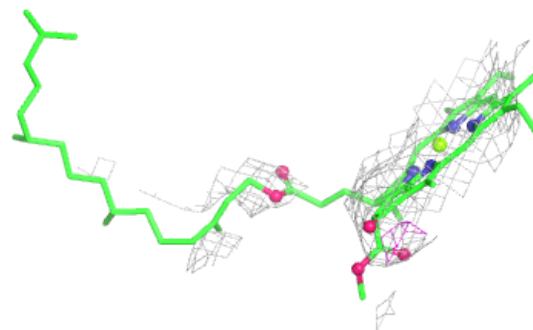


Electron density around DGD H 102:

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

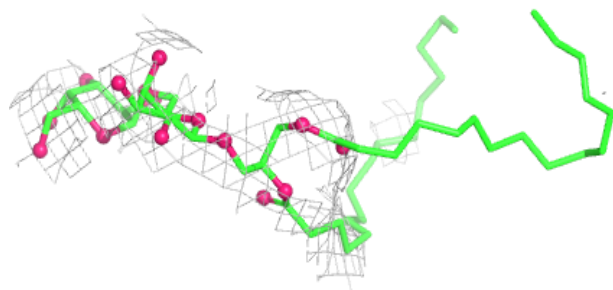
**Electron density around CLA D 403:**

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

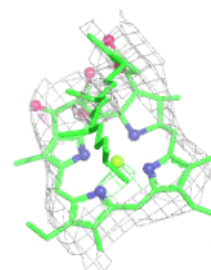
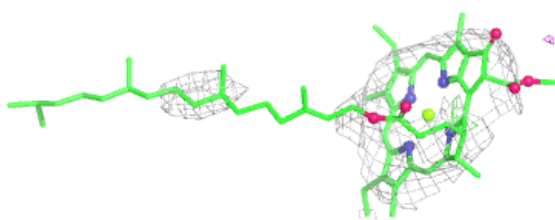
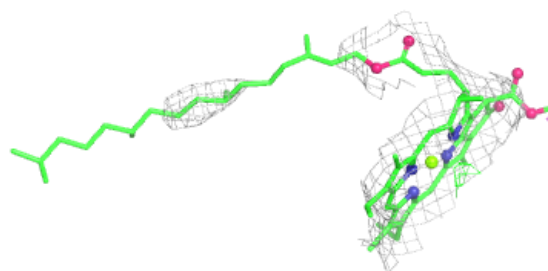


Electron density around DGD c 518:

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

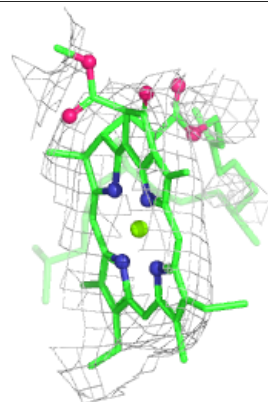
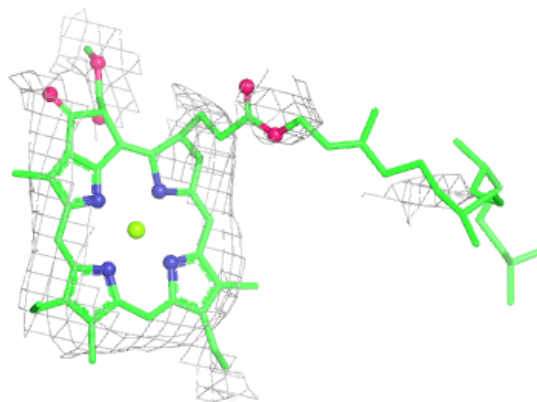
**Electron density around CLA b 610:**

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

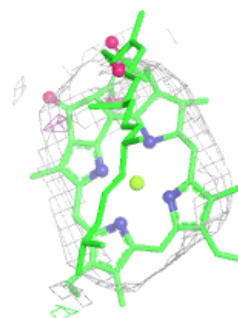
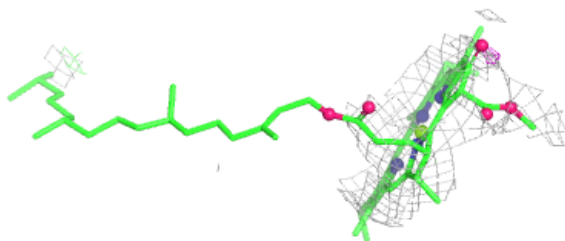
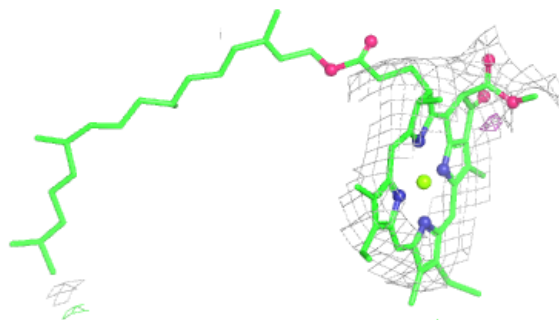


Electron density around CLA A 608:

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

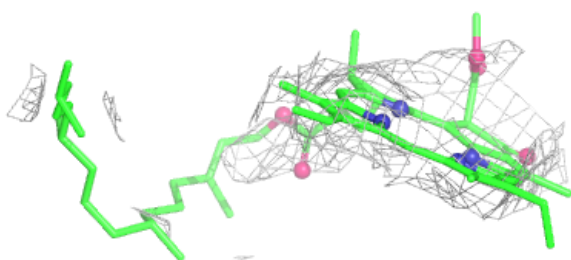
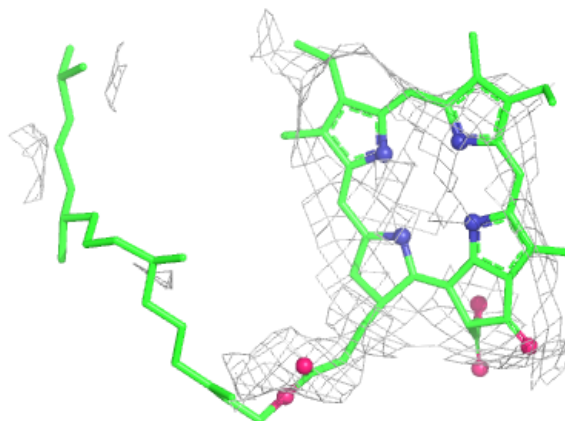
**Electron density around CLA b 612:**

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

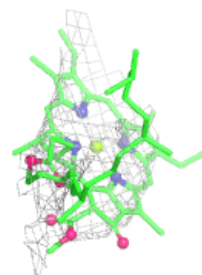
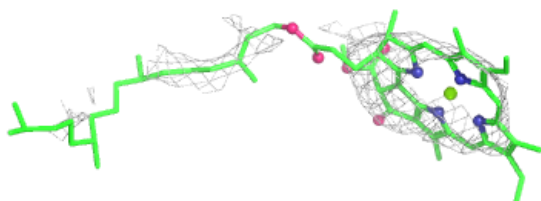
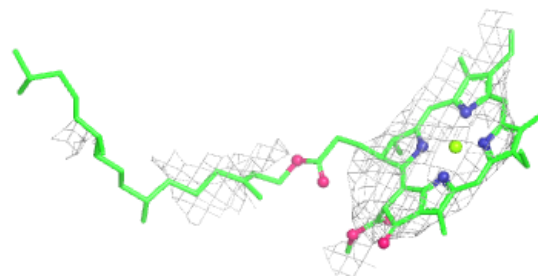


Electron density around PHO D 401:

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

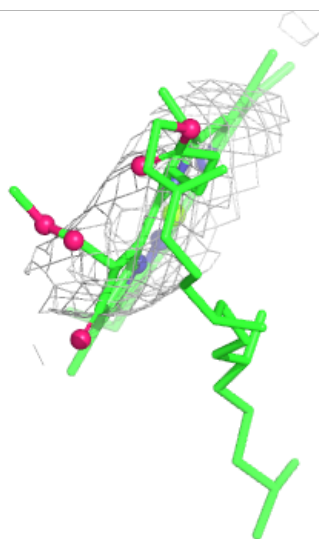
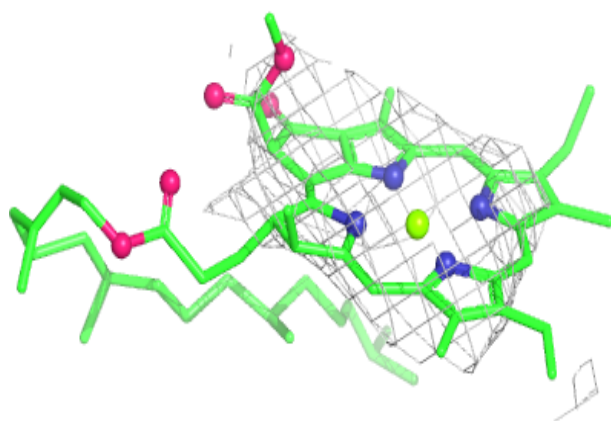
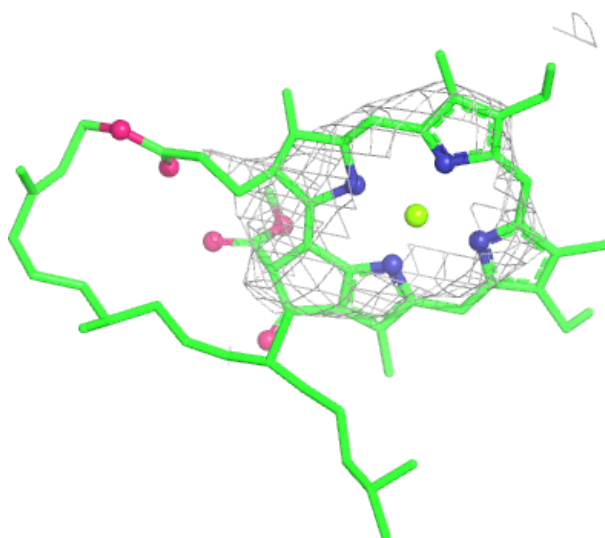
**Electron density around CLA a 604:**

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



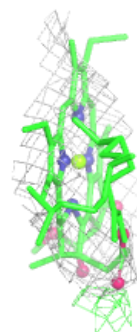
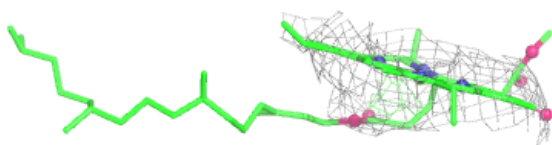
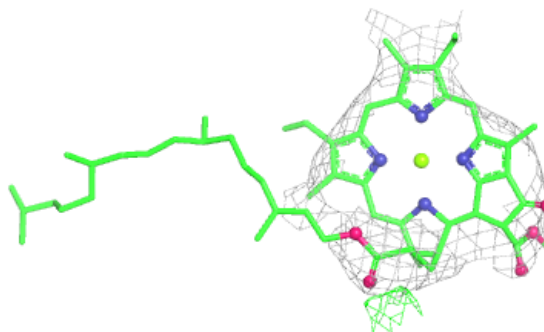
Electron density around CLA C 509:

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

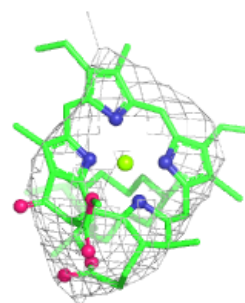
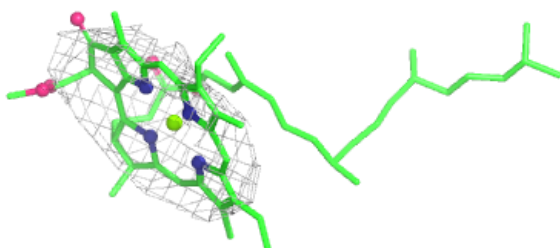
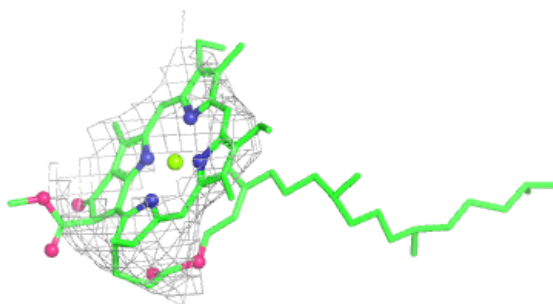


Electron density around CLA b 606:

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

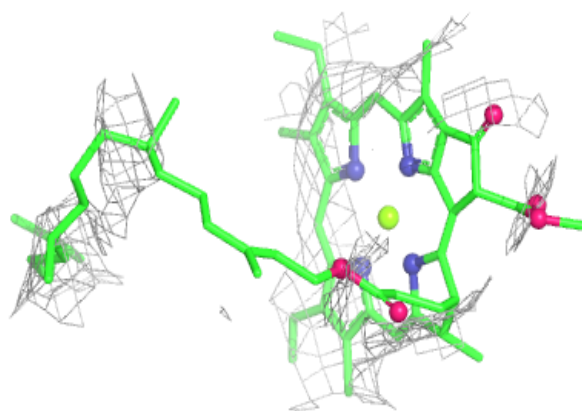
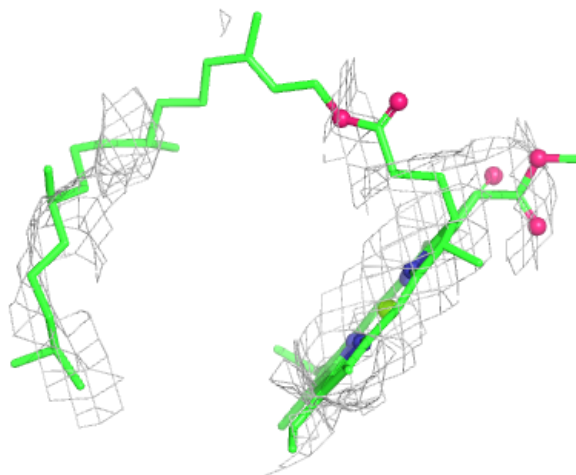
**Electron density around CLA c 506:**

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



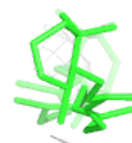
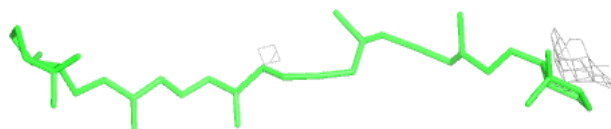
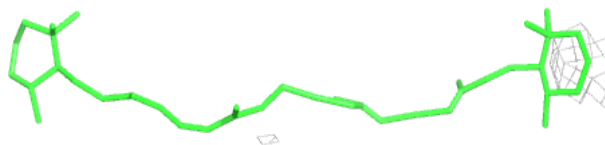
Electron density around CLA b 614:

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



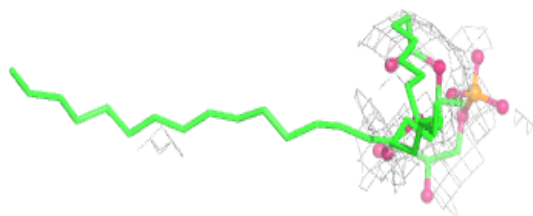
Electron density around BCR c 522:

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



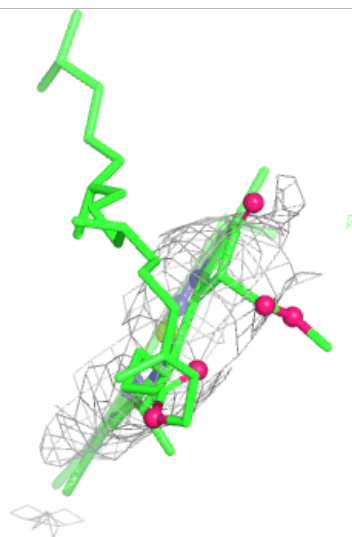
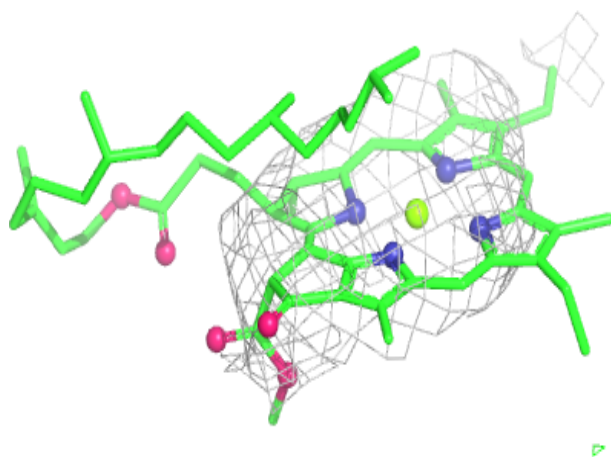
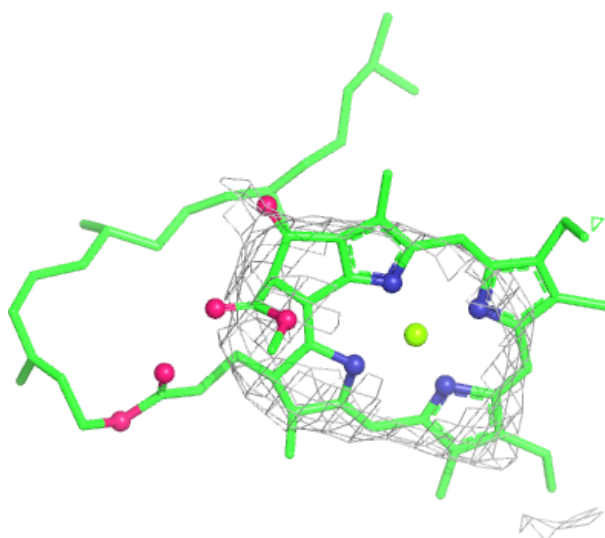
Electron density around LHG L 101:

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



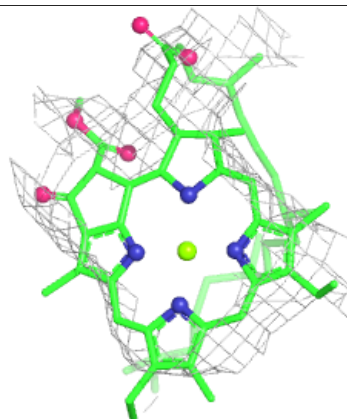
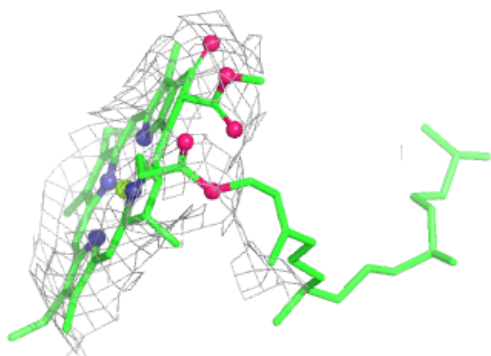
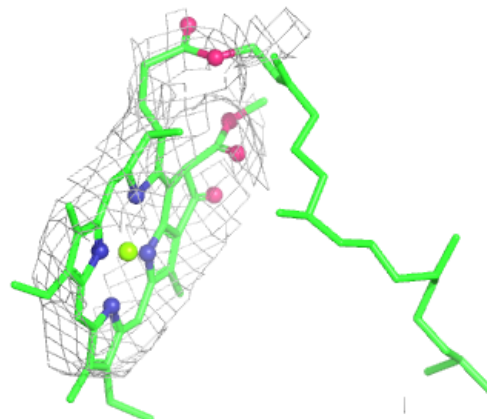
Electron density around CLA c 510:

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

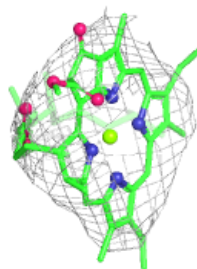
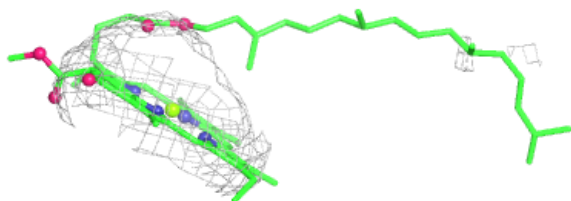
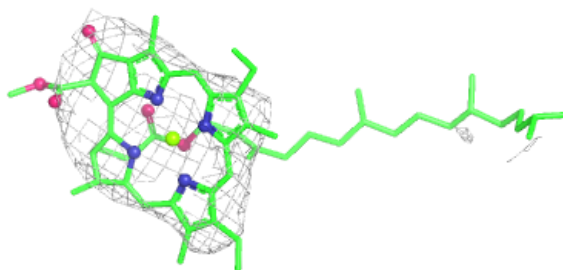


Electron density around CLA B 614:

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

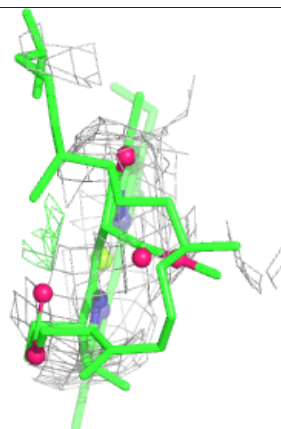
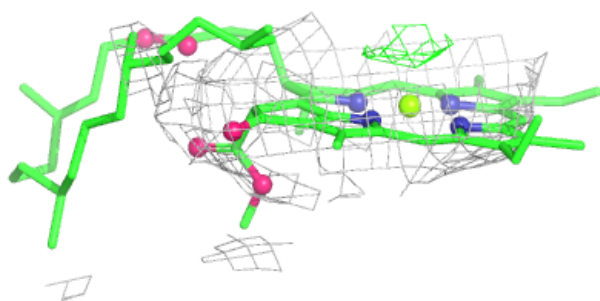
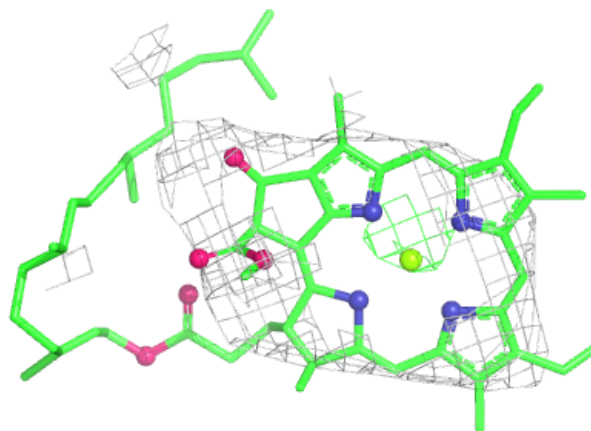
**Electron density around CLA B 609:**

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

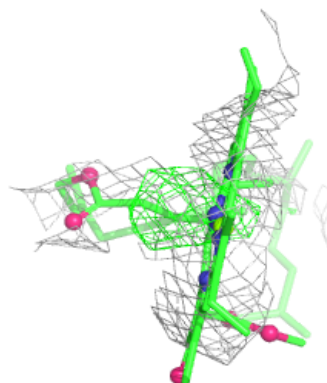
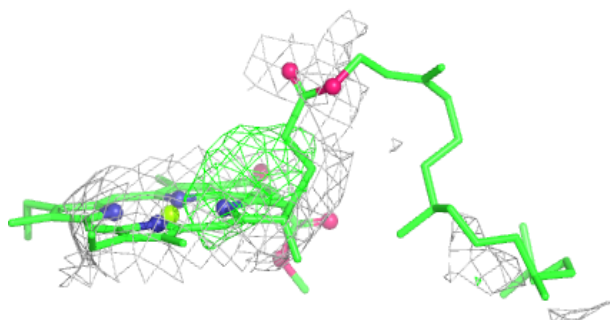
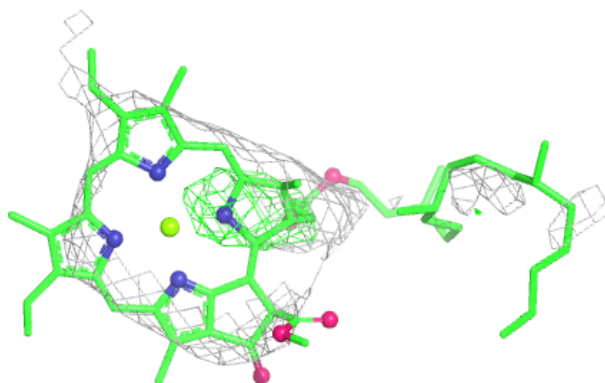


Electron density around CLA b 613:

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

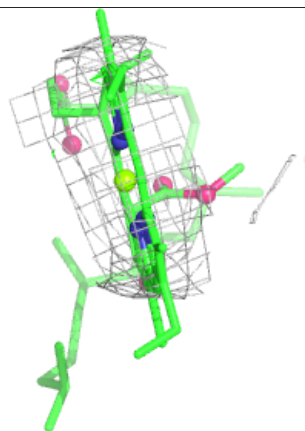
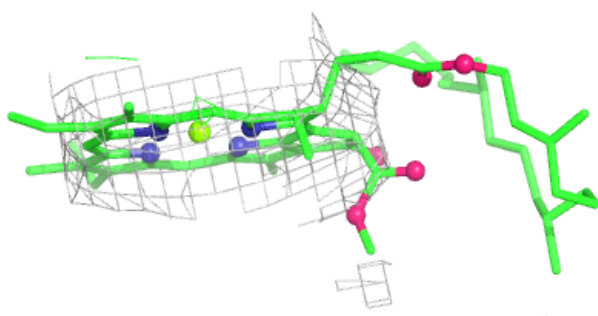
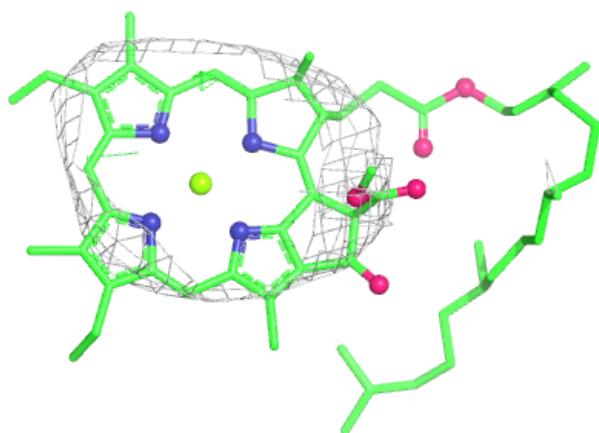
**Electron density around CLA b 615:**

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

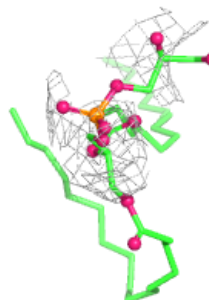
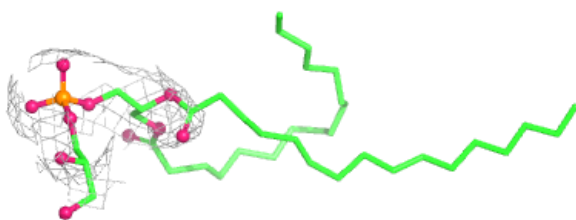
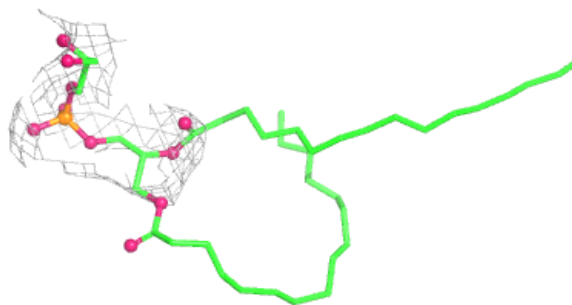


Electron density around CLA B 611:

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

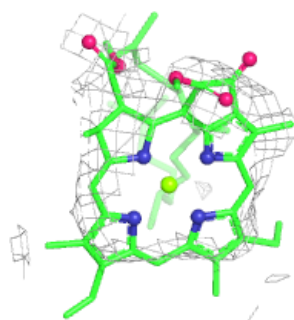
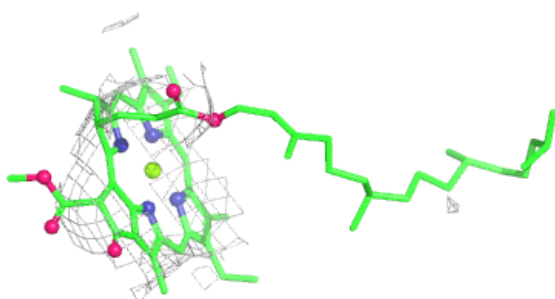
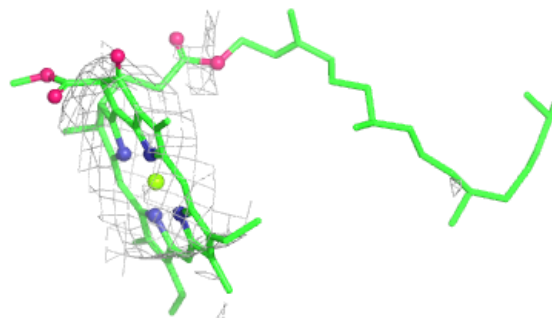
**Electron density around LHG B 622:**

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

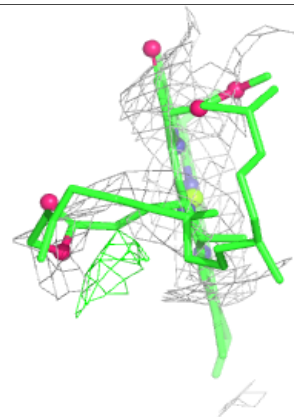
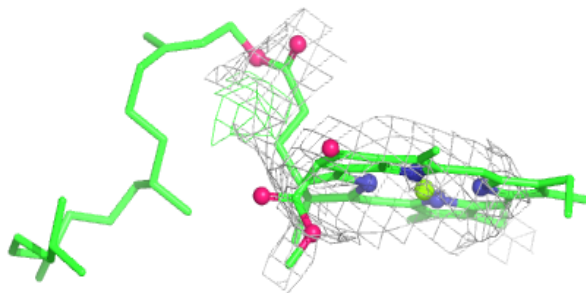
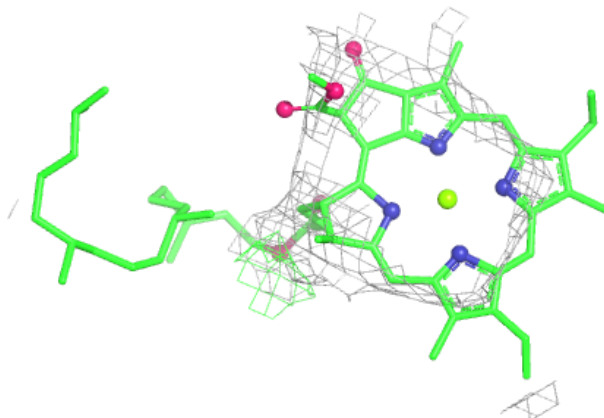


Electron density around CLA c 509:

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

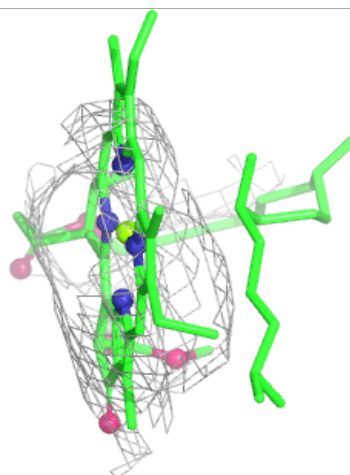
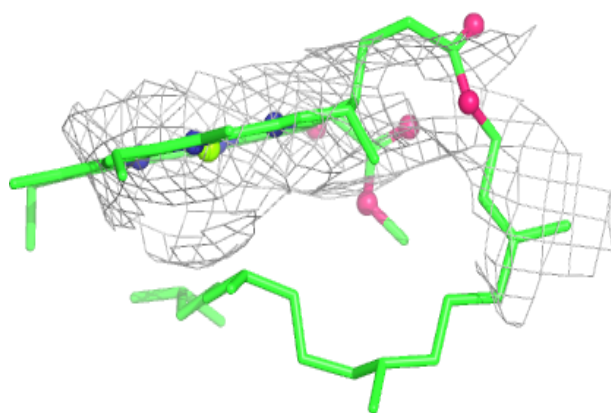
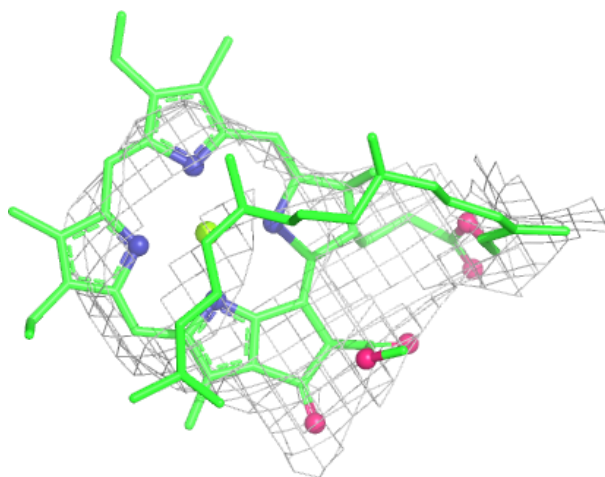
**Electron density around CLA B 613:**

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



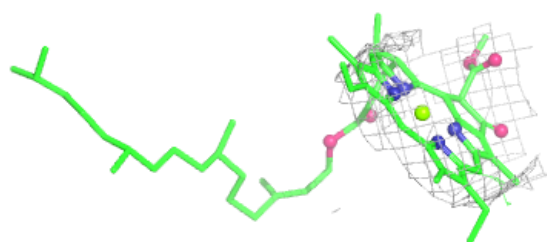
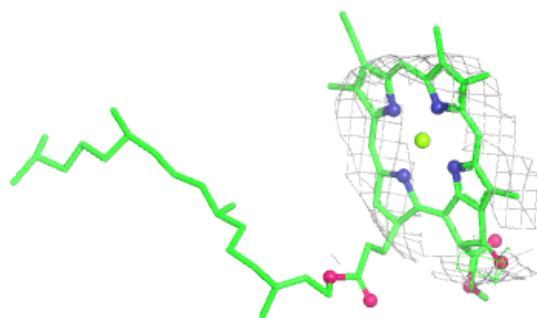
Electron density around CLA c 511:

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

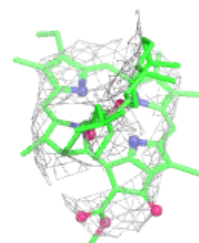
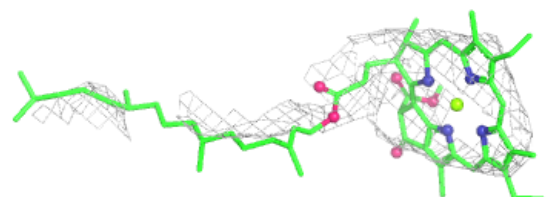
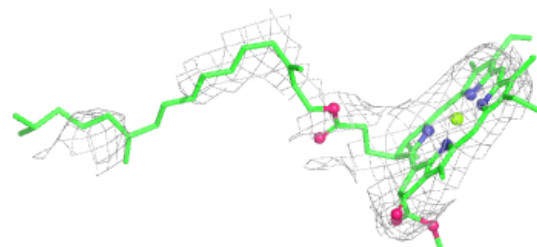


Electron density around CLA c 512:

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

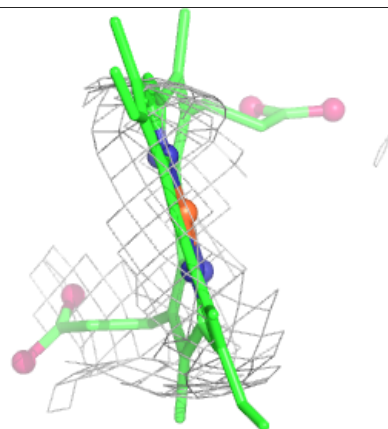
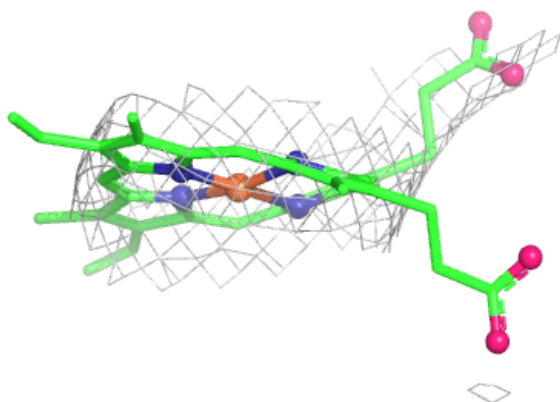
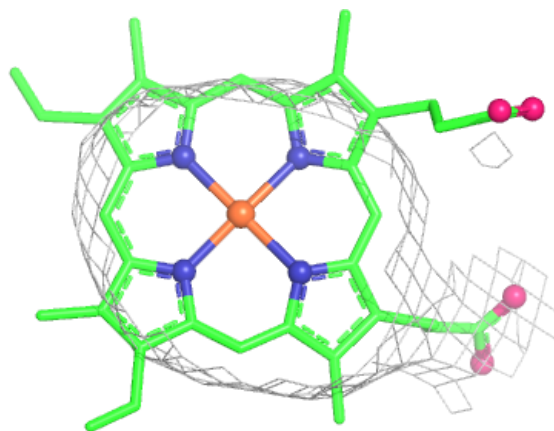
**Electron density around CLA C 502:**

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



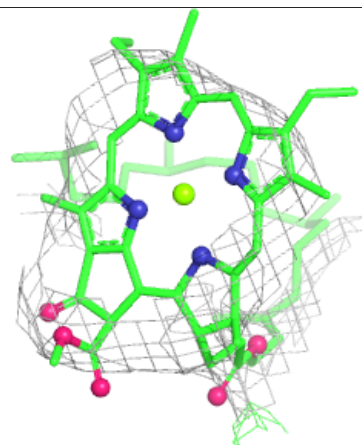
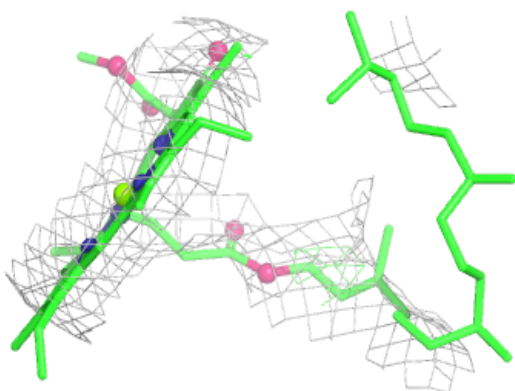
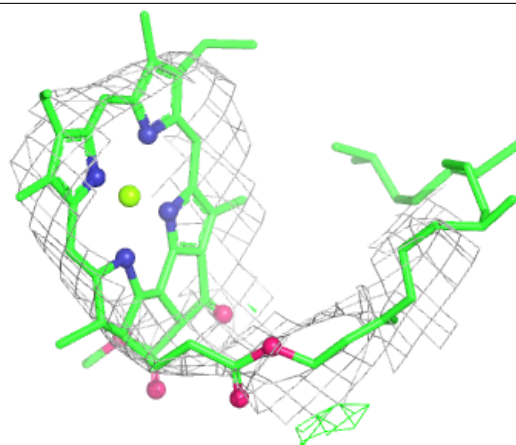
Electron density around HEM e 102:

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



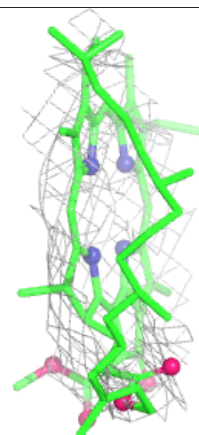
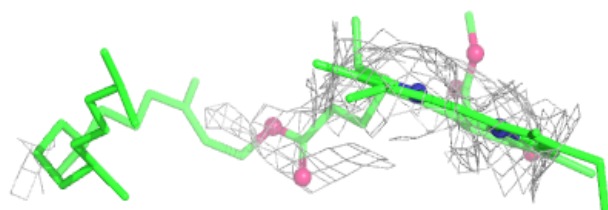
Electron density around CLA C 503:

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

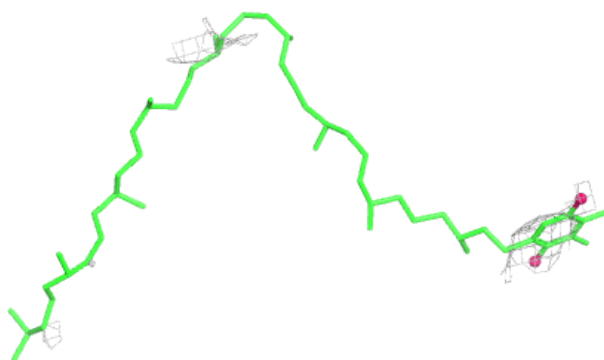


Electron density around PHO a 606:

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

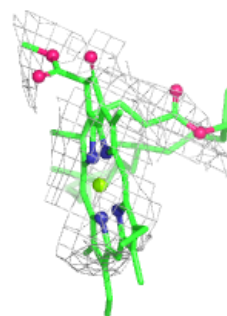
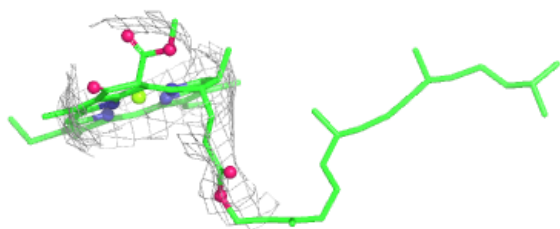
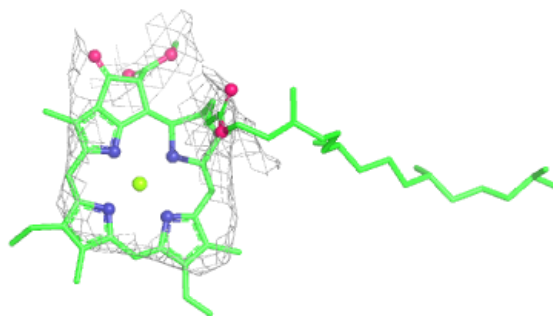
**Electron density around PL9 D 405:**

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

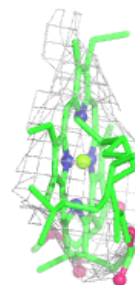
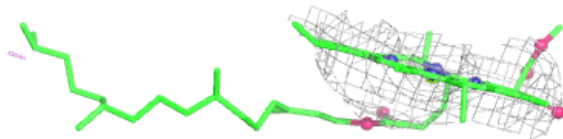
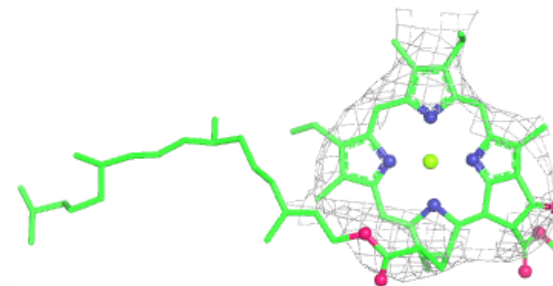


Electron density around CLA A 606:

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

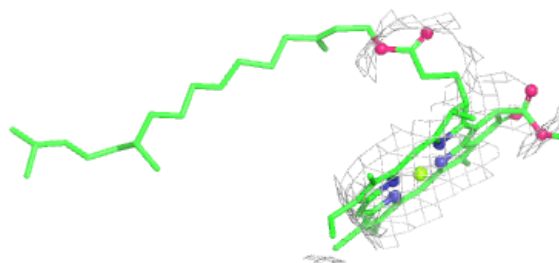
**Electron density around CLA B 604:**

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



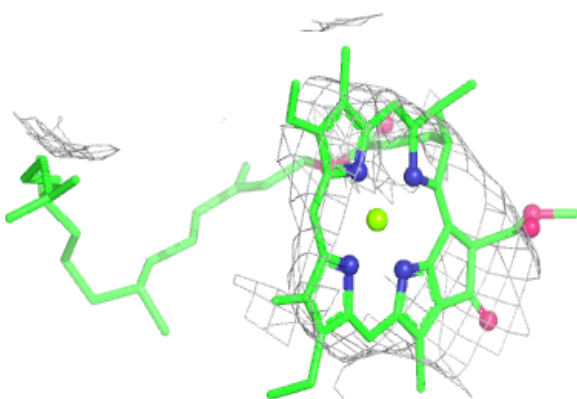
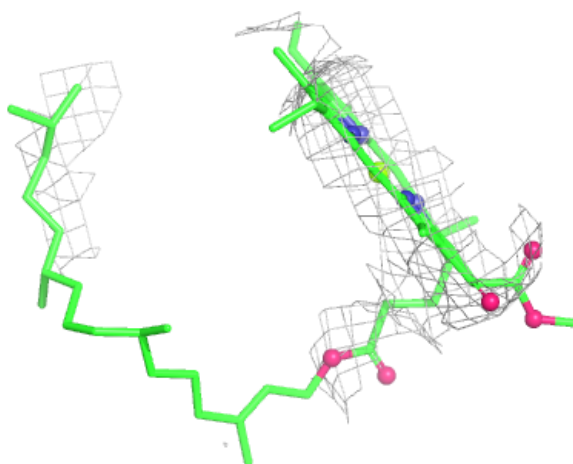
Electron density around CLA c 505:

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



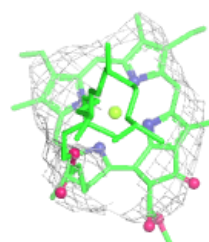
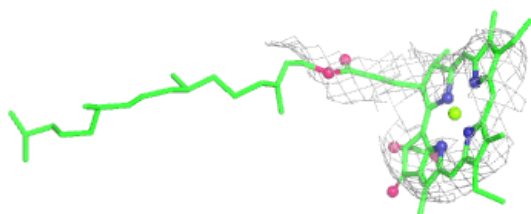
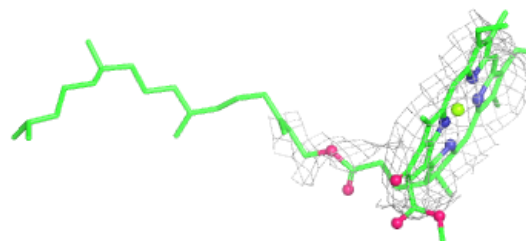
Electron density around CLA B 612:

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

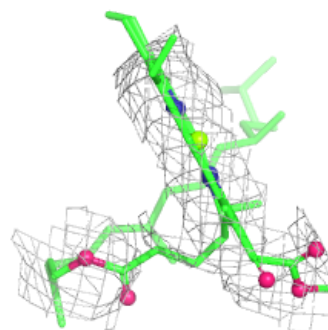
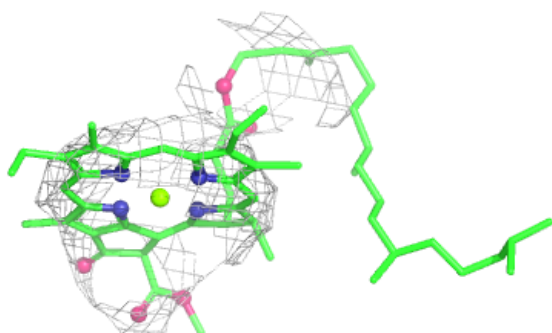
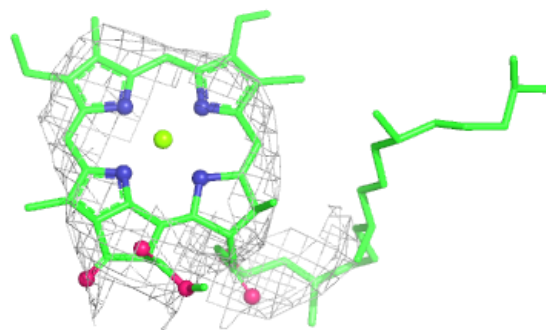


Electron density around CLA b 607:

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

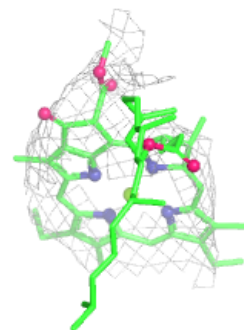
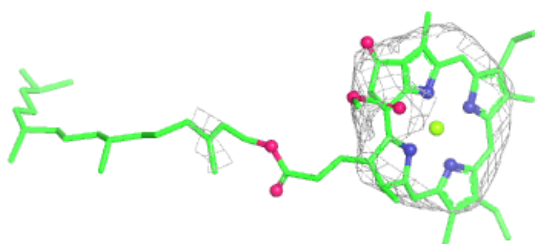
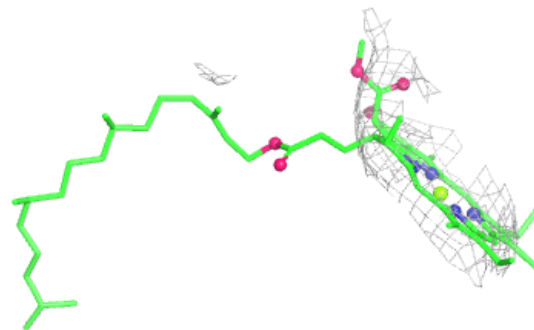
**Electron density around CLA a 613:**

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

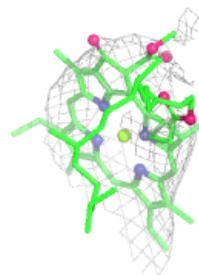
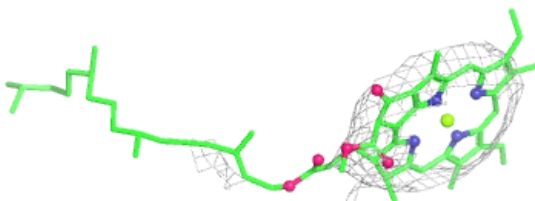
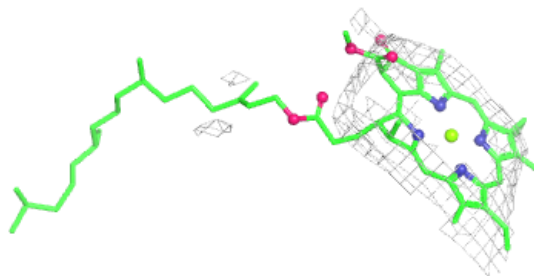


Electron density around CLA d 402:

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

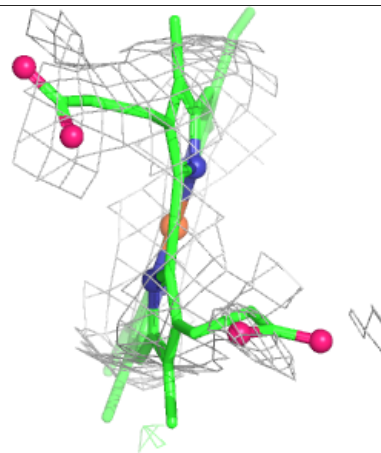
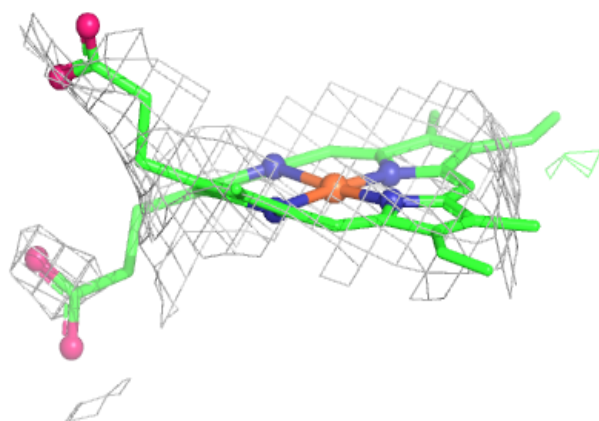
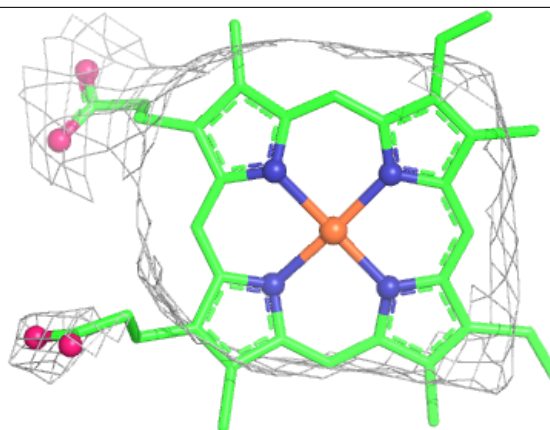
**Electron density around CLA A 605:**

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



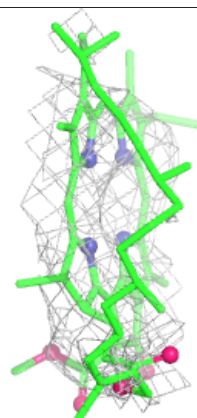
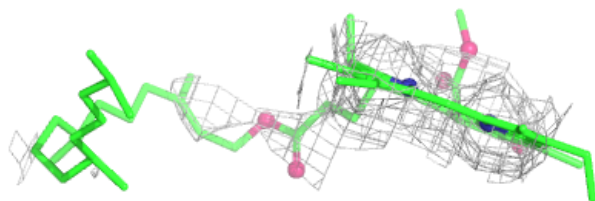
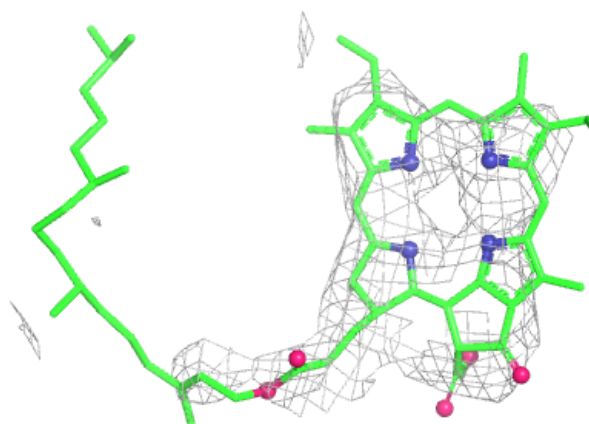
Electron density around HEM E 102:

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



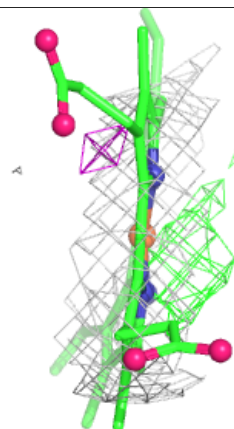
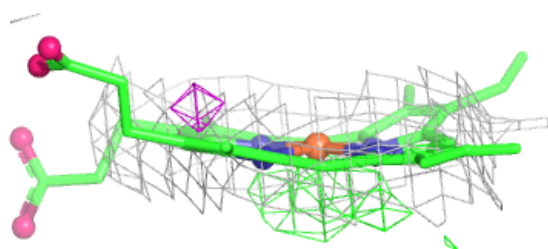
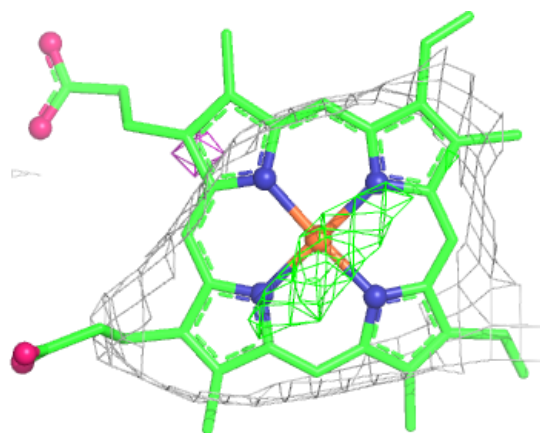
Electron density around PHO A 607:

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



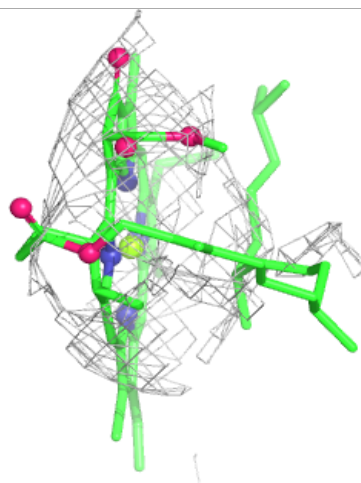
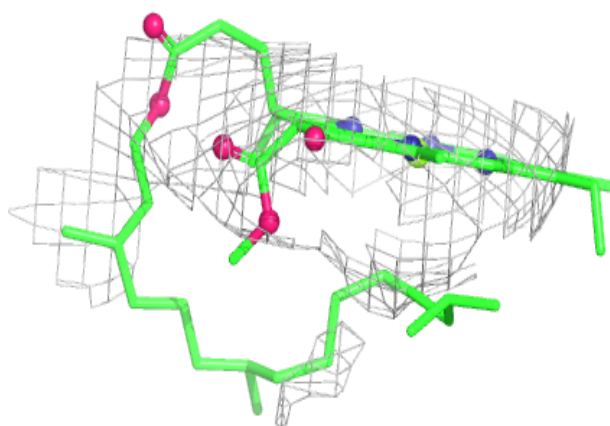
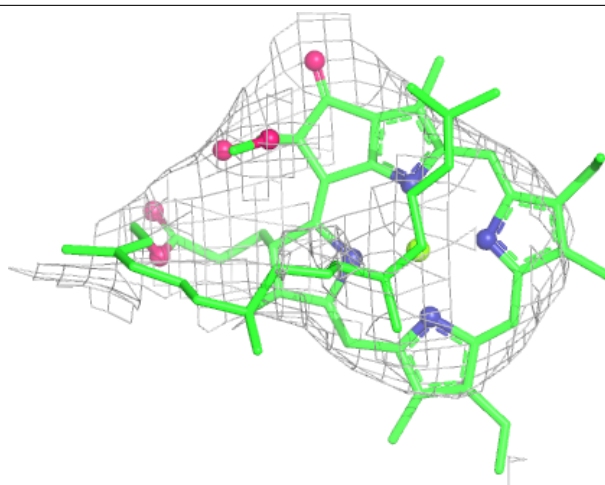
Electron density around HEM v 201:

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



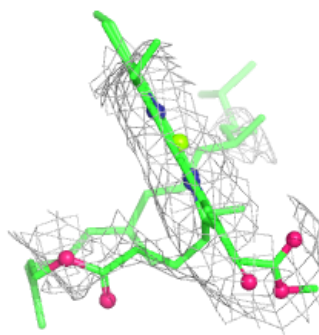
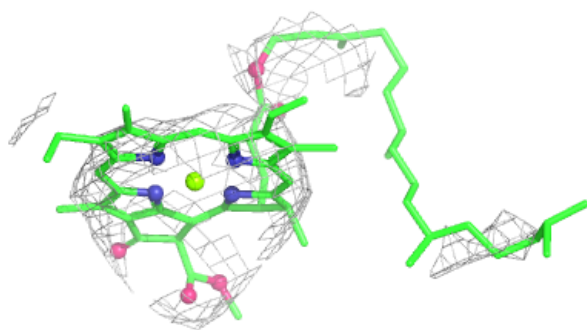
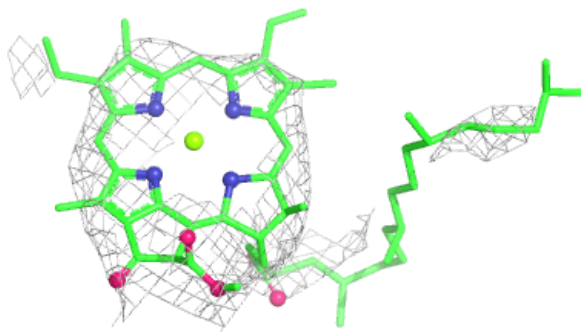
Electron density around CLA C 510:

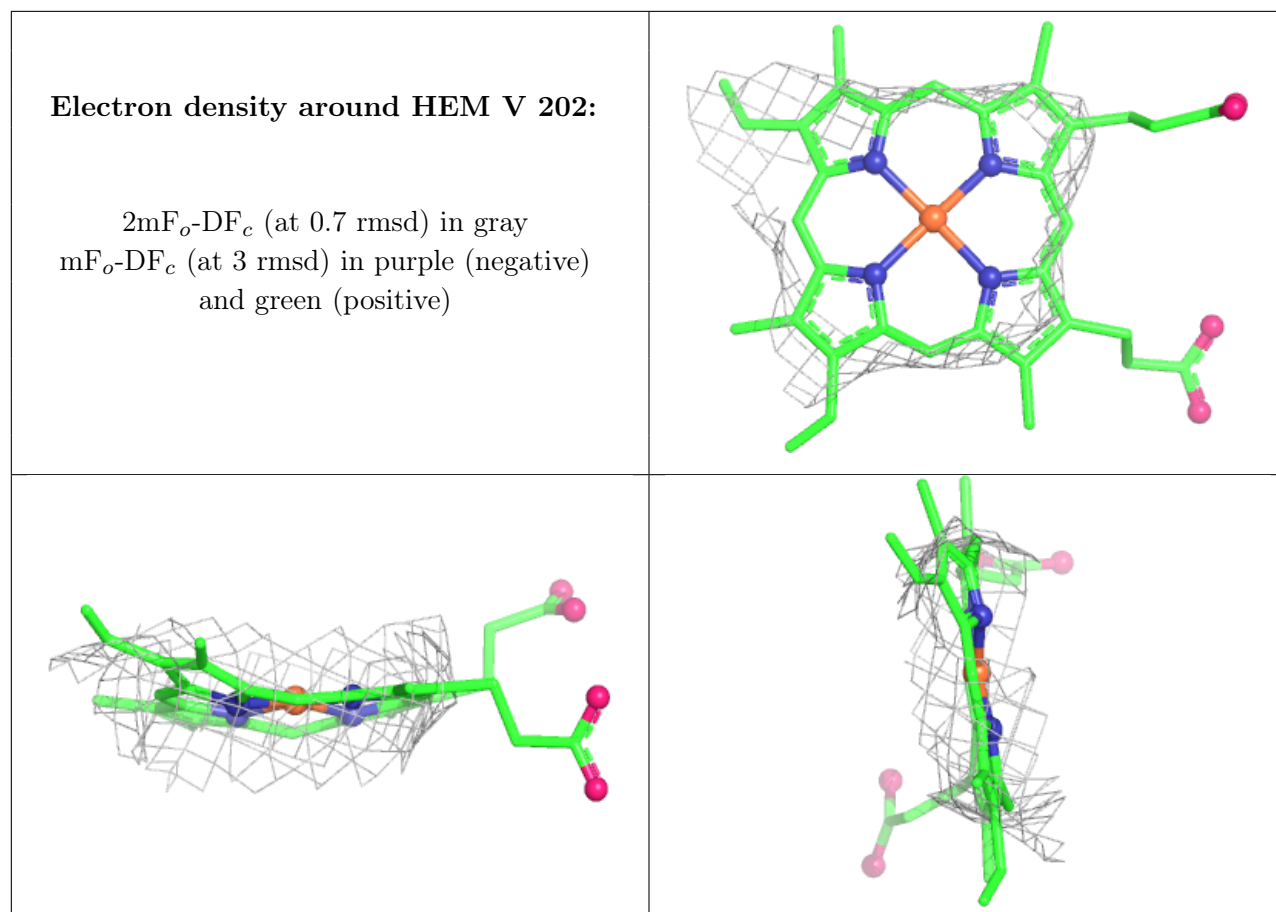
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.