



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:25 PM UTC

PDB ID : 4PBU / pdb_00004pbu
Title : Serial Time-resolved crystallography of Photosystem II using a femtosecond X-ray laser The S1 state
Authors : Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.; Zatsepin, N.; Rendek, K.N.; Hunter, M.; Shoeman, R.L.; White, T.A.; Wang, D.; James, D.; Yang, J.H.; Cobb, D.E.; Reeder, B.; Sierra, R.G.; Liu, H.; Barty, A.; Aquila, A.; Deponte, D.; Kirian, R.A.; Bari, S.; Bergkamp, J.J.; Beyerlein, K.; Bogan, M.J.; Caleman, C.; Chao, T.-C.; Conrad, C.E.; Davis, K.M.; Fleckenstein, H.; Galli, L.; Hau-Riege, S.P.; Kassemeyer, S.; Laksmono, H.; Liang, M.; Lomb, L.; Marchesini, S.; Martin, A.V.; Messerschmidt, M.; Milathianaki, D.; Nass, K.; Ros, A.; Roy-Chowdhury, S.; Schmidt, K.; Seibert, M.; Steinbrener, J.; Stellato, F.; Yan, L.; Yoon, C.; Moore, T.A.; Moore, A.L.; Pushkar, Y.; Williams, G.J.; Boutet, S.; Doak, R.B.; Weierstall, U.; Frank, M.; Chapman, H.N.; Spence, J.C.H.; Fromme, P.
Deposited on : 2014-04-13
Resolution : 5.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0

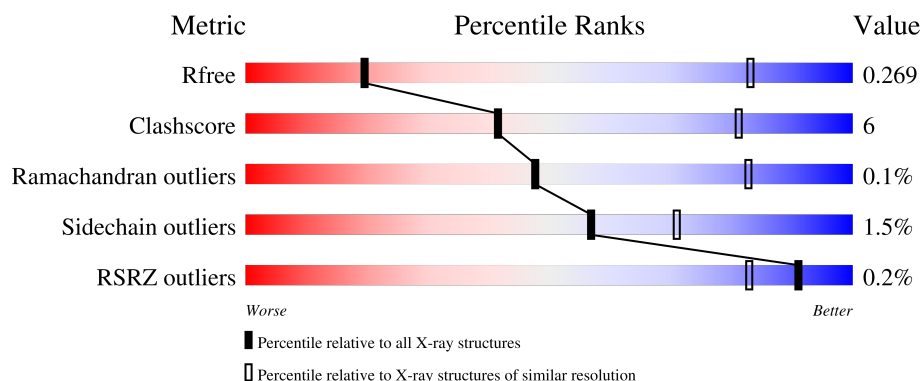
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)

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.

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

Mol	Chain	Length	Quality of chain
1	A	334	90% 10%
1	a	334	84% 15% .
2	B	504	91% 9%
2	b	504	92% 8%
3	C	455	88% 11% ..
3	c	455	87% 12%
4	D	342	90% 10%
4	d	342	87% 13%
5	E	81	81% 19%
5	e	81	84% 16%
6	F	34	82% 15% .
6	f	34	3% 71% 24% 6%
7	H	65	86% 12% .
7	h	65	89% 11%
8	I	38	89% 11%
8	i	38	87% 13%
9	J	40	82% 12% 5%
9	j	40	85% 15%
10	K	37	86% 11% .
10	k	37	73% 24% .
11	L	37	78% 19% .
11	l	37	89% 11%
12	M	34	3% 82% 18%
12	m	34	85% 15%
13	O	243	85% 14% .
13	o	243	88% 10% .

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Mol	Chain	Length	Quality of chain
14	T	30	
14	t	30	
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
22	CL	v	201	-	-	-	X
24	CLA	A	606	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	K	101	-	X	-	-
26	BCR	f	101	-	X	-	-
26	BCR	h	101	-	X	-	-
26	BCR	k	102	-	X	-	-
29	LHG	D	409	-	-	X	-
29	LHG	d	410	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	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 core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	455	Total	C	N	O	S	0	0	0
			3519	2303	589	614	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	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	0	0
			662	432	107	123				
5	e	81	Total	C	N	O		0	0	0
			662	432	107	123				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	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	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

- 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	40	Total	C	N	O	S	0	0	0
			288	192	44	49	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	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	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	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			

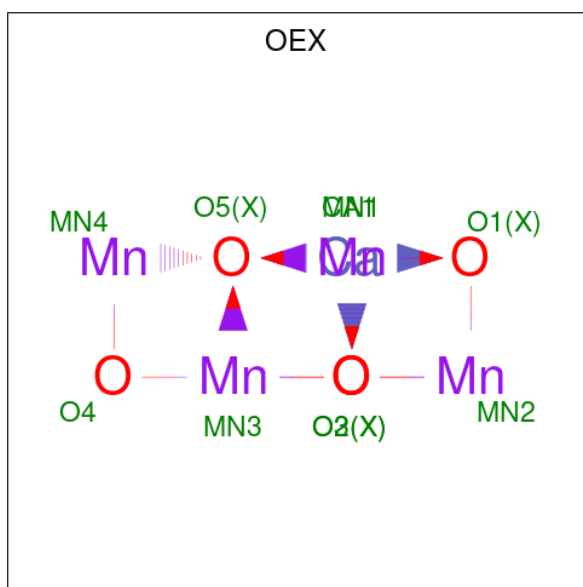
- Molecule 18 is a protein called Photosystem II reaction center X protein.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			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		

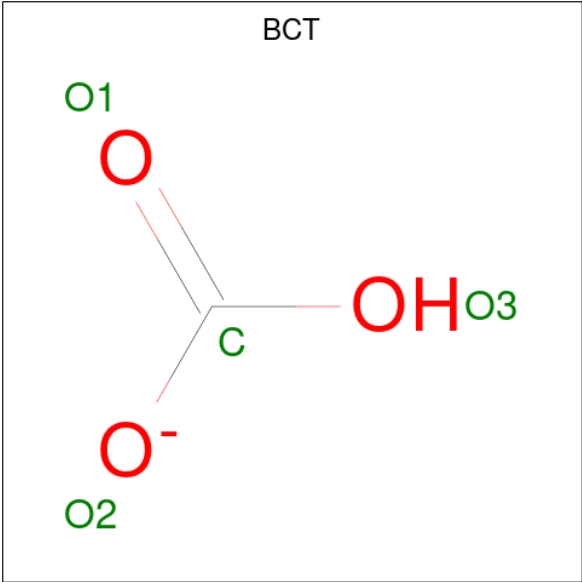
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

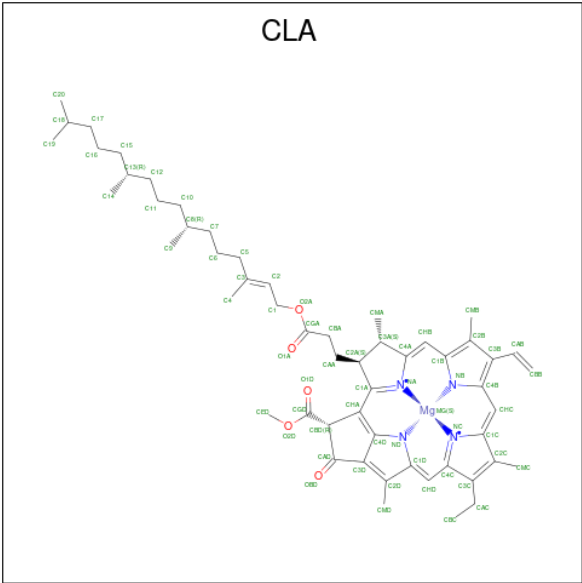
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	V	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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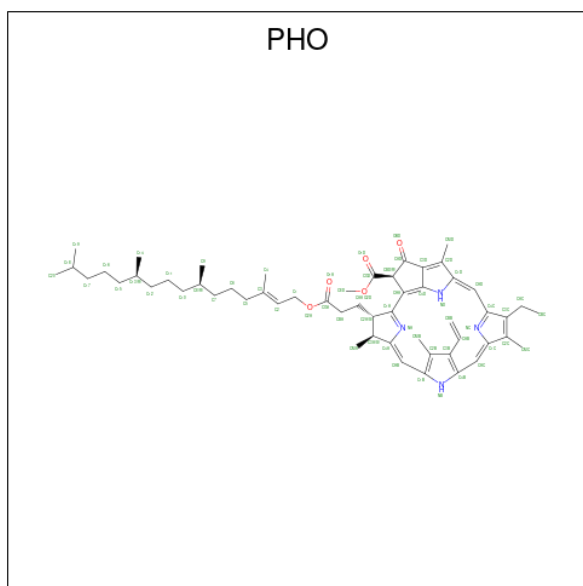
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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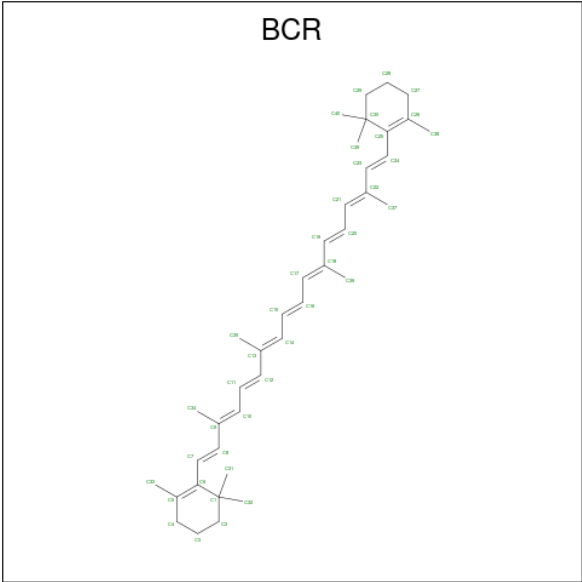
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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



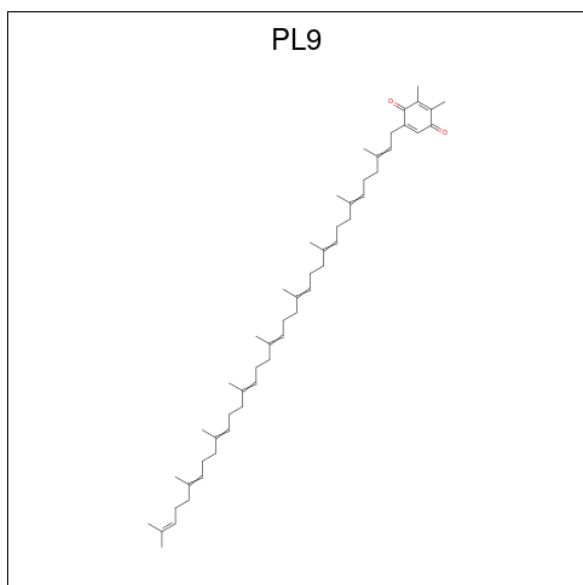
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

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

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



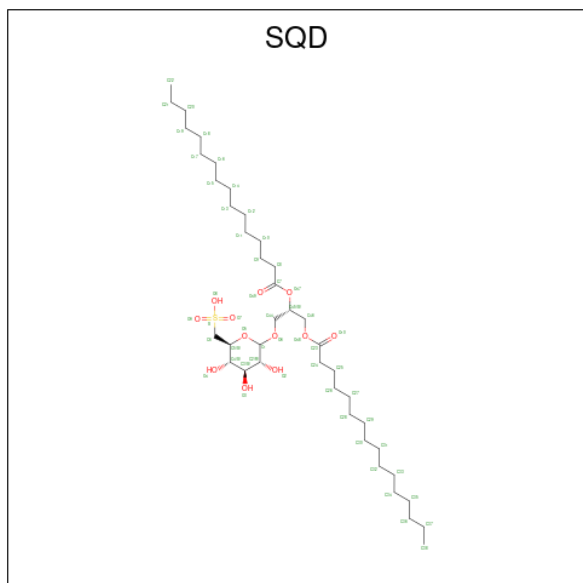
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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

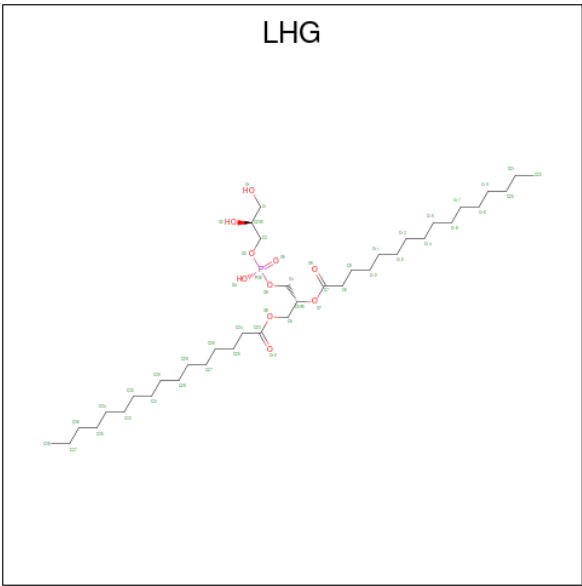
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG)

(formula: C₃₈H₇₅O₁₀P).



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

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

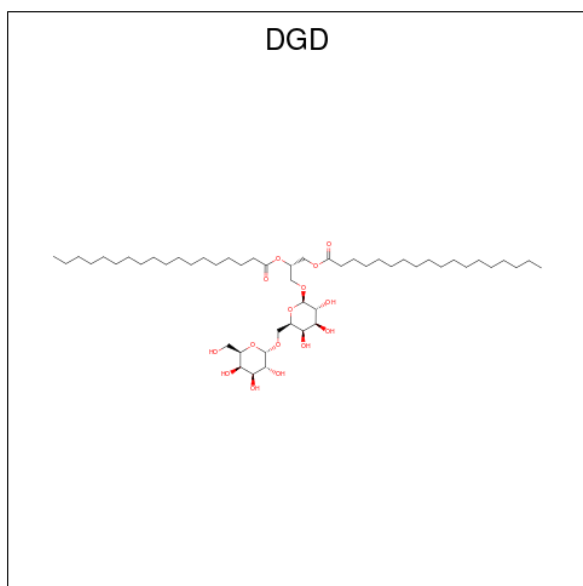
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total	Ca	0	0
			1	1		

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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



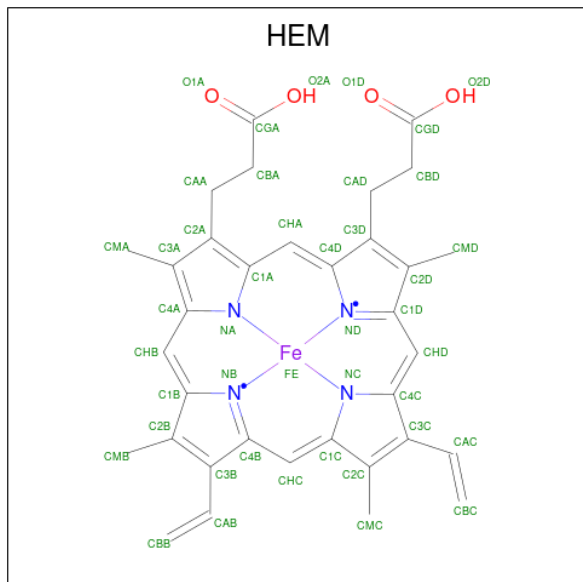
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	D	1	Total	C	O	0	0
			62	47	15		
31	H	1	Total	C	O	0	0
			62	47	15		

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

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



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

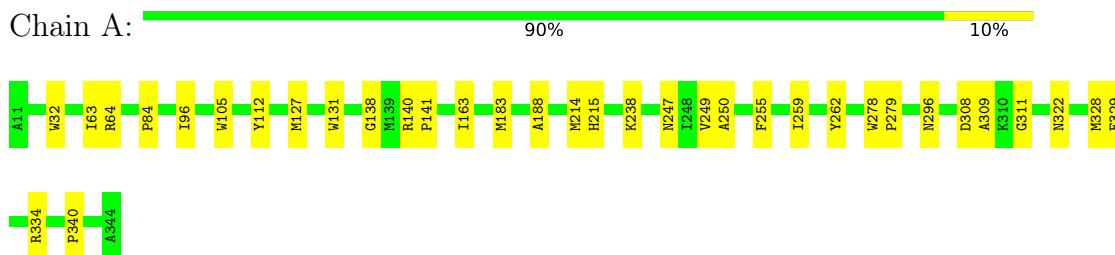
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	j	1	Total	Mg	0	0
			1	1		

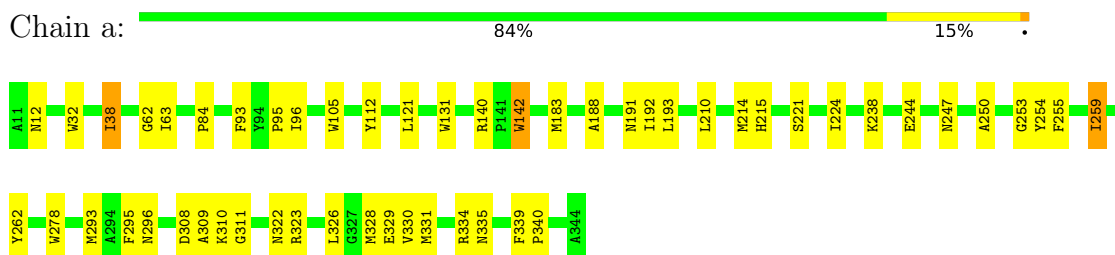
3 Residue-property plots [i](#)

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

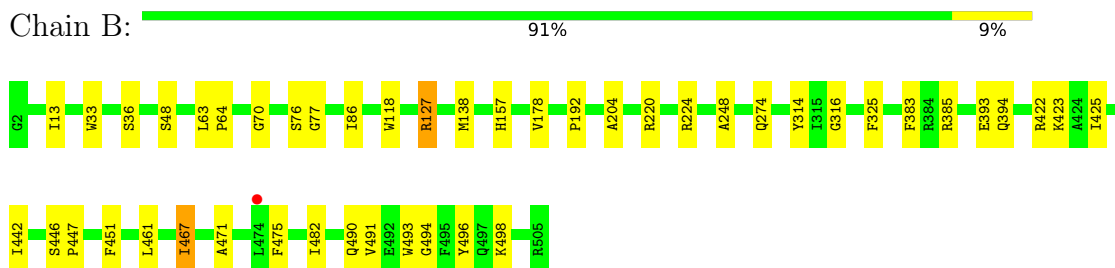
- Molecule 1: Photosystem Q(B) protein 1



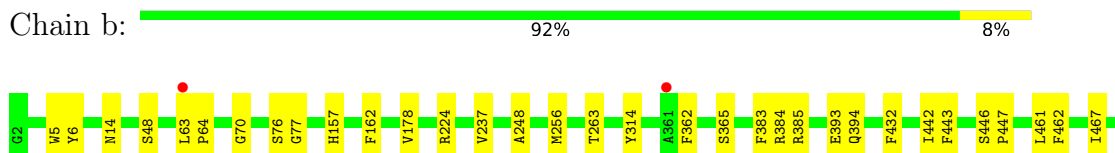
- Molecule 1: Photosystem Q(B) protein 1



- Molecule 2: Photosystem II core light harvesting protein



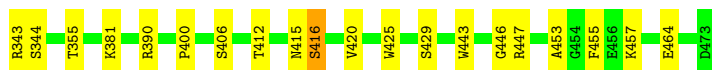
- Molecule 2: Photosystem II core light harvesting protein





• Molecule 3: Photosystem II CP43 protein

Chain C: 88% 11% ..



• Molecule 3: Photosystem II CP43 protein

Chain c: 87% 12%



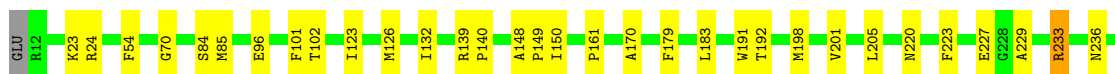
• Molecule 4: Photosystem II D2 protein

Chain D: 90% 10%



• Molecule 4: Photosystem II D2 protein

Chain d: 87% 13%



• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 81% 19%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 84% 16%



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 82% 15%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 3% 71% 24% 6%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 86% 12%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 89% 11%



- Molecule 8: Photosystem II reaction center protein I

Chain I: 89% 11%



- Molecule 8: Photosystem II reaction center protein I

Chain i: 87% 13%



- Molecule 9: Photosystem II reaction center protein J

Chain J: 82% 12% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain j: 85% 15%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 86% 11% .



- Molecule 10: Photosystem II reaction center protein K

Chain k: 73% 24% .



- Molecule 11: Photosystem II reaction center protein L

Chain L: 78% 19% .



- Molecule 11: Photosystem II reaction center protein L

Chain l: 89% 11%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 3% 82% 18%



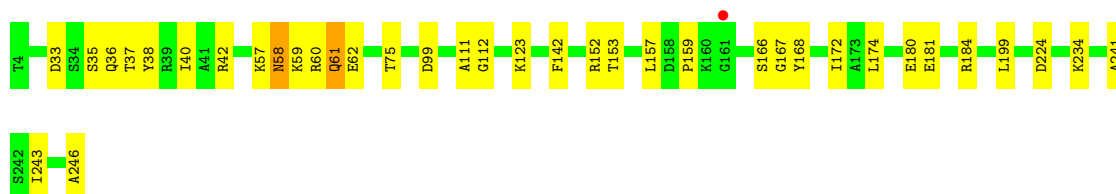
- Molecule 12: Photosystem II reaction center protein M

Chain m: 85% 15%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 85% 14%



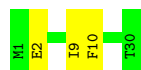
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 88% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 90% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 83% 17%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 85% 15%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  87% 13%



- Molecule 16: Cytochrome c-550

Chain V:  91% 9%



- Molecule 16: Cytochrome c-550

Chain v:  % 85% 15% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  83% 17%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  72% 28%



- Molecule 18: Photosystem II reaction center X protein

Chain X:  90% 10%

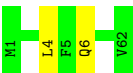


- Molecule 18: Photosystem II reaction center X protein

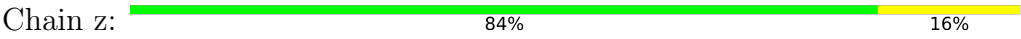
Chain x:  85% 15%



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.25Å 226.26Å 307.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.64 – 5.00 100.64 – 5.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.64-5.00) 100.0 (100.64-5.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.261 , 0.262 0.272 , 0.269	Depositor DCC
R_{free} test set	2056 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	285.1	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 133.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	48924	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/2705	0.80	0/3689
1	a	0.60	1/2705 (0.0%)	0.81	1/3689 (0.0%)
2	B	0.58	0/4109	0.79	0/5600
2	b	0.57	0/4109	0.76	0/5600
3	C	0.55	0/3599	0.78	0/4900
3	c	0.53	0/3633	0.79	0/4946
4	D	0.61	0/2821	0.78	0/3844
4	d	0.56	0/2812	0.77	0/3832
5	E	0.55	0/681	0.81	0/928
5	e	0.54	0/681	0.80	0/928
6	F	0.68	1/284 (0.4%)	0.73	0/387
6	f	0.55	0/265	0.77	0/360
7	H	0.58	0/524	0.77	0/713
7	h	0.54	0/524	0.73	0/713
8	I	0.57	0/319	0.74	0/429
8	i	0.57	0/319	0.77	0/429
9	J	0.59	0/278	0.82	0/376
9	j	0.49	0/294	0.84	0/396
10	K	0.57	0/303	0.81	0/416
10	k	0.63	1/303 (0.3%)	0.87	0/416
11	L	0.57	0/311	0.77	0/422
11	l	0.57	0/311	0.73	0/422
12	M	0.59	0/270	0.86	0/367
12	m	0.60	0/270	0.74	0/367
13	O	0.54	0/1896	0.74	0/2571
13	o	0.52	0/1896	0.75	0/2571
14	T	0.56	0/265	0.76	0/359
14	t	0.60	0/265	0.80	0/359
15	U	0.55	0/785	0.74	0/1064
15	u	0.55	0/785	0.72	0/1064
16	V	0.57	0/1085	0.78	0/1473
16	v	0.53	0/1085	0.82	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.58	0/216	0.83	0/289
17	y	0.52	0/216	0.97	0/289
18	X	0.53	0/290	0.83	0/392
18	x	0.53	0/290	0.85	0/392
19	Z	0.54	0/490	0.87	0/669
19	z	0.54	0/490	0.91	0/669
All	All	0.57	3/42484 (0.0%)	0.78	2/57803 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	28	VAL	CA-CB	5.69	1.57	1.54
1	a	38	ILE	CA-CB	5.51	1.57	1.54
10	k	28	ILE	CA-CB	5.33	1.56	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	v	105	ARG	N-CA-C	6.42	119.09	111.33
1	a	142	TRP	N-CA-C	5.90	120.17	112.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2620	0	2517	40	0
1	a	2620	0	2517	66	0
2	B	3969	0	3828	57	0
2	b	3969	0	3828	53	0
3	C	3486	0	3407	48	0
3	c	3519	0	3437	53	23
4	D	2726	0	2627	35	0
4	d	2717	0	2621	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	662	0	648	12	0
5	e	662	0	648	11	0
6	F	275	0	282	4	0
6	f	257	0	269	5	0
7	H	511	0	532	8	0
7	h	511	0	532	7	0
8	I	312	0	329	4	0
8	i	312	0	329	4	0
9	J	272	0	279	5	0
9	j	288	0	300	6	0
10	K	293	0	305	7	0
10	k	293	0	305	9	0
11	L	304	0	316	8	0
11	l	304	0	316	4	0
12	M	267	0	289	8	0
12	m	267	0	289	8	0
13	O	1865	0	1838	33	23
13	o	1865	0	1838	35	0
14	T	256	0	262	4	0
14	t	256	0	262	4	0
15	U	774	0	773	25	0
15	u	774	0	773	19	0
16	V	1064	0	1073	20	0
16	v	1064	0	1075	30	0
17	Y	215	0	246	3	0
17	y	215	0	246	9	0
18	X	287	0	317	4	0
18	x	287	0	317	10	0
19	Z	479	0	516	0	0
19	z	479	0	516	4	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	V	1	0	0	0	0
22	a	2	0	0	0	0
22	v	1	0	0	0	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	260	0	288	8	0
24	B	1040	0	1152	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	C	845	0	936	36	0
24	D	130	0	144	1	0
24	a	195	0	216	7	0
24	b	1040	0	1152	21	0
24	c	845	0	936	45	0
24	d	195	0	216	13	0
25	A	64	0	74	2	0
25	D	64	0	74	4	0
25	a	64	0	74	3	0
25	d	64	0	74	1	0
26	A	40	0	48	0	0
26	B	160	0	188	6	0
26	C	80	0	93	0	0
26	D	40	0	48	2	0
26	H	40	0	46	1	0
26	K	40	0	46	1	0
26	T	80	0	94	2	0
26	Y	40	0	47	1	0
26	a	40	0	48	1	0
26	b	80	0	92	5	0
26	c	80	0	95	3	0
26	f	40	0	46	0	0
26	h	40	0	46	1	0
26	k	80	0	90	5	0
27	A	55	0	80	9	0
27	D	55	0	80	1	0
27	a	55	0	80	8	0
27	d	55	0	80	1	0
28	A	108	0	156	6	0
28	F	43	0	53	0	0
28	L	54	0	78	5	0
28	a	108	0	156	7	0
28	d	43	0	53	1	0
28	l	54	0	78	7	0
29	A	42	0	57	3	0
29	B	49	0	74	3	0
29	D	147	0	222	25	0
29	a	42	0	57	5	0
29	b	49	0	74	6	0
29	d	147	0	222	26	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	c	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	C	186	0	246	6	0
31	D	62	0	82	3	0
31	H	62	0	82	2	0
31	c	124	0	164	0	0
31	d	62	0	82	2	0
31	h	62	0	82	1	0
31	j	62	0	82	2	0
32	E	43	0	30	0	0
32	V	43	0	30	9	0
32	e	43	0	30	0	0
32	v	43	0	30	8	0
33	j	1	0	0	0	0
All	All	48924	0	49705	629	23

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (629) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:37:CYS:SG	32:V:202:HEM:HAB	1.52	1.49
16:v:40:CYS:SG	32:v:202:HEM:HAC	1.53	1.46
16:V:37:CYS:SG	32:V:202:HEM:CAB	2.03	1.46
16:V:40:CYS:SG	32:V:202:HEM:CAC	2.03	1.44
16:V:40:CYS:SG	32:V:202:HEM:HAC	1.56	1.40
16:v:40:CYS:SG	32:v:202:HEM:CAC	2.12	1.36
16:v:37:CYS:SG	32:v:202:HEM:CAB	2.17	1.31
16:v:37:CYS:SG	32:v:202:HEM:HAB	1.73	1.28
1:A:214:MET:HG2	27:A:611:PL9:H102	1.20	1.18
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.24	1.14
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.28	1.11
2:b:383:PHE:CZ	13:o:167:GLY:HA2	1.98	0.98
10:K:17:ILE:H	10:K:17:ILE:HD13	1.29	0.97
29:D:409:LHG:H132	29:D:409:LHG:H372	1.48	0.92
24:C:510:CLA:H43	29:D:409:LHG:H383	1.53	0.91
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:510:CLA:C4	29:D:409:LHG:H383	2.03	0.88
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.09	0.88
1:A:214:MET:HG2	27:A:611:PL9:C10	2.02	0.88
3:c:457:LYS:NZ	4:d:227:GLU:O	2.08	0.88
16:v:40:CYS:HG	32:v:202:HEM:HAC	0.89	0.85
2:b:393:GLU:HB3	15:u:18:GLY:CA	2.07	0.84
2:b:162:PHE:O	24:b:607:CLA:HHD	1.77	0.84
4:d:233:ARG:HG2	4:d:233:ARG:HH11	1.42	0.84
29:D:409:LHG:H352	29:D:409:LHG:H151	1.59	0.82
24:c:905:CLA:H191	29:d:410:LHG:H341	1.61	0.82
6:f:41:GLN:OE1	9:j:31:GLY:HA3	1.80	0.82
24:c:909:CLA:HBC2	29:d:410:LHG:H352	1.60	0.82
2:b:383:PHE:CE2	13:o:167:GLY:HA2	2.14	0.82
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.61	0.82
1:a:250:ALA:CA	2:b:491:VAL:HG11	2.08	0.81
29:d:410:LHG:H322	29:d:410:LHG:H151	1.60	0.81
5:e:67:THR:H	5:e:75:GLN:HE22	1.25	0.81
24:c:911:CLA:H43	29:d:410:LHG:H383	1.65	0.77
2:b:442:ILE:HD11	13:o:174:LEU:HD23	1.66	0.77
2:b:442:ILE:HD11	13:o:174:LEU:CD2	2.16	0.76
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.68	0.76
13:o:156:PHE:HB3	13:o:225:MET:CE	2.17	0.74
2:B:467:ILE:HG13	4:D:126:MET:HE1	1.68	0.74
1:A:340:PRO:HD3	15:U:103:TYR:CZ	2.23	0.74
4:d:24:ARG:HH12	18:x:35:ASP:CG	1.95	0.74
24:C:508:CLA:H92	29:D:409:LHG:H371	1.69	0.73
28:a:411:SQD:H301	24:c:909:CLA:H71	1.67	0.73
13:O:57:LYS:O	13:O:58:ASN:HB2	1.87	0.73
3:C:381:LYS:NZ	13:O:99:ASP:OD2	2.20	0.73
31:C:518:DGD:HBH2	29:D:409:LHG:H223	1.70	0.72
29:D:409:LHG:H112	29:D:409:LHG:H382	1.71	0.72
1:A:340:PRO:HB3	15:U:103:TYR:CG	2.26	0.71
24:b:616:CLA:H2	24:b:617:CLA:HBB2	1.73	0.70
3:C:344:SER:O	13:O:75:THR:HG22	1.92	0.70
4:D:351:ALA:HA	15:U:101:GLY:O	1.92	0.70
1:A:334:ARG:HG3	13:O:157:LEU:HB2	1.73	0.69
13:o:57:LYS:O	13:o:58:ASN:HB2	1.91	0.69
3:C:321:ASP:OD2	15:U:99:ASN:HB2	1.92	0.68
3:c:447:ARG:NH2	4:d:229:ALA:HB1	2.08	0.68
4:d:24:ARG:HD3	18:x:37:VAL:HG22	1.74	0.68
2:B:393:GLU:HB3	15:U:18:GLY:CA	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:612:CLA:H142	29:B:621:LHG:H361	1.76	0.68
24:c:911:CLA:H41	29:d:410:LHG:H361	1.75	0.68
16:V:37:CYS:SG	32:V:202:HEM:C3B	2.85	0.68
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.24	0.67
1:a:250:ALA:HA	2:b:491:VAL:CG1	2.14	0.67
1:a:253:GLY:HA3	2:b:491:VAL:CG1	2.16	0.67
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.75	0.67
1:A:214:MET:CG	27:A:611:PL9:H102	2.12	0.67
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.75	0.67
24:c:911:CLA:C4	29:d:410:LHG:H383	2.24	0.67
13:o:156:PHE:HB3	13:o:225:MET:HE1	1.77	0.67
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.78	0.66
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.31	0.66
28:a:411:SQD:H252	29:d:410:LHG:H121	1.76	0.66
6:F:41:GLN:OE1	9:J:31:GLY:HA3	1.96	0.66
1:A:249:VAL:HG12	2:B:491:VAL:HG21	1.77	0.66
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.76	0.65
16:V:40:CYS:SG	32:V:202:HEM:CBC	2.81	0.65
1:a:247:ASN:HB3	2:b:482:ILE:HD11	1.77	0.65
16:v:40:CYS:SG	32:v:202:HEM:C3C	2.89	0.64
2:B:385:ARG:NE	15:U:14:ASP:OD1	2.26	0.64
24:C:506:CLA:HMC2	24:C:507:CLA:H102	1.79	0.64
1:a:296:ASN:HB2	3:c:400:PRO:O	1.97	0.63
1:a:308:ASP:HB2	5:e:52:PRO:O	1.98	0.63
3:c:72:LEU:HD11	3:c:108:THR:HB	1.80	0.63
28:L:101:SQD:H462	28:L:101:SQD:H1	1.79	0.63
27:A:611:PL9:H403	6:F:22:ALA:HB2	1.80	0.63
16:V:40:CYS:SG	32:V:202:HEM:C3C	2.90	0.63
3:c:381:LYS:NZ	13:o:99:ASP:OD2	2.24	0.63
1:A:308:ASP:HB2	5:E:52:PRO:O	1.98	0.62
24:d:404:CLA:H61	18:x:14:LEU:HD12	1.80	0.62
27:a:410:PL9:H512	28:d:407:SQD:H311	1.82	0.62
2:b:383:PHE:O	13:o:166:SER:HA	1.99	0.62
24:a:408:CLA:H203	24:c:907:CLA:H142	1.82	0.61
29:D:409:LHG:H112	29:D:409:LHG:C38	2.30	0.61
1:a:259:ILE:HA	29:a:413:LHG:H202	1.81	0.61
24:C:510:CLA:H41	29:D:409:LHG:H383	1.81	0.61
2:B:393:GLU:HB3	15:U:18:GLY:HA3	1.83	0.61
3:C:286:ALA:HB2	24:C:502:CLA:HMD2	1.80	0.61
10:k:35:LEU:HD13	17:y:32:GLY:HA3	1.82	0.61
5:e:53:ASP:HA	16:v:1:ALA:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:17:ILE:HD13	10:K:17:ILE:N	2.08	0.60
24:c:911:CLA:C4	29:d:410:LHG:C38	2.80	0.60
3:C:167:VAL:HG21	24:C:512:CLA:HBB	1.84	0.60
3:C:457:LYS:NZ	4:D:227:GLU:O	2.26	0.60
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.82	0.60
4:d:351:ALA:HA	15:u:101:GLY:O	2.01	0.60
1:a:121:LEU:HD11	24:c:906:CLA:H152	1.84	0.59
5:e:53:ASP:O	16:v:1:ALA:N	2.34	0.59
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.33	0.59
11:L:13:ASN:ND2	11:L:16:SER:H	2.01	0.59
28:l:101:SQD:H462	28:l:101:SQD:H1	1.83	0.59
16:v:37:CYS:SG	32:v:202:HEM:C3B	2.94	0.59
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.85	0.59
1:a:326:LEU:HD22	16:v:134:LYS:HB2	1.83	0.59
24:c:911:CLA:H43	29:d:410:LHG:C38	2.31	0.59
3:C:324:LEU:HB3	15:U:32:ILE:HD13	1.85	0.59
3:c:286:ALA:HB2	24:c:903:CLA:HMD2	1.83	0.59
4:d:24:ARG:NH1	18:x:35:ASP:OD2	2.36	0.59
24:A:606:CLA:HMB3	24:A:606:CLA:HBB1	1.84	0.58
3:C:381:LYS:CE	13:O:99:ASP:OD2	2.51	0.58
2:B:383:PHE:CE2	13:O:167:GLY:HA2	2.38	0.58
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.85	0.58
2:b:314:TYR:OH	13:o:176:GLN:NE2	2.23	0.58
28:A:612:SQD:H291	24:C:508:CLA:H71	1.84	0.58
1:a:326:LEU:CD2	16:v:134:LYS:HB2	2.34	0.58
3:c:344:SER:O	13:o:75:THR:HG22	2.04	0.58
16:v:40:CYS:HG	32:v:202:HEM:CAC	1.82	0.58
24:c:910:CLA:HMB1	24:c:910:CLA:HBB1	1.85	0.58
5:E:69:ARG:NH2	7:H:50:ASN:O	2.33	0.58
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.86	0.58
4:d:85:MET:CE	4:d:96:GLU:HG2	2.34	0.58
24:b:614:CLA:HMB1	24:b:614:CLA:HBB1	1.86	0.57
3:c:324:LEU:HB3	15:u:32:ILE:HD13	1.87	0.57
29:D:409:LHG:H372	29:D:409:LHG:C13	2.29	0.57
1:A:296:ASN:HB2	3:C:400:PRO:O	2.04	0.57
24:d:404:CLA:H162	7:h:33:VAL:HG13	1.85	0.57
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.87	0.57
24:c:906:CLA:HBB1	24:c:906:CLA:HMB3	1.87	0.57
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.40	0.57
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.35	0.56
11:l:21:LEU:HD13	28:l:101:SQD:H312	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:ILE:HG13	4:D:126:MET:CE	2.34	0.56
1:a:322:ASN:OD1	3:c:412:THR:HA	2.04	0.56
24:b:616:CLA:H2	24:b:617:CLA:CBB	2.35	0.56
10:k:21:LEU:HD13	17:y:24:MET:HE3	1.88	0.56
1:a:331:MET:SD	4:d:347:PRO:HB2	2.45	0.56
3:c:167:VAL:HG21	24:c:913:CLA:HHB	1.88	0.56
10:k:15:TYR:OH	19:z:58:ASN:ND2	2.37	0.56
26:B:622:BCR:HC41	28:a:402:SQD:H142	1.87	0.56
1:a:309:ALA:HB3	16:v:1:ALA:O	2.05	0.56
5:E:53:ASP:O	16:V:1:ALA:N	2.39	0.56
10:k:21:LEU:HD13	17:y:24:MET:CE	2.35	0.56
1:a:38:ILE:HG12	28:a:402:SQD:H151	1.86	0.56
1:A:63:ILE:HB	3:C:335:THR:HG21	1.87	0.56
26:B:619:BCR:H381	26:B:622:BCR:H341	1.87	0.56
3:C:390:ARG:HD2	16:V:101:PHE:CZ	2.41	0.56
10:K:17:ILE:H	10:K:17:ILE:CD1	2.00	0.55
26:c:915:BCR:HC32	8:i:23:PHE:HB3	1.89	0.55
4:d:236:ASN:O	4:d:239:GLN:HG2	2.07	0.55
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.88	0.55
24:a:407:CLA:HMB2	24:d:403:CLA:H122	1.87	0.55
2:b:393:GLU:HB3	15:u:18:GLY:HA3	1.88	0.55
13:o:42:ARG:O	13:o:241:ALA:HA	2.06	0.55
3:C:323:LYS:O	15:U:47:LYS:HD2	2.06	0.55
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.89	0.55
24:a:406:CLA:HMC3	24:a:406:CLA:HBC3	1.88	0.55
1:A:183:MET:HA	24:A:606:CLA:HMD1	1.89	0.55
28:A:612:SQD:H383	9:J:22:ILE:HD11	1.89	0.55
24:c:903:CLA:H61	24:c:913:CLA:H42	1.87	0.55
3:c:213:LEU:HD11	26:c:915:BCR:H373	1.89	0.55
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.90	0.54
24:a:407:CLA:H101	24:d:403:CLA:H152	1.89	0.54
1:a:131:TRP:CH2	24:c:906:CLA:HAA2	2.42	0.54
3:c:33:PHE:CE1	4:d:229:ALA:HB3	2.43	0.54
1:A:340:PRO:HD3	15:U:103:TYR:CE1	2.42	0.54
11:L:13:ASN:C	11:L:13:ASN:HD22	2.15	0.54
4:d:323:GLU:HB3	13:o:168:TYR:OH	2.07	0.54
29:d:410:LHG:H122	29:d:410:LHG:C37	2.38	0.54
3:c:459:ILE:H	4:d:223:PHE:HA	1.72	0.54
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.89	0.54
2:B:394:GLN:HG3	15:U:17:LEU:O	2.08	0.53
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:404:BCR:H313	31:D:406:DGD:HA91	1.89	0.53
28:A:612:SQD:H321	24:C:508:CLA:H193	1.91	0.53
1:a:63:ILE:HB	3:c:335:THR:HG21	1.89	0.53
4:d:272:LEU:C	4:d:272:LEU:HD23	2.33	0.53
4:D:312:GLU:HB2	13:O:159:PRO:CG	2.38	0.53
5:E:15:THR:HB	9:J:8:ILE:O	2.08	0.53
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.42	0.53
24:D:403:CLA:H121	18:X:18:ALA:HB2	1.90	0.53
7:H:65:LEU:HD12	7:H:66:GLY:H	1.73	0.53
1:a:214:MET:HG2	27:a:410:PL9:C10	2.38	0.53
3:c:339:LYS:NZ	15:u:99:ASN:O	2.41	0.53
2:b:432:PHE:O	13:o:178:LYS:NZ	2.38	0.53
24:B:609:CLA:HMB3	4:D:126:MET:HB3	1.91	0.53
25:a:412:PHO:HBC2	25:a:412:PHO:HHD	1.90	0.53
1:a:214:MET:HG2	27:a:410:PL9:H103	1.90	0.53
5:e:18:ARG:NH2	9:j:1:MET:SD	2.82	0.53
3:c:60:ILE:HG22	24:c:904:CLA:HHD	1.91	0.53
1:a:329:GLU:OE1	16:v:134:LYS:NZ	2.29	0.53
2:b:393:GLU:HB3	15:u:18:GLY:HA2	1.88	0.53
4:d:233:ARG:HH11	4:d:233:ARG:CG	2.18	0.53
2:B:475:PHE:CD1	4:D:140:PRO:HG3	2.44	0.52
1:a:210:LEU:HG	25:a:412:PHO:ND	2.24	0.52
3:c:443:TRP:CZ2	24:c:909:CLA:HMD1	2.44	0.52
3:C:443:TRP:CZ2	24:C:508:CLA:HMD1	2.43	0.52
1:a:310:LYS:NZ	5:e:58:GLN:O	2.38	0.52
24:b:612:CLA:H141	29:b:620:LHG:H382	1.91	0.52
24:C:504:CLA:H201	29:D:409:LHG:H342	1.90	0.52
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.92	0.52
19:z:2:THR:O	19:z:6:GLN:HB2	2.09	0.52
13:O:57:LYS:HE3	2:b:48:SER:O	2.10	0.52
4:d:351:ALA:N	15:u:101:GLY:O	2.42	0.52
2:B:446:SER:HB2	2:B:447:PRO:CD	2.38	0.52
3:C:326:ALA:HB2	15:U:98:TYR:CB	2.40	0.52
1:a:253:GLY:CA	2:b:491:VAL:HG12	2.20	0.52
24:B:603:CLA:H161	31:H:102:DGD:HAW1	1.92	0.52
1:a:340:PRO:HD3	15:u:103:TYR:CZ	2.45	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.51
24:B:609:CLA:HBB2	4:D:150:ILE:HD13	1.93	0.51
24:B:610:CLA:HMD1	7:H:27:THR:HB	1.92	0.51
2:B:385:ARG:HE	15:U:14:ASP:CG	2.15	0.51
2:B:48:SER:O	13:o:57:LYS:HE3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:340:PRO:HG3	3:c:317:PHE:CZ	2.45	0.51
3:c:334:PRO:HA	13:o:153:THR:OG1	2.11	0.51
2:B:248:ALA:HA	24:B:604:CLA:H42	1.92	0.51
24:d:404:CLA:H2	18:x:14:LEU:HA	1.91	0.51
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.45	0.51
2:B:76:SER:O	13:o:111:ALA:HA	2.11	0.51
3:c:321:ASP:OD2	15:u:99:ASN:HB2	2.11	0.51
24:c:902:CLA:C4D	24:c:904:CLA:H2	2.41	0.51
2:B:493:TRP:HB3	5:E:5:THR:HG23	1.93	0.51
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	1.91	0.51
13:o:58:ASN:HA	13:o:60:ARG:HH21	1.76	0.51
13:O:184:ARG:HA	15:U:9:LEU:CD1	2.41	0.50
2:b:383:PHE:CD1	13:o:166:SER:OG	2.64	0.50
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.93	0.50
2:B:325:PHE:CG	11:L:34:TYR:HB3	2.46	0.50
13:O:111:ALA:HB1	2:b:77:GLY:C	2.36	0.50
2:b:442:ILE:CD1	13:o:174:LEU:HD23	2.40	0.50
24:c:905:CLA:C19	29:d:410:LHG:H341	2.38	0.50
3:C:447:ARG:NH2	4:D:229:ALA:HB1	2.27	0.50
24:C:504:CLA:H191	29:D:409:LHG:H341	1.91	0.50
2:b:443:PHE:CE1	13:o:176:GLN:HG3	2.46	0.50
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.94	0.50
24:A:606:CLA:CB1	24:A:614:CLA:HAC2	2.42	0.50
29:D:409:LHG:H132	29:D:409:LHG:C37	2.33	0.50
1:a:311:GLY:HA3	16:v:125:ILE:HG21	1.93	0.50
3:c:390:ARG:HD3	16:v:100:ILE:HD12	1.94	0.50
3:C:326:ALA:HA	15:U:98:TYR:CD2	2.46	0.50
1:a:334:ARG:HD3	4:d:320:LEU:HD13	1.92	0.50
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.47	0.49
1:a:262:TYR:CE2	29:a:413:LHG:HC2	2.46	0.49
1:a:328:MET:HE1	4:d:183:LEU:HD22	1.93	0.49
1:A:334:ARG:HB2	13:O:157:LEU:HD12	1.94	0.49
16:V:37:CYS:SG	32:V:202:HEM:CBB	2.88	0.49
3:c:318:LEU:C	3:c:318:LEU:HD23	2.36	0.49
29:d:410:LHG:H122	29:d:410:LHG:H372	1.94	0.49
7:h:38:PHE:HB2	26:h:101:BCR:C10	2.42	0.49
3:C:390:ARG:HD3	16:V:90:GLU:O	2.13	0.49
4:d:198:MET:SD	24:d:401:CLA:HED2	2.52	0.49
24:A:614:CLA:HMB1	24:A:614:CLA:HBB1	1.95	0.49
1:a:238:LYS:HD2	14:t:30:THR:HG21	1.93	0.49
24:b:612:CLA:C14	29:b:620:LHG:H382	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:396:MET:HE1	16:v:47:LYS:O	2.13	0.49
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.47	0.49
27:A:611:PL9:H503	18:X:24:THR:HG21	1.94	0.49
2:B:36:SER:OG	26:B:619:BCR:H362	2.12	0.49
2:B:422:ARG:O	2:B:425:ILE:HG12	2.13	0.49
3:C:60:ILE:HG22	24:C:503:CLA:HHD	1.95	0.49
5:E:82:GLN:C	5:E:84:LYS:H	2.21	0.49
2:b:383:PHE:CE2	13:o:167:GLY:CA	2.93	0.49
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.94	0.49
24:c:905:CLA:H202	29:d:410:LHG:C17	2.42	0.49
1:a:311:GLY:C	16:v:125:ILE:CG2	2.86	0.49
24:c:907:CLA:HMC2	24:c:908:CLA:H102	1.93	0.49
1:A:247:ASN:HB3	2:B:482:ILE:HD11	1.94	0.49
29:D:409:LHG:H382	29:D:409:LHG:C11	2.42	0.49
24:d:404:CLA:C2	18:x:14:LEU:HA	2.43	0.49
2:B:383:PHE:O	13:O:166:SER:HA	2.12	0.48
24:B:604:CLA:HAB	24:B:606:CLA:H171	1.95	0.48
11:L:13:ASN:HD22	11:L:16:SER:H	1.60	0.48
1:a:224:ILE:HG23	2:b:484:PRO:HA	1.94	0.48
1:A:322:ASN:OD1	3:C:412:THR:HA	2.14	0.48
3:C:324:LEU:HD22	15:U:32:ILE:HD13	1.96	0.48
2:b:385:ARG:NE	15:u:14:ASP:OD1	2.30	0.48
2:B:471:ALA:HB1	4:D:140:PRO:HG2	1.94	0.48
17:Y:38:LEU:O	17:Y:42:ARG:HD3	2.13	0.48
28:A:613:SQD:H252	26:b:619:BCR:H373	1.95	0.48
1:a:330:VAL:HG21	4:d:328:TRP:CE2	2.49	0.48
24:c:911:CLA:H192	24:c:911:CLA:HBC3	1.94	0.48
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.96	0.48
7:h:12:ARG:HB3	7:h:13:PRO:HD3	1.96	0.48
17:y:22:LEU:HA	17:y:25:ILE:HD12	1.95	0.48
28:L:101:SQD:H462	28:L:101:SQD:C1	2.41	0.48
2:B:77:GLY:C	13:o:111:ALA:HB1	2.39	0.48
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.95	0.48
28:a:411:SQD:H321	24:c:909:CLA:H102	1.94	0.48
3:c:373:ASN:ND2	13:o:16:ALA:HA	2.29	0.48
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.49	0.48
3:C:324:LEU:HD13	15:U:32:ILE:HG21	1.96	0.48
1:a:215:HIS:HA	27:a:410:PL9:O1	2.14	0.48
1:a:221:SER:HA	4:d:139:ARG:HB2	1.95	0.48
1:A:334:ARG:NH2	13:O:159:PRO:HA	2.28	0.48
2:B:385:ARG:HB2	15:U:13:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:335:ASN:ND2	13:o:156:PHE:CE1	2.81	0.47
2:b:498:LYS:HA	4:d:24:ARG:HA	1.96	0.47
24:b:604:CLA:HAB	24:b:606:CLA:H171	1.95	0.47
13:o:156:PHE:HB3	13:o:225:MET:HE2	1.93	0.47
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.12	0.47
11:l:14:ARG:HD3	28:l:101:SQD:H241	1.96	0.47
2:B:442:ILE:HD11	13:O:174:LEU:CD2	2.43	0.47
2:b:365:SER:HB3	13:o:172:ILE:HD12	1.95	0.47
24:c:909:CLA:O1D	29:d:410:LHG:HC2	2.14	0.47
4:d:328:TRP:CZ3	16:v:135:VAL:HA	2.50	0.47
5:E:34:GLY:HA3	6:F:32:PHE:O	2.15	0.47
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.96	0.47
28:l:101:SQD:H1	28:l:101:SQD:C46	2.43	0.47
2:b:394:GLN:HG3	15:u:17:LEU:O	2.14	0.47
24:c:911:CLA:H41	29:d:410:LHG:C38	2.44	0.47
3:C:334:PRO:HA	13:O:153:THR:OG1	2.15	0.47
5:e:15:THR:HB	9:j:8:ILE:O	2.15	0.47
3:C:29:GLU:CD	3:C:29:GLU:H	2.22	0.47
3:C:78:GLU:OE2	16:V:106:ASN:ND2	2.48	0.47
24:C:508:CLA:O1D	29:D:409:LHG:HC2	2.15	0.47
1:a:84:PRO:HA	1:a:112:TYR:CG	2.50	0.47
1:a:262:TYR:CZ	29:a:413:LHG:HC32	2.50	0.47
2:b:248:ALA:HA	24:b:604:CLA:H42	1.96	0.47
3:c:26:ARG:HH21	17:y:46:LEU:C	2.20	0.47
24:d:404:CLA:H61	18:x:14:LEU:CD1	2.44	0.47
29:d:410:LHG:H222	31:j:101:DGD:HBH2	1.97	0.47
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.50	0.47
3:C:288:CYS:SG	31:C:516:DGD:HB32	2.55	0.47
3:C:415:ASN:O	3:C:416:SER:HB2	2.14	0.47
25:D:401:PHO:HBC2	25:D:401:PHO:HHD	1.97	0.47
2:b:237:VAL:HG11	24:b:611:CLA:H201	1.97	0.47
2:b:365:SER:CB	13:o:172:ILE:HD12	2.45	0.47
3:c:62:PHE:CE2	26:k:101:BCR:H331	2.50	0.47
24:C:504:CLA:H202	29:D:409:LHG:H172	1.97	0.47
13:O:42:ARG:O	13:O:241:ALA:HA	2.15	0.47
24:c:905:CLA:H101	31:j:101:DGD:HBH1	1.96	0.47
4:d:123:ILE:HD11	31:h:102:DGD:HAH1	1.97	0.47
1:A:309:ALA:HB3	16:V:1:ALA:O	2.14	0.47
2:b:475:PHE:CD1	4:d:140:PRO:HG3	2.50	0.47
24:b:605:CLA:H43	24:b:606:CLA:H2	1.96	0.47
4:d:201:VAL:HG11	24:d:401:CLA:C3D	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.46
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.50	0.46
3:c:33:PHE:CE1	4:d:229:ALA:CB	2.98	0.46
27:d:405:PL9:H411	11:l:29:LEU:HD23	1.97	0.46
10:k:31:LEU:HB3	26:k:101:BCR:C15	2.45	0.46
15:U:43:PRO:HD3	16:V:81:THR:HB	1.97	0.46
1:a:295:PHE:HD1	3:c:291:TRP:CD2	2.33	0.46
1:a:340:PRO:HB3	15:u:103:TYR:CG	2.50	0.46
24:c:907:CLA:H122	24:c:907:CLA:H162	1.75	0.46
4:d:84:SER:O	5:e:69:ARG:HB2	2.14	0.46
26:B:620:BCR:H24C	26:B:620:BCR:H371	1.78	0.46
3:C:25:ASN:HD21	3:C:31:SER:HA	1.79	0.46
3:C:429:SER:HB3	31:C:517:DGD:HBT2	1.98	0.46
3:C:453:ALA:O	8:I:33:LYS:HB3	2.16	0.46
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.98	0.46
24:b:616:CLA:H161	7:h:7:LEU:HD21	1.98	0.46
4:d:192:THR:HG23	24:d:403:CLA:HBC2	1.96	0.46
17:y:20:ALA:O	17:y:24:MET:HG2	2.15	0.46
1:A:340:PRO:HG3	3:C:317:PHE:CZ	2.50	0.46
24:A:606:CLA:CAD	24:A:614:CLA:HAC2	2.45	0.46
3:C:464:GLU:OE2	4:D:245:SER:OG	2.31	0.46
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.98	0.46
1:A:127:MET:CE	24:C:505:CLA:HBB1	2.45	0.46
4:d:205:LEU:HD13	25:d:402:PHO:HAB	1.96	0.46
3:C:332:GLN:O	15:U:94:GLY:HA2	2.16	0.46
4:D:272:LEU:C	4:D:272:LEU:HD23	2.40	0.46
3:c:79:LYS:HD2	16:v:35:TYR:CE1	2.50	0.46
13:o:129:THR:HA	13:o:141:ASP:O	2.16	0.46
24:C:508:CLA:HMB3	24:C:508:CLA:HBB1	1.97	0.46
26:b:618:BCR:H24C	26:b:618:BCR:H371	1.81	0.46
3:c:397:THR:HG21	16:v:40:CYS:SG	2.56	0.46
24:c:909:CLA:H92	29:d:410:LHG:H371	1.98	0.46
29:A:615:LHG:HC12	4:D:27:PHE:CD2	2.51	0.46
15:U:43:PRO:CD	16:V:81:THR:HB	2.46	0.46
27:a:410:PL9:H503	18:x:24:THR:OG1	2.16	0.46
2:b:384:ARG:NH1	15:u:102:LEU:HG	2.30	0.46
25:A:608:PHO:HAB	4:D:205:LEU:HD13	1.98	0.46
2:B:224:ARG:NH1	4:D:16:ASP:OD1	2.42	0.46
2:b:462:PHE:CE2	24:b:614:CLA:HMB3	2.51	0.46
12:M:11:THR:CG2	14:T:9:ILE:HD11	2.47	0.45
3:c:320:ARG:HD2	16:v:49:ASN:CG	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:43:ILE:O	9:j:35:GLY:HA3	2.16	0.45
1:A:64:ARG:O	13:O:152:ARG:NH1	2.45	0.45
3:C:381:LYS:HE3	13:O:99:ASP:OD2	2.14	0.45
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.98	0.45
24:A:609:CLA:H162	24:A:609:CLA:H122	1.76	0.45
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.97	0.45
1:a:278:TRP:CE2	28:a:411:SQD:H223	2.52	0.45
2:b:498:LYS:HE3	4:d:23:LYS:HB2	1.99	0.45
4:D:58:TRP:CD2	5:E:55:TYR:HD1	2.35	0.45
1:a:191:ASN:HB2	3:c:411:ALA:HB1	1.99	0.45
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.51	0.45
29:B:621:LHG:HC81	29:D:407:LHG:O9	2.16	0.45
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.49	0.45
11:L:24:ILE:HG13	12:M:18:PRO:HB2	1.98	0.45
12:M:3:VAL:HG11	14:T:2:GLU:CG	2.41	0.45
12:m:11:THR:CG2	14:t:9:ILE:HD11	2.47	0.45
27:A:611:PL9:H502	4:D:39:PRO:HG3	1.99	0.45
24:B:611:CLA:H152	24:B:611:CLA:OBD	2.17	0.45
24:C:504:CLA:H191	29:D:409:LHG:C34	2.47	0.45
5:E:70:PHE:HZ	7:H:51:SER:HB3	1.81	0.45
3:c:28:GLN:NE2	4:d:233:ARG:NE	2.65	0.45
4:d:266:TRP:CD1	29:d:409:LHG:HC31	2.52	0.45
4:d:312:GLU:HB2	13:o:159:PRO:CG	2.47	0.45
24:C:508:CLA:CBC	29:D:409:LHG:H341	2.47	0.45
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.99	0.45
1:A:311:GLY:HA3	16:V:125:ILE:HG21	1.99	0.45
26:K:101:BCR:H371	26:K:101:BCR:H24C	1.70	0.45
12:M:20:VAL:HG11	12:m:20:VAL:HG21	1.98	0.45
1:a:323:ARG:HD3	16:v:137:TYR:OXT	2.17	0.45
1:a:339:PHE:HB3	1:a:340:PRO:HD2	1.98	0.45
2:b:6:TYR:OH	29:d:408:LHG:HC2	2.16	0.45
1:A:329:GLU:OE1	16:V:134:LYS:NZ	2.41	0.45
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.83	0.45
4:D:70:GLY:O	9:J:37:GLY:HA3	2.16	0.45
4:D:323:GLU:CD	13:O:172:ILE:HD11	2.42	0.45
8:I:33:LYS:HB3	8:I:34:ARG:H	1.50	0.45
13:O:180:GLU:CD	13:O:180:GLU:H	2.24	0.45
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.81	0.45
29:b:620:LHG:HC81	29:d:408:LHG:O9	2.17	0.45
4:d:233:ARG:HG2	4:d:233:ARG:NH1	2.19	0.45
2:B:442:ILE:HD11	13:O:174:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.99	0.44
1:A:215:HIS:HA	27:A:611:PL9:O1	2.17	0.44
2:B:127:ARG:HH11	2:B:127:ARG:CG	2.18	0.44
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.98	0.44
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.44
24:b:607:CLA:H192	24:b:607:CLA:H161	1.62	0.44
4:d:24:ARG:NH1	18:x:35:ASP:CG	2.72	0.44
2:B:494:GLY:HA3	5:E:4:THR:O	2.16	0.44
24:B:607:CLA:H202	28:a:402:SQD:H302	2.00	0.44
4:D:209:LEU:HD23	4:D:209:LEU:C	2.42	0.44
10:K:17:ILE:N	10:K:17:ILE:CD1	2.76	0.44
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.89	0.44
24:c:906:CLA:HAA1	24:c:906:CLA:HBD	1.98	0.44
2:B:138:MET:HE3	24:B:616:CLA:CHD	2.47	0.44
4:D:323:GLU:HB3	13:O:168:TYR:OH	2.17	0.44
5:E:20:TRP:HZ2	9:J:13:VAL:HG13	1.83	0.44
24:a:406:CLA:CBD	24:d:401:CLA:HAC2	2.47	0.44
24:b:612:CLA:H71	29:b:620:LHG:H321	1.99	0.44
29:b:620:LHG:H311	12:m:18:PRO:HB3	2.00	0.44
1:A:262:TYR:CE2	29:A:615:LHG:HC31	2.52	0.44
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.53	0.44
24:a:407:CLA:HAB	24:d:403:CLA:H72	1.98	0.44
3:c:459:ILE:HB	4:d:223:PHE:CD1	2.52	0.44
4:d:101:PHE:HB3	31:d:406:DGD:HG2	1.99	0.44
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.44
4:d:233:ARG:CG	4:d:233:ARG:NH1	2.80	0.44
1:A:334:ARG:HD3	4:D:320:LEU:HD13	1.98	0.44
3:C:318:LEU:C	3:C:318:LEU:HD23	2.43	0.44
24:C:510:CLA:HBC3	24:C:510:CLA:H192	1.99	0.44
4:D:17:ILE:HD12	18:X:36:LYS:HE3	1.99	0.44
2:b:393:GLU:HB3	15:u:18:GLY:N	2.30	0.44
2:b:471:ALA:HB1	4:d:140:PRO:HG2	1.99	0.44
24:b:607:CLA:H72	26:b:619:BCR:H311	2.00	0.44
3:c:323:LYS:O	15:u:47:LYS:HD2	2.18	0.44
1:A:138:GLY:HA2	3:C:455:PHE:CZ	2.53	0.44
28:A:612:SQD:O7	3:C:28:GLN:NE2	2.37	0.44
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	1.99	0.44
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.53	0.44
24:c:914:CLA:HAB	26:c:918:BCR:H24C	1.99	0.44
1:A:215:HIS:ND1	27:A:611:PL9:O1	2.47	0.43
26:b:619:BCR:H24C	26:b:619:BCR:H371	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:LEU:HD22	29:D:407:LHG:H301	1.99	0.43
1:a:131:TRP:CZ3	24:c:906:CLA:CBA	3.01	0.43
1:a:323:ARG:NH1	16:v:135:VAL:O	2.50	0.43
24:C:508:CLA:OBD	29:D:409:LHG:HC31	2.19	0.43
13:O:111:ALA:HA	2:b:76:SER:O	2.18	0.43
2:b:157:HIS:CD2	2:b:157:HIS:C	2.96	0.43
16:v:57:GLU:CD	16:v:57:GLU:H	2.25	0.43
19:z:15:LEU:HD22	19:z:46:LEU:HD23	2.00	0.43
1:A:163:ILE:HD11	31:C:516:DGD:HA22	2.01	0.43
29:A:615:LHG:HC12	4:D:27:PHE:HD2	1.84	0.43
24:c:911:CLA:H51	29:d:410:LHG:H361	2.00	0.43
10:k:46:ARG:NH2	17:y:46:LEU:OXT	2.50	0.43
1:A:32:TRP:CD2	8:I:22:GLY:HA3	2.54	0.43
4:D:85:MET:CE	4:D:96:GLU:HG2	2.49	0.43
13:O:58:ASN:HA	13:O:60:ARG:NH2	2.33	0.43
3:c:42:LEU:HD21	24:c:912:CLA:H2A	2.01	0.43
5:e:52:PRO:HG3	9:j:36:LEU:HD21	2.00	0.43
28:l:101:SQD:H382	12:m:15:VAL:CG1	2.49	0.43
13:o:61:GLN:HG2	13:o:62:GLU:N	2.34	0.43
2:B:13:ILE:HG12	24:B:613:CLA:HAC2	2.00	0.43
3:C:339:LYS:NZ	15:U:94:GLY:O	2.49	0.43
4:D:125:PHE:CE2	25:D:401:PHO:HBD	2.54	0.43
2:b:462:PHE:CZ	24:b:614:CLA:HMB3	2.53	0.43
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.54	0.43
24:B:606:CLA:H62	24:B:606:CLA:H41	1.77	0.43
24:B:616:CLA:H2	24:B:617:CLA:CBB	2.48	0.43
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.43
10:K:10:LYS:HD2	10:K:10:LYS:N	2.34	0.43
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.51	0.43
1:a:262:TYR:HE2	29:a:413:LHG:HC2	1.84	0.43
1:a:334:ARG:HG3	13:o:157:LEU:HB2	2.00	0.43
24:b:615:CLA:H62	24:b:615:CLA:H41	1.62	0.43
24:B:612:CLA:H112	29:B:621:LHG:H342	2.01	0.43
3:c:390:ARG:HD2	16:v:101:PHE:CZ	2.54	0.43
4:d:70:GLY:O	9:j:37:GLY:HA3	2.19	0.43
8:i:33:LYS:HA	8:i:33:LYS:HD3	1.83	0.43
24:C:506:CLA:H162	24:C:506:CLA:H122	1.72	0.42
28:L:101:SQD:H341	28:L:101:SQD:H311	1.81	0.42
2:b:5:TRP:CZ2	29:b:620:LHG:H271	2.53	0.42
24:B:605:CLA:H43	24:B:606:CLA:H2	2.01	0.42
31:C:518:DGD:CGB	29:D:409:LHG:H202	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:37:CYS:CB	32:V:202:HEM:HAB	2.44	0.42
1:a:254:TYR:CD2	4:d:132:ILE:HG22	2.53	0.42
26:D:404:BCR:HC22	31:D:406:DGD:HA72	2.00	0.42
26:T:101:BCR:H341	26:b:618:BCR:H381	2.02	0.42
24:a:408:CLA:H122	24:a:408:CLA:H162	1.85	0.42
7:h:53:LEU:CD1	18:x:7:LEU:HA	2.48	0.42
11:l:14:ARG:HH12	28:l:101:SQD:H3	1.84	0.42
3:C:330:SER:O	13:O:123:LYS:NZ	2.43	0.42
4:D:310:GLU:HG3	13:O:224:ASP:OD2	2.20	0.42
15:U:104:LYS:HG3	16:V:45:ILE:CG2	2.49	0.42
27:a:410:PL9:H13	27:a:410:PL9:H172	1.69	0.42
3:c:397:THR:HB	16:v:39:SER:O	2.20	0.42
25:A:608:PHO:NC	25:A:608:PHO:ND	2.68	0.42
11:L:14:ARG:HH12	28:L:101:SQD:H3	1.85	0.42
13:O:59:LYS:HD2	13:O:61:GLN:CG	2.50	0.42
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.53	0.42
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.42
1:A:249:VAL:HG12	2:B:491:VAL:HG23	2.00	0.42
1:a:323:ARG:HB3	4:d:329:MET:HA	2.01	0.42
2:b:237:VAL:HG12	24:b:613:CLA:HMD1	2.01	0.42
2:B:498:LYS:HE3	4:D:23:LYS:HB2	2.00	0.42
1:a:142:TRP:HZ2	3:c:447:ARG:HB2	1.84	0.42
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.02	0.42
4:D:102:THR:OG1	31:D:406:DGD:HG31	2.19	0.42
2:b:256:MET:HA	2:b:263:THR:HG21	2.02	0.42
6:f:21:VAL:O	6:f:25:THR:HG23	2.20	0.42
3:C:205:ASP:HA	3:C:206:PRO:HD3	1.90	0.42
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.81	0.42
26:T:101:BCR:H24C	26:T:101:BCR:H371	1.89	0.42
8:i:2:GLU:O	8:i:6:ILE:HG12	2.20	0.42
10:k:34:ALA:HB1	26:k:101:BCR:C20	2.50	0.42
19:z:9:LEU:HD13	19:z:54:VAL:HG11	2.01	0.42
2:B:274:GLN:HG2	31:H:102:DGD:O5E	2.20	0.42
24:b:617:CLA:HBB1	24:b:617:CLA:HMB3	2.01	0.42
24:c:913:CLA:H121	24:c:914:CLA:H142	2.02	0.42
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.02	0.41
2:B:157:HIS:C	2:B:157:HIS:CD2	2.98	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
24:B:605:CLA:H141	24:B:605:CLA:H161	1.93	0.41
1:a:323:ARG:HH12	16:v:135:VAL:C	2.28	0.41
24:b:606:CLA:H122	24:b:611:CLA:HMA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:94:THR:HG22	24:c:902:CLA:HED1	2.02	0.41
3:c:406:SER:HA	3:c:420:VAL:HG23	2.02	0.41
24:c:911:CLA:C5	29:d:410:LHG:H361	2.50	0.41
31:C:518:DGD:HBN2	29:D:409:LHG:H202	2.01	0.41
27:D:405:PL9:H512	14:T:10:PHE:HB2	2.03	0.41
1:a:131:TRP:CZ2	24:c:906:CLA:HAA2	2.54	0.41
24:C:502:CLA:H61	24:C:512:CLA:H42	2.03	0.41
1:a:121:LEU:HD21	24:c:906:CLA:H172	2.02	0.41
3:c:447:ARG:HH21	4:d:229:ALA:HB1	1.83	0.41
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.51	0.41
24:A:609:CLA:C1B	8:I:12:VAL:HG22	2.50	0.41
2:B:204:ALA:CB	24:B:603:CLA:HAB	2.50	0.41
24:B:614:CLA:H162	24:B:614:CLA:H121	1.89	0.41
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.56	0.41
29:d:410:LHG:H242	29:d:410:LHG:H272	1.92	0.41
27:A:611:PL9:C22	25:D:401:PHO:HMA2	2.51	0.41
24:C:501:CLA:H42	24:C:502:CLA:HMD3	2.02	0.41
28:L:101:SQD:H381	12:M:16:LEU:HD23	2.03	0.41
26:a:409:BCR:H24C	26:a:409:BCR:H371	1.84	0.41
3:c:437:PHE:HA	24:c:909:CLA:HMC2	2.03	0.41
4:d:351:ALA:CA	15:u:101:GLY:O	2.66	0.41
12:m:3:VAL:HG11	14:t:2:GLU:CG	2.46	0.41
2:B:33:TRP:CD1	26:B:622:BCR:H381	2.55	0.41
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.94	0.41
3:C:343:ARG:HD2	13:O:75:THR:C	2.46	0.41
25:D:401:PHO:HBB1	25:D:401:PHO:HMB1	2.03	0.41
3:c:158:THR:O	3:c:251:HIS:HB3	2.21	0.41
3:c:170:ILE:HD13	24:c:913:CLA:H111	2.03	0.41
2:B:127:ARG:NH1	2:B:127:ARG:CG	2.81	0.41
2:B:220:ARG:HG3	7:H:20:LYS:HD3	2.03	0.41
29:D:409:LHG:H332	29:D:409:LHG:H302	1.88	0.41
1:a:62:GLY:O	3:c:337:LEU:HD11	2.21	0.41
27:a:410:PL9:H403	6:f:22:ALA:HB2	2.02	0.41
24:c:903:CLA:HMB2	24:c:905:CLA:HHC	2.02	0.41
2:B:451:PHE:CD1	2:B:451:PHE:C	2.98	0.41
24:B:611:CLA:HHC	24:B:611:CLA:CBB	2.50	0.41
24:B:617:CLA:HBB1	24:B:617:CLA:HMB3	2.03	0.41
3:C:425:TRP:CD1	24:C:504:CLA:HMA3	2.56	0.41
24:C:504:CLA:HAC2	10:K:26:PRO:O	2.20	0.41
24:C:507:CLA:H41	24:C:507:CLA:H61	1.93	0.41
11:L:7:ARG:HD2	28:l:101:SQD:O8	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:32:TRP:CD2	8:i:22:GLY:HA3	2.56	0.41
1:a:183:MET:HG2	24:d:401:CLA:HBC1	2.03	0.41
1:a:193:LEU:HD13	4:d:179:PHE:HB3	2.03	0.41
27:a:410:PL9:C25	29:a:413:LHG:H201	2.50	0.41
3:c:326:ALA:HB2	15:u:98:TYR:CB	2.50	0.41
3:c:447:ARG:NE	29:d:410:LHG:O2	2.44	0.41
24:c:909:CLA:OBD	29:d:410:LHG:HC31	2.20	0.41
24:c:912:CLA:HMB1	26:k:102:BCR:H382	2.03	0.41
1:A:141:PRO:HG3	3:C:446:GLY:C	2.45	0.41
24:C:509:CLA:HBB1	24:C:509:CLA:CMB	2.47	0.41
3:c:443:TRP:HH2	29:d:410:LHG:O7	2.03	0.41
4:d:102:THR:OG1	31:d:406:DGD:HG31	2.21	0.41
26:k:102:BCR:H24C	26:k:102:BCR:H371	1.80	0.41
13:o:51:LEU:HB3	13:o:65:PHE:HB3	2.02	0.41
13:o:58:ASN:HA	13:o:60:ARG:NH2	2.36	0.41
16:v:41:HIS:HA	16:v:45:ILE:O	2.21	0.41
2:B:385:ARG:HB2	15:U:13:VAL:CG1	2.51	0.40
2:b:63:LEU:N	2:b:64:PRO:HD2	2.36	0.40
24:b:607:CLA:H122	24:b:607:CLA:H162	1.51	0.40
24:c:910:CLA:H192	24:c:913:CLA:HMD1	2.02	0.40
24:B:612:CLA:HBC1	29:D:407:LHG:H321	2.03	0.40
3:C:406:SER:HA	3:C:420:VAL:HG23	2.03	0.40
13:O:112:GLY:HA2	2:b:76:SER:OG	2.21	0.40
17:Y:33:PRO:HD3	26:Y:101:BCR:C16	2.51	0.40
4:d:323:GLU:CD	13:o:172:ILE:HD11	2.45	0.40
28:A:612:SQD:H321	24:C:508:CLA:C19	2.51	0.40
3:C:324:LEU:O	15:U:98:TYR:HE1	2.05	0.40
3:C:338:GLY:HA3	3:C:341:LEU:O	2.21	0.40
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.03	0.40
1:a:340:PRO:HD3	15:u:103:TYR:CE1	2.57	0.40
25:a:412:PHO:ND	25:a:412:PHO:NC	2.70	0.40
3:c:31:SER:HB2	3:c:41:ARG:HG2	2.02	0.40
10:k:28:ILE:HG12	17:y:28:ILE:HG21	2.03	0.40
2:B:118:TRP:CZ2	11:L:4:ASN:HA	2.56	0.40
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.57	0.40
16:v:26:TYR:OH	16:v:122:GLU:OE2	2.36	0.40
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.04	0.40
24:A:609:CLA:H202	24:C:506:CLA:H101	2.02	0.40
2:B:192:PRO:HB3	7:H:49:TYR:CE2	2.57	0.40

All (23) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:37:THR:O	3:c:19:ASN:CG[2_455]	0.56	1.64
13:O:37:THR:O	3:c:19:ASN:ND2[2_455]	0.91	1.29
13:O:36:GLN:NE2	3:c:19:ASN:CA[2_455]	0.99	1.21
13:O:37:THR:N	3:c:19:ASN:OD1[2_455]	1.04	1.16
13:O:36:GLN:NE2	3:c:19:ASN:C[2_455]	1.05	1.15
13:O:35:SER:O	3:c:20:SER:OG[2_455]	1.43	0.77
13:O:36:GLN:NE2	3:c:19:ASN:N[2_455]	1.56	0.64
13:O:37:THR:C	3:c:19:ASN:OD1[2_455]	1.59	0.61
13:O:37:THR:O	3:c:19:ASN:CB[2_455]	1.60	0.60
13:O:37:THR:O	3:c:19:ASN:OD1[2_455]	1.73	0.47
13:O:36:GLN:OE1	3:c:20:SER:N[2_455]	1.77	0.43
13:O:36:GLN:CA	3:c:20:SER:CB[2_455]	1.77	0.43
13:O:36:GLN:CD	3:c:19:ASN:N[2_455]	1.89	0.31
13:O:36:GLN:C	3:c:19:ASN:OD1[2_455]	1.94	0.26
13:O:36:GLN:CD	3:c:19:ASN:C[2_455]	1.97	0.23
13:O:36:GLN:OE1	3:c:20:SER:O[2_455]	2.03	0.17
13:O:35:SER:C	3:c:20:SER:OG[2_455]	2.06	0.14
13:O:37:THR:CA	3:c:19:ASN:CG[2_455]	2.09	0.11
13:O:38:TYR:N	3:c:19:ASN:ND2[2_455]	2.12	0.08
13:O:33:ASP:OD2	3:c:23:ALA:CA[2_455]	2.14	0.06
13:O:246:ALA:OXT	3:c:19:ASN:CB[2_455]	2.14	0.06
13:O:36:GLN:NE2	3:c:19:ASN:CB[2_455]	2.17	0.03
13:O:35:SER:O	3:c:20:SER:CB[2_455]	2.18	0.02

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	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	36	72
1	a	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	36	72
2	B	502/504 (100%)	496 (99%)	6 (1%)	0	100	100
2	b	502/504 (100%)	492 (98%)	10 (2%)	0	100	100
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	43	77
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	339/342 (99%)	333 (98%)	6 (2%)	0	100	100
5	E	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
5	e	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/40 (90%)	36 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/34 (94%)	32 (100%)	0	0	100	100
12	m	32/34 (94%)	32 (100%)	0	0	100	100
13	O	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	30	67
13	o	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	30	67
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	28 (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
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
18	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
18	x	37/39 (95%)	35 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	5191/5276 (98%)	5072 (98%)	113 (2%)	6 (0%)	48	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416	SER
3	c	416	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	269/269 (100%)	268 (100%)	1 (0%)	84	83
1	a	269/269 (100%)	267 (99%)	2 (1%)	76	80
2	B	402/402 (100%)	399 (99%)	3 (1%)	76	80
2	b	402/402 (100%)	397 (99%)	5 (1%)	63	74
3	C	352/356 (99%)	345 (98%)	7 (2%)	48	66
3	c	356/356 (100%)	351 (99%)	5 (1%)	59	72
4	D	277/277 (100%)	275 (99%)	2 (1%)	76	80
4	d	276/277 (100%)	274 (99%)	2 (1%)	76	80
5	E	72/72 (100%)	71 (99%)	1 (1%)	59	72
5	e	72/72 (100%)	70 (97%)	2 (3%)	38	59
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	52
6	f	26/28 (93%)	25 (96%)	1 (4%)	29	51
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	35/35 (100%)	35 (100%)	0	100	100
8	i	35/35 (100%)	35 (100%)	0	100	100
9	J	26/28 (93%)	26 (100%)	0	100	100
9	j	28/28 (100%)	28 (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	35/35 (100%)	33 (94%)	2 (6%)	18	40
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	58
12	M	31/31 (100%)	30 (97%)	1 (3%)	34	55
12	m	31/31 (100%)	31 (100%)	0	100	100
13	O	206/206 (100%)	202 (98%)	4 (2%)	50	66
13	o	206/206 (100%)	201 (98%)	5 (2%)	43	63
14	T	27/27 (100%)	27 (100%)	0	100	100
14	t	27/27 (100%)	25 (93%)	2 (7%)	13	34
15	U	84/84 (100%)	83 (99%)	1 (1%)	63	74
15	u	84/84 (100%)	83 (99%)	1 (1%)	63	74
16	V	117/117 (100%)	116 (99%)	1 (1%)	70	77
16	v	117/117 (100%)	114 (97%)	3 (3%)	40	61
17	Y	22/22 (100%)	21 (96%)	1 (4%)	24	46
17	y	22/22 (100%)	22 (100%)	0	100	100
18	X	32/32 (100%)	32 (100%)	0	100	100
18	x	32/32 (100%)	31 (97%)	1 (3%)	35	56
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
19	z	52/52 (100%)	49 (94%)	3 (6%)	18	40
All	All	4305/4314 (100%)	4239 (98%)	66 (2%)	57	71

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LYS
2	B	86	ILE
2	B	127	ARG

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Mol	Chain	Res	Type
2	B	467	ILE
3	C	24	THR
3	C	25	ASN
3	C	29	GLU
3	C	142	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	11	GLU
4	D	90	LEU
5	E	71	GLU
6	F	44	GLN
7	H	12	ARG
7	H	65	LEU
10	K	13	GLU
10	K	17	ILE
11	L	1	MET
11	L	13	ASN
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
1	a	244	GLU
2	b	14	ASN
2	b	362	PHE
2	b	472	ARG
2	b	491	VAL
2	b	505	ARG
3	c	120	ILE
3	c	240	ILE
3	c	289	PHE
3	c	355	THR
3	c	416	SER
4	d	150	ILE
4	d	233	ARG

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Mol	Chain	Res	Type
5	e	59	GLU
5	e	60	GLN
6	f	44	GLN
10	k	13	GLU
10	k	17	ILE
11	l	1	MET
13	o	55	GLU
13	o	61	GLN
13	o	62	GLU
13	o	194	LYS
13	o	225	MET
14	t	1	MET
14	t	25	GLU
15	u	70	ARG
16	v	17	LYS
16	v	23	GLU
16	v	122	GLU
18	x	2	THR
19	z	1	MET
19	z	3	ILE
19	z	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	315	ASN
2	B	14	ASN
2	B	53	ASN
2	B	281	GLN
2	B	374	ASN
2	B	409	GLN
3	C	25	ASN
3	C	44	ASN
3	C	373	ASN
4	D	83	ASN
4	D	186	GLN
4	D	255	GLN
4	D	332	GLN
5	E	74	GLN
6	F	44	GLN

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Mol	Chain	Res	Type
10	K	40	GLN
11	L	13	ASN
12	M	33	GLN
13	O	124	ASN
13	O	147	ASN
16	V	34	GLN
1	a	165	GLN
1	a	315	ASN
2	b	53	ASN
2	b	281	GLN
2	b	497	GLN
3	c	19	ASN
3	c	28	GLN
3	c	201	ASN
3	c	373	ASN
4	d	83	ASN
4	d	186	GLN
4	d	255	GLN
4	d	332	GLN
5	e	74	GLN
5	e	75	GLN
6	f	44	GLN
13	o	61	GLN
13	o	82	GLN
13	o	124	ASN
13	o	147	ASN
15	u	78	ASN
15	u	81	HIS
16	v	34	GLN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 152 ligands modelled in this entry, 16 are monoatomic - leaving 136 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
24	CLA	B	605	-	69,73,73	2.37	16 (23%)	82,113,113	2.57	27 (32%)
26	BCR	B	618	-	41,41,41	3.49	14 (34%)	56,56,56	7.56	38 (67%)
26	BCR	D	404	-	41,41,41	3.62	14 (34%)	56,56,56	7.88	40 (71%)
32	HEM	V	202	16	50,50,50	1.86	10 (20%)	67,82,82	1.28	4 (5%)
24	CLA	c	909	-	69,73,73	2.37	19 (27%)	82,113,113	2.50	21 (25%)
24	CLA	b	607	-	69,73,73	2.56	19 (27%)	82,113,113	2.58	25 (30%)
28	SQD	a	402	-	52,54,54	1.01	2 (3%)	62,65,65	1.19	5 (8%)
24	CLA	C	502	-	69,73,73	2.20	17 (24%)	82,113,113	2.42	21 (25%)
24	CLA	c	907	-	69,73,73	2.42	19 (27%)	82,113,113	2.52	22 (26%)
26	BCR	k	102	-	41,41,41	3.62	14 (34%)	56,56,56	8.54	43 (76%)
28	SQD	d	407	-	41,43,54	1.13	2 (4%)	51,54,65	1.40	6 (11%)
24	CLA	c	911	-	69,73,73	2.25	17 (24%)	82,113,113	2.47	24 (29%)
26	BCR	b	619	-	41,41,41	3.62	15 (36%)	56,56,56	8.61	42 (75%)
25	PHO	a	412	-	58,69,69	2.67	11 (18%)	55,99,99	2.85	14 (25%)
26	BCR	k	101	-	41,41,41	3.68	14 (34%)	56,56,56	8.61	42 (75%)
24	CLA	a	406	-	69,73,73	2.11	20 (28%)	82,113,113	2.51	24 (29%)
32	HEM	v	202	16	50,50,50	1.89	10 (20%)	67,82,82	1.43	8 (11%)
24	CLA	B	611	-	69,73,73	2.27	18 (26%)	82,113,113	2.51	24 (29%)
24	CLA	B	609	-	69,73,73	2.09	17 (24%)	82,113,113	2.45	26 (31%)
31	DGD	C	516	-	63,63,67	0.88	3 (4%)	77,77,81	0.98	2 (2%)
26	BCR	f	101	-	41,41,41	3.64	15 (36%)	56,56,56	8.06	46 (82%)
24	CLA	b	605	-	69,73,73	2.39	20 (28%)	82,113,113	2.59	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PL9	D	405	-	55,55,55	0.83	2 (3%)	68,69,69	1.32	10 (14%)
31	DGD	C	518	-	63,63,67	0.80	3 (4%)	77,77,81	0.90	3 (3%)
27	PL9	a	410	-	55,55,55	0.71	2 (3%)	68,69,69	1.58	17 (25%)
24	CLA	a	407	-	69,73,73	2.20	17 (24%)	82,113,113	2.42	26 (31%)
26	BCR	B	619	-	41,41,41	3.49	14 (34%)	56,56,56	7.82	41 (73%)
26	BCR	C	515	-	41,41,41	3.63	14 (34%)	56,56,56	8.33	38 (67%)
28	SQD	L	101	-	52,54,54	1.03	3 (5%)	62,65,65	1.40	9 (14%)
29	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	4 (7%)
24	CLA	b	613	-	69,73,73	2.46	15 (21%)	82,113,113	2.50	24 (29%)
24	CLA	c	913	-	69,73,73	2.75	20 (28%)	82,113,113	2.49	26 (31%)
25	PHO	D	401	-	58,69,69	2.68	12 (20%)	55,99,99	2.86	15 (27%)
24	CLA	b	615	-	69,73,73	2.18	16 (23%)	82,113,113	2.68	27 (32%)
24	CLA	b	610	-	69,73,73	2.45	19 (27%)	82,113,113	2.32	21 (25%)
24	CLA	C	508	-	69,73,73	2.50	21 (30%)	82,113,113	2.42	19 (23%)
26	BCR	B	620	-	41,41,41	3.55	14 (34%)	56,56,56	8.51	42 (75%)
24	CLA	B	607	-	69,73,73	2.42	18 (26%)	82,113,113	2.56	26 (31%)
24	CLA	C	505	-	69,73,73	2.35	21 (30%)	82,113,113	2.35	22 (26%)
27	PL9	A	611	-	55,55,55	0.72	2 (3%)	68,69,69	1.55	12 (17%)
24	CLA	b	604	-	69,73,73	2.20	16 (23%)	82,113,113	2.41	24 (29%)
31	DGD	d	406	-	63,63,67	0.97	4 (6%)	77,77,81	0.95	4 (5%)
24	CLA	B	602	-	69,73,73	2.55	21 (30%)	82,113,113	2.60	23 (28%)
24	CLA	B	617	-	69,73,73	2.17	18 (26%)	82,113,113	2.47	26 (31%)
24	CLA	D	402	-	69,73,73	2.09	19 (27%)	82,113,113	2.38	27 (32%)
26	BCR	H	101	-	41,41,41	3.62	14 (34%)	56,56,56	8.34	41 (73%)
24	CLA	C	512	-	69,73,73	2.65	18 (26%)	82,113,113	2.40	26 (31%)
26	BCR	c	915	-	41,41,41	3.61	15 (36%)	56,56,56	8.67	38 (67%)
24	CLA	B	610	-	69,73,73	2.24	19 (27%)	82,113,113	2.43	23 (28%)
26	BCR	A	610	-	41,41,41	3.54	14 (34%)	56,56,56	7.79	37 (66%)
26	BCR	b	618	-	41,41,41	3.52	14 (34%)	56,56,56	8.04	44 (78%)
24	CLA	c	904	-	69,73,73	2.57	18 (26%)	82,113,113	2.48	23 (28%)
29	LHG	A	615	-	41,41,48	1.05	2 (4%)	44,47,54	1.08	3 (6%)
24	CLA	b	614	-	69,73,73	2.15	16 (23%)	82,113,113	2.53	24 (29%)
24	CLA	B	608	-	69,73,73	2.27	18 (26%)	82,113,113	2.41	23 (28%)
24	CLA	C	513	-	69,73,73	2.61	19 (27%)	82,113,113	2.43	24 (29%)
31	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.86	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SQD	F	101	-	41,43,54	1.16	3 (7%)	51,54,65	1.42	7 (13%)
24	CLA	A	606	-	69,73,73	2.13	17 (24%)	82,113,113	2.38	24 (29%)
24	CLA	c	908	-	69,73,73	2.45	19 (27%)	82,113,113	2.64	24 (29%)
31	DGD	c	917	-	63,63,67	0.88	2 (3%)	77,77,81	0.80	3 (3%)
24	CLA	A	614	-	69,73,73	1.97	18 (26%)	82,113,113	2.38	24 (29%)
25	PHO	A	608	-	58,69,69	2.53	12 (20%)	55,99,99	2.95	11 (20%)
24	CLA	B	612	-	69,73,73	2.11	16 (23%)	82,113,113	2.51	23 (28%)
24	CLA	c	910	-	69,73,73	2.39	19 (27%)	82,113,113	2.64	25 (30%)
24	CLA	b	609	-	69,73,73	2.34	20 (28%)	82,113,113	2.41	22 (26%)
29	LHG	d	410	-	48,48,48	0.92	2 (4%)	51,54,54	0.97	4 (7%)
24	CLA	C	503	-	69,73,73	2.47	18 (26%)	82,113,113	2.41	21 (25%)
24	CLA	d	404	-	69,73,73	2.39	21 (30%)	82,113,113	2.48	26 (31%)
24	CLA	B	614	-	69,73,73	2.26	18 (26%)	82,113,113	2.47	24 (29%)
24	CLA	b	616	-	69,73,73	2.33	15 (21%)	82,113,113	2.46	24 (29%)
29	LHG	b	620	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	3 (5%)
24	CLA	A	609	-	69,73,73	2.19	16 (23%)	82,113,113	2.55	24 (29%)
32	HEM	e	101	5,6	50,50,50	2.02	11 (22%)	67,82,82	1.27	4 (5%)
24	CLA	c	905	-	69,73,73	2.52	22 (31%)	82,113,113	2.56	23 (28%)
26	BCR	T	101	-	41,41,41	3.62	15 (36%)	56,56,56	7.16	39 (69%)
31	DGD	c	916	-	63,63,67	0.86	3 (4%)	77,77,81	0.90	3 (3%)
28	SQD	A	613	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
24	CLA	D	403	-	69,73,73	2.37	19 (27%)	82,113,113	2.50	22 (26%)
24	CLA	b	603	-	69,73,73	2.35	20 (28%)	82,113,113	2.33	22 (26%)
24	CLA	a	408	-	69,73,73	2.17	17 (24%)	82,113,113	2.45	26 (31%)
31	DGD	H	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.94	4 (5%)
32	HEM	E	101	5,6	50,50,50	1.98	10 (20%)	67,82,82	1.35	5 (7%)
24	CLA	d	403	-	69,73,73	2.11	17 (24%)	82,113,113	2.41	22 (26%)
24	CLA	B	603	-	69,73,73	2.34	19 (27%)	82,113,113	2.33	21 (25%)
24	CLA	B	606	-	69,73,73	2.31	17 (24%)	82,113,113	2.40	24 (29%)
24	CLA	C	504	-	69,73,73	2.36	19 (27%)	82,113,113	2.49	23 (28%)
24	CLA	d	401	-	69,73,73	2.30	16 (23%)	82,113,113	2.48	23 (28%)
28	SQD	l	101	-	52,54,54	0.99	3 (5%)	62,65,65	1.33	8 (12%)
29	LHG	B	621	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	4 (7%)
23	BCT	a	414	21	3,3,3	1.36	1 (33%)	2,3,3	0.72	0
26	BCR	K	101	-	41,41,41	3.58	14 (34%)	56,56,56	7.86	43 (76%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	a	413	-	41,41,48	1.05	2 (4%)	44,47,54	0.91	2 (4%)
24	CLA	b	606	-	69,73,73	2.30	20 (28%)	82,113,113	2.47	24 (29%)
24	CLA	C	507	-	69,73,73	2.45	20 (28%)	82,113,113	2.59	26 (31%)
24	CLA	B	604	-	69,73,73	2.19	18 (26%)	82,113,113	2.54	26 (31%)
24	CLA	b	617	-	69,73,73	2.29	19 (27%)	82,113,113	2.48	26 (31%)
29	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	3 (5%)
26	BCR	C	514	-	41,41,41	3.68	15 (36%)	56,56,56	8.55	36 (64%)
26	BCR	B	622	-	41,41,41	3.60	15 (36%)	56,56,56	7.70	36 (64%)
24	CLA	b	612	-	69,73,73	2.22	15 (21%)	82,113,113	2.46	24 (29%)
20	OEX	A	601	1,3	0,15,15	-	-	-	-	-
24	CLA	c	902	-	69,73,73	2.30	19 (27%)	82,113,113	2.67	25 (30%)
24	CLA	C	511	3	69,73,73	2.46	18 (26%)	82,113,113	2.60	23 (28%)
24	CLA	A	607	-	69,73,73	2.28	18 (26%)	82,113,113	2.56	25 (30%)
26	BCR	T	102	-	41,41,41	3.52	15 (36%)	56,56,56	7.29	38 (67%)
26	BCR	c	918	-	41,41,41	3.44	15 (36%)	56,56,56	7.70	36 (64%)
24	CLA	C	501	-	69,73,73	2.28	18 (26%)	82,113,113	2.53	23 (28%)
31	DGD	D	406	-	63,63,67	1.00	4 (6%)	77,77,81	1.03	6 (7%)
24	CLA	c	906	-	69,73,73	2.27	19 (27%)	82,113,113	2.45	22 (26%)
29	LHG	D	408	-	48,48,48	0.90	3 (6%)	51,54,54	0.85	2 (3%)
26	BCR	h	101	-	41,41,41	3.61	14 (34%)	56,56,56	8.48	42 (75%)
24	CLA	C	509	-	69,73,73	2.44	19 (27%)	82,113,113	2.60	27 (32%)
24	CLA	b	602	-	69,73,73	2.54	20 (28%)	82,113,113	2.49	26 (31%)
25	PHO	d	402	-	58,69,69	2.51	13 (22%)	55,99,99	2.81	13 (23%)
23	BCT	A	605	21	3,3,3	1.46	1 (33%)	2,3,3	0.26	0
24	CLA	b	611	-	69,73,73	2.35	18 (26%)	82,113,113	2.49	22 (26%)
24	CLA	b	608	-	69,73,73	2.38	17 (24%)	82,113,113	2.35	24 (29%)
31	DGD	j	101	-	63,63,67	0.88	3 (4%)	77,77,81	0.87	3 (3%)
24	CLA	B	613	-	69,73,73	2.35	19 (27%)	82,113,113	2.44	21 (25%)
24	CLA	C	510	-	69,73,73	2.31	20 (28%)	82,113,113	2.53	26 (31%)
27	PL9	d	405	-	55,55,55	0.82	2 (3%)	68,69,69	1.30	8 (11%)
24	CLA	C	506	-	69,73,73	2.33	20 (28%)	82,113,113	2.48	24 (29%)
31	DGD	C	517	-	63,63,67	0.89	2 (3%)	77,77,81	0.86	4 (5%)
28	SQD	a	411	-	52,54,54	0.93	2 (3%)	62,65,65	1.53	10 (16%)
26	BCR	a	409	-	41,41,41	3.48	14 (34%)	56,56,56	7.87	34 (60%)
24	CLA	B	616	-	69,73,73	2.44	20 (28%)	82,113,113	2.50	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	OEX	a	401	1,3	0,15,15	-	-	-		
29	LHG	d	409	-	48,48,48	0.85	2 (4%)	51,54,54	0.92	3 (5%)
24	CLA	c	912	3	69,73,73	2.57	20 (28%)	82,113,113	2.52	23 (28%)
24	CLA	c	914	-	69,73,73	2.75	21 (30%)	82,113,113	2.37	25 (30%)
29	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	0.91	3 (5%)
28	SQD	A	612	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)
24	CLA	c	903	-	69,73,73	2.29	17 (24%)	82,113,113	2.59	22 (26%)
26	BCR	Y	101	-	41,41,41	3.65	14 (34%)	56,56,56	8.11	36 (64%)
24	CLA	B	615	-	69,73,73	2.23	19 (27%)	82,113,113	2.51	27 (32%)

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
24	CLA	B	605	-	1/1/15/20	4/39/115/115	-
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
26	BCR	D	404	-	-	6/29/63/63	0/2/2/2
32	HEM	V	202	16	-	6/14/54/54	-
24	CLA	c	909	-	-	4/39/115/115	-
24	CLA	b	607	-	1/1/15/20	10/39/115/115	-
28	SQD	a	402	-	-	21/49/69/69	0/1/1/1
24	CLA	C	502	-	-	7/39/115/115	-
24	CLA	c	907	-	1/1/15/20	11/39/115/115	-
26	BCR	k	102	-	-	10/29/63/63	0/2/2/2
28	SQD	d	407	-	-	21/38/58/69	0/1/1/1
24	CLA	c	911	-	1/1/15/20	6/39/115/115	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	PHO	a	412	-	-	2/37/103/103	0/5/6/6
26	BCR	k	101	-	-	8/29/63/63	0/2/2/2
24	CLA	a	406	-	1/1/15/20	2/39/115/115	-
32	HEM	v	202	16	-	6/14/54/54	-
24	CLA	B	611	-	1/1/15/20	7/39/115/115	-
24	CLA	B	609	-	-	1/39/115/115	-
31	DGD	C	516	-	-	24/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	f	101	-	-	7/29/63/63	0/2/2/2
24	CLA	b	605	-	1/1/15/20	5/39/115/115	-
27	PL9	D	405	-	-	1/53/73/73	0/1/1/1
31	DGD	C	518	-	-	16/51/91/95	0/2/2/2
27	PL9	a	410	-	-	10/53/73/73	0/1/1/1
24	CLA	a	407	-	-	11/39/115/115	-
26	BCR	B	619	-	-	4/29/63/63	0/2/2/2
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
28	SQD	L	101	-	-	29/49/69/69	0/1/1/1
29	LHG	D	407	-	-	13/53/53/53	-
24	CLA	b	613	-	1/1/15/20	5/39/115/115	-
24	CLA	c	913	-	1/1/15/20	13/39/115/115	-
25	PHO	D	401	-	-	4/37/103/103	0/5/6/6
24	CLA	b	615	-	1/1/15/20	17/39/115/115	-
24	CLA	b	610	-	-	2/39/115/115	-
24	CLA	C	508	-	-	5/39/115/115	-
26	BCR	B	620	-	-	1/29/63/63	0/2/2/2
24	CLA	C	505	-	1/1/15/20	2/39/115/115	-
24	CLA	B	607	-	-	7/39/115/115	-
27	PL9	A	611	-	-	9/53/73/73	0/1/1/1
24	CLA	b	604	-	1/1/15/20	6/39/115/115	-
31	DGD	d	406	-	-	33/51/91/95	0/2/2/2
24	CLA	B	602	-	1/1/15/20	18/39/115/115	-
24	CLA	B	617	-	1/1/15/20	15/39/115/115	-
24	CLA	D	402	-	1/1/15/20	5/39/115/115	-
26	BCR	H	101	-	-	8/29/63/63	0/2/2/2
24	CLA	C	512	-	1/1/15/20	9/39/115/115	-
26	BCR	c	915	-	-	8/29/63/63	0/2/2/2
24	CLA	B	610	-	1/1/15/20	0/39/115/115	-
26	BCR	A	610	-	-	4/29/63/63	0/2/2/2
26	BCR	b	618	-	-	3/29/63/63	0/2/2/2
24	CLA	c	904	-	-	3/39/115/115	-
29	LHG	A	615	-	-	24/46/46/53	-
24	CLA	b	614	-	1/1/15/20	6/39/115/115	-
24	CLA	B	608	-	1/1/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	513	-	-	9/39/115/115	-
31	DGD	h	102	-	-	13/51/91/95	0/2/2/2
28	SQD	F	101	-	-	17/38/58/69	0/1/1/1
24	CLA	A	606	-	1/1/15/20	3/39/115/115	-
24	CLA	c	908	-	1/1/15/20	10/39/115/115	-
31	DGD	c	917	-	-	18/51/91/95	0/2/2/2
24	CLA	A	614	-	-	2/39/115/115	-
25	PHO	A	608	-	-	2/37/103/103	0/5/6/6
24	CLA	B	612	-	-	3/39/115/115	-
24	CLA	c	910	-	1/1/15/20	9/39/115/115	-
24	CLA	b	609	-	-	1/39/115/115	-
29	LHG	d	410	-	-	17/53/53/53	-
24	CLA	C	503	-	1/1/15/20	1/39/115/115	-
24	CLA	d	404	-	-	7/39/115/115	-
24	CLA	B	614	-	1/1/15/20	3/39/115/115	-
24	CLA	b	616	-	1/1/15/20	11/39/115/115	-
29	LHG	b	620	-	-	17/53/53/53	-
24	CLA	A	609	-	-	13/39/115/115	-
32	HEM	e	101	5,6	-	4/14/54/54	-
24	CLA	c	905	-	-	9/39/115/115	-
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
31	DGD	c	916	-	-	20/51/91/95	0/2/2/2
28	SQD	A	613	-	-	23/49/69/69	0/1/1/1
24	CLA	b	603	-	1/1/15/20	2/39/115/115	-
24	CLA	D	403	-	-	14/39/115/115	-
24	CLA	a	408	-	-	11/39/115/115	-
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
32	HEM	E	101	5,6	-	4/14/54/54	-
24	CLA	d	403	-	1/1/15/20	5/39/115/115	-
24	CLA	B	603	-	1/1/15/20	0/39/115/115	-
24	CLA	B	606	-	1/1/15/20	5/39/115/115	-
24	CLA	C	504	-	1/1/15/20	9/39/115/115	-
24	CLA	d	401	-	-	2/39/115/115	-
28	SQD	l	101	-	-	28/49/69/69	0/1/1/1
29	LHG	B	621	-	-	17/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	a	413	-	-	25/46/46/53	-
26	BCR	K	101	-	-	11/29/63/63	0/2/2/2
24	CLA	b	606	-	1/1/15/20	4/39/115/115	-
24	CLA	C	507	-	1/1/15/20	11/39/115/115	-
24	CLA	B	604	-	1/1/15/20	5/39/115/115	-
24	CLA	b	617	-	1/1/15/20	12/39/115/115	-
29	LHG	d	408	-	-	11/53/53/53	-
26	BCR	C	514	-	-	5/29/63/63	0/2/2/2
26	BCR	B	622	-	-	4/29/63/63	0/2/2/2
24	CLA	b	612	-	-	4/39/115/115	-
24	CLA	c	902	-	1/1/15/20	3/39/115/115	-
24	CLA	C	511	3	-	0/39/115/115	-
24	CLA	A	607	-	-	7/39/115/115	-
26	BCR	T	102	-	-	3/29/63/63	0/2/2/2
26	BCR	c	918	-	-	13/29/63/63	0/2/2/2
24	CLA	C	501	-	-	9/39/115/115	-
31	DGD	D	406	-	-	33/51/91/95	0/2/2/2
24	CLA	c	906	-	1/1/15/20	4/39/115/115	-
29	LHG	D	408	-	-	13/53/53/53	-
26	BCR	h	101	-	-	9/29/63/63	0/2/2/2
24	CLA	C	509	-	1/1/15/20	8/39/115/115	-
24	CLA	b	602	-	1/1/15/20	18/39/115/115	-
25	PHO	d	402	-	-	1/37/103/103	0/5/6/6
24	CLA	b	611	-	1/1/15/20	4/39/115/115	-
24	CLA	b	608	-	1/1/15/20	1/39/115/115	-
31	DGD	j	101	-	-	18/51/91/95	0/2/2/2
24	CLA	B	613	-	1/1/15/20	3/39/115/115	-
24	CLA	C	510	-	1/1/15/20	6/39/115/115	-
27	PL9	d	405	-	-	3/53/73/73	0/1/1/1
24	CLA	C	506	-	1/1/15/20	14/39/115/115	-
31	DGD	C	517	-	-	24/51/91/95	0/2/2/2
28	SQD	a	411	-	-	23/49/69/69	0/1/1/1
26	BCR	a	409	-	-	2/29/63/63	0/2/2/2
24	CLA	B	616	-	1/1/15/20	11/39/115/115	-
29	LHG	d	409	-	-	10/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	912	3	-	7/39/115/115	-
24	CLA	c	914	-	-	15/39/115/115	-
29	LHG	D	409	-	-	12/53/53/53	-
28	SQD	A	612	-	-	17/49/69/69	0/1/1/1
24	CLA	c	903	-	-	4/39/115/115	-
26	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
24	CLA	B	615	-	1/1/15/20	10/39/115/115	-

All (1773) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NA	14.06	2.39	2.06
24	c	914	CLA	MG-NC	12.56	2.36	2.06
24	b	613	CLA	MG-NA	12.54	2.36	2.06
24	c	913	CLA	MG-NA	12.23	2.35	2.06
24	B	605	CLA	MG-NA	12.05	2.34	2.06
24	B	616	CLA	MG-NA	11.79	2.34	2.06
24	b	607	CLA	MG-NA	11.61	2.33	2.06
24	C	513	CLA	MG-NA	11.55	2.33	2.06
24	C	511	CLA	MG-NA	11.41	2.33	2.06
24	C	507	CLA	MG-NA	11.40	2.33	2.06
24	d	401	CLA	MG-NA	11.29	2.33	2.06
24	B	607	CLA	MG-NA	11.19	2.32	2.06
24	C	503	CLA	MG-NC	11.10	2.32	2.06
24	B	613	CLA	MG-NA	10.93	2.32	2.06
24	A	607	CLA	MG-NA	10.92	2.32	2.06
24	b	609	CLA	MG-NA	10.67	2.31	2.06
24	C	509	CLA	MG-NA	10.32	2.30	2.06
24	B	602	CLA	MG-NA	10.25	2.30	2.06
24	C	508	CLA	MG-NA	10.15	2.30	2.06
24	b	610	CLA	MG-NC	10.00	2.30	2.06
24	c	904	CLA	MG-NA	9.99	2.30	2.06
24	b	616	CLA	MG-NA	9.92	2.29	2.06
24	B	614	CLA	MG-NA	9.84	2.29	2.06
24	b	602	CLA	MG-NC	9.83	2.29	2.06
24	c	910	CLA	MG-NA	9.80	2.29	2.06
24	C	506	CLA	MG-NA	9.74	2.29	2.06
24	B	606	CLA	MG-NA	9.67	2.29	2.06
24	b	617	CLA	MG-NA	9.52	2.28	2.06
24	c	904	CLA	MG-NC	9.49	2.28	2.06
25	D	401	PHO	C1D-C2D	9.42	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	MG-NA	9.40	2.28	2.06
24	C	505	CLA	MG-NA	9.38	2.28	2.06
24	c	912	CLA	MG-NC	9.37	2.28	2.06
25	a	412	PHO	C1D-C2D	9.33	1.49	1.39
24	D	403	CLA	MG-NA	9.32	2.28	2.06
25	a	412	PHO	C1B-C2B	9.28	1.49	1.39
25	A	608	PHO	C1B-C2B	9.26	1.49	1.39
24	B	603	CLA	MG-NA	9.24	2.28	2.06
24	b	605	CLA	MG-NA	9.23	2.28	2.06
24	b	604	CLA	MG-NA	9.15	2.28	2.06
24	C	501	CLA	MG-NA	9.15	2.28	2.06
24	c	902	CLA	MG-NA	9.14	2.28	2.06
24	B	608	CLA	MG-NA	9.08	2.27	2.06
24	c	909	CLA	MG-NA	9.08	2.27	2.06
24	C	510	CLA	MG-NA	9.03	2.27	2.06
24	d	404	CLA	MG-NA	9.02	2.27	2.06
24	c	907	CLA	MG-NA	8.97	2.27	2.06
24	b	603	CLA	MG-NC	8.96	2.27	2.06
26	c	918	BCR	C8-C9	-8.95	1.26	1.46
25	D	401	PHO	C1B-C2B	8.92	1.49	1.39
25	A	608	PHO	C1D-C2D	8.92	1.49	1.39
26	b	619	BCR	C8-C9	-8.90	1.26	1.46
26	B	622	BCR	C8-C9	-8.85	1.27	1.46
26	C	514	BCR	C8-C9	-8.83	1.27	1.46
26	C	514	BCR	C12-C13	-8.80	1.27	1.46
26	c	915	BCR	C8-C9	-8.79	1.27	1.46
24	c	905	CLA	MG-NC	8.76	2.27	2.06
24	b	608	CLA	MG-NA	8.75	2.27	2.06
26	D	404	BCR	C8-C9	-8.74	1.27	1.46
24	B	612	CLA	MG-NA	8.74	2.27	2.06
26	c	918	BCR	C12-C13	-8.73	1.27	1.46
26	K	101	BCR	C8-C9	-8.73	1.27	1.46
24	c	908	CLA	MG-NA	8.73	2.27	2.06
26	h	101	BCR	C8-C9	-8.73	1.27	1.46
26	k	101	BCR	C8-C9	-8.72	1.27	1.46
26	f	101	BCR	C8-C9	-8.70	1.27	1.46
26	H	101	BCR	C19-C18	-8.69	1.27	1.46
26	T	101	BCR	C8-C9	-8.68	1.27	1.46
26	f	101	BCR	C19-C18	-8.68	1.27	1.46
26	k	101	BCR	C12-C13	-8.67	1.27	1.46
26	C	515	BCR	C8-C9	-8.65	1.27	1.46
26	Y	101	BCR	C8-C9	-8.65	1.27	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	101	BCR	C19-C18	-8.64	1.27	1.46
26	k	101	BCR	C19-C18	-8.63	1.27	1.46
26	Y	101	BCR	C19-C18	-8.60	1.27	1.46
24	b	611	CLA	MG-NA	8.59	2.26	2.06
26	k	102	BCR	C8-C9	-8.59	1.27	1.46
24	c	908	CLA	MG-NC	8.58	2.26	2.06
26	B	620	BCR	C8-C9	-8.57	1.27	1.46
25	d	402	PHO	C1B-C2B	8.57	1.48	1.39
26	k	102	BCR	C19-C18	-8.56	1.27	1.46
26	Y	101	BCR	C12-C13	-8.56	1.27	1.46
25	d	402	PHO	C1D-C2D	8.55	1.48	1.39
24	b	612	CLA	MG-NA	8.55	2.26	2.06
26	B	622	BCR	C12-C13	-8.53	1.27	1.46
26	C	514	BCR	C19-C18	-8.53	1.27	1.46
26	T	101	BCR	C12-C13	-8.53	1.27	1.46
26	B	620	BCR	C12-C13	-8.53	1.27	1.46
26	c	918	BCR	C19-C18	-8.52	1.27	1.46
26	k	102	BCR	C12-C13	-8.51	1.27	1.46
26	C	515	BCR	C19-C18	-8.50	1.27	1.46
26	B	618	BCR	C8-C9	-8.50	1.27	1.46
26	H	101	BCR	C12-C13	-8.50	1.27	1.46
26	H	101	BCR	C8-C9	-8.49	1.27	1.46
24	c	906	CLA	MG-NA	8.48	2.26	2.06
26	b	618	BCR	C8-C9	-8.48	1.27	1.46
26	D	404	BCR	C19-C18	-8.47	1.27	1.46
26	b	619	BCR	C12-C13	-8.47	1.27	1.46
26	B	619	BCR	C8-C9	-8.47	1.27	1.46
26	b	619	BCR	C19-C18	-8.47	1.27	1.46
26	C	515	BCR	C12-C13	-8.46	1.27	1.46
24	B	604	CLA	MG-NA	8.46	2.26	2.06
26	T	102	BCR	C8-C9	-8.44	1.27	1.46
26	K	101	BCR	C19-C18	-8.44	1.27	1.46
26	A	610	BCR	C8-C9	-8.43	1.27	1.46
26	c	915	BCR	C19-C18	-8.42	1.27	1.46
26	b	618	BCR	C12-C13	-8.42	1.27	1.46
26	c	915	BCR	C12-C13	-8.39	1.28	1.46
26	h	101	BCR	C12-C13	-8.39	1.28	1.46
26	T	101	BCR	C19-C18	-8.39	1.28	1.46
26	D	404	BCR	C12-C13	-8.37	1.28	1.46
26	B	622	BCR	C19-C18	-8.35	1.28	1.46
26	f	101	BCR	C12-C13	-8.34	1.28	1.46
26	B	619	BCR	C19-C18	-8.32	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	102	BCR	C19-C18	-8.32	1.28	1.46
26	K	101	BCR	C12-C13	-8.30	1.28	1.46
24	c	903	CLA	MG-NA	8.29	2.26	2.06
26	B	618	BCR	C12-C13	-8.29	1.28	1.46
26	T	102	BCR	C12-C13	-8.26	1.28	1.46
26	A	610	BCR	C12-C13	-8.26	1.28	1.46
26	A	610	BCR	C19-C18	-8.24	1.28	1.46
26	a	409	BCR	C8-C9	-8.23	1.28	1.46
26	B	620	BCR	C19-C18	-8.20	1.28	1.46
26	B	619	BCR	C12-C13	-8.19	1.28	1.46
26	a	409	BCR	C12-C13	-8.18	1.28	1.46
26	b	618	BCR	C19-C18	-8.15	1.28	1.46
26	a	409	BCR	C19-C18	-8.13	1.28	1.46
24	C	502	CLA	MG-NA	8.07	2.25	2.06
26	B	618	BCR	C19-C18	-8.06	1.28	1.46
32	e	101	HEM	C3D-C2D	8.03	1.54	1.36
24	C	504	CLA	MG-NC	8.00	2.25	2.06
32	E	101	HEM	C3D-C2D	7.69	1.53	1.36
24	c	912	CLA	MG-NA	7.65	2.24	2.06
24	a	407	CLA	MG-NA	7.64	2.24	2.06
32	v	202	HEM	C3D-C2D	7.61	1.53	1.36
26	k	101	BCR	C20-C21	-7.60	1.19	1.43
24	d	403	CLA	MG-NA	7.60	2.24	2.06
24	a	408	CLA	MG-NA	7.59	2.24	2.06
26	f	101	BCR	C20-C21	-7.57	1.19	1.43
24	c	911	CLA	MG-NC	7.52	2.24	2.06
26	Y	101	BCR	C20-C21	-7.51	1.19	1.43
26	D	404	BCR	C20-C21	-7.47	1.20	1.43
26	k	102	BCR	C20-C21	-7.46	1.20	1.43
26	C	514	BCR	C20-C21	-7.45	1.20	1.43
26	k	101	BCR	C16-C17	-7.45	1.20	1.43
26	C	515	BCR	C20-C21	-7.43	1.20	1.43
24	B	611	CLA	MG-NA	7.43	2.23	2.06
26	H	101	BCR	C20-C21	-7.43	1.20	1.43
26	f	101	BCR	C16-C17	-7.43	1.20	1.43
26	C	514	BCR	C16-C17	-7.42	1.20	1.43
26	Y	101	BCR	C16-C17	-7.42	1.20	1.43
26	C	515	BCR	C16-C17	-7.39	1.20	1.43
26	h	101	BCR	C20-C21	-7.39	1.20	1.43
24	a	406	CLA	MG-NA	7.38	2.23	2.06
26	b	619	BCR	C20-C21	-7.38	1.20	1.43
24	b	615	CLA	MG-NC	7.38	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	915	BCR	C20-C21	-7.36	1.20	1.43
24	c	905	CLA	MG-NA	7.36	2.23	2.06
26	K	101	BCR	C20-C21	-7.35	1.20	1.43
26	h	101	BCR	C16-C17	-7.34	1.20	1.43
26	H	101	BCR	C16-C17	-7.33	1.20	1.43
26	k	102	BCR	C16-C17	-7.32	1.20	1.43
26	b	619	BCR	C16-C17	-7.31	1.20	1.43
26	T	101	BCR	C16-C17	-7.29	1.20	1.43
26	c	915	BCR	C16-C17	-7.28	1.20	1.43
26	B	622	BCR	C16-C17	-7.28	1.20	1.43
26	D	404	BCR	C16-C17	-7.28	1.20	1.43
26	T	101	BCR	C20-C21	-7.27	1.20	1.43
26	A	610	BCR	C20-C21	-7.26	1.20	1.43
26	B	620	BCR	C16-C17	-7.23	1.20	1.43
26	B	619	BCR	C20-C21	-7.22	1.20	1.43
26	A	610	BCR	C16-C17	-7.22	1.20	1.43
26	b	618	BCR	C20-C21	-7.21	1.20	1.43
26	K	101	BCR	C16-C17	-7.20	1.20	1.43
32	V	202	HEM	C3D-C2D	7.19	1.52	1.36
26	B	622	BCR	C20-C21	-7.18	1.20	1.43
24	A	606	CLA	MG-NA	7.18	2.23	2.06
26	T	102	BCR	C16-C17	-7.17	1.20	1.43
26	a	409	BCR	C16-C17	-7.17	1.21	1.43
26	c	918	BCR	C20-C21	-7.15	1.21	1.43
26	B	620	BCR	C20-C21	-7.15	1.21	1.43
26	B	618	BCR	C20-C21	-7.15	1.21	1.43
26	B	618	BCR	C16-C17	-7.10	1.21	1.43
26	T	102	BCR	C20-C21	-7.10	1.21	1.43
26	b	618	BCR	C16-C17	-7.09	1.21	1.43
24	B	615	CLA	MG-NC	7.05	2.23	2.06
26	B	619	BCR	C16-C17	-7.05	1.21	1.43
24	B	602	CLA	MG-NC	6.98	2.22	2.06
24	b	614	CLA	MG-NA	6.98	2.22	2.06
26	a	409	BCR	C20-C21	-6.98	1.21	1.43
24	c	909	CLA	MG-NC	6.97	2.22	2.06
24	b	602	CLA	MG-NA	6.87	2.22	2.06
24	C	513	CLA	MG-NC	6.80	2.22	2.06
24	C	504	CLA	MG-NA	6.79	2.22	2.06
25	a	412	PHO	C3B-C4B	6.78	1.48	1.41
24	B	617	CLA	MG-NA	6.71	2.22	2.06
24	c	913	CLA	MG-ND	-6.67	1.92	2.05
24	B	610	CLA	MG-NA	6.57	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	C3B-C4B	6.51	1.48	1.41
24	B	615	CLA	MG-NA	6.38	2.21	2.06
24	B	610	CLA	MG-NC	6.35	2.21	2.06
24	c	907	CLA	MG-ND	-6.25	1.93	2.05
24	B	609	CLA	MG-NA	6.22	2.21	2.06
24	b	605	CLA	MG-NC	6.17	2.20	2.06
25	d	402	PHO	C3B-C4B	6.11	1.47	1.41
24	B	611	CLA	MG-NC	6.08	2.20	2.06
24	b	610	CLA	MG-NA	6.08	2.20	2.06
24	c	912	CLA	MG-ND	6.07	2.17	2.05
24	D	403	CLA	MG-NC	6.06	2.20	2.06
24	A	609	CLA	MG-NC	6.00	2.20	2.06
24	b	607	CLA	MG-NC	5.99	2.20	2.06
25	D	401	PHO	C3B-C2B	5.98	1.48	1.40
24	b	608	CLA	MG-NC	5.96	2.20	2.06
26	T	101	BCR	C16-C15	-5.95	1.19	1.36
26	b	619	BCR	C16-C15	-5.94	1.19	1.36
26	C	514	BCR	C16-C15	-5.94	1.19	1.36
26	c	915	BCR	C16-C15	-5.92	1.20	1.36
24	D	402	CLA	MG-NA	5.91	2.20	2.06
26	C	515	BCR	C16-C15	-5.84	1.20	1.36
26	k	101	BCR	C16-C15	-5.84	1.20	1.36
26	k	102	BCR	C16-C15	-5.84	1.20	1.36
26	f	101	BCR	C16-C15	-5.83	1.20	1.36
26	B	622	BCR	C16-C15	-5.83	1.20	1.36
24	D	402	CLA	MG-NC	5.82	2.20	2.06
24	c	913	CLA	MG-NB	5.81	2.17	2.05
26	Y	101	BCR	C16-C15	-5.80	1.20	1.36
26	A	610	BCR	C16-C15	-5.79	1.20	1.36
26	K	101	BCR	C16-C15	-5.75	1.20	1.36
26	h	101	BCR	C16-C15	-5.73	1.20	1.36
26	D	404	BCR	C16-C15	-5.73	1.20	1.36
26	B	620	BCR	C16-C15	-5.73	1.20	1.36
26	B	618	BCR	C16-C15	-5.73	1.20	1.36
26	T	102	BCR	C16-C15	-5.72	1.20	1.36
26	H	101	BCR	C16-C15	-5.71	1.20	1.36
24	A	609	CLA	MG-NA	5.69	2.19	2.06
26	Y	101	BCR	C11-C12	-5.68	1.19	1.34
24	d	404	CLA	MG-NC	5.68	2.19	2.06
26	C	514	BCR	C11-C12	-5.67	1.19	1.34
24	C	503	CLA	MG-NA	5.67	2.19	2.06
25	D	401	PHO	C4D-CHA	5.67	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	610	BCR	C20-C19	-5.66	1.19	1.34
26	a	409	BCR	C16-C15	-5.65	1.20	1.36
26	k	101	BCR	C11-C12	-5.64	1.20	1.34
26	b	618	BCR	C16-C15	-5.62	1.20	1.36
26	k	101	BCR	C20-C19	-5.62	1.20	1.34
26	C	515	BCR	C20-C19	-5.61	1.20	1.34
26	k	102	BCR	C20-C19	-5.60	1.20	1.34
26	H	101	BCR	C20-C19	-5.60	1.20	1.34
26	c	918	BCR	C11-C12	-5.59	1.20	1.34
26	D	404	BCR	C20-C19	-5.58	1.20	1.34
26	Y	101	BCR	C20-C19	-5.57	1.20	1.34
26	B	620	BCR	C11-C12	-5.57	1.20	1.34
26	T	101	BCR	C11-C12	-5.57	1.20	1.34
26	f	101	BCR	C20-C19	-5.57	1.20	1.34
26	b	619	BCR	C11-C12	-5.55	1.20	1.34
26	C	514	BCR	C20-C19	-5.55	1.20	1.34
25	A	608	PHO	C3B-C2B	5.53	1.47	1.40
26	k	102	BCR	C11-C12	-5.53	1.20	1.34
26	c	915	BCR	C20-C19	-5.53	1.20	1.34
26	B	622	BCR	C11-C12	-5.53	1.20	1.34
26	D	404	BCR	C11-C12	-5.52	1.20	1.34
24	c	914	CLA	MG-NB	-5.50	1.94	2.05
26	f	101	BCR	C11-C12	-5.49	1.20	1.34
25	A	608	PHO	C3B-C4B	5.48	1.47	1.41
24	c	911	CLA	MG-NA	5.47	2.19	2.06
32	v	202	HEM	FE-ND	5.47	2.11	1.94
26	B	622	BCR	C20-C19	-5.47	1.20	1.34
26	T	101	BCR	C20-C19	-5.46	1.20	1.34
26	h	101	BCR	C20-C19	-5.46	1.20	1.34
24	b	611	CLA	MG-ND	-5.46	1.95	2.05
26	C	515	BCR	C11-C12	-5.46	1.20	1.34
24	c	914	CLA	MG-ND	5.46	2.16	2.05
24	C	508	CLA	C3C-C2C	5.45	1.48	1.36
26	T	102	BCR	C11-C12	-5.44	1.20	1.34
26	K	101	BCR	C11-C12	-5.43	1.20	1.34
25	d	402	PHO	C4D-CHA	5.43	1.47	1.39
26	h	101	BCR	C11-C12	-5.43	1.20	1.34
26	K	101	BCR	C20-C19	-5.42	1.20	1.34
26	b	618	BCR	C11-C12	-5.42	1.20	1.34
24	b	602	CLA	O2D-CGD	5.42	1.46	1.33
26	c	915	BCR	C11-C12	-5.42	1.20	1.34
26	H	101	BCR	C11-C12	-5.41	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	MG-NC	5.40	2.19	2.06
24	c	914	CLA	C3C-C2C	5.40	1.48	1.36
24	b	602	CLA	CHC-C1C	5.39	1.49	1.38
26	B	620	BCR	C20-C19	-5.39	1.20	1.34
24	c	905	CLA	C3C-C2C	5.39	1.48	1.36
26	a	409	BCR	C11-C12	-5.38	1.20	1.34
24	B	606	CLA	MG-NC	5.38	2.19	2.06
24	B	603	CLA	C3C-C2C	5.37	1.48	1.36
24	c	910	CLA	MG-ND	-5.37	1.95	2.05
24	c	905	CLA	MG-ND	-5.35	1.95	2.05
26	B	619	BCR	C20-C19	-5.35	1.20	1.34
24	c	913	CLA	C3C-C2C	5.33	1.48	1.36
25	a	412	PHO	C3B-C2B	5.33	1.47	1.40
24	b	612	CLA	MG-NC	5.32	2.18	2.06
24	C	512	CLA	C3C-C2C	5.32	1.48	1.36
26	B	619	BCR	C16-C15	-5.31	1.21	1.36
26	b	619	BCR	C20-C19	-5.31	1.20	1.34
24	C	503	CLA	C3C-C2C	5.31	1.48	1.36
24	B	603	CLA	CHC-C1C	5.31	1.49	1.38
26	B	619	BCR	C11-C12	-5.30	1.20	1.34
24	b	603	CLA	C3C-C2C	5.30	1.48	1.36
24	C	513	CLA	C3C-C2C	5.27	1.48	1.36
24	b	611	CLA	C3C-C2C	5.27	1.48	1.36
24	c	908	CLA	C3C-C2C	5.26	1.48	1.36
26	B	618	BCR	C11-C12	-5.26	1.21	1.34
24	b	608	CLA	C3C-C2C	5.26	1.48	1.36
25	d	402	PHO	C3B-C2B	5.25	1.47	1.40
26	c	918	BCR	C11-C10	-5.23	1.27	1.43
25	a	412	PHO	C4D-CHA	5.23	1.47	1.39
24	c	914	CLA	CHC-C1C	5.22	1.49	1.38
24	c	909	CLA	C3C-C2C	5.22	1.48	1.36
24	c	907	CLA	O2D-CGD	5.22	1.46	1.33
26	A	610	BCR	C11-C12	-5.22	1.21	1.34
25	A	608	PHO	C4D-CHA	5.22	1.47	1.39
24	c	904	CLA	C3C-C2C	5.22	1.48	1.36
26	T	102	BCR	C20-C19	-5.21	1.21	1.34
24	B	617	CLA	MG-NC	5.21	2.18	2.06
24	b	615	CLA	MG-NA	5.21	2.18	2.06
24	c	914	CLA	O2D-CGD	5.20	1.46	1.33
24	b	610	CLA	O2D-CGD	5.20	1.46	1.33
24	C	507	CLA	C3C-C2C	5.20	1.48	1.36
24	B	613	CLA	CHC-C1C	5.20	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	618	BCR	C20-C19	-5.19	1.21	1.34
26	H	101	BCR	C11-C10	-5.18	1.27	1.43
24	c	907	CLA	C3C-C2C	5.18	1.47	1.36
26	C	514	BCR	C11-C10	-5.18	1.27	1.43
24	B	602	CLA	O2D-CGD	5.18	1.46	1.33
24	d	404	CLA	C3C-C2C	5.18	1.47	1.36
24	B	616	CLA	C3C-C2C	5.18	1.47	1.36
24	c	909	CLA	O2D-CGD	5.17	1.45	1.33
26	D	404	BCR	C11-C10	-5.16	1.27	1.43
24	b	606	CLA	O2D-CGD	5.16	1.45	1.33
24	d	401	CLA	C3C-C2C	5.16	1.47	1.36
26	a	409	BCR	C20-C19	-5.16	1.21	1.34
24	C	502	CLA	CHC-C1C	5.16	1.48	1.38
24	b	607	CLA	C3C-C2C	5.15	1.47	1.36
24	C	509	CLA	MG-NB	-5.15	1.95	2.05
24	c	905	CLA	O2D-CGD	5.15	1.45	1.33
24	b	603	CLA	CHC-C1C	5.14	1.48	1.38
24	A	606	CLA	C3C-C2C	5.14	1.47	1.36
26	c	918	BCR	C15-C14	-5.13	1.27	1.43
24	c	903	CLA	O2D-CGD	5.12	1.45	1.33
24	B	607	CLA	C3C-C2C	5.12	1.47	1.36
26	C	515	BCR	C11-C10	-5.12	1.27	1.43
24	b	608	CLA	CHC-C1C	5.12	1.48	1.38
26	k	101	BCR	C11-C10	-5.11	1.27	1.43
24	C	512	CLA	CHC-C1C	5.11	1.48	1.38
24	c	904	CLA	CHC-C1C	5.11	1.48	1.38
24	c	913	CLA	O2D-CGD	5.11	1.45	1.33
24	B	611	CLA	C3C-C2C	5.10	1.47	1.36
24	B	602	CLA	C3C-C2C	5.10	1.47	1.36
26	b	619	BCR	C11-C10	-5.09	1.27	1.43
24	C	513	CLA	O2D-CGD	5.09	1.45	1.33
24	C	509	CLA	O2D-CGD	5.08	1.45	1.33
26	B	622	BCR	C11-C10	-5.08	1.27	1.43
24	b	610	CLA	CHC-C1C	5.08	1.48	1.38
24	b	617	CLA	CHC-C1C	5.07	1.48	1.38
24	c	906	CLA	CHC-C1C	5.07	1.48	1.38
26	k	101	BCR	C15-C14	-5.07	1.27	1.43
24	b	602	CLA	C3C-C2C	5.07	1.47	1.36
24	C	506	CLA	O2D-CGD	5.06	1.45	1.33
24	c	912	CLA	C3C-C2C	5.06	1.47	1.36
25	a	412	PHO	C3D-C4D	-5.06	1.34	1.41
26	T	101	BCR	C11-C10	-5.06	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	O2D-CGD	5.06	1.45	1.33
26	k	102	BCR	C11-C10	-5.06	1.27	1.43
24	c	911	CLA	O2D-CGD	5.06	1.45	1.33
26	c	918	BCR	C20-C19	-5.06	1.21	1.34
24	b	617	CLA	O2D-CGD	5.06	1.45	1.33
24	c	912	CLA	O2D-CGD	5.06	1.45	1.33
24	B	606	CLA	C3C-C2C	5.05	1.47	1.36
24	b	605	CLA	MG-ND	-5.05	1.95	2.05
24	C	507	CLA	CHC-C1C	5.05	1.48	1.38
24	b	610	CLA	C3C-C2C	5.05	1.47	1.36
24	C	508	CLA	MG-NB	5.05	2.15	2.05
26	T	101	BCR	C15-C14	-5.05	1.27	1.43
26	Y	101	BCR	C11-C10	-5.05	1.27	1.43
24	C	510	CLA	C3C-C2C	5.05	1.47	1.36
24	C	503	CLA	CHC-C1C	5.05	1.48	1.38
24	b	607	CLA	O2D-CGD	5.04	1.45	1.33
24	C	508	CLA	O2D-CGD	5.04	1.45	1.33
24	C	508	CLA	MG-NC	5.04	2.18	2.06
24	C	505	CLA	C3C-C2C	5.04	1.47	1.36
26	f	101	BCR	C15-C14	-5.04	1.27	1.43
24	B	602	CLA	CHC-C1C	5.04	1.48	1.38
26	C	514	BCR	C15-C14	-5.03	1.27	1.43
24	C	511	CLA	O2D-CGD	5.03	1.45	1.33
26	k	102	BCR	C15-C14	-5.03	1.27	1.43
24	C	513	CLA	CHC-C1C	5.03	1.48	1.38
24	c	911	CLA	C3C-C2C	5.03	1.47	1.36
24	D	403	CLA	C3C-C2C	5.02	1.47	1.36
24	b	604	CLA	C3C-C2C	5.02	1.47	1.36
26	f	101	BCR	C11-C10	-5.01	1.27	1.43
26	A	610	BCR	C11-C10	-5.01	1.27	1.43
26	B	618	BCR	C20-C19	-5.01	1.21	1.34
24	b	613	CLA	C3C-C2C	5.00	1.47	1.36
24	C	507	CLA	O2D-CGD	5.00	1.45	1.33
24	c	912	CLA	CHC-C1C	5.00	1.48	1.38
26	C	515	BCR	C15-C14	-5.00	1.27	1.43
24	b	604	CLA	O2D-CGD	5.00	1.45	1.33
24	b	605	CLA	C3C-C2C	4.99	1.47	1.36
24	C	512	CLA	O2D-CGD	4.99	1.45	1.33
24	c	913	CLA	CHC-C1C	4.99	1.48	1.38
26	H	101	BCR	C15-C14	-4.99	1.27	1.43
25	a	412	PHO	O2D-CGD	4.99	1.45	1.33
24	B	609	CLA	C3C-C2C	4.99	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	C3C-C2C	4.99	1.47	1.36
24	C	501	CLA	CHC-C1C	4.99	1.48	1.38
24	c	910	CLA	O2D-CGD	4.98	1.45	1.33
24	A	609	CLA	C3C-C2C	4.98	1.47	1.36
24	B	609	CLA	O2D-CGD	4.98	1.45	1.33
24	B	608	CLA	C3C-C2C	4.98	1.47	1.36
24	B	606	CLA	CHC-C1C	4.97	1.48	1.38
24	d	403	CLA	C3C-C2C	4.97	1.47	1.36
24	b	611	CLA	O2D-CGD	4.97	1.45	1.33
24	C	511	CLA	C3C-C2C	4.97	1.47	1.36
26	Y	101	BCR	C15-C14	-4.96	1.27	1.43
26	c	915	BCR	C11-C10	-4.96	1.27	1.43
24	b	614	CLA	O2D-CGD	4.96	1.45	1.33
26	K	101	BCR	C11-C10	-4.96	1.27	1.43
26	h	101	BCR	C11-C10	-4.96	1.27	1.43
24	C	502	CLA	O2D-CGD	4.95	1.45	1.33
26	h	101	BCR	C15-C14	-4.95	1.27	1.43
24	c	914	CLA	CHD-C1D	4.95	1.48	1.38
24	C	506	CLA	C3C-C2C	4.95	1.47	1.36
26	B	620	BCR	C11-C10	-4.95	1.27	1.43
24	B	617	CLA	C3C-C2C	4.94	1.47	1.36
26	b	618	BCR	C11-C10	-4.94	1.27	1.43
24	B	608	CLA	MG-NC	4.93	2.18	2.06
26	B	618	BCR	C11-C10	-4.93	1.27	1.43
26	T	102	BCR	C11-C10	-4.93	1.27	1.43
25	D	401	PHO	OBD-CAD	4.93	1.28	1.22
26	b	619	BCR	C15-C14	-4.93	1.27	1.43
25	d	402	PHO	O2D-CGD	4.92	1.45	1.33
24	a	407	CLA	MG-ND	-4.92	1.96	2.05
24	B	607	CLA	CHC-C1C	4.92	1.48	1.38
26	c	918	BCR	C23-C22	-4.92	1.35	1.46
26	C	515	BCR	C23-C22	-4.92	1.35	1.46
26	D	404	BCR	C15-C14	-4.92	1.27	1.43
24	C	506	CLA	CHC-C1C	4.92	1.48	1.38
24	C	509	CLA	C3C-C2C	4.92	1.47	1.36
24	B	614	CLA	C3C-C2C	4.92	1.47	1.36
26	B	622	BCR	C15-C14	-4.91	1.27	1.43
24	a	408	CLA	C3C-C2C	4.91	1.47	1.36
24	a	407	CLA	C3C-C2C	4.91	1.47	1.36
24	c	910	CLA	C3C-C2C	4.91	1.47	1.36
25	D	401	PHO	O2D-CGD	4.91	1.45	1.33
32	e	101	HEM	FE-ND	4.91	2.10	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	BCR	C23-C22	-4.91	1.35	1.46
24	b	614	CLA	C3C-C2C	4.91	1.47	1.36
24	c	903	CLA	MG-ND	-4.90	1.96	2.05
24	c	902	CLA	C3C-C2C	4.90	1.47	1.36
24	C	505	CLA	O2D-CGD	4.90	1.45	1.33
26	B	620	BCR	C15-C14	-4.90	1.28	1.43
24	D	402	CLA	C3C-C2C	4.90	1.47	1.36
26	a	409	BCR	C11-C10	-4.89	1.28	1.43
24	C	501	CLA	C3C-C2C	4.89	1.47	1.36
24	C	508	CLA	CHC-C1C	4.88	1.48	1.38
26	k	101	BCR	C23-C22	-4.88	1.35	1.46
24	C	509	CLA	CHD-C1D	4.88	1.47	1.38
24	B	607	CLA	O2D-CGD	4.87	1.45	1.33
26	K	101	BCR	C15-C14	-4.87	1.28	1.43
24	B	605	CLA	C3C-C2C	4.87	1.47	1.36
24	B	611	CLA	CHC-C1C	4.87	1.48	1.38
24	B	610	CLA	C3C-C2C	4.87	1.47	1.36
32	E	101	HEM	FE-NC	4.87	2.11	1.95
24	B	617	CLA	O2D-CGD	4.87	1.45	1.33
24	b	608	CLA	O2D-CGD	4.87	1.45	1.33
24	C	504	CLA	C3C-C2C	4.86	1.47	1.36
24	b	616	CLA	C3C-C2C	4.86	1.47	1.36
24	C	505	CLA	CHC-C1C	4.86	1.48	1.38
24	b	606	CLA	C3C-C2C	4.86	1.47	1.36
24	b	610	CLA	CHD-C1D	4.86	1.47	1.38
24	b	617	CLA	C3C-C2C	4.86	1.47	1.36
24	B	616	CLA	O2D-CGD	4.86	1.45	1.33
24	A	609	CLA	CHC-C1C	4.86	1.48	1.38
26	c	915	BCR	C15-C14	-4.86	1.28	1.43
26	h	101	BCR	C23-C22	-4.85	1.35	1.46
24	b	612	CLA	CHC-C1C	4.85	1.48	1.38
26	b	618	BCR	C23-C22	-4.85	1.35	1.46
24	B	614	CLA	CHC-C1C	4.85	1.48	1.38
24	b	607	CLA	CHC-C1C	4.84	1.48	1.38
24	A	606	CLA	O2D-CGD	4.84	1.45	1.33
24	C	510	CLA	O2D-CGD	4.84	1.45	1.33
26	B	619	BCR	C11-C10	-4.84	1.28	1.43
24	b	602	CLA	CHD-C1D	4.84	1.47	1.38
24	a	407	CLA	O2D-CGD	4.84	1.45	1.33
26	A	610	BCR	C15-C14	-4.84	1.28	1.43
26	D	404	BCR	C23-C22	-4.83	1.35	1.46
24	B	606	CLA	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	906	CLA	C3C-C2C	4.83	1.47	1.36
32	V	202	HEM	FE-ND	4.83	2.09	1.94
24	D	403	CLA	CHC-C1C	4.83	1.48	1.38
24	b	606	CLA	CHC-C1C	4.82	1.48	1.38
24	B	604	CLA	O2D-CGD	4.82	1.45	1.33
24	c	904	CLA	O2D-CGD	4.82	1.45	1.33
25	D	401	PHO	C3D-C4D	-4.82	1.34	1.41
24	B	611	CLA	CHD-C1D	4.82	1.47	1.38
32	E	101	HEM	FE-ND	4.81	2.09	1.94
24	A	614	CLA	C3C-C2C	4.81	1.47	1.36
26	a	409	BCR	C15-C14	-4.81	1.28	1.43
26	k	102	BCR	C23-C22	-4.81	1.35	1.46
26	Y	101	BCR	C23-C22	-4.81	1.35	1.46
24	C	502	CLA	C3C-C2C	4.81	1.47	1.36
24	b	613	CLA	O2D-CGD	4.80	1.45	1.33
24	d	404	CLA	CHC-C1C	4.80	1.48	1.38
32	e	101	HEM	FE-NB	4.80	2.09	1.94
24	a	406	CLA	C3C-C2C	4.79	1.47	1.36
24	B	613	CLA	O2D-CGD	4.79	1.45	1.33
24	b	612	CLA	O2D-CGD	4.79	1.45	1.33
26	K	101	BCR	C23-C22	-4.79	1.35	1.46
24	c	903	CLA	C3C-C2C	4.78	1.47	1.36
24	B	615	CLA	CHC-C1C	4.78	1.48	1.38
26	B	618	BCR	C23-C22	-4.77	1.35	1.46
26	C	514	BCR	C23-C22	-4.77	1.35	1.46
24	B	615	CLA	C3C-C2C	4.77	1.47	1.36
24	B	613	CLA	C3C-C2C	4.77	1.47	1.36
24	b	611	CLA	CHC-C1C	4.77	1.48	1.38
26	T	102	BCR	C15-C14	-4.77	1.28	1.43
24	b	615	CLA	C3C-C2C	4.77	1.47	1.36
24	A	614	CLA	MG-NA	4.76	2.17	2.06
24	C	513	CLA	CHD-C1D	4.76	1.47	1.38
24	B	615	CLA	O2D-CGD	4.76	1.44	1.33
24	B	602	CLA	O2A-CGA	4.75	1.47	1.33
24	b	605	CLA	CHC-C1C	4.75	1.48	1.38
26	a	409	BCR	C23-C22	-4.75	1.35	1.46
24	b	604	CLA	CHC-C1C	4.75	1.48	1.38
24	A	606	CLA	CHC-C1C	4.75	1.48	1.38
24	d	404	CLA	CHD-C1D	4.74	1.47	1.38
24	b	615	CLA	O2D-CGD	4.74	1.44	1.33
24	C	511	CLA	MG-NC	4.74	2.17	2.06
24	b	613	CLA	CHC-C1C	4.74	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	CHC-C1C	4.74	1.48	1.38
24	B	610	CLA	CHC-C1C	4.74	1.48	1.38
24	c	902	CLA	O2D-CGD	4.73	1.44	1.33
24	B	617	CLA	CHC-C1C	4.73	1.48	1.38
24	b	609	CLA	O2D-CGD	4.73	1.44	1.33
26	f	101	BCR	C23-C22	-4.72	1.35	1.46
24	b	602	CLA	O2A-CGA	4.72	1.47	1.33
24	a	408	CLA	O2D-CGD	4.72	1.44	1.33
24	b	605	CLA	O2D-CGD	4.72	1.44	1.33
26	H	101	BCR	C23-C22	-4.72	1.35	1.46
24	c	908	CLA	CHC-C1C	4.72	1.47	1.38
24	A	607	CLA	C3C-C2C	4.71	1.46	1.36
24	B	616	CLA	CHC-C1C	4.71	1.47	1.38
24	B	604	CLA	C3C-C2C	4.71	1.46	1.36
24	d	401	CLA	CHC-C1C	4.71	1.47	1.38
24	C	503	CLA	O2D-CGD	4.71	1.44	1.33
24	b	612	CLA	CHB-C1B	4.70	1.50	1.39
24	a	408	CLA	CHC-C1C	4.70	1.47	1.38
26	b	618	BCR	C15-C14	-4.70	1.28	1.43
24	B	608	CLA	O2D-CGD	4.70	1.44	1.33
24	C	511	CLA	CHC-C1C	4.69	1.47	1.38
24	b	607	CLA	CHD-C1D	4.69	1.47	1.38
24	B	609	CLA	MG-NC	4.69	2.17	2.06
24	b	614	CLA	CHC-C1C	4.68	1.47	1.38
24	c	912	CLA	CHD-C1D	4.68	1.47	1.38
24	b	616	CLA	CHC-C1C	4.67	1.47	1.38
24	A	609	CLA	C3D-C4D	-4.67	1.33	1.44
24	B	608	CLA	CHC-C1C	4.67	1.47	1.38
26	B	619	BCR	C15-C14	-4.67	1.28	1.43
24	c	902	CLA	CHB-C1B	4.66	1.49	1.39
24	c	905	CLA	CHC-C1C	4.66	1.47	1.38
24	c	902	CLA	MG-NC	4.66	2.17	2.06
24	C	504	CLA	O2D-CGD	4.65	1.44	1.33
24	b	614	CLA	MG-NC	4.65	2.17	2.06
24	D	403	CLA	O2D-CGD	4.65	1.44	1.33
26	B	618	BCR	C15-C14	-4.64	1.28	1.43
24	C	501	CLA	O2D-CGD	4.64	1.44	1.33
24	D	403	CLA	CHB-C1B	4.64	1.49	1.39
24	b	612	CLA	C3C-C2C	4.64	1.46	1.36
24	C	512	CLA	CHD-C1D	4.63	1.47	1.38
24	D	402	CLA	O2D-CGD	4.63	1.44	1.33
24	c	902	CLA	CHC-C1C	4.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	CHC-C1C	4.63	1.47	1.38
24	c	903	CLA	CHC-C1C	4.63	1.47	1.38
24	B	615	CLA	CHD-C1D	4.62	1.47	1.38
24	C	505	CLA	CHD-C1D	4.62	1.47	1.38
24	c	907	CLA	CHC-C1C	4.62	1.47	1.38
25	A	608	PHO	C3D-C4D	-4.62	1.35	1.41
24	c	913	CLA	CHD-C1D	4.62	1.47	1.38
24	c	909	CLA	CHC-C1C	4.62	1.47	1.38
26	b	619	BCR	C23-C22	-4.62	1.36	1.46
26	c	915	BCR	C23-C22	-4.61	1.36	1.46
24	A	607	CLA	O2D-CGD	4.61	1.44	1.33
24	a	406	CLA	O2D-CGD	4.61	1.44	1.33
24	C	504	CLA	CHC-C1C	4.61	1.47	1.38
24	d	404	CLA	O2D-CGD	4.61	1.44	1.33
24	C	510	CLA	CHB-C1B	4.60	1.49	1.39
24	c	908	CLA	CHB-C1B	4.60	1.49	1.39
24	c	911	CLA	CHC-C1C	4.60	1.47	1.38
24	B	612	CLA	C3C-C2C	4.60	1.46	1.36
24	C	501	CLA	CHD-C1D	4.59	1.47	1.38
24	C	507	CLA	CHD-C1D	4.59	1.47	1.38
24	B	608	CLA	CHB-C1B	4.59	1.49	1.39
28	F	101	SQD	O48-C23	4.59	1.46	1.33
26	B	619	BCR	C23-C22	-4.58	1.36	1.46
24	d	403	CLA	CHC-C1C	4.58	1.47	1.38
24	b	608	CLA	CHB-C1B	4.58	1.49	1.39
24	c	903	CLA	MG-NC	4.57	2.17	2.06
24	B	607	CLA	CHD-C1D	4.56	1.47	1.38
24	c	910	CLA	OBD-CAD	4.56	1.30	1.22
24	b	610	CLA	CHB-C1B	4.56	1.49	1.39
24	c	910	CLA	CHC-C1C	4.55	1.47	1.38
24	B	604	CLA	CHC-C1C	4.55	1.47	1.38
24	C	506	CLA	CHB-C1B	4.55	1.49	1.39
25	A	608	PHO	O2D-CGD	4.54	1.44	1.33
24	B	614	CLA	CHB-C1B	4.54	1.49	1.39
24	B	606	CLA	CHB-C1B	4.54	1.49	1.39
31	D	406	DGD	O1G-C1A	4.54	1.46	1.33
24	B	603	CLA	CHB-C1B	4.53	1.49	1.39
24	c	906	CLA	MG-NC	4.53	2.17	2.06
26	B	620	BCR	C23-C22	-4.53	1.36	1.46
24	c	906	CLA	CHD-C1D	4.52	1.47	1.38
24	B	611	CLA	O2D-CGD	4.52	1.44	1.33
24	c	912	CLA	CHB-C1B	4.51	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	CHB-C1B	4.51	1.49	1.39
24	B	607	CLA	MG-NC	4.51	2.17	2.06
31	D	406	DGD	O2G-C1B	4.51	1.47	1.34
24	b	602	CLA	CHC-C4B	4.51	1.49	1.39
24	c	914	CLA	MG-NA	4.51	2.17	2.06
24	c	904	CLA	CHD-C1D	4.50	1.47	1.38
24	b	615	CLA	CHD-C1D	4.50	1.47	1.38
24	c	906	CLA	CHB-C1B	4.49	1.49	1.39
24	b	613	CLA	CHB-C1B	4.49	1.49	1.39
29	A	615	LHG	O8-C23	4.49	1.46	1.33
24	C	511	CLA	CHB-C1B	4.49	1.49	1.39
28	a	402	SQD	O48-C23	4.49	1.46	1.33
24	b	603	CLA	CHD-C1D	4.49	1.47	1.38
28	F	101	SQD	O47-C7	4.49	1.47	1.34
24	B	612	CLA	O2D-CGD	4.49	1.44	1.33
24	B	602	CLA	CHD-C1D	4.48	1.47	1.38
26	T	102	BCR	C23-C22	-4.48	1.36	1.46
31	d	406	DGD	O2G-C1B	4.48	1.46	1.34
24	c	906	CLA	O2D-CGD	4.47	1.44	1.33
24	c	913	CLA	O2A-CGA	4.47	1.46	1.33
24	B	602	CLA	CHC-C4B	4.47	1.49	1.39
24	C	502	CLA	MG-NC	4.47	2.16	2.06
24	C	505	CLA	CHB-C1B	4.47	1.49	1.39
24	c	902	CLA	CHD-C1D	4.47	1.47	1.38
28	A	613	SQD	O48-C23	4.46	1.46	1.33
24	b	612	CLA	CHD-C1D	4.46	1.47	1.38
24	b	608	CLA	MG-NB	4.46	2.14	2.05
24	a	407	CLA	CHC-C1C	4.46	1.47	1.38
24	B	614	CLA	O2D-CGD	4.46	1.44	1.33
25	d	402	PHO	C3D-C2D	4.46	1.47	1.39
24	B	605	CLA	CHD-C1D	4.46	1.47	1.38
24	c	913	CLA	CHB-C1B	4.46	1.49	1.39
24	c	904	CLA	CHB-C1B	4.46	1.49	1.39
24	B	615	CLA	CHB-C1B	4.45	1.49	1.39
28	d	407	SQD	O47-C7	4.45	1.46	1.34
24	C	504	CLA	CHD-C1D	4.45	1.47	1.38
24	b	611	CLA	CHD-C1D	4.45	1.47	1.38
24	b	608	CLA	CHD-C1D	4.44	1.47	1.38
24	B	607	CLA	CHB-C1B	4.44	1.49	1.39
24	B	610	CLA	O2D-CGD	4.44	1.44	1.33
24	A	609	CLA	CHB-C1B	4.44	1.49	1.39
24	c	908	CLA	O2D-CGD	4.44	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	O2A-CGA	4.44	1.46	1.33
24	C	513	CLA	CHB-C1B	4.44	1.49	1.39
24	B	604	CLA	CHD-C1D	4.44	1.47	1.38
24	C	512	CLA	CHB-C1B	4.44	1.49	1.39
24	D	403	CLA	CHD-C1D	4.43	1.47	1.38
28	d	407	SQD	O48-C23	4.43	1.46	1.33
28	L	101	SQD	O47-C7	4.43	1.46	1.34
24	B	611	CLA	C3D-C4D	-4.43	1.34	1.44
24	B	603	CLA	CHD-C1D	4.42	1.47	1.38
24	C	510	CLA	C3D-C4D	-4.42	1.34	1.44
26	B	622	BCR	C23-C22	-4.42	1.36	1.46
26	A	610	BCR	C23-C22	-4.42	1.36	1.46
28	L	101	SQD	O48-C23	4.42	1.46	1.33
24	b	605	CLA	CHB-C1B	4.42	1.49	1.39
24	b	606	CLA	C3D-C4D	-4.41	1.34	1.44
24	c	914	CLA	CHB-C1B	4.41	1.49	1.39
24	c	907	CLA	C3D-C4D	-4.41	1.34	1.44
24	b	615	CLA	O2A-CGA	4.41	1.46	1.33
25	a	412	PHO	OBD-CAD	4.41	1.28	1.22
24	c	913	CLA	MG-NC	4.40	2.16	2.06
28	a	402	SQD	O47-C7	4.40	1.46	1.34
24	c	913	CLA	C3D-C4D	-4.40	1.34	1.44
24	B	605	CLA	O2D-CGD	4.40	1.44	1.33
25	a	412	PHO	C3D-C2D	4.40	1.47	1.39
24	C	506	CLA	CHD-C1D	4.40	1.47	1.38
24	C	504	CLA	CHB-C1B	4.39	1.49	1.39
24	C	507	CLA	CHB-C1B	4.39	1.49	1.39
24	C	508	CLA	CHB-C1B	4.39	1.49	1.39
24	D	403	CLA	C3D-C4D	-4.38	1.34	1.44
24	C	508	CLA	CHD-C1D	4.38	1.47	1.38
29	a	413	LHG	O8-C23	4.38	1.46	1.33
24	d	403	CLA	O2A-CGA	4.37	1.46	1.33
28	l	101	SQD	O47-C7	4.37	1.46	1.34
24	c	909	CLA	CHD-C1D	4.37	1.47	1.38
24	c	914	CLA	O2A-CGA	4.37	1.46	1.33
24	c	910	CLA	MG-NC	4.37	2.16	2.06
24	B	603	CLA	O2D-CGD	4.37	1.44	1.33
24	c	905	CLA	CHD-C1D	4.36	1.46	1.38
24	b	615	CLA	C3D-C4D	-4.36	1.34	1.44
24	B	608	CLA	CHD-C1D	4.36	1.46	1.38
24	C	510	CLA	CHC-C1C	4.36	1.47	1.38
24	b	602	CLA	CHB-C1B	4.35	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	903	CLA	CHB-C1B	4.35	1.49	1.39
32	E	101	HEM	FE-NA	4.35	2.09	1.95
24	C	510	CLA	CHD-C1D	4.35	1.46	1.38
24	a	408	CLA	CHB-C1B	4.34	1.49	1.39
24	A	609	CLA	O2D-CGD	4.34	1.43	1.33
24	C	506	CLA	O2A-CGA	4.34	1.46	1.33
24	B	616	CLA	CHD-C1D	4.34	1.46	1.38
24	c	908	CLA	O2A-CGA	4.34	1.46	1.33
24	b	611	CLA	MG-NC	4.34	2.16	2.06
31	d	406	DGD	O1G-C1A	4.34	1.46	1.33
24	b	612	CLA	C3D-C4D	-4.34	1.34	1.44
29	a	413	LHG	O7-C7	4.33	1.46	1.34
24	a	407	CLA	MG-NC	4.33	2.16	2.06
24	b	609	CLA	CHB-C1B	4.33	1.49	1.39
24	b	607	CLA	C3D-C4D	-4.33	1.34	1.44
24	A	607	CLA	CHC-C1C	4.33	1.47	1.38
24	B	605	CLA	CHB-C1B	4.32	1.49	1.39
24	c	902	CLA	O2A-CGA	4.32	1.45	1.33
24	B	605	CLA	CHC-C1C	4.32	1.47	1.38
24	c	914	CLA	C3D-C4D	-4.32	1.34	1.44
24	C	504	CLA	CHD-C4C	4.31	1.49	1.39
24	c	903	CLA	C3D-C4D	-4.31	1.34	1.44
24	b	609	CLA	CHD-C1D	4.31	1.46	1.38
24	b	615	CLA	CHB-C1B	4.31	1.49	1.39
24	C	506	CLA	C3D-C4D	-4.30	1.34	1.44
24	B	617	CLA	O2A-CGA	4.30	1.45	1.33
24	A	607	CLA	CHD-C1D	4.29	1.46	1.38
24	b	605	CLA	CHD-C1D	4.29	1.46	1.38
24	c	908	CLA	CHD-C1D	4.29	1.46	1.38
24	c	902	CLA	C3D-C4D	-4.29	1.34	1.44
24	a	408	CLA	O2A-CGA	4.29	1.45	1.33
24	C	513	CLA	CHC-C4B	4.29	1.49	1.39
24	c	909	CLA	CHB-C1B	4.28	1.49	1.39
28	A	613	SQD	O47-C7	4.28	1.46	1.34
24	a	407	CLA	C3D-C4D	-4.28	1.34	1.44
24	D	402	CLA	O2A-CGA	4.28	1.45	1.33
24	b	617	CLA	CHD-C1D	4.28	1.46	1.38
24	b	615	CLA	CHC-C1C	4.28	1.47	1.38
24	C	511	CLA	CHD-C1D	4.28	1.46	1.38
24	d	404	CLA	O2A-CGA	4.28	1.45	1.33
24	C	505	CLA	C3D-C4D	-4.28	1.34	1.44
25	D	401	PHO	C3D-C2D	4.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	CHB-C1B	4.27	1.49	1.39
24	B	612	CLA	CHC-C1C	4.27	1.47	1.38
24	a	407	CLA	CHB-C1B	4.27	1.49	1.39
24	B	609	CLA	C3D-C4D	-4.27	1.34	1.44
24	b	603	CLA	CHB-C1B	4.27	1.49	1.39
24	c	907	CLA	MG-NB	4.27	2.14	2.05
24	b	602	CLA	C3D-C4D	-4.27	1.34	1.44
24	B	609	CLA	CHD-C1D	4.26	1.46	1.38
24	d	401	CLA	CHB-C1B	4.26	1.49	1.39
24	B	610	CLA	CHB-C1B	4.26	1.49	1.39
24	C	513	CLA	C3D-C4D	-4.26	1.34	1.44
24	C	507	CLA	O2A-CGA	4.26	1.45	1.33
24	b	609	CLA	C3D-C4D	-4.26	1.34	1.44
24	B	604	CLA	CHB-C1B	4.26	1.49	1.39
24	C	503	CLA	CHD-C1D	4.26	1.46	1.38
24	C	509	CLA	O2A-CGA	4.26	1.45	1.33
24	C	512	CLA	C3D-C4D	-4.25	1.34	1.44
24	c	910	CLA	C3D-C4D	-4.25	1.34	1.44
24	C	512	CLA	O2A-CGA	4.25	1.45	1.33
24	A	609	CLA	CHD-C1D	4.25	1.46	1.38
24	C	502	CLA	CHD-C1D	4.24	1.46	1.38
24	c	911	CLA	CHD-C1D	4.24	1.46	1.38
24	c	907	CLA	CHB-C1B	4.24	1.48	1.39
24	c	905	CLA	MG-NB	4.24	2.14	2.05
24	b	617	CLA	CHB-C1B	4.23	1.48	1.39
24	d	404	CLA	C3D-C4D	-4.23	1.34	1.44
24	B	606	CLA	CHD-C1D	4.23	1.46	1.38
24	b	603	CLA	O2D-CGD	4.23	1.43	1.33
25	d	402	PHO	OBD-CAD	4.23	1.27	1.22
24	c	911	CLA	CHB-C1B	4.23	1.48	1.39
24	C	503	CLA	CHC-C4B	4.22	1.48	1.39
24	c	905	CLA	C3D-C4D	-4.22	1.34	1.44
24	B	608	CLA	C3D-C4D	-4.22	1.34	1.44
24	c	911	CLA	C3D-C4D	-4.22	1.34	1.44
24	b	614	CLA	C3D-C4D	-4.22	1.34	1.44
29	A	615	LHG	O7-C7	4.22	1.46	1.34
24	C	501	CLA	CHB-C1B	4.22	1.48	1.39
28	a	411	SQD	O48-C23	4.22	1.45	1.33
24	c	904	CLA	CHC-C4B	4.21	1.48	1.39
24	c	905	CLA	CHB-C1B	4.21	1.48	1.39
24	b	603	CLA	CHD-C4C	4.21	1.48	1.39
24	C	503	CLA	C3D-C4D	-4.21	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	910	CLA	CHD-C1D	4.20	1.46	1.38
25	d	402	PHO	C3D-C4D	-4.20	1.35	1.41
24	c	907	CLA	CHD-C1D	4.20	1.46	1.38
31	c	917	DGD	O1G-C1A	4.20	1.45	1.33
24	C	511	CLA	C3D-C4D	-4.20	1.34	1.44
24	b	603	CLA	MG-NA	4.19	2.16	2.06
24	D	402	CLA	CHC-C1C	4.19	1.46	1.38
24	C	503	CLA	O2A-CGA	4.19	1.45	1.33
24	B	610	CLA	CHD-C1D	4.19	1.46	1.38
24	B	605	CLA	C3D-C4D	-4.19	1.34	1.44
24	A	609	CLA	O2A-CGA	4.19	1.45	1.33
24	b	604	CLA	C3D-C4D	-4.19	1.34	1.44
24	c	904	CLA	C3D-C4D	-4.18	1.34	1.44
24	d	403	CLA	C3D-C4D	-4.18	1.34	1.44
24	c	907	CLA	O2A-CGA	4.18	1.45	1.33
24	A	614	CLA	O2D-CGD	4.18	1.43	1.33
24	C	502	CLA	C3D-C4D	-4.18	1.34	1.44
24	b	614	CLA	O2A-CGA	4.18	1.45	1.33
24	c	914	CLA	CHC-C4B	4.18	1.48	1.39
24	A	614	CLA	CHC-C1C	4.17	1.46	1.38
24	C	513	CLA	O2A-CGA	4.17	1.45	1.33
24	B	609	CLA	CHC-C1C	4.17	1.46	1.38
24	B	616	CLA	CHB-C1B	4.17	1.48	1.39
24	C	504	CLA	C3D-C4D	-4.17	1.34	1.44
24	c	912	CLA	O2A-CGA	4.16	1.45	1.33
24	C	505	CLA	CHC-C4B	4.15	1.48	1.39
24	b	614	CLA	CHB-C1B	4.15	1.48	1.39
24	c	914	CLA	CHD-C4C	4.15	1.48	1.39
24	b	613	CLA	C3D-C4D	-4.15	1.34	1.44
24	D	403	CLA	O2A-CGA	4.15	1.45	1.33
24	c	908	CLA	CHC-C4B	4.15	1.48	1.39
24	C	507	CLA	C3D-C4D	-4.15	1.34	1.44
24	C	501	CLA	CHD-C4C	4.15	1.48	1.39
24	c	909	CLA	C3D-C4D	-4.14	1.34	1.44
24	B	602	CLA	C3D-C4D	-4.14	1.34	1.44
24	c	912	CLA	C3D-C4D	-4.14	1.34	1.44
24	d	401	CLA	O2A-CGA	4.14	1.45	1.33
24	C	511	CLA	O2A-CGA	4.14	1.45	1.33
24	B	614	CLA	C3D-C4D	-4.14	1.34	1.44
24	c	910	CLA	CHB-C1B	4.14	1.48	1.39
24	B	617	CLA	CHB-C1B	4.13	1.48	1.39
31	C	517	DGD	O1G-C1A	4.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	O2A-CGA	4.13	1.45	1.33
24	C	509	CLA	MG-NC	4.13	2.16	2.06
26	c	918	BCR	C16-C17	-4.13	1.30	1.43
24	c	903	CLA	CHD-C1D	4.13	1.46	1.38
24	b	617	CLA	C3D-C4D	-4.13	1.34	1.44
24	C	512	CLA	CHD-C4C	4.12	1.48	1.39
24	C	509	CLA	C3D-C4D	-4.12	1.34	1.44
29	D	409	LHG	O8-C23	4.12	1.45	1.33
24	b	611	CLA	CHC-C4B	4.12	1.48	1.39
24	b	604	CLA	CHB-C1B	4.12	1.48	1.39
24	B	616	CLA	O2A-CGA	4.11	1.45	1.33
24	a	408	CLA	CHD-C1D	4.11	1.46	1.38
24	C	501	CLA	C3D-C4D	-4.11	1.34	1.44
24	d	404	CLA	CHB-C1B	4.11	1.48	1.39
24	b	603	CLA	C3D-C4D	-4.11	1.34	1.44
24	B	607	CLA	O2A-CGA	4.11	1.45	1.33
24	b	607	CLA	O2A-CGA	4.11	1.45	1.33
24	B	604	CLA	C3D-C4D	-4.11	1.34	1.44
24	B	611	CLA	CHB-C1B	4.11	1.48	1.39
24	b	611	CLA	C3D-C4D	-4.11	1.34	1.44
28	A	612	SQD	O47-C7	4.10	1.45	1.34
28	l	101	SQD	O48-C23	4.10	1.45	1.33
24	c	910	CLA	O2A-CGA	4.10	1.45	1.33
24	B	610	CLA	C3D-C4D	-4.10	1.35	1.44
24	B	603	CLA	CHC-C4B	4.10	1.48	1.39
24	b	602	CLA	CHD-C4C	4.10	1.48	1.39
24	b	616	CLA	CHB-C1B	4.10	1.48	1.39
24	a	406	CLA	OBD-CAD	4.10	1.29	1.22
24	c	911	CLA	O2A-CGA	4.10	1.45	1.33
24	c	913	CLA	CHC-C4B	4.09	1.48	1.39
24	A	606	CLA	CHB-C1B	4.09	1.48	1.39
24	C	508	CLA	C3D-C4D	-4.09	1.35	1.44
24	d	401	CLA	C3D-C4D	-4.09	1.35	1.44
24	d	404	CLA	CHD-C4C	4.09	1.48	1.39
24	C	503	CLA	CHB-C1B	4.08	1.48	1.39
24	B	615	CLA	C3D-C4D	-4.08	1.35	1.44
24	d	403	CLA	CHD-C1D	4.08	1.46	1.38
24	d	401	CLA	O2D-CGD	4.08	1.43	1.33
24	C	502	CLA	CHB-C1B	4.08	1.48	1.39
24	B	607	CLA	C3D-C4D	-4.08	1.35	1.44
24	c	906	CLA	CHD-C4C	4.08	1.48	1.39
24	b	616	CLA	CHD-C1D	4.07	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	CHB-C1B	4.07	1.48	1.39
24	b	616	CLA	C3D-C4D	-4.07	1.35	1.44
24	b	604	CLA	CHD-C1D	4.07	1.46	1.38
24	b	610	CLA	O2A-CGA	4.07	1.45	1.33
24	b	607	CLA	CHC-C4B	4.07	1.48	1.39
24	c	906	CLA	O2A-CGA	4.06	1.45	1.33
24	B	615	CLA	O2A-CGA	4.06	1.45	1.33
24	C	501	CLA	O2A-CGA	4.06	1.45	1.33
24	b	617	CLA	CHC-C4B	4.06	1.48	1.39
24	C	501	CLA	CHC-C4B	4.05	1.48	1.39
24	A	614	CLA	MG-NC	4.05	2.15	2.06
24	c	907	CLA	CHD-C4C	4.05	1.48	1.39
31	h	102	DGD	O1G-C1A	4.05	1.45	1.33
24	c	906	CLA	CHC-C4B	4.05	1.48	1.39
24	b	611	CLA	CHB-C1B	4.05	1.48	1.39
24	B	602	CLA	MG-NB	4.04	2.13	2.05
24	A	607	CLA	C3D-C4D	-4.04	1.35	1.44
24	C	510	CLA	MG-ND	-4.04	1.97	2.05
24	C	502	CLA	O2A-CGA	4.04	1.45	1.33
24	A	606	CLA	CHD-C1D	4.04	1.46	1.38
25	A	608	PHO	OBD-CAD	4.04	1.27	1.22
24	a	408	CLA	C3D-C4D	-4.03	1.35	1.44
24	B	604	CLA	O2A-CGA	4.03	1.45	1.33
28	a	411	SQD	O47-C7	4.03	1.45	1.34
24	C	501	CLA	MG-NC	4.03	2.15	2.06
24	c	906	CLA	C3D-C4D	-4.03	1.35	1.44
24	B	602	CLA	CHB-C1B	4.03	1.48	1.39
24	C	507	CLA	CHC-C4B	4.03	1.48	1.39
29	b	620	LHG	O8-C23	4.02	1.45	1.33
24	b	606	CLA	CHB-C1B	4.02	1.48	1.39
24	A	609	CLA	OBD-CAD	4.02	1.29	1.22
29	B	621	LHG	O8-C23	4.01	1.45	1.33
29	d	408	LHG	O8-C23	4.01	1.45	1.33
24	B	613	CLA	C3D-C4D	-4.01	1.35	1.44
24	C	508	CLA	O2A-CGA	4.01	1.45	1.33
24	B	612	CLA	CHD-C1D	4.01	1.46	1.38
24	C	504	CLA	O2A-CGA	4.00	1.45	1.33
24	B	608	CLA	CHD-C4C	4.00	1.48	1.39
31	j	101	DGD	O1G-C1A	4.00	1.45	1.33
24	b	612	CLA	O2A-CGA	4.00	1.45	1.33
28	A	612	SQD	O48-C23	4.00	1.45	1.33
24	B	613	CLA	CHD-C4C	4.00	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	609	CLA	CHC-C4B	4.00	1.48	1.39
24	B	603	CLA	MG-NC	3.99	2.15	2.06
24	b	613	CLA	CHD-C1D	3.99	1.46	1.38
24	B	612	CLA	CHB-C1B	3.99	1.48	1.39
24	b	608	CLA	C3D-C4D	-3.99	1.35	1.44
24	B	603	CLA	CHD-C4C	3.99	1.48	1.39
24	B	612	CLA	C3D-C4D	-3.99	1.35	1.44
24	C	506	CLA	CHD-C4C	3.98	1.48	1.39
24	b	613	CLA	O2A-CGA	3.98	1.45	1.33
24	b	607	CLA	CHD-C4C	3.98	1.48	1.39
24	d	403	CLA	MG-NC	3.98	2.15	2.06
24	b	603	CLA	OBD-CAD	3.98	1.29	1.22
24	c	912	CLA	CHD-C4C	3.98	1.48	1.39
24	b	606	CLA	MG-ND	-3.97	1.97	2.05
24	b	603	CLA	O2A-CGA	3.97	1.44	1.33
24	A	614	CLA	O2A-CGA	3.97	1.44	1.33
24	b	606	CLA	CHD-C1D	3.97	1.46	1.38
24	C	503	CLA	CHD-C4C	3.97	1.48	1.39
24	D	403	CLA	CHC-C4B	3.97	1.48	1.39
24	c	908	CLA	C3D-C4D	-3.97	1.35	1.44
31	h	102	DGD	O2G-C1B	3.97	1.45	1.34
24	B	611	CLA	CHC-C4B	3.96	1.48	1.39
29	D	407	LHG	O8-C23	3.96	1.44	1.33
31	C	518	DGD	O1G-C1A	3.96	1.44	1.33
24	B	607	CLA	CHC-C4B	3.96	1.48	1.39
24	C	509	CLA	OBD-CAD	3.96	1.29	1.22
24	b	603	CLA	CHC-C4B	3.96	1.48	1.39
31	H	102	DGD	O1G-C1A	3.96	1.44	1.33
24	b	610	CLA	CHD-C4C	3.96	1.48	1.39
24	C	505	CLA	CHD-C4C	3.96	1.48	1.39
24	C	510	CLA	O2A-CGA	3.95	1.44	1.33
24	B	603	CLA	C3D-C4D	-3.95	1.35	1.44
29	D	408	LHG	O8-C23	3.95	1.44	1.33
24	A	606	CLA	C3D-C4D	-3.95	1.35	1.44
24	B	613	CLA	CHD-C1D	3.94	1.46	1.38
25	a	412	PHO	C3A-C2A	-3.94	1.51	1.54
31	C	516	DGD	O2G-C1B	3.94	1.45	1.34
25	A	608	PHO	O2A-CGA	3.94	1.44	1.33
31	c	916	DGD	O1G-C1A	3.94	1.44	1.33
24	c	909	CLA	O2A-CGA	3.94	1.44	1.33
24	C	506	CLA	CHC-C4B	3.94	1.48	1.39
24	c	905	CLA	O2A-CGA	3.94	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	606	CLA	CHC-C4B	3.94	1.48	1.39
24	D	403	CLA	CHD-C4C	3.94	1.48	1.39
24	B	609	CLA	O2A-CGA	3.94	1.44	1.33
24	a	407	CLA	O2A-CGA	3.93	1.44	1.33
24	B	617	CLA	C3D-C4D	-3.93	1.35	1.44
24	b	614	CLA	OBD-CAD	3.93	1.29	1.22
24	C	508	CLA	CHC-C4B	3.93	1.48	1.39
24	B	602	CLA	CHD-C4C	3.93	1.48	1.39
24	C	510	CLA	OBD-CAD	3.92	1.29	1.22
24	d	403	CLA	O2D-CGD	3.91	1.42	1.33
29	d	410	LHG	O8-C23	3.91	1.44	1.33
24	a	406	CLA	CHC-C1C	3.91	1.46	1.38
24	C	507	CLA	CHD-C4C	3.91	1.48	1.39
31	C	516	DGD	O1G-C1A	3.91	1.44	1.33
24	B	616	CLA	CHD-C4C	3.91	1.48	1.39
24	C	512	CLA	CHC-C4B	3.90	1.48	1.39
24	B	607	CLA	CHD-C4C	3.90	1.48	1.39
24	d	404	CLA	CHC-C4B	3.90	1.48	1.39
24	C	513	CLA	CHD-C4C	3.89	1.48	1.39
24	C	505	CLA	O2A-CGA	3.89	1.44	1.33
24	b	610	CLA	C3D-C4D	-3.89	1.35	1.44
29	D	409	LHG	O7-C7	3.89	1.45	1.34
24	C	511	CLA	CHD-C4C	3.89	1.48	1.39
24	b	609	CLA	CHC-C4B	3.89	1.48	1.39
24	c	911	CLA	CHC-C4B	3.89	1.48	1.39
24	b	610	CLA	OBD-CAD	3.89	1.29	1.22
24	C	510	CLA	CHD-C4C	3.88	1.48	1.39
24	B	611	CLA	O2A-CGA	3.88	1.44	1.33
24	c	902	CLA	CHD-C4C	3.88	1.48	1.39
24	b	609	CLA	O2A-CGA	3.88	1.44	1.33
24	B	609	CLA	CHB-C1B	3.88	1.48	1.39
24	A	614	CLA	OBD-CAD	3.87	1.29	1.22
24	B	613	CLA	CHC-C4B	3.87	1.48	1.39
31	H	102	DGD	O2G-C1B	3.87	1.45	1.34
24	d	401	CLA	CHD-C1D	3.86	1.45	1.38
24	c	902	CLA	CHC-C4B	3.86	1.48	1.39
24	c	913	CLA	CHD-C4C	3.86	1.48	1.39
24	B	617	CLA	CHD-C1D	3.86	1.45	1.38
24	c	903	CLA	O2A-CGA	3.86	1.44	1.33
32	e	101	HEM	FE-NC	3.85	2.07	1.95
24	b	611	CLA	OBD-CAD	3.85	1.29	1.22
24	A	607	CLA	O2A-CGA	3.85	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	CHC-C4B	3.85	1.48	1.39
24	D	402	CLA	CHC-C4B	3.85	1.48	1.39
24	c	908	CLA	CHD-C4C	3.85	1.48	1.39
24	c	909	CLA	CHC-C4B	3.84	1.48	1.39
24	a	406	CLA	C3D-C4D	-3.84	1.35	1.44
25	a	412	PHO	O2A-CGA	3.84	1.44	1.33
24	A	606	CLA	CHD-C4C	3.84	1.47	1.39
24	b	603	CLA	MG-NB	3.84	2.13	2.05
24	B	606	CLA	C3D-C4D	-3.84	1.35	1.44
24	C	511	CLA	CHC-C4B	3.83	1.48	1.39
24	c	905	CLA	CHC-C4B	3.83	1.48	1.39
29	B	621	LHG	O7-C7	3.83	1.45	1.34
29	d	410	LHG	O7-C7	3.83	1.45	1.34
24	c	904	CLA	O2A-CGA	3.82	1.44	1.33
24	b	616	CLA	O2A-CGA	3.82	1.44	1.33
24	B	614	CLA	CHC-C4B	3.82	1.48	1.39
26	k	101	BCR	C21-C22	-3.82	1.27	1.35
24	b	609	CLA	OBD-CAD	3.81	1.29	1.22
24	a	406	CLA	CHD-C1D	3.81	1.45	1.38
24	B	617	CLA	OBD-CAD	3.80	1.29	1.22
24	c	911	CLA	CHD-C4C	3.80	1.47	1.39
24	C	502	CLA	CHC-C4B	3.80	1.47	1.39
24	b	615	CLA	CHD-C4C	3.80	1.47	1.39
24	B	605	CLA	O2A-CGA	3.80	1.44	1.33
24	b	609	CLA	CHD-C4C	3.80	1.47	1.39
24	a	406	CLA	O2A-CGA	3.80	1.44	1.33
24	c	914	CLA	OBD-CAD	3.80	1.29	1.22
24	D	402	CLA	CHB-C1B	3.80	1.47	1.39
24	b	613	CLA	CHC-C4B	3.79	1.47	1.39
24	b	615	CLA	CHC-C4B	3.79	1.47	1.39
24	c	903	CLA	OBD-CAD	3.79	1.29	1.22
24	b	605	CLA	O2A-CGA	3.79	1.44	1.33
24	B	614	CLA	CHD-C4C	3.79	1.47	1.39
24	B	610	CLA	CHC-C4B	3.79	1.47	1.39
24	c	912	CLA	OBD-CAD	3.79	1.29	1.22
24	C	509	CLA	CHD-C4C	3.79	1.47	1.39
24	A	606	CLA	OBD-CAD	3.78	1.29	1.22
31	C	517	DGD	O2G-C1B	3.78	1.44	1.34
24	C	508	CLA	CHD-C4C	3.78	1.47	1.39
24	b	608	CLA	CHD-C4C	3.78	1.47	1.39
24	b	611	CLA	CHD-C4C	3.77	1.47	1.39
24	c	907	CLA	CHC-C4B	3.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	912	CLA	CHC-C4B	3.77	1.47	1.39
24	b	605	CLA	C3D-C4D	-3.77	1.35	1.44
29	D	408	LHG	O7-C7	3.77	1.44	1.34
24	c	904	CLA	CHD-C4C	3.77	1.47	1.39
24	b	604	CLA	O2A-CGA	3.76	1.44	1.33
24	B	605	CLA	CHD-C4C	3.76	1.47	1.39
24	b	616	CLA	CHD-C4C	3.76	1.47	1.39
29	b	620	LHG	O7-C7	3.76	1.44	1.34
24	B	612	CLA	CHC-C4B	3.76	1.47	1.39
24	a	406	CLA	CHB-C1B	3.76	1.47	1.39
24	D	402	CLA	OBD-CAD	3.76	1.28	1.22
24	c	911	CLA	OBD-CAD	3.75	1.28	1.22
32	V	202	HEM	FE-NB	3.75	2.06	1.94
24	B	606	CLA	O2A-CGA	3.75	1.44	1.33
24	b	606	CLA	MG-NB	3.75	2.13	2.05
24	c	910	CLA	CHC-C4B	3.75	1.47	1.39
25	A	608	PHO	C3D-C2D	3.75	1.46	1.39
24	C	511	CLA	OBD-CAD	3.74	1.28	1.22
24	D	402	CLA	C3D-C4D	-3.74	1.35	1.44
24	a	408	CLA	CHD-C4C	3.74	1.47	1.39
24	B	609	CLA	CHD-C4C	3.73	1.47	1.39
26	c	918	BCR	C21-C22	-3.73	1.27	1.35
24	A	607	CLA	CHD-C4C	3.73	1.47	1.39
24	B	604	CLA	OBD-CAD	3.73	1.28	1.22
24	d	403	CLA	CHB-C1B	3.73	1.47	1.39
24	C	508	CLA	MG-ND	-3.73	1.98	2.05
24	c	906	CLA	OBD-CAD	3.73	1.28	1.22
24	B	603	CLA	OBD-CAD	3.73	1.28	1.22
24	B	607	CLA	OBD-CAD	3.72	1.28	1.22
24	A	607	CLA	CHB-C1B	3.72	1.47	1.39
24	b	614	CLA	CHC-C4B	3.72	1.47	1.39
24	B	616	CLA	MG-NC	3.72	2.15	2.06
24	a	407	CLA	CHD-C1D	3.72	1.45	1.38
24	b	604	CLA	OBD-CAD	3.72	1.28	1.22
24	B	614	CLA	CHD-C1D	3.71	1.45	1.38
24	d	403	CLA	CHC-C4B	3.71	1.47	1.39
24	B	616	CLA	CHC-C4B	3.71	1.47	1.39
24	B	606	CLA	CHC-C4B	3.71	1.47	1.39
24	B	613	CLA	O2A-CGA	3.71	1.44	1.33
25	D	401	PHO	O2A-CGA	3.70	1.44	1.33
24	B	616	CLA	C3D-C4D	-3.70	1.35	1.44
24	b	610	CLA	CHC-C4B	3.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	CLA	OBD-CAD	3.70	1.28	1.22
24	b	611	CLA	O2A-CGA	3.70	1.44	1.33
24	A	614	CLA	CHB-C1B	3.70	1.47	1.39
24	B	614	CLA	O2A-CGA	3.70	1.44	1.33
24	A	614	CLA	CHC-C4B	3.70	1.47	1.39
29	d	408	LHG	O7-C7	3.69	1.44	1.34
24	c	903	CLA	CHC-C4B	3.69	1.47	1.39
24	b	616	CLA	CHC-C4B	3.69	1.47	1.39
24	c	905	CLA	OBD-CAD	3.69	1.28	1.22
24	b	604	CLA	CHD-C4C	3.68	1.47	1.39
24	a	408	CLA	MG-NC	3.68	2.15	2.06
24	b	606	CLA	CHC-C4B	3.68	1.47	1.39
24	A	609	CLA	CHD-C4C	3.68	1.47	1.39
24	b	608	CLA	CHC-C4B	3.67	1.47	1.39
24	C	513	CLA	OBD-CAD	3.66	1.28	1.22
24	b	602	CLA	OBD-CAD	3.66	1.28	1.22
24	B	604	CLA	CHC-C4B	3.66	1.47	1.39
24	a	406	CLA	MG-NC	3.65	2.14	2.06
26	H	101	BCR	C21-C22	-3.65	1.27	1.35
24	a	407	CLA	CHC-C4B	3.65	1.47	1.39
24	A	607	CLA	OBD-CAD	3.65	1.28	1.22
24	B	615	CLA	CHD-C4C	3.64	1.47	1.39
24	B	611	CLA	CHD-C4C	3.64	1.47	1.39
24	C	513	CLA	MG-ND	-3.64	1.98	2.05
24	c	903	CLA	CHD-C4C	3.64	1.47	1.39
29	d	409	LHG	O8-C23	3.64	1.44	1.33
24	C	509	CLA	CHC-C4B	3.64	1.47	1.39
26	C	515	BCR	C21-C22	-3.64	1.27	1.35
24	b	606	CLA	O2A-CGA	3.63	1.43	1.33
31	c	916	DGD	O2G-C1B	3.63	1.44	1.34
24	b	614	CLA	CHD-C1D	3.62	1.45	1.38
24	B	602	CLA	OBD-CAD	3.62	1.28	1.22
24	C	504	CLA	OBD-CAD	3.62	1.28	1.22
31	j	101	DGD	O2G-C1B	3.62	1.44	1.34
26	f	101	BCR	C21-C22	-3.62	1.27	1.35
24	b	613	CLA	MG-ND	-3.62	1.98	2.05
26	D	404	BCR	C21-C22	-3.61	1.27	1.35
24	A	606	CLA	MG-ND	-3.61	1.98	2.05
24	D	402	CLA	CHD-C1D	3.61	1.45	1.38
24	C	501	CLA	OBD-CAD	3.60	1.28	1.22
24	c	902	CLA	OBD-CAD	3.60	1.28	1.22
24	c	908	CLA	OBD-CAD	3.60	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	BCR	C21-C22	-3.60	1.27	1.35
24	b	608	CLA	O2A-CGA	3.60	1.43	1.33
24	d	404	CLA	OBD-CAD	3.59	1.28	1.22
26	c	915	BCR	C17-C18	-3.59	1.27	1.35
24	C	510	CLA	CHC-C4B	3.59	1.47	1.39
24	B	610	CLA	OBD-CAD	3.59	1.28	1.22
26	Y	101	BCR	C21-C22	-3.59	1.27	1.35
26	h	101	BCR	C21-C22	-3.59	1.27	1.35
26	b	619	BCR	C21-C22	-3.58	1.27	1.35
24	d	401	CLA	CHC-C4B	3.58	1.47	1.39
24	C	512	CLA	MG-NC	3.58	2.14	2.06
24	C	502	CLA	OBD-CAD	3.58	1.28	1.22
24	b	613	CLA	OBD-CAD	3.57	1.28	1.22
24	b	613	CLA	C1B-C2B	3.57	1.51	1.43
24	c	905	CLA	CHD-C4C	3.57	1.47	1.39
26	K	101	BCR	C21-C22	-3.57	1.27	1.35
29	d	409	LHG	O7-C7	3.57	1.44	1.34
26	C	514	BCR	C17-C18	-3.57	1.27	1.35
24	B	604	CLA	CHD-C4C	3.57	1.47	1.39
24	b	612	CLA	CHD-C4C	3.56	1.47	1.39
24	A	614	CLA	CHD-C1D	3.56	1.45	1.38
26	B	622	BCR	C21-C22	-3.56	1.27	1.35
26	Y	101	BCR	C17-C18	-3.56	1.27	1.35
24	B	617	CLA	CHD-C4C	3.56	1.47	1.39
24	C	505	CLA	OBD-CAD	3.56	1.28	1.22
24	B	608	CLA	CHC-C4B	3.55	1.47	1.39
32	e	101	HEM	FE-NA	3.55	2.06	1.95
31	c	917	DGD	O2G-C1B	3.55	1.44	1.34
26	k	101	BCR	C17-C18	-3.55	1.27	1.35
24	A	614	CLA	C3D-C4D	-3.55	1.36	1.44
24	b	616	CLA	OBD-CAD	3.55	1.28	1.22
26	f	101	BCR	C17-C18	-3.55	1.27	1.35
24	b	607	CLA	OBD-CAD	3.54	1.28	1.22
26	C	514	BCR	C21-C22	-3.54	1.27	1.35
24	c	911	CLA	MG-ND	-3.54	1.98	2.05
24	b	606	CLA	CHD-C4C	3.54	1.47	1.39
24	a	408	CLA	CHC-C4B	3.53	1.47	1.39
24	d	401	CLA	CHD-C4C	3.52	1.47	1.39
26	k	102	BCR	C17-C18	-3.51	1.27	1.35
24	C	507	CLA	OBD-CAD	3.51	1.28	1.22
24	C	508	CLA	OBD-CAD	3.51	1.28	1.22
24	C	502	CLA	CHD-C4C	3.50	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	OBD-CAD	3.50	1.28	1.22
24	C	504	CLA	CHC-C4B	3.50	1.47	1.39
26	B	619	BCR	C21-C22	-3.50	1.27	1.35
26	b	618	BCR	C17-C18	-3.50	1.27	1.35
24	a	406	CLA	CHD-C4C	3.50	1.47	1.39
24	C	506	CLA	OBD-CAD	3.49	1.28	1.22
26	B	622	BCR	C17-C18	-3.49	1.27	1.35
24	B	612	CLA	MG-NC	3.49	2.14	2.06
24	b	617	CLA	OBD-CAD	3.49	1.28	1.22
25	d	402	PHO	O2A-CGA	3.49	1.43	1.33
24	A	606	CLA	O2A-CGA	3.48	1.43	1.33
24	B	616	CLA	OBD-CAD	3.48	1.28	1.22
24	c	907	CLA	OBD-CAD	3.48	1.28	1.22
24	B	612	CLA	CHD-C4C	3.48	1.47	1.39
24	B	610	CLA	CHD-C4C	3.48	1.47	1.39
24	b	617	CLA	CHD-C4C	3.48	1.47	1.39
26	D	404	BCR	C17-C18	-3.47	1.27	1.35
24	D	402	CLA	CHD-C4C	3.47	1.47	1.39
26	B	620	BCR	C21-C22	-3.47	1.27	1.35
24	B	611	CLA	OBD-CAD	3.47	1.28	1.22
26	C	515	BCR	C17-C18	-3.46	1.27	1.35
24	b	614	CLA	CHD-C4C	3.46	1.47	1.39
24	B	603	CLA	O2A-CGA	3.46	1.43	1.33
24	a	407	CLA	CHD-C4C	3.46	1.47	1.39
24	B	612	CLA	O2A-CGA	3.46	1.43	1.33
24	B	615	CLA	CHC-C4B	3.45	1.47	1.39
24	c	913	CLA	OBD-CAD	3.45	1.28	1.22
26	c	915	BCR	C21-C22	-3.45	1.27	1.35
26	b	619	BCR	C17-C18	-3.44	1.27	1.35
26	h	101	BCR	C17-C18	-3.44	1.27	1.35
26	T	101	BCR	C17-C18	-3.44	1.27	1.35
24	c	910	CLA	CHD-C4C	3.44	1.47	1.39
24	B	605	CLA	CHC-C4B	3.43	1.47	1.39
24	B	606	CLA	OBD-CAD	3.42	1.28	1.22
24	B	613	CLA	OBD-CAD	3.42	1.28	1.22
26	A	610	BCR	C17-C18	-3.42	1.27	1.35
24	b	605	CLA	OBD-CAD	3.42	1.28	1.22
24	b	605	CLA	CHD-C4C	3.40	1.46	1.39
24	b	612	CLA	CHC-C4B	3.39	1.47	1.39
24	A	614	CLA	CHD-C4C	3.39	1.46	1.39
31	C	518	DGD	O2G-C1B	3.39	1.43	1.34
24	C	505	CLA	MG-NC	3.39	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	618	BCR	C21-C22	-3.39	1.28	1.35
24	c	909	CLA	OBD-CAD	3.38	1.28	1.22
24	B	615	CLA	OBD-CAD	3.38	1.28	1.22
24	B	608	CLA	OBD-CAD	3.38	1.28	1.22
24	B	609	CLA	OBD-CAD	3.38	1.28	1.22
26	k	102	BCR	C21-C22	-3.37	1.28	1.35
24	b	608	CLA	C3D-C2D	3.37	1.48	1.39
26	K	101	BCR	C17-C18	-3.37	1.28	1.35
26	H	101	BCR	C17-C18	-3.35	1.28	1.35
24	B	606	CLA	CHD-C4C	3.35	1.46	1.39
26	A	610	BCR	C21-C22	-3.35	1.28	1.35
24	b	604	CLA	CHC-C4B	3.35	1.46	1.39
24	B	603	CLA	C1B-C2B	3.35	1.51	1.43
24	b	608	CLA	OBD-CAD	3.35	1.28	1.22
24	b	605	CLA	CHC-C4B	3.35	1.46	1.39
26	b	618	BCR	C21-C22	-3.35	1.28	1.35
24	a	406	CLA	CHC-C4B	3.34	1.46	1.39
25	D	401	PHO	C3A-C2A	-3.34	1.51	1.54
24	B	614	CLA	MG-NC	3.33	2.14	2.06
24	b	615	CLA	OBD-CAD	3.33	1.28	1.22
24	B	616	CLA	C1B-C2B	3.32	1.50	1.43
24	d	401	CLA	OBD-CAD	3.32	1.28	1.22
24	C	512	CLA	OBD-CAD	3.31	1.28	1.22
26	a	409	BCR	C17-C18	-3.30	1.28	1.35
24	c	909	CLA	CHD-C4C	3.30	1.46	1.39
24	A	607	CLA	CHC-C4B	3.28	1.46	1.39
24	B	610	CLA	MG-NB	3.28	2.12	2.05
26	c	918	BCR	C16-C15	-3.28	1.27	1.36
24	B	609	CLA	CHC-C4B	3.28	1.46	1.39
32	V	202	HEM	CAB-C3B	3.27	1.56	1.47
24	B	608	CLA	O2A-CGA	3.27	1.42	1.33
26	B	620	BCR	C17-C18	-3.27	1.28	1.35
24	C	506	CLA	MG-NC	3.27	2.14	2.06
32	v	202	HEM	CAB-C3B	3.26	1.56	1.47
26	T	102	BCR	C17-C18	-3.26	1.28	1.35
24	B	614	CLA	OBD-CAD	3.25	1.28	1.22
26	c	918	BCR	C17-C18	-3.25	1.28	1.35
24	b	612	CLA	OBD-CAD	3.25	1.28	1.22
24	c	904	CLA	OBD-CAD	3.24	1.28	1.22
32	v	202	HEM	CAC-C3C	3.24	1.56	1.47
24	B	612	CLA	OBD-CAD	3.24	1.28	1.22
26	a	409	BCR	C21-C22	-3.22	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C1B-C2B	3.22	1.50	1.43
32	v	202	HEM	FE-NA	3.22	2.05	1.95
24	d	403	CLA	CHD-C4C	3.22	1.46	1.39
26	T	102	BCR	C21-C22	-3.21	1.28	1.35
24	b	613	CLA	CHD-C4C	3.21	1.46	1.39
24	b	608	CLA	C1B-C2B	3.20	1.50	1.43
24	b	602	CLA	MG-NB	-3.20	1.99	2.05
24	d	403	CLA	OBD-CAD	3.20	1.28	1.22
29	D	407	LHG	O7-C7	3.19	1.43	1.34
24	C	504	CLA	MG-NB	3.16	2.12	2.05
26	B	618	BCR	C17-C18	-3.16	1.28	1.35
24	d	404	CLA	MG-NB	-3.15	1.99	2.05
32	V	202	HEM	CAC-C3C	3.14	1.55	1.47
24	C	508	CLA	C3D-C2D	3.14	1.47	1.39
24	B	603	CLA	C3D-C2D	3.13	1.47	1.39
32	v	202	HEM	FE-NC	3.11	2.05	1.95
32	E	101	HEM	CAB-C3B	3.10	1.55	1.47
24	C	510	CLA	MG-NB	3.10	2.11	2.05
24	a	407	CLA	OBD-CAD	3.09	1.27	1.22
24	A	606	CLA	MG-NC	3.09	2.13	2.06
24	B	617	CLA	C3D-C2D	3.09	1.47	1.39
24	C	511	CLA	C1B-C2B	3.09	1.50	1.43
32	e	101	HEM	CAB-C3B	3.08	1.55	1.47
24	B	604	CLA	MG-NC	3.08	2.13	2.06
24	B	603	CLA	MG-NB	3.08	2.11	2.05
24	C	505	CLA	C1B-C2B	3.08	1.50	1.43
24	d	404	CLA	C3D-C2D	3.07	1.47	1.39
24	b	606	CLA	OBD-CAD	3.07	1.27	1.22
24	C	513	CLA	C3D-C2D	3.06	1.47	1.39
24	b	617	CLA	C3D-C2D	3.06	1.47	1.39
26	B	619	BCR	C17-C18	-3.06	1.28	1.35
24	b	616	CLA	C3D-C2D	3.06	1.47	1.39
24	b	616	CLA	C1B-C2B	3.06	1.50	1.43
24	c	908	CLA	C1B-C2B	3.05	1.50	1.43
24	B	611	CLA	MG-ND	-3.05	1.99	2.05
24	C	511	CLA	C3D-C2D	3.04	1.47	1.39
24	b	603	CLA	C1B-C2B	3.04	1.50	1.43
24	c	906	CLA	C1B-C2B	3.04	1.50	1.43
24	B	610	CLA	C1B-C2B	3.03	1.50	1.43
24	B	604	CLA	C3D-C2D	3.03	1.47	1.39
32	e	101	HEM	CAC-C3C	3.02	1.55	1.47
24	b	614	CLA	C1B-C2B	3.02	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	CLA	C1B-C2B	3.01	1.50	1.43
24	C	504	CLA	C3D-C2D	3.00	1.47	1.39
24	b	606	CLA	C1B-C2B	3.00	1.50	1.43
24	B	614	CLA	C3D-C2D	3.00	1.47	1.39
24	a	406	CLA	MG-ND	-3.00	1.99	2.05
24	B	605	CLA	OBD-CAD	3.00	1.27	1.22
24	D	403	CLA	C1B-C2B	2.99	1.50	1.43
24	a	406	CLA	MG-NB	-2.99	1.99	2.05
24	C	512	CLA	C3D-C2D	2.99	1.47	1.39
24	d	401	CLA	C1B-C2B	2.99	1.50	1.43
24	C	503	CLA	OBD-CAD	2.98	1.27	1.22
24	c	909	CLA	C3D-C2D	2.98	1.47	1.39
24	b	612	CLA	C3D-C2D	2.98	1.47	1.39
24	A	607	CLA	C3D-C2D	2.98	1.47	1.39
24	c	902	CLA	C1B-C2B	2.98	1.50	1.43
24	c	908	CLA	C3D-C2D	2.97	1.47	1.39
24	b	610	CLA	C3D-C2D	2.97	1.47	1.39
24	A	614	CLA	C1B-C2B	2.97	1.50	1.43
32	E	101	HEM	FE-NB	2.97	2.04	1.94
24	b	610	CLA	C1B-C2B	2.97	1.50	1.43
24	b	616	CLA	C4D-CHA	2.96	1.48	1.38
24	a	407	CLA	C3D-C2D	2.96	1.47	1.39
24	c	914	CLA	C3D-C2D	2.96	1.47	1.39
24	B	604	CLA	C1B-C2B	2.96	1.50	1.43
24	C	507	CLA	C1B-C2B	2.96	1.50	1.43
24	C	511	CLA	C4D-CHA	2.95	1.48	1.38
24	C	504	CLA	MG-ND	-2.95	1.99	2.05
24	c	913	CLA	C1B-C2B	2.95	1.50	1.43
24	B	611	CLA	C3D-C2D	2.95	1.47	1.39
24	C	501	CLA	C3D-C2D	2.95	1.47	1.39
24	C	501	CLA	C1B-C2B	2.95	1.50	1.43
24	c	912	CLA	C3D-C2D	2.94	1.47	1.39
24	D	402	CLA	C1B-C2B	2.94	1.50	1.43
24	c	908	CLA	C4D-CHA	2.94	1.48	1.38
24	A	614	CLA	C3D-C2D	2.94	1.47	1.39
24	c	905	CLA	C3D-C2D	2.94	1.47	1.39
32	E	101	HEM	CAC-C3C	2.93	1.55	1.47
24	A	607	CLA	C1B-C2B	2.93	1.50	1.43
27	a	410	PL9	C6-C5	2.93	1.49	1.35
24	C	507	CLA	C4D-CHA	2.93	1.48	1.38
24	c	904	CLA	C4D-CHA	2.93	1.48	1.38
24	B	610	CLA	C3D-C2D	2.93	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	611	PL9	C6-C5	2.93	1.49	1.35
32	V	202	HEM	FE-NA	2.93	2.04	1.95
24	B	615	CLA	C1B-C2B	2.92	1.50	1.43
24	C	512	CLA	C1B-C2B	2.92	1.50	1.43
24	c	912	CLA	C1B-C2B	2.91	1.50	1.43
32	v	202	HEM	FE-NB	2.91	2.03	1.94
24	b	607	CLA	C3D-C2D	2.90	1.46	1.39
24	D	403	CLA	C3D-C2D	2.90	1.46	1.39
24	c	903	CLA	C3D-C2D	2.90	1.46	1.39
24	c	910	CLA	C1B-C2B	2.90	1.49	1.43
24	b	605	CLA	C1B-C2B	2.90	1.49	1.43
24	B	613	CLA	C4B-NB	-2.90	1.34	1.37
24	b	602	CLA	C4D-CHA	2.89	1.48	1.38
24	B	609	CLA	C3D-C2D	2.89	1.46	1.39
24	b	613	CLA	C3D-C2D	2.89	1.46	1.39
24	b	602	CLA	C3D-C2D	2.89	1.46	1.39
24	b	617	CLA	MG-NC	2.88	2.13	2.06
24	B	616	CLA	C3D-C2D	2.88	1.46	1.39
24	B	606	CLA	C1B-C2B	2.88	1.49	1.43
27	d	405	PL9	C6-C5	2.88	1.49	1.35
24	c	912	CLA	C4D-CHA	2.87	1.48	1.38
24	c	913	CLA	C4D-CHA	2.86	1.48	1.38
24	C	505	CLA	C3D-C2D	2.86	1.46	1.39
24	b	607	CLA	MG-ND	-2.86	2.00	2.05
24	B	602	CLA	C4D-CHA	2.85	1.48	1.38
24	C	503	CLA	C1B-C2B	2.85	1.49	1.43
24	B	606	CLA	C3D-C2D	2.85	1.46	1.39
24	C	503	CLA	C4D-CHA	2.85	1.48	1.38
24	C	507	CLA	C3D-C2D	2.85	1.46	1.39
27	D	405	PL9	C6-C5	2.85	1.49	1.35
24	a	408	CLA	C3D-C2D	2.84	1.46	1.39
24	B	609	CLA	MG-NB	-2.84	2.00	2.05
24	C	501	CLA	C4D-CHA	2.84	1.48	1.38
24	C	507	CLA	MG-NC	2.84	2.13	2.06
24	B	608	CLA	C3D-C2D	2.84	1.46	1.39
24	c	913	CLA	C3D-C2D	2.84	1.46	1.39
24	d	403	CLA	C3D-C2D	2.84	1.46	1.39
24	C	509	CLA	C1B-C2B	2.83	1.49	1.43
24	B	607	CLA	C1B-C2B	2.83	1.49	1.43
24	b	603	CLA	C3D-C2D	2.83	1.46	1.39
24	C	513	CLA	C4D-CHA	2.82	1.48	1.38
24	C	510	CLA	C3D-C2D	2.82	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C4D-CHA	2.82	1.48	1.38
24	c	906	CLA	C3D-C2D	2.81	1.46	1.39
24	c	904	CLA	C3D-C2D	2.81	1.46	1.39
24	A	606	CLA	C3D-C2D	2.81	1.46	1.39
24	b	607	CLA	C1B-C2B	2.81	1.49	1.43
24	B	615	CLA	C3D-C2D	2.81	1.46	1.39
24	c	903	CLA	C4D-CHA	2.81	1.48	1.38
25	A	608	PHO	CBD-CGD	-2.81	1.49	1.52
24	b	614	CLA	C3D-C2D	2.80	1.46	1.39
24	b	604	CLA	C3D-C2D	2.80	1.46	1.39
24	b	605	CLA	C3D-C2D	2.80	1.46	1.39
24	b	612	CLA	C1B-C2B	2.80	1.49	1.43
24	a	407	CLA	C4D-CHA	2.80	1.48	1.38
24	d	401	CLA	MG-ND	-2.79	2.00	2.05
24	C	502	CLA	C3D-C2D	2.79	1.46	1.39
24	A	609	CLA	C3D-C2D	2.79	1.46	1.39
24	b	615	CLA	C3D-C2D	2.79	1.46	1.39
24	c	902	CLA	C4D-CHA	2.78	1.47	1.38
24	b	611	CLA	C4D-CHA	2.78	1.47	1.38
24	A	614	CLA	C4B-NB	-2.78	1.34	1.37
24	C	509	CLA	C3D-C2D	2.78	1.46	1.39
24	C	504	CLA	C4D-CHA	2.78	1.47	1.38
24	C	509	CLA	C4D-CHA	2.77	1.47	1.38
24	C	506	CLA	C3D-C2D	2.77	1.46	1.39
24	c	909	CLA	C1B-C2B	2.77	1.49	1.43
26	c	918	BCR	C24-C25	-2.77	1.35	1.45
24	c	907	CLA	C1B-C2B	2.77	1.49	1.43
24	c	912	CLA	MG-NB	-2.77	2.00	2.05
24	b	604	CLA	C1B-C2B	2.77	1.49	1.43
24	D	403	CLA	MG-NB	-2.76	2.00	2.05
24	B	611	CLA	C1B-C2B	2.76	1.49	1.43
24	B	613	CLA	C3D-C2D	2.76	1.46	1.39
24	c	903	CLA	C1B-C2B	2.76	1.49	1.43
24	b	609	CLA	C3D-C2D	2.76	1.46	1.39
24	c	910	CLA	C3D-C2D	2.75	1.46	1.39
24	A	609	CLA	C1B-C2B	2.75	1.49	1.43
24	b	612	CLA	C4D-CHA	2.75	1.47	1.38
24	C	513	CLA	C1B-C2B	2.75	1.49	1.43
24	B	605	CLA	C4D-CHA	2.75	1.47	1.38
24	a	407	CLA	C1B-C2B	2.75	1.49	1.43
24	b	608	CLA	C4D-CHA	2.75	1.47	1.38
24	d	404	CLA	C1B-C2B	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	C4D-CHA	2.74	1.47	1.38
24	C	504	CLA	C1B-C2B	2.74	1.49	1.43
24	b	615	CLA	C1B-C2B	2.74	1.49	1.43
24	b	605	CLA	C4D-CHA	2.74	1.47	1.38
24	c	911	CLA	C4D-CHA	2.74	1.47	1.38
24	C	503	CLA	C3D-C2D	2.74	1.46	1.39
24	d	401	CLA	C3D-C2D	2.74	1.46	1.39
24	B	607	CLA	C3D-C2D	2.74	1.46	1.39
24	b	617	CLA	C4D-CHA	2.74	1.47	1.38
24	A	607	CLA	C4B-NB	-2.74	1.34	1.37
24	c	904	CLA	C1B-C2B	2.74	1.49	1.43
24	b	610	CLA	C4D-CHA	2.73	1.47	1.38
24	c	914	CLA	C4D-CHA	2.73	1.47	1.38
24	B	612	CLA	C3D-C2D	2.72	1.46	1.39
24	b	609	CLA	C4D-CHA	2.71	1.47	1.38
24	b	602	CLA	C1C-C2C	2.71	1.50	1.44
24	C	506	CLA	C4D-CHA	2.71	1.47	1.38
24	b	609	CLA	C1B-C2B	2.71	1.49	1.43
24	B	613	CLA	C1B-C2B	2.71	1.49	1.43
24	C	505	CLA	MG-ND	-2.71	2.00	2.05
24	B	614	CLA	C1B-C2B	2.70	1.49	1.43
24	c	902	CLA	C3D-C2D	2.69	1.46	1.39
24	c	906	CLA	C4D-CHA	2.69	1.47	1.38
24	B	614	CLA	C4D-CHA	2.69	1.47	1.38
24	b	607	CLA	C4D-CHA	2.69	1.47	1.38
24	c	910	CLA	C4D-CHA	2.68	1.47	1.38
24	b	611	CLA	C3D-C2D	2.68	1.46	1.39
24	a	406	CLA	C1B-C2B	2.68	1.49	1.43
24	A	609	CLA	MG-NB	-2.67	2.00	2.05
24	C	505	CLA	C4D-CHA	2.67	1.47	1.38
24	C	510	CLA	C1B-C2B	2.67	1.49	1.43
24	c	914	CLA	C1B-C2B	2.67	1.49	1.43
26	K	101	BCR	C24-C25	-2.67	1.35	1.45
24	c	907	CLA	C4D-CHA	2.67	1.47	1.38
24	B	616	CLA	C4D-CHA	2.67	1.47	1.38
24	B	617	CLA	C1B-C2B	2.67	1.49	1.43
24	C	506	CLA	C1B-C2B	2.67	1.49	1.43
24	B	611	CLA	C4D-CHA	2.66	1.47	1.38
26	C	515	BCR	C24-C25	-2.66	1.36	1.45
24	C	503	CLA	C1C-C2C	2.66	1.49	1.44
24	c	911	CLA	C1B-C2B	2.66	1.49	1.43
24	b	607	CLA	MG-NB	2.65	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C4D-CHA	2.65	1.47	1.38
24	a	406	CLA	C4B-NB	-2.65	1.34	1.37
26	C	514	BCR	C24-C25	-2.65	1.36	1.45
24	B	603	CLA	C4D-CHA	2.64	1.47	1.38
31	H	102	DGD	O5D-C1E	2.64	1.44	1.40
24	c	905	CLA	C4D-CHA	2.64	1.47	1.38
24	B	607	CLA	C4D-CHA	2.63	1.47	1.38
24	b	611	CLA	C1B-C2B	2.63	1.49	1.43
24	B	610	CLA	C4D-CHA	2.63	1.47	1.38
24	d	404	CLA	C4D-CHA	2.63	1.47	1.38
24	B	602	CLA	C3D-C2D	2.63	1.46	1.39
24	b	606	CLA	C4D-CHA	2.63	1.47	1.38
24	b	609	CLA	C4B-NB	-2.63	1.34	1.37
24	C	505	CLA	MG-NB	2.63	2.11	2.05
24	C	510	CLA	C4D-CHA	2.62	1.47	1.38
26	H	101	BCR	C24-C25	-2.62	1.36	1.45
24	b	607	CLA	C1D-C2D	2.62	1.50	1.45
24	B	602	CLA	C1D-C2D	2.62	1.50	1.45
26	k	101	BCR	C24-C25	-2.62	1.36	1.45
24	c	907	CLA	C3D-C2D	2.61	1.46	1.39
24	b	617	CLA	C1B-C2B	2.61	1.49	1.43
26	h	101	BCR	C24-C25	-2.61	1.36	1.45
24	b	617	CLA	C4B-NB	-2.61	1.34	1.37
24	B	602	CLA	C1B-C2B	2.61	1.49	1.43
24	c	911	CLA	C3D-C2D	2.61	1.46	1.39
24	C	508	CLA	C1B-C2B	2.61	1.49	1.43
24	B	609	CLA	C4D-CHA	2.60	1.47	1.38
24	B	617	CLA	C4D-CHA	2.60	1.47	1.38
24	B	617	CLA	C4B-NB	-2.60	1.34	1.37
24	a	408	CLA	C4D-CHA	2.60	1.47	1.38
26	Y	101	BCR	C24-C25	-2.60	1.36	1.45
24	b	615	CLA	C4D-CHA	2.60	1.47	1.38
24	D	402	CLA	C3D-C2D	2.60	1.46	1.39
24	b	606	CLA	C3D-C2D	2.60	1.46	1.39
24	a	406	CLA	C3D-C2D	2.60	1.46	1.39
24	A	607	CLA	C4D-CHA	2.60	1.47	1.38
24	b	604	CLA	C4B-NB	-2.60	1.34	1.37
26	B	618	BCR	C24-C25	-2.60	1.36	1.45
26	c	915	BCR	C24-C25	-2.59	1.36	1.45
26	k	102	BCR	C24-C25	-2.59	1.36	1.45
24	B	605	CLA	C3D-C2D	2.59	1.46	1.39
24	B	615	CLA	C1C-NC	-2.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C4D-CHA	2.58	1.47	1.38
24	b	614	CLA	C4D-CHA	2.58	1.47	1.38
24	C	508	CLA	C4D-CHA	2.58	1.47	1.38
26	T	102	BCR	C24-C25	-2.57	1.36	1.45
24	c	908	CLA	C1C-C2C	2.57	1.49	1.44
26	b	619	BCR	C24-C25	-2.57	1.36	1.45
24	C	511	CLA	MG-NB	-2.57	2.00	2.05
24	B	608	CLA	C1B-C2B	2.57	1.49	1.43
24	B	606	CLA	C4D-CHA	2.57	1.47	1.38
24	B	607	CLA	C1D-C2D	2.57	1.50	1.45
26	B	620	BCR	C24-C25	-2.57	1.36	1.45
24	C	504	CLA	C4B-NB	-2.56	1.34	1.37
26	A	610	BCR	C24-C25	-2.56	1.36	1.45
24	C	502	CLA	C1B-C2B	2.56	1.49	1.43
24	a	406	CLA	C4D-CHA	2.56	1.47	1.38
26	B	622	BCR	C24-C25	-2.56	1.36	1.45
26	D	404	BCR	C24-C25	-2.56	1.36	1.45
24	c	907	CLA	MG-NC	2.56	2.12	2.06
24	b	602	CLA	C1B-C2B	2.55	1.49	1.43
24	B	602	CLA	C1C-C2C	2.55	1.49	1.44
24	A	609	CLA	C4D-CHA	2.55	1.47	1.38
24	b	604	CLA	C4D-CHA	2.55	1.47	1.38
24	D	402	CLA	C4D-CHA	2.55	1.47	1.38
24	A	606	CLA	C1B-C2B	2.55	1.49	1.43
24	B	608	CLA	C1B-NB	-2.54	1.34	1.37
24	c	914	CLA	C1C-C2C	2.54	1.49	1.44
24	C	507	CLA	MG-NB	-2.54	2.00	2.05
24	D	402	CLA	MG-ND	-2.53	2.00	2.05
24	b	610	CLA	C1D-C2D	2.53	1.50	1.45
24	b	606	CLA	MG-NC	2.53	2.12	2.06
24	B	612	CLA	C1B-C2B	2.53	1.49	1.43
26	b	618	BCR	C24-C25	-2.52	1.36	1.45
24	B	615	CLA	C4D-CHA	2.52	1.47	1.38
24	A	606	CLA	C4D-CHA	2.52	1.47	1.38
24	b	602	CLA	C1D-C2D	2.52	1.50	1.45
24	A	614	CLA	C4D-CHA	2.51	1.47	1.38
24	c	909	CLA	C4D-CHA	2.51	1.47	1.38
24	C	507	CLA	C1C-C2C	2.51	1.49	1.44
26	f	101	BCR	C24-C25	-2.50	1.36	1.45
24	c	905	CLA	C1B-C2B	2.50	1.49	1.43
24	B	612	CLA	C4D-CHA	2.50	1.47	1.38
24	b	613	CLA	C4D-CHA	2.50	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	BCR	C24-C25	-2.49	1.36	1.45
24	d	403	CLA	C4D-CHA	2.49	1.46	1.38
24	B	608	CLA	C4D-CHA	2.48	1.46	1.38
24	c	904	CLA	C1C-C2C	2.48	1.49	1.44
24	c	906	CLA	C1C-C2C	2.47	1.49	1.44
24	B	613	CLA	C4D-CHA	2.47	1.46	1.38
32	V	202	HEM	CMA-C3A	2.47	1.55	1.50
24	d	404	CLA	C1D-C2D	2.47	1.50	1.45
24	C	510	CLA	C4B-NB	-2.46	1.34	1.37
24	C	513	CLA	C1C-C2C	2.46	1.49	1.44
24	B	610	CLA	MG-ND	-2.46	2.00	2.05
24	C	501	CLA	C1D-C2D	2.45	1.50	1.45
24	C	512	CLA	C1C-C2C	2.45	1.49	1.44
24	B	603	CLA	C1D-C2D	2.45	1.50	1.45
24	c	914	CLA	C1D-C2D	2.45	1.50	1.45
24	d	403	CLA	C1B-C2B	2.45	1.48	1.43
24	c	907	CLA	C1D-C2D	2.44	1.50	1.45
24	c	909	CLA	C1C-NC	-2.43	1.34	1.37
32	V	202	HEM	FE-NC	2.43	2.03	1.95
24	b	603	CLA	C1D-C2D	2.42	1.50	1.45
24	b	611	CLA	C4C-C3C	2.42	1.49	1.45
24	c	902	CLA	C1D-C2D	2.42	1.50	1.45
25	d	402	PHO	C3A-C2A	-2.42	1.52	1.54
24	A	607	CLA	MG-NB	-2.42	2.01	2.05
24	d	404	CLA	MG-ND	2.41	2.10	2.05
32	V	202	HEM	CMB-C2B	2.41	1.55	1.50
24	c	905	CLA	C1C-C2C	2.41	1.49	1.44
24	C	506	CLA	MG-ND	-2.41	2.01	2.05
24	C	509	CLA	C4B-NB	-2.40	1.34	1.37
32	E	101	HEM	CMA-C3A	2.39	1.55	1.50
24	d	404	CLA	C4C-C3C	2.38	1.49	1.45
26	B	619	BCR	C24-C25	-2.38	1.36	1.45
24	c	910	CLA	C1C-C2C	2.37	1.49	1.44
24	d	401	CLA	C4D-CHA	2.37	1.46	1.38
24	C	513	CLA	C1D-C2D	2.36	1.50	1.45
24	B	604	CLA	C4D-CHA	2.36	1.46	1.38
31	h	102	DGD	O5D-C1E	2.36	1.44	1.40
24	c	908	CLA	C4B-NB	-2.35	1.34	1.37
31	j	101	DGD	O2G-C2G	-2.35	1.41	1.46
24	b	617	CLA	C1C-C2C	2.35	1.49	1.44
24	C	506	CLA	C1D-C2D	2.35	1.50	1.45
24	b	605	CLA	C1D-C2D	2.34	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C1D-C2D	2.34	1.50	1.45
32	e	101	HEM	CMB-C2B	2.34	1.55	1.50
24	B	610	CLA	C4B-NB	-2.33	1.34	1.37
26	a	409	BCR	C24-C25	-2.33	1.37	1.45
32	V	202	HEM	CMC-C2C	2.32	1.55	1.50
24	B	613	CLA	C1B-NB	-2.32	1.34	1.37
27	A	611	PL9	C2-C3	2.32	1.40	1.34
24	b	610	CLA	C4C-C3C	2.32	1.49	1.45
24	c	907	CLA	C1C-C2C	2.31	1.49	1.44
24	C	504	CLA	C1D-C2D	2.31	1.49	1.45
32	e	101	HEM	CMA-C3A	2.30	1.55	1.50
24	C	508	CLA	C4C-C3C	2.30	1.48	1.45
24	A	607	CLA	C1D-C2D	2.29	1.49	1.45
24	B	615	CLA	C1B-NB	-2.29	1.34	1.37
24	a	406	CLA	C1D-C2D	2.29	1.49	1.45
25	d	402	PHO	CBD-CGD	-2.29	1.49	1.52
24	C	502	CLA	C4B-NB	-2.29	1.34	1.37
24	B	602	CLA	MG-ND	-2.29	2.01	2.05
24	B	610	CLA	C1D-C2D	2.29	1.49	1.45
24	C	506	CLA	C1C-C2C	2.29	1.49	1.44
25	d	402	PHO	C4B-NB	-2.28	1.34	1.38
24	C	501	CLA	C1C-C2C	2.28	1.49	1.44
24	c	904	CLA	C1D-C2D	2.28	1.49	1.45
24	b	607	CLA	C1C-C2C	2.28	1.49	1.44
24	c	913	CLA	C1C-C2C	2.27	1.49	1.44
24	d	401	CLA	C1D-C2D	2.27	1.49	1.45
24	A	614	CLA	C1D-C2D	2.26	1.49	1.45
24	C	512	CLA	C4C-C3C	2.26	1.48	1.45
24	b	605	CLA	C1C-C2C	2.25	1.49	1.44
26	B	622	BCR	C8-C7	-2.25	1.26	1.33
24	C	510	CLA	C1D-C2D	2.25	1.49	1.45
24	c	906	CLA	C1D-C2D	2.25	1.49	1.45
32	v	202	HEM	CMC-C2C	2.24	1.55	1.50
24	c	909	CLA	C1C-C2C	2.24	1.49	1.44
24	C	510	CLA	MG-NC	2.24	2.11	2.06
24	C	507	CLA	C3B-C2B	2.23	1.48	1.41
31	D	406	DGD	O5D-C1E	2.23	1.43	1.40
24	B	609	CLA	C1B-C2B	2.23	1.48	1.43
24	B	613	CLA	MG-NB	2.23	2.10	2.05
27	d	405	PL9	C2-C3	2.23	1.40	1.34
24	b	606	CLA	C3B-C4B	2.23	1.49	1.42
24	c	908	CLA	C1D-C2D	2.23	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C1C-C2C	2.22	1.49	1.44
31	d	406	DGD	O5D-C1E	2.22	1.43	1.40
24	D	403	CLA	C1C-C2C	2.21	1.49	1.44
24	d	404	CLA	C1C-C2C	2.21	1.49	1.44
24	C	509	CLA	C4C-C3C	2.21	1.48	1.45
24	B	616	CLA	C4B-NB	-2.21	1.35	1.37
32	E	101	HEM	CMB-C2B	2.21	1.55	1.50
24	c	911	CLA	C1D-C2D	2.20	1.49	1.45
24	b	604	CLA	C1B-NB	-2.20	1.35	1.37
31	C	518	DGD	O2G-C2G	-2.20	1.41	1.46
24	B	608	CLA	C1D-C2D	2.20	1.49	1.45
28	L	101	SQD	O6-C1	2.20	1.43	1.40
24	C	509	CLA	C1D-C2D	2.20	1.49	1.45
23	A	605	BCT	O1-C	2.20	1.33	1.25
24	c	914	CLA	C4C-C3C	2.19	1.48	1.45
24	B	614	CLA	C1C-C2C	2.19	1.49	1.44
24	D	402	CLA	C1D-ND	-2.19	1.35	1.37
24	b	610	CLA	C4B-NB	-2.19	1.35	1.37
24	C	505	CLA	C1C-C2C	2.19	1.49	1.44
24	b	603	CLA	C3B-C4B	2.19	1.49	1.42
24	C	507	CLA	C4B-NB	-2.19	1.35	1.37
24	D	403	CLA	C4C-C3C	2.19	1.48	1.45
24	b	611	CLA	C1C-C2C	2.18	1.49	1.44
24	b	603	CLA	C1C-C2C	2.18	1.48	1.44
24	B	607	CLA	C1C-C2C	2.18	1.48	1.44
24	B	615	CLA	C1D-C2D	2.18	1.49	1.45
24	b	603	CLA	MG-ND	-2.18	2.01	2.05
24	B	616	CLA	C1C-C2C	2.18	1.48	1.44
24	B	616	CLA	C1B-NB	-2.18	1.35	1.37
24	c	904	CLA	C4C-C3C	2.18	1.48	1.45
24	a	407	CLA	C1D-C2D	2.18	1.49	1.45
24	c	906	CLA	C4B-NB	-2.18	1.35	1.37
24	b	602	CLA	C3B-C4B	2.18	1.49	1.42
24	d	404	CLA	C4B-NB	-2.18	1.35	1.37
24	c	905	CLA	C1D-C2D	2.18	1.49	1.45
26	T	102	BCR	C8-C7	-2.17	1.26	1.33
24	B	605	CLA	MG-NC	2.17	2.11	2.06
24	A	607	CLA	C1B-NB	-2.17	1.35	1.37
24	C	508	CLA	C1D-C2D	2.17	1.49	1.45
24	B	608	CLA	C1D-ND	-2.17	1.35	1.37
24	C	513	CLA	C3B-C2B	2.16	1.48	1.41
24	B	605	CLA	C1D-C2D	2.16	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	C4B-NB	-2.15	1.35	1.37
24	b	610	CLA	C1C-C2C	2.15	1.48	1.44
24	C	507	CLA	C1D-C2D	2.15	1.49	1.45
24	C	510	CLA	C1C-C2C	2.15	1.48	1.44
24	c	912	CLA	C1D-C2D	2.15	1.49	1.45
24	c	905	CLA	C1C-NC	-2.14	1.34	1.37
24	B	611	CLA	C3B-C4B	2.14	1.49	1.42
24	c	913	CLA	C4C-C3C	2.14	1.48	1.45
24	A	614	CLA	C1D-ND	-2.14	1.35	1.37
28	l	101	SQD	O6-C1	2.13	1.43	1.40
24	B	611	CLA	C1C-NC	-2.13	1.34	1.37
31	D	406	DGD	O3G-C1D	2.13	1.43	1.40
24	C	505	CLA	C4C-C3C	2.13	1.48	1.45
24	a	408	CLA	C1D-C2D	2.13	1.49	1.45
24	c	913	CLA	C1D-C2D	2.13	1.49	1.45
24	c	905	CLA	C4C-C3C	2.13	1.48	1.45
24	d	403	CLA	C1C-C2C	2.13	1.48	1.44
24	c	903	CLA	C1C-C2C	2.13	1.48	1.44
24	b	609	CLA	C1D-C2D	2.12	1.49	1.45
24	b	609	CLA	C1B-NB	-2.12	1.35	1.37
24	B	609	CLA	C4B-NB	-2.12	1.35	1.37
24	D	402	CLA	C4C-C3C	2.12	1.48	1.45
24	C	511	CLA	C1C-C2C	2.12	1.48	1.44
24	b	605	CLA	C1C-NC	-2.11	1.34	1.37
24	b	615	CLA	C1C-C2C	2.11	1.48	1.44
24	b	617	CLA	C1C-NC	-2.10	1.34	1.37
24	C	512	CLA	C1D-C2D	2.10	1.49	1.45
27	a	410	PL9	C2-C3	2.10	1.39	1.34
24	b	608	CLA	C1B-NB	-2.10	1.35	1.37
24	d	403	CLA	C1D-C2D	2.10	1.49	1.45
24	C	505	CLA	C1B-NB	-2.10	1.35	1.37
24	c	909	CLA	C4C-C3C	2.10	1.48	1.45
24	B	616	CLA	C1D-C2D	2.10	1.49	1.45
25	A	608	PHO	C3A-C2A	-2.10	1.52	1.54
24	B	604	CLA	C1C-NC	-2.10	1.34	1.37
24	c	909	CLA	C1D-C2D	2.09	1.49	1.45
24	c	910	CLA	C1C-NC	-2.09	1.34	1.37
31	C	516	DGD	O5D-C1E	2.08	1.43	1.40
24	b	606	CLA	C1C-C2C	2.08	1.48	1.44
24	D	403	CLA	C1C-NC	-2.08	1.34	1.37
32	e	101	HEM	CMC-C2C	2.08	1.55	1.50
26	c	915	BCR	C8-C7	-2.08	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C1C-C2C	2.08	1.48	1.44
24	B	603	CLA	C3B-C2B	2.08	1.48	1.41
24	B	607	CLA	C4C-C3C	2.08	1.48	1.45
26	c	918	BCR	C8-C7	-2.08	1.26	1.33
24	c	910	CLA	C1D-C2D	2.07	1.49	1.45
26	C	514	BCR	C8-C7	-2.07	1.26	1.33
24	c	912	CLA	C3B-C2B	2.07	1.48	1.41
24	b	609	CLA	MG-ND	-2.07	2.01	2.05
31	c	916	DGD	O5D-C1E	2.07	1.43	1.40
26	b	619	BCR	C8-C7	-2.07	1.27	1.33
24	b	614	CLA	C1C-C2C	2.06	1.48	1.44
32	v	202	HEM	CMD-C2D	2.06	1.55	1.50
24	b	609	CLA	C1C-C2C	2.06	1.48	1.44
24	b	606	CLA	C4B-NB	-2.06	1.35	1.37
24	b	602	CLA	C4C-C3C	2.06	1.48	1.45
24	A	606	CLA	C1B-NB	-2.06	1.35	1.37
24	b	609	CLA	C3B-C4B	2.05	1.48	1.42
24	c	902	CLA	C4C-C3C	2.05	1.48	1.45
24	B	617	CLA	MG-NB	2.05	2.09	2.05
24	B	606	CLA	MG-ND	-2.05	2.01	2.05
24	B	602	CLA	C3B-C4B	2.05	1.48	1.42
24	C	508	CLA	C3B-C2B	2.05	1.48	1.41
24	C	506	CLA	C4B-NB	-2.04	1.35	1.37
24	B	606	CLA	C3B-C4B	2.04	1.48	1.42
24	B	612	CLA	MG-ND	-2.04	2.01	2.05
26	f	101	BCR	C8-C7	-2.04	1.27	1.33
24	B	616	CLA	C4C-C3C	2.04	1.48	1.45
24	C	505	CLA	C1D-C2D	2.04	1.49	1.45
24	B	617	CLA	C3B-C2B	2.04	1.48	1.41
24	c	902	CLA	C1C-C2C	2.04	1.48	1.44
24	B	604	CLA	C1D-C2D	2.03	1.49	1.45
24	C	503	CLA	C3B-C2B	2.03	1.48	1.41
24	B	615	CLA	C4B-NB	-2.03	1.35	1.37
24	c	902	CLA	C3B-C2B	2.03	1.48	1.41
24	a	406	CLA	C1C-NC	-2.03	1.34	1.37
24	c	912	CLA	C1C-C2C	2.03	1.48	1.44
24	c	905	CLA	C4B-NB	-2.03	1.35	1.37
24	C	506	CLA	C4C-C3C	2.03	1.48	1.45
24	B	613	CLA	C1C-C2C	2.03	1.48	1.44
24	C	511	CLA	C4C-C3C	2.03	1.48	1.45
24	c	906	CLA	C4C-C3C	2.02	1.48	1.45
26	T	101	BCR	C8-C7	-2.02	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C3B-C2B	2.02	1.48	1.41
31	d	406	DGD	O3G-C1D	2.02	1.43	1.40
29	D	408	LHG	O7-C5	-2.02	1.41	1.46
24	B	614	CLA	C1C-NC	-2.02	1.34	1.37
32	e	101	HEM	CMD-C2D	2.02	1.54	1.50
24	C	501	CLA	C4B-NB	-2.01	1.35	1.37
24	B	614	CLA	MG-ND	2.01	2.09	2.05
24	B	613	CLA	C1D-C2D	2.01	1.49	1.45
24	B	602	CLA	C4C-C3C	2.01	1.48	1.45
24	c	914	CLA	C3B-C2B	2.01	1.47	1.41
27	D	405	PL9	C2-C3	2.01	1.39	1.34
28	F	101	SQD	O6-C1	2.01	1.43	1.40
24	C	502	CLA	C1D-C2D	2.01	1.49	1.45
24	c	908	CLA	C1A-CHA	2.01	1.51	1.43
23	a	414	BCT	O1-C	2.01	1.32	1.25
32	v	202	HEM	CMA-C3A	2.01	1.54	1.50
24	D	402	CLA	C4B-NB	-2.01	1.35	1.37
25	D	401	PHO	CBD-CGD	-2.00	1.50	1.52
32	E	101	HEM	CMD-C2D	2.00	1.54	1.50
24	a	408	CLA	C1C-C2C	2.00	1.48	1.44
24	B	604	CLA	C1C-C2C	2.00	1.48	1.44

All (2793) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	BCR	C20-C21-C22	30.76	170.41	127.28
26	H	101	BCR	C20-C21-C22	27.39	165.69	127.28
26	c	915	BCR	C20-C21-C22	27.33	165.60	127.28
26	k	101	BCR	C16-C17-C18	27.12	165.32	127.28
26	h	101	BCR	C20-C21-C22	27.12	165.32	127.28
26	B	620	BCR	C20-C21-C22	27.04	165.20	127.28
26	C	514	BCR	C15-C16-C17	26.79	178.33	123.52
26	C	515	BCR	C20-C21-C22	26.17	163.98	127.28
26	Y	101	BCR	C20-C21-C22	26.00	163.75	127.28
26	B	620	BCR	C16-C17-C18	25.86	163.55	127.28
26	b	619	BCR	C16-C17-C18	25.79	163.45	127.28
26	A	610	BCR	C20-C21-C22	25.67	163.28	127.28
26	C	514	BCR	C16-C17-C18	25.57	163.14	127.28
26	b	618	BCR	C16-C17-C18	25.56	163.12	127.28
26	c	915	BCR	C16-C17-C18	25.49	163.03	127.28
26	B	620	BCR	C15-C16-C17	25.34	175.36	123.52
26	H	101	BCR	C15-C16-C17	25.31	175.30	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	915	BCR	C15-C16-C17	24.78	174.22	123.52
26	k	101	BCR	C15-C16-C17	24.72	174.09	123.52
26	B	618	BCR	C16-C17-C18	24.65	161.85	127.28
26	h	101	BCR	C15-C16-C17	24.54	173.73	123.52
26	k	102	BCR	C15-C16-C17	24.11	172.85	123.52
26	k	102	BCR	C20-C21-C22	23.93	160.84	127.28
26	k	102	BCR	C16-C17-C18	23.91	160.81	127.28
26	Y	101	BCR	C16-C17-C18	23.77	160.61	127.28
26	C	515	BCR	C15-C16-C17	23.72	172.06	123.52
26	f	101	BCR	C16-C17-C18	23.63	160.42	127.28
26	C	514	BCR	C20-C21-C22	23.46	160.19	127.28
26	f	101	BCR	C15-C16-C17	23.24	171.07	123.52
26	D	404	BCR	C15-C16-C17	23.22	171.03	123.52
26	D	404	BCR	C20-C21-C22	22.89	159.38	127.28
26	k	101	BCR	C20-C21-C22	22.84	159.31	127.28
26	B	622	BCR	C16-C17-C18	22.76	159.20	127.28
26	D	404	BCR	C16-C17-C18	22.72	159.14	127.28
26	a	409	BCR	C16-C17-C18	22.62	159.01	127.28
26	K	101	BCR	C15-C16-C17	22.36	169.26	123.52
26	B	619	BCR	C20-C21-C22	22.33	158.59	127.28
26	c	918	BCR	C16-C15-C14	22.33	169.20	123.52
26	a	409	BCR	C15-C16-C17	22.10	168.74	123.52
26	a	409	BCR	C20-C21-C22	22.00	158.13	127.28
26	A	610	BCR	C16-C17-C18	21.97	158.09	127.28
26	c	915	BCR	C16-C15-C14	21.91	168.36	123.52
26	T	102	BCR	C16-C17-C18	21.83	157.89	127.28
26	C	515	BCR	C16-C15-C14	21.80	168.12	123.52
26	h	101	BCR	C16-C17-C18	21.45	157.36	127.28
26	K	101	BCR	C20-C21-C22	21.37	157.25	127.28
26	b	618	BCR	C20-C21-C22	21.34	157.21	127.28
26	T	101	BCR	C15-C16-C17	21.18	166.87	123.52
26	C	515	BCR	C16-C17-C18	21.04	156.79	127.28
26	B	619	BCR	C16-C17-C18	20.95	156.66	127.28
26	B	622	BCR	C15-C16-C17	20.93	166.34	123.52
26	H	101	BCR	C16-C17-C18	20.91	156.60	127.28
26	c	918	BCR	C20-C21-C22	20.82	156.47	127.28
26	C	514	BCR	C16-C15-C14	20.72	165.92	123.52
26	Y	101	BCR	C15-C16-C17	20.68	165.83	123.52
26	c	918	BCR	C16-C17-C18	20.61	156.18	127.28
26	T	101	BCR	C16-C15-C14	20.36	165.19	123.52
26	D	404	BCR	C16-C15-C14	20.15	164.75	123.52
26	T	102	BCR	C15-C16-C17	20.15	164.74	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	BCR	C15-C16-C17	19.96	164.36	123.52
26	c	918	BCR	C15-C16-C17	19.93	164.31	123.52
26	B	622	BCR	C20-C21-C22	19.73	154.95	127.28
26	B	618	BCR	C15-C16-C17	19.70	163.82	123.52
26	h	101	BCR	C21-C20-C19	19.26	179.01	123.20
26	K	101	BCR	C16-C15-C14	19.18	162.77	123.52
26	K	101	BCR	C16-C17-C18	19.08	154.03	127.28
26	f	101	BCR	C20-C21-C22	18.93	153.83	127.28
26	T	102	BCR	C20-C21-C22	18.70	153.50	127.28
26	B	618	BCR	C20-C21-C22	18.41	153.09	127.28
26	B	620	BCR	C16-C15-C14	18.38	161.13	123.52
26	k	102	BCR	C21-C20-C19	18.35	176.37	123.20
26	C	514	BCR	C21-C20-C19	18.25	176.07	123.20
26	h	101	BCR	C16-C15-C14	18.19	160.74	123.52
26	B	622	BCR	C16-C15-C14	18.17	160.69	123.52
26	c	915	BCR	C21-C20-C19	18.15	175.79	123.20
26	A	610	BCR	C15-C16-C17	18.12	160.59	123.52
26	k	102	BCR	C16-C15-C14	17.81	159.97	123.52
26	T	101	BCR	C16-C17-C18	17.56	151.91	127.28
26	C	515	BCR	C21-C20-C19	17.55	174.04	123.20
26	k	101	BCR	C16-C15-C14	17.31	158.93	123.52
26	k	101	BCR	C21-C20-C19	17.28	173.27	123.20
26	f	101	BCR	C16-C15-C14	17.11	158.53	123.52
26	b	619	BCR	C21-C20-C19	16.94	172.30	123.20
26	b	618	BCR	C15-C16-C17	16.72	157.73	123.52
26	Y	101	BCR	C16-C15-C14	16.51	157.30	123.52
26	a	409	BCR	C16-C15-C14	16.49	157.26	123.52
26	c	918	BCR	C21-C20-C19	16.39	170.69	123.20
26	T	102	BCR	C16-C15-C14	16.20	156.66	123.52
26	H	101	BCR	C21-C20-C19	16.12	169.92	123.20
26	H	101	BCR	C16-C15-C14	16.07	156.40	123.52
26	B	619	BCR	C15-C16-C17	16.01	156.29	123.52
26	b	618	BCR	C19-C18-C17	15.91	144.03	119.01
26	B	619	BCR	C16-C15-C14	15.85	155.95	123.52
26	Y	101	BCR	C21-C20-C19	15.74	168.81	123.20
26	B	619	BCR	C21-C20-C19	15.73	168.78	123.20
26	c	918	BCR	C11-C12-C13	15.57	169.06	126.36
26	B	618	BCR	C19-C18-C17	15.05	142.68	119.01
26	b	619	BCR	C16-C15-C14	14.85	153.90	123.52
26	K	101	BCR	C21-C20-C19	14.79	166.05	123.20
26	C	515	BCR	C11-C10-C9	14.73	147.93	127.28
26	A	610	BCR	C16-C15-C14	14.60	153.39	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	918	BCR	C10-C11-C12	14.54	165.34	123.20
26	K	101	BCR	C15-C14-C13	14.40	147.47	127.28
26	k	101	BCR	C20-C19-C18	14.35	165.72	126.36
26	B	620	BCR	C21-C20-C19	14.35	164.77	123.20
26	T	101	BCR	C20-C21-C22	14.24	147.25	127.28
26	B	618	BCR	C16-C15-C14	14.13	152.43	123.52
26	H	101	BCR	C11-C10-C9	14.12	147.09	127.28
26	f	101	BCR	C7-C8-C9	13.97	146.90	126.23
26	B	619	BCR	C19-C18-C17	13.94	140.93	119.01
26	B	622	BCR	C21-C20-C19	13.87	163.40	123.20
26	B	619	BCR	C15-C14-C13	13.79	146.62	127.28
26	B	622	BCR	C10-C11-C12	13.76	163.06	123.20
26	A	610	BCR	C21-C20-C19	13.71	162.93	123.20
26	b	618	BCR	C11-C10-C9	13.64	146.41	127.28
26	D	404	BCR	C21-C20-C19	13.62	162.68	123.20
26	B	619	BCR	C11-C10-C9	13.53	146.26	127.28
26	Y	101	BCR	C11-C10-C9	13.33	145.97	127.28
26	k	102	BCR	C20-C19-C18	13.22	162.60	126.36
26	k	102	BCR	C10-C11-C12	13.22	161.49	123.20
26	c	918	BCR	C20-C19-C18	13.18	162.51	126.36
26	b	619	BCR	C15-C14-C13	13.03	145.54	127.28
26	C	514	BCR	C20-C19-C18	13.00	162.02	126.36
26	b	619	BCR	C11-C10-C9	12.91	145.38	127.28
26	C	514	BCR	C10-C11-C12	12.87	160.49	123.20
26	B	620	BCR	C19-C18-C17	12.86	139.24	119.01
26	B	620	BCR	C11-C10-C9	12.84	145.28	127.28
26	k	102	BCR	C11-C10-C9	12.83	145.27	127.28
26	B	622	BCR	C20-C19-C18	12.74	161.31	126.36
26	b	618	BCR	C21-C20-C19	12.69	159.98	123.20
26	C	515	BCR	C20-C19-C18	12.68	161.14	126.36
26	c	915	BCR	C10-C11-C12	12.66	159.89	123.20
26	T	101	BCR	C10-C11-C12	12.65	159.85	123.20
26	k	102	BCR	C15-C14-C13	12.59	144.94	127.28
26	K	101	BCR	C20-C19-C18	12.55	160.78	126.36
26	T	101	BCR	C11-C10-C9	12.46	144.75	127.28
26	b	618	BCR	C16-C15-C14	12.45	148.99	123.52
26	k	101	BCR	C19-C18-C17	12.40	138.51	119.01
26	h	101	BCR	C15-C14-C13	12.39	144.66	127.28
24	c	908	CLA	C4A-NA-C1A	12.35	112.31	106.68
26	b	619	BCR	C10-C11-C12	12.34	158.95	123.20
26	Y	101	BCR	C19-C18-C17	12.31	138.37	119.01
26	f	101	BCR	C21-C20-C19	12.23	158.65	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	BCR	C19-C18-C17	12.17	138.15	119.01
26	T	102	BCR	C21-C20-C19	12.14	158.38	123.20
26	k	101	BCR	C7-C8-C9	12.13	144.18	126.23
26	A	610	BCR	C19-C18-C17	12.12	138.08	119.01
26	B	618	BCR	C21-C20-C19	12.06	158.14	123.20
26	k	101	BCR	C11-C10-C9	12.04	144.17	127.28
26	c	918	BCR	C7-C8-C9	11.95	143.92	126.23
26	K	101	BCR	C19-C18-C17	11.88	137.70	119.01
26	f	101	BCR	C19-C18-C17	11.87	137.69	119.01
26	a	409	BCR	C11-C10-C9	11.87	143.92	127.28
26	h	101	BCR	C11-C10-C9	11.87	143.92	127.28
26	T	101	BCR	C11-C12-C13	11.85	158.86	126.36
26	T	102	BCR	C19-C18-C17	11.82	137.60	119.01
24	C	511	CLA	C4A-NA-C1A	11.77	112.05	106.68
26	a	409	BCR	C10-C11-C12	11.75	157.25	123.20
26	H	101	BCR	C15-C14-C13	11.75	143.75	127.28
26	b	618	BCR	C15-C14-C13	11.74	143.75	127.28
26	C	515	BCR	C15-C14-C13	11.73	143.73	127.28
26	K	101	BCR	C10-C11-C12	11.62	156.88	123.20
26	Y	101	BCR	C15-C14-C13	11.60	143.54	127.28
26	a	409	BCR	C15-C14-C13	11.59	143.54	127.28
26	K	101	BCR	C11-C12-C13	11.59	158.16	126.36
26	A	610	BCR	C11-C10-C9	11.57	143.50	127.28
24	C	507	CLA	C4A-NA-C1A	11.56	111.95	106.68
26	a	409	BCR	C19-C18-C17	11.52	137.13	119.01
26	b	619	BCR	C7-C8-C9	11.52	143.27	126.23
26	T	102	BCR	C15-C14-C13	11.51	143.41	127.28
26	h	101	BCR	C20-C19-C18	11.48	157.85	126.36
26	c	915	BCR	C15-C14-C13	11.46	143.35	127.28
26	Y	101	BCR	C20-C19-C18	11.44	157.72	126.36
26	f	101	BCR	C11-C10-C9	11.43	143.31	127.28
26	B	618	BCR	C12-C13-C14	11.37	136.90	119.01
24	b	605	CLA	C4A-NA-C1A	11.35	111.86	106.68
26	a	409	BCR	C23-C22-C21	11.32	136.82	119.01
26	k	101	BCR	C10-C11-C12	11.32	156.01	123.20
26	c	915	BCR	C20-C19-C18	11.28	157.28	126.36
26	a	409	BCR	C21-C20-C19	11.28	155.87	123.20
26	B	622	BCR	C15-C14-C13	11.27	143.08	127.28
26	B	618	BCR	C11-C10-C9	11.23	143.03	127.28
26	H	101	BCR	C20-C19-C18	11.19	157.04	126.36
26	B	622	BCR	C11-C12-C13	11.17	157.00	126.36
26	b	618	BCR	C10-C11-C12	11.10	155.38	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	912	CLA	C4A-NA-C1A	11.06	111.72	106.68
26	T	101	BCR	C20-C19-C18	11.04	156.63	126.36
26	k	102	BCR	C11-C12-C13	11.02	156.57	126.36
26	k	102	BCR	C19-C18-C17	11.01	136.33	119.01
26	A	610	BCR	C15-C14-C13	11.01	142.72	127.28
26	B	618	BCR	C20-C19-C18	11.00	156.52	126.36
26	T	101	BCR	C21-C20-C19	10.98	155.00	123.20
26	B	619	BCR	C20-C19-C18	10.97	156.45	126.36
26	B	620	BCR	C10-C11-C12	10.95	154.92	123.20
26	f	101	BCR	C20-C19-C18	10.93	156.34	126.36
26	C	515	BCR	C10-C11-C12	10.90	154.78	123.20
26	C	514	BCR	C11-C12-C13	10.89	156.24	126.36
26	B	622	BCR	C19-C18-C17	10.88	136.12	119.01
26	h	101	BCR	C10-C11-C12	10.85	154.63	123.20
26	h	101	BCR	C11-C12-C13	10.81	156.00	126.36
26	A	610	BCR	C23-C22-C21	10.78	135.97	119.01
24	B	605	CLA	C4A-NA-C1A	10.78	111.60	106.68
26	k	101	BCR	C15-C14-C13	10.77	142.39	127.28
26	D	404	BCR	C15-C14-C13	10.75	142.35	127.28
26	a	409	BCR	C11-C12-C13	10.75	155.84	126.36
26	b	619	BCR	C11-C12-C13	10.66	155.58	126.36
26	A	610	BCR	C12-C13-C14	10.56	135.63	119.01
26	D	404	BCR	C11-C10-C9	10.56	142.09	127.28
24	c	904	CLA	C4A-NA-C1A	10.55	111.49	106.68
26	B	622	BCR	C11-C10-C9	10.53	142.05	127.28
26	B	620	BCR	C15-C14-C13	10.49	141.99	127.28
26	f	101	BCR	C11-C12-C13	10.49	155.12	126.36
26	b	618	BCR	C7-C8-C9	10.48	141.75	126.23
26	b	618	BCR	C12-C13-C14	10.48	135.50	119.01
26	H	101	BCR	C19-C18-C17	10.44	135.43	119.01
25	A	608	PHO	C3B-C4B-NB	10.44	114.27	107.46
26	T	102	BCR	C11-C12-C13	10.40	154.89	126.36
26	B	620	BCR	C11-C12-C13	10.36	154.77	126.36
26	A	610	BCR	C10-C11-C12	10.35	153.19	123.20
26	b	618	BCR	C20-C19-C18	10.35	154.74	126.36
24	B	616	CLA	C4A-NA-C1A	10.33	111.39	106.68
26	k	102	BCR	C7-C8-C9	10.33	141.51	126.23
26	f	101	BCR	C29-C30-C25	10.28	125.38	110.44
26	C	514	BCR	C19-C18-C17	10.25	135.13	119.01
26	H	101	BCR	C10-C11-C12	10.23	152.83	123.20
26	c	915	BCR	C11-C12-C13	10.20	154.33	126.36
26	c	915	BCR	C11-C10-C9	10.11	141.46	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	102	BCR	C20-C19-C18	10.07	153.96	126.36
24	C	513	CLA	C4A-NA-C1A	10.01	111.25	106.68
24	c	902	CLA	C4A-NA-C1A	10.01	111.25	106.68
26	T	101	BCR	C15-C14-C13	10.00	141.31	127.28
26	A	610	BCR	C11-C12-C13	9.99	153.76	126.36
26	a	409	BCR	C12-C13-C14	9.99	134.72	119.01
24	B	602	CLA	C4A-NA-C1A	9.98	111.23	106.68
24	b	612	CLA	C4A-NA-C1A	9.97	111.23	106.68
26	C	514	BCR	C7-C8-C9	9.93	140.92	126.23
24	b	613	CLA	C4A-NA-C1A	9.91	111.20	106.68
26	C	514	BCR	C15-C14-C13	9.90	141.17	127.28
24	c	910	CLA	C4A-NA-C1A	9.87	111.18	106.68
26	k	101	BCR	C11-C12-C13	9.85	153.36	126.36
24	b	616	CLA	C4A-NA-C1A	9.80	111.15	106.68
24	C	509	CLA	C4A-NA-C1A	9.79	111.15	106.68
26	b	618	BCR	C23-C22-C21	9.79	134.40	119.01
26	T	102	BCR	C12-C13-C14	9.77	134.38	119.01
24	b	607	CLA	C4A-NA-C1A	9.74	111.12	106.68
26	D	404	BCR	C20-C19-C18	9.74	153.07	126.36
24	c	906	CLA	C4A-NA-C1A	9.70	111.11	106.68
26	h	101	BCR	C24-C23-C22	9.70	140.59	126.23
24	c	913	CLA	C4A-NA-C1A	9.70	111.11	106.68
26	T	102	BCR	C11-C10-C9	9.68	140.85	127.28
26	b	619	BCR	C20-C19-C18	9.67	152.88	126.36
26	D	404	BCR	C11-C12-C13	9.66	152.86	126.36
24	C	504	CLA	C4A-NA-C1A	9.65	111.08	106.68
26	f	101	BCR	C10-C11-C12	9.63	151.12	123.20
26	B	618	BCR	C11-C12-C13	9.62	152.75	126.36
24	C	506	CLA	C4A-NA-C1A	9.62	111.07	106.68
24	c	903	CLA	C4A-NA-C1A	9.62	111.07	106.68
26	B	620	BCR	C20-C19-C18	9.61	152.71	126.36
26	T	102	BCR	C10-C11-C12	9.61	151.03	123.20
26	a	409	BCR	C7-C8-C9	9.59	140.42	126.23
26	f	101	BCR	C15-C14-C13	9.56	140.69	127.28
26	h	101	BCR	C19-C18-C17	9.55	134.03	119.01
26	H	101	BCR	C11-C12-C13	9.51	152.44	126.36
26	K	101	BCR	C7-C8-C9	9.51	140.30	126.23
26	T	101	BCR	C19-C18-C17	9.50	133.95	119.01
24	C	505	CLA	C4A-NA-C1A	9.48	111.01	106.68
24	B	613	CLA	C4A-NA-C1A	9.47	111.00	106.68
24	C	510	CLA	C4A-NA-C1A	9.46	110.99	106.68
26	B	620	BCR	C7-C8-C9	9.44	140.20	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C4A-NA-C1A	9.43	110.98	106.68
25	A	608	PHO	C2D-C1D-ND	9.41	116.23	109.43
25	d	402	PHO	C3B-C4B-NB	9.41	113.59	107.46
26	D	404	BCR	C30-C25-C26	-9.40	109.80	122.64
24	b	611	CLA	C4A-NA-C1A	9.38	110.96	106.68
26	h	101	BCR	C7-C8-C9	9.35	140.07	126.23
26	c	915	BCR	C19-C18-C17	9.35	133.71	119.01
26	C	515	BCR	C19-C18-C17	9.34	133.70	119.01
26	K	101	BCR	C12-C13-C14	9.31	133.66	119.01
26	C	515	BCR	C12-C13-C14	9.30	133.63	119.01
26	B	618	BCR	C10-C11-C12	9.29	150.11	123.20
24	b	602	CLA	C4A-NA-C1A	9.28	110.91	106.68
24	B	610	CLA	C4A-NA-C1A	9.26	110.90	106.68
24	b	608	CLA	C4A-NA-C1A	9.23	110.89	106.68
26	B	619	BCR	C12-C13-C14	9.22	133.51	119.01
26	c	915	BCR	C7-C8-C9	9.21	139.86	126.23
24	D	403	CLA	C4A-NA-C1A	9.20	110.88	106.68
26	D	404	BCR	C19-C18-C17	9.20	133.48	119.01
26	H	101	BCR	C12-C13-C14	9.20	133.48	119.01
26	a	409	BCR	C24-C23-C22	9.19	139.83	126.23
25	D	401	PHO	C3B-C4B-NB	9.17	113.44	107.46
24	b	614	CLA	C4A-NA-C1A	9.09	110.83	106.68
26	T	101	BCR	C7-C8-C9	9.08	139.67	126.23
26	B	620	BCR	C36-C18-C17	-9.08	108.10	122.82
26	K	101	BCR	C11-C10-C9	9.07	140.00	127.28
24	B	612	CLA	C4A-NA-C1A	9.05	110.81	106.68
24	C	512	CLA	C4A-NA-C1A	9.05	110.81	106.68
26	B	619	BCR	C36-C18-C19	-9.04	104.28	118.09
26	B	622	BCR	C7-C8-C9	9.04	139.60	126.23
25	d	402	PHO	O2D-CGD-CBD	9.03	120.87	110.95
25	a	412	PHO	O2D-CGD-CBD	9.00	120.84	110.95
24	C	501	CLA	C4A-NA-C1A	8.96	110.77	106.68
24	B	607	CLA	C4A-NA-C1A	8.94	110.76	106.68
24	c	909	CLA	C4A-NA-C1A	8.93	110.75	106.68
24	B	614	CLA	C4A-NA-C1A	8.92	110.75	106.68
24	C	503	CLA	C4A-NA-C1A	8.88	110.73	106.68
26	D	404	BCR	C29-C30-C25	8.87	123.32	110.44
26	B	619	BCR	C24-C23-C22	8.85	139.32	126.23
26	a	409	BCR	C20-C19-C18	8.85	150.62	126.36
24	C	508	CLA	C4A-NA-C1A	8.80	110.69	106.68
24	B	611	CLA	C4A-NA-C1A	8.78	110.69	106.68
26	A	610	BCR	C20-C19-C18	8.76	150.37	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	515	BCR	C11-C12-C13	8.76	150.37	126.36
24	A	609	CLA	C1D-ND-C4D	-8.75	100.17	106.31
24	b	617	CLA	C4A-NA-C1A	8.70	110.65	106.68
26	B	619	BCR	C23-C22-C21	8.70	132.69	119.01
24	c	905	CLA	C4A-NA-C1A	8.64	110.62	106.68
26	b	618	BCR	C36-C18-C19	-8.59	104.96	118.09
26	c	918	BCR	C11-C10-C9	8.58	139.31	127.28
26	Y	101	BCR	C11-C12-C13	8.56	149.84	126.36
26	k	102	BCR	C23-C22-C21	8.55	132.46	119.01
24	b	615	CLA	C1D-ND-C4D	-8.55	100.31	106.31
26	H	101	BCR	C23-C22-C21	8.51	132.40	119.01
26	B	620	BCR	C23-C22-C21	8.49	132.37	119.01
26	D	404	BCR	C32-C1-C6	8.49	123.56	110.24
26	B	618	BCR	C15-C14-C13	8.49	139.18	127.28
26	c	915	BCR	C24-C23-C22	8.49	138.79	126.23
26	Y	101	BCR	C10-C11-C12	8.47	147.74	123.20
24	B	617	CLA	C4A-NA-C1A	8.41	110.51	106.68
26	A	610	BCR	C37-C22-C21	-8.39	109.22	122.82
26	B	619	BCR	C10-C11-C12	8.38	147.47	123.20
25	D	401	PHO	C2D-C1D-ND	8.37	115.48	109.43
26	B	622	BCR	C24-C23-C22	8.34	138.58	126.23
26	C	514	BCR	C11-C10-C9	8.34	138.97	127.28
24	c	914	CLA	C4A-NA-C1A	8.31	110.47	106.68
24	b	610	CLA	C4A-NA-C1A	8.31	110.47	106.68
24	c	909	CLA	C1D-ND-C4D	-8.26	100.52	106.31
25	a	412	PHO	C2D-C1D-ND	8.26	115.40	109.43
24	c	911	CLA	C4A-NA-C1A	8.24	110.44	106.68
26	A	610	BCR	C27-C26-C25	8.24	133.83	122.70
25	d	402	PHO	C2D-C1D-ND	8.23	115.38	109.43
25	D	401	PHO	C2B-C1B-NB	8.23	115.38	109.43
24	c	903	CLA	C1D-ND-C4D	-8.22	100.54	106.31
24	c	907	CLA	CMD-C2D-C1D	8.20	139.18	124.73
26	b	619	BCR	C23-C22-C21	8.17	131.86	119.01
24	c	905	CLA	C1D-ND-C4D	-8.15	100.59	106.31
24	d	401	CLA	C1D-ND-C4D	-8.14	100.60	106.31
24	c	907	CLA	C4A-NA-C1A	8.14	110.39	106.68
25	a	412	PHO	C3B-C4B-NB	8.13	112.77	107.46
24	c	902	CLA	CMD-C2D-C1D	8.13	139.04	124.73
26	K	101	BCR	C23-C22-C21	8.12	131.78	119.01
24	B	602	CLA	CMD-C2D-C1D	8.11	139.01	124.73
24	B	611	CLA	C1D-ND-C4D	-8.10	100.63	106.31
26	H	101	BCR	C7-C8-C9	8.06	138.16	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C7-C8-C9	8.06	138.15	126.23
26	A	610	BCR	C7-C8-C9	8.05	138.15	126.23
24	B	615	CLA	C4A-NA-C1A	8.05	110.35	106.68
24	a	406	CLA	C1D-ND-C4D	-8.05	100.67	106.31
24	A	609	CLA	C4A-NA-C1A	8.01	110.33	106.68
24	B	607	CLA	CMD-C2D-C1D	8.00	138.81	124.73
26	b	618	BCR	C11-C12-C13	7.97	148.22	126.36
24	B	604	CLA	C1D-ND-C4D	-7.93	100.75	106.31
24	B	606	CLA	C4A-NA-C1A	7.91	110.29	106.68
26	B	618	BCR	C35-C13-C12	-7.91	106.01	118.09
24	B	608	CLA	C4A-NA-C1A	7.91	110.29	106.68
26	f	101	BCR	C30-C25-C26	-7.90	111.84	122.64
24	d	404	CLA	C4A-NA-C1A	7.88	110.27	106.68
24	B	604	CLA	C4A-NA-C1A	7.87	110.27	106.68
24	A	606	CLA	C1D-ND-C4D	-7.86	100.80	106.31
26	f	101	BCR	C23-C22-C21	7.86	131.37	119.01
26	k	101	BCR	C36-C18-C19	-7.85	106.10	118.09
24	c	902	CLA	C1D-ND-C4D	-7.82	100.83	106.31
24	c	910	CLA	C1D-ND-C4D	-7.80	100.84	106.31
24	A	607	CLA	C4A-NA-C1A	7.79	110.23	106.68
24	C	502	CLA	C4A-NA-C1A	7.79	110.23	106.68
26	Y	101	BCR	C33-C5-C6	7.78	132.98	124.48
26	Y	101	BCR	C7-C8-C9	7.78	137.75	126.23
24	b	607	CLA	CMD-C2D-C1D	7.78	138.42	124.73
26	D	404	BCR	C12-C13-C14	7.77	131.23	119.01
24	B	609	CLA	C1D-ND-C4D	-7.76	100.86	106.31
26	k	101	BCR	C12-C13-C14	7.75	131.20	119.01
24	a	408	CLA	C4A-NA-C1A	7.74	110.21	106.68
26	D	404	BCR	C10-C11-C12	7.74	145.63	123.20
26	T	101	BCR	C33-C5-C6	7.71	132.89	124.48
26	c	915	BCR	C23-C22-C21	7.70	131.12	119.01
26	Y	101	BCR	C33-C5-C4	-7.67	97.23	113.60
26	k	102	BCR	C12-C13-C14	7.67	131.07	119.01
24	D	403	CLA	C1D-ND-C4D	-7.65	100.94	106.31
25	A	608	PHO	C2B-C1B-NB	7.65	114.96	109.43
24	C	503	CLA	CMD-C2D-C1D	7.64	138.19	124.73
26	b	618	BCR	C40-C30-C25	7.63	122.21	110.24
24	c	907	CLA	C1D-ND-C4D	-7.62	100.96	106.31
24	c	911	CLA	C1D-ND-C4D	-7.60	100.98	106.31
26	B	618	BCR	C8-C9-C10	7.60	130.96	119.01
24	C	507	CLA	CMD-C2D-C1D	7.59	138.09	124.73
24	C	509	CLA	CMD-C2D-C1D	7.56	138.04	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	101	BCR	C8-C7-C6	7.55	147.17	127.00
24	B	603	CLA	C4A-NA-C1A	7.55	110.12	106.68
24	C	508	CLA	C1D-ND-C4D	-7.55	101.02	106.31
26	b	618	BCR	C24-C23-C22	7.55	137.40	126.23
26	B	618	BCR	C36-C18-C19	-7.54	106.57	118.09
24	C	510	CLA	CMD-C2D-C1D	7.53	137.99	124.73
26	B	619	BCR	C30-C25-C26	-7.47	112.44	122.64
26	B	618	BCR	C36-C18-C17	-7.45	110.75	122.82
24	C	506	CLA	CMD-C2D-C1D	7.45	137.84	124.73
26	h	101	BCR	C12-C13-C14	7.44	130.71	119.01
24	B	615	CLA	C1D-ND-C4D	-7.43	101.10	106.31
24	b	611	CLA	C1D-ND-C4D	-7.43	101.10	106.31
24	B	614	CLA	CMD-C2D-C1D	7.43	137.81	124.73
24	C	501	CLA	CMD-C2D-C1D	7.41	137.78	124.73
24	b	613	CLA	C1D-ND-C4D	-7.39	101.12	106.31
24	d	404	CLA	CMD-C2D-C1D	7.38	137.72	124.73
24	b	602	CLA	CMD-C2D-C1D	7.37	137.70	124.73
24	c	910	CLA	CMD-C2D-C1D	7.37	137.70	124.73
24	B	606	CLA	C1D-ND-C4D	-7.36	101.15	106.31
25	d	402	PHO	C2B-C1B-NB	7.36	114.75	109.43
26	c	915	BCR	C12-C13-C14	7.35	130.56	119.01
24	b	614	CLA	C1D-ND-C4D	-7.34	101.16	106.31
26	b	619	BCR	C12-C13-C14	7.33	130.54	119.01
26	b	618	BCR	C36-C18-C17	-7.29	111.00	122.82
24	c	911	CLA	CMD-C2D-C1D	7.29	137.57	124.73
26	k	101	BCR	C33-C5-C6	7.29	132.44	124.48
26	h	101	BCR	C23-C22-C21	7.28	130.46	119.01
24	C	510	CLA	C1D-ND-C4D	-7.26	101.22	106.31
24	b	606	CLA	CMD-C2D-C1D	7.26	137.51	124.73
24	d	404	CLA	C1D-ND-C4D	-7.23	101.24	106.31
24	a	408	CLA	C1D-ND-C4D	-7.23	101.24	106.31
26	Y	101	BCR	C12-C13-C14	7.23	130.37	119.01
26	B	622	BCR	C33-C5-C6	7.22	132.37	124.48
24	c	914	CLA	CMD-C2D-C1D	7.21	137.42	124.73
24	B	605	CLA	CMD-C2D-C1D	7.20	137.40	124.73
25	a	412	PHO	C2B-C1B-NB	7.19	114.63	109.43
24	c	908	CLA	CMD-C2D-C1D	7.18	137.38	124.73
24	c	905	CLA	CMD-C2D-C1D	7.17	137.35	124.73
26	T	101	BCR	C8-C7-C6	7.14	146.08	127.00
26	B	618	BCR	C24-C23-C22	7.14	136.80	126.23
24	a	406	CLA	CMD-C2D-C1D	7.12	137.27	124.73
25	A	608	PHO	O2D-CGD-CBD	7.12	118.77	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	C4A-NA-C1A	7.11	109.92	106.68
26	A	610	BCR	C36-C18-C17	-7.10	111.31	122.82
24	D	403	CLA	CMD-C2D-C1D	7.09	137.21	124.73
24	c	904	CLA	CMD-C2D-C1D	7.08	137.20	124.73
26	f	101	BCR	C32-C1-C6	7.06	121.32	110.24
26	H	101	BCR	C36-C18-C19	-7.06	107.30	118.09
24	C	504	CLA	CMD-C2D-C1D	7.06	137.17	124.73
24	c	913	CLA	CMD-C2D-C1D	7.06	137.16	124.73
24	B	612	CLA	C1D-ND-C4D	-7.06	101.36	106.31
26	Y	101	BCR	C36-C18-C19	-7.05	107.32	118.09
26	B	620	BCR	C12-C13-C14	7.02	130.05	119.01
24	C	509	CLA	C1D-ND-C4D	-7.02	101.39	106.31
26	T	102	BCR	C23-C22-C21	6.99	130.00	119.01
26	T	102	BCR	C36-C18-C17	-6.98	111.51	122.82
26	Y	101	BCR	C29-C30-C25	6.98	120.58	110.44
26	f	101	BCR	C36-C18-C19	-6.97	107.44	118.09
24	B	607	CLA	C1D-ND-C4D	-6.96	101.43	106.31
24	d	401	CLA	C4A-NA-C1A	6.96	109.85	106.68
24	a	407	CLA	CMD-C2D-C1D	6.96	136.98	124.73
24	C	502	CLA	C1D-ND-C4D	-6.95	101.43	106.31
24	b	614	CLA	CMD-C2D-C1D	6.95	136.97	124.73
24	b	605	CLA	CMD-C2D-C1D	6.94	136.95	124.73
24	B	617	CLA	C1D-ND-C4D	-6.93	101.45	106.31
24	C	502	CLA	CMD-C2D-C1D	6.92	136.92	124.73
26	T	101	BCR	C12-C13-C14	6.92	129.90	119.01
26	c	918	BCR	C19-C18-C17	6.92	129.89	119.01
24	b	611	CLA	CMD-C2D-C1D	6.91	136.89	124.73
24	c	906	CLA	CMD-C2D-C1D	6.90	136.88	124.73
24	b	612	CLA	C1D-ND-C4D	-6.89	101.48	106.31
24	A	607	CLA	C1D-ND-C4D	-6.87	101.50	106.31
26	f	101	BCR	C8-C9-C10	6.85	129.78	119.01
24	b	609	CLA	C1D-ND-C4D	-6.83	101.52	106.31
26	B	622	BCR	C12-C13-C14	6.83	129.75	119.01
24	B	614	CLA	C1D-ND-C4D	-6.82	101.53	106.31
25	D	401	PHO	O2D-CGD-CBD	6.81	118.43	110.95
24	B	611	CLA	CMD-C2D-C1D	6.80	136.71	124.73
24	B	602	CLA	C1D-ND-C4D	-6.80	101.54	106.31
26	K	101	BCR	C36-C18-C19	-6.80	107.70	118.09
24	A	607	CLA	CMD-C2D-C1D	6.77	136.66	124.73
24	C	513	CLA	CMD-C2D-C1D	6.76	136.64	124.73
24	b	607	CLA	C1D-ND-C4D	-6.76	101.57	106.31
24	C	505	CLA	CMD-C2D-C1D	6.76	136.62	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	BCR	C36-C18-C17	-6.76	111.87	122.82
26	C	515	BCR	C24-C23-C22	6.75	136.21	126.23
25	A	608	PHO	C4D-ND-C1D	-6.72	100.82	108.87
26	T	102	BCR	C24-C23-C22	6.72	136.17	126.23
26	A	610	BCR	C35-C13-C14	-6.71	111.94	122.82
26	C	514	BCR	C33-C5-C6	6.70	131.79	124.48
24	b	603	CLA	C1D-ND-C4D	-6.70	101.61	106.31
24	B	613	CLA	C1D-ND-C4D	-6.69	101.62	106.31
26	C	514	BCR	C38-C26-C27	-6.68	99.34	113.60
24	b	609	CLA	CMD-C2D-C1D	6.67	136.47	124.73
24	c	912	CLA	C1D-ND-C4D	-6.66	101.64	106.31
24	B	608	CLA	C1D-ND-C4D	-6.65	101.65	106.31
26	b	618	BCR	C29-C30-C25	6.64	120.09	110.44
25	D	401	PHO	C3D-C4D-ND	6.64	116.22	107.71
24	b	606	CLA	C1D-ND-C4D	-6.63	101.66	106.31
24	d	403	CLA	C4A-NA-C1A	6.62	109.70	106.68
24	C	512	CLA	CMD-C2D-C1D	6.62	136.39	124.73
24	C	511	CLA	C1D-ND-C4D	-6.62	101.67	106.31
24	d	403	CLA	C1D-ND-C4D	-6.62	101.67	106.31
24	B	603	CLA	CMD-C2D-C1D	6.61	136.38	124.73
26	H	101	BCR	C32-C1-C6	6.61	120.61	110.24
25	A	608	PHO	C3D-C4D-ND	6.59	116.15	107.71
24	b	604	CLA	C1D-ND-C4D	-6.58	101.69	106.31
26	k	102	BCR	C37-C22-C21	-6.58	112.16	122.82
24	b	615	CLA	CMD-C2D-C1D	6.58	136.31	124.73
26	B	619	BCR	C23-C24-C25	6.58	144.56	127.00
24	c	913	CLA	C1D-ND-C4D	-6.57	101.70	106.31
24	C	511	CLA	CMD-C2D-C1D	6.54	136.25	124.73
24	b	603	CLA	C4A-NA-C1A	6.53	109.66	106.68
26	a	409	BCR	C36-C18-C17	-6.53	112.24	122.82
26	H	101	BCR	C8-C9-C10	6.53	129.28	119.01
26	B	618	BCR	C23-C22-C21	6.52	129.27	119.01
24	c	912	CLA	CMD-C2D-C1D	6.51	136.20	124.73
26	K	101	BCR	C8-C7-C6	6.51	144.39	127.00
24	b	610	CLA	CMD-C2D-C1D	6.50	136.17	124.73
24	B	610	CLA	CMD-C2D-C1D	6.49	136.16	124.73
25	a	412	PHO	C3D-C4D-ND	6.49	116.02	107.71
24	b	606	CLA	C4A-NA-C1A	6.49	109.64	106.68
24	A	614	CLA	C2C-C1C-NC	6.48	116.79	109.98
24	B	616	CLA	CMD-C2D-C1D	6.47	136.11	124.73
26	C	515	BCR	C23-C22-C21	6.46	129.18	119.01
24	C	506	CLA	C1D-ND-C4D	-6.45	101.78	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	CMD-C2D-C1D	6.45	136.09	124.73
24	B	615	CLA	CMD-C2D-C1D	6.42	136.04	124.73
26	B	619	BCR	C11-C12-C13	6.42	143.97	126.36
25	a	412	PHO	C4D-ND-C1D	-6.42	101.19	108.87
24	b	617	CLA	CMD-C2D-C1D	6.41	136.02	124.73
24	c	906	CLA	C1D-ND-C4D	-6.41	101.81	106.31
24	d	401	CLA	C2D-C1D-ND	6.40	116.47	110.13
26	k	101	BCR	C23-C22-C21	6.40	129.08	119.01
24	B	610	CLA	C1D-ND-C4D	-6.39	101.83	106.31
26	H	101	BCR	C37-C22-C21	-6.39	112.47	122.82
24	b	617	CLA	C1D-ND-C4D	-6.38	101.84	106.31
26	a	409	BCR	C37-C22-C21	-6.37	112.49	122.82
24	B	616	CLA	C1D-ND-C4D	-6.37	101.84	106.31
24	A	609	CLA	CMD-C2D-C1D	6.37	135.94	124.73
24	D	402	CLA	CMD-C2D-C1D	6.37	135.94	124.73
26	b	619	BCR	C33-C5-C6	6.36	131.42	124.48
26	k	101	BCR	C8-C7-C6	6.35	143.96	127.00
24	b	604	CLA	CMD-C2D-C1D	6.34	135.90	124.73
26	k	101	BCR	C33-C5-C4	-6.34	100.08	113.60
26	k	102	BCR	C8-C7-C6	6.34	143.93	127.00
25	D	401	PHO	C4D-ND-C1D	-6.33	101.28	108.87
24	B	612	CLA	CMD-C2D-C1D	6.31	135.84	124.73
24	D	402	CLA	C1D-ND-C4D	-6.31	101.89	106.31
24	D	402	CLA	C4A-NA-C1A	6.29	109.55	106.68
24	C	513	CLA	C1D-ND-C4D	-6.28	101.90	106.31
24	C	508	CLA	CMD-C2D-C1D	6.28	135.79	124.73
26	C	515	BCR	C31-C1-C6	6.26	120.06	110.24
26	C	514	BCR	C24-C23-C22	6.25	135.48	126.23
24	b	602	CLA	C1D-ND-C4D	-6.23	101.94	106.31
26	f	101	BCR	C40-C30-C39	6.22	126.44	108.63
24	D	402	CLA	C2D-C1D-ND	6.21	116.28	110.13
24	b	616	CLA	C1D-ND-C4D	-6.21	101.95	106.31
26	T	101	BCR	C24-C23-C22	6.20	135.41	126.23
26	k	101	BCR	C29-C30-C25	6.20	119.45	110.44
24	b	603	CLA	CMD-C2D-C1D	6.20	135.65	124.73
26	B	622	BCR	C23-C22-C21	6.19	128.75	119.01
24	B	604	CLA	CMD-C2D-C1D	6.19	135.63	124.73
24	B	603	CLA	C1D-ND-C4D	-6.19	101.97	106.31
24	b	610	CLA	C1D-ND-C4D	-6.18	101.97	106.31
26	Y	101	BCR	C37-C22-C21	-6.16	112.83	122.82
24	A	606	CLA	C4A-NA-C1A	6.16	109.49	106.68
24	b	612	CLA	CMD-C2D-C1D	6.14	135.55	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	101	BCR	C12-C13-C14	6.14	128.67	119.01
24	B	605	CLA	C1D-ND-C4D	-6.14	102.00	106.31
26	k	102	BCR	C36-C18-C17	-6.14	112.88	122.82
24	A	607	CLA	C2C-C1C-NC	6.13	116.42	109.98
24	c	903	CLA	CMD-C2D-C1D	6.13	135.52	124.73
26	B	618	BCR	C7-C8-C9	6.13	135.30	126.23
26	A	610	BCR	C38-C26-C27	-6.13	100.53	113.60
26	T	101	BCR	C36-C18-C17	-6.11	112.91	122.82
24	B	617	CLA	CMD-C2D-C1D	6.11	135.48	124.73
24	C	504	CLA	C1D-ND-C4D	-6.11	102.03	106.31
24	C	501	CLA	O2D-CGD-CBD	6.09	121.88	111.23
24	a	407	CLA	C4A-NA-C1A	6.08	109.45	106.68
24	c	914	CLA	C1D-ND-C4D	-6.08	102.05	106.31
24	a	406	CLA	C2C-C1C-NC	6.06	116.35	109.98
26	a	409	BCR	C37-C22-C23	-6.06	108.84	118.09
24	B	605	CLA	C2C-C1C-NC	6.05	116.34	109.98
26	B	619	BCR	C8-C9-C10	6.05	128.53	119.01
24	b	608	CLA	CMD-C2D-C1D	6.05	135.38	124.73
26	C	514	BCR	C38-C26-C25	6.04	131.08	124.48
24	b	614	CLA	C2D-C1D-ND	6.04	116.11	110.13
26	B	619	BCR	C29-C30-C25	6.04	119.21	110.44
24	c	909	CLA	CMD-C2D-C1D	6.03	135.35	124.73
24	a	407	CLA	C1D-ND-C4D	-6.03	102.08	106.31
24	a	406	CLA	C2D-C1D-ND	6.02	116.08	110.13
24	c	909	CLA	C2D-C1D-ND	6.02	116.08	110.13
26	C	514	BCR	C8-C7-C6	6.02	143.07	127.00
26	A	610	BCR	C8-C9-C10	6.00	128.45	119.01
24	B	609	CLA	C2C-C1C-NC	6.00	116.28	109.98
26	h	101	BCR	C39-C30-C25	5.99	119.64	110.24
24	b	605	CLA	C1D-ND-C4D	-5.98	102.11	106.31
26	B	620	BCR	C8-C9-C10	5.98	128.42	119.01
24	A	606	CLA	C2D-C1D-ND	5.98	116.05	110.13
26	H	101	BCR	C30-C25-C26	-5.98	114.46	122.64
24	B	608	CLA	CMD-C2D-C1D	5.98	135.26	124.73
24	c	903	CLA	C2D-C1D-ND	5.98	116.04	110.13
24	C	512	CLA	C1D-ND-C4D	-5.97	102.12	106.31
24	B	614	CLA	C2D-C1D-ND	5.97	116.03	110.13
26	c	918	BCR	C15-C14-C13	5.96	135.63	127.28
26	h	101	BCR	C8-C7-C6	5.95	142.90	127.00
24	B	613	CLA	CMD-C2D-C1D	5.95	135.21	124.73
24	A	609	CLA	C2D-C1D-ND	5.94	116.01	110.13
26	C	515	BCR	C7-C8-C9	5.93	135.01	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	622	BCR	C8-C7-C6	5.92	142.82	127.00
24	c	904	CLA	C1D-ND-C4D	-5.91	102.16	106.31
24	d	401	CLA	CMD-C2D-C1D	5.90	135.12	124.73
26	Y	101	BCR	C30-C25-C26	-5.90	114.57	122.64
24	b	615	CLA	C2D-C1D-ND	5.90	115.96	110.13
24	a	407	CLA	C2C-C1C-NC	5.88	116.16	109.98
24	B	617	CLA	C2D-C1D-ND	5.87	115.94	110.13
26	T	101	BCR	C2-C1-C6	5.85	118.94	110.44
24	A	614	CLA	C2D-C1D-ND	5.85	115.91	110.13
26	C	514	BCR	C36-C18-C17	-5.83	113.36	122.82
24	C	501	CLA	C1D-ND-C4D	-5.82	102.23	106.31
26	b	619	BCR	C37-C22-C21	-5.82	113.39	122.82
24	d	403	CLA	C2C-C1C-NC	5.81	116.09	109.98
24	B	612	CLA	C2D-C1D-ND	5.81	115.87	110.13
24	c	905	CLA	C2D-C1D-ND	5.81	115.87	110.13
24	C	503	CLA	C1D-ND-C4D	-5.79	102.25	106.31
24	B	606	CLA	CMD-C2D-C1D	5.78	134.91	124.73
26	k	102	BCR	C38-C26-C27	-5.77	101.30	113.60
26	B	622	BCR	C36-C18-C17	-5.76	113.48	122.82
26	h	101	BCR	C36-C18-C17	-5.76	113.48	122.82
26	c	918	BCR	C38-C26-C25	5.76	130.77	124.48
24	A	614	CLA	C3D-C2D-C1D	-5.76	97.97	105.83
24	c	908	CLA	C1D-ND-C4D	-5.76	102.27	106.31
24	B	606	CLA	C2D-C1D-ND	5.76	115.82	110.13
24	d	401	CLA	C2C-C1C-NC	5.74	116.02	109.98
26	k	102	BCR	C33-C5-C6	5.74	130.75	124.48
24	b	604	CLA	C4A-NA-C1A	5.74	109.30	106.68
25	d	402	PHO	C4D-ND-C1D	-5.74	102.00	108.87
24	B	602	CLA	O2D-CGD-CBD	5.73	121.25	111.23
26	k	102	BCR	C38-C26-C25	5.72	130.73	124.48
24	A	614	CLA	CMD-C2D-C1D	5.72	134.80	124.73
24	a	408	CLA	CMD-C2D-C1D	5.70	134.77	124.73
26	a	409	BCR	C27-C26-C25	5.70	130.41	122.70
28	a	411	SQD	O6-C1-C2	5.70	116.93	108.27
24	b	611	CLA	C2D-C1D-ND	5.69	115.76	110.13
26	C	514	BCR	C29-C30-C25	5.69	118.70	110.44
25	d	402	PHO	C3D-C4D-ND	5.68	114.99	107.71
26	b	619	BCR	C33-C5-C4	-5.68	101.48	113.60
24	b	617	CLA	C2D-C1D-ND	5.67	115.74	110.13
24	A	614	CLA	C1D-ND-C4D	-5.67	102.33	106.31
26	C	514	BCR	C12-C13-C14	5.66	127.92	119.01
24	B	614	CLA	C3D-C2D-C1D	-5.65	98.12	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	101	BCR	C24-C23-C22	5.64	134.57	126.23
24	B	611	CLA	C2D-C1D-ND	5.63	115.70	110.13
26	c	915	BCR	C8-C9-C10	5.63	127.86	119.01
24	a	407	CLA	C3D-C2D-C1D	-5.62	98.16	105.83
26	B	618	BCR	C34-C9-C10	-5.62	113.72	122.82
24	b	616	CLA	CMD-C2D-C1D	5.62	134.62	124.73
26	T	102	BCR	C35-C13-C14	-5.61	113.72	122.82
26	D	404	BCR	C23-C22-C21	5.61	127.83	119.01
26	b	618	BCR	C30-C25-C26	-5.59	114.99	122.64
24	B	616	CLA	C2D-C1D-ND	5.59	115.66	110.13
24	c	910	CLA	C2D-C1D-ND	5.59	115.66	110.13
24	a	406	CLA	C4A-NA-C1A	5.58	109.23	106.68
26	Y	101	BCR	C8-C7-C6	5.58	141.91	127.00
24	B	604	CLA	C2C-C1C-NC	5.58	115.84	109.98
26	H	101	BCR	C33-C5-C6	5.58	130.57	124.48
24	b	613	CLA	CMD-C2D-C1D	5.57	134.53	124.73
24	B	609	CLA	C2D-C1D-ND	5.56	115.63	110.13
24	b	606	CLA	C2D-C1D-ND	5.56	115.63	110.13
24	D	402	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
32	V	202	HEM	C4D-ND-C1D	5.55	111.78	105.21
24	b	604	CLA	C2C-C1C-NC	5.55	115.81	109.98
26	K	101	BCR	C37-C22-C21	-5.55	113.83	122.82
26	b	618	BCR	C27-C26-C25	5.54	130.19	122.70
26	T	102	BCR	C7-C8-C9	5.54	134.43	126.23
24	d	401	CLA	C3D-C2D-C1D	-5.53	98.28	105.83
26	A	610	BCR	C30-C25-C26	-5.53	115.08	122.64
24	C	507	CLA	C1D-ND-C4D	-5.53	102.44	106.31
24	c	903	CLA	O2D-CGD-CBD	5.52	120.89	111.23
26	C	515	BCR	C8-C7-C6	5.52	141.73	127.00
24	a	408	CLA	C2D-C1D-ND	5.51	115.58	110.13
24	B	604	CLA	C2D-C1D-ND	5.51	115.58	110.13
32	v	202	HEM	C4D-ND-C1D	5.50	111.72	105.21
26	T	102	BCR	C8-C9-C10	5.50	127.67	119.01
24	b	602	CLA	O2D-CGD-CBD	5.50	120.84	111.23
26	K	101	BCR	C23-C24-C25	5.49	141.66	127.00
26	c	915	BCR	C36-C18-C17	-5.49	113.93	122.82
24	A	606	CLA	CMD-C2D-C1D	5.48	134.39	124.73
26	h	101	BCR	C8-C9-C10	5.48	127.63	119.01
24	B	609	CLA	CMD-C2D-C1D	5.48	134.38	124.73
26	b	618	BCR	C38-C26-C27	-5.47	101.92	113.60
24	b	614	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
24	b	613	CLA	C2D-C1D-ND	5.47	115.54	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	618	BCR	C34-C9-C8	-5.47	109.74	118.09
24	a	408	CLA	C2C-C1C-NC	5.46	115.72	109.98
24	c	914	CLA	C3B-C2B-C1B	-5.46	100.74	107.17
24	D	403	CLA	C2D-C1D-ND	5.46	115.53	110.13
24	B	615	CLA	C2D-C1D-ND	5.45	115.52	110.13
24	a	406	CLA	C3D-C2D-C1D	-5.44	98.40	105.83
24	C	504	CLA	C2C-C1C-NC	5.43	115.68	109.98
26	H	101	BCR	C35-C13-C12	-5.42	109.81	118.09
24	b	612	CLA	C2D-C1D-ND	5.42	115.49	110.13
24	B	613	CLA	C2D-C1D-ND	5.41	115.48	110.13
24	b	616	CLA	C2D-C1D-ND	5.41	115.48	110.13
24	b	615	CLA	O2D-CGD-CBD	5.41	120.68	111.23
24	d	403	CLA	C2D-C1D-ND	5.40	115.47	110.13
26	B	620	BCR	C37-C22-C23	-5.39	109.86	118.09
26	c	915	BCR	C23-C24-C25	5.38	141.38	127.00
24	C	509	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
24	B	608	CLA	C2D-C1D-ND	5.38	115.45	110.13
24	A	609	CLA	C2C-C1C-NC	5.38	115.63	109.98
24	C	509	CLA	C2C-C1C-NC	5.38	115.63	109.98
26	b	618	BCR	C37-C22-C23	-5.38	109.87	118.09
26	b	619	BCR	C29-C30-C25	5.38	118.25	110.44
26	H	101	BCR	C29-C30-C25	5.38	118.25	110.44
24	B	609	CLA	C2B-C1B-NB	5.38	115.90	110.33
24	c	902	CLA	C2C-C1C-NC	5.38	115.63	109.98
24	C	507	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
24	C	502	CLA	C2D-C1D-ND	5.37	115.44	110.13
26	C	515	BCR	C35-C13-C12	-5.36	109.89	118.09
24	B	610	CLA	C2C-C1C-NC	5.36	115.61	109.98
24	b	606	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
24	D	402	CLA	C2C-C1C-NC	5.35	115.60	109.98
24	c	902	CLA	C2D-C1D-ND	5.35	115.42	110.13
24	b	608	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
24	b	614	CLA	C2C-C1C-NC	5.34	115.59	109.98
24	a	407	CLA	C2D-C1D-ND	5.32	115.39	110.13
24	B	608	CLA	C2C-C1C-NC	5.32	115.57	109.98
24	c	907	CLA	C2D-C1D-ND	5.32	115.39	110.13
24	B	612	CLA	C2C-C1C-NC	5.31	115.56	109.98
26	b	619	BCR	C36-C18-C19	-5.31	109.98	118.09
26	B	618	BCR	C2-C1-C6	5.30	118.14	110.44
26	A	610	BCR	C24-C23-C22	5.30	134.08	126.23
24	C	511	CLA	C2D-C1D-ND	5.30	115.37	110.13
24	b	608	CLA	C2D-C1D-ND	5.30	115.37	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
24	B	616	CLA	C3B-C2B-C1B	-5.30	100.93	107.17
24	C	505	CLA	C1D-ND-C4D	-5.30	102.60	106.31
24	b	605	CLA	C2C-C1C-NC	5.29	115.54	109.98
26	f	101	BCR	C23-C24-C25	5.29	141.13	127.00
26	D	404	BCR	C39-C30-C29	-5.28	88.67	108.95
26	f	101	BCR	C37-C22-C21	-5.28	114.26	122.82
26	B	619	BCR	C38-C26-C27	-5.27	102.35	113.60
26	C	515	BCR	C29-C30-C25	5.27	118.09	110.44
24	c	911	CLA	C2D-C1D-ND	5.27	115.34	110.13
26	Y	101	BCR	C8-C9-C10	5.27	127.29	119.01
24	d	404	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
24	b	603	CLA	C2D-C1D-ND	5.26	115.34	110.13
24	b	609	CLA	C2D-C1D-ND	5.26	115.33	110.13
26	b	619	BCR	C38-C26-C25	5.26	130.22	124.48
24	B	616	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
26	H	101	BCR	C33-C5-C4	-5.25	102.40	113.60
24	C	508	CLA	C2D-C1D-ND	5.25	115.32	110.13
24	B	612	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
26	Y	101	BCR	C36-C18-C17	-5.24	114.32	122.82
26	Y	101	BCR	C4-C5-C6	5.24	129.79	122.70
24	B	603	CLA	C2D-C1D-ND	5.24	115.31	110.13
32	E	101	HEM	C4D-ND-C1D	5.24	111.41	105.21
26	b	618	BCR	C35-C13-C12	-5.24	110.09	118.09
26	K	101	BCR	C8-C9-C10	5.23	127.24	119.01
24	C	501	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
26	B	619	BCR	C40-C30-C25	5.22	118.42	110.24
24	b	616	CLA	C3B-C2B-C1B	-5.21	101.02	107.17
24	C	512	CLA	O2D-CGD-CBD	5.21	120.34	111.23
24	b	606	CLA	C2C-C1C-NC	5.21	115.46	109.98
26	D	404	BCR	C24-C23-C22	5.21	133.94	126.23
26	D	404	BCR	C8-C7-C6	5.20	140.90	127.00
26	C	514	BCR	C2-C1-C6	5.20	117.99	110.44
24	A	614	CLA	C1C-C2C-C3C	-5.20	101.52	106.98
24	b	615	CLA	C2C-C1C-NC	5.19	115.44	109.98
24	b	609	CLA	O2D-CGD-CBD	5.19	120.30	111.23
24	A	607	CLA	C2D-C1D-ND	5.19	115.26	110.13
26	a	409	BCR	C30-C25-C26	-5.19	115.54	122.64
26	D	404	BCR	C4-C5-C6	5.19	129.72	122.70
26	b	618	BCR	C35-C13-C14	-5.19	114.41	122.82
24	B	602	CLA	C2D-C1D-ND	5.19	115.26	110.13
24	C	506	CLA	O2D-CGD-CBD	5.19	120.30	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	909	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
24	C	510	CLA	C2C-C1C-NC	5.17	115.41	109.98
26	T	102	BCR	C39-C30-C25	5.17	118.34	110.24
24	b	608	CLA	C1D-ND-C4D	-5.17	102.69	106.31
24	b	610	CLA	C2C-C1C-NC	5.16	115.41	109.98
24	C	510	CLA	C2D-C1D-ND	5.16	115.24	110.13
24	c	903	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
26	C	515	BCR	C36-C18-C19	-5.16	110.21	118.09
24	a	406	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
24	d	404	CLA	C2B-C1B-NB	5.16	115.67	110.33
24	b	617	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
26	b	618	BCR	C33-C5-C4	-5.15	102.61	113.60
24	b	611	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
32	e	101	HEM	C4D-ND-C1D	5.15	111.31	105.21
26	k	101	BCR	C24-C23-C22	5.14	133.85	126.23
24	C	513	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
24	c	904	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
24	d	404	CLA	C2D-C1D-ND	5.14	115.21	110.13
24	b	602	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
24	c	902	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
26	b	618	BCR	C8-C9-C10	5.13	127.08	119.01
24	b	617	CLA	O2D-CGD-CBD	5.13	120.20	111.23
24	c	907	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
24	B	614	CLA	C2C-C1C-NC	5.13	115.37	109.98
26	a	409	BCR	C35-C13-C14	-5.13	114.51	122.82
24	d	403	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
24	B	610	CLA	C2D-C1D-ND	5.12	115.20	110.13
26	c	918	BCR	C8-C7-C6	5.12	140.68	127.00
24	C	507	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
26	B	622	BCR	C37-C22-C21	-5.12	114.52	122.82
26	a	409	BCR	C8-C9-C10	5.12	127.06	119.01
24	c	908	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
26	H	101	BCR	C34-C9-C10	-5.11	114.53	122.82
24	b	604	CLA	C2D-C1D-ND	5.11	115.18	110.13
24	A	606	CLA	C2B-C1B-NB	5.10	115.62	110.33
24	A	607	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
26	k	101	BCR	C2-C1-C6	5.10	117.84	110.44
26	T	102	BCR	C38-C26-C27	-5.09	102.74	113.60
26	f	101	BCR	C39-C30-C29	-5.09	89.41	108.95
26	C	514	BCR	C27-C26-C25	5.09	129.58	122.70
24	B	615	CLA	C2C-C1C-NC	5.09	115.33	109.98
24	b	607	CLA	CHD-C1D-ND	-5.08	117.65	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	O2D-CGD-CBD	5.08	120.11	111.23
24	c	913	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
24	c	906	CLA	C3B-C2B-C1B	-5.08	101.19	107.17
24	C	503	CLA	C3B-C2B-C1B	-5.08	101.19	107.17
26	K	101	BCR	C36-C18-C17	-5.08	114.59	122.82
24	A	609	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
26	b	619	BCR	C38-C26-C27	-5.07	102.78	113.60
24	B	617	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
24	B	602	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
26	B	619	BCR	C27-C26-C25	5.06	129.54	122.70
24	c	908	CLA	C2D-C1D-ND	5.06	115.13	110.13
24	c	912	CLA	C2D-C1D-ND	5.06	115.13	110.13
24	C	503	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
24	B	603	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
26	B	618	BCR	C38-C26-C27	-5.05	102.84	113.60
24	c	913	CLA	O2D-CGD-CBD	5.05	120.05	111.23
26	k	102	BCR	C33-C5-C4	-5.04	102.84	113.60
24	B	617	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
24	B	607	CLA	C2D-C1D-ND	5.04	115.11	110.13
24	C	506	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
24	A	607	CLA	C2B-C1B-NB	5.04	115.55	110.33
24	b	616	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
24	C	506	CLA	C2C-C1C-NC	5.04	115.27	109.98
26	B	622	BCR	C36-C18-C19	-5.03	110.40	118.09
24	c	908	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
24	B	602	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
24	c	904	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
24	B	604	CLA	O2D-CGD-CBD	5.01	120.00	111.23
26	Y	101	BCR	C23-C22-C21	5.01	126.89	119.01
26	D	404	BCR	C7-C8-C9	5.01	133.65	126.23
24	b	605	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	D	403	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	c	905	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	C	502	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
26	B	619	BCR	C37-C22-C21	-5.00	114.72	122.82
26	D	404	BCR	C8-C9-C10	5.00	126.87	119.01
26	B	620	BCR	C24-C23-C22	4.99	133.62	126.23
24	c	910	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
24	B	615	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
24	A	614	CLA	C4A-NA-C1A	4.99	108.96	106.68
24	b	605	CLA	C2D-C1D-ND	4.99	115.06	110.13
26	Y	101	BCR	C23-C24-C25	4.99	140.32	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C4A-NA-C1A	4.99	108.95	106.68
24	C	504	CLA	O2D-CGD-CBD	4.98	119.94	111.23
24	c	902	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
24	c	908	CLA	C2C-C1C-NC	4.98	115.21	109.98
24	c	903	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
24	A	606	CLA	C2C-C1C-NC	4.98	115.21	109.98
24	d	404	CLA	C2C-C1C-NC	4.98	115.21	109.98
24	A	607	CLA	C1C-C2C-C3C	-4.97	101.75	106.98
24	c	910	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
24	c	904	CLA	C2D-C1D-ND	4.97	115.05	110.13
24	C	505	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
24	A	607	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
26	T	102	BCR	C23-C24-C25	4.96	140.24	127.00
24	c	910	CLA	O2D-CGD-CBD	4.96	119.89	111.23
26	k	101	BCR	C37-C22-C21	-4.96	114.79	122.82
24	c	911	CLA	C2C-C1C-NC	4.95	115.19	109.98
26	B	619	BCR	C36-C18-C17	-4.95	114.79	122.82
24	C	501	CLA	C2C-C1C-NC	4.95	115.18	109.98
24	B	611	CLA	C2B-C1B-NB	4.95	115.46	110.33
24	B	608	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
24	C	502	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
24	b	604	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
24	C	506	CLA	C2D-C1D-ND	4.95	115.02	110.13
24	B	613	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
26	B	622	BCR	C23-C24-C25	4.95	140.21	127.00
26	C	515	BCR	C38-C26-C25	4.94	129.88	124.48
24	A	606	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
24	B	609	CLA	O2D-CGD-CBD	4.94	119.86	111.23
24	b	613	CLA	C3C-C4C-NC	4.94	116.75	110.43
26	B	619	BCR	C35-C13-C14	-4.94	114.82	122.82
24	A	607	CLA	O2D-CGD-CBD	4.93	119.86	111.23
24	C	501	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
24	C	511	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
24	C	511	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
24	B	606	CLA	C2C-C1C-NC	4.93	115.16	109.98
26	c	918	BCR	C38-C26-C27	-4.93	103.09	113.60
24	b	609	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
24	C	512	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
26	B	619	BCR	C2-C1-C6	4.92	117.59	110.44
26	b	619	BCR	C8-C7-C6	4.92	140.15	127.00
24	a	408	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
24	A	607	CLA	C3B-C4B-NB	4.92	114.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	905	CLA	O2D-CGD-CBD	4.92	119.83	111.23
24	A	606	CLA	C3B-C2B-C1B	-4.92	101.38	107.17
24	b	603	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
24	C	510	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
26	h	101	BCR	C37-C22-C21	-4.91	114.87	122.82
26	k	101	BCR	C38-C26-C27	-4.90	103.14	113.60
26	f	101	BCR	C36-C18-C17	-4.90	114.88	122.82
24	B	607	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
24	A	609	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
24	b	607	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
24	B	615	CLA	C2B-C1B-NB	4.90	115.40	110.33
24	c	907	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
24	b	613	CLA	C2C-C1C-NC	4.89	115.12	109.98
26	A	610	BCR	C36-C18-C19	-4.89	110.61	118.09
24	A	614	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
24	c	910	CLA	C2C-C1C-NC	4.89	115.12	109.98
24	B	611	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
24	C	504	CLA	C2D-C1D-ND	4.89	114.96	110.13
26	B	620	BCR	C33-C5-C4	-4.89	103.18	113.60
26	a	409	BCR	C36-C18-C19	-4.88	110.63	118.09
24	c	906	CLA	C2D-C1D-ND	4.88	114.96	110.13
24	B	610	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
24	c	912	CLA	C3B-C2B-C1B	-4.87	101.42	107.17
24	b	615	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	d	403	CLA	C2B-C1B-NB	4.87	115.38	110.33
24	B	609	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
24	b	603	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
24	c	913	CLA	C2D-C1D-ND	4.87	114.94	110.13
24	B	606	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
24	C	505	CLA	C2C-C1C-NC	4.86	115.09	109.98
24	b	611	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
24	C	509	CLA	C2D-C1D-ND	4.86	114.94	110.13
28	A	612	SQD	O6-C1-C2	4.86	115.65	108.27
24	b	607	CLA	C2D-C1D-ND	4.85	114.93	110.13
24	B	613	CLA	O2D-CGD-CBD	4.85	119.71	111.23
24	B	607	CLA	C2C-C1C-NC	4.85	115.08	109.98
26	B	622	BCR	C2-C1-C6	4.85	117.48	110.44
24	b	608	CLA	C2C-C1C-NC	4.85	115.08	109.98
24	b	612	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
24	A	609	CLA	C2B-C1B-NB	4.84	115.35	110.33
24	c	909	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
24	C	504	CLA	C3D-C2D-C1D	-4.84	99.23	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	b	609	CLA	C2C-C1C-NC	4.84	115.06	109.98
24	D	403	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
24	b	607	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
24	c	903	CLA	C2B-C1B-NB	4.82	115.33	110.33
24	B	615	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
24	C	511	CLA	C2C-C1C-NC	4.81	115.03	109.98
26	K	101	BCR	C35-C13-C12	-4.80	110.75	118.09
24	C	507	CLA	C2D-C1D-ND	4.80	114.88	110.13
24	C	508	CLA	C2C-C1C-NC	4.80	115.02	109.98
24	d	404	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
26	a	409	BCR	C35-C13-C12	-4.80	110.76	118.09
24	b	616	CLA	C2B-C1B-NB	4.79	115.30	110.33
24	C	502	CLA	C2C-C1C-NC	4.79	115.01	109.98
26	k	102	BCR	C39-C30-C25	4.79	117.75	110.24
24	c	913	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
24	C	509	CLA	O2D-CGD-CBD	4.78	119.59	111.23
24	B	611	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
24	C	512	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
24	c	910	CLA	C2B-C1B-NB	4.78	115.29	110.33
24	c	911	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
24	d	401	CLA	C1C-C2C-C3C	-4.78	101.95	106.98
26	c	915	BCR	C2-C1-C6	4.78	117.38	110.44
24	d	401	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
26	k	102	BCR	C36-C18-C19	-4.78	110.79	118.09
24	B	605	CLA	C3D-C2D-C1D	-4.77	99.31	105.83
24	c	906	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
24	C	503	CLA	C2D-C1D-ND	4.77	114.85	110.13
26	C	514	BCR	C35-C13-C12	-4.77	110.80	118.09
24	B	606	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
26	a	409	BCR	C2-C1-C6	4.77	117.36	110.44
24	C	512	CLA	C2D-C1D-ND	4.77	114.84	110.13
24	B	605	CLA	C2D-C1D-ND	4.76	114.84	110.13
26	f	101	BCR	C24-C23-C22	4.76	133.28	126.23
24	B	611	CLA	C2C-C1C-NC	4.76	114.98	109.98
26	b	618	BCR	C37-C22-C21	-4.76	115.11	122.82
24	a	408	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
26	h	101	BCR	C23-C24-C25	4.76	139.70	127.00
24	c	912	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
24	B	609	CLA	C3B-C4B-NB	4.75	114.77	110.53
24	C	509	CLA	C2B-C1B-NB	4.75	115.25	110.33
24	c	905	CLA	C2B-C1B-NB	4.74	115.25	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	l	101	SQD	O6-C1-C2	4.74	115.48	108.27
24	B	613	CLA	C2C-C1C-NC	4.74	114.96	109.98
24	b	611	CLA	C2B-C1B-NB	4.74	115.24	110.33
26	T	102	BCR	C38-C26-C25	4.74	129.66	124.48
24	c	906	CLA	O2D-CGD-CBD	4.74	119.51	111.23
24	b	611	CLA	C2C-C1C-NC	4.73	114.95	109.98
24	B	602	CLA	C2B-C1B-NB	4.73	115.23	110.33
27	a	410	PL9	C7-C3-C4	4.73	120.81	116.91
26	c	918	BCR	C24-C23-C22	4.72	133.22	126.23
24	B	615	CLA	O2D-CGD-CBD	4.72	119.48	111.23
26	T	102	BCR	C36-C18-C19	-4.72	110.88	118.09
24	c	905	CLA	C2C-C1C-NC	4.71	114.93	109.98
24	B	612	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
26	c	918	BCR	C2-C1-C6	4.71	117.28	110.44
24	B	612	CLA	C3C-C4C-NC	4.71	116.46	110.43
24	C	510	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
24	c	914	CLA	C2B-C1B-NB	4.71	115.21	110.33
24	b	612	CLA	C2C-C1C-NC	4.70	114.92	109.98
24	b	616	CLA	C2C-C1C-NC	4.69	114.91	109.98
26	B	622	BCR	C33-C5-C4	-4.69	103.59	113.60
24	c	908	CLA	O2D-CGD-CBD	4.69	119.43	111.23
26	c	915	BCR	C27-C26-C25	4.69	129.04	122.70
26	B	620	BCR	C29-C30-C25	4.68	117.24	110.44
24	c	905	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
24	B	604	CLA	C1C-C2C-C3C	-4.68	102.06	106.98
24	B	617	CLA	C2C-C1C-NC	4.68	114.90	109.98
26	B	620	BCR	C8-C7-C6	4.68	139.50	127.00
24	B	616	CLA	C2C-C1C-NC	4.68	114.89	109.98
24	b	604	CLA	O2D-CGD-CBD	4.68	119.40	111.23
24	C	513	CLA	C2D-C1D-ND	4.68	114.75	110.13
24	C	502	CLA	C2B-C1B-NB	4.67	115.17	110.33
24	b	617	CLA	C3C-C4C-NC	4.67	116.41	110.43
24	B	610	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
24	C	513	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	C	501	CLA	C2D-C1D-ND	4.66	114.74	110.13
24	C	507	CLA	C2C-C1C-NC	4.66	114.88	109.98
24	C	508	CLA	O2D-CGD-CBD	4.66	119.38	111.23
24	D	402	CLA	C3C-C4C-NC	4.66	116.40	110.43
26	k	101	BCR	C30-C25-C26	-4.66	116.27	122.64
24	D	403	CLA	C2C-C1C-NC	4.66	114.88	109.98
24	c	902	CLA	C1C-C2C-C3C	-4.66	102.08	106.98
24	a	408	CLA	C2B-C1B-NB	4.65	115.15	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	B	607	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
24	b	612	CLA	O2D-CGD-CBD	4.65	119.35	111.23
24	B	610	CLA	O2D-CGD-CBD	4.64	119.35	111.23
24	c	913	CLA	C2C-C1C-NC	4.64	114.86	109.98
24	b	602	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
26	B	620	BCR	C34-C9-C8	-4.64	111.00	118.09
26	k	101	BCR	C1-C6-C5	-4.64	116.30	122.64
24	c	909	CLA	C2C-C1C-NC	4.64	114.85	109.98
26	D	404	BCR	C35-C13-C12	-4.63	111.01	118.09
24	B	603	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
24	C	504	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
24	c	909	CLA	C2B-C1B-NB	4.63	115.12	110.33
26	D	404	BCR	C23-C24-C25	4.62	139.35	127.00
24	b	613	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
26	k	102	BCR	C24-C23-C22	4.62	133.07	126.23
24	B	605	CLA	C3C-C4C-NC	4.61	116.34	110.43
24	a	406	CLA	C2B-C1B-NB	4.61	115.11	110.33
24	B	605	CLA	C1C-C2C-C3C	-4.61	102.13	106.98
24	c	912	CLA	C2C-C1C-NC	4.61	114.83	109.98
24	c	914	CLA	O2D-CGD-CBD	4.61	119.29	111.23
24	b	602	CLA	C2B-C1B-NB	4.61	115.11	110.33
26	B	618	BCR	C37-C22-C23	-4.61	111.04	118.09
24	b	605	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
24	a	407	CLA	C1C-C2C-C3C	-4.61	102.13	106.98
24	B	604	CLA	C3B-C4B-NB	4.61	114.64	110.53
24	b	615	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
24	b	613	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
26	T	101	BCR	C23-C22-C21	4.60	126.25	119.01
26	D	404	BCR	C36-C18-C17	-4.60	115.36	122.82
24	B	604	CLA	C3B-C2B-C1B	-4.59	101.75	107.17
24	B	608	CLA	C3B-C4B-NB	4.59	114.63	110.53
26	c	915	BCR	C40-C30-C25	4.59	117.44	110.24
26	k	101	BCR	C36-C18-C17	-4.58	115.39	122.82
24	C	503	CLA	C2C-C1C-NC	4.58	114.79	109.98
26	b	618	BCR	C23-C24-C25	4.58	139.23	127.00
24	b	602	CLA	C2D-C1D-ND	4.58	114.66	110.13
24	B	609	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
24	B	606	CLA	C3C-C4C-NC	4.58	116.29	110.43
24	b	603	CLA	O2D-CGD-CBD	4.57	119.23	111.23
24	b	607	CLA	C2C-C1C-NC	4.57	114.79	109.98
24	B	612	CLA	C2B-C1B-NB	4.57	115.06	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	514	BCR	C32-C1-C6	4.57	117.41	110.24
24	c	914	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
26	B	619	BCR	C8-C7-C6	4.56	139.19	127.00
24	b	606	CLA	C3B-C2B-C1B	-4.56	101.79	107.17
24	C	505	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
26	b	619	BCR	C39-C30-C25	4.56	117.39	110.24
24	c	907	CLA	C2C-C1C-NC	4.56	114.77	109.98
24	C	504	CLA	C3B-C2B-C1B	-4.56	101.80	107.17
24	d	403	CLA	C3B-C2B-C1B	-4.55	101.80	107.17
26	a	409	BCR	C8-C7-C6	4.55	139.16	127.00
24	C	505	CLA	O2D-CGD-CBD	4.55	119.19	111.23
24	B	616	CLA	C2B-C1B-NB	4.55	115.05	110.33
24	b	617	CLA	C2B-C1B-NB	4.55	115.05	110.33
24	b	606	CLA	C3C-C4C-NC	4.55	116.25	110.43
24	a	408	CLA	O2D-CGD-CBD	4.55	119.18	111.23
24	A	614	CLA	O2D-CGD-CBD	4.54	119.17	111.23
24	B	608	CLA	C2B-C1B-NB	4.54	115.04	110.33
26	D	404	BCR	C36-C18-C19	-4.54	111.15	118.09
24	b	605	CLA	C3C-C4C-NC	4.54	116.25	110.43
24	b	604	CLA	C1C-C2C-C3C	-4.54	102.21	106.98
24	a	407	CLA	C3C-C4C-NC	4.54	116.24	110.43
26	k	102	BCR	C2-C1-C6	4.53	117.02	110.44
24	c	911	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	D	402	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	d	403	CLA	C1C-C2C-C3C	-4.52	102.22	106.98
26	B	620	BCR	C2-C1-C6	4.52	117.01	110.44
26	C	514	BCR	C33-C5-C4	-4.52	103.95	113.60
26	f	101	BCR	C38-C26-C27	-4.52	103.95	113.60
24	b	604	CLA	C2B-C1B-NB	4.52	115.02	110.33
24	b	616	CLA	O2D-CGD-CBD	4.52	119.13	111.23
26	Y	101	BCR	C1-C6-C5	-4.52	116.46	122.64
24	C	508	CLA	C3B-C2B-C1B	-4.52	101.85	107.17
31	D	406	DGD	O2G-C1B-C2B	4.52	121.25	111.48
24	B	617	CLA	C3C-C4C-NC	4.51	116.21	110.43
24	B	604	CLA	C2B-C1B-NB	4.51	115.00	110.33
26	C	514	BCR	C30-C25-C26	-4.51	116.47	122.64
24	b	603	CLA	C2B-C1B-NB	4.51	115.00	110.33
24	C	508	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
24	C	507	CLA	O2D-CGD-CBD	4.51	119.11	111.23
24	c	904	CLA	C2B-C1B-NB	4.50	115.00	110.33
24	c	903	CLA	C2C-C1C-NC	4.50	114.71	109.98
24	c	910	CLA	C3C-C4C-NC	4.50	116.20	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	C3C-C4C-NC	4.50	116.19	110.43
26	B	618	BCR	C30-C25-C26	-4.49	116.50	122.64
24	b	610	CLA	C2D-C1D-ND	4.49	114.57	110.13
26	k	102	BCR	C8-C9-C10	4.49	126.07	119.01
26	c	915	BCR	C37-C22-C21	-4.49	115.55	122.82
24	C	509	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
24	a	406	CLA	CAC-C3C-C4C	4.49	130.63	124.79
24	D	403	CLA	C2B-C1B-NB	4.48	114.98	110.33
24	C	511	CLA	C2B-C1B-NB	4.48	114.98	110.33
24	b	607	CLA	O2D-CGD-CBD	4.48	119.06	111.23
26	C	515	BCR	C38-C26-C27	-4.47	104.06	113.60
24	b	617	CLA	C2C-C1C-NC	4.47	114.67	109.98
24	d	404	CLA	C1C-C2C-C3C	-4.46	102.28	106.98
24	B	614	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
26	h	101	BCR	C30-C25-C26	-4.46	116.54	122.64
26	K	101	BCR	C35-C13-C14	-4.46	115.59	122.82
26	B	618	BCR	C29-C30-C25	4.46	116.91	110.44
24	C	501	CLA	O2D-CGD-O1D	-4.46	115.17	123.85
24	b	613	CLA	O2D-CGD-CBD	4.45	119.01	111.23
26	b	619	BCR	C23-C24-C25	4.44	138.86	127.00
26	c	918	BCR	C23-C24-C25	4.44	138.85	127.00
26	T	101	BCR	C33-C5-C4	-4.43	104.15	113.60
24	C	506	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
24	c	914	CLA	C2D-C1D-ND	4.43	114.51	110.13
24	a	406	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
24	c	909	CLA	C3C-C4C-NC	4.43	116.10	110.43
24	B	609	CLA	C1C-C2C-C3C	-4.42	102.33	106.98
24	b	610	CLA	O2D-CGD-CBD	4.42	118.96	111.23
26	C	515	BCR	C37-C22-C21	-4.42	115.66	122.82
24	a	407	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
24	C	513	CLA	O2D-CGD-CBD	4.41	118.94	111.23
26	a	409	BCR	C29-C30-C25	4.41	116.85	110.44
26	B	620	BCR	C23-C24-C25	4.41	138.78	127.00
26	h	101	BCR	C4-C5-C6	4.40	128.65	122.70
24	b	615	CLA	C2B-C1B-NB	4.40	114.89	110.33
26	C	514	BCR	C23-C24-C25	4.40	138.74	127.00
24	c	907	CLA	C2B-C1B-NB	4.40	114.88	110.33
26	T	101	BCR	C38-C26-C27	-4.39	104.23	113.60
26	a	409	BCR	C23-C24-C25	4.39	138.73	127.00
24	B	604	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	B	602	CLA	C2C-C1C-NC	4.39	114.59	109.98
26	Y	101	BCR	C34-C9-C10	-4.39	115.71	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
24	B	617	CLA	C2B-C1B-NB	4.38	114.87	110.33
24	a	408	CLA	C3C-C4C-NC	4.37	116.03	110.43
24	c	902	CLA	O2D-CGD-CBD	4.37	118.87	111.23
24	C	503	CLA	C2B-C1B-NB	4.37	114.86	110.33
24	C	513	CLA	C2B-C1B-NB	4.36	114.85	110.33
24	B	604	CLA	C3D-C4D-ND	4.36	117.08	109.99
24	b	610	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
24	d	403	CLA	C3B-C4B-NB	4.36	114.42	110.53
28	d	407	SQD	O47-C7-C8	4.35	120.90	111.48
24	c	912	CLA	C2B-C1B-NB	4.35	114.84	110.33
28	A	612	SQD	O47-C7-C8	4.35	120.89	111.48
26	D	404	BCR	C34-C9-C10	-4.35	115.77	122.82
24	d	401	CLA	C2B-C1B-NB	4.35	114.84	110.33
26	T	102	BCR	C29-C30-C25	4.35	116.76	110.44
24	C	501	CLA	C2B-C1B-NB	4.35	114.84	110.33
24	B	616	CLA	C3C-C4C-NC	4.35	116.00	110.43
28	L	101	SQD	O6-C1-C2	4.35	114.88	108.27
26	H	101	BCR	C8-C7-C6	4.35	138.61	127.00
26	c	915	BCR	C30-C25-C26	-4.34	116.70	122.64
24	C	509	CLA	C1C-C2C-C3C	-4.34	102.41	106.98
24	C	508	CLA	C3D-C4D-ND	4.34	117.04	109.99
26	T	102	BCR	C8-C7-C6	4.34	138.59	127.00
26	k	102	BCR	C23-C24-C25	4.34	138.59	127.00
26	B	620	BCR	C30-C25-C26	-4.34	116.71	122.64
24	b	610	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
24	c	908	CLA	C1C-C2C-C3C	-4.33	102.42	106.98
24	B	612	CLA	O2D-CGD-CBD	4.33	118.81	111.23
24	c	902	CLA	C2B-C1B-NB	4.33	114.82	110.33
24	A	609	CLA	C1C-C2C-C3C	-4.33	102.42	106.98
24	C	505	CLA	C2D-C1D-ND	4.33	114.41	110.13
26	b	619	BCR	C24-C23-C22	4.33	132.64	126.23
24	c	904	CLA	C2C-C1C-NC	4.33	114.53	109.98
26	T	101	BCR	C27-C26-C25	4.33	128.55	122.70
24	C	512	CLA	C2C-C1C-NC	4.32	114.52	109.98
26	B	619	BCR	C33-C5-C6	4.32	129.20	124.48
24	C	510	CLA	C2B-C1B-NB	4.32	114.81	110.33
24	d	401	CLA	C3C-C4C-NC	4.31	115.95	110.43
24	c	903	CLA	C3C-C4C-NC	4.31	115.95	110.43
24	B	605	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
28	d	407	SQD	O6-C1-C2	4.31	114.81	108.27
26	C	514	BCR	C36-C18-C19	-4.31	111.51	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	101	BCR	C40-C30-C25	4.30	116.99	110.24
24	c	909	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	A	614	CLA	C3C-C4C-NC	4.30	115.94	110.43
26	h	101	BCR	C35-C13-C12	-4.30	111.52	118.09
26	k	101	BCR	C35-C13-C14	-4.30	115.86	122.82
31	C	516	DGD	O2G-C1B-C2B	4.30	120.77	111.48
31	d	406	DGD	O2G-C1B-C2B	4.29	120.77	111.48
32	E	101	HEM	CBD-CAD-C3D	-4.29	100.67	112.53
24	c	906	CLA	C2C-C1C-NC	4.29	114.49	109.98
24	B	608	CLA	C1C-C2C-C3C	-4.29	102.47	106.98
24	b	614	CLA	C3B-C2B-C1B	-4.29	102.12	107.17
24	b	615	CLA	C3B-C4B-NB	4.28	114.36	110.53
28	F	101	SQD	O6-C1-C2	4.28	114.78	108.27
24	d	403	CLA	C3C-C4C-NC	4.28	115.91	110.43
26	H	101	BCR	C28-C27-C26	4.28	121.68	114.06
24	b	615	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
24	A	614	CLA	C2B-C1B-NB	4.27	114.75	110.33
26	c	915	BCR	C29-C30-C25	4.27	116.64	110.44
24	C	511	CLA	O2D-CGD-CBD	4.26	118.69	111.23
24	B	614	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
26	b	619	BCR	C39-C30-C29	-4.26	92.59	108.95
24	B	606	CLA	C2B-C1B-NB	4.26	114.74	110.33
26	B	618	BCR	C38-C26-C25	4.26	129.13	124.48
24	B	603	CLA	C2C-C1C-NC	4.26	114.45	109.98
26	Y	101	BCR	C35-C13-C14	-4.25	115.92	122.82
26	T	102	BCR	C2-C1-C6	4.25	116.62	110.44
24	B	607	CLA	O2D-CGD-O1D	-4.25	115.57	123.85
26	A	610	BCR	C23-C24-C25	4.25	138.35	127.00
26	h	101	BCR	C28-C27-C26	4.25	121.63	114.06
26	B	620	BCR	C33-C5-C6	4.24	129.11	124.48
26	k	101	BCR	C38-C26-C25	4.24	129.11	124.48
24	c	902	CLA	CHD-C1D-ND	-4.23	118.84	124.80
26	c	918	BCR	C33-C5-C4	-4.23	104.57	113.60
24	A	609	CLA	O2D-CGD-CBD	4.23	118.62	111.23
26	c	918	BCR	C37-C22-C21	-4.23	115.97	122.82
24	c	913	CLA	C2B-C1B-NB	4.22	114.71	110.33
26	h	101	BCR	C38-C26-C27	-4.22	104.61	113.60
24	C	508	CLA	C2B-C1B-NB	4.21	114.70	110.33
24	b	615	CLA	C3D-C4D-ND	4.21	116.83	109.99
26	B	619	BCR	C35-C13-C12	-4.21	111.66	118.09
24	B	604	CLA	C3C-C4C-NC	4.21	115.82	110.43
26	b	618	BCR	C33-C5-C6	4.21	129.07	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	C1C-C2C-C3C	-4.21	102.56	106.98
26	B	619	BCR	C33-C5-C4	-4.20	104.63	113.60
26	T	101	BCR	C30-C25-C26	-4.20	116.90	122.64
26	c	918	BCR	C29-C30-C25	4.20	116.54	110.44
24	a	406	CLA	C3B-C4B-NB	4.20	114.28	110.53
24	b	612	CLA	C3C-C4C-NC	4.19	115.80	110.43
24	c	912	CLA	O2D-CGD-CBD	4.19	118.55	111.23
24	b	612	CLA	C3B-C2B-C1B	-4.18	102.24	107.17
24	b	603	CLA	C2C-C1C-NC	4.18	114.38	109.98
24	C	506	CLA	C3C-C4C-NC	4.18	115.78	110.43
24	b	605	CLA	C2B-C1B-NB	4.18	114.66	110.33
26	h	101	BCR	C34-C9-C10	-4.18	116.05	122.82
24	a	407	CLA	O2D-CGD-CBD	4.17	118.52	111.23
24	C	504	CLA	CHD-C1D-ND	-4.17	118.94	124.80
24	b	604	CLA	CHD-C1D-ND	-4.17	118.94	124.80
24	b	609	CLA	C2B-C1B-NB	4.16	114.64	110.33
24	B	613	CLA	C3C-C4C-NC	4.16	115.76	110.43
26	B	618	BCR	C23-C24-C25	4.16	138.11	127.00
24	C	502	CLA	O2D-CGD-CBD	4.16	118.50	111.23
26	b	618	BCR	C4-C5-C6	4.16	128.32	122.70
24	B	607	CLA	CHD-C1D-ND	-4.15	118.96	124.80
26	C	515	BCR	C36-C18-C17	-4.15	116.09	122.82
26	T	102	BCR	C37-C22-C23	-4.15	111.75	118.09
24	c	907	CLA	CHD-C1D-ND	-4.15	118.96	124.80
24	C	503	CLA	CHD-C1D-ND	-4.15	118.96	124.80
24	C	510	CLA	C3B-C4B-NB	4.15	114.23	110.53
24	C	507	CLA	C1C-C2C-C3C	-4.15	102.62	106.98
24	C	507	CLA	C2B-C1B-NB	4.14	114.62	110.33
24	C	501	CLA	CHD-C1D-ND	-4.14	118.97	124.80
24	A	606	CLA	C3C-C4C-NC	4.14	115.73	110.43
26	D	404	BCR	C33-C5-C4	-4.14	104.77	113.60
24	a	406	CLA	C3C-C4C-NC	4.14	115.73	110.43
24	c	905	CLA	C3D-C4D-ND	4.14	116.71	109.99
24	c	914	CLA	C2C-C1C-NC	4.13	114.32	109.98
24	A	606	CLA	C3B-C4B-NB	4.13	114.22	110.53
24	A	609	CLA	C3D-C4D-ND	4.13	116.69	109.99
26	k	102	BCR	C32-C1-C6	4.13	116.71	110.24
24	b	605	CLA	O2D-CGD-CBD	4.12	118.44	111.23
24	c	911	CLA	O2D-CGD-CBD	4.12	118.43	111.23
24	B	609	CLA	C3C-C4C-NC	4.11	115.70	110.43
24	c	911	CLA	C2B-C1B-NB	4.11	114.59	110.33
26	c	915	BCR	C31-C1-C6	4.11	116.68	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	CHD-C1D-ND	-4.11	119.03	124.80
24	B	614	CLA	C2B-C1B-NB	4.10	114.58	110.33
24	c	906	CLA	C2B-C1B-NB	4.10	114.58	110.33
24	b	606	CLA	C4-C3-C5	4.10	122.35	115.23
26	f	101	BCR	C32-C1-C2	-4.10	93.21	108.95
24	B	611	CLA	C3C-C4C-NC	4.10	115.68	110.43
24	b	608	CLA	C3C-C4C-NC	4.09	115.67	110.43
24	c	905	CLA	C1C-C2C-C3C	-4.09	102.68	106.98
26	h	101	BCR	C1-C6-C5	-4.09	117.05	122.64
24	C	502	CLA	C3C-C4C-NC	4.09	115.67	110.43
24	C	512	CLA	C2B-C1B-NB	4.08	114.56	110.33
26	C	515	BCR	C31-C1-C2	-4.08	93.28	108.95
26	C	515	BCR	C2-C1-C6	4.08	116.37	110.44
24	B	609	CLA	C3D-C4D-ND	4.08	116.62	109.99
26	b	619	BCR	C32-C1-C6	4.08	116.64	110.24
24	C	513	CLA	C2C-C1C-NC	4.07	114.26	109.98
24	b	609	CLA	C3C-C4C-NC	4.06	115.64	110.43
28	a	411	SQD	O47-C7-C8	4.06	120.27	111.48
24	b	609	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
26	K	101	BCR	C30-C25-C26	-4.06	117.09	122.64
26	b	618	BCR	C8-C7-C6	4.06	137.83	127.00
26	T	102	BCR	C35-C13-C12	-4.05	111.90	118.09
26	C	514	BCR	C23-C22-C21	4.05	125.38	119.01
26	k	102	BCR	C35-C13-C12	-4.05	111.91	118.09
26	T	102	BCR	C39-C30-C29	-4.05	93.41	108.95
24	a	408	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
26	C	514	BCR	C32-C1-C2	-4.04	93.44	108.95
24	d	404	CLA	C3B-C4B-NB	4.04	114.14	110.53
26	B	619	BCR	C40-C30-C29	-4.04	93.44	108.95
24	b	616	CLA	C3C-C4C-NC	4.04	115.60	110.43
26	b	619	BCR	C8-C9-C10	4.04	125.36	119.01
24	C	510	CLA	CHD-C1D-ND	-4.04	119.12	124.80
24	b	607	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
24	B	603	CLA	O2D-CGD-CBD	4.03	118.28	111.23
26	B	618	BCR	C8-C7-C6	4.03	137.78	127.00
24	d	404	CLA	CHD-C1D-ND	-4.03	119.13	124.80
24	C	511	CLA	C3C-C4C-NC	4.03	115.60	110.43
24	c	911	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
24	b	606	CLA	C2B-C1B-NB	4.03	114.51	110.33
24	B	617	CLA	O2D-CGD-CBD	4.03	118.27	111.23
24	C	504	CLA	C2B-C1B-NB	4.03	114.50	110.33
24	b	607	CLA	C2B-C1B-NB	4.03	114.50	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	907	CLA	C3C-C4C-NC	4.03	115.59	110.43
26	c	915	BCR	C8-C7-C6	4.02	137.75	127.00
24	B	610	CLA	C3C-C4C-NC	4.02	115.58	110.43
24	C	503	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
24	a	408	CLA	C3B-C4B-NB	4.02	114.12	110.53
24	B	614	CLA	CHD-C1D-ND	-4.02	119.15	124.80
24	b	603	CLA	CHD-C1D-ND	-4.01	119.15	124.80
24	c	913	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
24	D	403	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
24	B	607	CLA	C2B-C1B-NB	4.00	114.48	110.33
24	b	602	CLA	C2C-C1C-NC	4.00	114.19	109.98
24	C	503	CLA	C3C-C4C-NC	4.00	115.55	110.43
24	c	911	CLA	C3C-C4C-NC	4.00	115.55	110.43
24	b	614	CLA	C3B-C4B-NB	3.99	114.09	110.53
24	b	608	CLA	C3B-C2B-C1B	-3.99	102.46	107.17
24	b	614	CLA	C2B-C1B-NB	3.99	114.47	110.33
24	b	613	CLA	C3D-C4D-ND	3.99	116.47	109.99
24	d	404	CLA	C3D-C4D-ND	3.99	116.47	109.99
24	b	605	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
24	C	510	CLA	C3D-C4D-ND	3.98	116.46	109.99
26	h	101	BCR	C33-C5-C4	-3.98	105.10	113.60
26	f	101	BCR	C38-C26-C25	3.98	128.83	124.48
24	B	602	CLA	C1C-C2C-C3C	-3.98	102.80	106.98
24	c	907	CLA	O2D-CGD-CBD	3.98	118.18	111.23
24	A	607	CLA	C3C-C4C-NC	3.98	115.52	110.43
24	b	611	CLA	C3C-C4C-NC	3.97	115.52	110.43
24	B	614	CLA	C3C-C4C-NC	3.97	115.52	110.43
26	c	915	BCR	C1-C6-C5	-3.97	117.22	122.64
24	B	613	CLA	CHD-C1D-ND	-3.97	119.22	124.80
24	C	509	CLA	C3C-C4C-NC	3.96	115.51	110.43
24	b	608	CLA	O2D-CGD-CBD	3.96	118.15	111.23
24	B	608	CLA	C3B-C2B-C1B	-3.96	102.50	107.17
24	B	607	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
29	A	615	LHG	O7-C7-C8	3.95	120.04	111.48
26	a	409	BCR	C34-C9-C8	-3.95	112.05	118.09
24	c	908	CLA	C3C-C4C-NC	3.95	115.49	110.43
24	b	611	CLA	O2D-CGD-CBD	3.95	118.14	111.23
24	d	404	CLA	O2D-CGD-CBD	3.95	118.14	111.23
26	h	101	BCR	C32-C1-C6	3.94	116.43	110.24
26	h	101	BCR	C29-C30-C25	3.94	116.17	110.44
24	C	510	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
24	A	614	CLA	C3B-C4B-NB	3.94	114.05	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	C3C-C4C-NC	3.94	115.48	110.43
28	L	101	SQD	O47-C7-C8	3.94	120.01	111.48
26	B	618	BCR	C27-C26-C25	3.94	128.03	122.70
24	a	406	CLA	C3D-C4D-ND	3.94	116.39	109.99
24	C	505	CLA	C3C-C4C-NC	3.94	115.47	110.43
26	B	622	BCR	C31-C1-C6	3.94	116.42	110.24
26	C	515	BCR	C8-C9-C10	3.93	125.19	119.01
24	C	507	CLA	CHD-C1D-ND	-3.93	119.28	124.80
24	C	503	CLA	O2D-CGD-CBD	3.93	118.09	111.23
26	f	101	BCR	C2-C1-C6	3.93	116.14	110.44
24	A	609	CLA	C3B-C4B-NB	3.93	114.03	110.53
24	a	408	CLA	C3D-C4D-ND	3.92	116.36	109.99
26	T	101	BCR	C8-C9-C10	3.92	125.18	119.01
24	c	906	CLA	C3C-C4C-NC	3.92	115.45	110.43
24	C	506	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
24	b	610	CLA	C3D-C4D-ND	3.92	116.36	109.99
24	D	403	CLA	C3D-C4D-ND	3.92	116.35	109.99
26	C	515	BCR	C35-C13-C14	-3.92	116.47	122.82
24	c	902	CLA	C3D-C4D-ND	3.91	116.35	109.99
24	c	910	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
24	B	606	CLA	O2D-CGD-CBD	3.91	118.06	111.23
24	b	606	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
26	Y	101	BCR	C27-C26-C25	3.90	127.98	122.70
24	B	610	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
26	k	102	BCR	C27-C26-C25	3.89	127.96	122.70
24	C	508	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
24	c	908	CLA	CHD-C1D-ND	-3.89	119.33	124.80
26	h	101	BCR	C38-C26-C25	3.89	128.73	124.48
24	c	912	CLA	C3C-C4C-NC	3.89	115.41	110.43
26	b	619	BCR	C30-C25-C26	-3.89	117.32	122.64
24	B	615	CLA	C3D-C4D-ND	3.89	116.31	109.99
26	D	404	BCR	C38-C26-C27	-3.89	105.31	113.60
24	b	604	CLA	C4-C3-C5	3.88	121.97	115.23
24	b	614	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
24	C	511	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
26	c	915	BCR	C34-C9-C8	-3.88	112.17	118.09
24	C	508	CLA	C3C-C4C-NC	3.87	115.39	110.43
26	h	101	BCR	C39-C30-C29	-3.87	94.08	108.95
24	b	610	CLA	C3C-C4C-NC	3.87	115.39	110.43
24	a	407	CLA	C2B-C1B-NB	3.87	114.34	110.33
24	C	510	CLA	O2D-CGD-CBD	3.87	117.99	111.23
24	b	612	CLA	C2B-C1B-NB	3.87	114.34	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	622	BCR	C40-C30-C25	3.87	116.31	110.24
26	K	101	BCR	C2-C1-C6	3.87	116.05	110.44
24	b	604	CLA	C3D-C4D-ND	3.86	116.27	109.99
24	A	607	CLA	C3D-C4D-ND	3.86	116.27	109.99
24	c	903	CLA	C3D-C4D-ND	3.86	116.26	109.99
24	b	607	CLA	C3D-C4D-ND	3.86	116.26	109.99
24	c	911	CLA	C3D-C4D-ND	3.86	116.26	109.99
26	k	101	BCR	C34-C9-C8	-3.86	112.19	118.09
24	d	401	CLA	C3B-C4B-NB	3.86	113.97	110.53
24	C	513	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
26	c	915	BCR	C35-C13-C14	-3.85	116.57	122.82
24	C	505	CLA	C2B-C1B-NB	3.85	114.32	110.33
26	K	101	BCR	C32-C1-C6	3.85	116.28	110.24
24	B	604	CLA	CHD-C1D-ND	-3.85	119.38	124.80
24	c	904	CLA	C3C-C4C-NC	3.85	115.36	110.43
24	D	402	CLA	C2B-C1B-NB	3.85	114.32	110.33
24	B	607	CLA	O2D-CGD-CBD	3.84	117.95	111.23
26	b	619	BCR	C2-C1-C6	3.84	116.02	110.44
24	B	617	CLA	CHD-C1D-ND	-3.84	119.40	124.80
24	B	603	CLA	C3C-C4C-NC	3.84	115.35	110.43
24	b	616	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
26	C	515	BCR	C33-C5-C6	3.84	128.67	124.48
24	B	607	CLA	C3C-C4C-NC	3.84	115.34	110.43
26	h	101	BCR	C2-C1-C6	3.83	116.01	110.44
24	c	905	CLA	C3C-C4C-NC	3.83	115.34	110.43
24	c	914	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
26	T	102	BCR	C4-C5-C6	3.83	127.87	122.70
24	B	606	CLA	C4-C3-C5	3.82	121.86	115.23
24	b	615	CLA	C3C-C4C-NC	3.82	115.33	110.43
24	b	609	CLA	C3B-C4B-NB	3.82	113.94	110.53
24	C	510	CLA	C3C-C4C-NC	3.82	115.32	110.43
24	C	504	CLA	C3B-C4B-NB	3.81	113.93	110.53
24	B	605	CLA	C3B-C4B-NB	3.81	113.93	110.53
24	B	615	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
24	b	604	CLA	C3B-C4B-NB	3.80	113.92	110.53
24	C	512	CLA	C3C-C4C-NC	3.80	115.30	110.43
26	Y	101	BCR	C38-C26-C27	-3.80	105.50	113.60
24	b	613	CLA	CAC-C3C-C4C	3.80	129.73	124.79
24	B	610	CLA	C2B-C1B-NB	3.79	114.26	110.33
24	B	613	CLA	C2B-C1B-NB	3.79	114.26	110.33
24	A	606	CLA	C3D-C4D-ND	3.78	116.14	109.99
24	B	611	CLA	C3D-C4D-ND	3.78	116.14	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	C3D-C4D-ND	3.78	116.14	109.99
24	c	907	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
26	H	101	BCR	C23-C24-C25	3.78	137.09	127.00
24	B	606	CLA	C3D-C4D-ND	3.78	116.13	109.99
24	a	407	CLA	C3B-C4B-NB	3.78	113.90	110.53
24	A	606	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
26	H	101	BCR	C24-C23-C22	3.77	131.81	126.23
24	c	903	CLA	C3B-C4B-NB	3.77	113.90	110.53
26	H	101	BCR	C35-C13-C14	-3.77	116.71	122.82
24	A	609	CLA	C3C-C4C-NC	3.77	115.26	110.43
29	b	620	LHG	O7-C7-C8	3.77	119.63	111.48
26	T	101	BCR	C35-C13-C14	-3.77	116.71	122.82
24	B	616	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
24	c	902	CLA	C3B-C4B-NB	3.77	113.89	110.53
24	b	603	CLA	C1C-C2C-C3C	-3.76	103.02	106.98
24	b	613	CLA	C4C-C3C-C2C	-3.76	101.41	106.89
24	B	608	CLA	C3D-C4D-ND	3.76	116.10	109.99
24	B	610	CLA	C3D-C4D-ND	3.75	116.09	109.99
26	D	404	BCR	C27-C26-C25	3.75	127.78	122.70
26	c	915	BCR	C36-C18-C19	-3.75	112.36	118.09
24	B	613	CLA	C3D-C4D-ND	3.75	116.08	109.99
24	b	604	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
24	c	909	CLA	O2D-CGD-CBD	3.75	117.78	111.23
28	L	101	SQD	C3-C4-C5	3.74	117.02	110.23
24	D	402	CLA	C3B-C4B-NB	3.74	113.87	110.53
24	b	602	CLA	C3C-C4C-NC	3.74	115.22	110.43
24	b	607	CLA	O2D-CGD-O1D	-3.74	116.58	123.85
24	b	614	CLA	CHD-C1D-ND	-3.73	119.55	124.80
26	f	101	BCR	C31-C1-C6	3.73	116.10	110.24
26	k	101	BCR	C27-C26-C25	3.73	127.75	122.70
24	c	910	CLA	C3B-C4B-NB	3.73	113.86	110.53
24	c	902	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
26	C	515	BCR	C33-C5-C4	-3.73	105.64	113.60
24	C	506	CLA	CHD-C1D-ND	-3.73	119.55	124.80
24	C	513	CLA	C3C-C4C-NC	3.73	115.21	110.43
24	C	509	CLA	C3B-C4B-NB	3.73	113.86	110.53
24	B	611	CLA	O2D-CGD-CBD	3.73	117.75	111.23
28	F	101	SQD	O47-C7-C8	3.73	119.54	111.48
24	b	609	CLA	C3D-C4D-ND	3.72	116.04	109.99
24	D	402	CLA	CHD-C1D-ND	-3.72	119.56	124.80
24	b	610	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
24	B	603	CLA	CHD-C1D-ND	-3.72	119.56	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	C3B-C4B-NB	3.72	113.85	110.53
24	c	904	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
26	B	620	BCR	C27-C26-C25	3.71	127.72	122.70
24	B	615	CLA	C3C-C4C-NC	3.71	115.19	110.43
31	C	517	DGD	O2G-C1B-C2B	3.71	119.51	111.48
24	c	910	CLA	C3D-C4D-ND	3.71	116.02	109.99
24	d	403	CLA	C3D-C4D-ND	3.70	116.01	109.99
26	B	620	BCR	C4-C5-C6	3.70	127.71	122.70
26	A	610	BCR	C35-C13-C12	-3.70	112.44	118.09
24	b	603	CLA	C3D-C4D-ND	3.70	116.00	109.99
24	D	403	CLA	C3B-C4B-NB	3.69	113.83	110.53
24	c	908	CLA	C2B-C1B-NB	3.69	114.16	110.33
26	f	101	BCR	C34-C9-C10	-3.69	116.84	122.82
24	C	508	CLA	C3B-C4B-NB	3.69	113.82	110.53
26	b	619	BCR	C35-C13-C12	-3.69	112.46	118.09
24	c	912	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
28	l	101	SQD	O47-C7-C8	3.69	119.45	111.48
26	c	918	BCR	C36-C18-C17	-3.68	116.85	122.82
24	c	913	CLA	C3C-C4C-NC	3.68	115.15	110.43
24	b	611	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
26	c	918	BCR	C23-C22-C21	3.68	124.80	119.01
24	c	914	CLA	CHD-C1D-ND	-3.68	119.62	124.80
24	b	603	CLA	C3C-C4C-NC	3.68	115.14	110.43
24	b	602	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
24	B	612	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
24	B	602	CLA	C3C-C4C-NC	3.67	115.14	110.43
24	B	607	CLA	C3D-C4D-ND	3.67	115.96	109.99
24	b	606	CLA	CHD-C1D-ND	-3.67	119.63	124.80
24	C	512	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	b	614	CLA	C3D-C4D-ND	3.67	115.95	109.99
24	B	605	CLA	O2D-CGD-CBD	3.67	117.65	111.23
26	h	101	BCR	C36-C18-C19	-3.67	112.48	118.09
26	k	102	BCR	C40-C30-C25	3.67	115.99	110.24
24	B	603	CLA	C2B-C1B-NB	3.66	114.12	110.33
24	c	906	CLA	CHD-C1D-ND	-3.66	119.65	124.80
24	b	612	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
27	D	405	PL9	C40-C39-C41	3.65	121.57	115.23
24	C	505	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
28	a	402	SQD	O47-C7-C8	3.65	119.37	111.48
24	B	612	CLA	C3D-C4D-ND	3.65	115.92	109.99
24	c	905	CLA	CHD-C1D-ND	-3.65	119.67	124.80
24	c	909	CLA	C4C-C3C-C2C	-3.64	101.59	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	C3B-C4B-NB	3.64	113.78	110.53
24	C	509	CLA	C3D-C4D-ND	3.64	115.91	109.99
24	b	608	CLA	CHD-C1D-ND	-3.63	119.69	124.80
27	d	405	PL9	C40-C39-C41	3.63	121.53	115.23
24	B	603	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
26	T	102	BCR	C30-C25-C26	-3.63	117.68	122.64
24	C	502	CLA	C3D-C4D-ND	3.63	115.89	109.99
24	C	502	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	b	605	CLA	CAC-C3C-C4C	3.63	129.51	124.79
26	B	619	BCR	C37-C22-C23	-3.63	112.55	118.09
26	H	101	BCR	C38-C26-C27	-3.63	105.87	113.60
24	c	911	CLA	C3B-C4B-NB	3.62	113.77	110.53
24	b	608	CLA	C3B-C4B-NB	3.62	113.76	110.53
26	D	404	BCR	C1-C6-C5	-3.62	117.69	122.64
26	T	102	BCR	C27-C26-C25	3.62	127.59	122.70
24	B	615	CLA	C3B-C4B-NB	3.62	113.76	110.53
24	D	403	CLA	C3C-C4C-NC	3.61	115.06	110.43
24	B	603	CLA	C3D-C4D-ND	3.61	115.86	109.99
26	H	101	BCR	C27-C26-C25	3.60	127.58	122.70
24	c	902	CLA	C3C-C4C-NC	3.60	115.05	110.43
32	v	202	HEM	CBD-CAD-C3D	-3.60	102.57	112.53
24	c	909	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
24	b	612	CLA	C3D-C4D-ND	3.60	115.83	109.99
24	c	907	CLA	C3D-C4D-ND	3.59	115.83	109.99
24	b	607	CLA	C3C-C4C-NC	3.59	115.03	110.43
26	Y	101	BCR	C2-C1-C6	3.59	115.66	110.44
24	B	611	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
26	D	404	BCR	C32-C1-C2	-3.59	95.17	108.95
26	b	619	BCR	C35-C13-C14	-3.59	117.00	122.82
24	a	407	CLA	C3D-C4D-ND	3.59	115.82	109.99
28	A	612	SQD	O9-S-C6	3.59	112.11	106.76
24	d	403	CLA	CHD-C1D-ND	-3.59	119.76	124.80
24	c	908	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
26	k	102	BCR	C35-C13-C14	-3.58	117.02	122.82
24	C	507	CLA	C3C-C4C-NC	3.58	115.01	110.43
24	B	614	CLA	C3B-C4B-NB	3.58	113.72	110.53
24	B	613	CLA	CAC-C3C-C4C	3.57	129.44	124.79
24	b	612	CLA	C3B-C4B-NB	3.57	113.72	110.53
24	c	909	CLA	C3B-C4B-NB	3.56	113.71	110.53
26	K	101	BCR	C24-C23-C22	3.56	131.51	126.23
24	D	402	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
26	B	620	BCR	C36-C18-C19	-3.56	112.65	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	C3D-C4D-ND	3.56	115.77	109.99
24	a	408	CLA	CHD-C1D-ND	-3.55	119.80	124.80
24	b	617	CLA	CHD-C1D-ND	-3.55	119.80	124.80
24	c	914	CLA	C3D-C4D-ND	3.55	115.75	109.99
24	b	617	CLA	C4C-C3C-C2C	-3.54	101.73	106.89
28	a	411	SQD	O9-S-C6	3.54	112.05	106.76
24	b	608	CLA	C1C-C2C-C3C	-3.54	103.25	106.98
27	A	611	PL9	C20-C19-C21	3.54	121.37	115.23
24	b	615	CLA	C1-C2-C3	-3.54	120.40	126.20
26	k	101	BCR	C23-C24-C25	3.54	136.45	127.00
26	k	101	BCR	C4-C5-C6	3.54	127.48	122.70
26	B	620	BCR	C35-C13-C14	-3.54	117.09	122.82
24	B	617	CLA	C4C-C3C-C2C	-3.54	101.75	106.89
26	B	618	BCR	C35-C13-C14	-3.53	117.09	122.82
24	B	616	CLA	C3B-C4B-NB	3.53	113.68	110.53
24	B	606	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
26	K	101	BCR	C38-C26-C27	-3.53	106.07	113.60
24	B	611	CLA	C3B-C4B-NB	3.52	113.68	110.53
24	c	904	CLA	CHD-C1D-ND	-3.52	119.84	124.80
24	c	914	CLA	C3C-C4C-NC	3.52	114.94	110.43
24	c	913	CLA	C3D-C4D-ND	3.52	115.71	109.99
26	T	102	BCR	C1-C6-C5	-3.52	117.83	122.64
24	B	604	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
24	B	612	CLA	CHD-C1D-ND	-3.51	119.86	124.80
24	C	501	CLA	C3C-C4C-NC	3.51	114.93	110.43
24	c	904	CLA	O2D-CGD-CBD	3.51	117.36	111.23
24	c	912	CLA	C3D-C4D-ND	3.51	115.69	109.99
26	C	515	BCR	C40-C30-C25	3.51	115.74	110.24
26	c	918	BCR	C33-C5-C6	3.51	128.31	124.48
24	c	903	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
24	c	906	CLA	C3D-C4D-ND	3.51	115.69	109.99
24	B	608	CLA	CHD-C1D-ND	-3.50	119.88	124.80
24	B	605	CLA	C2B-C1B-NB	3.50	113.95	110.33
24	B	612	CLA	C3B-C4B-NB	3.49	113.65	110.53
24	b	605	CLA	C3B-C4B-NB	3.49	113.65	110.53
26	A	610	BCR	C34-C9-C8	-3.49	112.75	118.09
24	A	609	CLA	C4-C3-C5	3.49	121.28	115.23
32	V	202	HEM	CBD-CAD-C3D	-3.48	102.91	112.53
25	a	412	PHO	O2D-CGD-O1D	-3.47	117.09	123.85
24	B	608	CLA	C3C-C4C-NC	3.47	114.88	110.43
24	c	905	CLA	C3B-C4B-NB	3.47	113.63	110.53
24	C	504	CLA	C3D-C4D-ND	3.46	115.62	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	C2B-C1B-NB	3.46	113.92	110.33
24	c	907	CLA	C3B-C4B-NB	3.46	113.62	110.53
24	B	605	CLA	CED-O2D-CGD	3.46	123.76	115.92
24	B	614	CLA	C3D-C4D-ND	3.46	115.61	109.99
26	B	622	BCR	C35-C13-C12	-3.46	112.81	118.09
24	d	401	CLA	O2D-CGD-CBD	3.46	117.27	111.23
24	A	614	CLA	CHD-C1D-ND	-3.45	119.94	124.80
24	b	613	CLA	C3B-C4B-NB	3.45	113.61	110.53
29	D	407	LHG	O8-C23-C24	3.45	122.34	111.83
24	C	511	CLA	C1-O2A-CGA	3.44	124.99	116.65
26	c	915	BCR	C33-C5-C6	3.44	128.24	124.48
24	b	606	CLA	C3D-C4D-ND	3.44	115.58	109.99
24	b	610	CLA	CHD-C1D-ND	-3.44	119.97	124.80
24	b	613	CLA	C2B-C1B-NB	3.43	113.89	110.33
24	A	607	CLA	CHD-C1D-ND	-3.43	119.97	124.80
24	B	606	CLA	C4C-C3C-C2C	-3.43	101.90	106.89
26	B	620	BCR	C35-C13-C12	-3.42	112.86	118.09
26	H	101	BCR	C36-C18-C17	-3.42	117.27	122.82
24	b	602	CLA	CHD-C1D-ND	-3.42	119.99	124.80
26	c	915	BCR	C35-C13-C12	-3.42	112.87	118.09
24	b	611	CLA	C3D-C4D-ND	3.42	115.54	109.99
24	c	906	CLA	C1C-C2C-C3C	-3.42	103.39	106.98
24	b	606	CLA	CMB-C2B-C1B	3.41	130.62	125.42
24	b	602	CLA	O2A-CGA-CBA	3.41	122.24	111.83
26	K	101	BCR	C31-C1-C6	3.41	115.59	110.24
24	a	406	CLA	CHD-C1D-ND	-3.41	120.00	124.80
24	b	617	CLA	C3D-C4D-ND	3.41	115.52	109.99
24	b	614	CLA	O2D-CGD-CBD	3.40	117.18	111.23
26	A	610	BCR	C30-C25-C24	3.40	124.87	115.65
24	b	608	CLA	C2B-C1B-NB	3.40	113.85	110.33
24	b	609	CLA	CHD-C1D-ND	-3.39	120.03	124.80
24	C	502	CLA	CAC-C3C-C4C	3.39	129.20	124.79
24	C	513	CLA	C3D-C4D-ND	3.39	115.49	109.99
24	C	505	CLA	C3D-C4D-ND	3.38	115.48	109.99
26	b	618	BCR	C1-C6-C5	-3.38	118.01	122.64
28	A	613	SQD	O47-C7-C8	3.38	118.80	111.48
26	c	915	BCR	C33-C5-C4	-3.38	106.39	113.60
24	B	615	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
24	D	402	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
24	C	511	CLA	C3D-C4D-ND	3.37	115.47	109.99
26	k	101	BCR	C35-C13-C12	-3.37	112.94	118.09
24	A	614	CLA	C3D-C4D-ND	3.37	115.47	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	614	CLA	CBC-CAC-C3C	-3.36	103.30	112.42
26	B	618	BCR	C32-C1-C6	3.36	115.51	110.24
24	B	617	CLA	CAC-C3C-C4C	3.36	129.16	124.79
24	C	506	CLA	C2B-C1B-NB	3.36	113.81	110.33
24	b	606	CLA	CAC-C3C-C4C	3.35	129.15	124.79
24	b	608	CLA	C4-C3-C5	3.35	121.04	115.23
24	D	403	CLA	CHD-C1D-ND	-3.35	120.09	124.80
26	b	619	BCR	C34-C9-C8	-3.35	112.98	118.09
29	d	410	LHG	O7-C7-C8	3.34	118.71	111.48
26	f	101	BCR	C27-C26-C25	3.34	127.22	122.70
32	e	101	HEM	CBD-CAD-C3D	-3.34	103.30	112.53
24	b	615	CLA	C4-C3-C5	3.34	121.02	115.23
24	b	616	CLA	C3B-C4B-NB	3.34	113.51	110.53
24	b	610	CLA	CAC-C3C-C4C	3.33	129.13	124.79
26	B	620	BCR	C37-C22-C21	-3.33	117.42	122.82
26	c	915	BCR	C31-C1-C2	-3.33	96.15	108.95
26	f	101	BCR	C35-C13-C14	-3.33	117.42	122.82
24	b	602	CLA	C3D-C4D-ND	3.33	115.40	109.99
24	B	613	CLA	C1C-C2C-C3C	-3.33	103.48	106.98
24	B	615	CLA	C4-C3-C5	3.33	121.00	115.23
24	d	403	CLA	C4-C3-C5	3.33	121.00	115.23
24	a	407	CLA	CMB-C2B-C1B	3.32	130.48	125.42
26	B	619	BCR	C34-C9-C8	-3.32	113.02	118.09
26	B	622	BCR	C35-C13-C14	-3.32	117.44	122.82
24	c	905	CLA	C4-C3-C5	3.31	120.98	115.23
26	K	101	BCR	C33-C5-C4	-3.31	106.53	113.60
24	A	607	CLA	CAC-C3C-C4C	3.31	129.10	124.79
26	B	619	BCR	C38-C26-C25	3.31	128.10	124.48
24	B	611	CLA	C4C-C3C-C2C	-3.31	102.08	106.89
24	C	506	CLA	C3D-C4D-ND	3.30	115.36	109.99
24	B	609	CLA	CHD-C1D-ND	-3.30	120.16	124.80
24	D	403	CLA	O2D-CGD-CBD	3.30	117.00	111.23
26	K	101	BCR	C27-C26-C25	3.30	127.16	122.70
24	C	505	CLA	CHD-C1D-ND	-3.30	120.16	124.80
24	D	402	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
24	b	605	CLA	C4C-C3C-C2C	-3.29	102.10	106.89
24	d	403	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
24	A	609	CLA	CHD-C1D-ND	-3.29	120.17	124.80
26	A	610	BCR	C40-C30-C25	3.29	115.40	110.24
28	a	411	SQD	C1-C2-C3	-3.28	103.10	110.01
24	C	508	CLA	CHD-C1D-ND	-3.28	120.18	124.80
24	B	617	CLA	C3B-C4B-NB	3.28	113.46	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
27	a	410	PL9	C7-C3-C2	-3.28	119.52	123.39
26	c	918	BCR	C32-C1-C6	3.28	115.38	110.24
29	a	413	LHG	O7-C7-C8	3.28	118.57	111.48
24	b	617	CLA	C3B-C4B-NB	3.27	113.45	110.53
26	c	918	BCR	C39-C30-C25	3.27	115.37	110.24
24	C	501	CLA	C3D-C4D-ND	3.27	115.30	109.99
24	B	610	CLA	CHD-C1D-ND	-3.27	120.20	124.80
28	A	612	SQD	C1-C2-C3	-3.27	103.14	110.01
26	c	918	BCR	C4-C5-C6	3.26	127.11	122.70
24	c	913	CLA	CMB-C2B-C1B	3.26	130.38	125.42
24	c	910	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
26	D	404	BCR	C37-C22-C21	-3.26	117.54	122.82
26	k	102	BCR	C30-C25-C26	-3.26	118.19	122.64
24	C	502	CLA	CHD-C1D-ND	-3.26	120.22	124.80
26	T	101	BCR	C34-C9-C8	-3.25	113.12	118.09
26	c	915	BCR	C38-C26-C27	-3.25	106.66	113.60
24	D	402	CLA	O2D-CGD-CBD	3.25	116.92	111.23
24	c	903	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
26	c	918	BCR	C12-C13-C14	3.25	124.12	119.01
24	B	616	CLA	CHD-C1D-ND	-3.25	120.23	124.80
26	b	619	BCR	C4-C5-C6	3.25	127.09	122.70
24	C	512	CLA	C3D-C4D-ND	3.25	115.26	109.99
26	T	101	BCR	C36-C18-C19	-3.24	113.13	118.09
24	b	617	CLA	CAC-C3C-C4C	3.24	129.01	124.79
24	c	908	CLA	CMB-C2B-C1B	3.24	130.35	125.42
24	d	401	CLA	CHD-C1D-ND	-3.24	120.24	124.80
24	C	508	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
24	B	616	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
24	b	606	CLA	CMC-C2C-C1C	3.23	130.09	125.03
24	B	610	CLA	CAC-C3C-C4C	3.23	129.00	124.79
24	D	402	CLA	C3D-C4D-ND	3.23	115.24	109.99
24	B	604	CLA	CMC-C2C-C1C	3.23	130.08	125.03
24	c	911	CLA	CHD-C1D-ND	-3.22	120.27	124.80
28	A	613	SQD	O6-C1-C2	3.22	113.16	108.27
24	B	608	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
24	C	507	CLA	CBC-CAC-C3C	-3.21	103.72	112.42
26	k	102	BCR	C31-C1-C6	3.21	115.28	110.24
24	B	616	CLA	O2D-CGD-CBD	3.21	116.84	111.23
24	C	502	CLA	C3B-C4B-NB	3.21	113.39	110.53
24	B	602	CLA	C3D-C4D-ND	3.20	115.19	109.99
26	f	101	BCR	C40-C30-C29	-3.20	96.67	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C1-C2-C3	-3.20	120.96	126.20
24	B	608	CLA	CED-O2D-CGD	3.20	123.17	115.92
26	H	101	BCR	C4-C5-C6	3.20	127.02	122.70
24	B	605	CLA	C3D-C4D-ND	3.19	115.18	109.99
24	b	614	CLA	C4C-C3C-C2C	-3.19	102.24	106.89
24	C	512	CLA	C4-C3-C5	3.19	120.77	115.23
25	d	402	PHO	CMB-C2B-C3B	3.19	131.06	124.68
26	b	618	BCR	C40-C30-C29	-3.19	96.69	108.95
24	B	615	CLA	CHD-C1D-ND	-3.19	120.31	124.80
24	B	612	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
26	B	620	BCR	C30-C25-C24	3.19	124.30	115.65
25	D	401	PHO	C1-C2-C3	-3.18	120.98	126.20
31	h	102	DGD	O2G-C1B-C2B	3.18	118.36	111.48
24	C	511	CLA	CMB-C2B-C1B	3.17	130.25	125.42
26	b	619	BCR	C27-C26-C25	3.17	126.99	122.70
24	b	611	CLA	C4C-C3C-C2C	-3.17	102.27	106.89
26	k	101	BCR	C8-C9-C10	3.17	124.00	119.01
24	B	613	CLA	C4-C3-C5	3.17	120.73	115.23
24	B	613	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
24	a	407	CLA	CAC-C3C-C4C	3.17	128.91	124.79
28	L	101	SQD	O7-S-C6	3.17	111.48	106.76
29	D	409	LHG	O7-C7-C8	3.16	118.32	111.48
24	b	614	CLA	C1-C2-C3	-3.16	121.02	126.20
24	C	513	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
26	c	918	BCR	C36-C18-C19	-3.16	113.27	118.09
24	b	608	CLA	C4C-C3C-C2C	-3.15	102.30	106.89
24	b	612	CLA	C1-C2-C3	-3.15	121.03	126.20
26	A	610	BCR	C33-C5-C4	-3.15	106.88	113.60
24	b	617	CLA	C1C-C2C-C3C	-3.15	103.67	106.98
26	T	102	BCR	C34-C9-C8	-3.15	113.28	118.09
24	c	912	CLA	C3B-C4B-NB	3.14	113.34	110.53
24	B	608	CLA	CBC-CAC-C3C	-3.14	103.90	112.42
26	A	610	BCR	C33-C5-C6	3.14	127.91	124.48
24	b	616	CLA	CHD-C1D-ND	-3.14	120.39	124.80
26	k	102	BCR	C29-C30-C25	3.14	115.00	110.44
26	D	404	BCR	C3-C2-C1	3.13	125.52	114.43
24	B	612	CLA	C1-C2-C3	-3.13	121.07	126.20
24	B	607	CLA	C3B-C4B-NB	3.13	113.32	110.53
25	D	401	PHO	C4-C3-C5	3.13	120.66	115.23
24	b	602	CLA	C1-O2A-CGA	3.13	124.22	116.65
24	b	608	CLA	C3D-C4D-ND	3.13	115.07	109.99
26	a	409	BCR	C33-C5-C4	-3.12	106.94	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	404	BCR	C35-C13-C14	-3.12	117.76	122.82
24	d	401	CLA	CBC-CAC-C3C	-3.12	103.96	112.42
26	h	101	BCR	C35-C13-C14	-3.12	117.76	122.82
24	A	606	CLA	O2D-CGD-CBD	3.12	116.68	111.23
26	c	915	BCR	C37-C22-C23	-3.11	113.33	118.09
26	C	514	BCR	C37-C22-C21	-3.11	117.77	122.82
26	b	618	BCR	C38-C26-C25	3.11	127.88	124.48
31	C	518	DGD	O3G-C3G-C2G	-3.11	103.26	110.82
24	C	502	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
24	B	603	CLA	C4-C3-C5	3.10	120.61	115.23
26	C	515	BCR	C34-C9-C8	-3.10	113.35	118.09
24	C	511	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
26	C	515	BCR	C30-C25-C26	-3.10	118.40	122.64
24	c	903	CLA	C1-C2-C3	-3.10	121.12	126.20
24	B	602	CLA	O2A-CGA-CBA	3.10	121.28	111.83
24	c	904	CLA	C4C-C3C-C2C	-3.10	102.39	106.89
26	A	610	BCR	C8-C7-C6	3.10	135.27	127.00
24	b	613	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
24	b	606	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
26	B	622	BCR	C3-C4-C5	3.09	119.56	114.06
29	B	621	LHG	O7-C7-C8	3.09	118.16	111.48
24	C	504	CLA	C3C-C4C-NC	3.09	114.38	110.43
26	f	101	BCR	C34-C9-C8	-3.09	113.38	118.09
29	A	615	LHG	O8-C23-C24	3.08	121.24	111.83
26	A	610	BCR	C31-C1-C6	3.08	115.07	110.24
24	b	610	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
26	T	101	BCR	C35-C13-C12	-3.08	113.39	118.09
26	B	619	BCR	C1-C6-C5	-3.08	118.43	122.64
24	b	605	CLA	C3D-C4D-ND	3.08	114.99	109.99
24	B	616	CLA	C3D-C4D-ND	3.07	114.98	109.99
28	l	101	SQD	O7-S-C6	3.07	111.34	106.76
24	C	513	CLA	CHD-C1D-ND	-3.07	120.48	124.80
24	C	506	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
24	c	904	CLA	C3D-C4D-ND	3.07	114.98	109.99
24	B	606	CLA	CMB-C2B-C1B	3.07	130.09	125.42
24	b	608	CLA	CAC-C3C-C4C	3.07	128.78	124.79
24	c	903	CLA	CHD-C1D-ND	-3.07	120.49	124.80
31	c	916	DGD	O2G-C1B-C2B	3.07	118.11	111.48
24	C	509	CLA	CMB-C2B-C1B	3.07	130.09	125.42
24	C	509	CLA	CHD-C1D-ND	-3.06	120.49	124.80
26	K	101	BCR	C40-C30-C25	3.06	115.05	110.24
24	c	912	CLA	CHD-C1D-ND	-3.06	120.49	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	905	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
24	b	610	CLA	C3B-C4B-NB	3.05	113.26	110.53
24	B	617	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
24	C	506	CLA	C4-C3-C5	3.05	120.53	115.23
24	d	404	CLA	C3C-C4C-NC	3.05	114.34	110.43
26	f	101	BCR	C33-C5-C4	-3.05	107.09	113.60
26	f	101	BCR	C4-C5-C6	3.05	126.82	122.70
26	a	409	BCR	C38-C26-C27	-3.04	107.10	113.60
24	c	907	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
28	F	101	SQD	O48-C23-C24	3.04	121.11	111.83
28	A	613	SQD	O48-C23-C24	3.04	121.10	111.83
24	b	616	CLA	C3D-C4D-ND	3.04	114.93	109.99
24	B	615	CLA	CAC-C3C-C4C	3.04	128.74	124.79
24	b	613	CLA	C4-C3-C5	3.03	120.49	115.23
24	A	607	CLA	C4-C3-C5	3.03	120.49	115.23
27	a	410	PL9	C25-C24-C26	3.03	120.49	115.23
24	B	610	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
29	D	407	LHG	O8-C23-O10	-3.03	116.06	123.63
24	B	603	CLA	C4C-C3C-C2C	-3.03	102.49	106.89
24	a	407	CLA	CHD-C1D-ND	-3.02	120.55	124.80
27	A	611	PL9	C32-C33-C34	-3.02	120.70	127.62
24	b	603	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	a	408	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
24	c	906	CLA	CAC-C3C-C4C	3.01	128.71	124.79
24	A	607	CLA	CMC-C2C-C1C	3.01	129.74	125.03
26	k	101	BCR	C39-C30-C29	-3.01	97.40	108.95
24	c	906	CLA	C4C-C3C-C2C	-3.01	102.52	106.89
24	b	611	CLA	C3B-C4B-NB	3.00	113.21	110.53
24	b	607	CLA	C3B-C4B-NB	3.00	113.21	110.53
24	d	403	CLA	O2D-CGD-CBD	3.00	116.47	111.23
31	H	102	DGD	O1G-C1A-C2A	3.00	120.98	111.83
24	C	507	CLA	C4-C3-C5	3.00	120.43	115.23
24	b	602	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
26	H	101	BCR	C32-C1-C31	-2.99	100.06	108.63
24	C	512	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
24	c	904	CLA	C1-C2-C3	-2.99	121.30	126.20
24	c	912	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
24	C	504	CLA	CAC-C3C-C4C	2.99	128.68	124.79
24	b	605	CLA	CMC-C2C-C1C	2.98	129.70	125.03
24	c	913	CLA	CHD-C1D-ND	-2.98	120.60	124.80
26	B	622	BCR	C1-C6-C5	-2.98	118.56	122.64
24	C	503	CLA	C3D-C4D-ND	2.98	114.83	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	CAC-C3C-C4C	2.98	128.67	124.79
24	b	615	CLA	CHD-C1D-ND	-2.98	120.61	124.80
24	B	609	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
24	b	616	CLA	CMC-C2C-C1C	2.98	129.69	125.03
29	d	408	LHG	O7-C7-C8	2.98	117.92	111.48
26	c	918	BCR	C1-C6-C5	-2.97	118.57	122.64
24	B	615	CLA	CBC-CAC-C3C	-2.97	104.38	112.42
24	B	615	CLA	C4C-C3C-C2C	-2.97	102.58	106.89
26	B	618	BCR	C39-C30-C25	2.96	114.89	110.24
24	c	911	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
24	c	912	CLA	C4-C3-C5	2.96	120.37	115.23
26	a	409	BCR	C33-C5-C6	2.96	127.72	124.48
24	B	607	CLA	O1D-CGD-CBD	-2.96	118.68	124.52
26	T	102	BCR	C37-C22-C21	-2.96	118.02	122.82
24	C	513	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
24	c	908	CLA	C3D-C4D-ND	2.96	114.79	109.99
24	B	617	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
24	C	501	CLA	CMB-C2B-C1B	2.95	129.91	125.42
24	B	616	CLA	CMB-C2B-C1B	2.95	129.91	125.42
24	c	902	CLA	CMB-C2B-C1B	2.95	129.91	125.42
24	B	604	CLA	C4-C3-C5	2.95	120.35	115.23
24	C	505	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
26	b	618	BCR	C32-C1-C6	2.94	114.86	110.24
24	B	605	CLA	CMB-C2B-C1B	2.94	129.90	125.42
24	C	504	CLA	C4-C3-C5	2.94	120.33	115.23
25	A	608	PHO	C4B-NB-C1B	-2.94	104.53	108.82
24	a	406	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
24	A	606	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
26	H	101	BCR	C39-C30-C29	-2.93	97.69	108.95
24	B	611	CLA	CHD-C1D-ND	-2.93	120.68	124.80
24	c	909	CLA	CHD-C1D-ND	-2.93	120.68	124.80
29	d	408	LHG	O8-C23-C24	2.93	120.77	111.83
26	h	101	BCR	C27-C26-C25	2.93	126.67	122.70
26	B	620	BCR	C39-C30-C25	2.93	114.83	110.24
24	C	503	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
24	B	612	CLA	CMC-C2C-C1C	2.92	129.60	125.03
31	H	102	DGD	O2G-C1B-C2B	2.92	117.79	111.48
24	c	913	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
25	a	412	PHO	C4-C3-C5	2.91	120.28	115.23
24	D	403	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
26	T	101	BCR	C29-C30-C25	2.91	114.67	110.44
24	c	907	CLA	CED-O2D-CGD	2.91	122.52	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	618	BCR	C2-C1-C6	2.91	114.66	110.44
26	K	101	BCR	C31-C1-C2	-2.91	97.79	108.95
24	B	608	CLA	O2D-CGD-CBD	2.91	116.31	111.23
24	c	908	CLA	C4-C3-C5	2.91	120.27	115.23
24	a	407	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
28	a	402	SQD	O48-C23-C24	2.90	120.69	111.83
24	B	611	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	c	906	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	C	505	CLA	CMC-C2C-C1C	2.90	129.57	125.03
28	A	612	SQD	C45-O47-C7	-2.90	110.86	117.80
31	H	102	DGD	O1G-C1A-O1A	-2.90	116.38	123.63
25	d	402	PHO	O2D-CGD-O1D	-2.90	118.21	123.85
25	D	401	PHO	CMB-C2B-C3B	2.89	130.47	124.68
24	C	511	CLA	CHD-C1D-ND	-2.89	120.73	124.80
24	b	605	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
28	A	613	SQD	O9-S-C6	2.89	111.07	106.76
24	c	914	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
24	b	609	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
24	C	504	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
26	C	514	BCR	C39-C30-C29	-2.88	97.89	108.95
24	c	910	CLA	CHD-C1D-ND	-2.88	120.75	124.80
26	b	619	BCR	C1-C6-C5	-2.88	118.70	122.64
26	f	101	BCR	C37-C22-C23	-2.88	113.69	118.09
24	B	605	CLA	C4C-C3C-C2C	-2.88	102.71	106.89
24	B	607	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
24	B	603	CLA	C3B-C4B-NB	2.87	113.09	110.53
26	Y	101	BCR	C35-C13-C12	-2.87	113.70	118.09
24	C	509	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
24	b	616	CLA	C4C-C3C-C2C	-2.86	102.72	106.89
24	c	902	CLA	C4-C3-C5	2.86	120.20	115.23
25	A	608	PHO	O1D-CGD-CBD	-2.86	120.38	124.72
26	K	101	BCR	C29-C30-C25	2.86	114.59	110.44
28	a	402	SQD	O9-S-C6	2.86	111.03	106.76
24	b	612	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
26	D	404	BCR	C2-C1-C6	2.86	114.59	110.44
24	a	406	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
24	B	605	CLA	CHD-C1D-ND	-2.86	120.78	124.80
27	A	611	PL9	C30-C29-C31	2.86	120.18	115.23
24	b	611	CLA	CHD-C1D-ND	-2.85	120.79	124.80
24	b	602	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
24	C	502	CLA	CMB-C2B-C1B	2.85	129.76	125.42
27	A	611	PL9	C25-C24-C26	2.85	120.17	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	C3B-C4B-NB	2.85	113.07	110.53
24	C	512	CLA	CHD-C1D-ND	-2.84	120.80	124.80
24	b	616	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	c	907	CLA	CMB-C2B-C1B	2.84	129.75	125.42
24	C	506	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
24	a	407	CLA	CBC-CAC-C3C	-2.84	104.72	112.42
24	B	609	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
24	b	609	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
28	l	101	SQD	O48-C23-C24	2.83	120.47	111.83
24	B	607	CLA	C4-C3-C5	2.83	120.14	115.23
24	A	614	CLA	C4-C3-C5	2.83	120.14	115.23
24	c	906	CLA	C3B-C4B-NB	2.83	113.05	110.53
26	T	101	BCR	C23-C24-C25	2.83	134.55	127.00
24	c	910	CLA	C4-C3-C5	2.83	120.13	115.23
28	a	411	SQD	C1-O5-C5	-2.83	108.20	113.72
27	A	611	PL9	C7-C3-C4	2.83	119.24	116.91
24	d	403	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
24	b	612	CLA	CBC-CAC-C3C	-2.82	104.77	112.42
26	A	610	BCR	C29-C30-C25	2.82	114.53	110.44
26	B	619	BCR	C1-C6-C7	2.82	123.30	115.65
24	C	510	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
24	b	603	CLA	C3B-C4B-NB	2.82	113.05	110.53
28	L	101	SQD	O48-C23-C24	2.82	120.42	111.83
26	K	101	BCR	C37-C22-C23	-2.82	113.79	118.09
24	c	908	CLA	C3B-C4B-NB	2.81	113.04	110.53
26	h	101	BCR	C37-C22-C23	-2.81	113.79	118.09
24	a	408	CLA	CAC-C3C-C4C	2.81	128.45	124.79
27	D	405	PL9	C53-C6-C1	2.81	121.03	115.28
24	b	613	CLA	C1-C2-C3	-2.81	121.60	126.20
27	A	611	PL9	C15-C14-C16	2.80	120.10	115.23
24	B	603	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
28	l	101	SQD	C1-O5-C5	-2.80	108.25	113.72
24	c	908	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
24	A	606	CLA	CAC-C3C-C4C	2.80	128.44	124.79
24	c	913	CLA	C1-O2A-CGA	2.80	123.43	116.65
24	b	612	CLA	CHD-C1D-ND	-2.80	120.86	124.80
26	T	101	BCR	C1-C6-C5	-2.80	118.81	122.64
24	D	402	CLA	CAC-C3C-C4C	2.80	128.43	124.79
24	B	614	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
24	C	507	CLA	C3D-C4D-ND	2.80	114.53	109.99
24	b	607	CLA	C4-C3-C5	2.79	120.08	115.23
24	C	502	CLA	O2D-CGD-O1D	-2.79	118.41	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	C1-C2-C3	-2.79	121.63	126.20
24	b	616	CLA	CAC-C3C-C4C	2.79	128.42	124.79
28	a	411	SQD	O5-C1-C2	-2.79	104.64	110.37
26	C	515	BCR	C23-C24-C25	2.79	134.44	127.00
24	c	903	CLA	CAC-C3C-C4C	2.79	128.41	124.79
26	Y	101	BCR	C39-C30-C29	-2.79	98.25	108.95
24	a	407	CLA	C4-C3-C5	2.78	120.06	115.23
24	b	617	CLA	O1D-CGD-CBD	-2.78	119.03	124.52
24	b	604	CLA	CMC-C2C-C1C	2.78	129.38	125.03
24	B	609	CLA	O2A-CGA-CBA	2.78	120.32	111.83
24	c	912	CLA	C1-O2A-CGA	2.78	123.38	116.65
24	B	608	CLA	C4-C3-C5	2.78	120.05	115.23
24	b	607	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
24	b	603	CLA	C4-C3-C5	2.78	120.05	115.23
25	D	401	PHO	O1D-CGD-CBD	-2.77	120.52	124.72
24	b	617	CLA	O2A-CGA-CBA	2.77	120.29	111.83
26	c	918	BCR	C30-C25-C26	-2.77	118.85	122.64
24	b	615	CLA	CED-O2D-CGD	2.77	122.20	115.92
26	h	101	BCR	C40-C30-C39	-2.77	100.71	108.63
24	B	613	CLA	CED-O2D-CGD	2.77	122.19	115.92
26	B	618	BCR	C4-C5-C6	2.76	126.44	122.70
24	b	602	CLA	CMB-C2B-C1B	2.76	129.62	125.42
31	j	101	DGD	O1G-C1A-C2A	2.76	120.24	111.83
24	c	904	CLA	C3B-C4B-NB	2.75	112.99	110.53
26	c	918	BCR	C39-C30-C29	-2.75	98.38	108.95
27	a	410	PL9	C37-C38-C39	-2.75	121.33	127.62
24	B	613	CLA	C3B-C4B-NB	2.75	112.98	110.53
24	b	610	CLA	CMB-C2B-C1B	2.75	129.60	125.42
26	B	618	BCR	C39-C30-C29	-2.75	98.41	108.95
24	b	615	CLA	CMB-C2B-C1B	2.75	129.60	125.42
26	k	102	BCR	C4-C5-C6	2.74	126.41	122.70
28	d	407	SQD	C44-O6-C1	-2.74	107.91	113.80
24	B	611	CLA	O2A-CGA-CBA	2.74	120.20	111.83
24	c	912	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
24	A	607	CLA	CBC-CAC-C3C	-2.74	104.99	112.42
24	A	614	CLA	CAC-C3C-C4C	2.74	128.35	124.79
27	d	405	PL9	C53-C6-C1	2.74	120.89	115.28
24	b	607	CLA	C1-C2-C3	-2.74	121.71	126.20
24	c	909	CLA	CMB-C2B-C1B	2.74	129.59	125.42
24	b	615	CLA	O2A-CGA-CBA	2.74	120.18	111.83
26	f	101	BCR	C35-C13-C12	-2.74	113.91	118.09
31	h	102	DGD	O1G-C1A-C2A	2.74	120.18	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	O2D-CGD-CBD	2.74	116.01	111.23
32	V	202	HEM	C1B-NB-C4B	2.73	108.44	105.21
24	B	617	CLA	O2A-CGA-CBA	2.73	120.17	111.83
24	B	602	CLA	C4C-C3C-C2C	-2.73	102.91	106.89
28	d	407	SQD	O48-C23-C24	2.73	120.16	111.83
27	A	611	PL9	C53-C6-C1	2.73	120.86	115.28
24	B	606	CLA	CHD-C1D-ND	-2.73	120.96	124.80
24	b	606	CLA	C3B-C4B-NB	2.73	112.96	110.53
24	d	401	CLA	CHD-C4C-C3C	-2.73	120.80	124.77
28	d	407	SQD	O9-S-C6	2.73	110.83	106.76
24	b	609	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
24	b	603	CLA	C4C-C3C-C2C	-2.72	102.92	106.89
24	b	607	CLA	O1D-CGD-CBD	-2.72	119.15	124.52
24	C	501	CLA	CAC-C3C-C4C	2.72	128.33	124.79
24	b	613	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	B	605	CLA	C4-C3-C5	2.72	119.95	115.23
24	B	607	CLA	CMB-C2B-C1B	2.72	129.56	125.42
24	B	607	CLA	C1-C2-C3	-2.72	121.74	126.20
24	C	504	CLA	C1-O2A-CGA	2.72	123.23	116.65
24	a	408	CLA	CMC-C2C-C1C	2.72	129.28	125.03
24	C	510	CLA	CHD-C4C-C3C	-2.72	120.81	124.77
24	b	615	CLA	CAC-C3C-C4C	2.72	128.32	124.79
24	B	602	CLA	CMC-C2C-C1C	2.72	129.28	125.03
27	A	611	PL9	C35-C34-C36	2.71	119.94	115.23
24	C	511	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
31	D	406	DGD	O5D-C1E-C2E	2.71	112.39	108.27
24	B	612	CLA	CAC-C3C-C4C	2.71	128.32	124.79
31	c	917	DGD	O2G-C1B-C2B	2.71	117.34	111.48
24	B	602	CLA	CMB-C2B-C1B	2.71	129.54	125.42
31	d	406	DGD	O1G-C1A-C2A	2.71	120.09	111.83
24	c	904	CLA	C4-C3-C5	2.71	119.92	115.23
25	D	401	PHO	C4B-NB-C1B	-2.70	104.88	108.82
24	C	508	CLA	C4-C3-C5	2.70	119.91	115.23
27	a	410	PL9	C35-C34-C36	2.69	119.90	115.23
26	B	619	BCR	C34-C9-C10	-2.69	118.46	122.82
27	A	611	PL9	C37-C38-C39	-2.69	121.46	127.62
24	B	610	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
24	B	615	CLA	CMB-C2B-C1B	2.69	129.51	125.42
26	C	514	BCR	C39-C30-C25	2.69	114.45	110.24
24	b	612	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
28	F	101	SQD	O7-S-C6	2.69	110.77	106.76
24	B	602	CLA	C4D-C3D-CAD	2.68	111.02	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	CAC-C3C-C4C	2.68	128.28	124.79
24	c	910	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
24	c	909	CLA	C4-C3-C5	2.68	119.88	115.23
24	c	910	CLA	C4D-C3D-CAD	2.68	111.01	108.11
26	B	622	BCR	C31-C1-C2	-2.68	98.68	108.95
24	c	911	CLA	C4D-C3D-CAD	2.68	111.01	108.11
24	A	609	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
24	A	606	CLA	CHD-C1D-ND	-2.67	121.04	124.80
28	L	101	SQD	C4-C3-C2	2.67	115.52	110.83
31	D	406	DGD	O1G-C1A-C2A	2.67	119.98	111.83
26	c	918	BCR	C40-C30-C25	2.67	114.43	110.24
24	B	610	CLA	C1-C2-C3	-2.67	121.82	126.20
27	a	410	PL9	C20-C19-C21	2.67	119.86	115.23
31	C	518	DGD	O1G-C1A-C2A	2.67	119.98	111.83
24	D	403	CLA	CAC-C3C-C4C	2.67	128.26	124.79
24	B	609	CLA	CAC-C3C-C4C	2.66	128.26	124.79
24	B	608	CLA	C4C-C3C-C2C	-2.66	103.02	106.89
24	C	501	CLA	C1-O2A-CGA	2.66	123.09	116.65
26	K	101	BCR	C34-C9-C8	-2.66	114.02	118.09
25	A	608	PHO	CMB-C2B-C3B	2.66	130.00	124.68
24	B	609	CLA	O1D-CGD-CBD	-2.66	119.28	124.52
26	B	622	BCR	C30-C25-C26	-2.66	119.01	122.64
24	B	604	CLA	C4C-C3C-C2C	-2.66	103.03	106.89
24	c	905	CLA	CAC-C3C-C4C	2.66	128.25	124.79
25	d	402	PHO	O1D-CGD-CBD	-2.65	120.70	124.72
24	c	911	CLA	C4-C3-C5	2.65	119.83	115.23
26	f	101	BCR	C3-C2-C1	2.65	123.80	114.43
31	C	517	DGD	O2G-C1B-O1B	-2.65	117.52	123.70
26	c	918	BCR	C8-C9-C10	2.64	123.17	119.01
24	b	614	CLA	CAC-C3C-C4C	2.64	128.23	124.79
28	A	612	SQD	O8-S-C6	2.64	111.07	105.97
27	a	410	PL9	C30-C29-C31	2.64	119.81	115.23
26	D	404	BCR	C30-C25-C24	2.64	122.81	115.65
27	a	410	PL9	C40-C39-C41	2.64	119.81	115.23
26	B	620	BCR	C40-C30-C39	-2.64	101.08	108.63
24	C	505	CLA	C3B-C4B-NB	2.64	112.89	110.53
24	B	612	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
26	K	101	BCR	C33-C5-C6	2.64	127.36	124.48
26	h	101	BCR	C30-C25-C24	2.64	122.80	115.65
24	C	507	CLA	C3B-C4B-NB	2.64	112.88	110.53
24	C	510	CLA	CMC-C2C-C1C	2.64	129.15	125.03
24	c	913	CLA	C4-C3-C5	2.64	119.80	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	602	CLA	CMC-C2C-C1C	2.64	129.15	125.03
24	A	609	CLA	CMB-C2B-C1B	2.64	129.43	125.42
24	b	608	CLA	CED-O2D-CGD	2.64	121.89	115.92
24	c	906	CLA	CMC-C2C-C1C	2.63	129.15	125.03
24	B	612	CLA	CHD-C4C-C3C	-2.63	120.93	124.77
27	A	611	PL9	C40-C39-C41	2.63	119.80	115.23
24	c	914	CLA	O2A-CGA-CBA	2.63	119.86	111.83
27	a	410	PL9	C53-C6-C1	2.63	120.67	115.28
32	v	202	HEM	C1B-NB-C4B	2.63	108.32	105.21
24	b	605	CLA	O2A-CGA-CBA	2.63	119.86	111.83
24	c	914	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
28	a	402	SQD	O6-C1-C2	2.63	112.26	108.27
24	d	404	CLA	CMB-C2B-C1B	2.63	129.42	125.42
24	D	402	CLA	C4-C3-C5	2.62	119.78	115.23
24	b	612	CLA	CMC-C2C-C1C	2.62	129.13	125.03
24	b	615	CLA	CBC-CAC-C3C	-2.62	105.33	112.42
26	H	101	BCR	C29-C28-C27	-2.62	105.53	111.28
24	C	507	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
26	T	101	BCR	C37-C22-C23	-2.61	114.10	118.09
24	A	606	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
24	A	609	CLA	CAC-C3C-C4C	2.61	128.18	124.79
24	D	403	CLA	CED-O2D-CGD	2.61	121.83	115.92
24	b	617	CLA	CED-O2D-CGD	2.61	121.83	115.92
26	H	101	BCR	C39-C30-C25	2.60	114.33	110.24
24	b	608	CLA	C4B-C3B-C2B	-2.60	104.06	107.30
24	C	509	CLA	CAC-C3C-C4C	2.60	128.18	124.79
24	c	908	CLA	O2A-CGA-CBA	2.60	119.77	111.83
24	b	613	CLA	CMB-C2B-C1B	2.60	129.38	125.42
26	C	515	BCR	C1-C6-C5	-2.60	119.08	122.64
24	c	903	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
24	D	403	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
26	B	622	BCR	C1-C6-C7	2.60	122.69	115.65
24	b	607	CLA	C1-O2A-CGA	2.60	122.94	116.65
24	b	615	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
24	C	512	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
24	d	401	CLA	C4-C3-C5	2.59	119.73	115.23
24	C	507	CLA	O1D-CGD-CBD	-2.59	119.40	124.52
24	B	603	CLA	C1-C2-C3	-2.59	121.95	126.20
24	C	511	CLA	C4-C3-C5	2.59	119.72	115.23
27	a	410	PL9	C32-C33-C34	-2.59	121.70	127.62
24	C	503	CLA	C4-C3-C5	2.59	119.72	115.23
26	k	102	BCR	C30-C25-C24	2.59	122.66	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	CMB-C2B-C1B	2.58	129.35	125.42
28	a	402	SQD	C3-C4-C5	2.58	114.91	110.23
24	C	501	CLA	CBC-CAC-C3C	-2.58	105.43	112.42
28	a	411	SQD	O48-C23-C24	2.58	119.69	111.83
24	d	404	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
24	b	605	CLA	CED-O2D-CGD	2.57	121.75	115.92
24	d	401	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
32	v	202	HEM	C3B-C4B-NB	-2.57	107.62	109.47
24	b	614	CLA	CHD-C4C-C3C	-2.57	121.03	124.77
24	d	404	CLA	O1D-CGD-CBD	-2.56	119.46	124.52
24	C	502	CLA	C4-C3-C5	2.56	119.68	115.23
24	b	602	CLA	O1D-CGD-CBD	-2.56	119.46	124.52
28	A	612	SQD	C44-O6-C1	-2.56	108.30	113.80
24	C	503	CLA	C3B-C4B-NB	2.56	112.82	110.53
28	F	101	SQD	O9-S-C6	2.56	110.58	106.76
24	C	506	CLA	CAC-C3C-C4C	2.56	128.12	124.79
24	c	902	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
26	B	618	BCR	C2-C3-C4	2.56	116.90	111.28
24	D	402	CLA	CHD-C4C-C3C	-2.56	121.05	124.77
24	A	609	CLA	CED-O2D-CGD	2.55	121.70	115.92
31	C	516	DGD	O3G-C3G-C2G	-2.55	104.61	110.82
26	B	620	BCR	C1-C6-C5	-2.55	119.15	122.64
24	C	509	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
26	H	101	BCR	C30-C25-C24	2.55	122.56	115.65
24	c	913	CLA	O2A-CGA-CBA	2.55	119.60	111.83
24	c	907	CLA	C4D-C3D-CAD	2.55	110.87	108.11
24	b	604	CLA	C4C-C3C-C2C	-2.55	103.19	106.89
26	B	619	BCR	C4-C5-C6	2.54	126.14	122.70
26	c	918	BCR	C27-C26-C25	2.54	126.14	122.70
24	b	611	CLA	CMB-C2B-C1B	2.54	129.29	125.42
26	B	618	BCR	C1-C6-C5	-2.54	119.16	122.64
24	C	509	CLA	O2A-CGA-CBA	2.54	119.58	111.83
24	C	513	CLA	CMC-C2C-C1C	2.54	129.00	125.03
32	v	202	HEM	C2A-C1A-NA	-2.54	107.34	110.15
24	B	616	CLA	C4-C3-C5	2.53	119.63	115.23
24	B	614	CLA	CHD-C4C-C3C	-2.53	121.08	124.77
26	b	619	BCR	C37-C22-C23	-2.53	114.22	118.09
26	b	618	BCR	C40-C30-C39	-2.53	101.39	108.63
24	c	902	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
24	C	501	CLA	CMC-C2C-C1C	2.53	128.99	125.03
29	a	413	LHG	O8-C23-C24	2.53	119.54	111.83
24	B	614	CLA	O2D-CGD-O1D	-2.53	118.93	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	101	BCR	C3-C4-C5	2.53	118.56	114.06
24	b	603	CLA	O2A-CGA-CBA	2.53	119.53	111.83
24	b	613	CLA	O2A-CGA-CBA	2.52	119.53	111.83
27	A	611	PL9	C10-C9-C11	2.52	119.60	115.23
24	C	509	CLA	C4D-C3D-CAD	2.52	110.84	108.11
24	c	902	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
26	K	101	BCR	C34-C9-C10	-2.52	118.73	122.82
24	c	909	CLA	C1-C2-C3	-2.52	122.07	126.20
28	a	411	SQD	C44-O6-C1	-2.52	108.40	113.80
26	K	101	BCR	C4-C5-C6	2.52	126.11	122.70
27	D	405	PL9	C7-C3-C4	2.52	118.98	116.91
28	A	612	SQD	C1-O5-C5	-2.52	108.81	113.72
24	C	512	CLA	O2A-CGA-CBA	2.51	119.49	111.83
26	k	101	BCR	C32-C1-C6	2.51	114.17	110.24
24	B	611	CLA	C4-C3-C5	2.51	119.58	115.23
29	D	407	LHG	O7-C7-C8	2.50	116.90	111.48
26	T	101	BCR	C38-C26-C25	2.50	127.22	124.48
29	d	410	LHG	O8-C23-C24	2.50	119.46	111.83
25	a	412	PHO	C4D-CHA-CBD	2.50	109.66	108.45
24	B	615	CLA	C1-O2A-CGA	2.50	122.71	116.65
24	D	402	CLA	CMC-C2C-C1C	2.50	128.94	125.03
24	C	512	CLA	C3B-C4B-NB	2.50	112.76	110.53
24	b	614	CLA	O2A-CGA-CBA	2.50	119.45	111.83
26	B	620	BCR	C31-C1-C6	2.50	114.16	110.24
24	b	613	CLA	CMC-C2C-C1C	2.50	128.93	125.03
25	A	608	PHO	CMA-C3A-C4A	-2.50	109.23	114.61
24	c	908	CLA	CBC-CAC-C3C	-2.49	105.66	112.42
24	B	610	CLA	CMB-C2B-C1B	2.49	129.22	125.42
24	b	607	CLA	CMB-C2B-C1B	2.49	129.22	125.42
24	a	406	CLA	O2D-CGD-CBD	2.49	115.59	111.23
25	a	412	PHO	CMB-C2B-C3B	2.49	129.67	124.68
24	C	501	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
24	C	503	CLA	CMC-C2C-C1C	2.49	128.93	125.03
24	b	609	CLA	C4-C3-C5	2.49	119.55	115.23
24	b	606	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
24	B	614	CLA	C4-C3-C5	2.49	119.54	115.23
26	T	101	BCR	C1-C6-C7	2.48	122.39	115.65
24	c	907	CLA	CMD-C2D-C3D	-2.48	121.99	127.69
24	b	605	CLA	CHD-C1D-ND	-2.48	121.31	124.80
26	A	610	BCR	C34-C9-C10	-2.48	118.80	122.82
26	C	515	BCR	C27-C26-C25	2.48	126.06	122.70
24	B	606	CLA	C3B-C4B-NB	2.48	112.75	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C3B-C4B-NB	2.48	112.75	110.53
24	c	908	CLA	CMC-C2C-C1C	2.48	128.91	125.03
26	T	101	BCR	C40-C30-C25	2.48	114.13	110.24
26	T	101	BCR	C37-C22-C21	-2.48	118.80	122.82
24	B	617	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
24	D	403	CLA	C4-C3-C5	2.48	119.53	115.23
24	A	607	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
24	B	613	CLA	CMC-C2C-C1C	2.47	128.90	125.03
24	b	603	CLA	C1-C2-C3	-2.47	122.15	126.20
24	c	906	CLA	CED-O2D-CGD	2.47	121.52	115.92
24	B	602	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
24	b	614	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
24	C	513	CLA	O2A-CGA-CBA	2.47	119.37	111.83
24	d	403	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
24	c	914	CLA	CMC-C2C-C1C	2.47	128.89	125.03
26	f	101	BCR	C28-C27-C26	2.46	118.45	114.06
24	B	607	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
25	D	401	PHO	CED-O2D-CGD	2.46	121.50	115.92
24	c	913	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
29	d	410	LHG	O4-P-O5	2.46	123.88	112.44
24	b	604	CLA	C5-C3-C2	-2.46	115.65	121.17
24	c	903	CLA	CMB-C2B-C1B	2.46	129.16	125.42
24	B	607	CLA	O2A-CGA-CBA	2.46	119.33	111.83
25	a	412	PHO	C1-C2-C3	-2.46	122.17	126.20
26	B	618	BCR	C37-C22-C21	-2.46	118.84	122.82
24	C	507	CLA	CMB-C2B-C1B	2.45	129.16	125.42
24	b	603	CLA	C1-O2A-CGA	2.45	122.58	116.65
24	B	609	CLA	C4B-C3B-C2B	-2.45	104.25	107.30
24	B	602	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
25	A	608	PHO	CBC-CAC-C3C	-2.45	109.37	112.87
24	a	408	CLA	C1-C2-C3	-2.45	122.19	126.20
27	D	405	PL9	C7-C3-C2	-2.44	120.51	123.39
24	B	604	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
24	D	402	CLA	CHB-C1B-C2B	-2.44	120.35	127.43
24	c	913	CLA	C3B-C4B-NB	2.44	112.71	110.53
24	B	612	CLA	CMB-C2B-C1B	2.44	129.13	125.42
24	B	602	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
24	C	512	CLA	CED-O2D-CGD	2.43	121.44	115.92
32	v	202	HEM	C3B-C2B-C1B	2.43	108.24	106.41
24	C	506	CLA	C3B-C4B-NB	2.43	112.70	110.53
24	A	607	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
26	B	620	BCR	C32-C1-C2	-2.43	99.62	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
24	b	613	CLA	CHD-C4C-C3C	-2.43	121.23	124.77
24	B	614	CLA	O2A-CGA-CBA	2.43	119.23	111.83
26	T	101	BCR	C3-C4-C5	2.43	118.38	114.06
25	d	402	PHO	C4B-NB-C1B	-2.43	105.28	108.82
24	A	609	CLA	CMC-C2C-C1C	2.43	128.82	125.03
24	C	510	CLA	CAC-C3C-C4C	2.43	127.94	124.79
24	B	617	CLA	C1-O2A-CGA	2.42	122.52	116.65
24	B	606	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
24	c	910	CLA	CMC-C2C-C1C	2.42	128.82	125.03
26	h	101	BCR	C28-C29-C30	2.42	123.00	114.43
26	T	101	BCR	C32-C1-C6	2.42	114.04	110.24
24	C	511	CLA	CAC-C3C-C4C	2.42	127.94	124.79
24	b	613	CLA	CED-O2D-CGD	2.42	121.40	115.92
26	H	101	BCR	C28-C29-C30	2.42	122.98	114.43
24	b	609	CLA	CAC-C3C-C4C	2.42	127.93	124.79
24	a	408	CLA	CHD-C4C-C3C	-2.41	121.25	124.77
28	a	411	SQD	O8-S-C6	2.41	110.63	105.97
26	Y	101	BCR	C30-C25-C24	2.41	122.19	115.65
24	C	513	CLA	CAC-C3C-C4C	2.41	127.93	124.79
24	a	408	CLA	C4-C3-C5	2.41	119.41	115.23
24	A	614	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
24	b	604	CLA	CAC-C3C-C4C	2.41	127.93	124.79
24	B	614	CLA	CBC-CAC-C3C	-2.41	105.88	112.42
24	b	616	CLA	C4-C3-C5	2.41	119.41	115.23
24	a	408	CLA	O2A-CGA-CBA	2.41	119.18	111.83
24	b	611	CLA	O2A-CGA-CBA	2.41	119.18	111.83
29	d	409	LHG	O8-C23-C24	2.41	119.17	111.83
24	C	505	CLA	CED-O2D-CGD	2.41	121.38	115.92
26	K	101	BCR	C1-C6-C5	-2.40	119.35	122.64
24	C	504	CLA	C4B-C3B-C2B	-2.40	104.31	107.30
32	e	101	HEM	CHC-C1C-NC	2.40	127.07	124.45
24	b	615	CLA	CHB-C4A-NA	2.40	127.86	124.40
32	E	101	HEM	CMD-C2D-C1D	2.40	128.79	125.03
29	D	408	LHG	O8-C23-C24	2.40	119.16	111.83
24	C	507	CLA	CMC-C2C-C1C	2.40	128.78	125.03
24	c	910	CLA	CED-O2D-CGD	2.40	121.36	115.92
24	b	615	CLA	O2A-CGA-O1A	-2.40	117.64	123.63
24	C	512	CLA	CAC-C3C-C4C	2.40	127.91	124.79
24	a	406	CLA	C7-C6-C5	-2.39	106.88	113.26
24	C	512	CLA	C1-O2A-CGA	2.39	122.44	116.65
24	B	614	CLA	C1-C2-C3	-2.39	122.28	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	401	PHO	O2D-CGD-O1D	-2.39	119.19	123.85
31	D	406	DGD	O6D-C5D-C6D	2.39	111.43	106.69
24	c	914	CLA	C4D-C3D-CAD	2.39	110.70	108.11
26	f	101	BCR	C1-C6-C5	-2.39	119.37	122.64
24	B	610	CLA	CED-O2D-CGD	2.39	121.33	115.92
24	C	513	CLA	C4-C3-C5	2.39	119.37	115.23
24	c	904	CLA	C4D-CHA-C1A	2.38	124.09	121.24
31	c	917	DGD	O1G-C1A-C2A	2.38	119.10	111.83
24	C	502	CLA	CMC-C2C-C1C	2.38	128.76	125.03
24	b	602	CLA	C4D-C3D-CAD	2.38	110.69	108.11
24	b	614	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
24	A	607	CLA	C4C-C3C-C2C	-2.38	103.43	106.89
24	d	404	CLA	C4C-C3C-C2C	-2.38	103.43	106.89
24	B	604	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
24	c	910	CLA	C1-O2A-CGA	2.37	122.40	116.65
24	C	509	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
26	k	102	BCR	C31-C1-C2	-2.37	99.84	108.95
24	B	612	CLA	CBC-CAC-C3C	-2.37	105.99	112.42
24	c	908	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
24	b	608	CLA	C1-C2-C3	-2.37	122.32	126.20
27	D	405	PL9	C27-C28-C29	-2.37	122.21	127.62
24	B	602	CLA	C3B-C4B-NB	2.36	112.64	110.53
24	c	911	CLA	CAC-C3C-C4C	2.36	127.86	124.79
24	C	513	CLA	C4D-C3D-CAD	2.36	110.67	108.11
27	A	611	PL9	C45-C44-C46	2.36	119.33	115.23
24	b	607	CLA	CAC-C3C-C4C	2.36	127.86	124.79
26	C	514	BCR	C3-C4-C5	2.36	118.26	114.06
31	h	102	DGD	O1G-C1A-O1A	-2.36	117.73	123.63
24	d	401	CLA	C1-O2A-CGA	2.36	122.36	116.65
31	D	406	DGD	O6E-C5E-C6E	2.36	112.28	106.44
24	c	913	CLA	C1-C2-C3	-2.36	122.34	126.20
24	C	513	CLA	CHD-C4C-NC	-2.36	120.58	124.23
24	c	912	CLA	CMB-C2B-C1B	2.35	129.00	125.42
24	d	403	CLA	O2A-CGA-CBA	2.35	119.01	111.83
24	a	407	CLA	C1-C2-C3	-2.35	122.34	126.20
24	D	403	CLA	CMB-C2B-C1B	2.35	129.00	125.42
24	B	611	CLA	CHB-C4A-NA	2.35	127.79	124.40
31	c	916	DGD	O3G-C3G-C2G	-2.34	105.12	110.82
31	j	101	DGD	O1G-C1A-O1A	-2.34	117.77	123.63
26	k	101	BCR	C1-C6-C7	2.34	122.00	115.65
24	C	508	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
26	k	101	BCR	C31-C1-C2	-2.34	99.96	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	CHD-C4C-C3C	-2.34	121.36	124.77
24	b	605	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
24	A	609	CLA	O2A-CGA-CBA	2.34	118.97	111.83
24	C	510	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
24	b	610	CLA	C7-C6-C5	-2.34	107.03	113.26
24	C	510	CLA	O2A-CGA-CBA	2.34	118.97	111.83
31	D	406	DGD	O2G-C1B-O1B	-2.34	118.24	123.70
26	C	515	BCR	C37-C22-C23	-2.34	114.52	118.09
24	C	508	CLA	CAC-C3C-C4C	2.34	127.83	124.79
24	C	510	CLA	C4B-C3B-C2B	-2.34	104.40	107.30
29	d	408	LHG	O8-C23-O10	-2.34	117.79	123.63
24	a	406	CLA	CHC-C1C-C2C	-2.33	120.31	126.95
24	C	504	CLA	CMC-C2C-C1C	2.33	128.68	125.03
24	d	401	CLA	CMB-C2B-C1B	2.33	128.97	125.42
26	a	409	BCR	C1-C6-C5	-2.33	119.45	122.64
24	b	602	CLA	CED-O2D-CGD	2.33	121.20	115.92
24	A	614	CLA	CMC-C2C-C1C	2.33	128.67	125.03
24	c	905	CLA	C7-C6-C5	-2.33	107.06	113.26
24	A	614	CLA	C4C-C3C-C2C	-2.33	103.50	106.89
26	k	101	BCR	C30-C25-C24	2.33	121.96	115.65
24	d	404	CLA	C4-C3-C5	2.33	119.27	115.23
24	d	404	CLA	C1-O2A-CGA	2.32	122.28	116.65
24	B	605	CLA	CAC-C3C-C4C	2.32	127.81	124.79
26	T	102	BCR	C34-C9-C10	-2.32	119.05	122.82
26	b	618	BCR	C1-C6-C7	2.32	121.95	115.65
26	B	619	BCR	C29-C28-C27	-2.32	106.17	111.28
24	c	911	CLA	O2A-CGA-CBA	2.32	118.91	111.83
27	d	405	PL9	C15-C14-C16	2.32	119.25	115.23
24	c	906	CLA	CBC-CAC-C3C	-2.32	106.14	112.42
26	c	915	BCR	C40-C30-C29	-2.32	100.05	108.95
24	B	603	CLA	C1-O2A-CGA	2.32	122.26	116.65
26	B	622	BCR	C27-C26-C25	2.32	125.83	122.70
24	A	609	CLA	C1-O2A-CGA	2.32	122.26	116.65
28	A	612	SQD	O48-C23-C24	2.32	118.90	111.83
24	a	407	CLA	C1-O2A-CGA	2.32	122.26	116.65
24	a	406	CLA	CHD-C4C-NC	-2.32	120.64	124.23
24	c	905	CLA	C4B-C3B-C2B	-2.31	104.42	107.30
24	A	614	CLA	CHD-C4C-C3C	-2.31	121.40	124.77
24	c	909	CLA	CED-O2D-CGD	2.31	121.16	115.92
24	d	403	CLA	CHD-C4C-C3C	-2.31	121.40	124.77
24	B	603	CLA	CED-O2D-CGD	2.31	121.15	115.92
24	B	613	CLA	O2D-CGD-O1D	-2.31	119.35	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	905	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
24	c	904	CLA	CAC-C3C-C4C	2.31	127.79	124.79
24	b	611	CLA	C4-C3-C5	2.31	119.23	115.23
24	B	616	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
26	D	404	BCR	C37-C22-C23	-2.30	114.57	118.09
26	b	619	BCR	C32-C1-C2	-2.30	100.10	108.95
24	c	903	CLA	O2A-CGA-CBA	2.30	118.86	111.83
24	B	605	CLA	O2A-CGA-CBA	2.30	118.86	111.83
24	C	504	CLA	C4C-C3C-C2C	-2.30	103.54	106.89
24	c	914	CLA	CED-O2D-CGD	2.30	121.13	115.92
24	B	611	CLA	CAC-C3C-C4C	2.30	127.78	124.79
26	A	610	BCR	C37-C22-C23	-2.30	114.58	118.09
24	b	617	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
26	Y	101	BCR	C28-C27-C26	2.30	118.15	114.06
25	a	412	PHO	CMA-C3A-C4A	-2.30	109.66	114.61
27	D	405	PL9	C35-C34-C36	2.30	119.21	115.23
24	b	607	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
24	b	604	CLA	CBC-CAC-C3C	-2.29	106.20	112.42
24	C	501	CLA	C1-C2-C3	-2.29	122.44	126.20
26	f	101	BCR	C30-C25-C24	2.29	121.87	115.65
24	b	610	CLA	C1-C2-C3	-2.29	122.44	126.20
24	c	910	CLA	O2A-CGA-CBA	2.29	118.82	111.83
24	c	910	CLA	CMB-C2B-C1B	2.29	128.91	125.42
24	c	902	CLA	CMC-C2C-C1C	2.29	128.61	125.03
27	D	405	PL9	C7-C8-C9	-2.29	122.89	126.83
24	b	611	CLA	CAC-C3C-C4C	2.29	127.77	124.79
24	a	408	CLA	CED-O2D-CGD	2.29	121.10	115.92
24	b	602	CLA	C4-C3-C5	2.29	119.20	115.23
29	d	409	LHG	O7-C7-C8	2.28	116.42	111.48
31	j	101	DGD	O2G-C1B-C2B	2.28	116.42	111.48
24	c	911	CLA	C1-C2-C3	-2.28	122.45	126.20
31	d	406	DGD	O2G-C1B-O1B	-2.28	118.37	123.70
24	c	905	CLA	C4D-C3D-CAD	2.28	110.58	108.11
24	a	407	CLA	CED-O2D-CGD	2.28	121.09	115.92
26	k	102	BCR	C39-C30-C29	-2.28	100.20	108.95
32	E	101	HEM	C3B-C2B-C1B	2.28	108.12	106.41
24	b	607	CLA	O2A-CGA-CBA	2.28	118.78	111.83
27	a	410	PL9	C42-C43-C44	-2.27	122.42	127.62
24	b	611	CLA	C4D-C3D-CAD	2.27	110.58	108.11
24	B	615	CLA	CMC-C2C-C1C	2.27	128.59	125.03
24	b	617	CLA	C1-O2A-CGA	2.27	122.15	116.65
24	B	606	CLA	CED-O2D-CGD	2.27	121.07	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	O2A-CGA-CBA	2.27	118.76	111.83
28	F	101	SQD	O48-C23-O10	-2.27	117.95	123.63
24	C	509	CLA	CHD-C4C-NC	-2.27	120.71	124.23
24	A	606	CLA	CMB-C2B-C3B	2.27	131.89	126.55
24	c	904	CLA	CHD-C4C-NC	-2.27	120.71	124.23
24	d	404	CLA	CBC-CAC-C3C	-2.27	106.27	112.42
24	C	506	CLA	CMC-C2C-C1C	2.27	128.58	125.03
27	D	405	PL9	C10-C9-C11	2.27	119.16	115.23
29	D	409	LHG	O4-P-O5	2.26	122.98	112.44
24	B	608	CLA	C1-O2A-CGA	2.26	122.13	116.65
26	C	514	BCR	C40-C30-C29	-2.26	100.26	108.95
24	d	403	CLA	CMC-C2C-C1C	2.26	128.57	125.03
32	e	101	HEM	C1B-NB-C4B	2.26	107.89	105.21
24	b	605	CLA	C4-C3-C5	2.26	119.15	115.23
24	B	606	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
27	d	405	PL9	C20-C19-C21	2.26	119.15	115.23
27	a	410	PL9	C22-C23-C24	-2.26	122.46	127.62
24	b	609	CLA	O2A-CGA-CBA	2.26	118.71	111.83
24	b	606	CLA	C1-C2-C3	-2.25	122.51	126.20
26	A	610	BCR	C2-C1-C6	2.25	113.71	110.44
26	k	102	BCR	C37-C22-C23	-2.25	114.65	118.09
26	k	102	BCR	C34-C9-C8	-2.25	114.65	118.09
24	C	505	CLA	CMB-C2B-C1B	2.25	128.85	125.42
24	B	616	CLA	C1-O2A-CGA	2.25	122.10	116.65
29	d	409	LHG	O8-C23-O10	-2.25	118.00	123.63
24	D	402	CLA	O2A-CGA-CBA	2.25	118.69	111.83
24	c	906	CLA	C1-O2A-CGA	2.25	122.09	116.65
24	b	608	CLA	CMC-C2C-C1C	2.25	128.55	125.03
29	A	615	LHG	O8-C23-O10	-2.25	118.01	123.63
24	a	406	CLA	C4-C3-C5	2.25	119.13	115.23
24	B	616	CLA	CED-O2D-CGD	2.24	121.01	115.92
24	b	612	CLA	C7-C6-C5	-2.24	107.28	113.26
24	b	608	CLA	CBC-CAC-C3C	-2.24	106.34	112.42
26	b	619	BCR	C2-C3-C4	2.24	116.21	111.28
24	C	507	CLA	CED-O2D-CGD	2.24	121.00	115.92
28	L	101	SQD	O9-S-C6	2.24	110.10	106.76
24	b	603	CLA	CMB-C2B-C3B	2.24	131.82	126.55
24	b	606	CLA	CHD-C4C-C3C	-2.24	121.51	124.77
26	K	101	BCR	C1-C6-C7	2.23	121.71	115.65
24	c	910	CLA	CAC-C3C-C4C	2.23	127.69	124.79
24	c	914	CLA	C1-O2A-CGA	2.23	122.05	116.65
26	D	404	BCR	C38-C26-C25	2.23	126.92	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	613	SQD	C3-C4-C5	2.23	114.27	110.23
24	c	913	CLA	C4D-C3D-CAD	2.23	110.53	108.11
24	c	911	CLA	O2D-CGD-O1D	-2.23	119.52	123.85
29	D	407	LHG	O4-P-O5	2.23	122.80	112.44
24	B	609	CLA	C4-C3-C5	2.22	119.09	115.23
24	b	614	CLA	C1-O2A-CGA	2.22	122.03	116.65
24	b	615	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
24	b	604	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
24	c	910	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
24	c	905	CLA	CHD-C4C-NC	-2.22	120.79	124.23
24	A	607	CLA	CED-O2D-CGD	2.22	120.95	115.92
24	A	606	CLA	C4-C3-C5	2.22	119.08	115.23
27	d	405	PL9	C7-C8-C9	-2.22	123.01	126.83
24	b	609	CLA	CMC-C2C-C1C	2.22	128.50	125.03
25	D	401	PHO	CAC-C3C-C4C	2.22	129.73	124.03
24	b	603	CLA	CED-O2D-CGD	2.21	120.94	115.92
28	A	612	SQD	O48-C23-O10	-2.21	118.09	123.63
32	v	202	HEM	C3D-C4D-ND	-2.21	107.74	110.17
24	B	607	CLA	C1-O2A-CGA	2.21	122.01	116.65
24	B	617	CLA	CED-O2D-CGD	2.21	120.93	115.92
24	B	613	CLA	O2A-CGA-CBA	2.21	118.58	111.83
24	D	402	CLA	CED-O2D-CGD	2.21	120.93	115.92
24	c	913	CLA	CAC-C3C-C4C	2.21	127.67	124.79
24	c	912	CLA	O2A-CGA-CBA	2.21	118.57	111.83
27	a	410	PL9	C45-C44-C46	2.21	119.06	115.23
29	D	409	LHG	O8-C23-C24	2.21	118.57	111.83
24	C	503	CLA	C4D-CHA-C1A	2.21	123.88	121.24
24	C	505	CLA	C1-O2A-CGA	2.21	122.00	116.65
26	C	515	BCR	C4-C5-C6	2.21	125.69	122.70
27	a	410	PL9	C10-C9-C11	2.21	119.06	115.23
24	B	609	CLA	C11-C12-C13	-2.21	108.64	115.97
24	A	606	CLA	C1D-CHD-C4C	-2.20	121.33	126.02
24	c	903	CLA	C4-C3-C5	2.20	119.05	115.23
24	b	617	CLA	CMC-C2C-C1C	2.20	128.48	125.03
24	b	613	CLA	CHD-C1D-ND	-2.20	121.70	124.80
24	b	604	CLA	O2A-CGA-CBA	2.20	118.55	111.83
26	C	514	BCR	C2-C3-C4	2.20	116.12	111.28
24	A	607	CLA	C1-O2A-CGA	2.20	121.98	116.65
24	c	904	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
24	c	902	CLA	O2A-CGA-CBA	2.20	118.54	111.83
24	A	606	CLA	O2A-CGA-CBA	2.20	118.54	111.83
24	b	609	CLA	O2A-CGA-O1A	-2.20	118.13	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	CED-O2D-CGD	2.20	120.90	115.92
24	B	605	CLA	C4B-C3B-C2B	-2.20	104.57	107.30
31	d	406	DGD	O5D-C1E-C2E	2.20	111.61	108.27
24	B	615	CLA	CED-O2D-CGD	2.19	120.89	115.92
26	B	619	BCR	C28-C29-C30	2.19	122.19	114.43
24	b	615	CLA	C4D-C3D-CAD	2.19	110.49	108.11
24	b	604	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
24	A	606	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
24	c	907	CLA	CMC-C2C-C1C	2.19	128.46	125.03
24	A	606	CLA	CMC-C2C-C1C	2.19	128.46	125.03
29	b	620	LHG	O7-C7-O9	-2.19	118.59	123.70
24	C	511	CLA	CED-O2D-CGD	2.19	120.88	115.92
24	B	609	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
24	C	502	CLA	CHD-C4C-C3C	-2.19	121.59	124.77
24	B	605	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
24	c	911	CLA	C4B-C3B-C2B	-2.18	104.59	107.30
26	k	102	BCR	C34-C9-C10	-2.18	119.28	122.82
28	L	101	SQD	O5-C1-C2	-2.18	105.89	110.37
24	c	907	CLA	C4-C3-C5	2.18	119.01	115.23
24	B	605	CLA	CMC-C2C-C1C	2.18	128.44	125.03
24	B	607	CLA	C4D-C3D-CAD	2.18	110.47	108.11
24	C	510	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
24	B	614	CLA	CMC-C2C-C1C	2.18	128.44	125.03
26	B	620	BCR	C3-C2-C1	2.18	122.14	114.43
24	d	404	CLA	CAC-C3C-C4C	2.18	127.62	124.79
26	A	610	BCR	C28-C27-C26	-2.18	110.18	114.06
25	a	412	PHO	C4B-NB-C1B	-2.17	105.65	108.82
24	c	914	CLA	C4-C3-C5	2.17	119.00	115.23
24	B	617	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
24	B	602	CLA	C1-O2A-CGA	2.17	121.90	116.65
24	B	604	CLA	O2A-CGA-CBA	2.17	118.44	111.83
24	c	912	CLA	C4D-C3D-CAD	2.17	110.46	108.11
24	B	617	CLA	CMB-C2B-C1B	2.17	128.72	125.42
31	H	102	DGD	O6E-C5E-C6E	2.16	111.81	106.44
24	c	904	CLA	O2A-CGA-CBA	2.16	118.43	111.83
24	B	617	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
26	c	915	BCR	C39-C30-C25	2.16	113.63	110.24
24	C	509	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
26	B	618	BCR	C33-C5-C4	-2.16	108.99	113.60
25	d	402	PHO	CMA-C3A-C4A	-2.16	109.96	114.61
26	D	404	BCR	C24-C25-C26	2.16	126.53	121.56
28	L	101	SQD	O47-C7-O49	-2.16	118.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	CLA	CAA-CBA-CGA	-2.16	107.08	113.21
32	v	202	HEM	C1D-C2D-C3D	-2.16	104.71	106.98
24	b	605	CLA	CMB-C2B-C1B	2.16	128.70	125.42
24	B	617	CLA	CHD-C4C-C3C	-2.15	121.63	124.77
24	B	610	CLA	CBC-CAC-C3C	-2.15	106.58	112.42
24	c	912	CLA	CAC-C3C-C4C	2.15	127.59	124.79
25	d	402	PHO	CBC-CAC-C3C	-2.15	109.79	112.87
24	B	605	CLA	CHB-C1B-NB	-2.15	120.82	124.05
24	B	605	CLA	CHD-C4C-NC	-2.15	120.90	124.23
24	a	407	CLA	O2A-CGA-CBA	2.15	118.39	111.83
28	a	411	SQD	C45-O47-C7	-2.15	112.65	117.80
24	B	609	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
24	c	908	CLA	CHB-C1B-NB	-2.15	120.83	124.05
24	A	614	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
24	c	903	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
26	b	619	BCR	C3-C2-C1	2.15	122.03	114.43
27	D	405	PL9	C2-C1-C6	2.14	121.55	119.00
29	D	408	LHG	O7-C7-C8	2.14	116.12	111.48
24	b	616	CLA	O2A-CGA-CBA	2.14	118.37	111.83
27	a	410	PL9	C27-C28-C29	-2.14	122.72	127.62
27	d	405	PL9	C35-C34-C36	2.14	118.94	115.23
26	B	620	BCR	C40-C30-C25	2.14	113.60	110.24
24	A	609	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
24	C	503	CLA	CED-O2D-CGD	2.14	120.76	115.92
24	C	511	CLA	C4D-C3D-CAD	2.14	110.43	108.11
28	A	612	SQD	O5-C1-C2	-2.14	105.98	110.37
24	b	602	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
24	B	605	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	B	614	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	c	913	CLA	CED-O2D-CGD	2.13	120.75	115.92
26	T	101	BCR	C2-C3-C4	2.13	115.97	111.28
24	b	617	CLA	CMB-C2B-C3B	2.13	131.56	126.55
24	A	614	CLA	CMB-C2B-C1B	2.13	128.66	125.42
24	C	509	CLA	C1-O2A-CGA	2.13	121.81	116.65
24	c	902	CLA	C4D-C3D-CAD	2.13	110.42	108.11
24	B	611	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
24	C	504	CLA	C7-C6-C5	-2.13	107.59	113.26
24	C	506	CLA	O2A-CGA-CBA	2.13	118.32	111.83
26	b	618	BCR	C32-C1-C31	-2.13	102.54	108.63
25	d	402	PHO	CMC-C2C-C1C	2.13	128.56	124.73
24	C	512	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
24	C	506	CLA	C1-C2-C3	-2.13	122.72	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	913	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
24	A	614	CLA	C4B-C3B-C2B	-2.12	104.66	107.30
26	H	101	BCR	C40-C30-C29	-2.12	100.79	108.95
32	V	202	HEM	C1D-C2D-C3D	-2.12	104.75	106.98
31	C	518	DGD	O1G-C1A-O1A	-2.12	118.32	123.63
24	B	609	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
24	a	408	CLA	CBC-CAC-C3C	-2.12	106.67	112.42
24	c	902	CLA	C1-O2A-CGA	2.12	121.78	116.65
24	C	506	CLA	CMB-C2B-C1B	2.12	128.65	125.42
26	B	620	BCR	C1-C6-C7	2.12	121.40	115.65
24	b	610	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
26	b	618	BCR	C31-C1-C6	2.12	113.56	110.24
24	C	508	CLA	O2D-CGD-O1D	-2.11	119.73	123.85
24	a	406	CLA	CMB-C2B-C1B	2.11	128.64	125.42
24	a	406	CLA	O2A-CGA-CBA	2.11	118.28	111.83
24	C	507	CLA	C1-O2A-CGA	2.11	121.76	116.65
28	l	101	SQD	O8-S-C6	2.11	110.05	105.97
24	D	403	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
24	B	604	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
26	K	101	BCR	C30-C25-C24	2.11	121.37	115.65
24	b	608	CLA	C1-O2A-CGA	2.11	121.76	116.65
26	k	101	BCR	C28-C27-C26	2.11	117.81	114.06
24	c	906	CLA	O2A-CGA-CBA	2.11	118.26	111.83
26	T	102	BCR	C33-C5-C6	-2.11	122.19	124.48
24	c	905	CLA	CMC-C2C-C1C	2.11	128.32	125.03
24	b	612	CLA	CMB-C2B-C1B	2.10	128.62	125.42
26	B	622	BCR	C37-C22-C23	-2.10	114.88	118.09
24	a	406	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
24	D	402	CLA	C4D-CHA-C1A	2.10	123.75	121.24
24	c	907	CLA	O2A-CGA-CBA	2.10	118.24	111.83
24	b	602	CLA	CAC-C3C-C4C	2.10	127.52	124.79
24	C	501	CLA	C4-C3-C5	2.10	118.87	115.23
24	b	611	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
24	C	503	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
24	C	510	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
24	C	506	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
29	b	620	LHG	O8-C23-C24	2.10	118.23	111.83
29	d	410	LHG	O8-C23-O10	-2.10	118.38	123.63
24	B	606	CLA	C1-C2-C3	-2.10	122.76	126.20
24	D	402	CLA	C4B-C3B-C2B	-2.10	104.70	107.30
29	B	621	LHG	O4-P-O5	2.10	122.19	112.44
24	B	604	CLA	CAC-C3C-C4C	2.10	127.52	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C4B-C3B-C2B	-2.09	104.70	107.30
26	K	101	BCR	C29-C28-C27	-2.09	106.67	111.28
28	d	407	SQD	O47-C45-C46	2.09	115.85	108.34
24	B	615	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
26	K	101	BCR	C38-C26-C25	2.09	126.77	124.48
27	d	405	PL9	C25-C24-C26	2.09	118.86	115.23
24	C	507	CLA	CHB-C1B-NB	-2.09	120.91	124.05
24	a	407	CLA	CHC-C1C-C2C	-2.09	121.01	126.95
24	d	404	CLA	CMC-C2C-C1C	2.09	128.29	125.03
26	c	918	BCR	C35-C13-C12	-2.08	114.90	118.09
24	A	607	CLA	CHC-C1C-C2C	-2.08	121.02	126.95
24	a	408	CLA	C4B-C3B-C2B	-2.08	104.71	107.30
24	d	403	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
24	b	617	CLA	CBC-CAC-C3C	-2.08	106.77	112.42
24	B	606	CLA	CHD-C4C-C3C	-2.08	121.74	124.77
24	c	914	CLA	CMB-C2B-C1B	2.08	128.59	125.42
26	h	101	BCR	C1-C6-C7	2.08	121.29	115.65
26	T	102	BCR	C31-C1-C2	-2.08	100.97	108.95
26	k	102	BCR	C2-C3-C4	2.08	115.85	111.28
24	b	611	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
24	A	609	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	B	606	CLA	CAC-C3C-C4C	2.07	127.49	124.79
27	a	410	PL9	C15-C14-C16	2.07	118.83	115.23
24	d	404	CLA	CED-O2D-CGD	2.07	120.61	115.92
24	B	603	CLA	O2A-CGA-CBA	2.07	118.15	111.83
26	b	619	BCR	C28-C27-C26	2.07	117.75	114.06
24	B	615	CLA	C4B-C3B-C2B	-2.07	104.73	107.30
24	b	608	CLA	CHD-C4C-C3C	-2.07	121.76	124.77
24	C	512	CLA	CMB-C2B-C1B	2.07	128.57	125.42
24	B	617	CLA	C4-C3-C5	2.07	118.81	115.23
24	C	505	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
31	c	916	DGD	C2G-O2G-C1B	-2.07	112.85	117.80
31	C	517	DGD	O1G-C1A-C2A	2.07	118.13	111.83
24	C	509	CLA	CHC-C1C-C2C	-2.06	121.08	126.95
24	b	605	CLA	C4B-C3B-C2B	-2.06	104.74	107.30
26	H	101	BCR	C1-C6-C5	-2.06	119.82	122.64
24	d	404	CLA	C4B-C3B-C2B	-2.06	104.74	107.30
26	B	622	BCR	C38-C26-C27	-2.06	109.20	113.60
24	B	615	CLA	O2A-CGA-CBA	2.06	118.11	111.83
24	B	604	CLA	CHD-C4C-C3C	-2.06	121.77	124.77
24	B	615	CLA	C1-C2-C3	-2.06	122.82	126.20
26	a	409	BCR	C31-C1-C2	-2.06	101.05	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	914	CLA	CAC-C3C-C4C	2.06	127.47	124.79
24	c	914	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
24	B	614	CLA	C4B-C3B-C2B	-2.06	104.75	107.30
24	d	404	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
27	d	405	PL9	C10-C9-C11	2.06	118.80	115.23
25	a	412	PHO	O2A-CGA-CBA	2.05	118.10	111.83
24	b	616	CLA	C1D-CHD-C4C	-2.05	121.66	126.02
24	C	509	CLA	C1-C2-C3	-2.05	122.83	126.20
26	b	618	BCR	C30-C25-C24	2.05	121.22	115.65
24	C	507	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
24	C	512	CLA	CMC-C2C-C1C	2.05	128.24	125.03
32	E	101	HEM	C1B-NB-C4B	2.05	107.63	105.21
24	A	607	CLA	CMB-C2B-C3B	2.05	131.36	126.55
24	C	503	CLA	CMB-C2B-C3B	2.05	131.36	126.55
24	A	606	CLA	CHC-C1C-C2C	-2.05	121.13	126.95
24	B	604	CLA	C4D-C3D-CAD	2.04	110.33	108.11
24	B	604	CLA	O1D-CGD-CBD	-2.04	120.48	124.52
24	c	913	CLA	CMC-C2C-C1C	2.04	128.23	125.03
26	B	622	BCR	C34-C9-C8	-2.04	114.97	118.09
24	B	611	CLA	CAA-CBA-CGA	-2.04	107.40	113.21
24	b	605	CLA	C6-C5-C3	-2.04	108.49	113.47
28	A	613	SQD	O5-C1-C2	-2.04	106.17	110.37
24	B	608	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
29	B	621	LHG	O7-C7-O9	-2.04	118.93	123.70
24	b	616	CLA	C4D-CHA-C1A	2.04	123.68	121.24
24	c	902	CLA	CAC-C3C-C4C	2.04	127.44	124.79
28	F	101	SQD	C3-C4-C5	2.04	113.93	110.23
24	C	510	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
24	c	914	CLA	C3B-C4B-NB	2.04	112.35	110.53
24	d	401	CLA	CMC-C2C-C1C	2.04	128.22	125.03
24	C	513	CLA	CMB-C2B-C1B	2.04	128.52	125.42
24	b	614	CLA	CED-O2D-CGD	2.04	120.54	115.92
28	l	101	SQD	O47-C7-O49	-2.04	118.94	123.70
24	D	402	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
24	B	607	CLA	CAC-C3C-C4C	2.03	127.44	124.79
24	c	909	CLA	CAC-C3C-C2C	2.03	131.30	127.56
24	C	511	CLA	CMC-C2C-C1C	2.03	128.21	125.03
25	D	401	PHO	CMA-C3A-C4A	-2.03	110.23	114.61
24	b	610	CLA	CMC-C2C-C1C	2.03	128.21	125.03
24	B	609	CLA	C11-C10-C8	-2.03	109.22	115.97
24	C	504	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
24	d	401	CLA	O2D-CGD-O1D	-2.03	119.90	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	CMC-C2C-C1C	2.03	128.20	125.03
24	c	908	CLA	C1-O2A-CGA	2.03	121.56	116.65
24	c	909	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
26	b	618	BCR	C28-C29-C30	2.03	121.60	114.43
24	B	612	CLA	C1D-CHD-C4C	-2.03	121.72	126.02
24	a	407	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
26	B	620	BCR	C31-C1-C2	-2.02	101.18	108.95
27	D	405	PL9	C51-C49-C50	2.02	119.24	114.59
24	c	912	CLA	CMC-C2C-C1C	2.02	128.19	125.03
24	a	408	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
24	B	616	CLA	C11-C10-C8	-2.02	109.25	115.97
24	b	614	CLA	C4-C3-C5	2.02	118.73	115.23
24	C	505	CLA	C4D-C3D-CAD	2.02	110.30	108.11
24	C	510	CLA	C1-C2-C3	-2.02	122.89	126.20
31	C	517	DGD	O1G-C1A-O1A	-2.02	118.58	123.63
24	C	509	CLA	C4-C3-C5	2.02	118.73	115.23
24	b	616	CLA	C1-O2A-CGA	2.01	121.53	116.65
24	C	507	CLA	CMD-C2D-C3D	-2.01	123.07	127.69
24	c	911	CLA	CMC-C2C-C1C	2.01	128.18	125.03
24	C	512	CLA	C4D-C3D-CAD	2.01	110.29	108.11
31	c	917	DGD	O1G-C1A-O1A	-2.01	118.59	123.63
24	C	510	CLA	C4-C3-C5	2.01	118.72	115.23
24	b	606	CLA	CED-O2D-CGD	2.01	120.48	115.92
24	b	612	CLA	O2A-CGA-CBA	2.01	117.97	111.83
24	a	407	CLA	CMC-C2C-C1C	2.01	128.18	125.03
29	B	621	LHG	O8-C23-C24	2.01	117.97	111.83
24	B	610	CLA	C4B-C3B-C2B	-2.01	104.80	107.30
24	C	513	CLA	CED-O2D-CGD	2.01	120.47	115.92
24	C	506	CLA	C4D-C3D-CAD	2.01	110.29	108.11
24	b	606	CLA	OBD-CAD-C3D	-2.01	123.72	128.42
24	b	602	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
24	c	911	CLA	CMB-C2B-C1B	2.01	128.48	125.42
24	c	904	CLA	CMC-C2C-C1C	2.01	128.17	125.03
24	b	607	CLA	CHD-C4C-NC	-2.01	121.12	124.23
28	l	101	SQD	C4-C3-C2	2.01	114.36	110.83
24	b	617	CLA	C4-C3-C5	2.01	118.71	115.23
24	B	605	CLA	C4D-C3D-CAD	2.01	110.28	108.11
26	f	101	BCR	C31-C1-C2	-2.01	101.25	108.95
24	D	403	CLA	O2A-CGA-CBA	2.00	117.95	111.83
24	b	616	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
27	a	410	PL9	C17-C18-C19	-2.00	123.04	127.62
24	a	408	CLA	CMB-C2B-C1B	2.00	128.47	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CMC-C2C-C1C	2.00	128.16	125.03
24	B	608	CLA	CHB-C4A-NA	2.00	127.29	124.40
26	k	101	BCR	C3-C4-C5	2.00	117.62	114.06
24	B	610	CLA	CMC-C2C-C1C	2.00	128.16	125.03

All (45) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	606	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	608	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	512	CLA	ND
24	D	402	CLA	ND
24	a	406	CLA	ND
24	b	602	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	611	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	c	902	CLA	ND
24	c	906	CLA	ND
24	c	907	CLA	ND
24	c	908	CLA	ND
24	c	910	CLA	ND
24	c	911	CLA	ND
24	c	913	CLA	ND
24	d	403	CLA	ND

All (1196) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	a	407	CLA	C2B-C3B-CAB-CBB
24	a	407	CLA	C4B-C3B-CAB-CBB
24	b	602	CLA	C2-C1-O2A-CGA
24	b	602	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	C11-C12-C13-C15
24	b	615	CLA	CAD-CBD-CGD-O1D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	c	903	CLA	CAD-CBD-CGD-O2D
24	c	908	CLA	CHA-CBD-CGD-O1D
24	c	913	CLA	C2B-C3B-CAB-CBB
24	c	913	CLA	C4B-C3B-CAB-CBB
26	B	618	BCR	C10-C11-C12-C13
26	C	514	BCR	C14-C15-C16-C17
26	C	514	BCR	C18-C19-C20-C21
26	C	515	BCR	C14-C15-C16-C17
26	C	515	BCR	C18-C19-C20-C21
26	D	404	BCR	C14-C15-C16-C17
26	D	404	BCR	C22-C23-C24-C25
26	D	404	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	H	101	BCR	C10-C11-C12-C13
26	H	101	BCR	C18-C19-C20-C21
26	K	101	BCR	C10-C11-C12-C13
26	K	101	BCR	C17-C18-C19-C20
26	K	101	BCR	C18-C19-C20-C21
26	b	619	BCR	C10-C11-C12-C13
26	c	915	BCR	C11-C12-C13-C14
26	c	915	BCR	C14-C15-C16-C17
26	c	915	BCR	C15-C16-C17-C18
26	c	915	BCR	C18-C19-C20-C21
26	c	918	BCR	C9-C10-C11-C12
26	c	918	BCR	C10-C11-C12-C13
26	c	918	BCR	C11-C12-C13-C14
26	c	918	BCR	C14-C15-C16-C17
26	c	918	BCR	C17-C18-C19-C20
26	c	918	BCR	C18-C19-C20-C21
26	f	101	BCR	C14-C15-C16-C17
26	f	101	BCR	C21-C22-C23-C24
26	f	101	BCR	C37-C22-C23-C24
26	f	101	BCR	C22-C23-C24-C25
26	h	101	BCR	C14-C15-C16-C17
26	h	101	BCR	C18-C19-C20-C21
26	k	102	BCR	C10-C11-C12-C13
26	k	102	BCR	C20-C21-C22-C23
26	k	102	BCR	C20-C21-C22-C37
27	A	611	PL9	C18-C19-C21-C22
27	A	611	PL9	C20-C19-C21-C22
28	A	613	SQD	O6-C44-C45-O47
28	L	101	SQD	O5-C1-O6-C44
28	L	101	SQD	C8-C7-O47-C45
28	L	101	SQD	O5-C5-C6-S
28	a	402	SQD	O6-C44-C45-O47
28	d	407	SQD	C46-C45-O47-C7
28	d	407	SQD	C8-C7-O47-C45
28	l	101	SQD	C8-C7-O47-C45
28	l	101	SQD	O5-C5-C6-S
29	A	615	LHG	O9-C7-O7-C5
29	A	615	LHG	C8-C7-O7-C5
29	B	621	LHG	C4-O6-P-O3
29	B	621	LHG	C4-O6-P-O4
29	B	621	LHG	C4-O6-P-O5
29	D	408	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	D	408	LHG	O2-C2-C3-O3
29	D	408	LHG	C3-O3-P-O5
29	D	408	LHG	C3-O3-P-O6
29	D	408	LHG	C4-O6-P-O4
29	a	413	LHG	O1-C1-C2-O2
29	a	413	LHG	C1-C2-C3-O3
29	b	620	LHG	C4-O6-P-O3
29	b	620	LHG	C4-O6-P-O4
29	b	620	LHG	C4-O6-P-O5
29	d	409	LHG	C1-C2-C3-O3
29	d	409	LHG	C3-O3-P-O5
29	d	409	LHG	C4-O6-P-O4
31	D	406	DGD	C2B-C1B-O2G-C2G
31	D	406	DGD	C2D-C1D-O3G-C3G
31	d	406	DGD	C2B-C1B-O2G-C2G
31	d	406	DGD	C2D-C1D-O3G-C3G
32	v	202	HEM	C2C-C3C-CAC-CBC
28	F	101	SQD	O10-C23-O48-C46
29	A	615	LHG	O10-C23-O8-C6
28	F	101	SQD	C24-C23-O48-C46
29	A	615	LHG	C24-C23-O8-C6
24	b	602	CLA	O1A-CGA-O2A-C1
28	L	101	SQD	O49-C7-O47-C45
28	d	407	SQD	O49-C7-O47-C45
31	D	406	DGD	O1B-C1B-O2G-C2G
31	d	406	DGD	O1B-C1B-O2G-C2G
24	B	615	CLA	C3-C5-C6-C7
24	b	605	CLA	C3-C5-C6-C7
24	B	617	CLA	CBA-CGA-O2A-C1
24	b	602	CLA	CBA-CGA-O2A-C1
24	C	513	CLA	CBD-CGD-O2D-CED
24	c	914	CLA	CBD-CGD-O2D-CED
24	B	606	CLA	C4-C3-C5-C6
24	B	606	CLA	C2-C3-C5-C6
24	C	513	CLA	O1D-CGD-O2D-CED
24	B	602	CLA	C3-C5-C6-C7
26	D	404	BCR	C15-C16-C17-C18
26	c	918	BCR	C19-C20-C21-C22
28	l	101	SQD	O49-C7-O47-C45
24	b	615	CLA	C3-C5-C6-C7
29	a	413	LHG	O2-C2-C3-O3
29	d	409	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	B	617	CLA	O1A-CGA-O2A-C1
31	d	406	DGD	O1A-C1A-O1G-C1G
31	D	406	DGD	O6E-C5E-C6E-O5E
24	b	602	CLA	C3-C5-C6-C7
31	d	406	DGD	C2A-C1A-O1G-C1G
24	b	606	CLA	C4-C3-C5-C6
27	A	611	PL9	C9-C11-C12-C13
27	A	611	PL9	C14-C16-C17-C18
27	A	611	PL9	C19-C21-C22-C23
27	A	611	PL9	C24-C26-C27-C28
27	a	410	PL9	C9-C11-C12-C13
27	a	410	PL9	C14-C16-C17-C18
27	a	410	PL9	C24-C26-C27-C28
24	c	902	CLA	O1D-CGD-O2D-CED
28	F	101	SQD	O5-C1-O6-C44
31	D	406	DGD	O6E-C1E-O5D-C6D
31	d	406	DGD	O6D-C1D-O3G-C3G
31	d	406	DGD	O6E-C1E-O5D-C6D
24	C	508	CLA	CBD-CGD-O2D-CED
26	C	515	BCR	C15-C16-C17-C18
26	h	101	BCR	C19-C20-C21-C22
29	D	408	LHG	C1-C2-C3-O3
28	l	101	SQD	C24-C23-O48-C46
24	c	914	CLA	O1D-CGD-O2D-CED
24	b	615	CLA	C4-C3-C5-C6
24	b	606	CLA	C2-C3-C5-C6
24	b	615	CLA	C2-C3-C5-C6
24	B	602	CLA	C11-C10-C8-C9
24	C	501	CLA	C11-C12-C13-C14
24	C	502	CLA	C14-C13-C15-C16
24	C	504	CLA	C11-C12-C13-C14
24	C	509	CLA	C6-C7-C8-C9
24	b	602	CLA	C11-C10-C8-C9
24	c	905	CLA	C11-C12-C13-C14
24	c	907	CLA	C6-C7-C8-C9
28	F	101	SQD	C2-C1-O6-C44
31	D	406	DGD	C2E-C1E-O5D-C6D
31	d	406	DGD	C2E-C1E-O5D-C6D
26	B	618	BCR	C11-C12-C13-C35
26	K	101	BCR	C36-C18-C19-C20
26	c	915	BCR	C11-C12-C13-C35
26	c	918	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
26	c	918	BCR	C36-C18-C19-C20
28	d	407	SQD	C23-C24-C25-C26
31	c	917	DGD	C1A-C2A-C3A-C4A
28	l	101	SQD	O10-C23-O48-C46
31	D	406	DGD	C1A-C2A-C3A-C4A
31	j	101	DGD	C1A-C2A-C3A-C4A
24	b	607	CLA	O1D-CGD-O2D-CED
24	c	912	CLA	O1D-CGD-O2D-CED
29	D	408	LHG	O1-C1-C2-O2
24	c	902	CLA	CBD-CGD-O2D-CED
24	b	607	CLA	C12-C13-C15-C16
26	C	514	BCR	C15-C16-C17-C18
26	C	514	BCR	C19-C20-C21-C22
26	c	918	BCR	C15-C16-C17-C18
26	k	102	BCR	C19-C20-C21-C22
27	a	410	PL9	C19-C21-C22-C23
31	D	406	DGD	C4E-C5E-C6E-O5E
28	a	402	SQD	C23-C24-C25-C26
29	D	407	LHG	C23-C24-C25-C26
31	d	406	DGD	C1B-C2B-C3B-C4B
24	A	609	CLA	C10-C11-C12-C13
24	B	616	CLA	C5-C6-C7-C8
24	d	403	CLA	C15-C16-C17-C18
26	k	101	BCR	C10-C11-C12-C13
24	A	609	CLA	C13-C15-C16-C17
24	B	602	CLA	C10-C11-C12-C13
24	B	615	CLA	C5-C6-C7-C8
24	b	607	CLA	C15-C16-C17-C18
24	c	907	CLA	C10-C11-C12-C13
28	A	613	SQD	C23-C24-C25-C26
29	A	615	LHG	C7-C8-C9-C10
31	C	517	DGD	C1B-C2B-C3B-C4B
31	D	406	DGD	C1B-C2B-C3B-C4B
31	D	406	DGD	O6D-C1D-O3G-C3G
31	c	917	DGD	C3B-C4B-C5B-C6B
24	B	607	CLA	C13-C15-C16-C17
24	B	615	CLA	C10-C11-C12-C13
24	C	509	CLA	C8-C10-C11-C12
24	b	602	CLA	C10-C11-C12-C13
24	b	614	CLA	C8-C10-C11-C12
29	d	410	LHG	C10-C11-C12-C13
24	C	506	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	a	408	CLA	C10-C11-C12-C13
24	b	602	CLA	C8-C10-C11-C12
24	b	615	CLA	C8-C10-C11-C12
24	c	914	CLA	C10-C11-C12-C13
24	D	403	CLA	C8-C10-C11-C12
28	L	101	SQD	C7-C8-C9-C10
24	A	607	CLA	C13-C15-C16-C17
24	B	607	CLA	C15-C16-C17-C18
24	D	403	CLA	C10-C11-C12-C13
24	a	407	CLA	C15-C16-C17-C18
24	b	615	CLA	C13-C15-C16-C17
24	c	912	CLA	CBD-CGD-O2D-CED
24	c	910	CLA	C13-C15-C16-C17
26	c	915	BCR	C19-C20-C21-C22
26	h	101	BCR	C15-C16-C17-C18
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C2A-CAA-CBA-CGA
24	C	509	CLA	C13-C15-C16-C17
24	b	607	CLA	C8-C10-C11-C12
24	b	617	CLA	C15-C16-C17-C18
24	A	609	CLA	C15-C16-C17-C18
24	B	612	CLA	C15-C16-C17-C18
24	B	617	CLA	C10-C11-C12-C13
24	C	501	CLA	C15-C16-C17-C18
24	C	506	CLA	C10-C11-C12-C13
24	b	612	CLA	C13-C15-C16-C17
28	d	407	SQD	C24-C23-O48-C46
24	b	609	CLA	C13-C15-C16-C17
24	A	607	CLA	C16-C17-C18-C20
26	B	619	BCR	C20-C21-C22-C37
26	C	515	BCR	C20-C21-C22-C37
26	H	101	BCR	C20-C21-C22-C37
26	c	915	BCR	C20-C21-C22-C37
26	c	918	BCR	C20-C21-C22-C37
26	h	101	BCR	C20-C21-C22-C37
26	B	620	BCR	C37-C22-C23-C24
26	K	101	BCR	C7-C8-C9-C34
26	B	618	BCR	C11-C12-C13-C14
29	D	407	LHG	O1-C1-C2-C3
29	a	413	LHG	O1-C1-C2-C3
28	l	101	SQD	C46-C45-O47-C7
24	a	406	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	c	918	BCR	C13-C14-C15-C16
24	C	506	CLA	C16-C17-C18-C19
24	a	407	CLA	C16-C17-C18-C20
24	a	408	CLA	C16-C17-C18-C19
24	b	602	CLA	C16-C17-C18-C19
24	b	602	CLA	C16-C17-C18-C20
24	c	910	CLA	C16-C17-C18-C19
24	c	910	CLA	C16-C17-C18-C20
24	c	912	CLA	C16-C17-C18-C19
24	b	615	CLA	C15-C16-C17-C18
26	B	619	BCR	C20-C21-C22-C23
26	C	514	BCR	C20-C21-C22-C23
26	H	101	BCR	C20-C21-C22-C23
26	K	101	BCR	C20-C21-C22-C23
26	c	915	BCR	C20-C21-C22-C23
26	c	918	BCR	C20-C21-C22-C23
24	B	614	CLA	C15-C16-C17-C18
24	b	613	CLA	C13-C15-C16-C17
24	b	616	CLA	C5-C6-C7-C8
24	c	907	CLA	C15-C16-C17-C18
24	B	617	CLA	C2-C1-O2A-CGA
24	D	403	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C19
24	b	617	CLA	C16-C17-C18-C20
24	c	909	CLA	C16-C17-C18-C19
24	b	616	CLA	C13-C15-C16-C17
28	A	612	SQD	C11-C12-C13-C14
28	A	613	SQD	C15-C16-C17-C18
28	l	101	SQD	C15-C16-C17-C18
31	C	516	DGD	C4B-C5B-C6B-C7B
28	F	101	SQD	C29-C30-C31-C32
28	F	101	SQD	C34-C35-C36-C37
28	a	402	SQD	C34-C35-C36-C37
28	a	411	SQD	C29-C30-C31-C32
29	B	621	LHG	C12-C13-C14-C15
29	a	413	LHG	C11-C10-C9-C8
29	b	620	LHG	C14-C15-C16-C17
29	b	620	LHG	C28-C29-C30-C31
29	d	410	LHG	C15-C16-C17-C18
31	C	518	DGD	C9B-CAB-CBB-CCB
31	D	406	DGD	CCA-CDA-CEA-CFA
31	c	917	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
31	d	406	DGD	C8B-C9B-CAB-CBB
31	j	101	DGD	C6A-C7A-C8A-C9A
28	a	411	SQD	C26-C27-C28-C29
28	l	101	SQD	C10-C11-C12-C13
29	A	615	LHG	C14-C15-C16-C17
29	A	615	LHG	C24-C25-C26-C27
31	D	406	DGD	C7B-C8B-C9B-CAB
28	A	612	SQD	C15-C16-C17-C18
28	F	101	SQD	C26-C27-C28-C29
28	l	101	SQD	C11-C10-C9-C8
29	b	620	LHG	C13-C14-C15-C16
31	d	406	DGD	CCB-CDB-CEB-CFB
31	h	102	DGD	CCA-CDA-CEA-CFA
28	A	612	SQD	C12-C13-C14-C15
28	A	612	SQD	C28-C29-C30-C31
29	d	410	LHG	C17-C18-C19-C20
29	d	410	LHG	C31-C32-C33-C34
31	C	517	DGD	C9A-CAA-CBA-CCA
31	d	406	DGD	C2A-C3A-C4A-C5A
31	d	406	DGD	CCA-CDA-CEA-CFA
24	b	610	CLA	C4B-C3B-CAB-CBB
31	C	517	DGD	C1A-C2A-C3A-C4A
28	a	402	SQD	C28-C29-C30-C31
28	a	411	SQD	C27-C28-C29-C30
28	a	411	SQD	C33-C34-C35-C36
31	d	406	DGD	C6A-C7A-C8A-C9A
24	a	407	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20
24	c	903	CLA	C16-C17-C18-C19
24	c	909	CLA	C16-C17-C18-C20
25	a	412	PHO	C2C-C3C-CAC-CBC
31	D	406	DGD	C2A-C3A-C4A-C5A
24	B	617	CLA	C8-C10-C11-C12
24	a	408	CLA	C15-C16-C17-C18
31	C	516	DGD	O6D-C5D-C6D-O5D
28	d	407	SQD	C24-C25-C26-C27
29	b	620	LHG	C25-C26-C27-C28
31	c	916	DGD	C4B-C5B-C6B-C7B
31	c	917	DGD	C3A-C4A-C5A-C6A
31	d	406	DGD	C9B-CAB-CBB-CCB
29	d	408	LHG	C30-C31-C32-C33
31	D	406	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
28	d	407	SQD	O10-C23-O48-C46
28	l	101	SQD	C24-C25-C26-C27
29	D	407	LHG	C32-C33-C34-C35
29	a	413	LHG	C24-C25-C26-C27
31	d	406	DGD	C1A-C2A-C3A-C4A
26	k	102	BCR	C15-C16-C17-C18
24	a	408	CLA	C16-C17-C18-C20
24	c	903	CLA	C16-C17-C18-C20
24	C	506	CLA	O1D-CGD-O2D-CED
28	a	411	SQD	C11-C12-C13-C14
29	a	413	LHG	C14-C15-C16-C17
31	D	406	DGD	CBA-CCA-CDA-CEA
31	c	916	DGD	C8A-C9A-CAA-CBA
31	c	917	DGD	CBA-CCA-CDA-CEA
28	A	612	SQD	C16-C17-C18-C19
28	a	402	SQD	C26-C27-C28-C29
29	D	407	LHG	C29-C30-C31-C32
31	C	517	DGD	C6B-C7B-C8B-C9B
28	A	613	SQD	C24-C23-O48-C46
28	l	101	SQD	C12-C13-C14-C15
28	l	101	SQD	C17-C18-C19-C20
28	l	101	SQD	C18-C19-C20-C21
28	l	101	SQD	C27-C28-C29-C30
31	C	516	DGD	C6A-C7A-C8A-C9A
31	C	516	DGD	C5B-C6B-C7B-C8B
31	C	517	DGD	CBB-CCB-CDB-CEB
29	a	413	LHG	C23-C24-C25-C26
28	A	613	SQD	C16-C17-C18-C19
28	A	613	SQD	C26-C27-C28-C29
28	L	101	SQD	C11-C10-C9-C8
28	L	101	SQD	C24-C25-C26-C27
28	d	407	SQD	C31-C32-C33-C34
29	b	620	LHG	C27-C28-C29-C30
29	d	410	LHG	C12-C13-C14-C15
29	d	410	LHG	C18-C19-C20-C21
31	C	516	DGD	C4A-C5A-C6A-C7A
31	C	517	DGD	CAA-CBA-CCA-CDA
31	C	517	DGD	C9B-CAB-CBB-CCB
31	D	406	DGD	C8B-C9B-CAB-CBB
31	c	916	DGD	C2B-C3B-C4B-C5B
31	d	406	DGD	C3B-C4B-C5B-C6B
31	j	101	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
28	A	612	SQD	C9-C10-C11-C12
28	a	402	SQD	C16-C17-C18-C19
29	d	410	LHG	C9-C10-C11-C12
28	F	101	SQD	C24-C25-C26-C27
28	L	101	SQD	C31-C32-C33-C34
28	L	101	SQD	C34-C35-C36-C37
25	D	401	PHO	C2C-C3C-CAC-CBC
28	F	101	SQD	C31-C32-C33-C34
28	d	407	SQD	C25-C26-C27-C28
29	a	413	LHG	C11-C12-C13-C14
29	b	620	LHG	C29-C30-C31-C32
29	d	410	LHG	C13-C14-C15-C16
31	C	517	DGD	C3A-C4A-C5A-C6A
31	h	102	DGD	C6A-C7A-C8A-C9A
24	C	507	CLA	C16-C17-C18-C19
24	b	617	CLA	C16-C17-C18-C19
28	L	101	SQD	C10-C11-C12-C13
31	j	101	DGD	CBB-CCB-CDB-CEB
28	F	101	SQD	C8-C7-O47-C45
24	B	605	CLA	C13-C15-C16-C17
31	C	518	DGD	C2A-C3A-C4A-C5A
29	A	615	LHG	C26-C27-C28-C29
24	b	616	CLA	C10-C11-C12-C13
29	A	615	LHG	C25-C26-C27-C28
29	a	413	LHG	C18-C19-C20-C21
27	A	611	PL9	C4-C3-C7-C8
28	l	101	SQD	C29-C30-C31-C32
29	a	413	LHG	C13-C14-C15-C16
31	C	516	DGD	CAB-CBB-CCB-CDB
31	D	406	DGD	CCB-CDB-CEB-CFB
31	H	102	DGD	C7A-C8A-C9A-CAA
26	Y	101	BCR	C10-C11-C12-C13
26	h	101	BCR	C10-C11-C12-C13
26	k	101	BCR	C18-C19-C20-C21
28	L	101	SQD	C11-C12-C13-C14
29	B	621	LHG	C13-C14-C15-C16
31	d	406	DGD	C3A-C4A-C5A-C6A
28	a	411	SQD	C24-C25-C26-C27
28	d	407	SQD	C26-C27-C28-C29
29	D	408	LHG	C16-C17-C18-C19
28	l	101	SQD	C14-C15-C16-C17
29	A	615	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	K	101	BCR	C6-C7-C8-C9
26	k	102	BCR	C6-C7-C8-C9
28	a	402	SQD	C10-C11-C12-C13
29	d	408	LHG	C25-C26-C27-C28
24	b	607	CLA	C10-C11-C12-C13
31	C	517	DGD	CAB-CBB-CCB-CDB
31	H	102	DGD	CBA-CCA-CDA-CEA
31	d	406	DGD	C7B-C8B-C9B-CAB
28	d	407	SQD	C27-C28-C29-C30
28	l	101	SQD	C32-C33-C34-C35
29	b	620	LHG	C32-C33-C34-C35
31	j	101	DGD	C2A-C3A-C4A-C5A
28	a	411	SQD	C25-C26-C27-C28
29	B	621	LHG	C11-C12-C13-C14
29	a	413	LHG	C16-C17-C18-C19
26	H	101	BCR	C15-C16-C17-C18
26	h	101	BCR	C9-C10-C11-C12
26	k	101	BCR	C19-C20-C21-C22
24	c	912	CLA	C16-C17-C18-C20
28	a	411	SQD	C9-C10-C11-C12
29	D	409	LHG	C29-C30-C31-C32
29	d	410	LHG	C34-C35-C36-C37
31	c	916	DGD	C9A-CAA-CBA-CCA
31	c	916	DGD	O6D-C5D-C6D-O5D
24	C	506	CLA	C13-C15-C16-C17
29	D	408	LHG	C32-C33-C34-C35
28	A	613	SQD	C28-C29-C30-C31
31	c	917	DGD	CCA-CDA-CEA-CFA
24	D	403	CLA	C16-C17-C18-C20
24	d	404	CLA	C16-C17-C18-C19
28	a	411	SQD	C16-C17-C18-C19
32	V	202	HEM	C2B-C3B-CAB-CBB
32	V	202	HEM	C2C-C3C-CAC-CBC
31	H	102	DGD	C9B-CAB-CBB-CCB
29	A	615	LHG	C13-C14-C15-C16
29	d	408	LHG	C29-C30-C31-C32
31	C	517	DGD	C3B-C4B-C5B-C6B
24	C	504	CLA	C13-C15-C16-C17
31	C	516	DGD	C8B-C9B-CAB-CBB
31	C	518	DGD	C6B-C7B-C8B-C9B
28	l	101	SQD	C7-C8-C9-C10
28	L	101	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
32	V	202	HEM	C4B-C3B-CAB-CBB
32	v	202	HEM	C4C-C3C-CAC-CBC
24	C	506	CLA	C16-C17-C18-C20
24	C	507	CLA	C16-C17-C18-C20
31	c	917	DGD	CAA-CBA-CCA-CDA
28	A	613	SQD	O10-C23-O48-C46
28	L	101	SQD	C18-C19-C20-C21
28	a	411	SQD	C14-C15-C16-C17
28	l	101	SQD	C16-C17-C18-C19
28	l	101	SQD	C28-C29-C30-C31
29	a	413	LHG	O7-C5-C6-O8
29	b	620	LHG	C12-C13-C14-C15
31	d	406	DGD	C5A-C6A-C7A-C8A
31	d	406	DGD	CAA-CBA-CCA-CDA
29	D	407	LHG	C24-C25-C26-C27
29	d	409	LHG	C11-C10-C9-C8
31	d	406	DGD	C4B-C5B-C6B-C7B
24	C	501	CLA	C13-C15-C16-C17
24	b	617	CLA	C5-C6-C7-C8
31	j	101	DGD	C7A-C8A-C9A-CAA
28	F	101	SQD	C30-C31-C32-C33
29	D	409	LHG	C15-C16-C17-C18
24	A	607	CLA	C16-C17-C18-C19
24	B	605	CLA	C16-C17-C18-C20
28	A	612	SQD	C30-C31-C32-C33
31	C	517	DGD	C4A-C5A-C6A-C7A
28	A	612	SQD	C32-C33-C34-C35
24	c	911	CLA	C4-C3-C5-C6
24	c	911	CLA	C2-C3-C5-C6
28	F	101	SQD	O49-C7-O47-C45
31	c	917	DGD	C8A-C9A-CAA-CBA
24	b	604	CLA	CBD-CGD-O2D-CED
24	c	911	CLA	O1D-CGD-O2D-CED
31	C	516	DGD	C3B-C4B-C5B-C6B
24	c	908	CLA	O1D-CGD-O2D-CED
24	C	507	CLA	C5-C6-C7-C8
24	a	408	CLA	C8-C10-C11-C12
24	b	604	CLA	C5-C6-C7-C8
31	C	518	DGD	CBA-CCA-CDA-CEA
29	A	615	LHG	C27-C28-C29-C30
24	b	602	CLA	C1A-C2A-CAA-CBA
24	c	914	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	d	404	CLA	C8-C10-C11-C12
29	d	409	LHG	C32-C33-C34-C35
31	c	916	DGD	C6A-C7A-C8A-C9A
28	a	402	SQD	C11-C12-C13-C14
28	L	101	SQD	C32-C33-C34-C35
28	F	101	SQD	C23-C24-C25-C26
24	B	602	CLA	C11-C10-C8-C7
24	B	617	CLA	C11-C12-C13-C15
24	C	506	CLA	C11-C12-C13-C15
24	C	508	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C10-C8-C7
24	b	602	CLA	C11-C10-C8-C7
24	b	605	CLA	C6-C7-C8-C10
24	b	607	CLA	C11-C12-C13-C15
24	b	612	CLA	C12-C13-C15-C16
28	d	407	SQD	C32-C33-C34-C35
24	A	609	CLA	C16-C17-C18-C19
24	b	616	CLA	C16-C17-C18-C19
29	D	409	LHG	C10-C11-C12-C13
28	A	612	SQD	C34-C35-C36-C37
24	a	408	CLA	C13-C15-C16-C17
29	B	621	LHG	C7-C8-C9-C10
31	j	101	DGD	C3B-C4B-C5B-C6B
27	a	410	PL9	C13-C14-C16-C17
24	D	403	CLA	C13-C15-C16-C17
24	c	910	CLA	C15-C16-C17-C18
24	C	501	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C14
24	D	403	CLA	C11-C10-C8-C9
24	b	607	CLA	C11-C12-C13-C14
24	b	611	CLA	C11-C12-C13-C14
24	b	617	CLA	C11-C12-C13-C14
24	c	905	CLA	C11-C10-C8-C9
24	c	908	CLA	C11-C10-C8-C9
24	d	401	CLA	C2C-C3C-CAC-CBC
24	C	512	CLA	CBA-CGA-O2A-C1
31	j	101	DGD	C2A-C1A-O1G-C1G
31	c	916	DGD	O6E-C5E-C6E-O5E
24	c	904	CLA	O1D-CGD-O2D-CED
28	L	101	SQD	C27-C28-C29-C30
28	A	613	SQD	O6-C44-C45-C46
31	d	406	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	C9A-CAA-CBA-CCA
25	D	401	PHO	O1D-CGD-O2D-CED
29	A	615	LHG	C15-C16-C17-C18
29	a	413	LHG	C15-C16-C17-C18
24	b	605	CLA	C15-C16-C17-C18
24	b	616	CLA	C8-C10-C11-C12
24	c	905	CLA	C10-C11-C12-C13
24	c	912	CLA	C13-C15-C16-C17
24	a	408	CLA	CBA-CGA-O2A-C1
31	C	516	DGD	O6E-C5E-C6E-O5E
24	b	603	CLA	C16-C17-C18-C19
24	b	614	CLA	C16-C17-C18-C19
24	c	907	CLA	C16-C17-C18-C19
31	C	516	DGD	C8A-C9A-CAA-CBA
31	D	406	DGD	C3A-C4A-C5A-C6A
24	C	509	CLA	C10-C11-C12-C13
24	b	615	CLA	C10-C11-C12-C13
24	c	910	CLA	C10-C11-C12-C13
27	a	410	PL9	C15-C14-C16-C17
31	c	916	DGD	C4D-C5D-C6D-O5D
24	A	609	CLA	C16-C17-C18-C20
24	C	512	CLA	O1A-CGA-O2A-C1
28	L	101	SQD	C13-C14-C15-C16
29	d	410	LHG	C27-C28-C29-C30
31	D	406	DGD	C9A-CAA-CBA-CCA
31	D	406	DGD	C4B-C5B-C6B-C7B
31	C	518	DGD	C6A-C7A-C8A-C9A
24	A	609	CLA	C5-C6-C7-C8
24	B	613	CLA	C13-C15-C16-C17
24	a	408	CLA	O1A-CGA-O2A-C1
28	A	613	SQD	C18-C19-C20-C21
24	B	607	CLA	O1D-CGD-O2D-CED
31	H	102	DGD	CBB-CCB-CDB-CEB
26	k	102	BCR	C9-C10-C11-C12
24	B	605	CLA	C16-C17-C18-C19
24	b	616	CLA	C16-C17-C18-C20
24	d	404	CLA	C16-C17-C18-C20
29	a	413	LHG	C7-C8-C9-C10
31	c	917	DGD	C9A-CAA-CBA-CCA
31	h	102	DGD	CAA-CBA-CCA-CDA
26	k	101	BCR	C20-C21-C22-C23
24	c	911	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	L	101	SQD	C24-C23-O48-C46
28	a	411	SQD	C30-C31-C32-C33
29	d	409	LHG	C16-C17-C18-C19
29	a	413	LHG	C19-C20-C21-C22
31	h	102	DGD	C9A-CAA-CBA-CCA
29	a	413	LHG	C28-C29-C30-C31
24	B	617	CLA	C16-C17-C18-C20
28	L	101	SQD	C28-C29-C30-C31
28	a	411	SQD	C12-C13-C14-C15
29	a	413	LHG	C26-C27-C28-C29
31	C	516	DGD	C7B-C8B-C9B-CAB
31	C	517	DGD	C8B-C9B-CAB-CBB
31	D	406	DGD	CAA-CBA-CCA-CDA
28	F	101	SQD	C35-C36-C37-C38
28	a	411	SQD	C19-C20-C21-C22
28	d	407	SQD	C35-C36-C37-C38
28	A	612	SQD	C27-C28-C29-C30
31	h	102	DGD	CBB-CCB-CDB-CEB
29	A	615	LHG	C11-C10-C9-C8
28	a	402	SQD	C19-C20-C21-C22
28	a	411	SQD	C35-C36-C37-C38
28	a	402	SQD	C13-C14-C15-C16
29	B	621	LHG	C32-C33-C34-C35
31	d	406	DGD	CAB-CBB-CCB-CDB
24	C	507	CLA	C2A-CAA-CBA-CGA
28	A	613	SQD	C19-C20-C21-C22
29	d	410	LHG	C19-C20-C21-C22
28	d	407	SQD	C34-C35-C36-C37
28	A	612	SQD	C35-C36-C37-C38
28	L	101	SQD	C35-C36-C37-C38
28	a	402	SQD	C29-C30-C31-C32
31	h	102	DGD	C5B-C6B-C7B-C8B
24	B	602	CLA	CBA-CGA-O2A-C1
29	a	413	LHG	C25-C26-C27-C28
29	d	410	LHG	C35-C36-C37-C38
28	a	411	SQD	C23-C24-C25-C26
29	d	408	LHG	C7-C8-C9-C10
24	C	512	CLA	O1D-CGD-O2D-CED
24	B	604	CLA	C16-C17-C18-C20
24	c	912	CLA	CBA-CGA-O2A-C1
28	l	101	SQD	C19-C20-C21-C22
28	A	612	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	d	408	LHG	C24-C25-C26-C27
24	B	615	CLA	C11-C12-C13-C14
24	B	615	CLA	C14-C13-C15-C16
24	B	617	CLA	C11-C12-C13-C14
24	C	507	CLA	C11-C10-C8-C9
24	C	508	CLA	C11-C10-C8-C9
24	a	407	CLA	C11-C12-C13-C14
24	b	605	CLA	C6-C7-C8-C9
24	c	913	CLA	C11-C10-C8-C9
29	d	410	LHG	C16-C17-C18-C19
31	d	406	DGD	C6B-C7B-C8B-C9B
24	D	402	CLA	C4B-C3B-CAB-CBB
29	D	407	LHG	C27-C28-C29-C30
31	C	516	DGD	C6B-C7B-C8B-C9B
31	D	406	DGD	C5A-C6A-C7A-C8A
31	D	406	DGD	C6A-C7A-C8A-C9A
31	H	102	DGD	C6B-C7B-C8B-C9B
24	b	603	CLA	C16-C17-C18-C20
31	C	516	DGD	CAA-CBA-CCA-CDA
28	a	402	SQD	C9-C10-C11-C12
31	C	517	DGD	C7B-C8B-C9B-CAB
31	j	101	DGD	CDB-CEB-CFB-CGB
29	A	615	LHG	C19-C20-C21-C22
31	H	102	DGD	CDB-CEB-CFB-CGB
31	c	916	DGD	CDA-CEA-CFA-CGA
24	A	609	CLA	C11-C10-C8-C7
24	B	602	CLA	C6-C7-C8-C10
24	B	615	CLA	C11-C12-C13-C15
24	C	501	CLA	C11-C12-C13-C15
24	C	501	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C10-C8-C7
24	C	513	CLA	C6-C7-C8-C10
24	D	403	CLA	C6-C7-C8-C10
24	a	407	CLA	C11-C10-C8-C7
24	a	407	CLA	C11-C12-C13-C15
24	b	617	CLA	C11-C12-C13-C15
24	c	905	CLA	C11-C10-C8-C7
24	c	907	CLA	C11-C10-C8-C7
24	c	908	CLA	C11-C10-C8-C7
24	c	913	CLA	C11-C10-C8-C7
24	d	404	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	B	609	CLA	C13-C15-C16-C17
31	C	517	DGD	CDB-CEB-CFB-CGB
31	C	516	DGD	C4D-C5D-C6D-O5D
28	A	613	SQD	O5-C1-O6-C44
31	j	101	DGD	O1A-C1A-O1G-C1G
28	A	612	SQD	C19-C20-C21-C22
26	B	622	BCR	C13-C14-C15-C16
26	K	101	BCR	C19-C20-C21-C22
26	a	409	BCR	C19-C20-C21-C22
24	b	614	CLA	C16-C17-C18-C20
31	d	406	DGD	C8A-C9A-CAA-CBA
31	C	516	DGD	C5A-C6A-C7A-C8A
24	c	914	CLA	C8-C10-C11-C12
28	A	613	SQD	C25-C26-C27-C28
28	l	101	SQD	C35-C36-C37-C38
24	B	616	CLA	C13-C15-C16-C17
27	a	410	PL9	C39-C41-C42-C43
28	L	101	SQD	C44-C45-C46-O48
28	d	407	SQD	C44-C45-C46-O48
28	l	101	SQD	C44-C45-C46-O48
29	a	413	LHG	C4-C5-C6-O8
31	D	406	DGD	O1G-C1G-C2G-C3G
29	D	407	LHG	C25-C26-C27-C28
28	d	407	SQD	C33-C34-C35-C36
31	c	916	DGD	C2A-C3A-C4A-C5A
24	B	602	CLA	C16-C17-C18-C20
24	c	914	CLA	C16-C17-C18-C19
28	A	613	SQD	C31-C32-C33-C34
29	b	620	LHG	C26-C27-C28-C29
31	C	518	DGD	C8B-C9B-CAB-CBB
31	c	917	DGD	C2B-C3B-C4B-C5B
31	h	102	DGD	CDB-CEB-CFB-CGB
24	a	406	CLA	C4C-C3C-CAC-CBC
28	a	402	SQD	C15-C16-C17-C18
28	a	411	SQD	C10-C11-C12-C13
31	j	101	DGD	C9B-CAB-CBB-CCB
26	B	618	BCR	C1-C6-C7-C8
31	c	916	DGD	CAB-CBB-CCB-CDB
24	B	616	CLA	C10-C11-C12-C13
24	C	508	CLA	C5-C6-C7-C8
31	c	916	DGD	C5B-C6B-C7B-C8B
31	c	917	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
24	c	907	CLA	C13-C15-C16-C17
28	A	613	SQD	C32-C33-C34-C35
29	D	409	LHG	C12-C13-C14-C15
24	C	501	CLA	C16-C17-C18-C19
24	C	502	CLA	C16-C17-C18-C20
24	B	602	CLA	CAA-CBA-CGA-O2A
28	L	101	SQD	O47-C45-C46-O48
28	d	407	SQD	O47-C45-C46-O48
28	l	101	SQD	O47-C45-C46-O48
27	a	410	PL9	C4-C3-C7-C8
31	C	518	DGD	C3B-C4B-C5B-C6B
24	a	408	CLA	C3-C5-C6-C7
28	A	613	SQD	C35-C36-C37-C38
26	B	622	BCR	C18-C19-C20-C21
26	D	404	BCR	C18-C19-C20-C21
31	D	406	DGD	CAB-CBB-CCB-CDB
24	B	617	CLA	C16-C17-C18-C19
31	D	406	DGD	C5B-C6B-C7B-C8B
31	d	406	DGD	C4A-C5A-C6A-C7A
24	B	612	CLA	C14-C13-C15-C16
24	D	403	CLA	C6-C7-C8-C9
24	b	612	CLA	C14-C13-C15-C16
24	c	907	CLA	C11-C10-C8-C9
28	L	101	SQD	O10-C23-O48-C46
26	A	610	BCR	C14-C15-C16-C17
31	c	916	DGD	CAA-CBA-CCA-CDA
28	d	407	SQD	C28-C29-C30-C31
24	A	614	CLA	C2C-C3C-CAC-CBC
24	c	907	CLA	C3-C5-C6-C7
26	B	619	BCR	C19-C20-C21-C22
31	h	102	DGD	O2G-C1B-C2B-C3B
24	C	510	CLA	C2-C3-C5-C6
24	B	604	CLA	C16-C17-C18-C19
24	c	907	CLA	C16-C17-C18-C20
28	l	101	SQD	C30-C31-C32-C33
24	B	602	CLA	C15-C16-C17-C18
24	B	607	CLA	C8-C10-C11-C12
29	B	621	LHG	C33-C34-C35-C36
26	k	101	BCR	C20-C21-C22-C37
24	B	602	CLA	C16-C17-C18-C19
24	C	501	CLA	C16-C17-C18-C20
24	C	502	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	B	612	CLA	C12-C13-C15-C16
24	B	615	CLA	C12-C13-C15-C16
24	B	616	CLA	C11-C10-C8-C7
24	B	617	CLA	C12-C13-C15-C16
24	C	504	CLA	C12-C13-C15-C16
24	a	407	CLA	C6-C7-C8-C10
24	b	602	CLA	C6-C7-C8-C10
28	a	402	SQD	C24-C25-C26-C27
29	B	621	LHG	C14-C15-C16-C17
29	D	409	LHG	C13-C14-C15-C16
29	b	620	LHG	C31-C32-C33-C34
31	h	102	DGD	CDA-CEA-CFA-CGA
26	K	101	BCR	C7-C8-C9-C10
24	c	904	CLA	CBA-CGA-O2A-C1
24	c	914	CLA	CBA-CGA-O2A-C1
31	C	517	DGD	C2G-C3G-O3G-C1D
31	C	517	DGD	C5D-C6D-O5D-C1E
31	c	917	DGD	C2G-C3G-O3G-C1D
31	c	917	DGD	C5D-C6D-O5D-C1E
31	c	917	DGD	C8B-C9B-CAB-CBB
24	C	508	CLA	O1D-CGD-O2D-CED
28	L	101	SQD	C16-C17-C18-C19
29	a	413	LHG	C17-C18-C19-C20
31	j	101	DGD	C6B-C7B-C8B-C9B
24	D	402	CLA	C2C-C3C-CAC-CBC
29	B	621	LHG	C34-C35-C36-C37
29	D	407	LHG	C13-C14-C15-C16
24	B	602	CLA	O1A-CGA-O2A-C1
24	c	912	CLA	O1A-CGA-O2A-C1
32	E	101	HEM	C2C-C3C-CAC-CBC
32	v	202	HEM	C2B-C3B-CAB-CBB
29	d	410	LHG	O1-C1-C2-C3
28	a	402	SQD	C18-C19-C20-C21
31	C	517	DGD	C8A-C9A-CAA-CBA
31	H	102	DGD	CCB-CDB-CEB-CFB
29	d	410	LHG	C32-C33-C34-C35
26	B	622	BCR	C14-C15-C16-C17
24	b	608	CLA	C3-C5-C6-C7
29	A	615	LHG	O6-C4-C5-O7
24	C	510	CLA	C4-C3-C5-C6
28	a	402	SQD	C31-C32-C33-C34
29	D	407	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	d	406	DGD	O1G-C1G-C2G-O2G
24	B	617	CLA	C14-C13-C15-C16
24	a	407	CLA	C6-C7-C8-C9
29	D	409	LHG	C16-C17-C18-C19
29	D	409	LHG	C17-C18-C19-C20
24	c	904	CLA	O1A-CGA-O2A-C1
29	B	621	LHG	C24-C25-C26-C27
29	D	408	LHG	C11-C10-C9-C8
31	C	518	DGD	C4A-C5A-C6A-C7A
24	C	503	CLA	C8-C10-C11-C12
28	A	613	SQD	C24-C25-C26-C27
28	a	402	SQD	C25-C26-C27-C28
24	c	914	CLA	O1A-CGA-O2A-C1
26	f	101	BCR	C13-C14-C15-C16
28	A	613	SQD	C2-C1-O6-C44
24	b	615	CLA	O1D-CGD-O2D-CED
31	H	102	DGD	CCA-CDA-CEA-CFA
28	F	101	SQD	C11-C10-C9-C8
24	c	902	CLA	C13-C15-C16-C17
28	A	613	SQD	C29-C30-C31-C32
24	B	611	CLA	C16-C17-C18-C19
24	c	911	CLA	C16-C17-C18-C19
24	B	614	CLA	C13-C15-C16-C17
31	c	916	DGD	C5A-C6A-C7A-C8A
28	A	613	SQD	C27-C28-C29-C30
24	B	605	CLA	C3-C5-C6-C7
24	C	510	CLA	O1D-CGD-O2D-CED
24	b	604	CLA	C16-C17-C18-C20
24	D	403	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	C1A-C2A-CAA-CBA
28	d	407	SQD	O47-C7-C8-C9
31	d	406	DGD	C7A-C8A-C9A-CAA
31	C	517	DGD	C5A-C6A-C7A-C8A
29	D	409	LHG	C27-C28-C29-C30
31	H	102	DGD	C5B-C6B-C7B-C8B
24	A	607	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C10
24	C	509	CLA	C6-C7-C8-C10
24	D	403	CLA	C11-C12-C13-C15
24	D	403	CLA	C12-C13-C15-C16
24	b	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	b	617	CLA	C11-C10-C8-C7
24	c	905	CLA	C12-C13-C15-C16
24	c	907	CLA	C6-C7-C8-C10
24	c	908	CLA	C11-C12-C13-C15
24	d	404	CLA	C11-C12-C13-C15
24	b	607	CLA	C16-C17-C18-C19
24	c	914	CLA	C16-C17-C18-C20
31	D	406	DGD	CDB-CEB-CFB-CGB
28	a	411	SQD	C31-C32-C33-C34
29	A	615	LHG	C10-C11-C12-C13
29	D	408	LHG	C26-C27-C28-C29
31	C	518	DGD	C9A-CAA-CBA-CCA
29	d	409	LHG	C26-C27-C28-C29
29	B	621	LHG	C31-C32-C33-C34
31	C	517	DGD	CBA-CCA-CDA-CEA
24	c	913	CLA	O1A-CGA-O2A-C1
24	B	616	CLA	C16-C17-C18-C20
24	B	611	CLA	C8-C10-C11-C12
24	A	607	CLA	C11-C10-C8-C9
24	C	504	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C9
24	b	602	CLA	C6-C7-C8-C9
28	A	613	SQD	C9-C10-C11-C12
24	A	609	CLA	O1D-CGD-O2D-CED
29	d	408	LHG	C15-C16-C17-C18
29	A	615	LHG	O7-C5-C6-O8
31	D	406	DGD	O1G-C1G-C2G-O2G
28	F	101	SQD	C28-C29-C30-C31
24	b	612	CLA	O1D-CGD-O2D-CED
31	D	406	DGD	CBB-CCB-CDB-CEB
28	a	402	SQD	O6-C44-C45-C46
24	C	513	CLA	C3-C5-C6-C7
24	B	608	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	CAD-CBD-CGD-O2D
24	c	905	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	O1D-CGD-O2D-CED
24	c	913	CLA	CBA-CGA-O2A-C1
31	C	517	DGD	CDA-CEA-CFA-CGA
28	L	101	SQD	C19-C20-C21-C22
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	611	CLA	CHA-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	602	CLA	CAD-CBD-CGD-O1D
24	b	605	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CAD-CBD-CGD-O1D
24	b	617	CLA	CHA-CBD-CGD-O1D
24	c	903	CLA	CAD-CBD-CGD-O1D
24	c	905	CLA	CAD-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O2D
24	c	910	CLA	CHA-CBD-CGD-O1D
29	D	408	LHG	C3-O3-P-O4
29	d	409	LHG	C3-O3-P-O4
29	d	409	LHG	C3-O3-P-O6
24	b	610	CLA	C2B-C3B-CAB-CBB
26	D	404	BCR	C23-C24-C25-C30
26	k	101	BCR	C5-C6-C7-C8
26	A	610	BCR	C36-C18-C19-C20
26	k	102	BCR	C36-C18-C19-C20
29	D	409	LHG	C2-C3-O3-P
29	d	410	LHG	C2-C3-O3-P
31	C	516	DGD	CBA-CCA-CDA-CEA
31	c	916	DGD	CCA-CDA-CEA-CFA
24	c	911	CLA	C16-C17-C18-C20
29	D	407	LHG	C33-C34-C35-C36
28	l	101	SQD	C13-C14-C15-C16
29	B	621	LHG	C26-C27-C28-C29
31	C	516	DGD	CDA-CEA-CFA-CGA
31	H	102	DGD	CDA-CEA-CFA-CGA
28	L	101	SQD	C46-C45-O47-C7
31	j	101	DGD	O6D-C5D-C6D-O5D
26	f	101	BCR	C10-C11-C12-C13
27	d	405	PL9	C39-C41-C42-C43
28	A	612	SQD	C23-C24-C25-C26
24	B	611	CLA	C16-C17-C18-C20
24	C	512	CLA	C16-C17-C18-C19
29	d	410	LHG	C25-C26-C27-C28
24	A	609	CLA	C11-C10-C8-C9
24	B	616	CLA	C11-C10-C8-C9
24	B	617	CLA	C6-C7-C8-C9
24	C	513	CLA	C6-C7-C8-C9
24	a	407	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	607	CLA	C14-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C10
24	C	506	CLA	C12-C13-C15-C16
26	B	622	BCR	C20-C21-C22-C23
31	c	916	DGD	C8B-C9B-CAB-CBB
31	j	101	DGD	C5A-C6A-C7A-C8A
26	b	619	BCR	C22-C23-C24-C25
24	C	502	CLA	C16-C17-C18-C19
26	T	102	BCR	C14-C15-C16-C17
26	b	618	BCR	C14-C15-C16-C17
28	a	402	SQD	C2-C1-O6-C44
31	C	517	DGD	C2E-C1E-O5D-C6D
25	A	608	PHO	C4-C3-C5-C6
29	B	621	LHG	C25-C26-C27-C28
24	B	616	CLA	C16-C17-C18-C19
31	H	102	DGD	O2G-C1B-C2B-C3B
24	d	401	CLA	C4C-C3C-CAC-CBC
28	L	101	SQD	C14-C15-C16-C17
31	d	406	DGD	CDA-CEA-CFA-CGA
24	c	910	CLA	C2-C1-O2A-CGA
24	b	604	CLA	C16-C17-C18-C19
24	c	908	CLA	C5-C6-C7-C8
28	a	402	SQD	C27-C28-C29-C30
31	c	917	DGD	C4A-C5A-C6A-C7A
24	b	613	CLA	C10-C11-C12-C13
26	k	102	BCR	C17-C18-C19-C20
31	c	916	DGD	C5D-C6D-O5D-C1E
31	C	516	DGD	C1B-C2B-C3B-C4B
28	a	402	SQD	O5-C1-O6-C44
25	A	608	PHO	C2-C3-C5-C6
27	a	410	PL9	C2-C3-C7-C8
24	B	602	CLA	C6-C7-C8-C9
24	B	616	CLA	C14-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C9
24	d	404	CLA	C6-C7-C8-C9
29	B	621	LHG	C11-C10-C9-C8
24	d	403	CLA	C4B-C3B-CAB-CBB
24	c	913	CLA	C15-C16-C17-C18
28	a	411	SQD	C24-C23-O48-C46
32	E	101	HEM	C4C-C3C-CAC-CBC
32	V	202	HEM	C4C-C3C-CAC-CBC
32	v	202	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	a	411	SQD	C34-C35-C36-C37
31	h	102	DGD	CCB-CDB-CEB-CFB
24	A	609	CLA	C12-C13-C15-C16
24	c	914	CLA	C11-C10-C8-C7
24	b	613	CLA	C3-C5-C6-C7
31	C	518	DGD	C7A-C8A-C9A-CAA
24	C	512	CLA	C16-C17-C18-C20
31	c	916	DGD	C4A-C5A-C6A-C7A
24	C	510	CLA	O1A-CGA-O2A-C1
29	a	413	LHG	O10-C23-O8-C6
24	c	913	CLA	C3A-C2A-CAA-CBA
24	C	510	CLA	C8-C10-C11-C12
26	b	618	BCR	C16-C17-C18-C36
24	A	606	CLA	C2C-C3C-CAC-CBC
31	c	916	DGD	C7A-C8A-C9A-CAA
29	d	408	LHG	C32-C33-C34-C35
24	D	402	CLA	C2-C1-O2A-CGA
26	T	101	BCR	C13-C14-C15-C16
26	Y	101	BCR	C15-C16-C17-C18
28	a	411	SQD	O10-C23-O48-C46
29	A	615	LHG	C17-C18-C19-C20
24	B	611	CLA	C13-C15-C16-C17
26	A	610	BCR	C17-C18-C19-C20
27	A	611	PL9	C2-C3-C7-C8
24	b	613	CLA	CBA-CGA-O2A-C1
27	D	405	PL9	C39-C41-C42-C43
31	C	518	DGD	CAB-CBB-CCB-CDB
24	B	611	CLA	C14-C13-C15-C16
24	b	602	CLA	C11-C12-C13-C14
24	b	614	CLA	C11-C12-C13-C14
24	b	614	CLA	C14-C13-C15-C16
24	b	615	CLA	C6-C7-C8-C9
24	b	617	CLA	C14-C13-C15-C16
24	c	913	CLA	C6-C7-C8-C9
24	c	914	CLA	C11-C10-C8-C9
24	c	914	CLA	C11-C12-C13-C14
31	C	517	DGD	C4B-C5B-C6B-C7B
28	A	613	SQD	C10-C11-C12-C13
31	C	516	DGD	C2B-C3B-C4B-C5B
29	a	413	LHG	C24-C23-O8-C6
24	B	606	CLA	CBD-CGD-O2D-CED
29	b	620	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	c	913	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C16-C17-C18-C19
24	b	611	CLA	C15-C16-C17-C18
26	B	618	BCR	C5-C6-C7-C8
26	H	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30
26	T	102	BCR	C1-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C30
26	k	101	BCR	C1-C6-C7-C8
24	C	510	CLA	CBA-CGA-O2A-C1
29	A	615	LHG	C9-C10-C11-C12
29	D	409	LHG	C28-C29-C30-C31
31	C	516	DGD	CBB-CCB-CDB-CEB
32	E	101	HEM	CAD-CBD-CGD-O1D
24	C	513	CLA	C4-C3-C5-C6
24	B	611	CLA	C12-C13-C15-C16
24	C	502	CLA	C12-C13-C15-C16
24	C	504	CLA	C11-C10-C8-C7
24	a	408	CLA	C11-C10-C8-C7
24	b	616	CLA	C11-C10-C8-C7
24	c	914	CLA	C6-C7-C8-C10
24	B	617	CLA	C13-C15-C16-C17
28	A	612	SQD	O6-C44-C45-O47
31	H	102	DGD	O1G-C1G-C2G-O2G
31	c	917	DGD	CBB-CCB-CDB-CEB
28	d	407	SQD	C11-C10-C9-C8
32	e	101	HEM	CAA-CBA-CGA-O1A
32	V	202	HEM	CAD-CBD-CGD-O2D
32	v	202	HEM	CAD-CBD-CGD-O2D
24	d	403	CLA	C13-C15-C16-C17
29	d	408	LHG	C26-C27-C28-C29
31	H	102	DGD	CAA-CBA-CCA-CDA
24	A	607	CLA	C6-C7-C8-C9
31	d	406	DGD	CBB-CCB-CDB-CEB
24	c	914	CLA	C5-C6-C7-C8
24	C	507	CLA	C4-C3-C5-C6
24	b	606	CLA	C13-C15-C16-C17
26	a	409	BCR	C14-C15-C16-C17
28	d	407	SQD	C29-C30-C31-C32
31	c	917	DGD	C2E-C1E-O5D-C6D
31	H	102	DGD	O1G-C1G-C2G-C3G
32	E	101	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	V	202	HEM	CAD-CBD-CGD-O1D
32	e	101	HEM	CAA-CBA-CGA-O2A
24	b	613	CLA	O1A-CGA-O2A-C1
24	c	913	CLA	C3-C5-C6-C7
24	C	501	CLA	C2A-CAA-CBA-CGA
24	B	616	CLA	C4B-C3B-CAB-CBB
32	v	202	HEM	CAD-CBD-CGD-O1D
29	d	408	LHG	C23-C24-C25-C26
25	D	401	PHO	CHA-CBD-CGD-O1D
25	a	412	PHO	CHA-CBD-CGD-O1D
29	b	620	LHG	C30-C31-C32-C33
29	A	615	LHG	O6-C4-C5-C6
31	C	516	DGD	O6E-C1E-O5D-C6D
31	c	917	DGD	O6E-C1E-O5D-C6D
24	c	908	CLA	C15-C16-C17-C18
24	b	615	CLA	C6-C7-C8-C10
24	c	905	CLA	C11-C12-C13-C15
29	D	407	LHG	C31-C32-C33-C34
24	B	604	CLA	C6-C7-C8-C9
24	b	615	CLA	C11-C12-C13-C14
24	b	617	CLA	C11-C10-C8-C9
24	c	905	CLA	C14-C13-C15-C16
24	c	910	CLA	C14-C13-C15-C16
28	F	101	SQD	C45-C44-O6-C1
31	D	406	DGD	C2G-C3G-O3G-C1D
24	B	604	CLA	C13-C15-C16-C17
24	C	509	CLA	C2-C1-O2A-CGA
24	d	403	CLA	C2-C1-O2A-CGA
31	j	101	DGD	C8A-C9A-CAA-CBA
31	C	518	DGD	O1A-C1A-O1G-C1G
31	h	102	DGD	C9B-CAB-CBB-CCB
26	A	610	BCR	C18-C19-C20-C21
31	C	518	DGD	C2A-C1A-O1G-C1G
26	B	619	BCR	C14-C15-C16-C17
24	B	602	CLA	CAA-CBA-CGA-O1A
31	j	101	DGD	C2B-C3B-C4B-C5B
24	c	908	CLA	C2A-CAA-CBA-CGA
29	D	408	LHG	C13-C14-C15-C16
24	A	609	CLA	C4-C3-C5-C6
27	d	405	PL9	C43-C44-C46-C47
24	B	607	CLA	C16-C17-C18-C20
26	b	618	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	a	413	LHG	O6-C4-C5-O7
28	a	411	SQD	C7-C8-C9-C10
31	C	517	DGD	O6E-C1E-O5D-C6D
24	b	604	CLA	C13-C15-C16-C17
29	A	615	LHG	C4-C5-C6-O8
28	L	101	SQD	C33-C34-C35-C36
24	A	609	CLA	O1A-CGA-O2A-C1
26	H	101	BCR	C9-C10-C11-C12
31	j	101	DGD	CDA-CEA-CFA-CGA
28	L	101	SQD	C17-C18-C19-C20
31	D	406	DGD	O2G-C2G-C3G-O3G
26	k	102	BCR	C14-C15-C16-C17
24	B	607	CLA	C11-C12-C13-C14
24	c	908	CLA	C11-C12-C13-C14
24	d	404	CLA	C11-C12-C13-C14
31	C	518	DGD	O6D-C5D-C6D-O5D
24	C	512	CLA	CAA-CBA-CGA-O2A
29	a	413	LHG	O6-C4-C5-C6
24	A	614	CLA	C4C-C3C-CAC-CBC
24	A	607	CLA	C6-C7-C8-C10
24	B	604	CLA	C6-C7-C8-C10
24	B	615	CLA	C11-C10-C8-C7
24	C	504	CLA	C11-C12-C13-C15
24	D	402	CLA	C12-C13-C15-C16
24	b	615	CLA	C11-C12-C13-C15
24	b	617	CLA	C12-C13-C15-C16
24	c	907	CLA	C12-C13-C15-C16
24	c	910	CLA	C12-C13-C15-C16
24	B	608	CLA	C2B-C3B-CAB-CBB
24	B	614	CLA	C2B-C3B-CAB-CBB
24	D	402	CLA	C2B-C3B-CAB-CBB
24	c	906	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
26	T	102	BCR	C5-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C26
29	d	408	LHG	C11-C12-C13-C14
29	b	620	LHG	C35-C36-C37-C38
27	d	405	PL9	C45-C44-C46-C47
31	d	406	DGD	O1G-C1A-C2A-C3A
24	c	906	CLA	C2-C3-C5-C6
24	c	909	CLA	C10-C11-C12-C13
29	D	407	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
24	C	513	CLA	C16-C17-C18-C20
29	A	615	LHG	O7-C7-C8-C9
24	b	602	CLA	C4-C3-C5-C6
24	c	906	CLA	C4-C3-C5-C6
28	l	101	SQD	O48-C23-C24-C25
24	B	606	CLA	C13-C15-C16-C17
28	A	612	SQD	C18-C19-C20-C21
24	c	909	CLA	C13-C15-C16-C17
32	e	101	HEM	CAD-CBD-CGD-O1D
32	e	101	HEM	CAD-CBD-CGD-O2D
24	D	403	CLA	C11-C12-C13-C14
24	B	602	CLA	C4B-C3B-CAB-CBB
29	D	409	LHG	C33-C34-C35-C36
31	c	916	DGD	O6E-C1E-O5D-C6D
24	c	913	CLA	CAA-CBA-CGA-O2A
26	k	101	BCR	C11-C12-C13-C14
26	K	101	BCR	C9-C10-C11-C12
26	f	101	BCR	C9-C10-C11-C12
28	a	411	SQD	O48-C23-C24-C25
31	C	518	DGD	O1G-C1A-C2A-C3A
31	D	406	DGD	O1G-C1A-C2A-C3A
24	b	615	CLA	C2-C1-O2A-CGA
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C15
24	b	616	CLA	C12-C13-C15-C16
28	A	613	SQD	C11-C12-C13-C14
29	d	408	LHG	C13-C14-C15-C16
24	A	606	CLA	C4C-C3C-CAC-CBC
29	D	409	LHG	C19-C20-C21-C22
24	b	617	CLA	C8-C10-C11-C12
28	L	101	SQD	C45-C46-O48-C23
26	K	101	BCR	C14-C15-C16-C17
24	C	512	CLA	CAA-CBA-CGA-O1A
31	h	102	DGD	O1B-C1B-C2B-C3B
24	A	609	CLA	CBA-CGA-O2A-C1
27	A	611	PL9	C26-C27-C28-C29
24	C	504	CLA	C11-C10-C8-C9
24	C	505	CLA	C14-C13-C15-C16
24	C	513	CLA	C11-C12-C13-C14
24	D	403	CLA	C14-C13-C15-C16
24	a	408	CLA	C11-C10-C8-C9
24	b	616	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	616	CLA	C14-C13-C15-C16
24	c	914	CLA	C6-C7-C8-C9
29	B	621	LHG	C5-C6-O8-C23
24	C	507	CLA	C2-C3-C5-C6
24	B	613	CLA	O1A-CGA-O2A-C1
24	B	613	CLA	C8-C10-C11-C12
31	D	406	DGD	O1A-C1A-C2A-C3A
24	B	616	CLA	C15-C16-C17-C18
28	A	612	SQD	C45-C44-O6-C1
31	C	516	DGD	C5D-C6D-O5D-C1E
31	h	102	DGD	C2G-C3G-O3G-C1D
29	D	407	LHG	C11-C10-C9-C8
28	l	101	SQD	O10-C23-C24-C25
31	C	518	DGD	O1A-C1A-C2A-C3A
24	b	604	CLA	C2A-CAA-CBA-CGA
24	b	611	CLA	C16-C17-C18-C20
24	c	913	CLA	CAA-CBA-CGA-O1A
27	a	410	PL9	C45-C44-C46-C47
24	C	506	CLA	C15-C16-C17-C18
29	A	615	LHG	O9-C7-C8-C9
24	A	606	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
25	D	401	PHO	CAD-CBD-CGD-O2D
25	d	402	PHO	CAD-CBD-CGD-O2D
31	C	517	DGD	C6A-C7A-C8A-C9A
24	c	906	CLA	CAA-CBA-CGA-O2A
31	j	101	DGD	O1G-C1A-C2A-C3A
31	C	516	DGD	C3A-C4A-C5A-C6A
24	B	602	CLA	C2-C1-O2A-CGA
31	C	516	DGD	C9A-CAA-CBA-CCA
24	b	611	CLA	C16-C17-C18-C19
28	a	411	SQD	O10-C23-C24-C25
31	d	406	DGD	O1A-C1A-C2A-C3A
24	B	602	CLA	C8-C10-C11-C12
29	b	620	LHG	O7-C7-C8-C9

There are no ring outliers.

110 monomers are involved in 277 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	605	CLA	2	0
26	B	618	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	404	BCR	2	0
32	V	202	HEM	9	0
24	c	909	CLA	8	0
24	b	607	CLA	4	0
28	a	402	SQD	3	0
24	C	502	CLA	3	0
24	c	907	CLA	3	0
26	k	102	BCR	2	0
28	d	407	SQD	1	0
24	c	911	CLA	9	0
26	b	619	BCR	3	0
25	a	412	PHO	3	0
26	k	101	BCR	3	0
24	a	406	CLA	2	0
32	v	202	HEM	8	0
24	B	611	CLA	4	0
24	B	609	CLA	2	0
31	C	516	DGD	2	0
24	b	605	CLA	1	0
27	D	405	PL9	1	0
31	C	518	DGD	3	0
27	a	410	PL9	8	0
24	a	407	CLA	3	0
26	B	619	BCR	2	0
28	L	101	SQD	5	0
29	D	407	LHG	3	0
24	b	613	CLA	1	0
24	c	913	CLA	5	0
25	D	401	PHO	4	0
24	b	615	CLA	1	0
24	C	508	CLA	9	0
26	B	620	BCR	1	0
24	B	607	CLA	1	0
24	C	505	CLA	3	0
27	A	611	PL9	9	0
24	b	604	CLA	2	0
31	d	406	DGD	2	0
24	B	617	CLA	4	0
26	H	101	BCR	1	0
24	C	512	CLA	2	0
26	c	915	BCR	2	0
24	B	610	CLA	1	0

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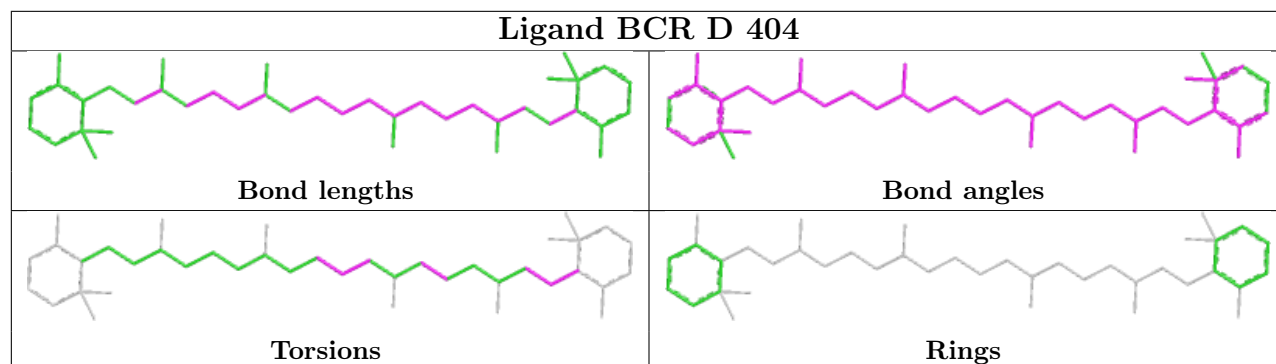
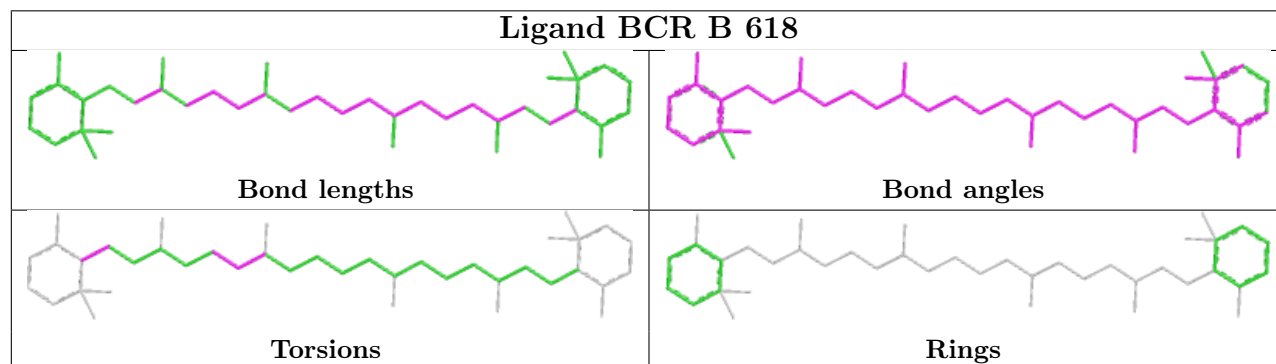
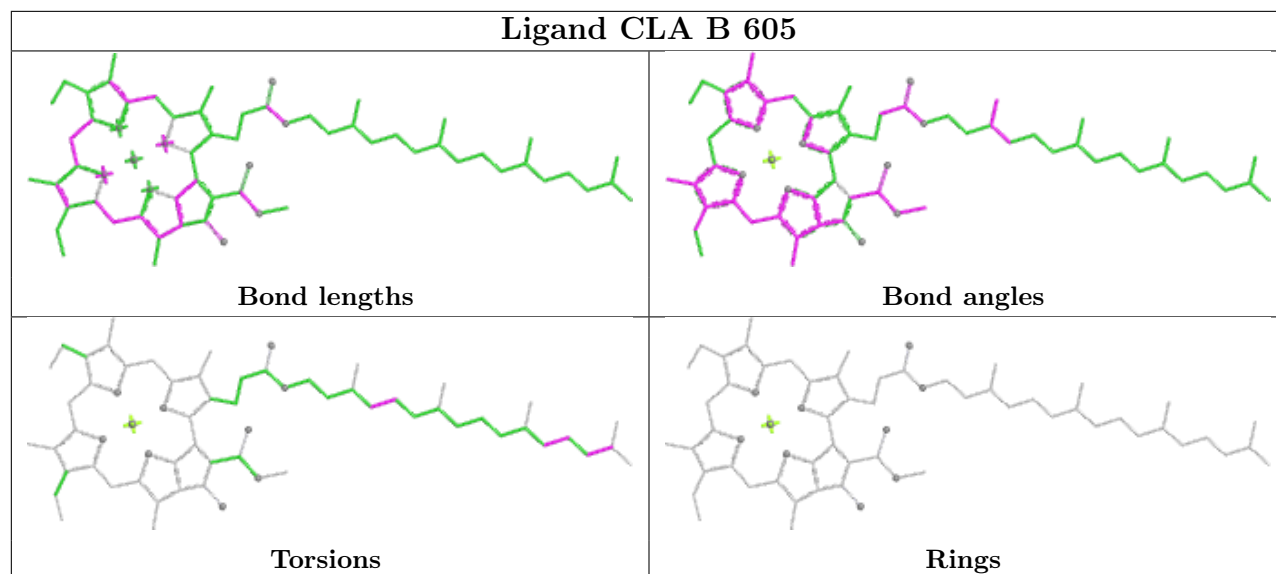
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	618	BCR	2	0
24	c	904	CLA	2	0
29	A	615	LHG	3	0
24	b	614	CLA	3	0
31	h	102	DGD	1	0
24	A	606	CLA	4	0
24	c	908	CLA	1	0
24	A	614	CLA	3	0
25	A	608	PHO	2	0
24	B	612	CLA	3	0
24	c	910	CLA	2	0
29	d	410	LHG	23	0
24	C	503	CLA	2	0
24	d	404	CLA	5	0
24	B	614	CLA	2	0
24	b	616	CLA	3	0
29	b	620	LHG	6	0
24	A	609	CLA	3	0
24	c	905	CLA	5	0
26	T	101	BCR	2	0
28	A	613	SQD	1	0
24	D	403	CLA	1	0
24	a	408	CLA	2	0
31	H	102	DGD	2	0
24	d	403	CLA	4	0
24	B	603	CLA	2	0
24	B	606	CLA	4	0
24	C	504	CLA	6	0
24	d	401	CLA	4	0
28	l	101	SQD	7	0
29	B	621	LHG	3	0
26	K	101	BCR	1	0
29	a	413	LHG	5	0
24	b	606	CLA	3	0
24	C	507	CLA	2	0
24	B	604	CLA	2	0
24	b	617	CLA	3	0
29	d	408	LHG	2	0
26	B	622	BCR	3	0
24	b	612	CLA	3	0
24	c	902	CLA	2	0
24	C	511	CLA	1	0

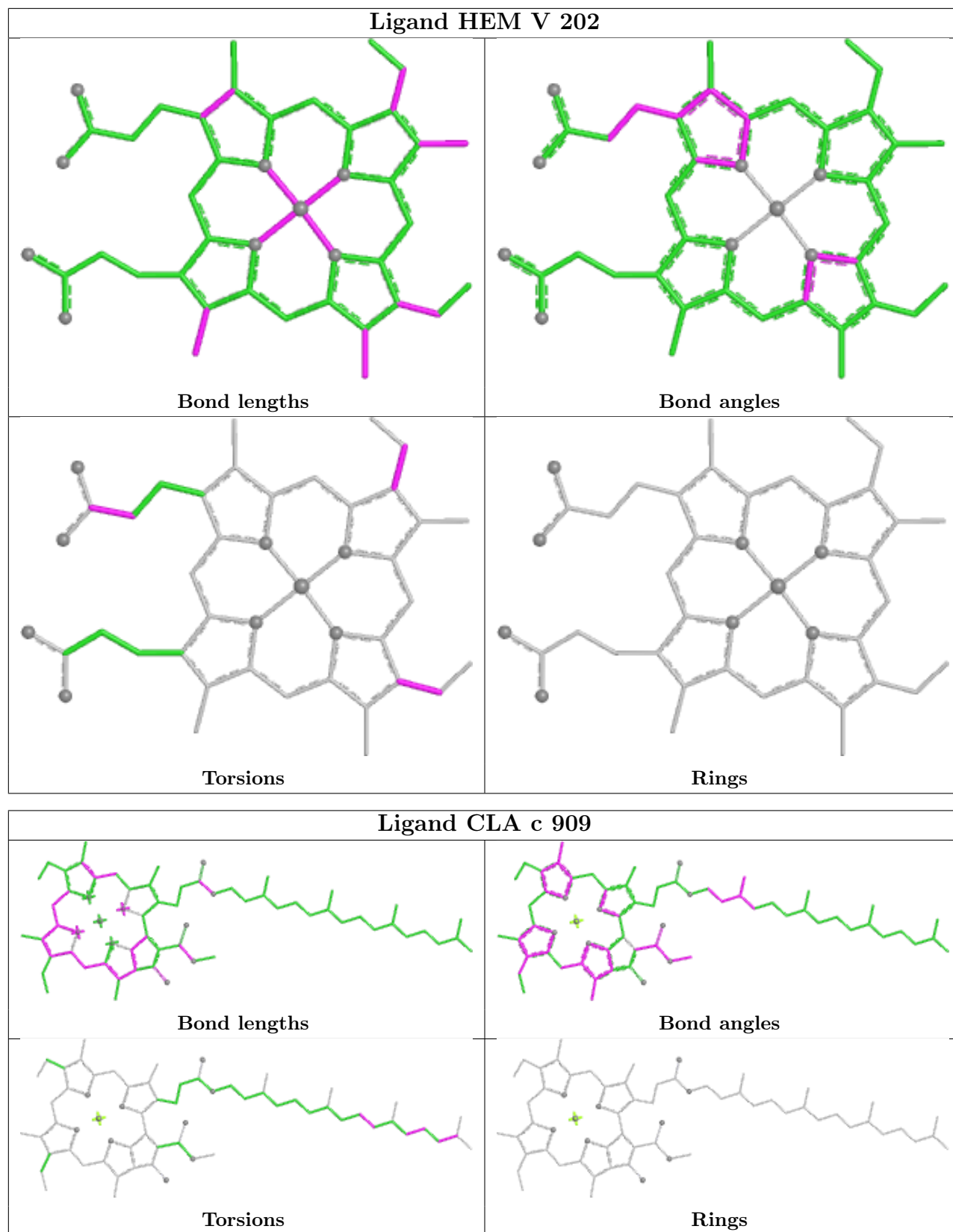
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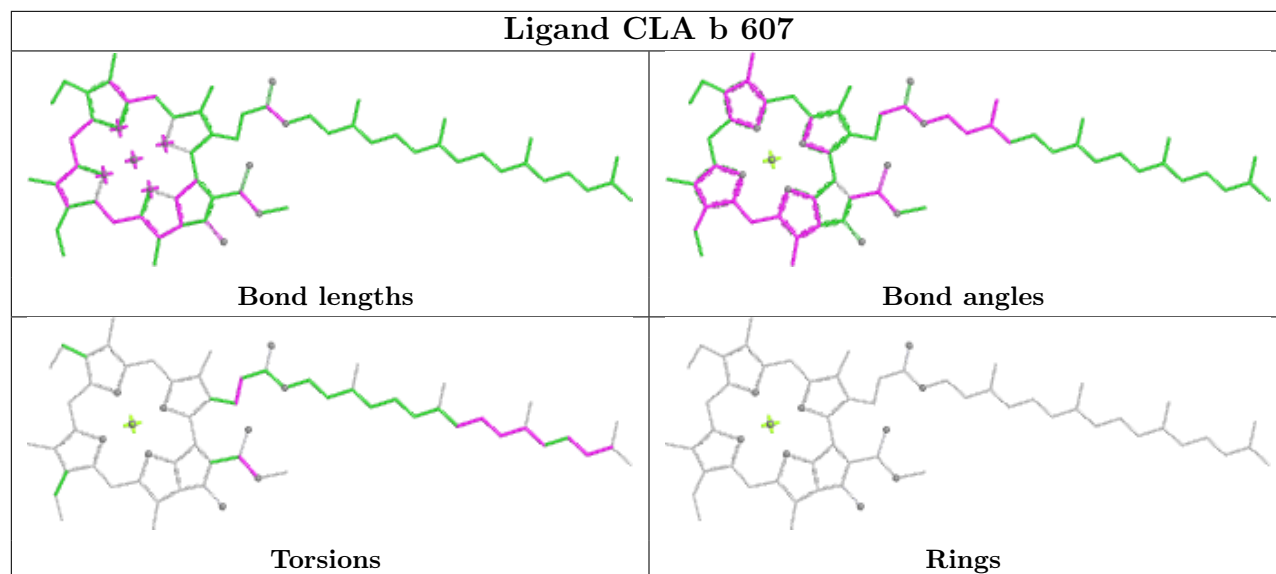
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	918	BCR	1	0
24	C	501	CLA	2	0
31	D	406	DGD	3	0
24	c	906	CLA	7	0
26	h	101	BCR	1	0
24	C	509	CLA	3	0
25	d	402	PHO	1	0
24	b	611	CLA	2	0
31	j	101	DGD	2	0
24	B	613	CLA	1	0
24	C	510	CLA	4	0
27	d	405	PL9	1	0
24	C	506	CLA	3	0
31	C	517	DGD	1	0
28	a	411	SQD	4	0
26	a	409	BCR	1	0
24	B	616	CLA	3	0
29	d	409	LHG	1	0
24	c	912	CLA	2	0
24	c	914	CLA	2	0
29	D	409	LHG	22	0
28	A	612	SQD	5	0
24	c	903	CLA	3	0
26	Y	101	BCR	1	0

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

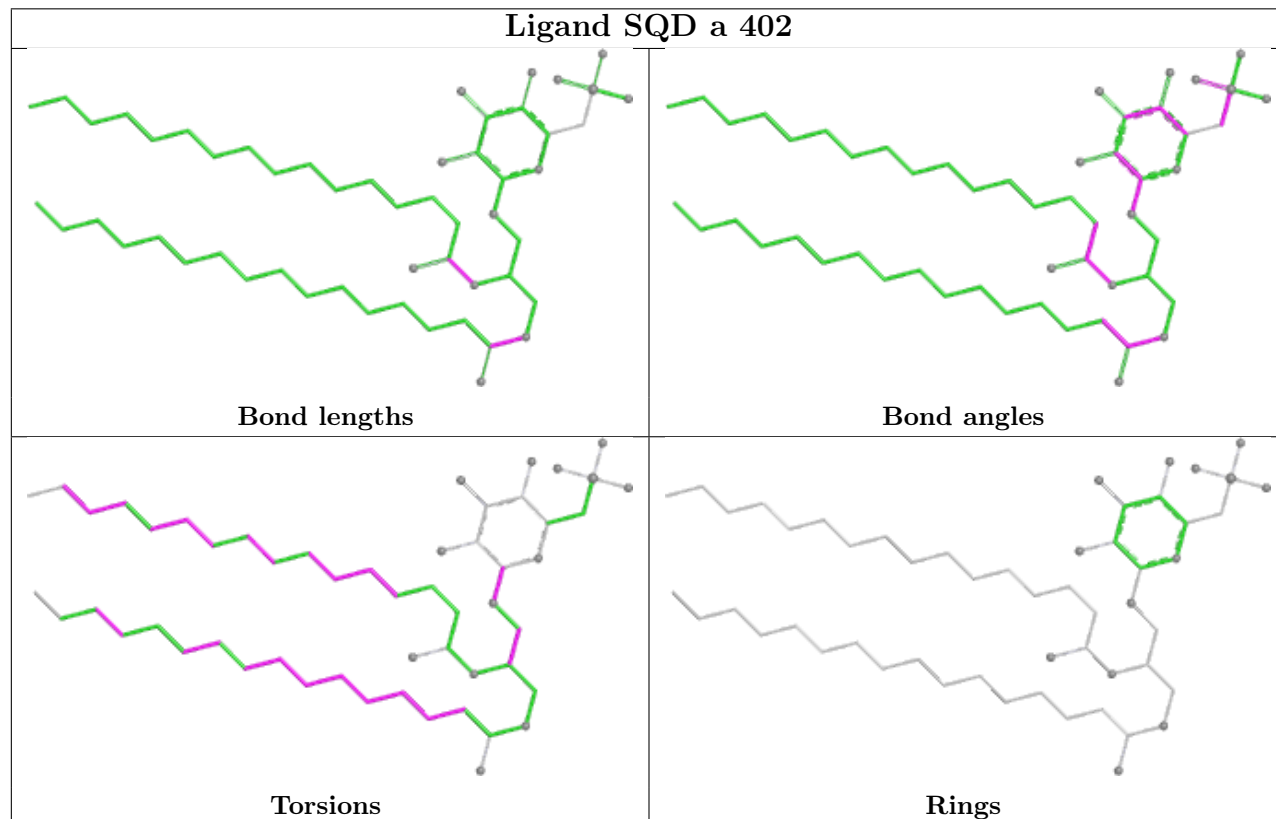


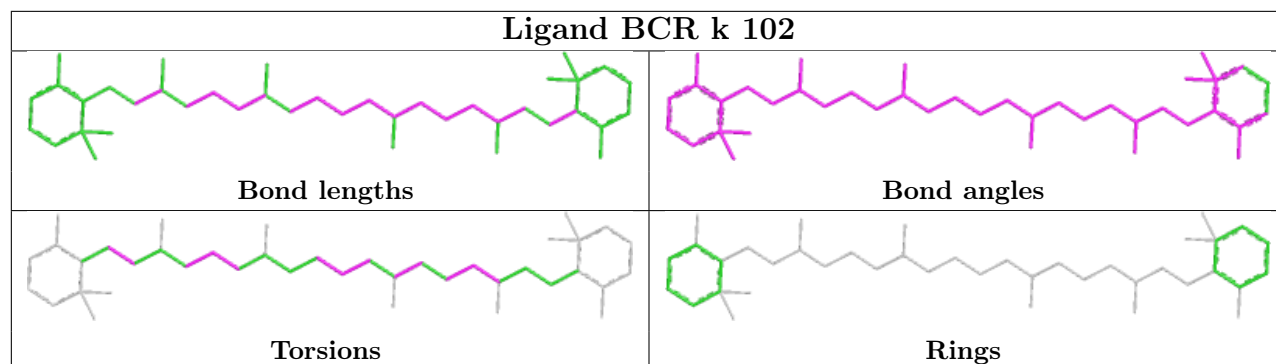
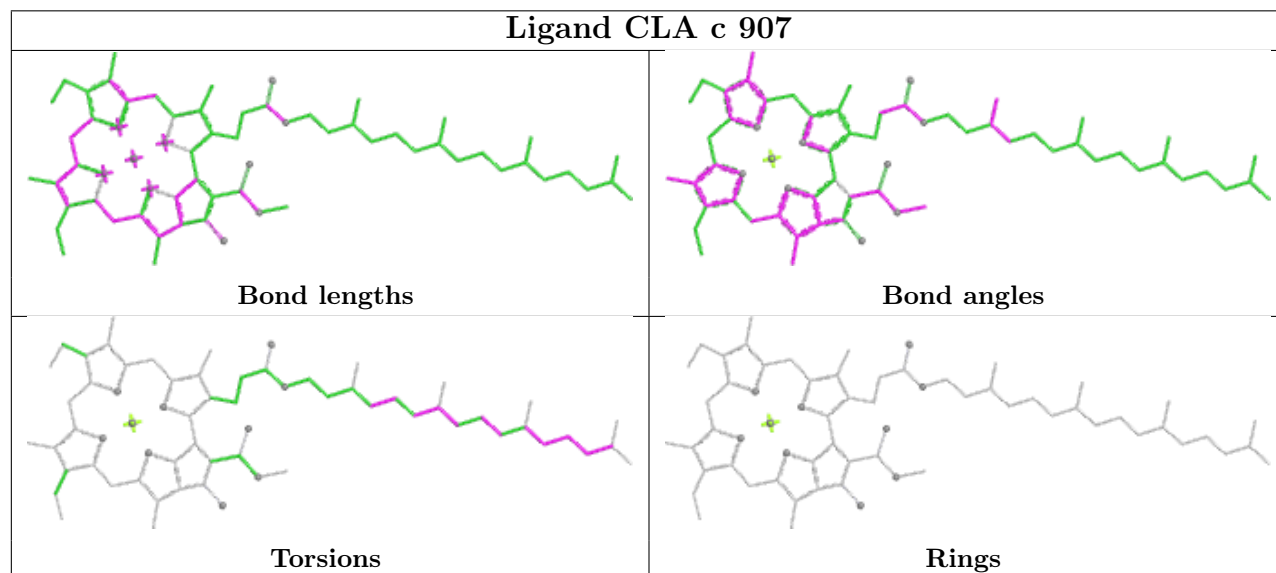
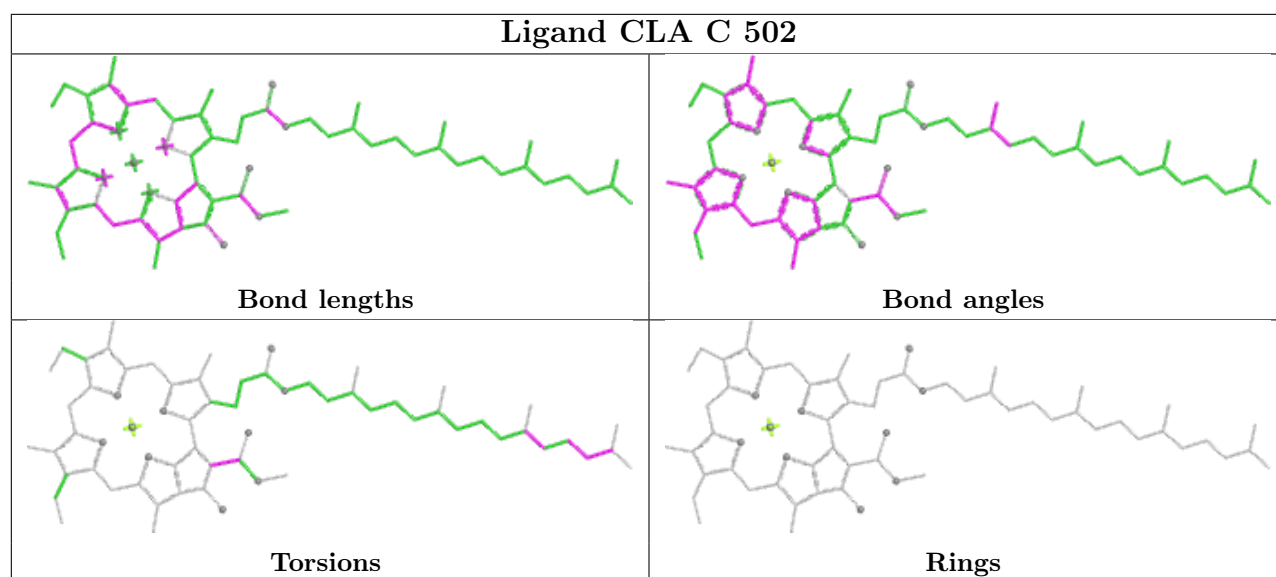


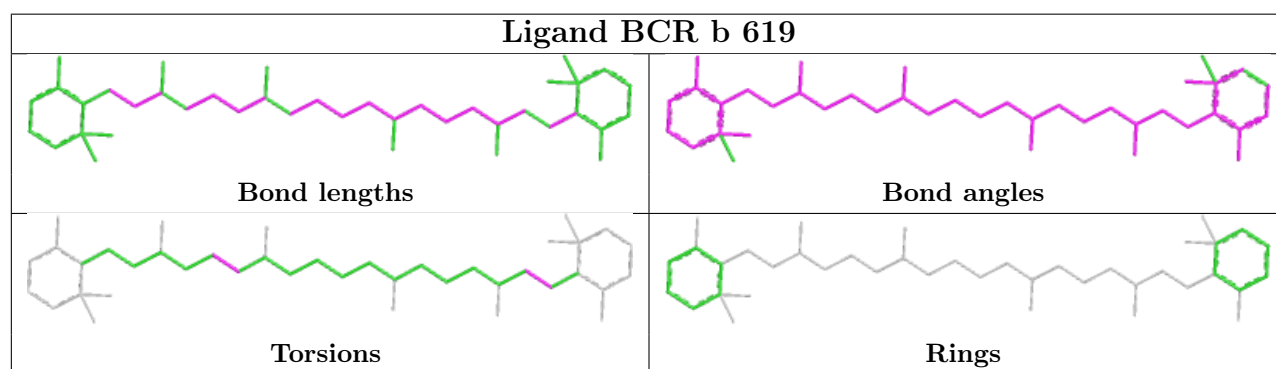
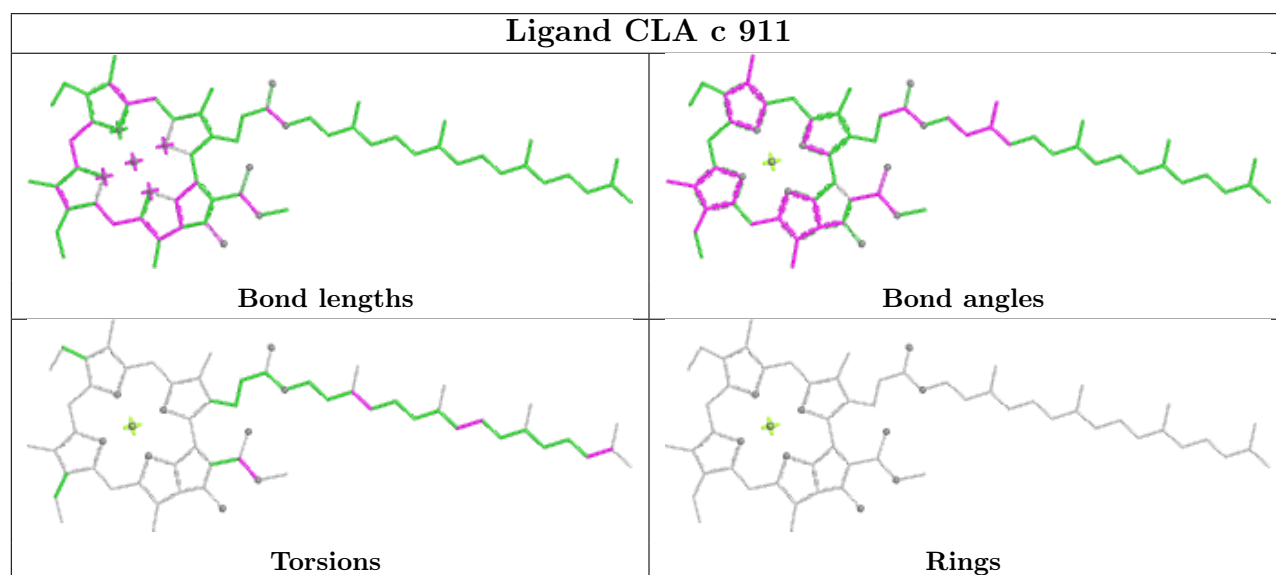
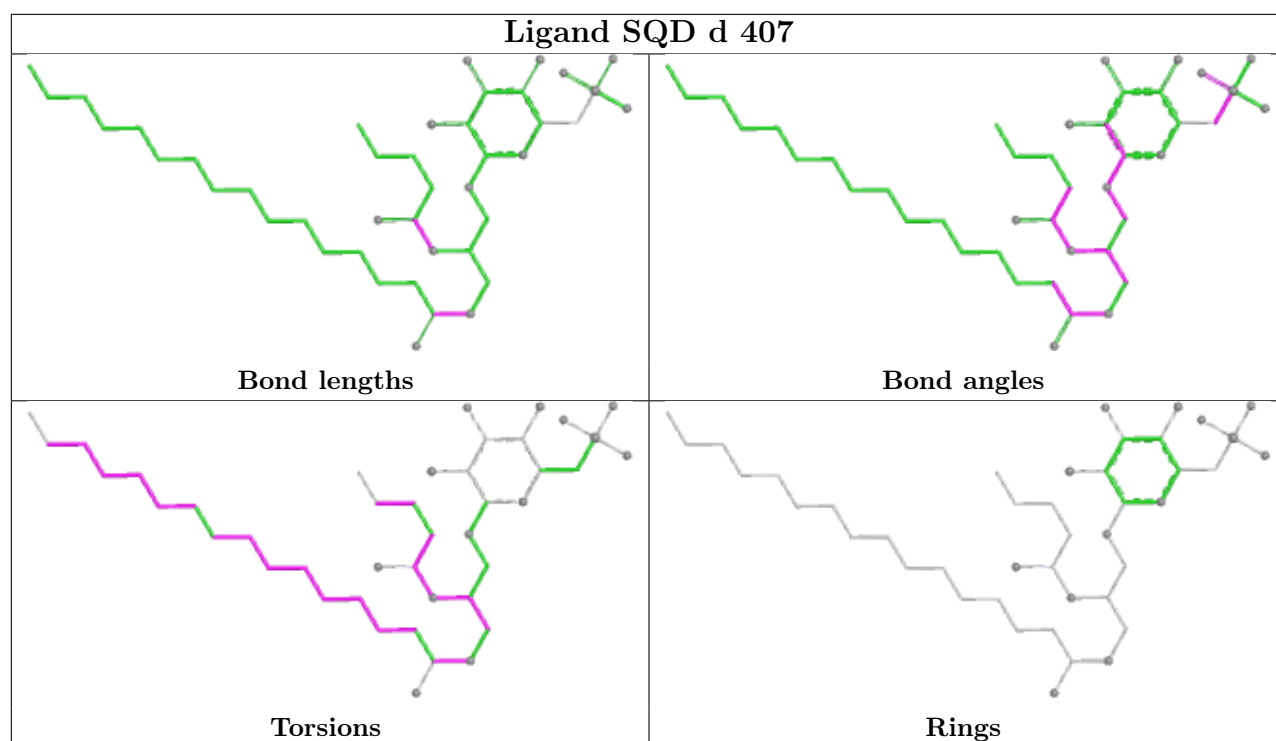
Ligand CLA b 607

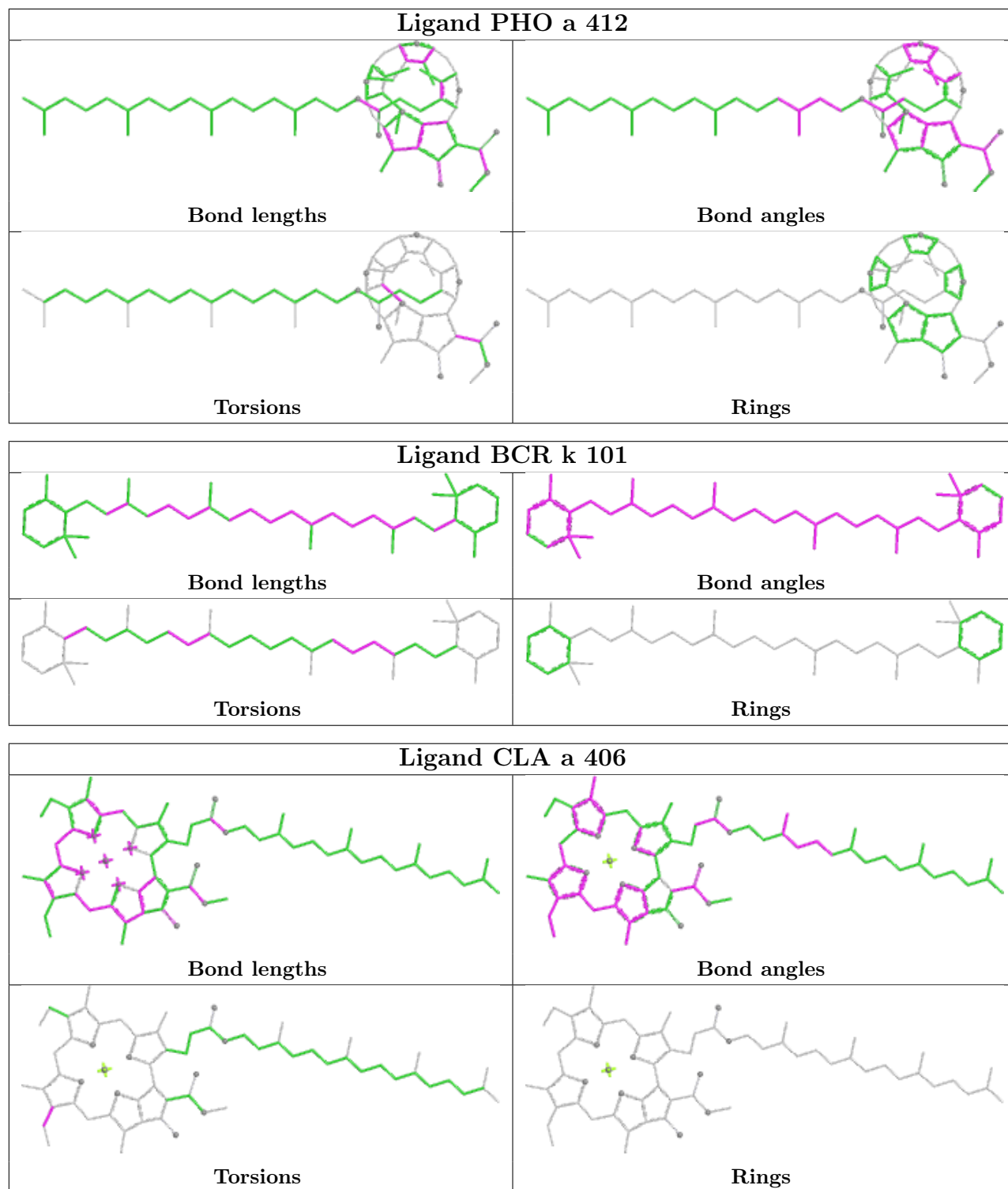


Ligand SQD a 402

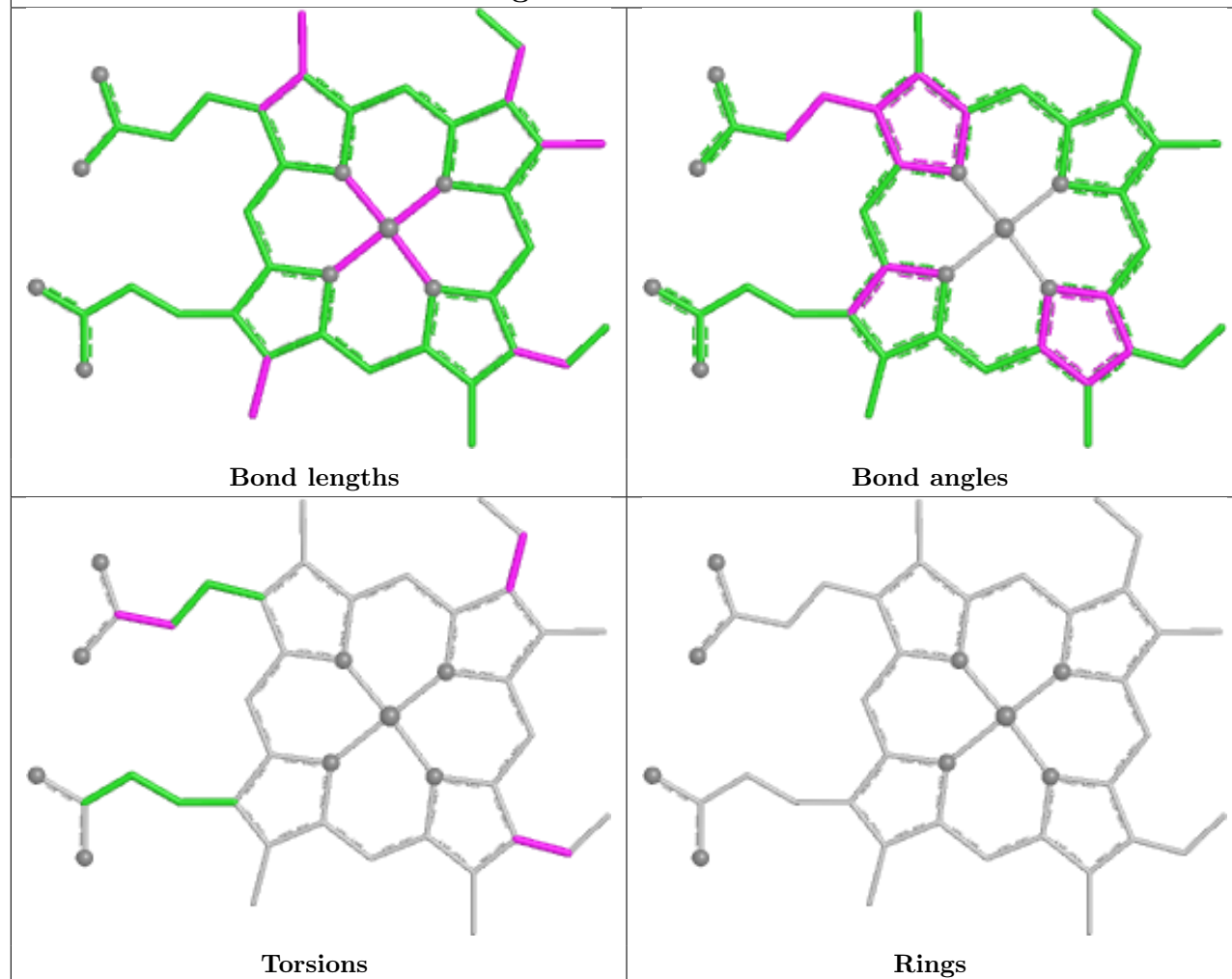




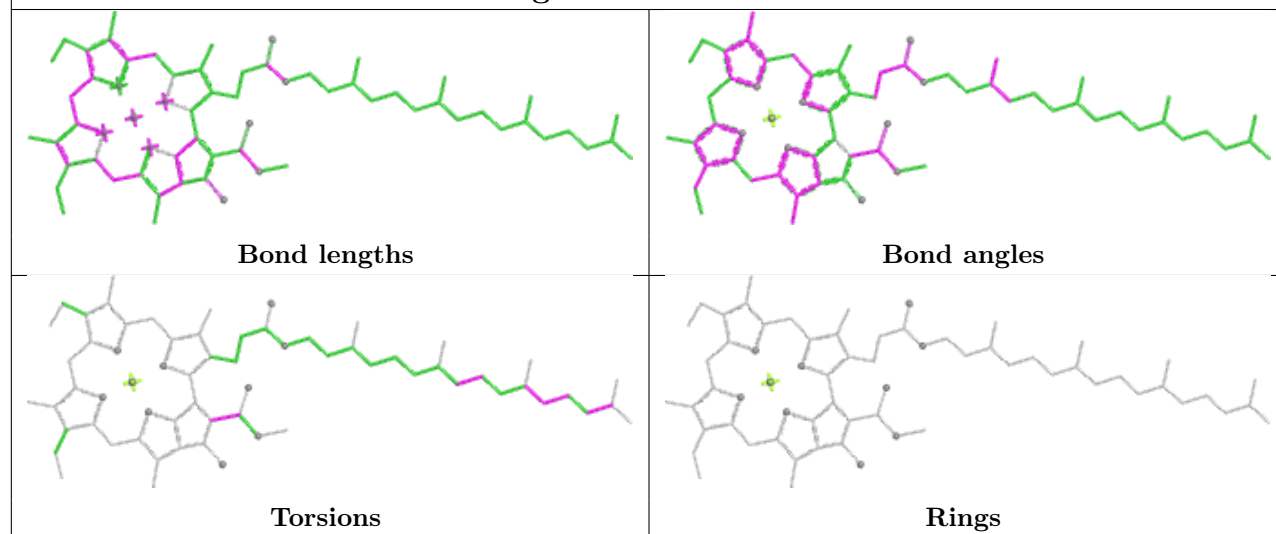


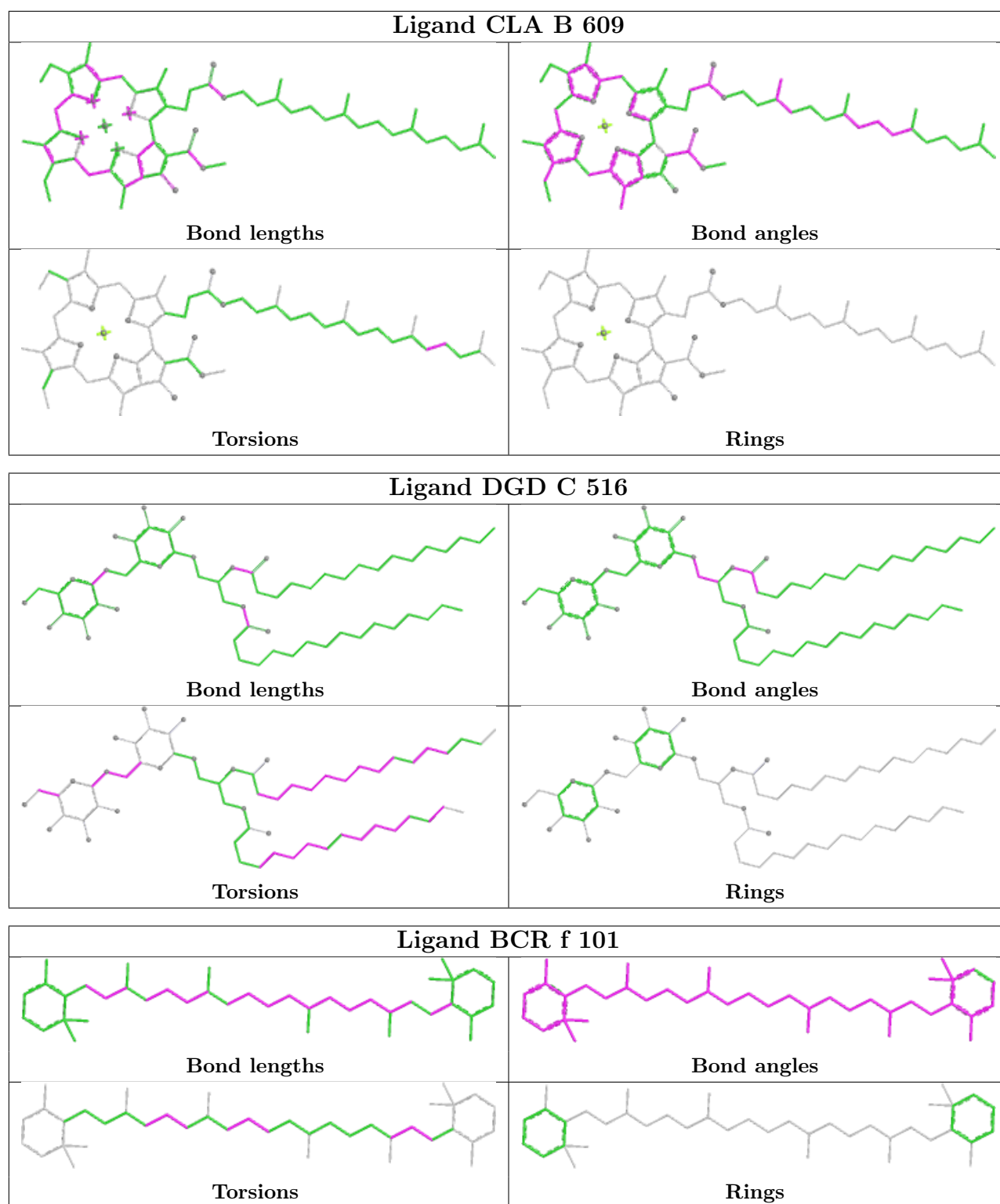


Ligand HEM v 202

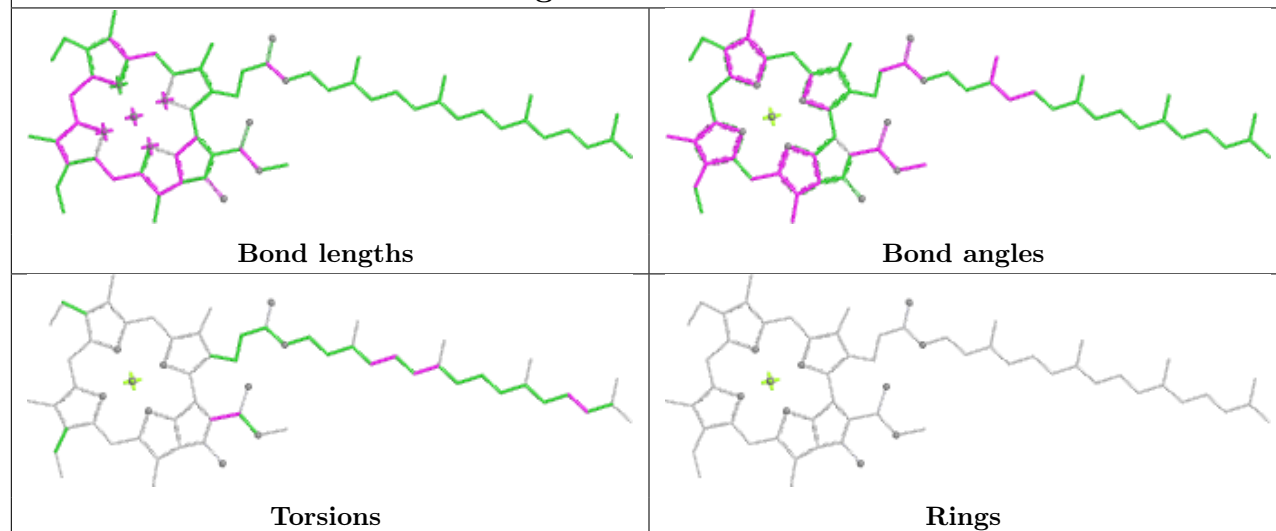


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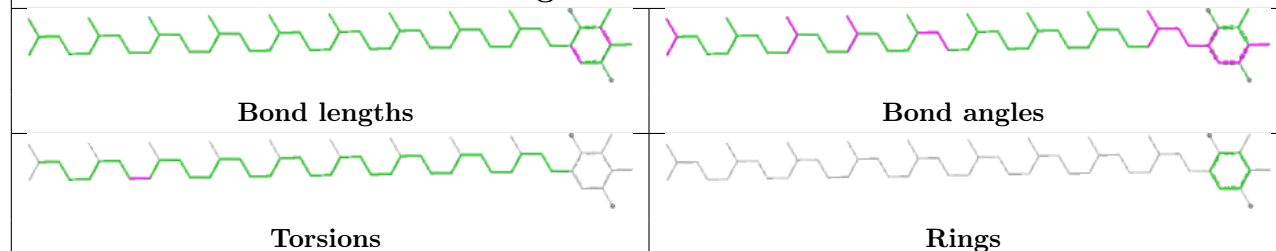




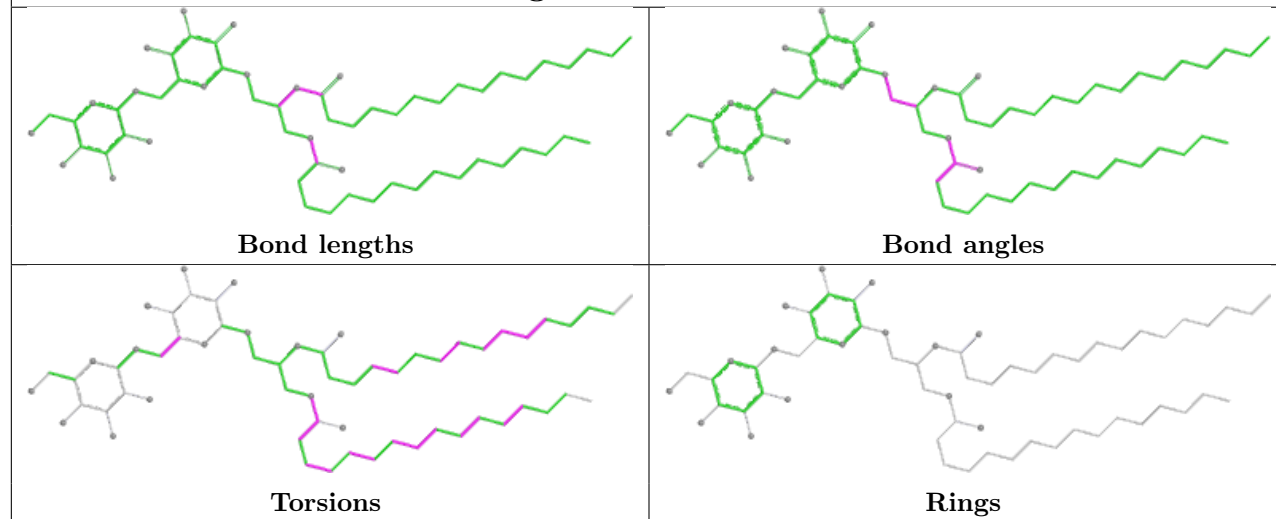
Ligand CLA b 605



Ligand PL9 D 405

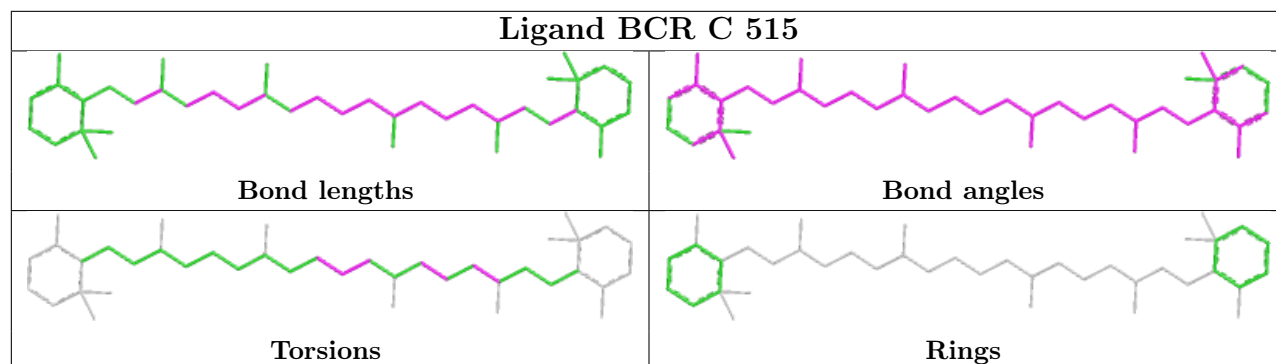
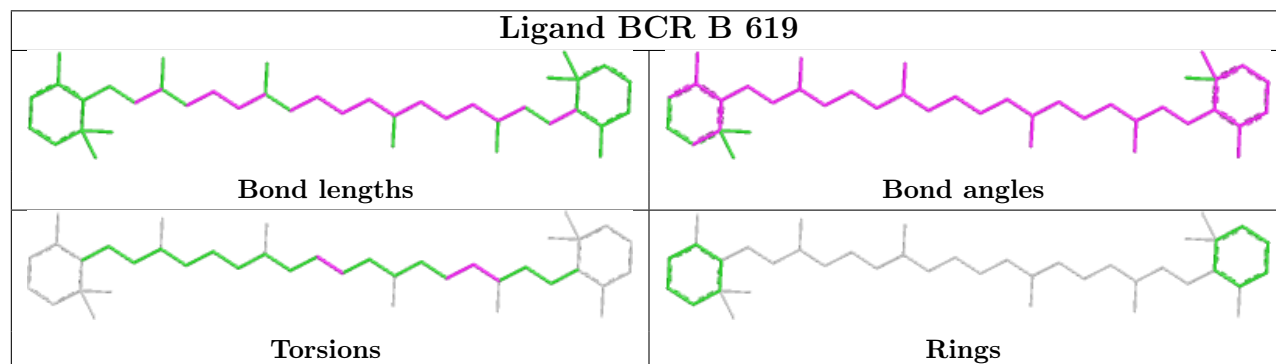
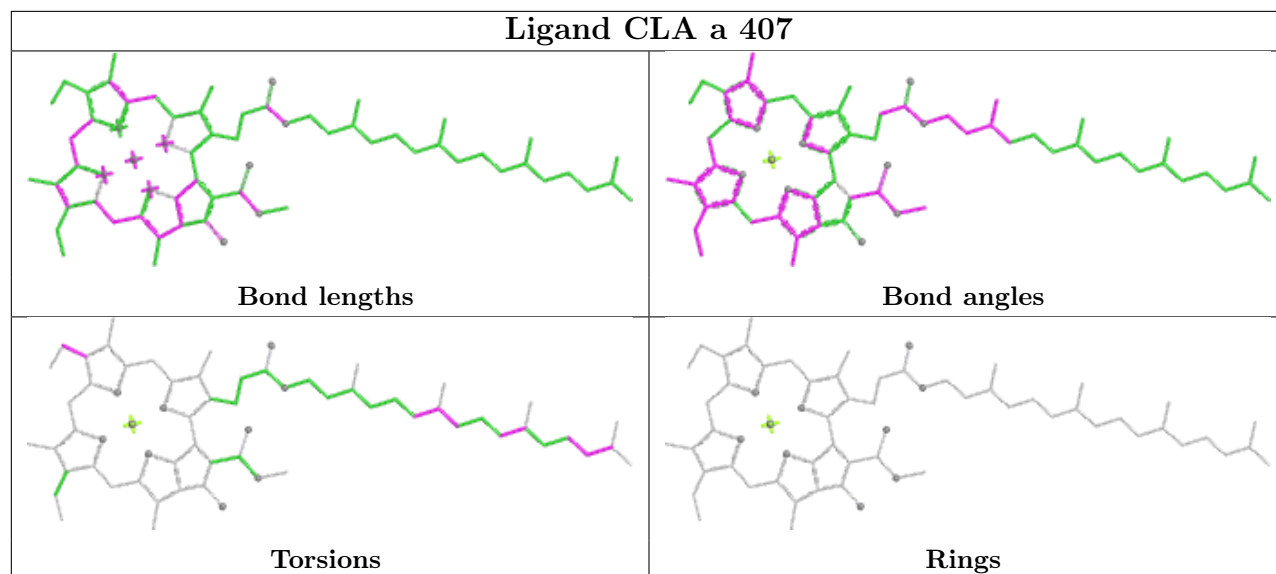


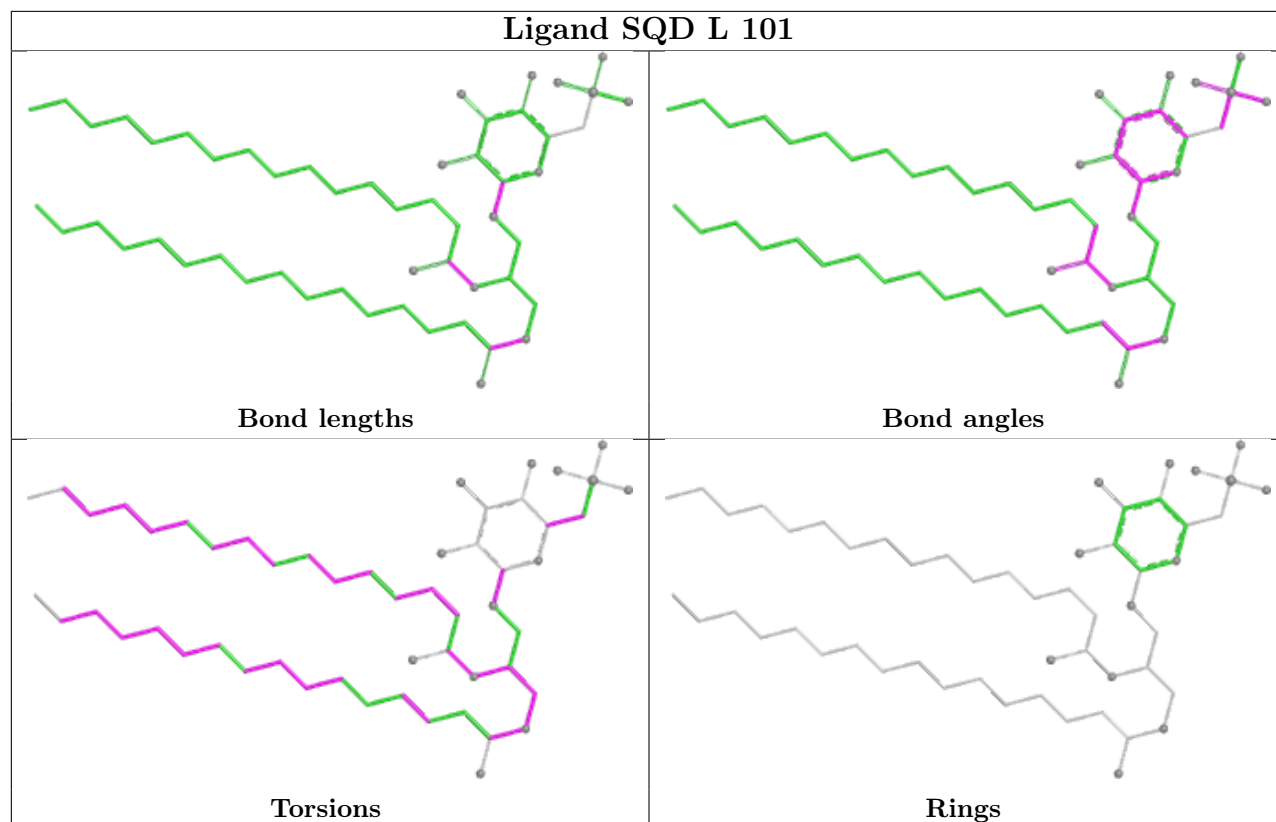
Ligand DGD C 518

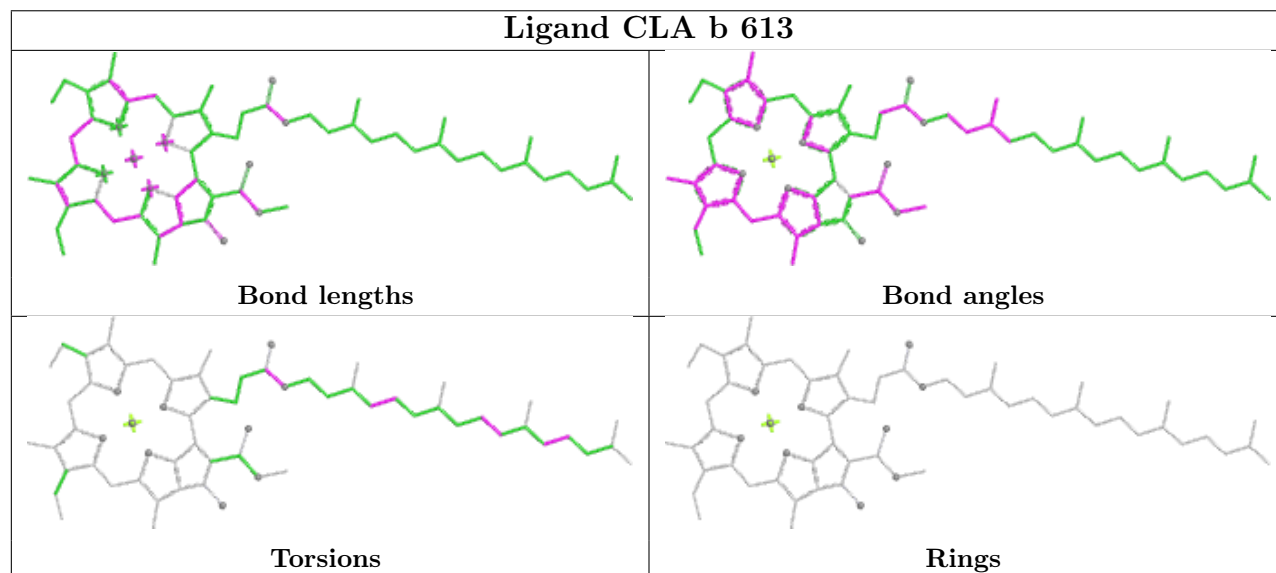
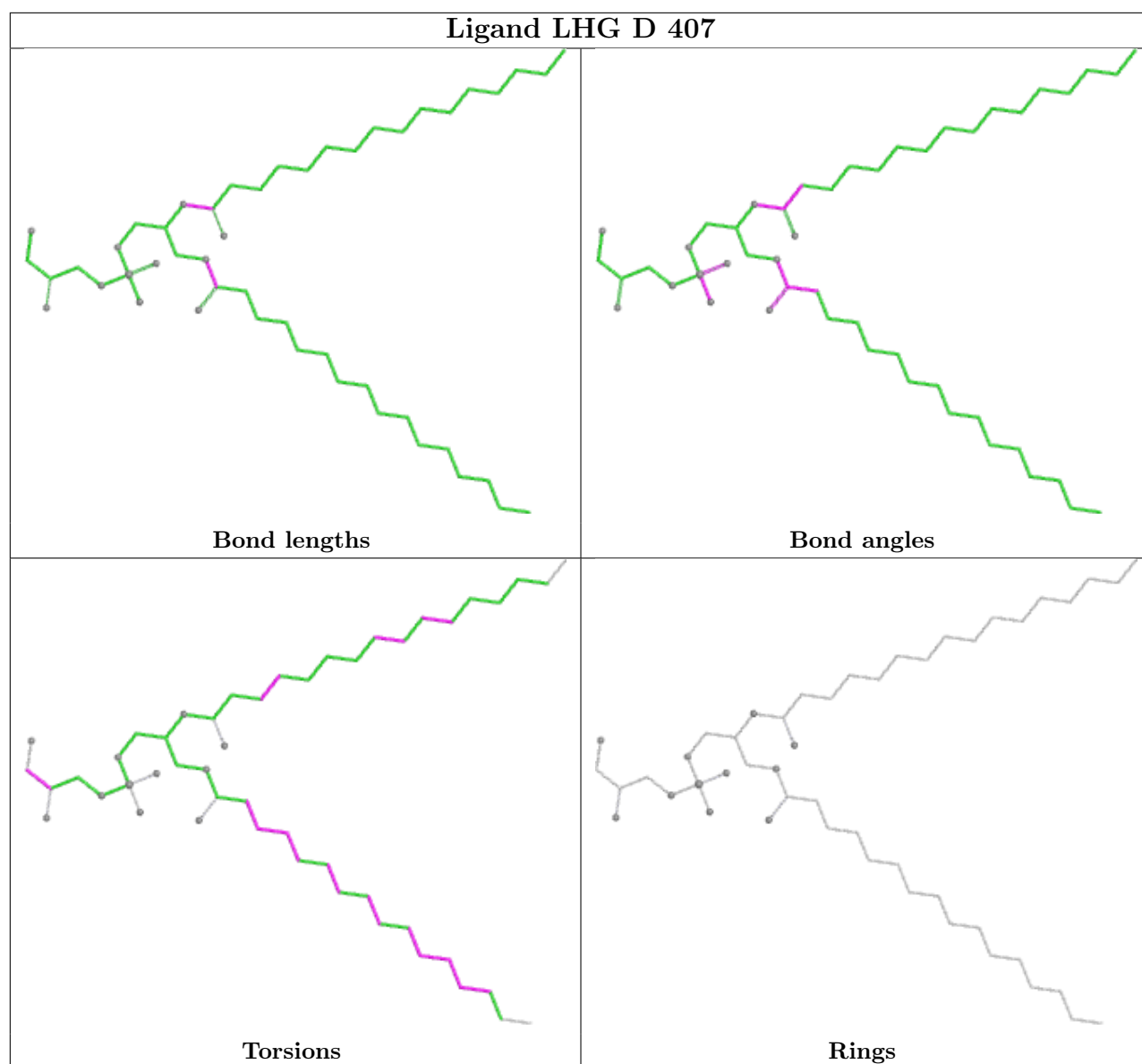


Ligand PL9 a 410

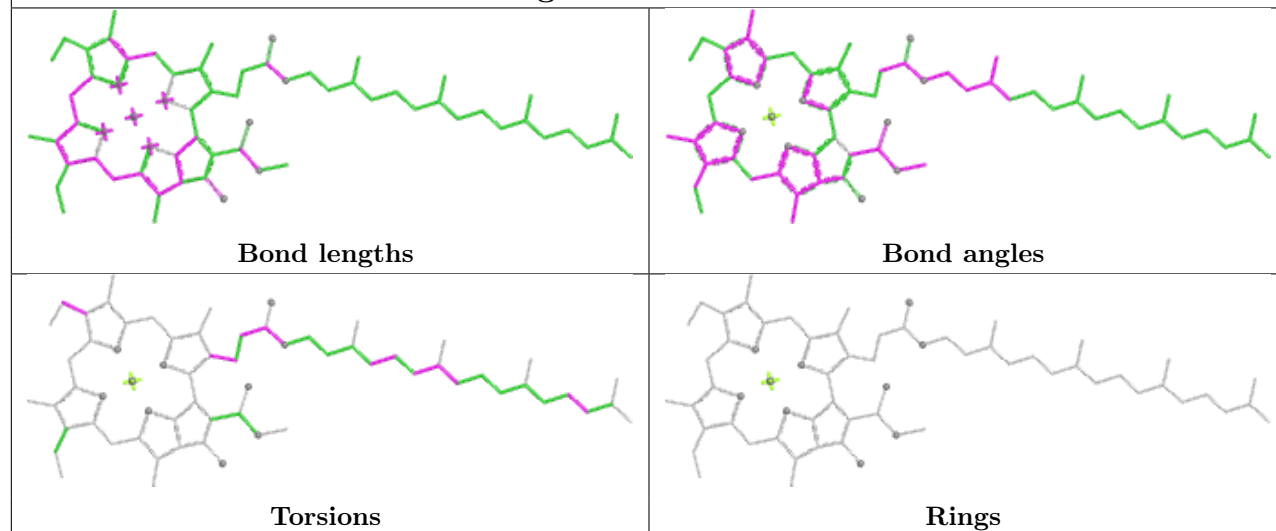




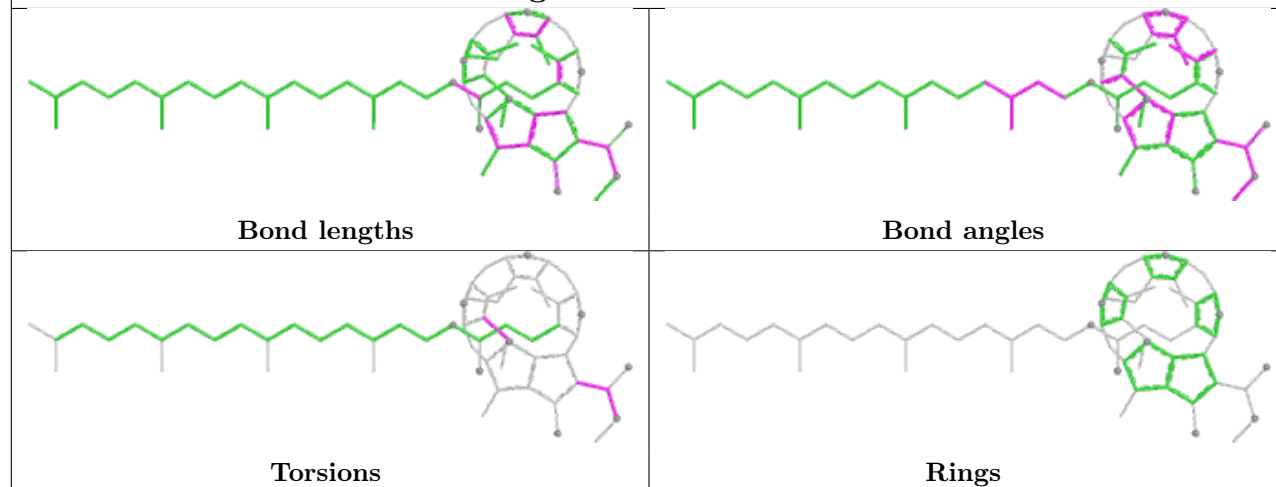




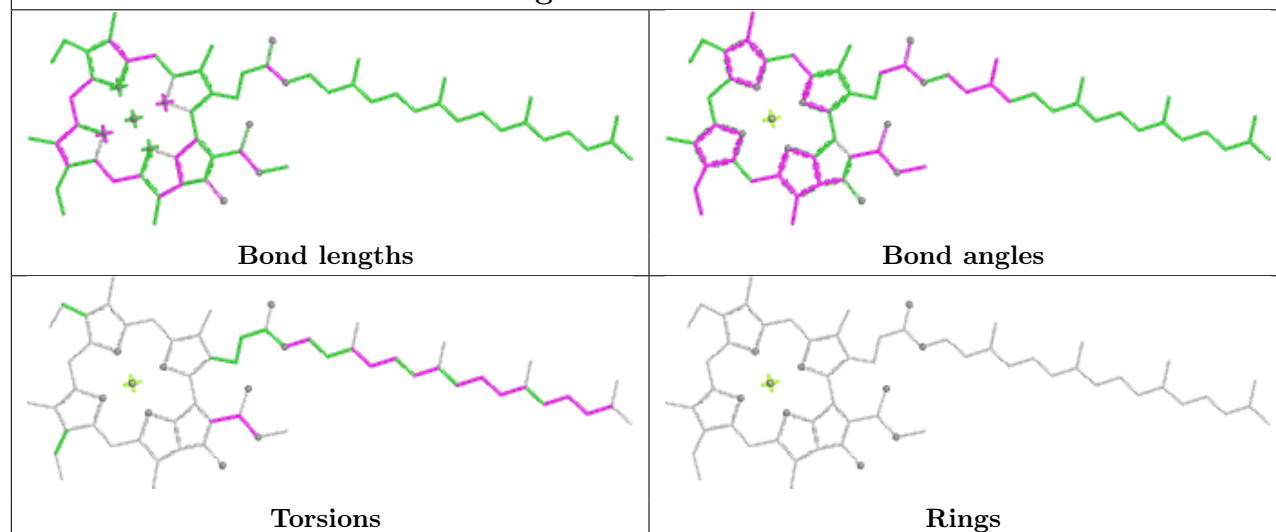
Ligand CLA c 913

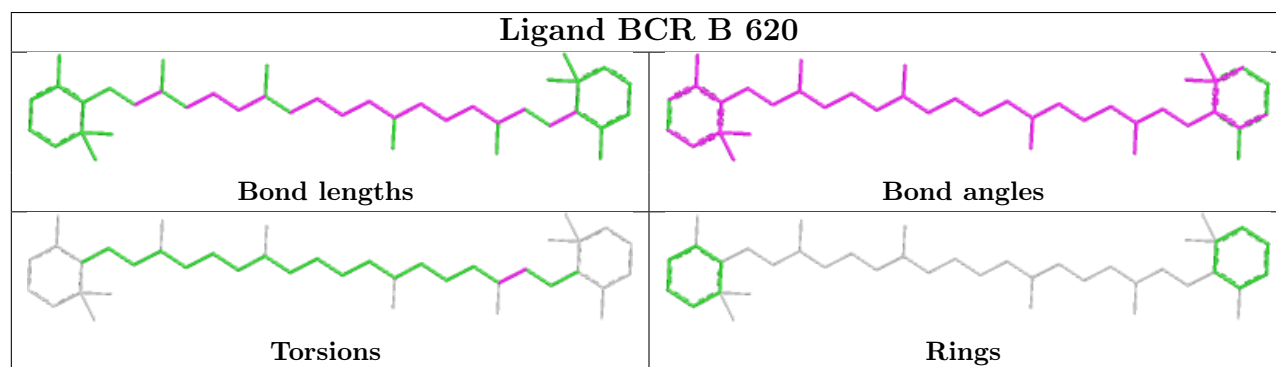
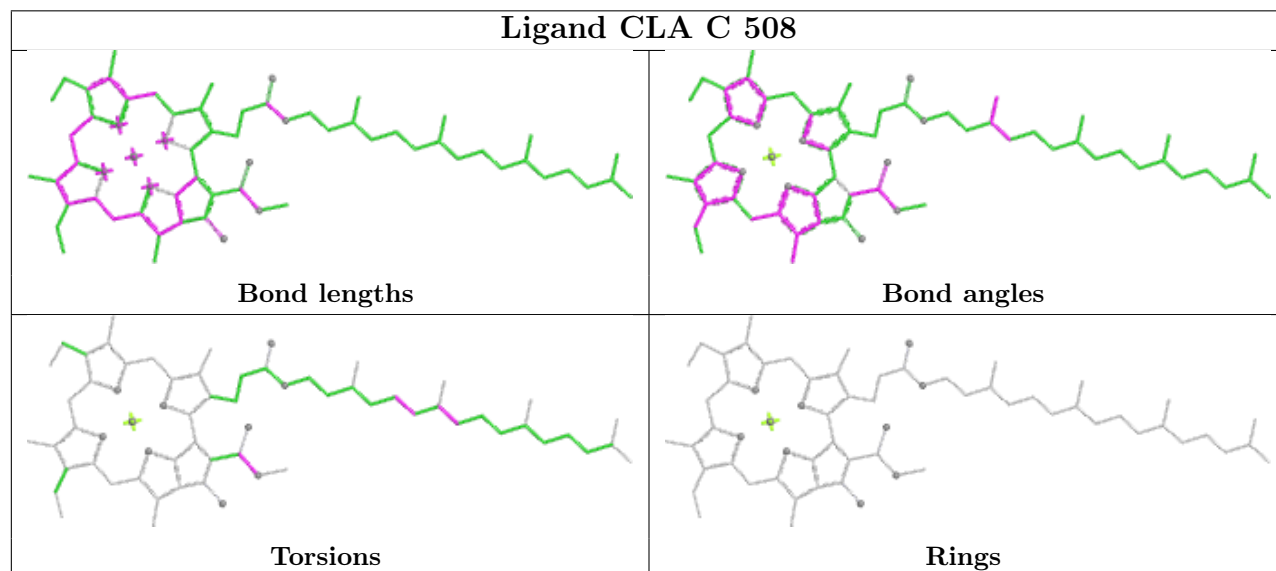
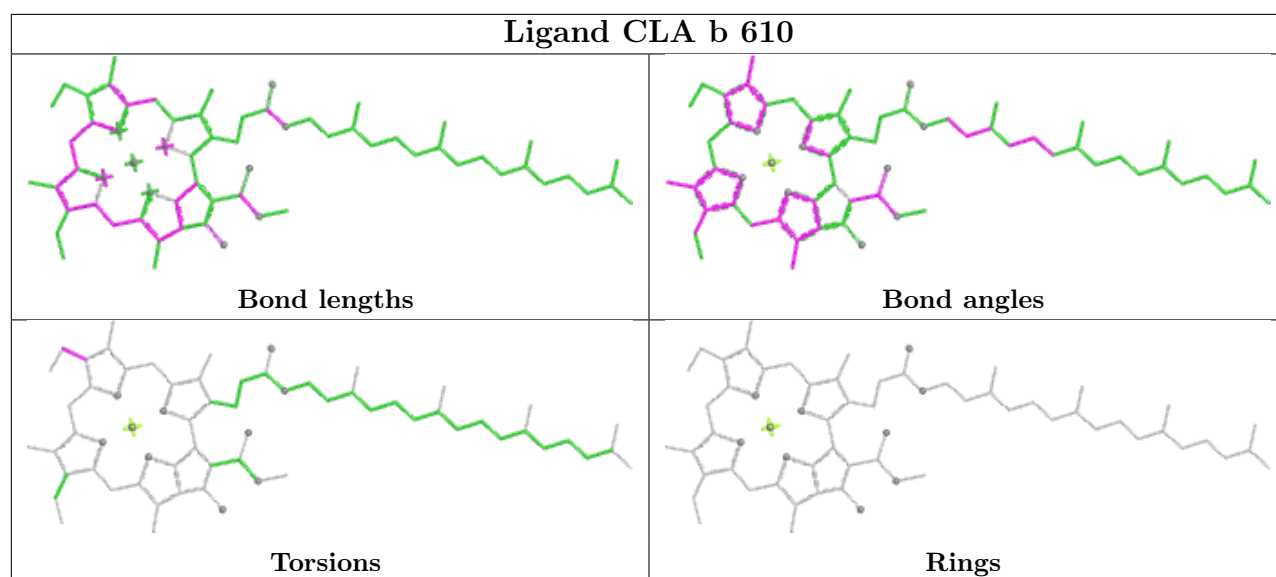


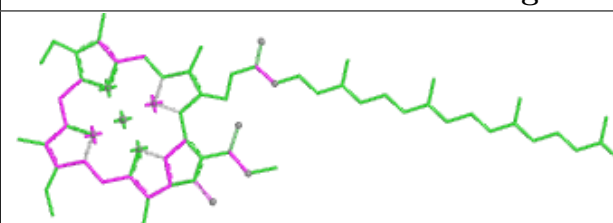
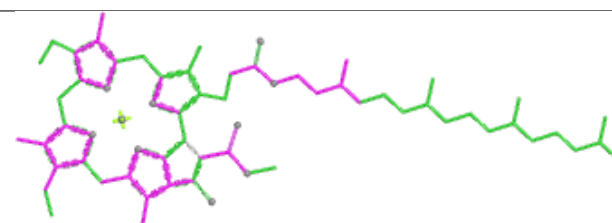
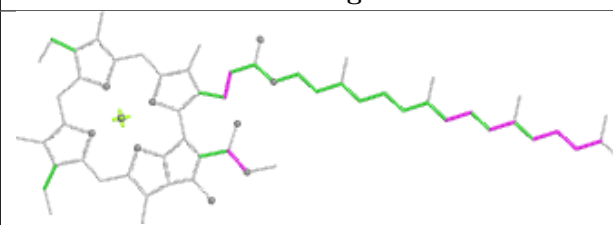
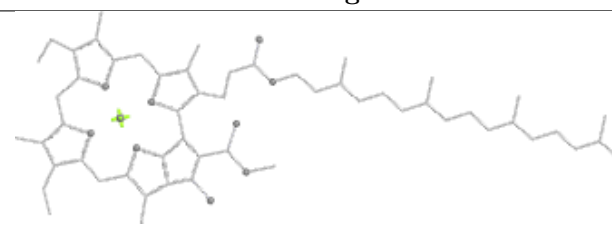
Ligand PHO D 401

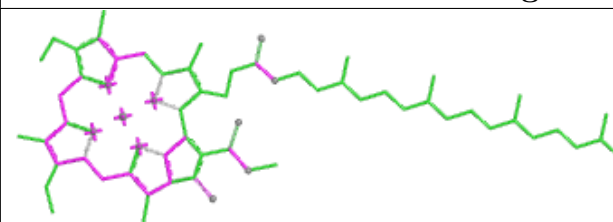
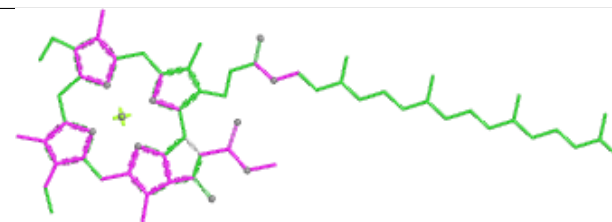
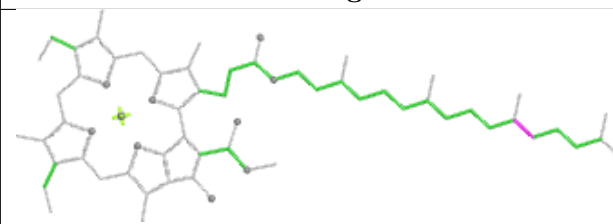
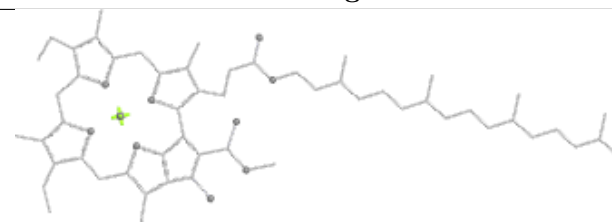


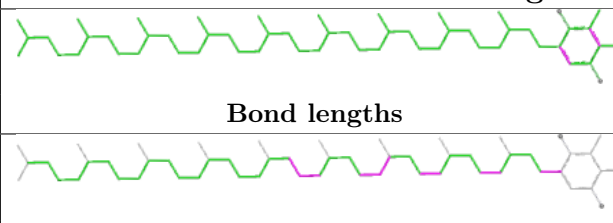
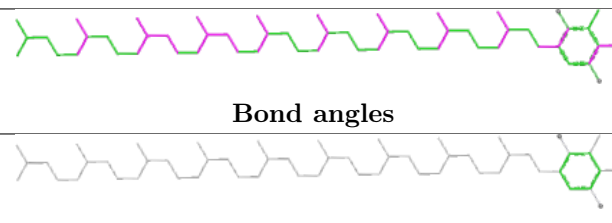
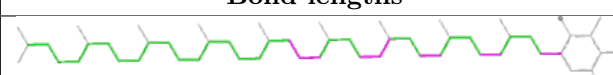
Ligand CLA b 615



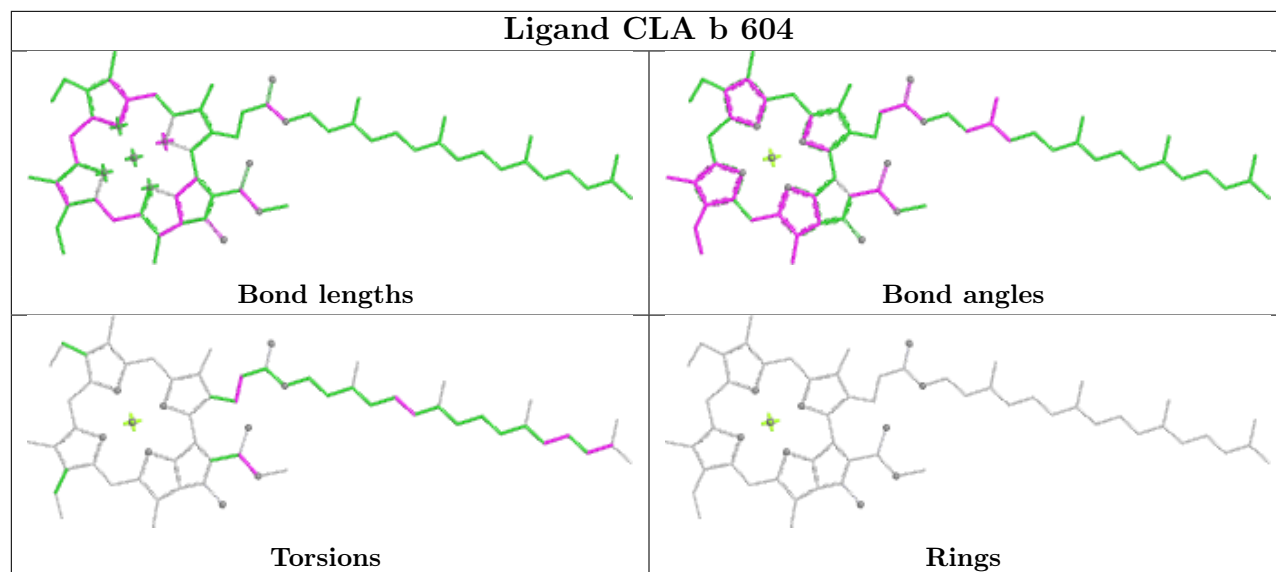


Ligand CLA B 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

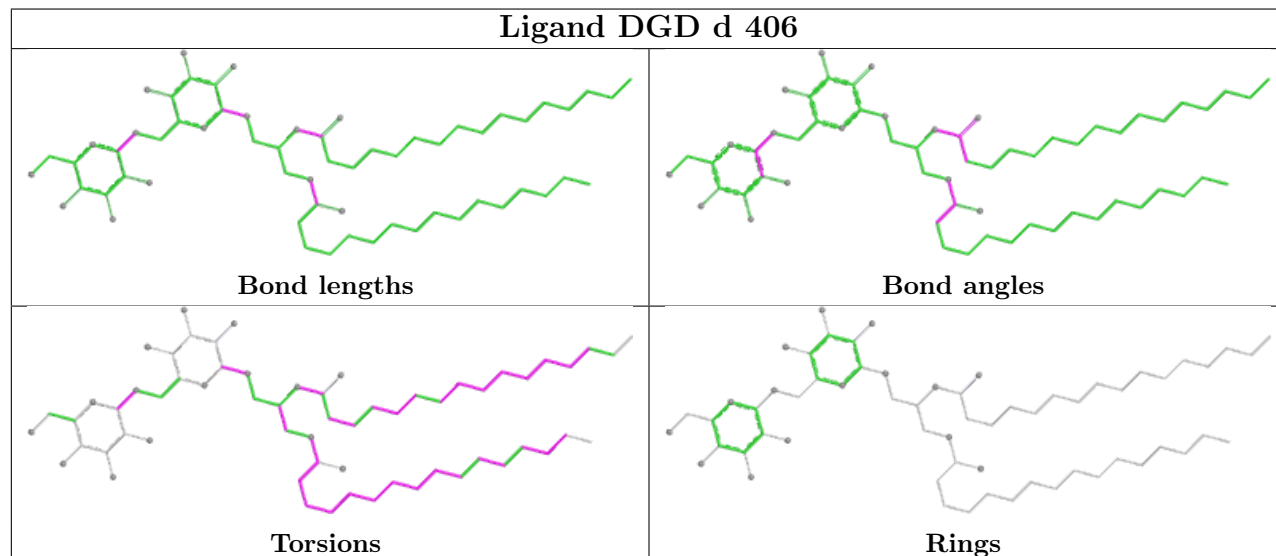
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

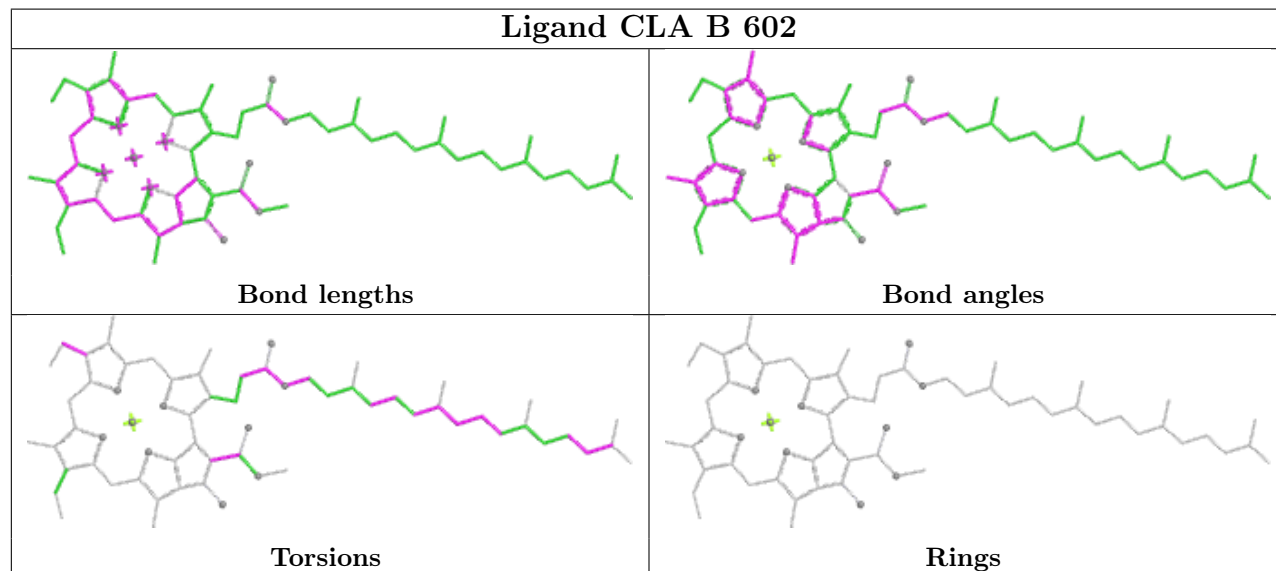
Ligand CLA b 604

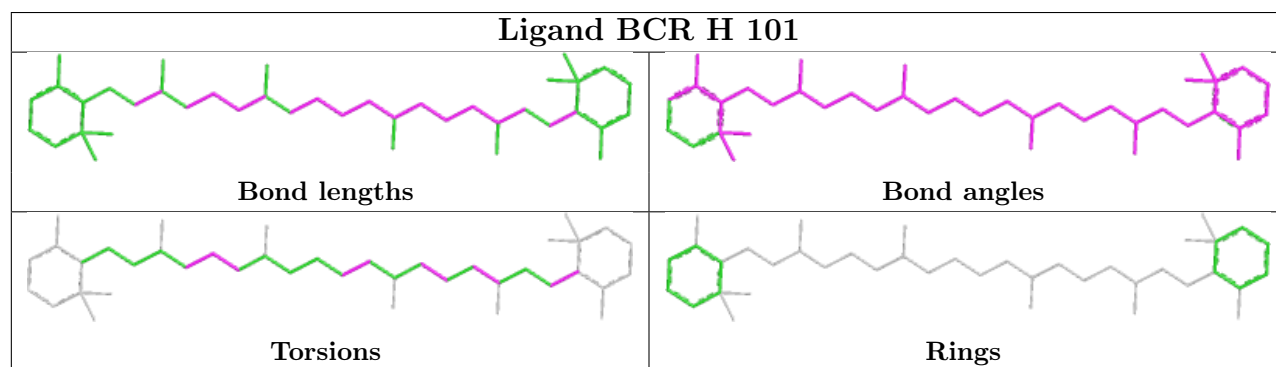
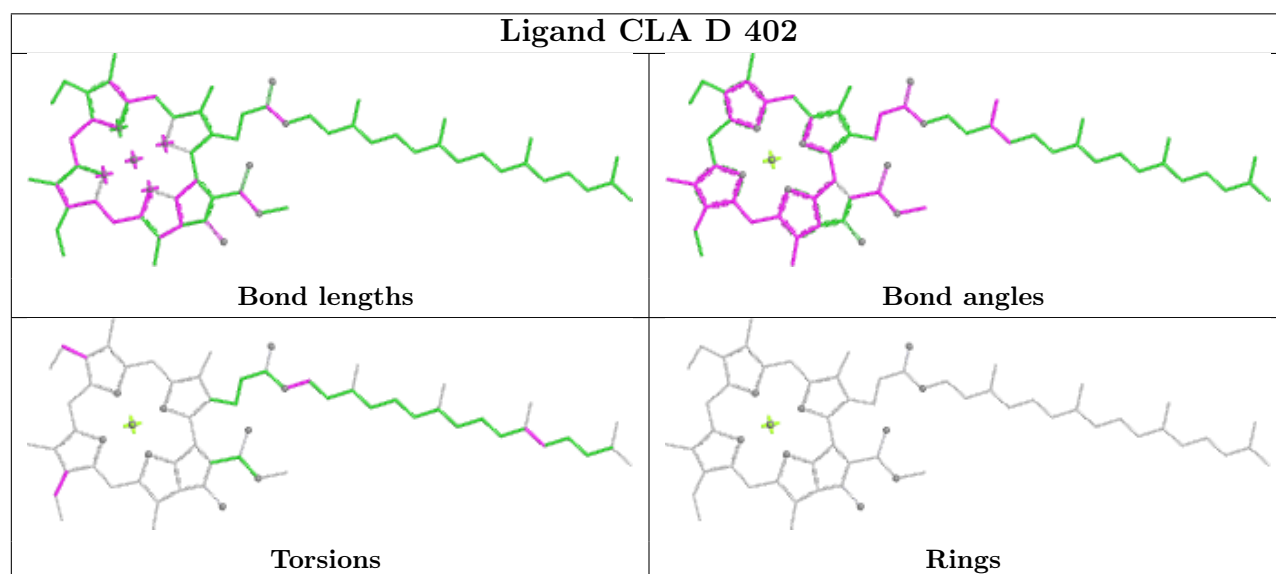
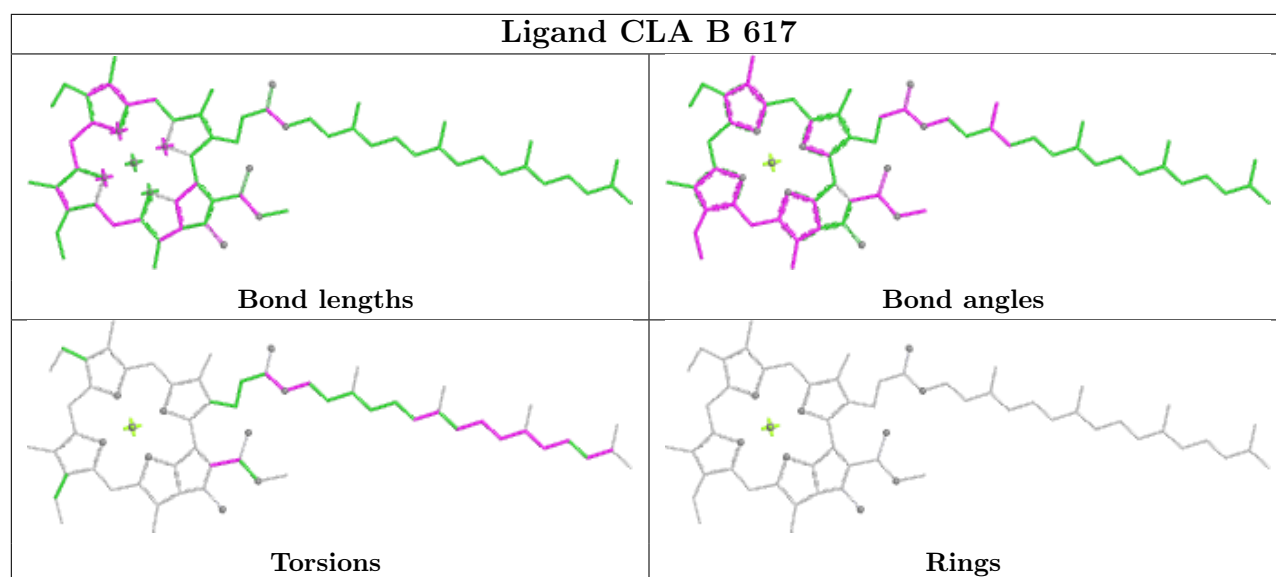


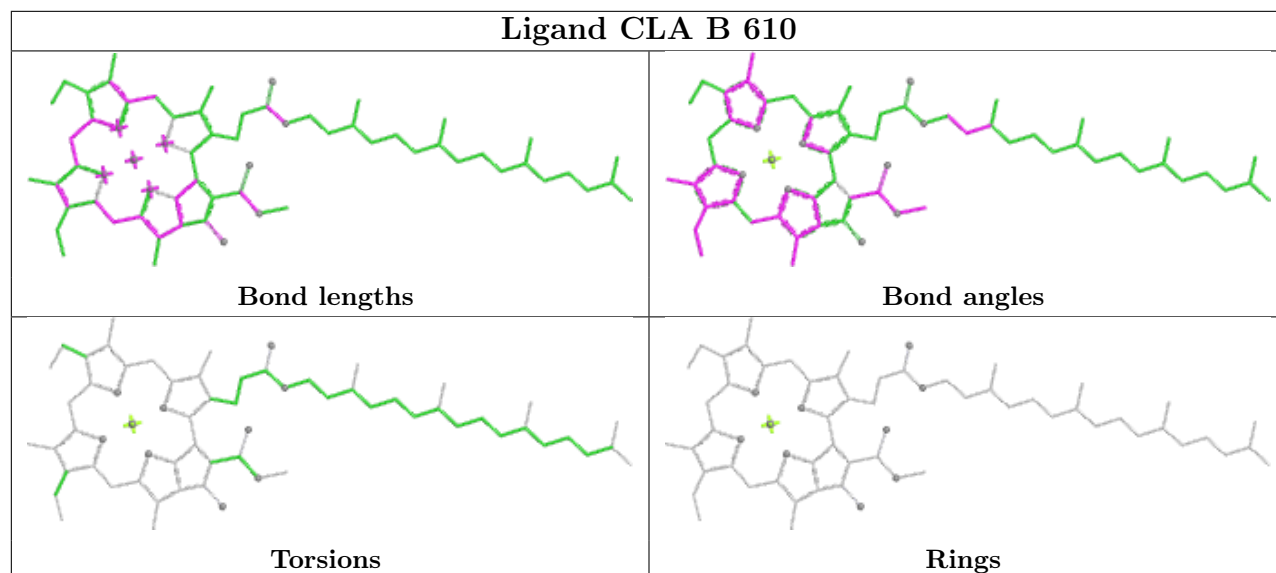
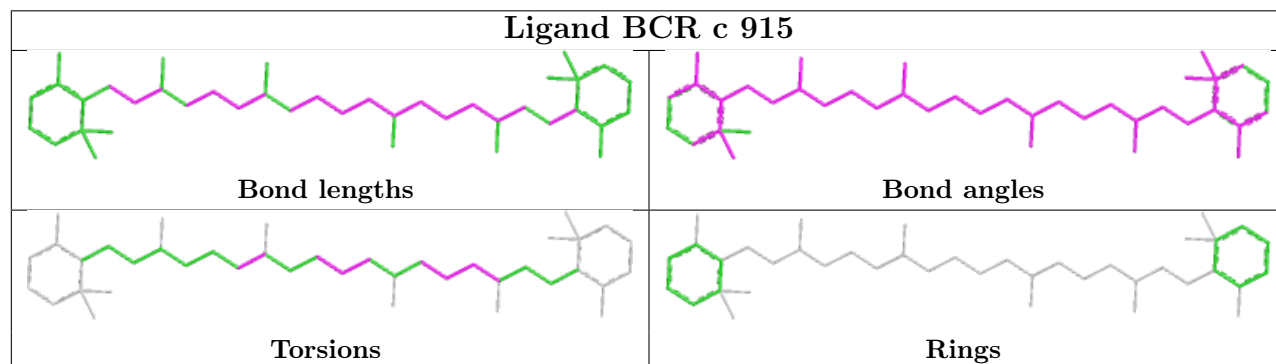
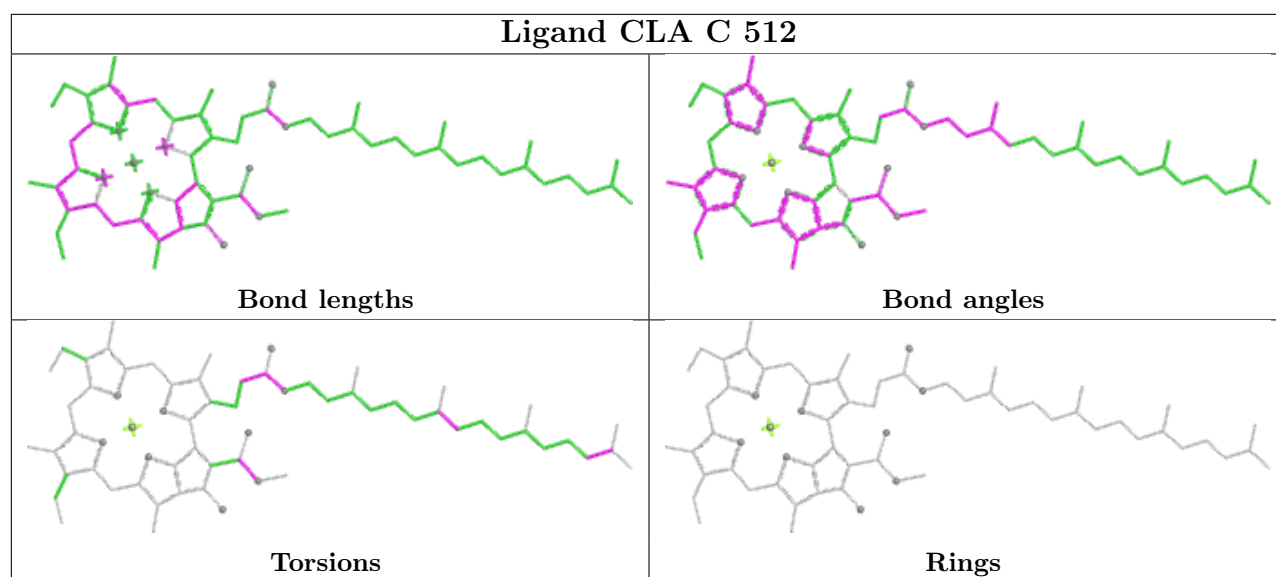
Ligand DGD d 406

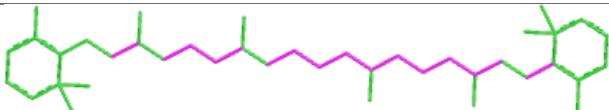
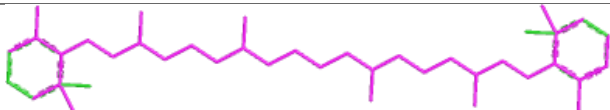
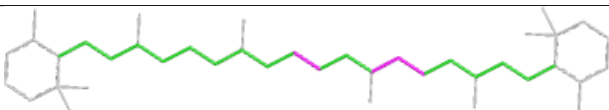
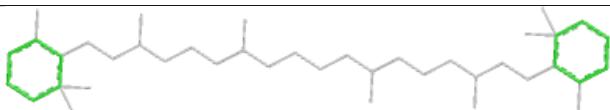


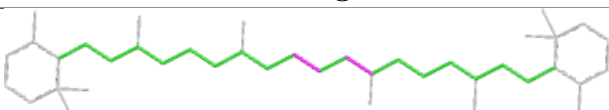
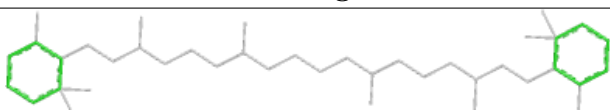
Ligand CLA B 602

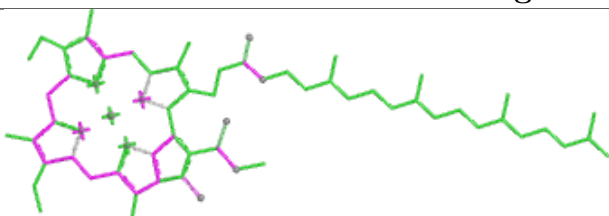
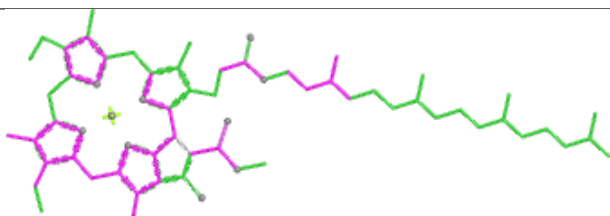
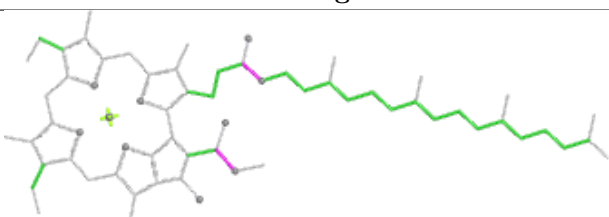
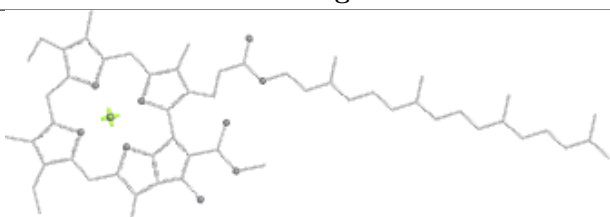


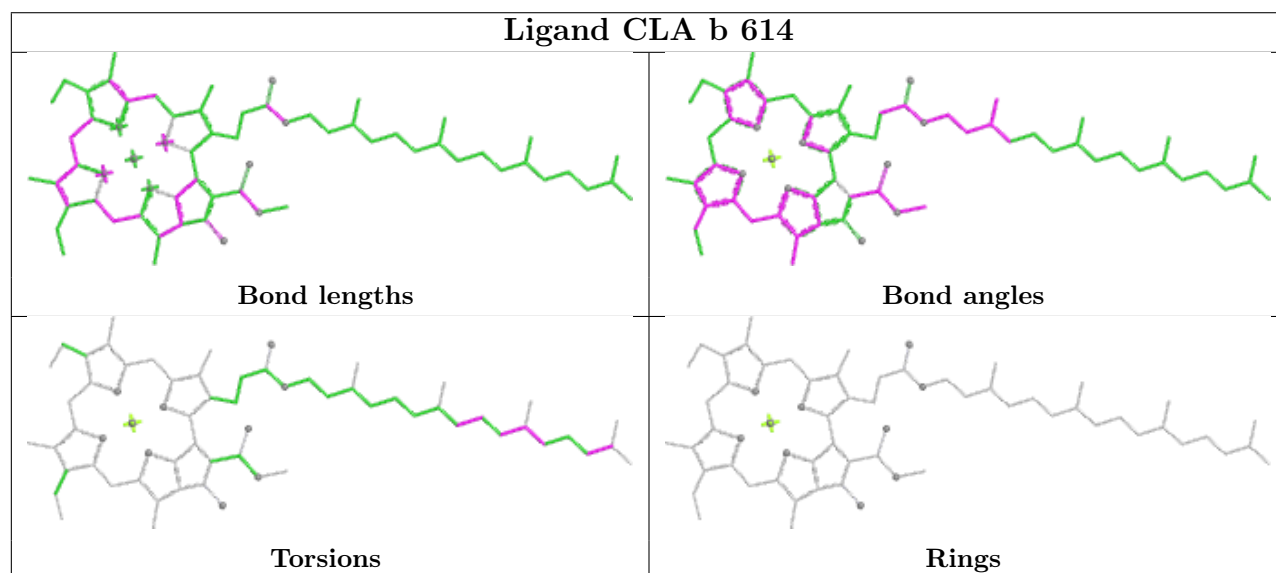
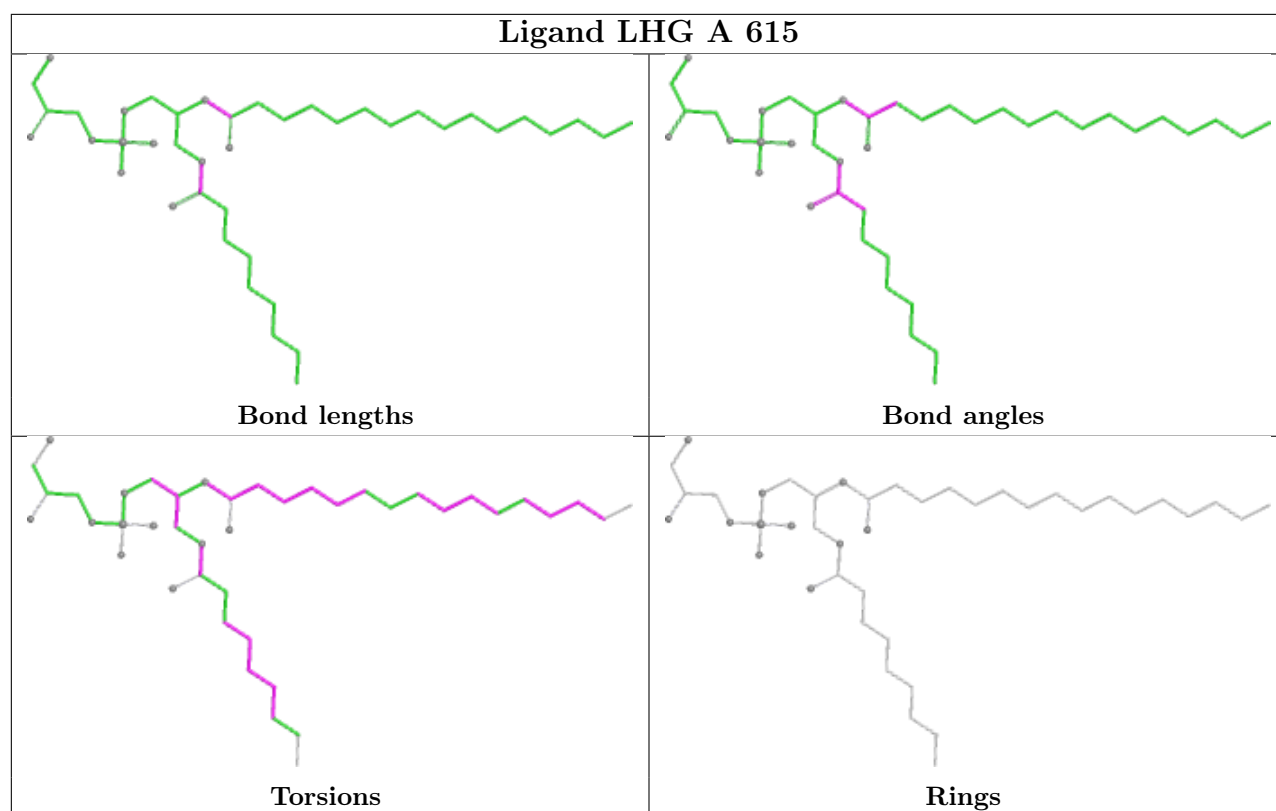


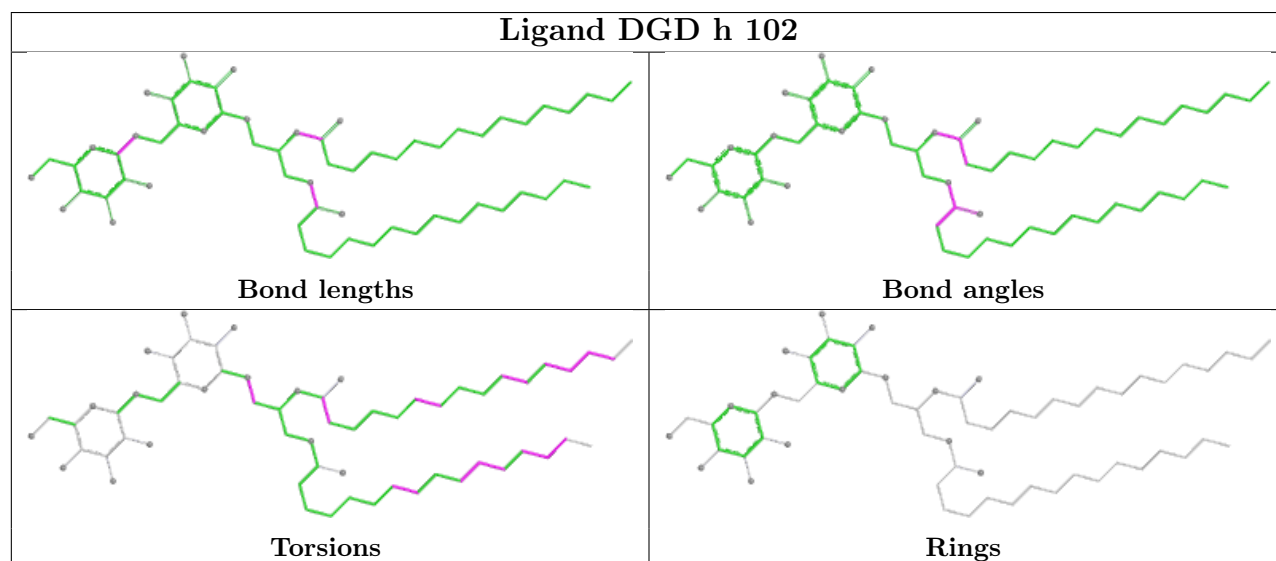
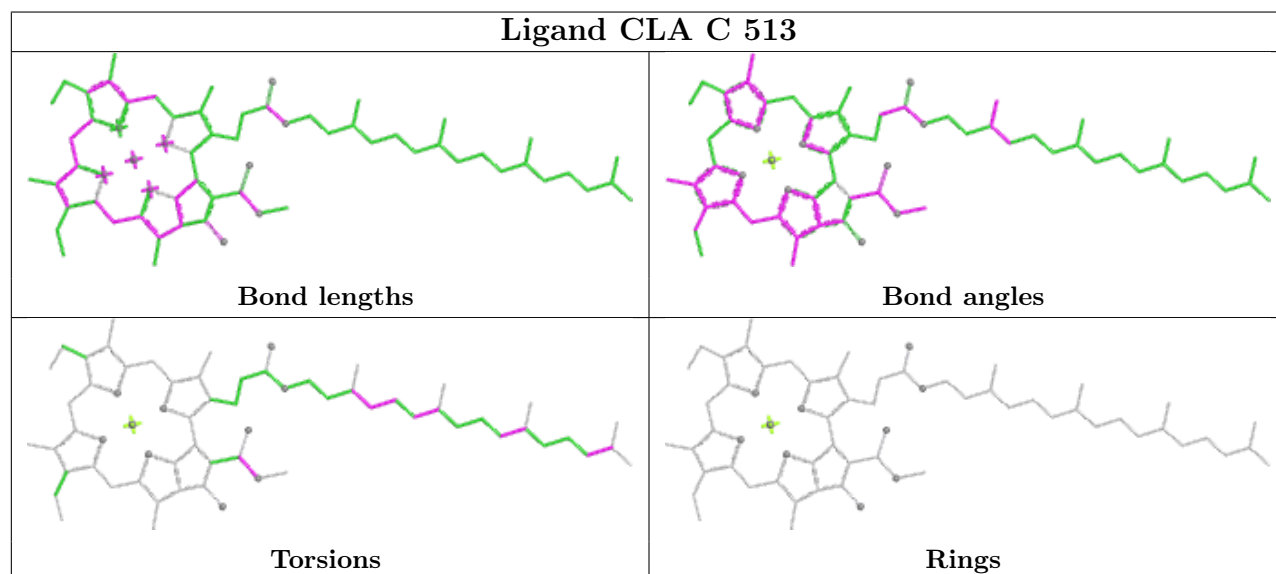
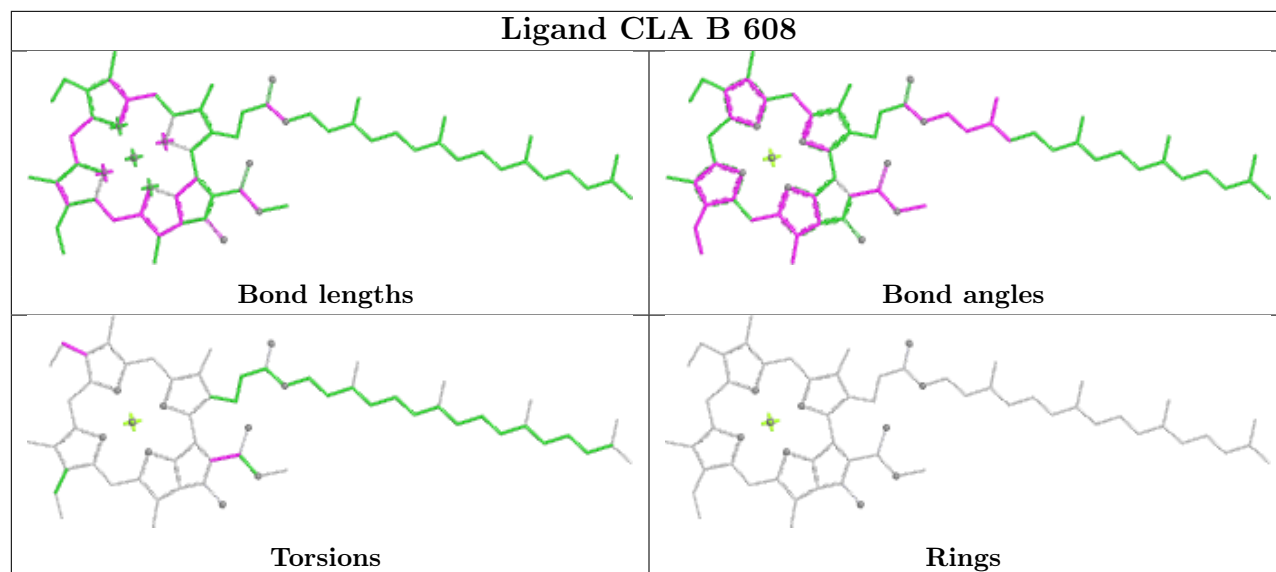


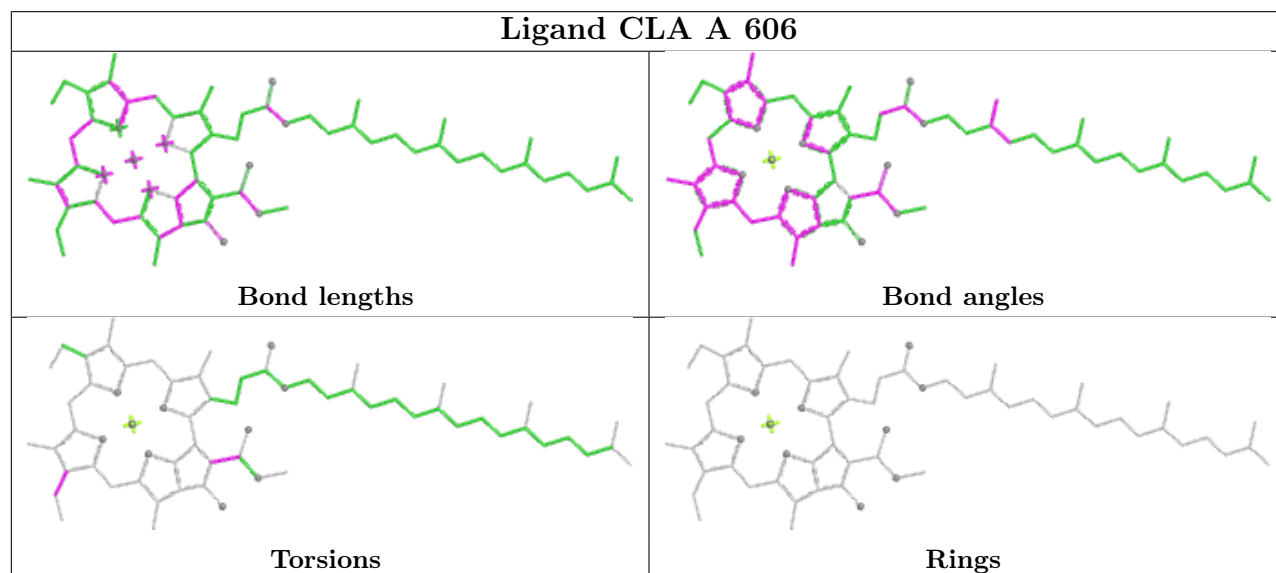
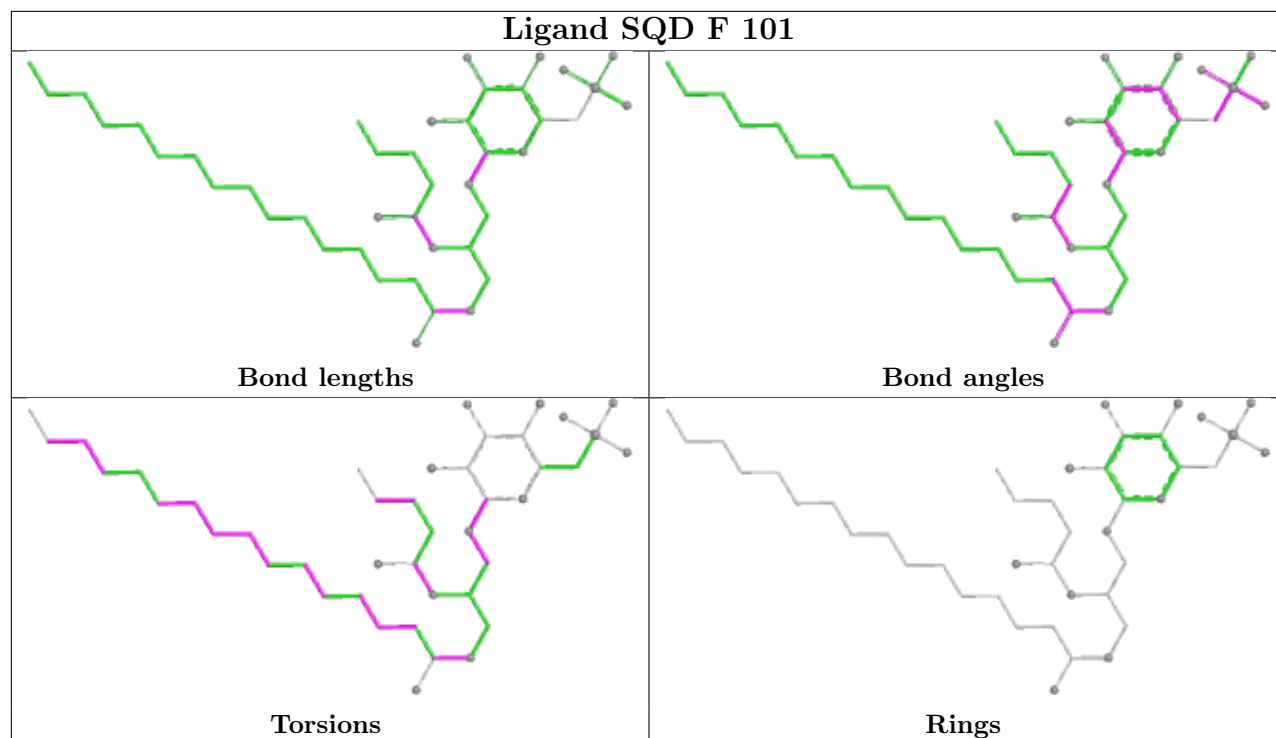
Ligand BCR A 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

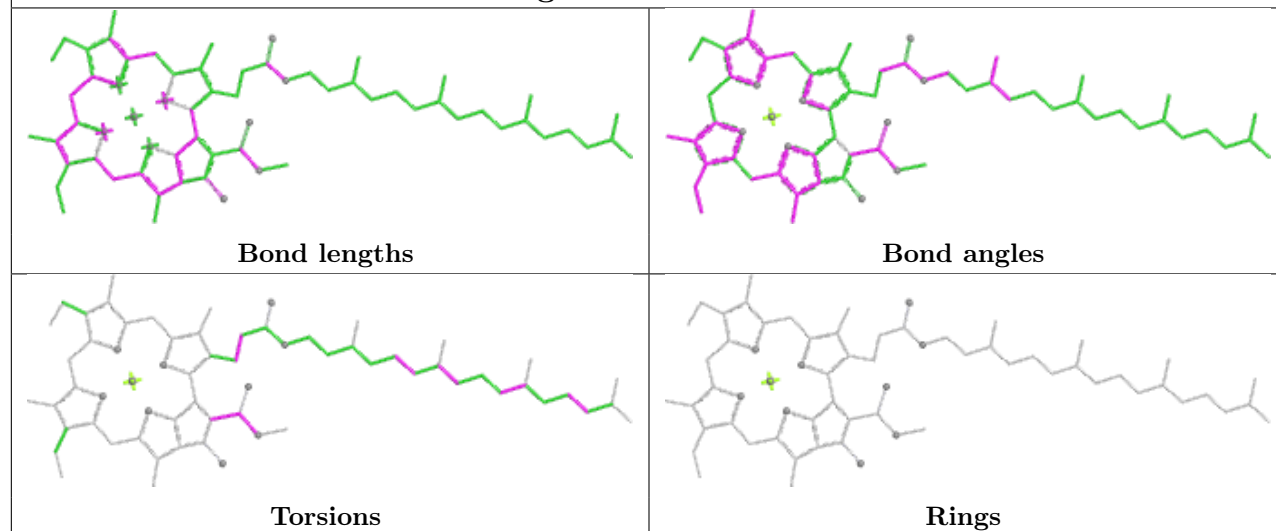
Ligand CLA c 904	
	
Bond lengths	Bond angles
	
Torsions	Rings



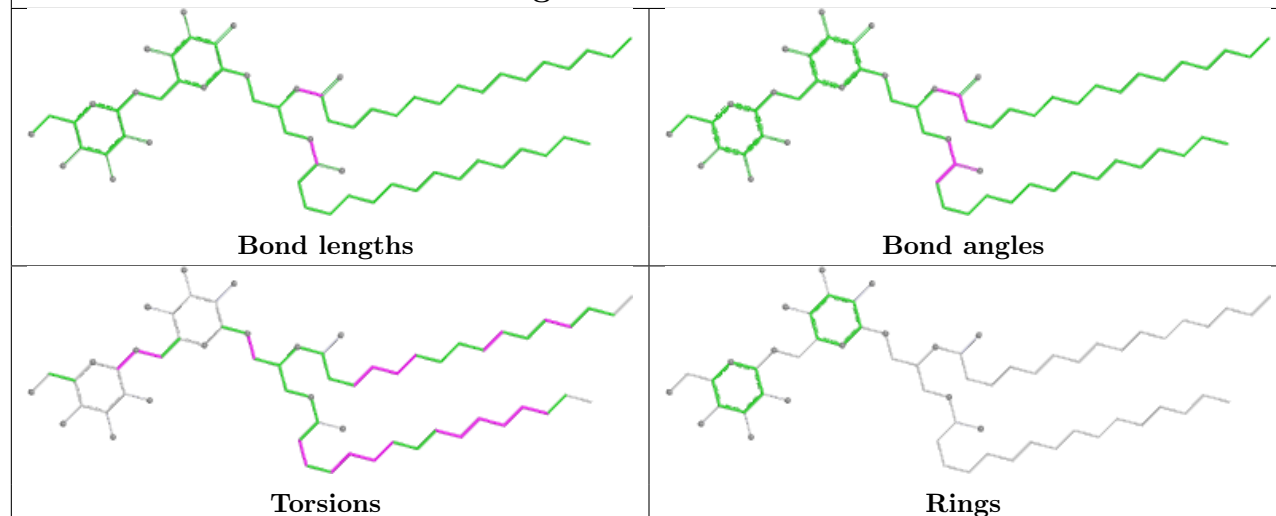




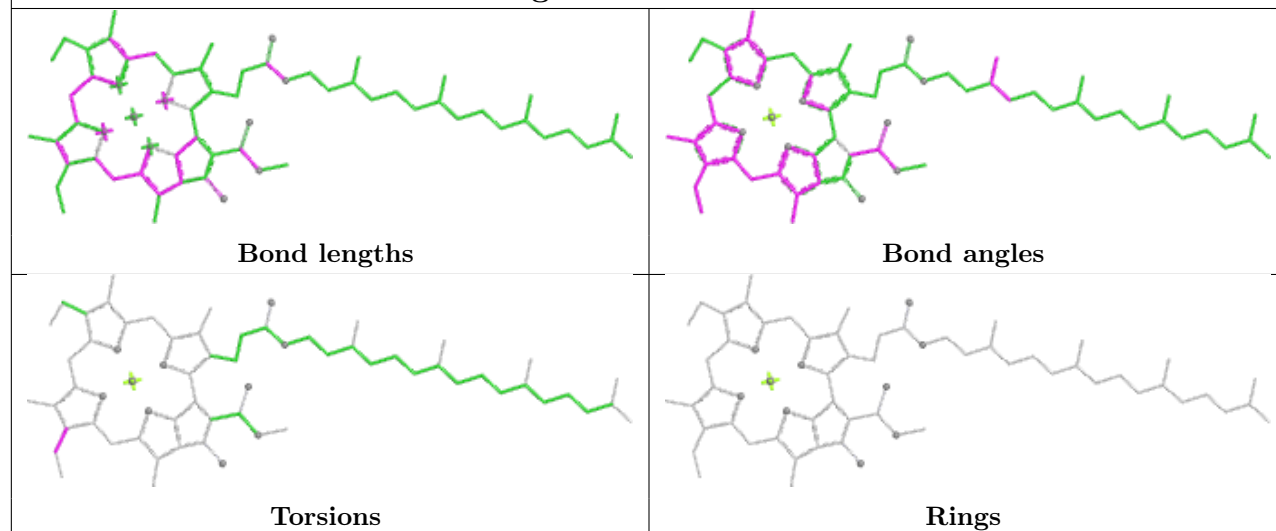
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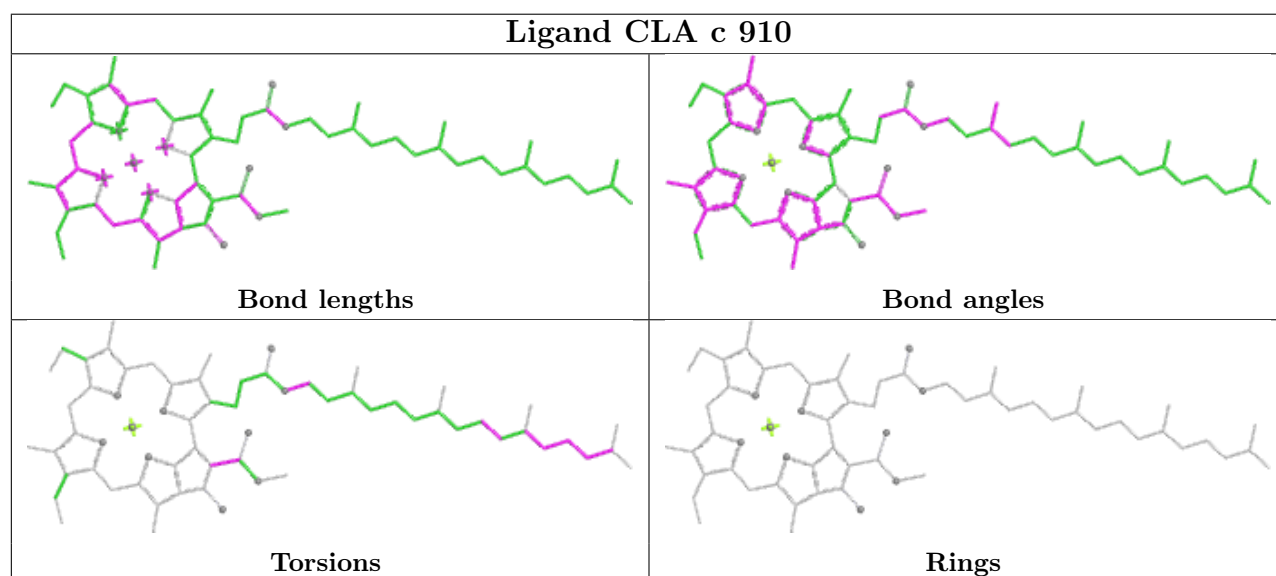
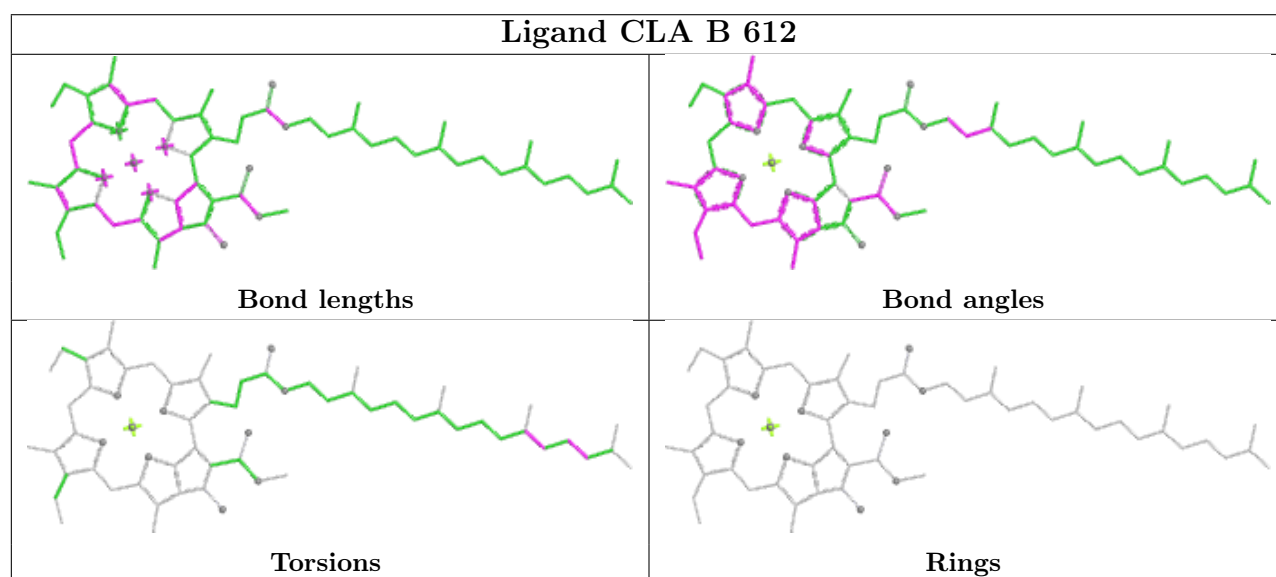
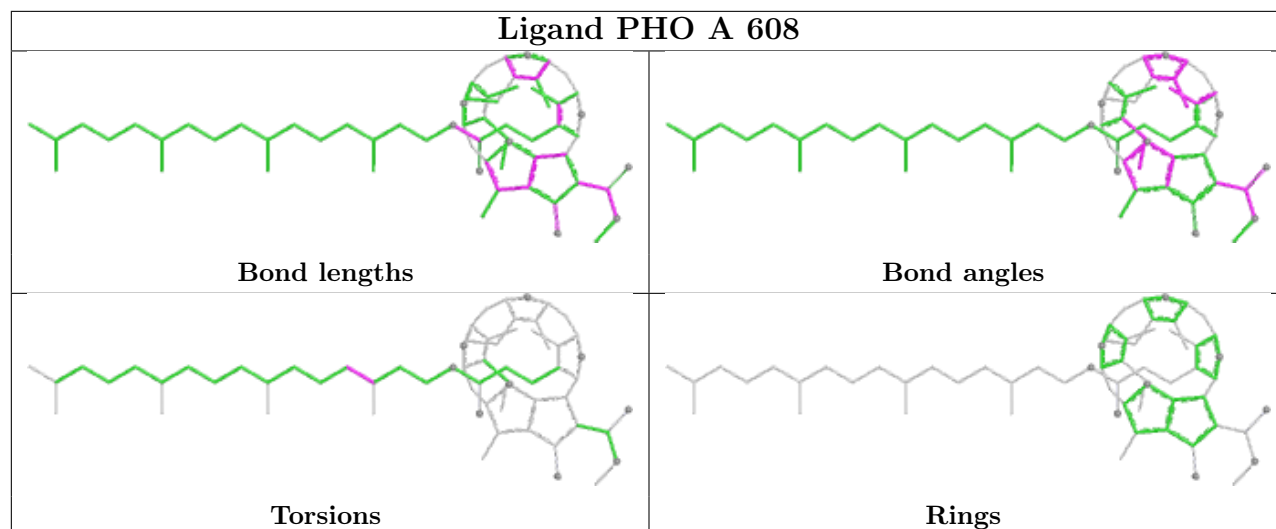


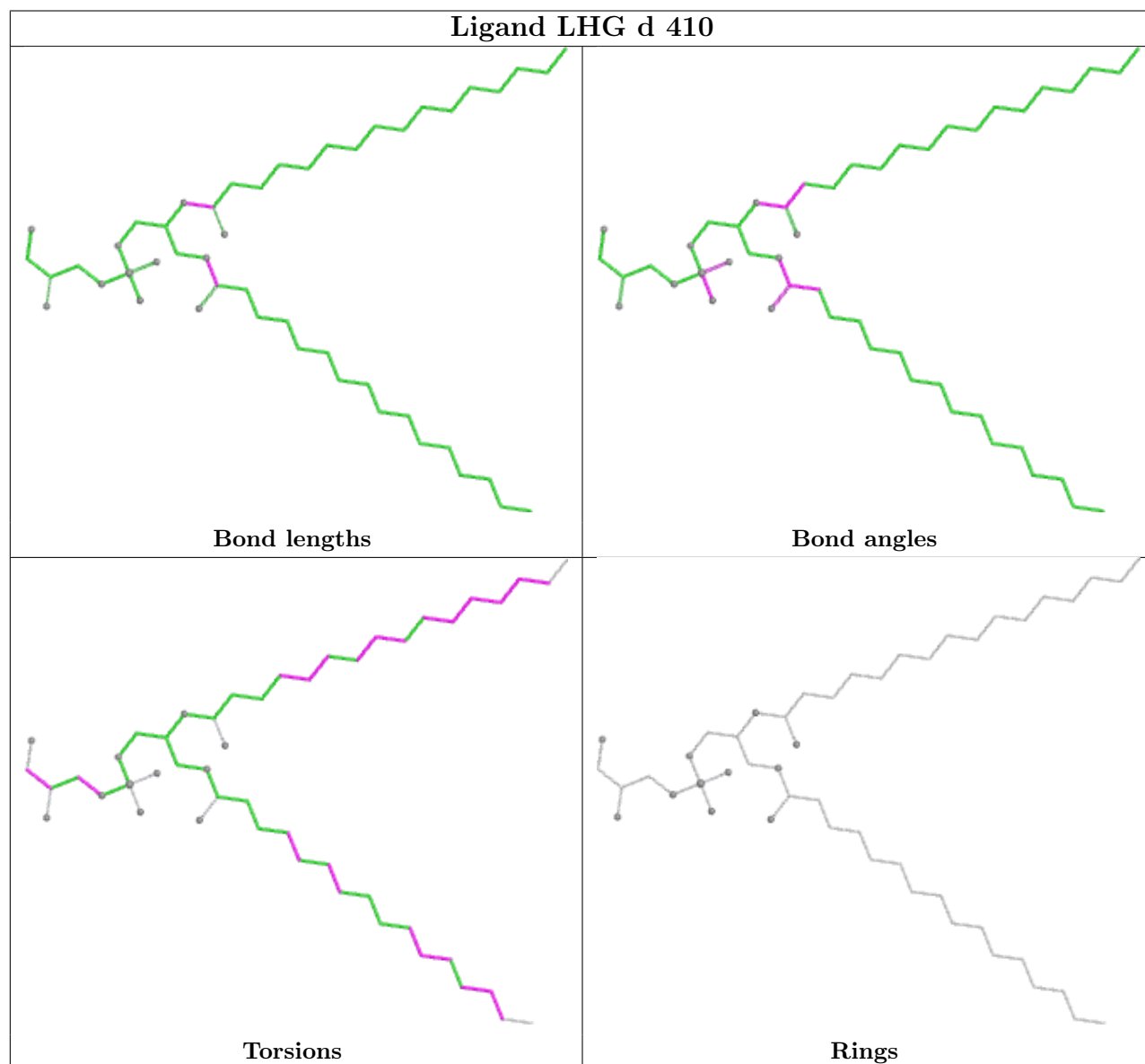
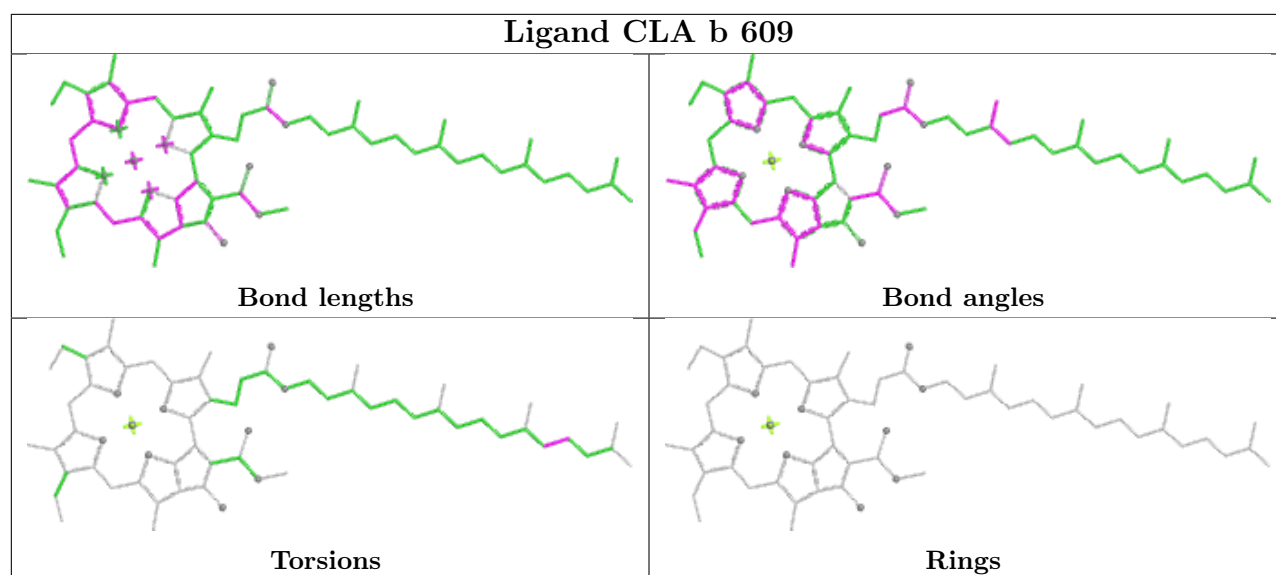
Ligand DGD c 917

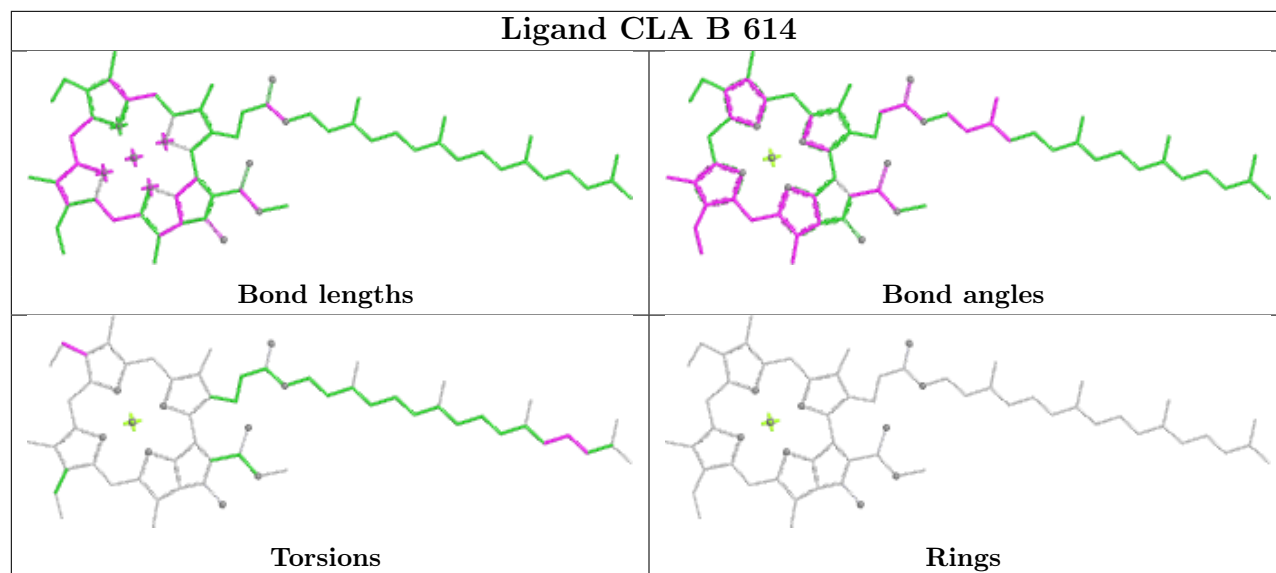
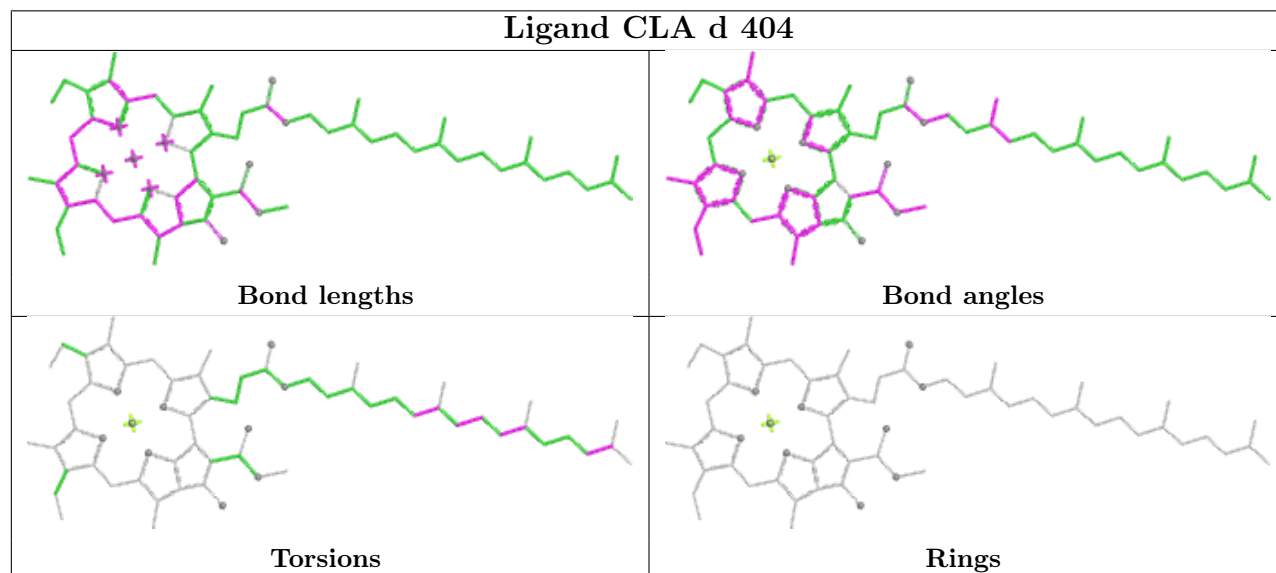
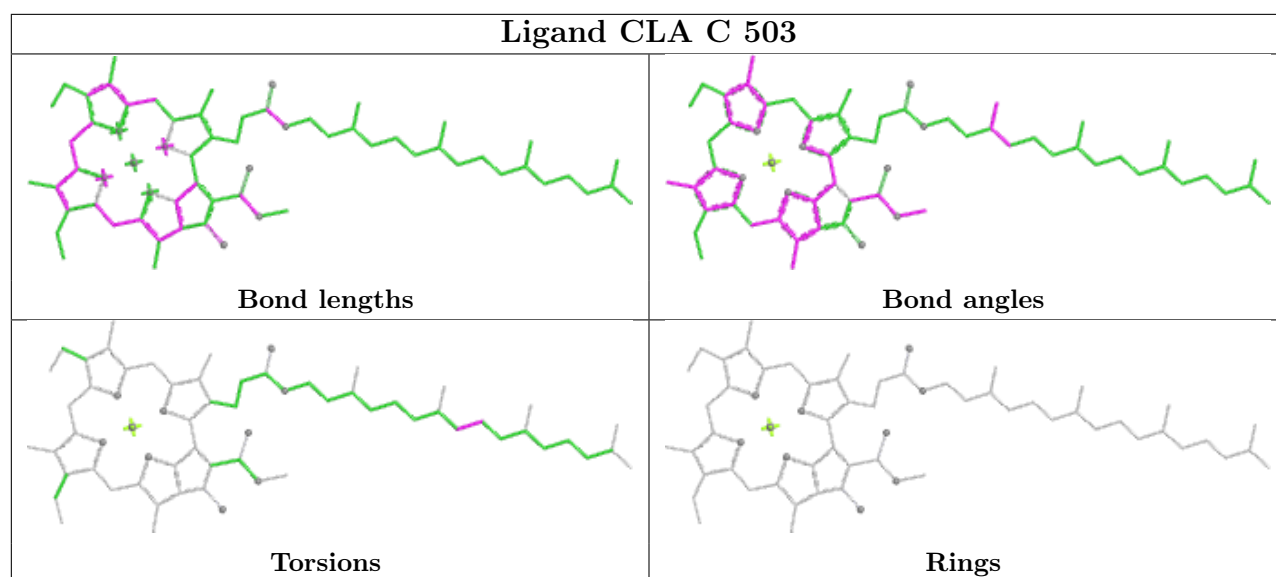


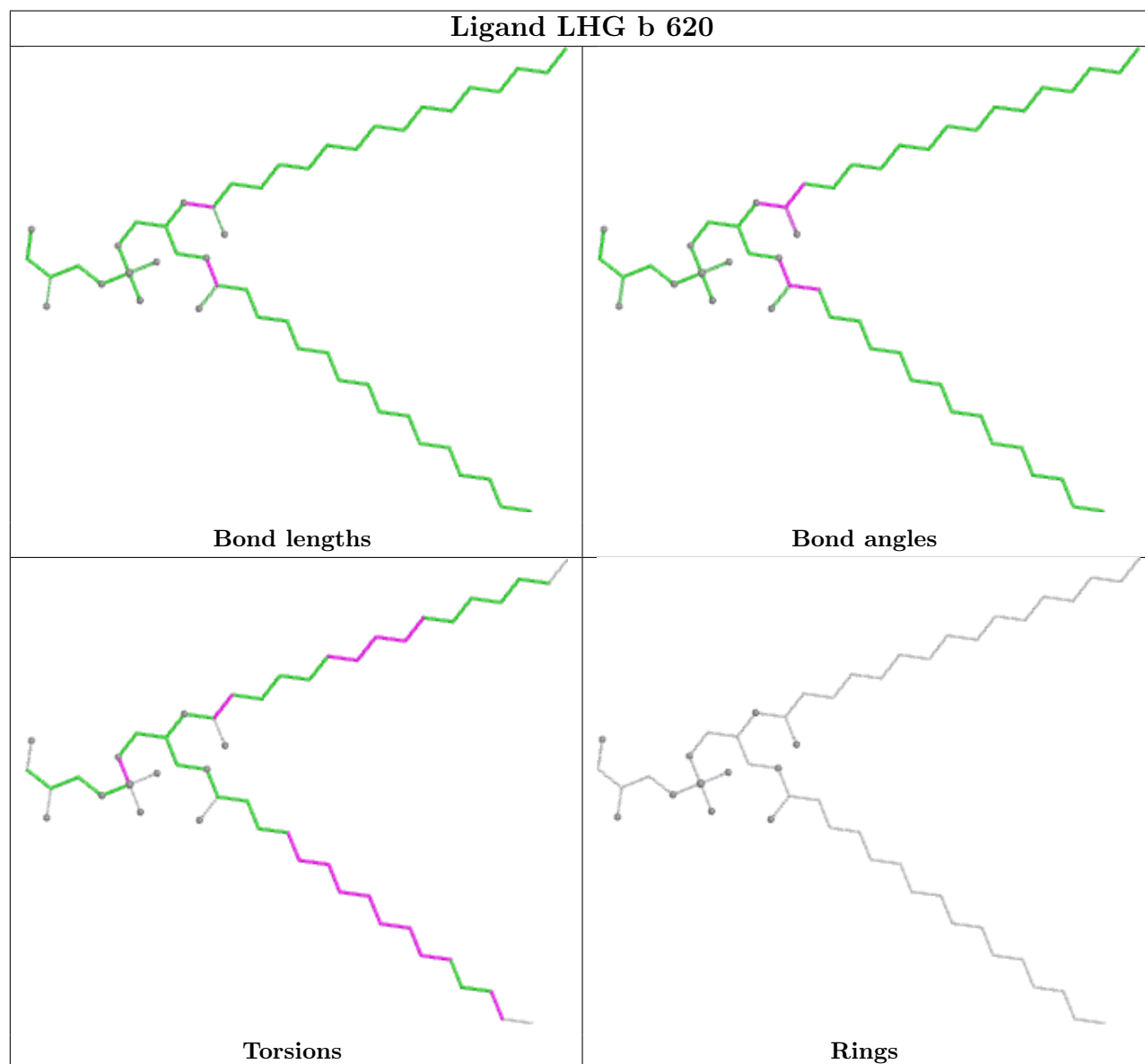
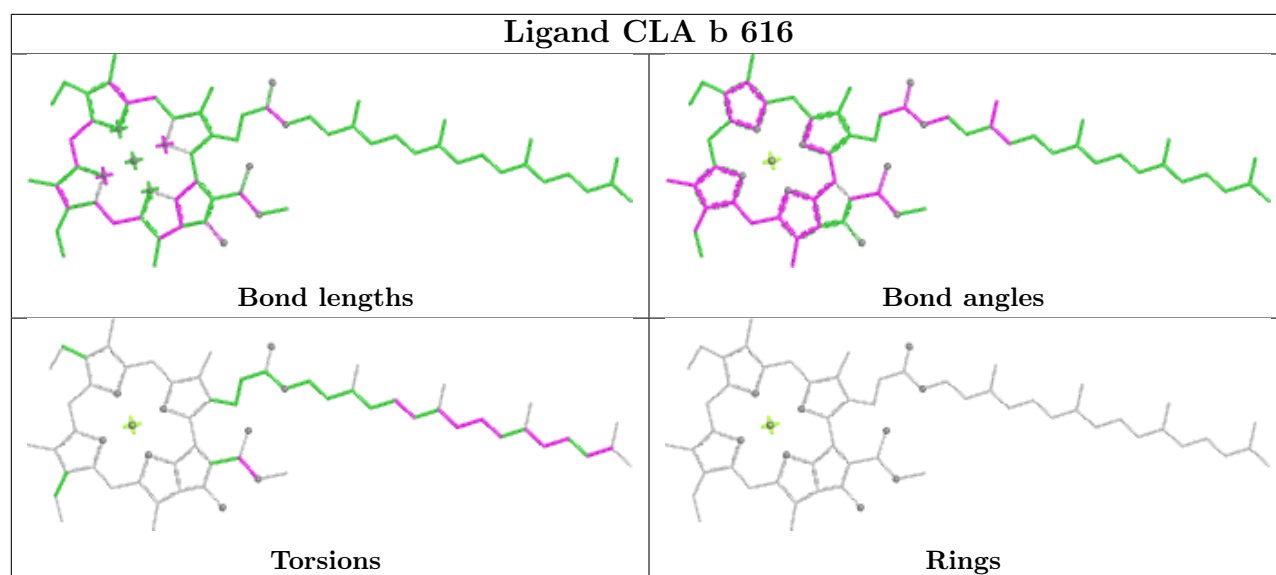
Ligand CLA A 614



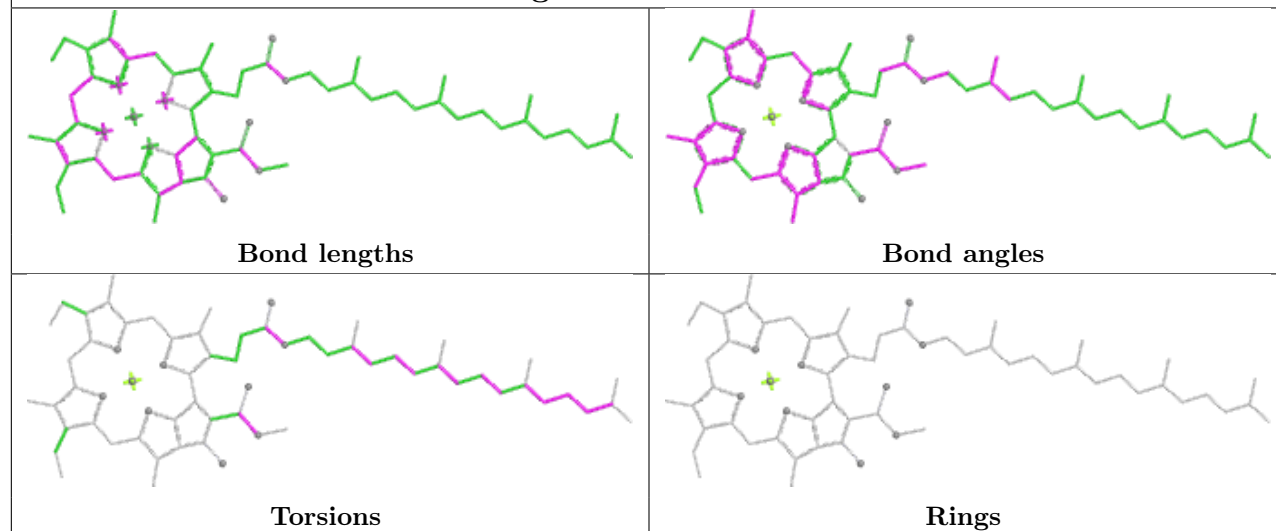




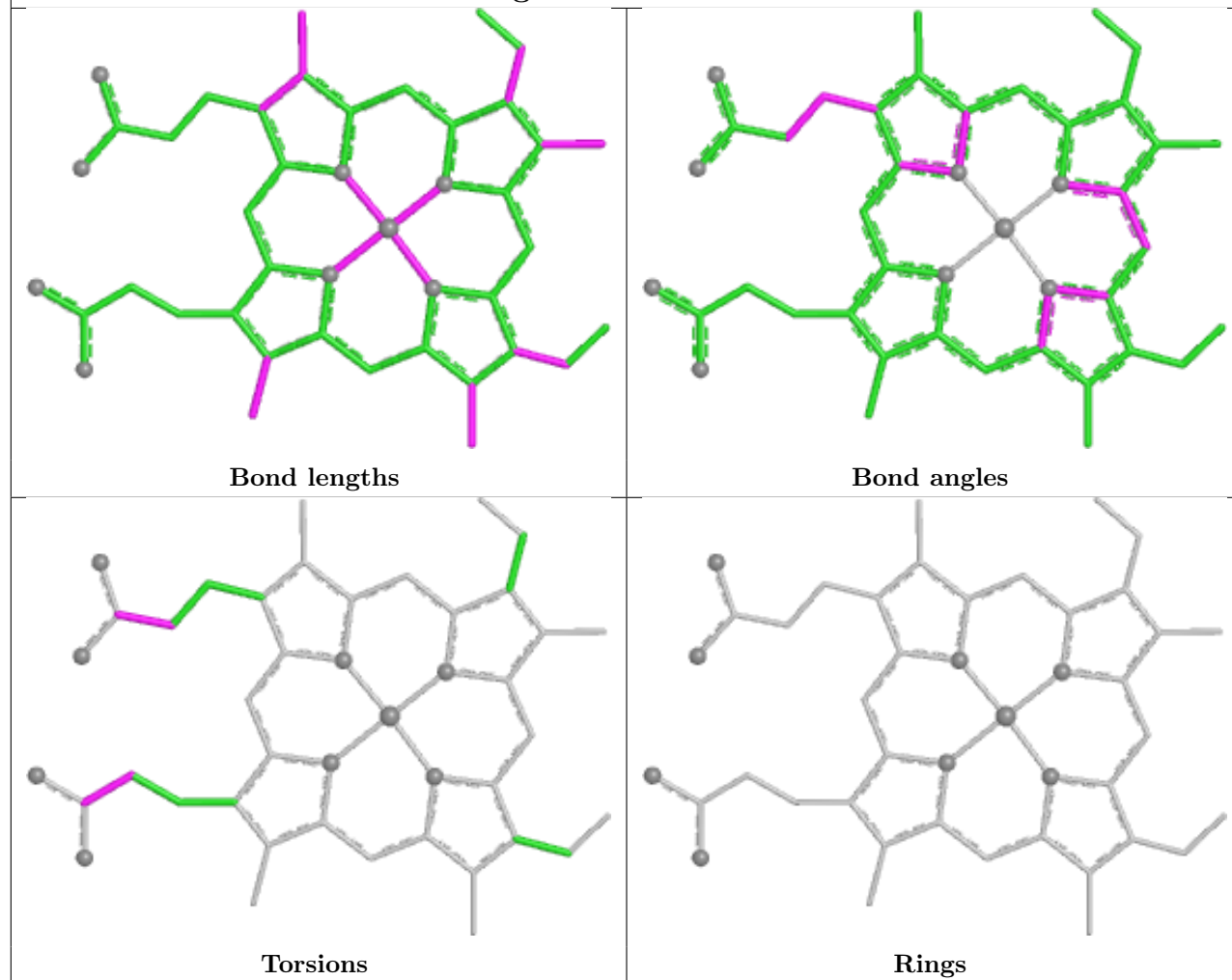


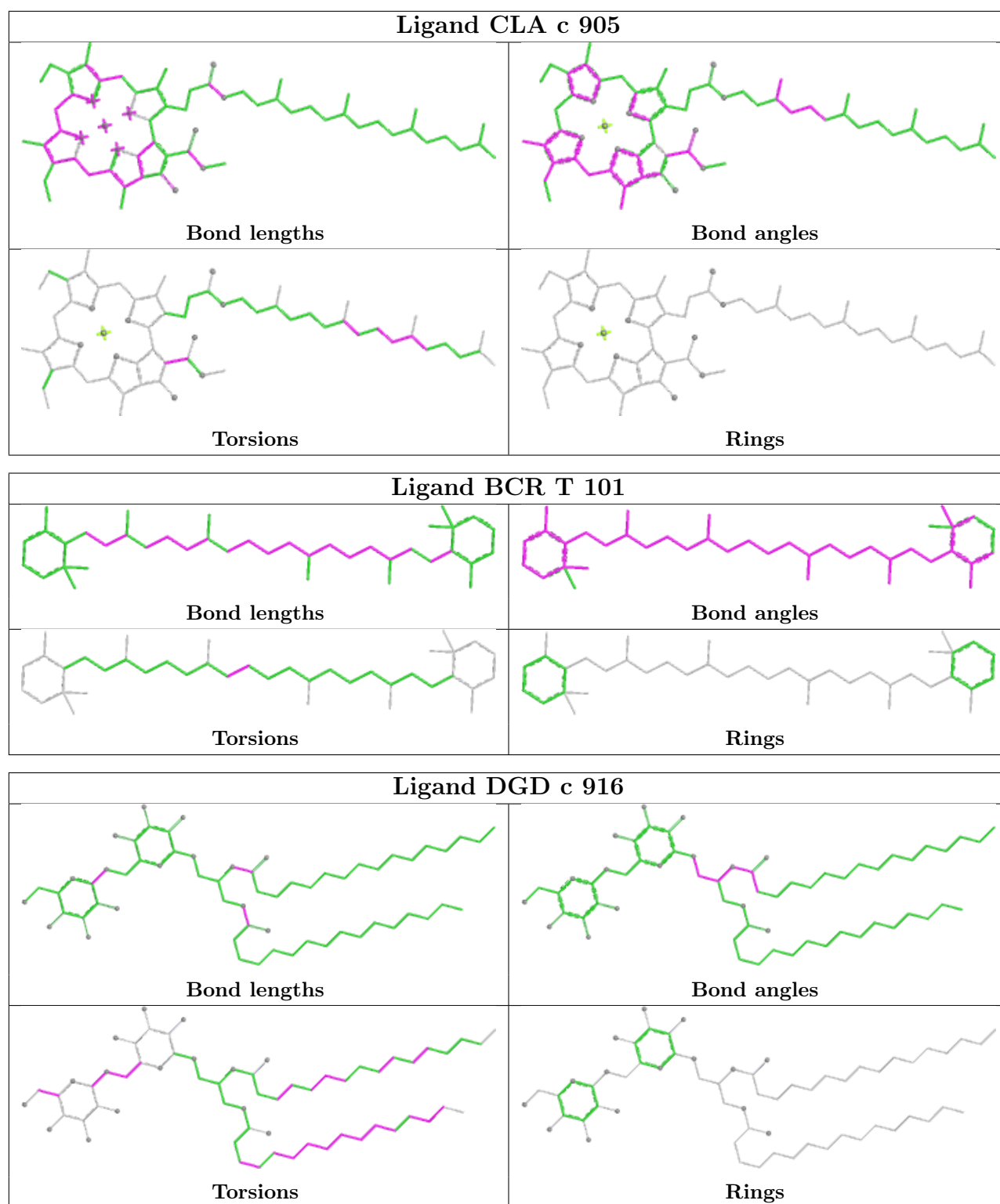


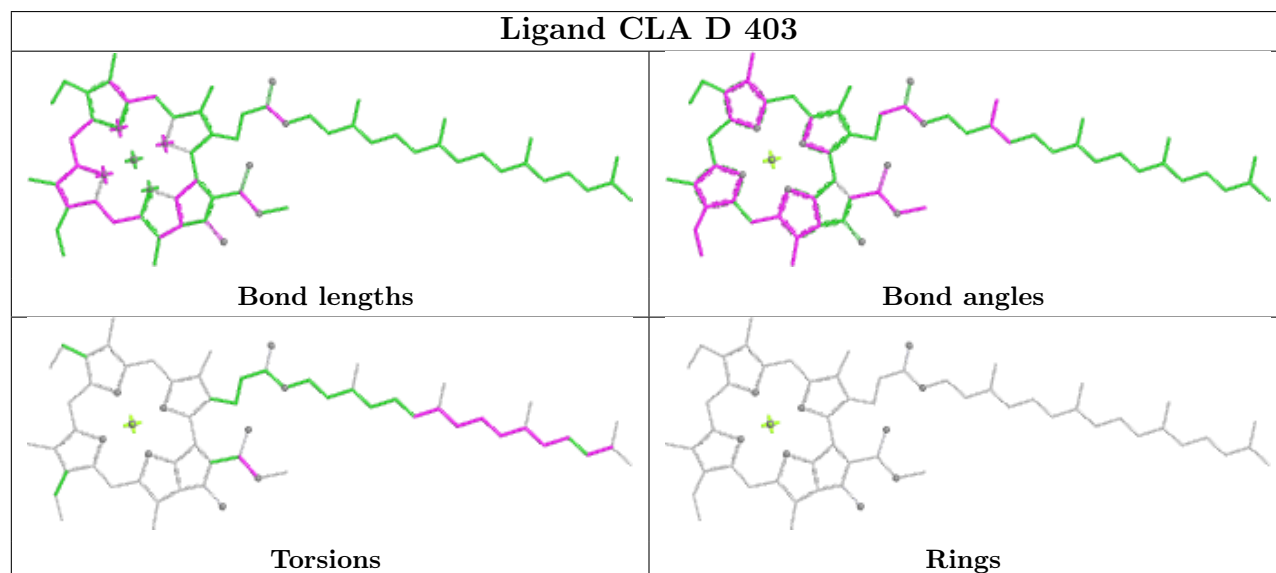
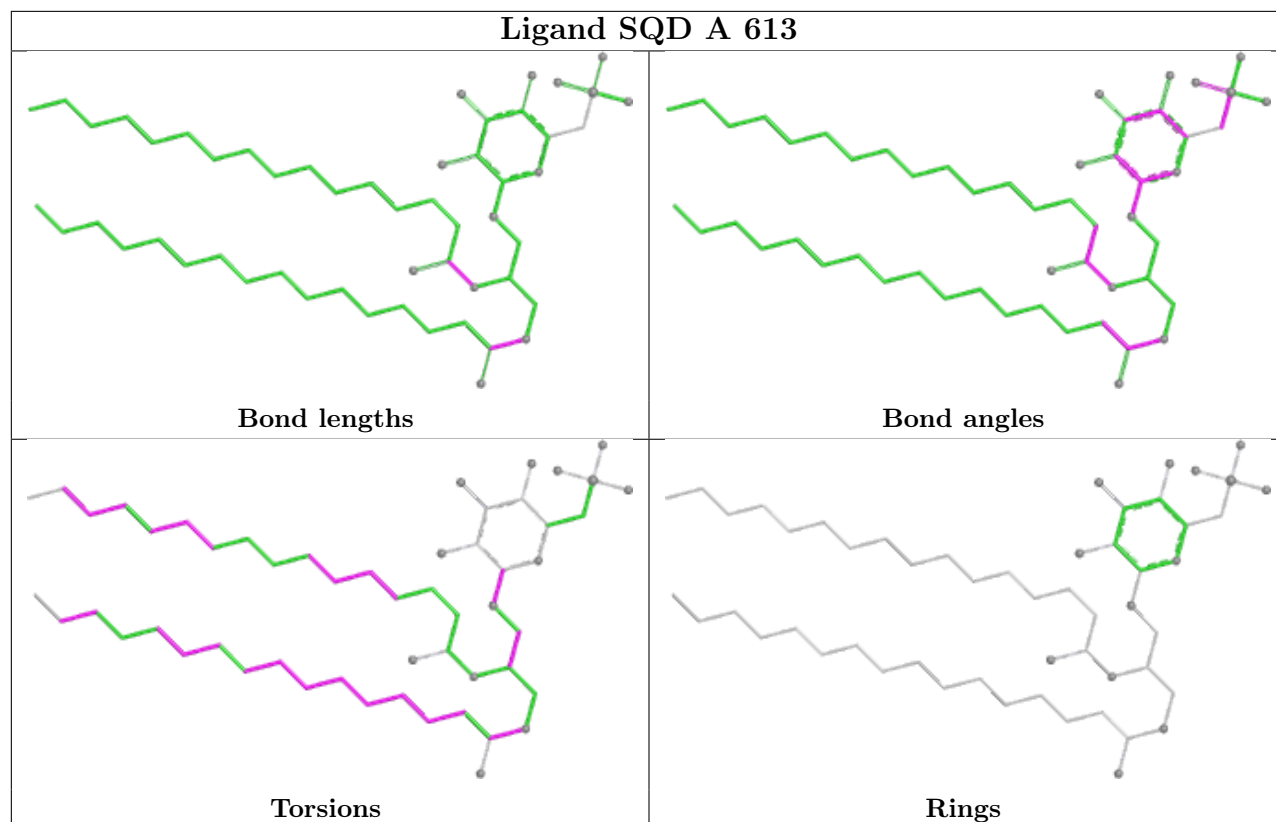
Ligand CLA A 609



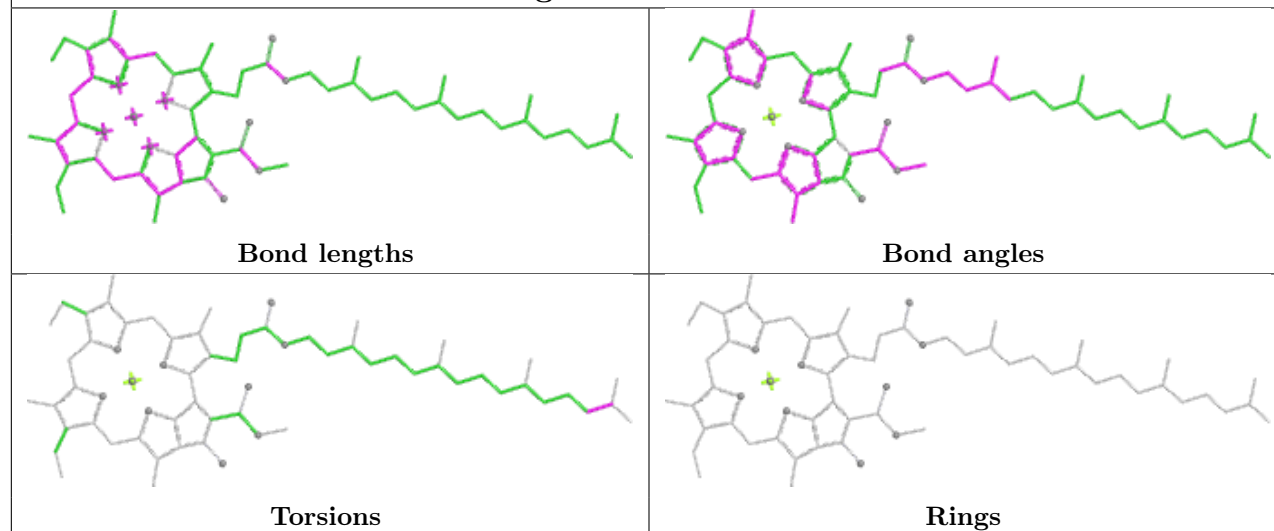
Ligand HEM e 101



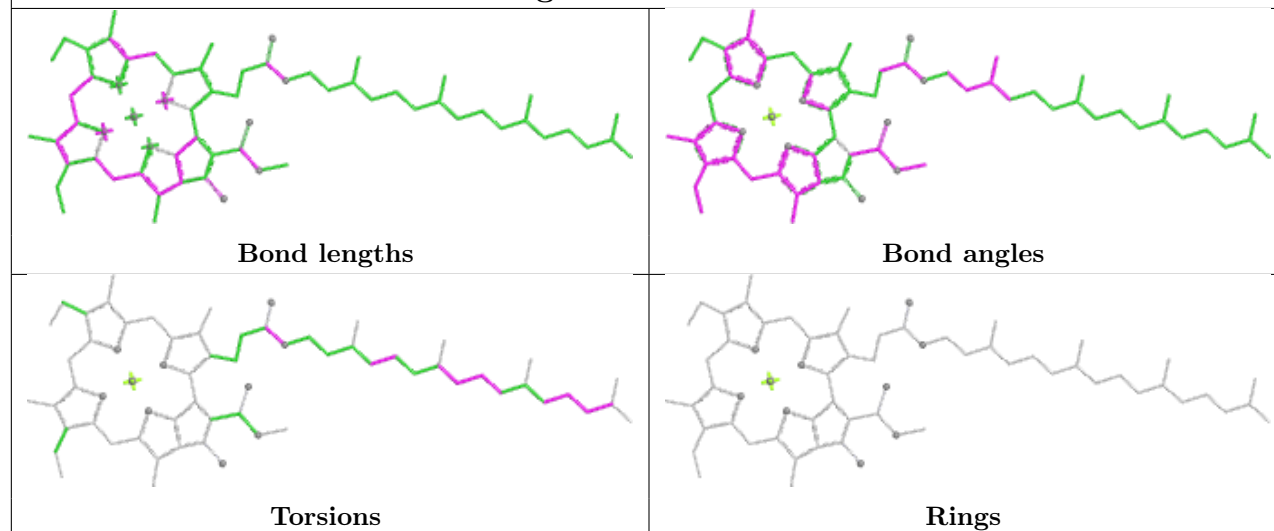




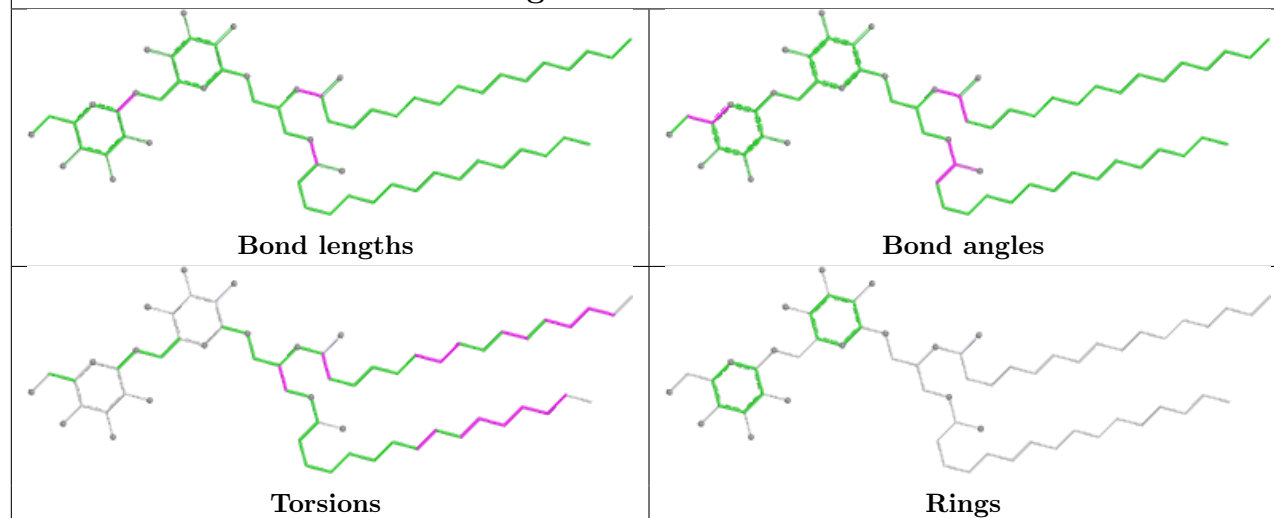
Ligand CLA b 603

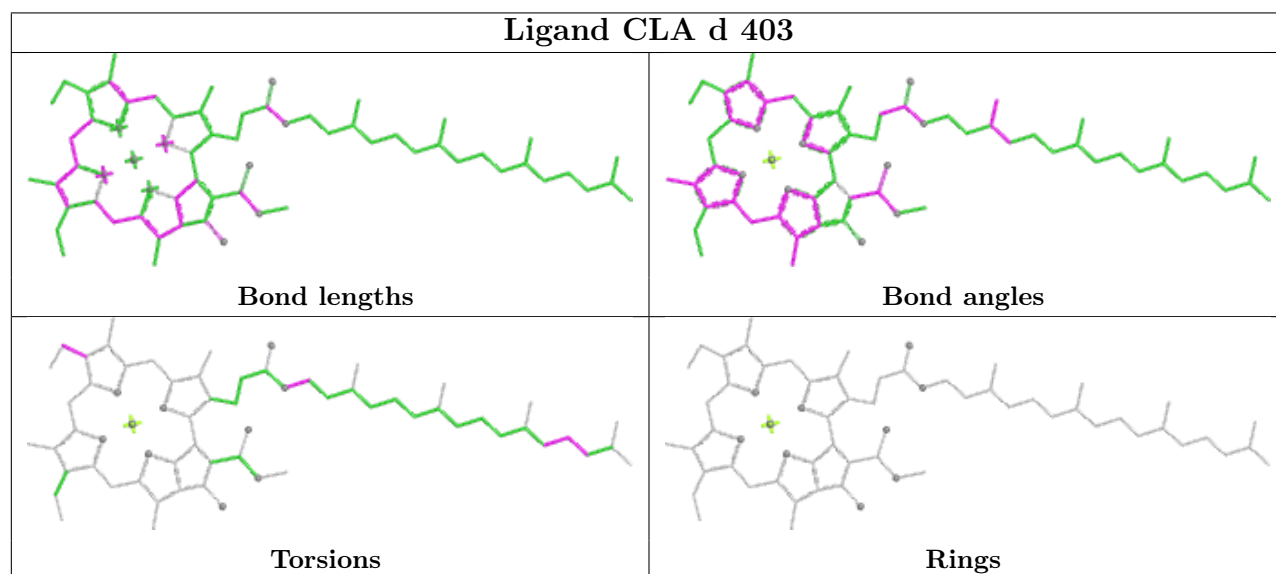
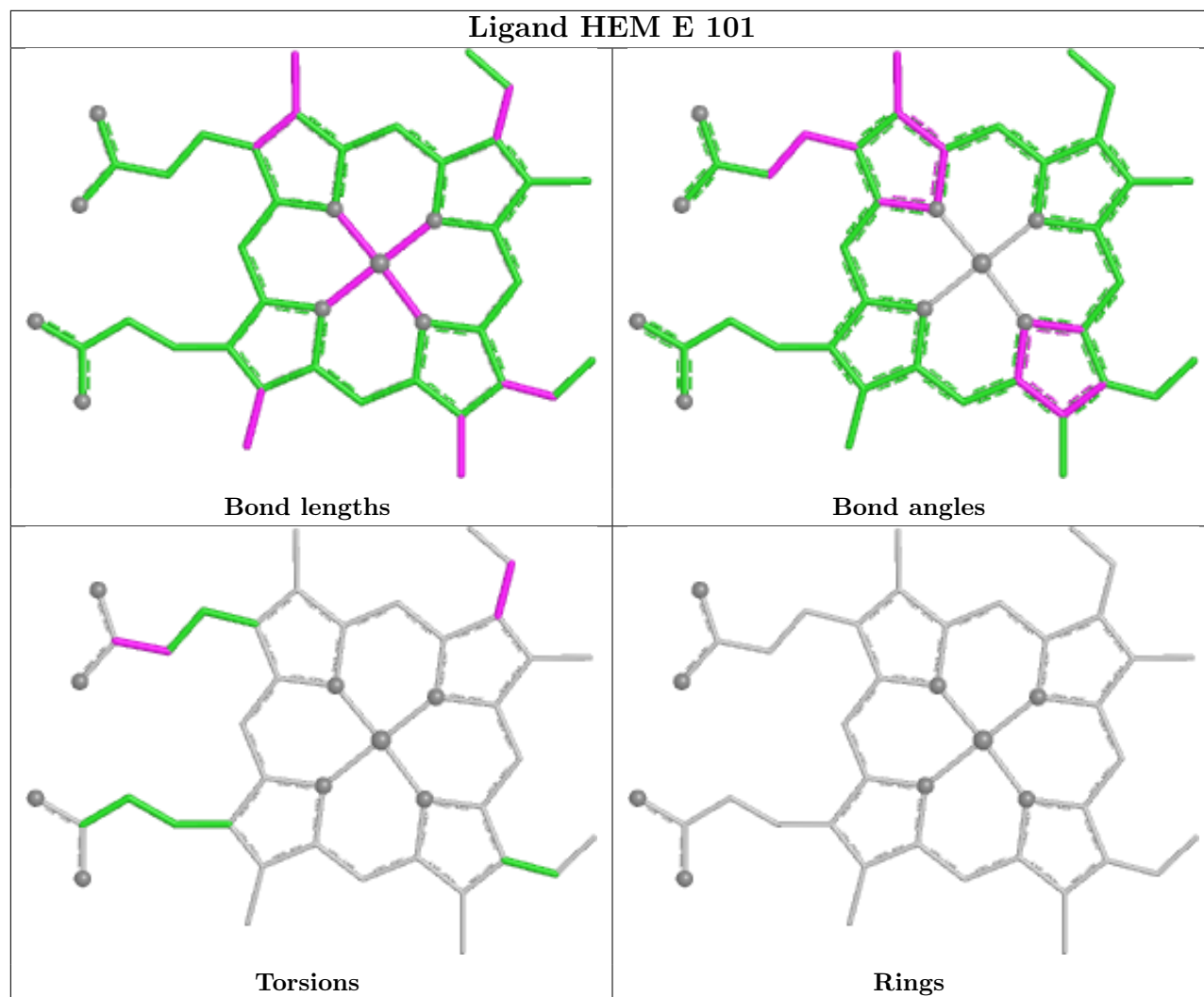


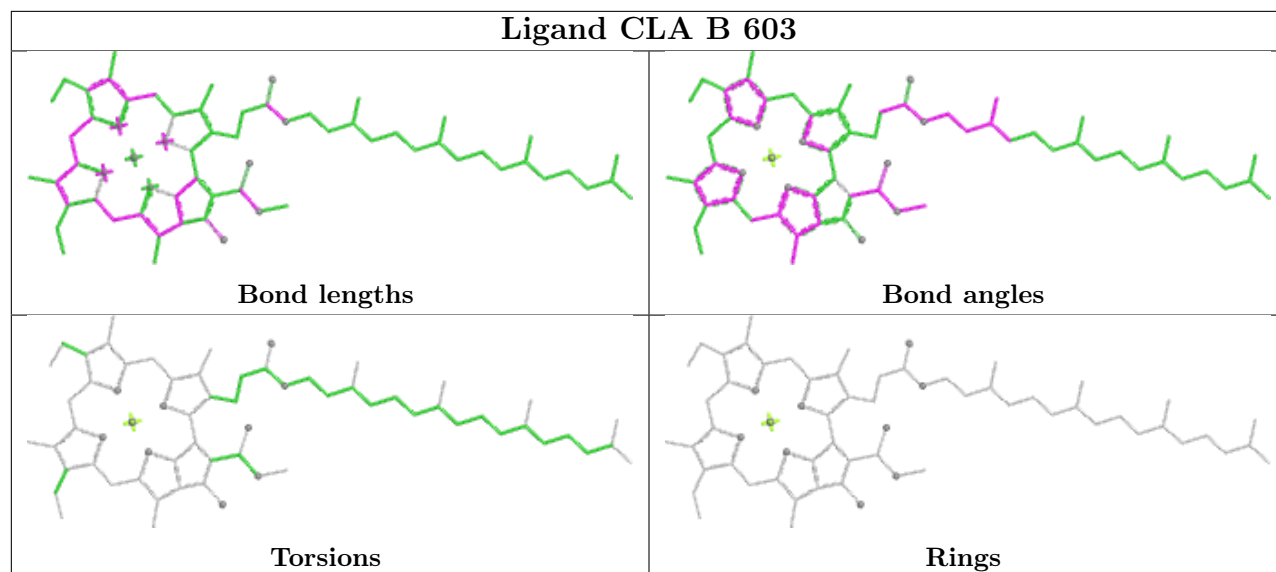
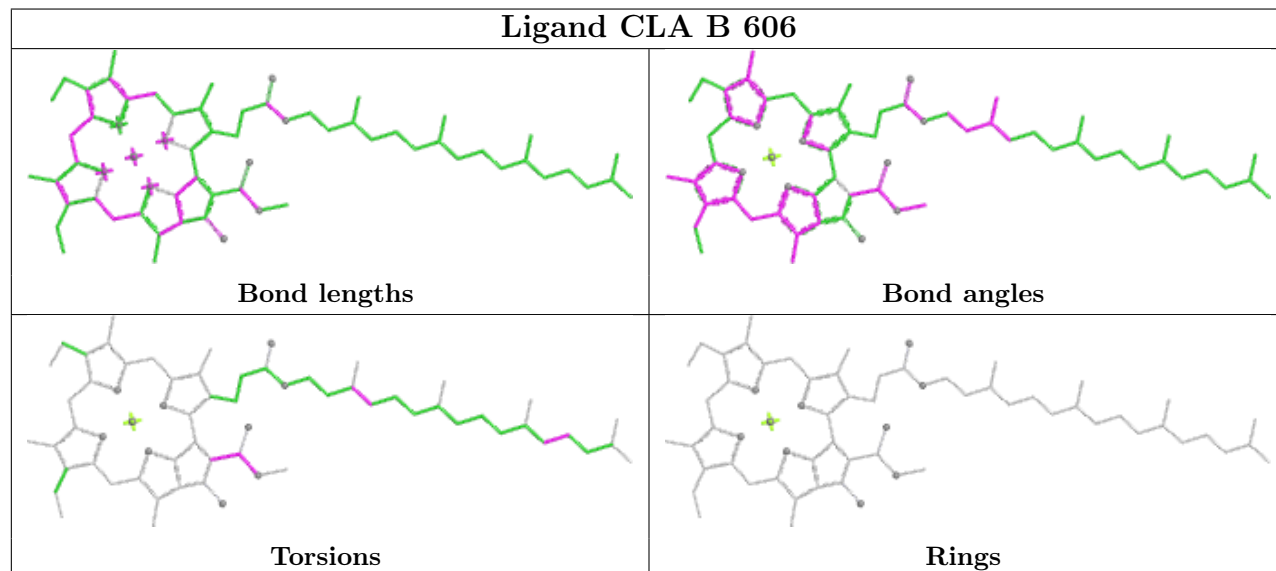
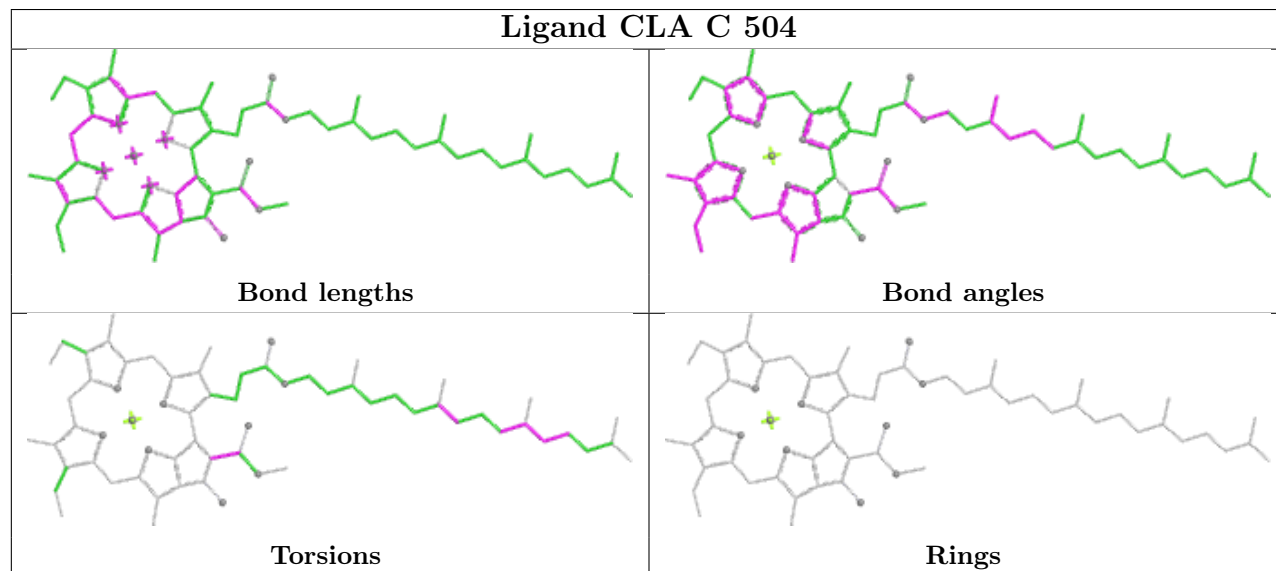
Ligand CLA a 408



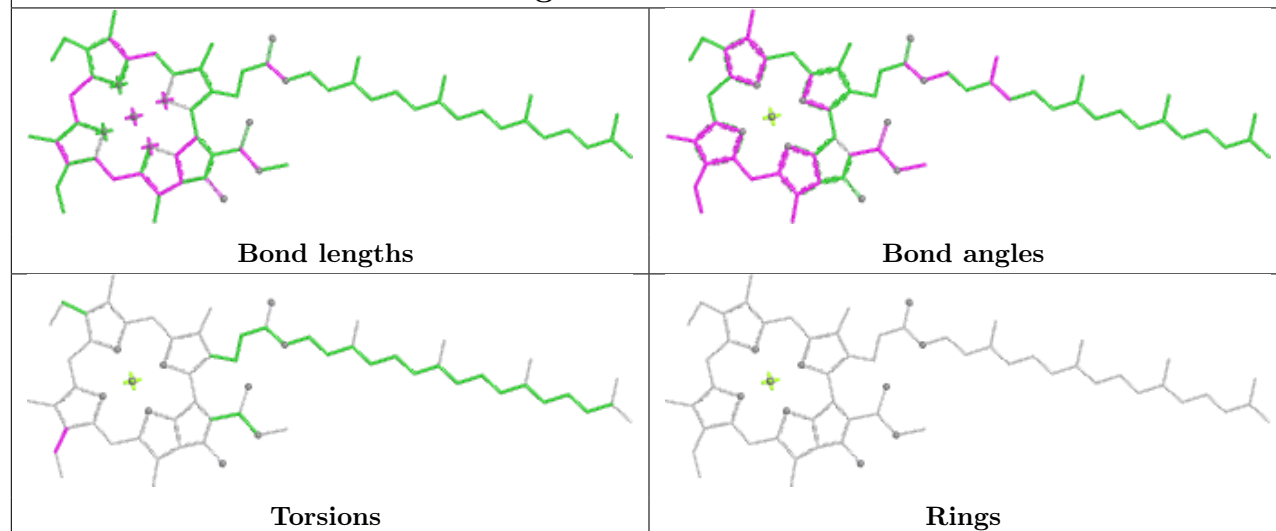
Ligand DGD H 102



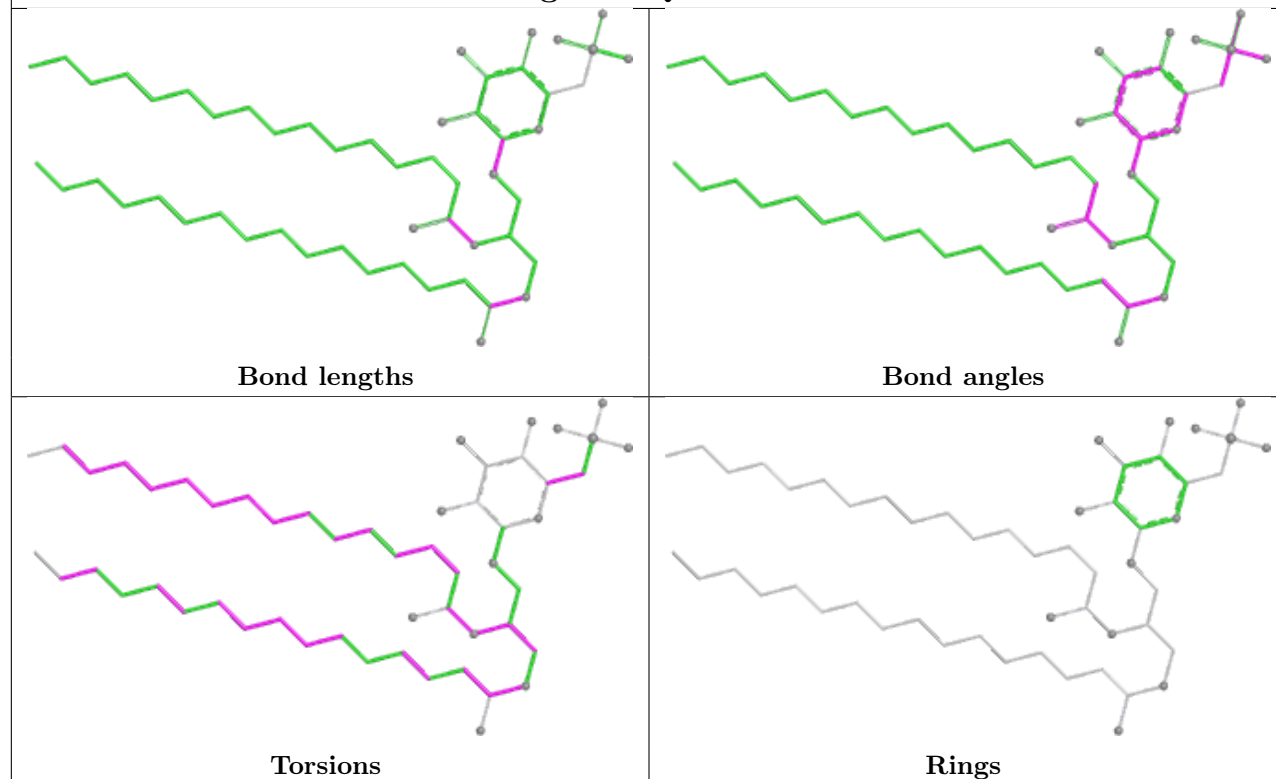


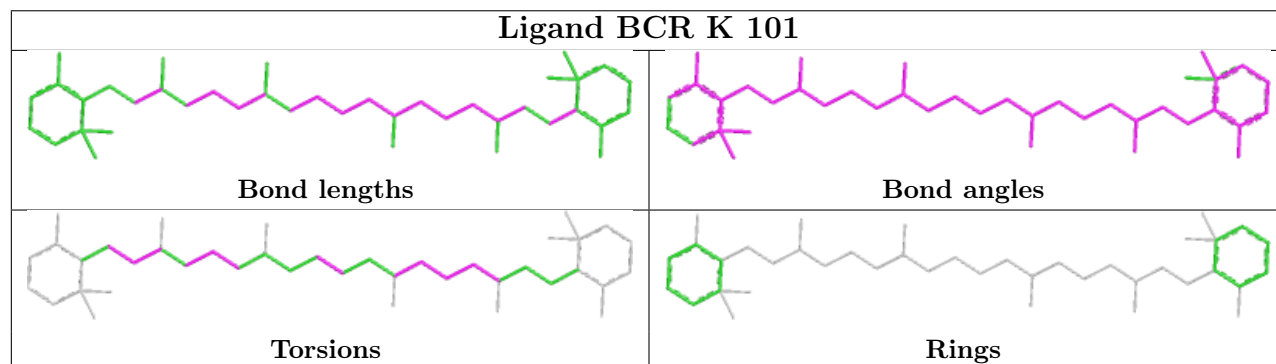
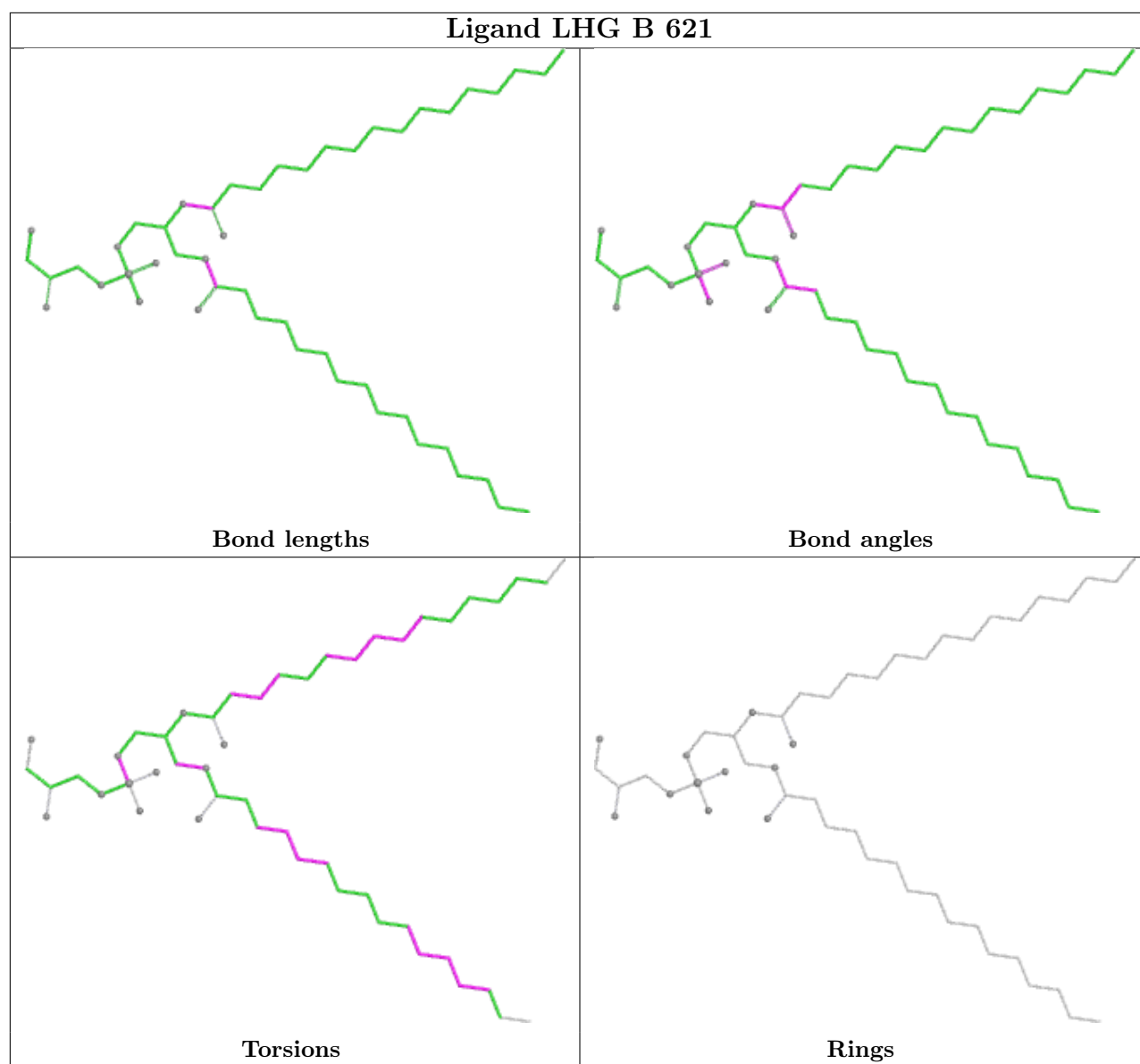
Ligand CLA B 603**Ligand CLA B 606****Ligand CLA C 504**

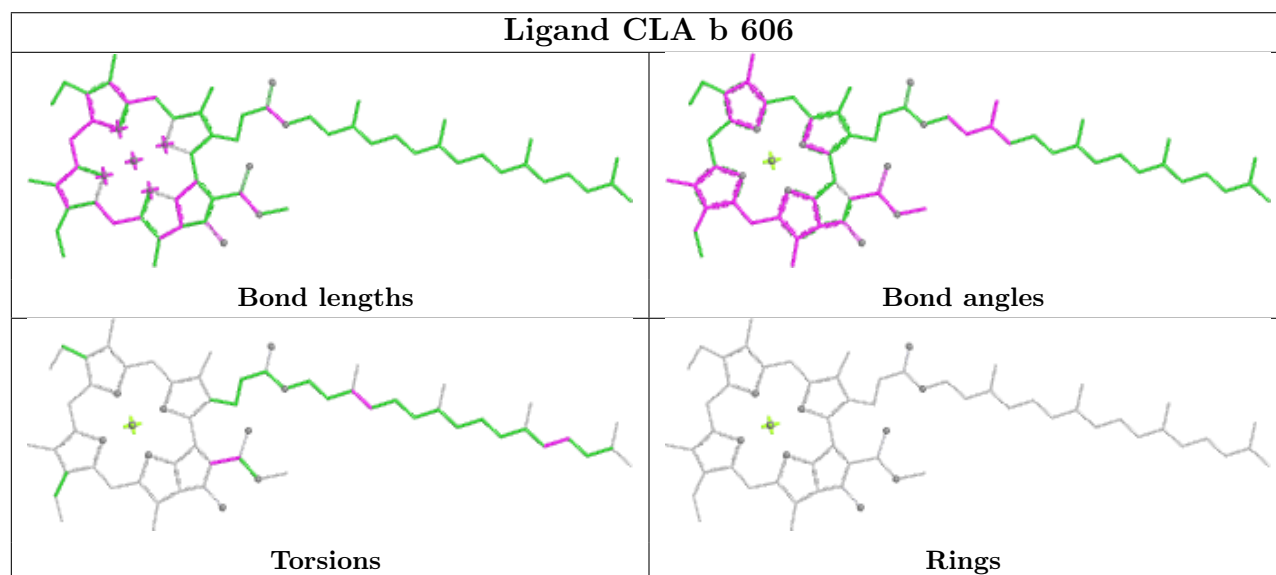
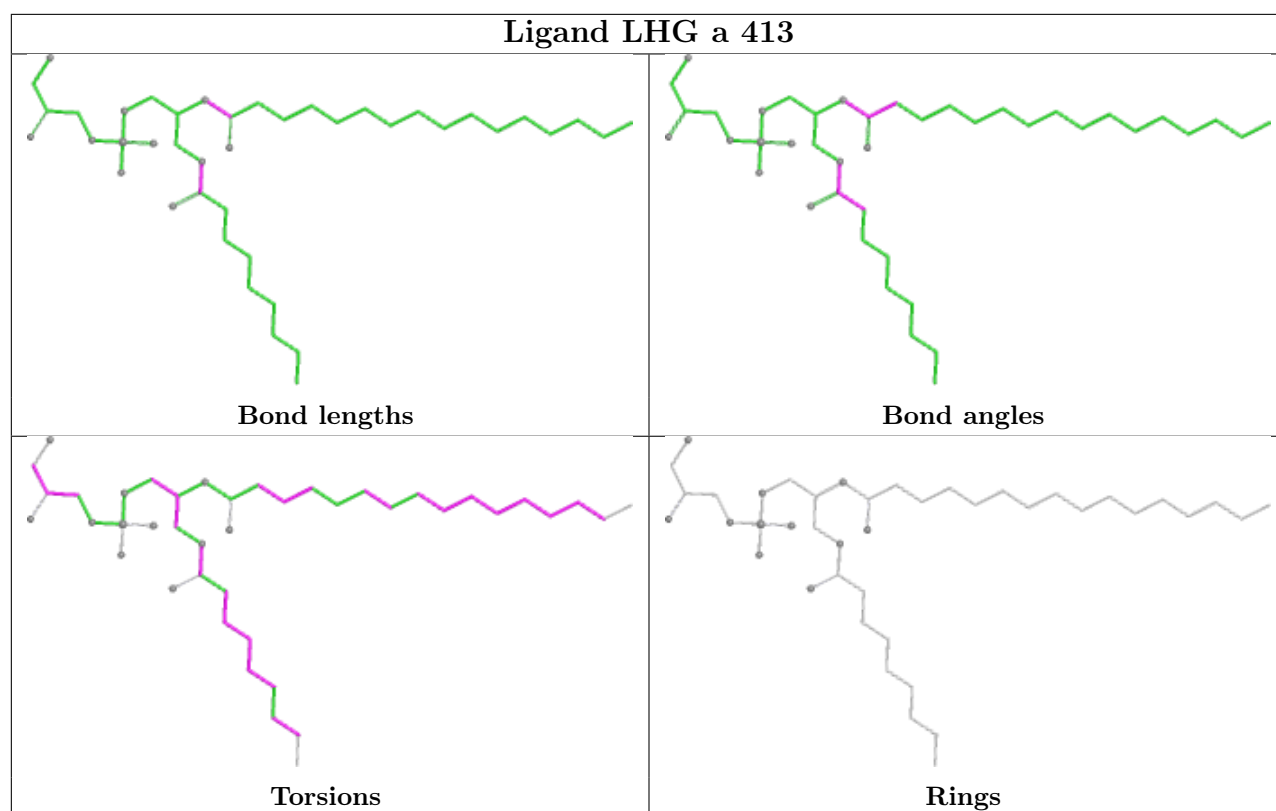
Ligand CLA d 401



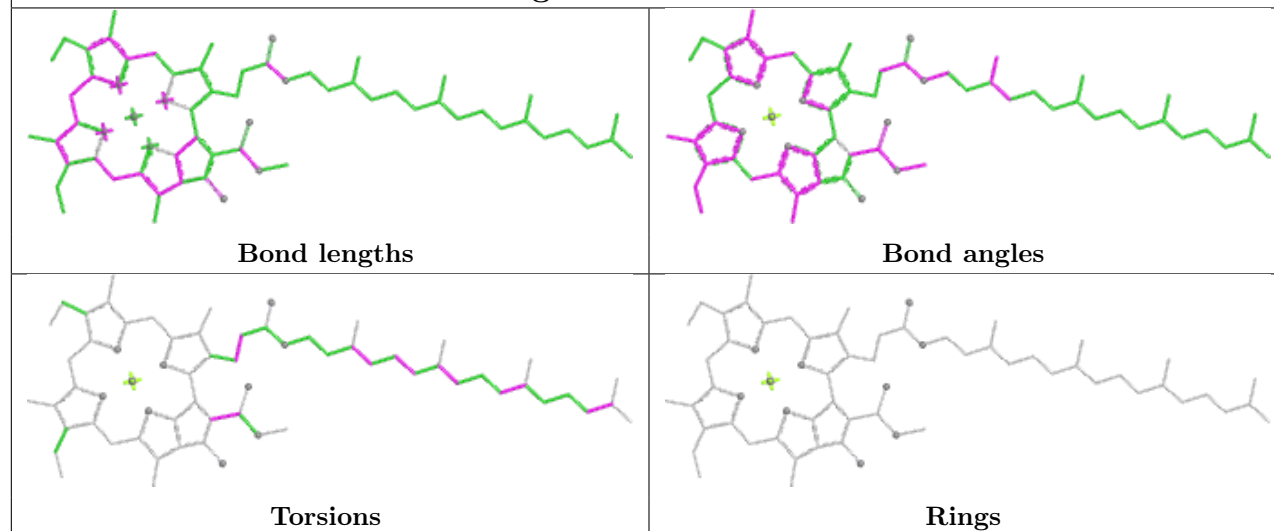
Ligand SQD l 101



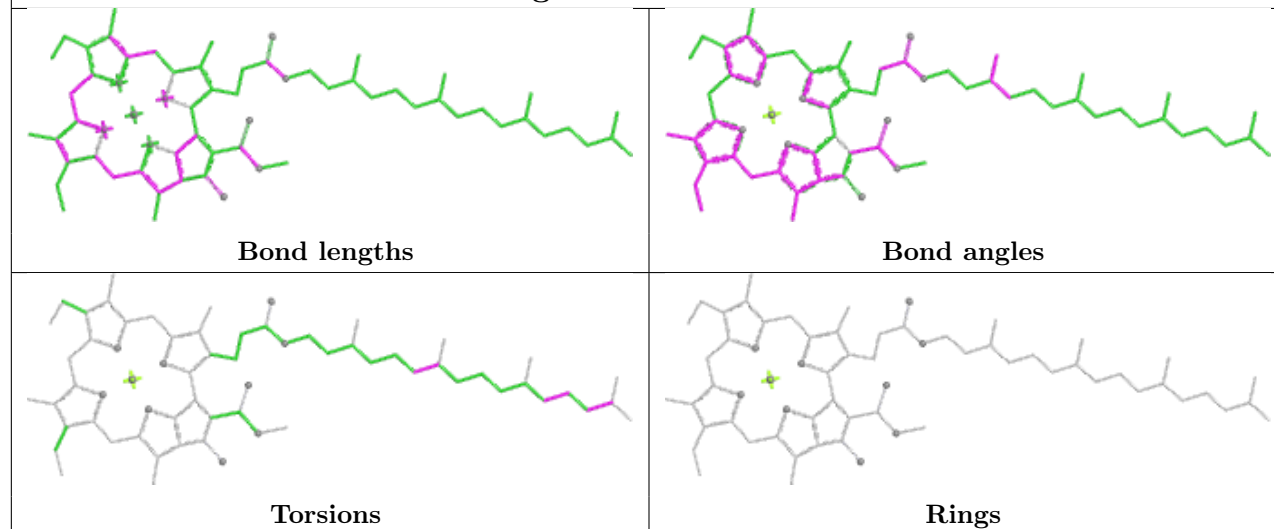




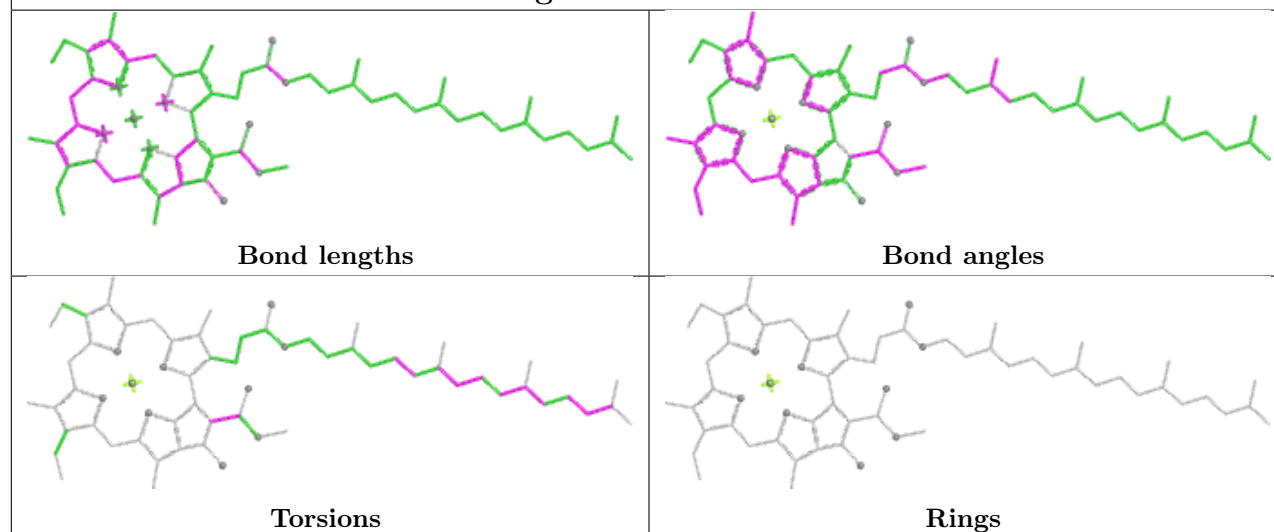
Ligand CLA C 507



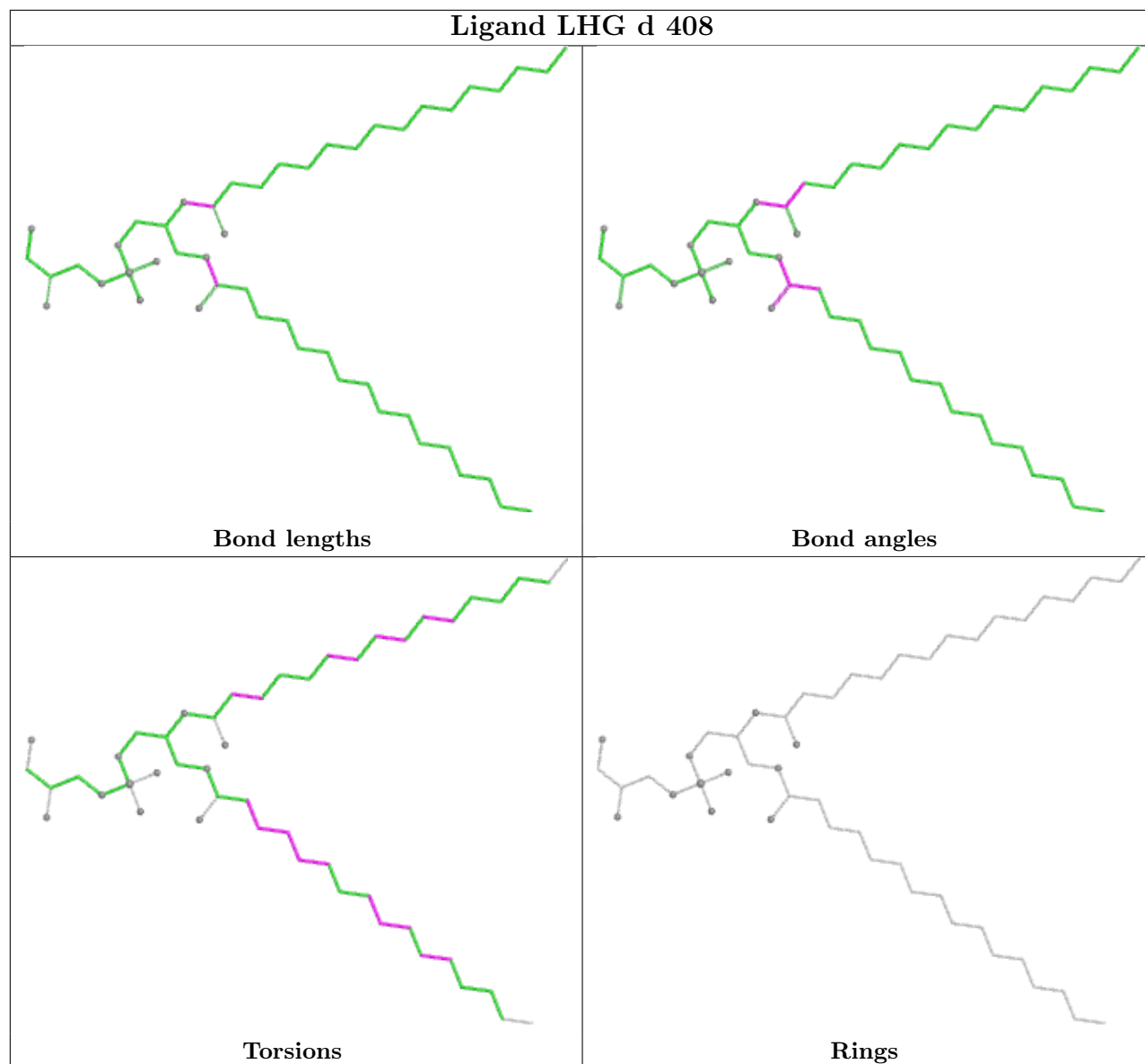
Ligand CLA B 604



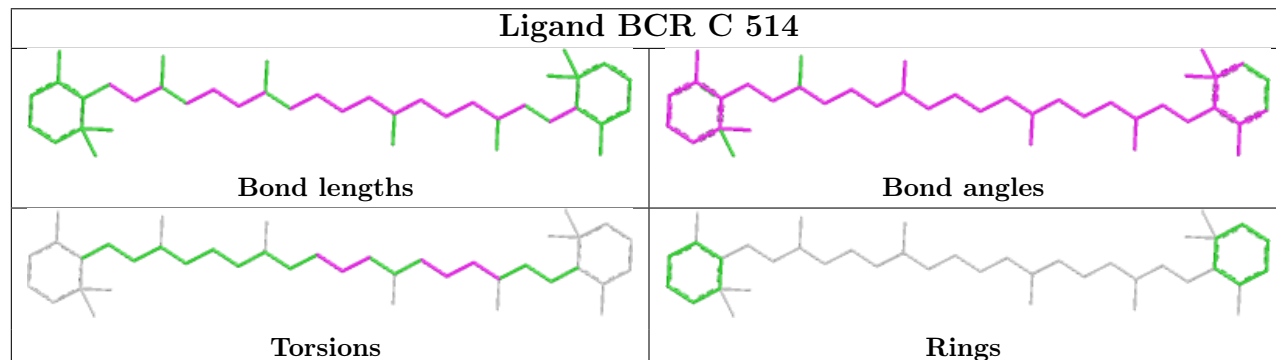
Ligand CLA b 617

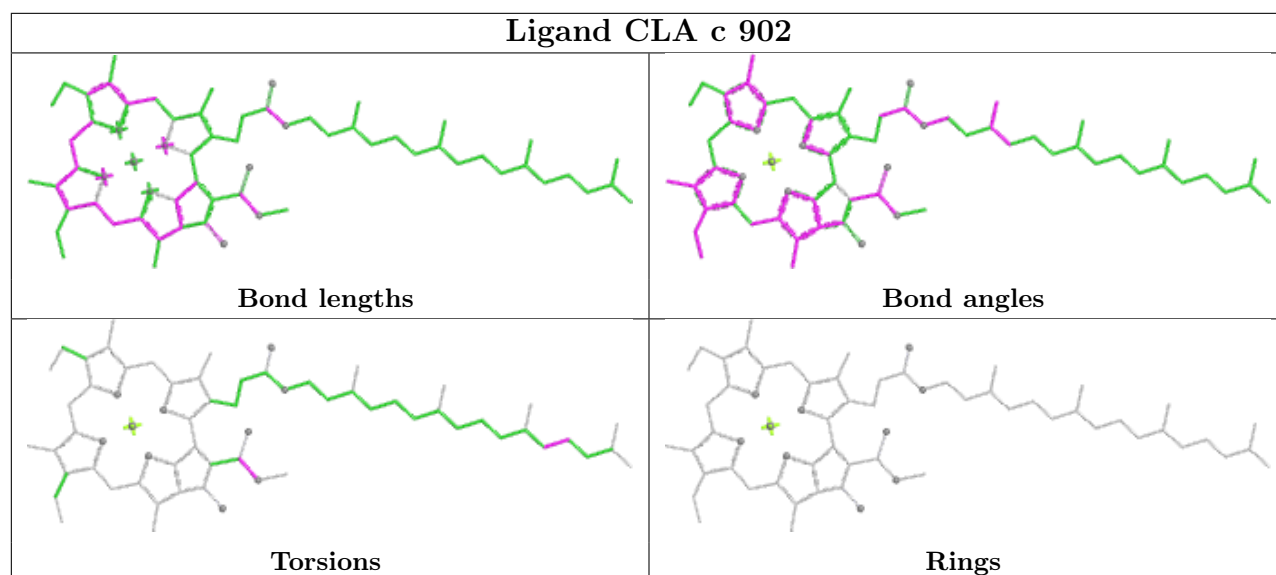
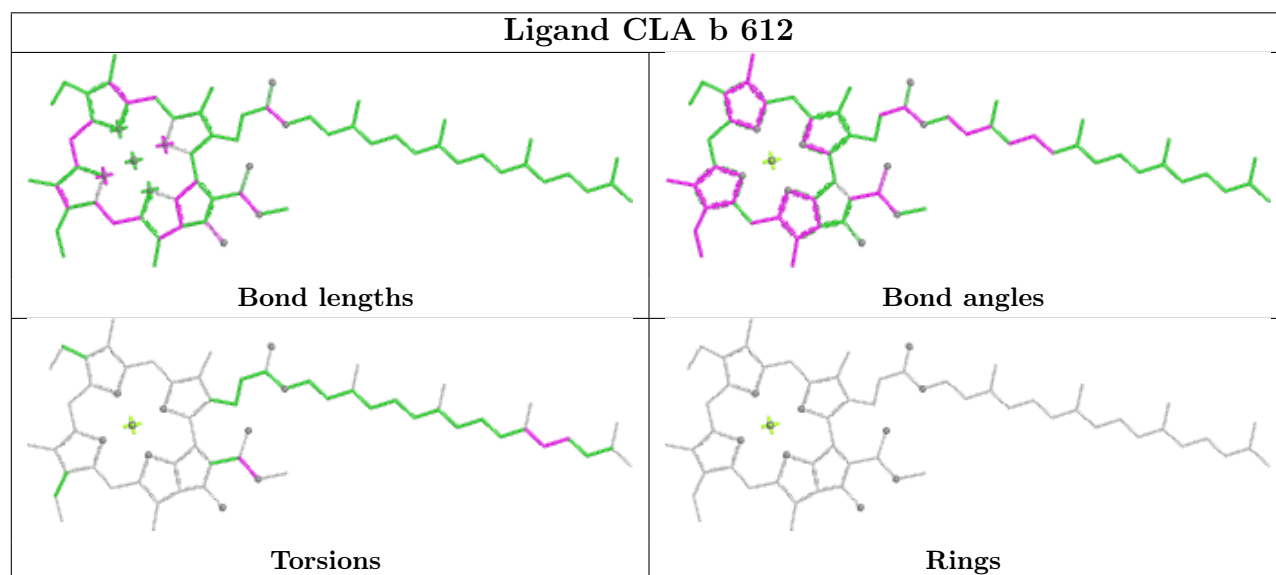
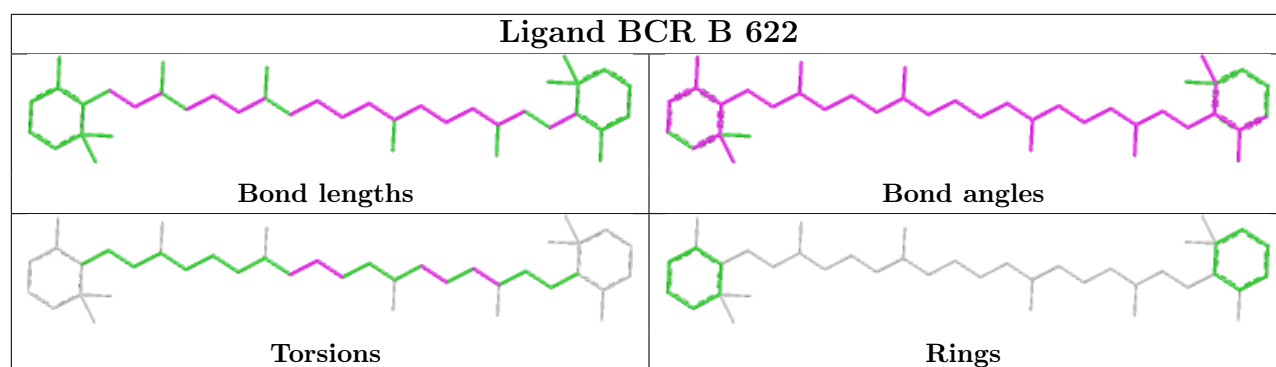


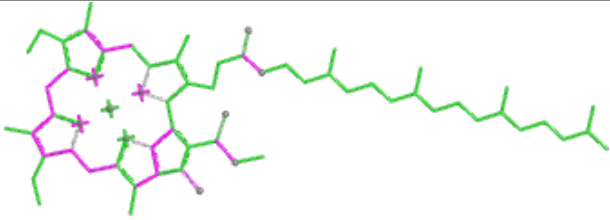
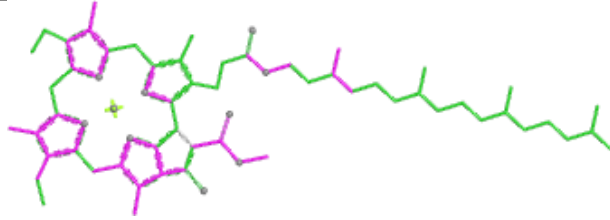
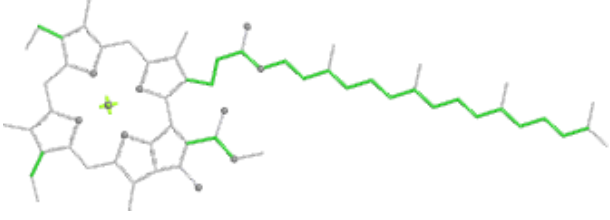
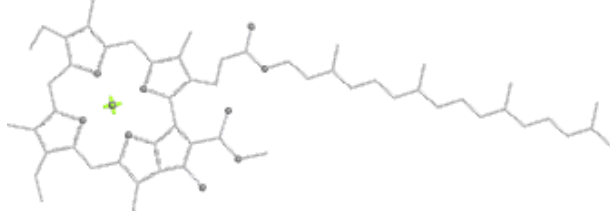
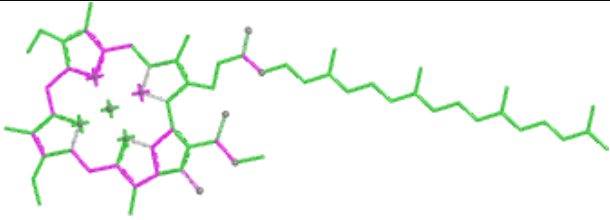
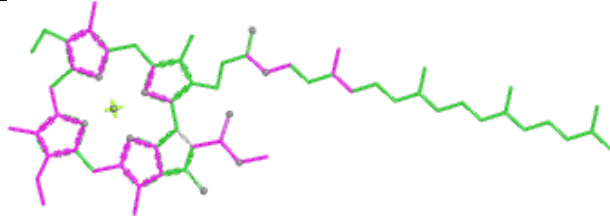
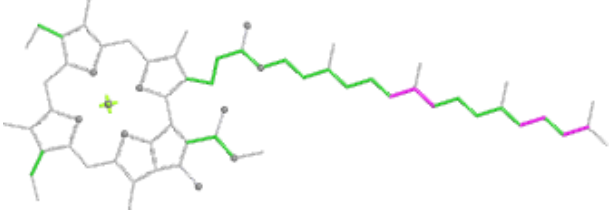
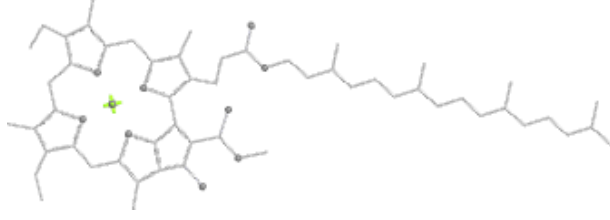
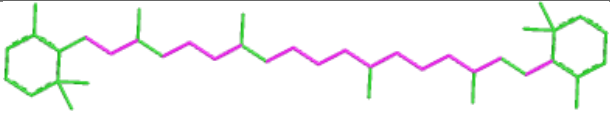
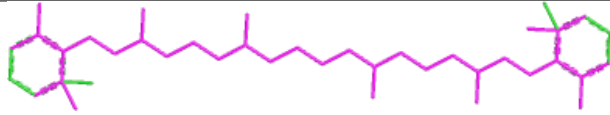
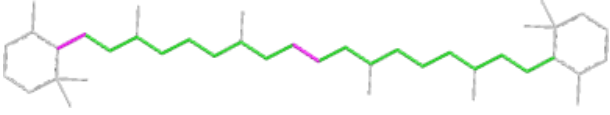
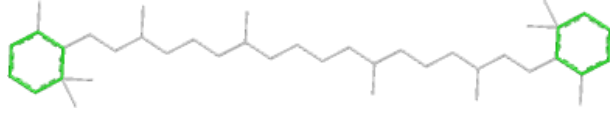
Ligand LHG d 408



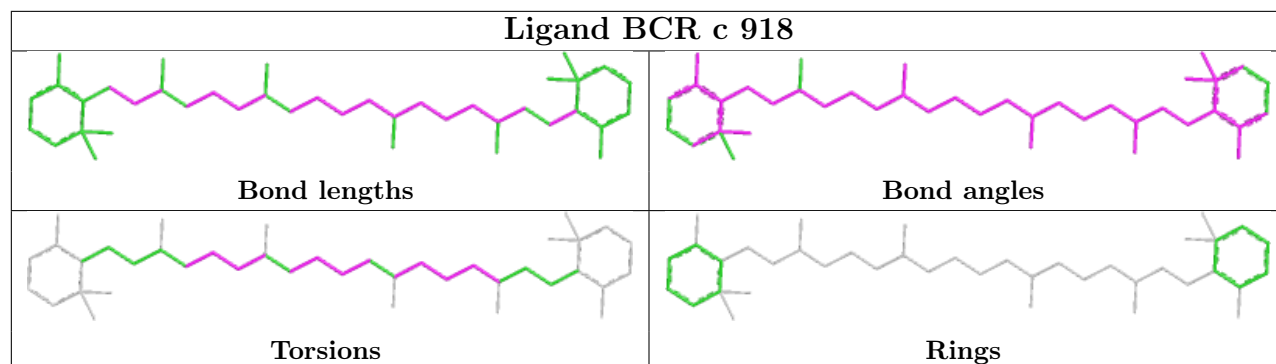
Ligand BCR C 514



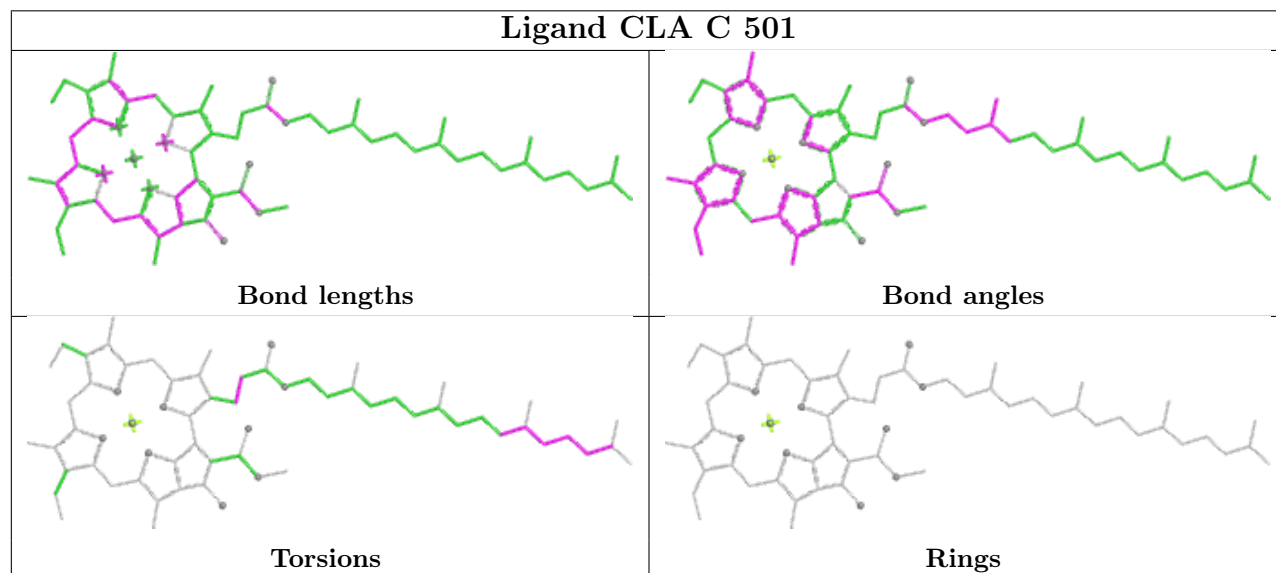


Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

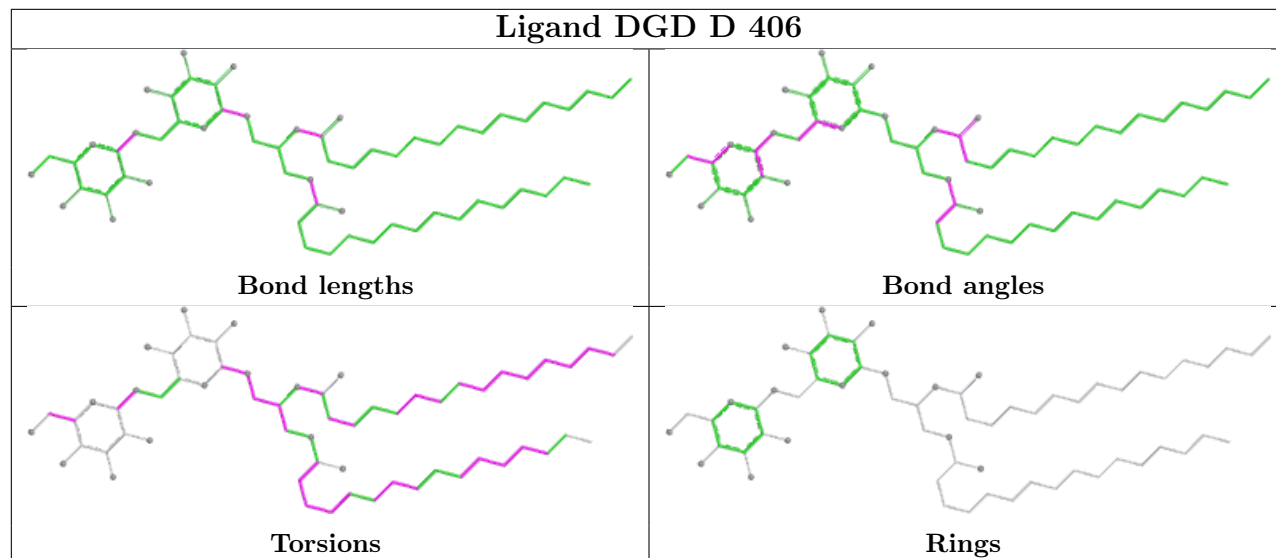
Ligand BCR c 918

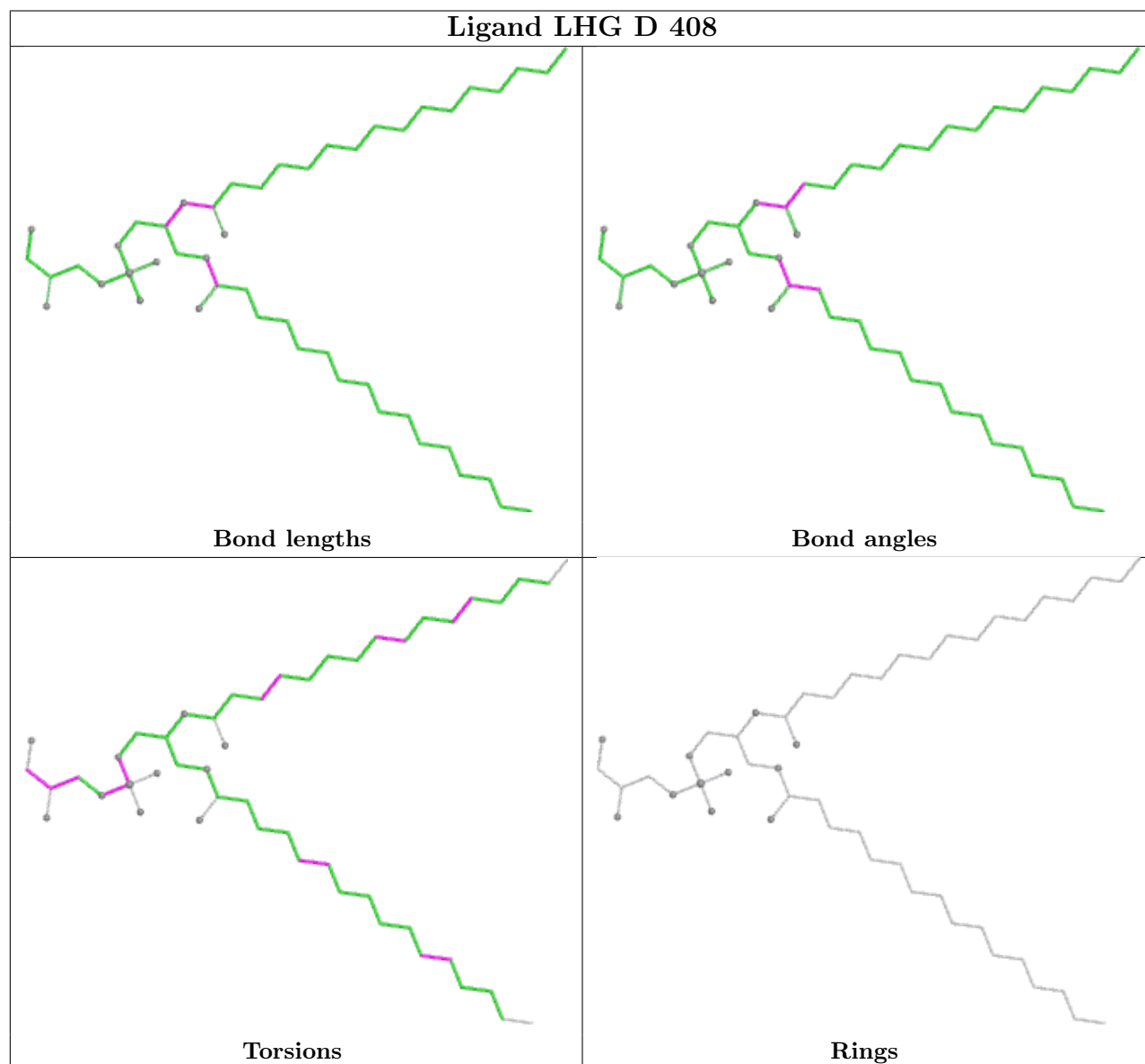
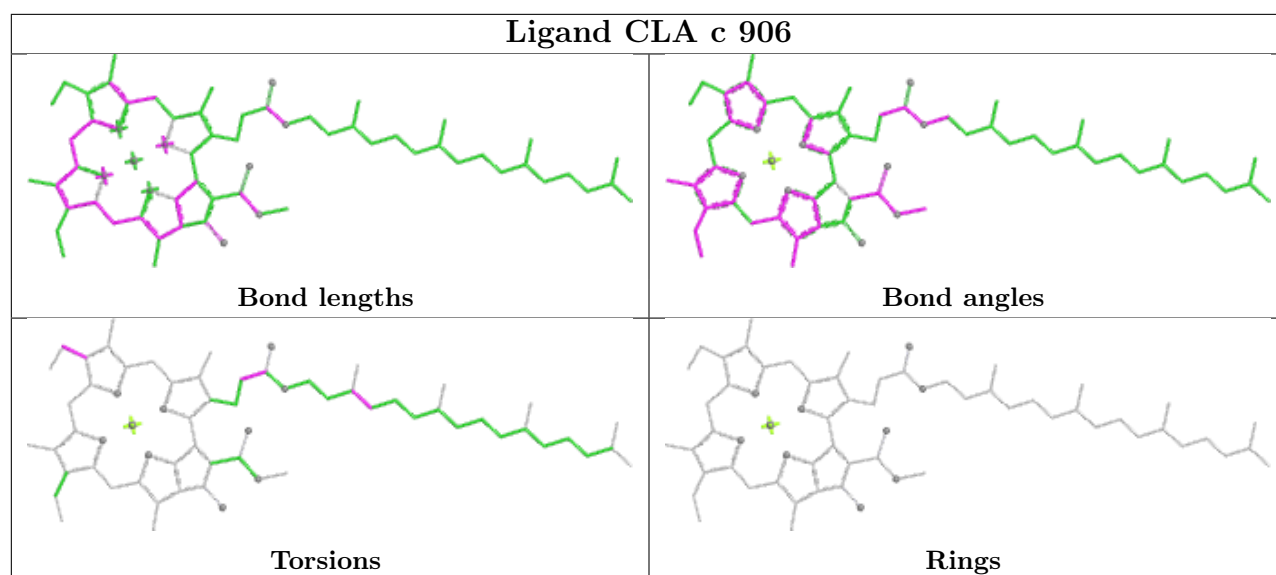


Ligand CLA C 501

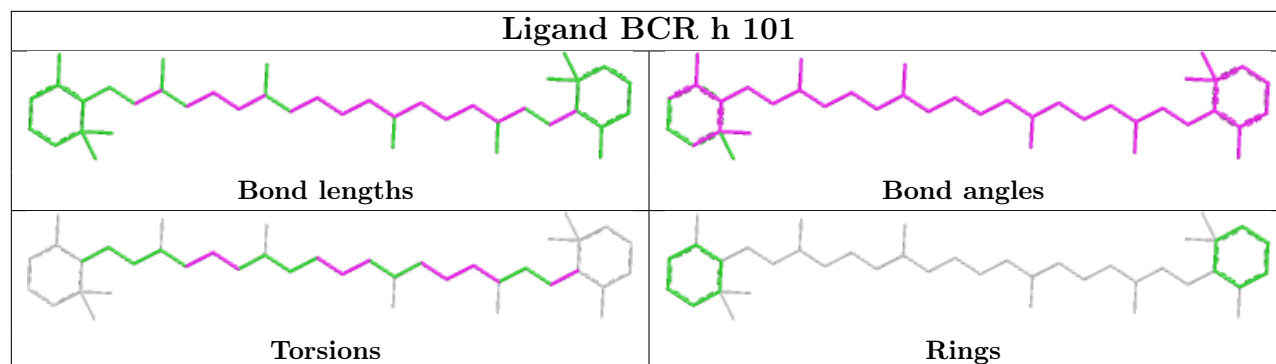


Ligand DGD D 406

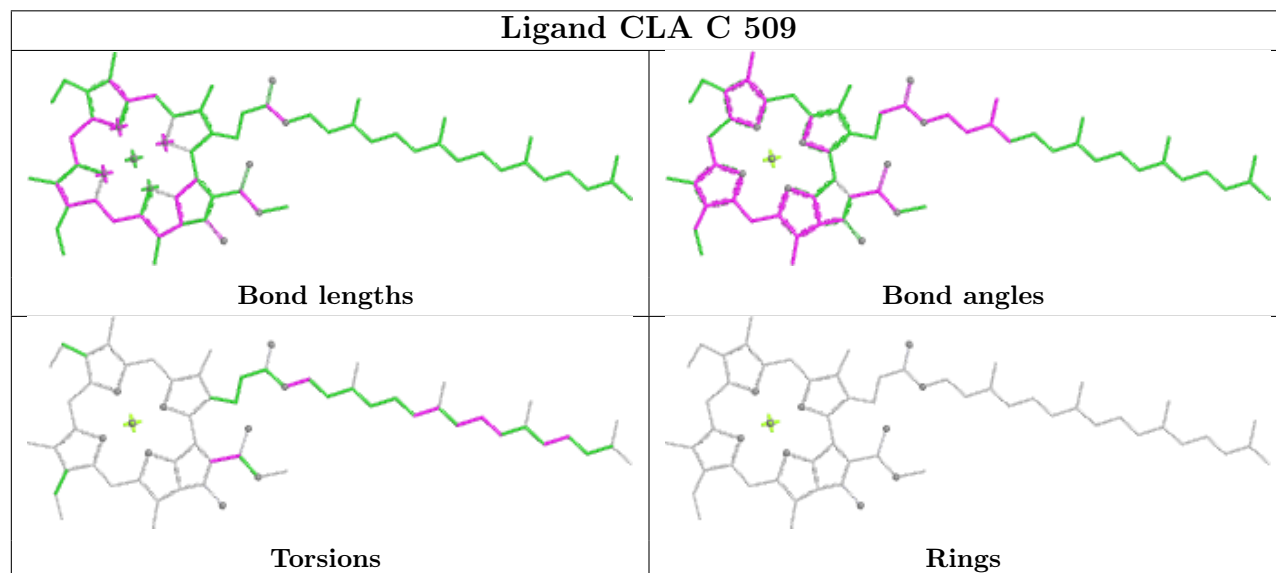




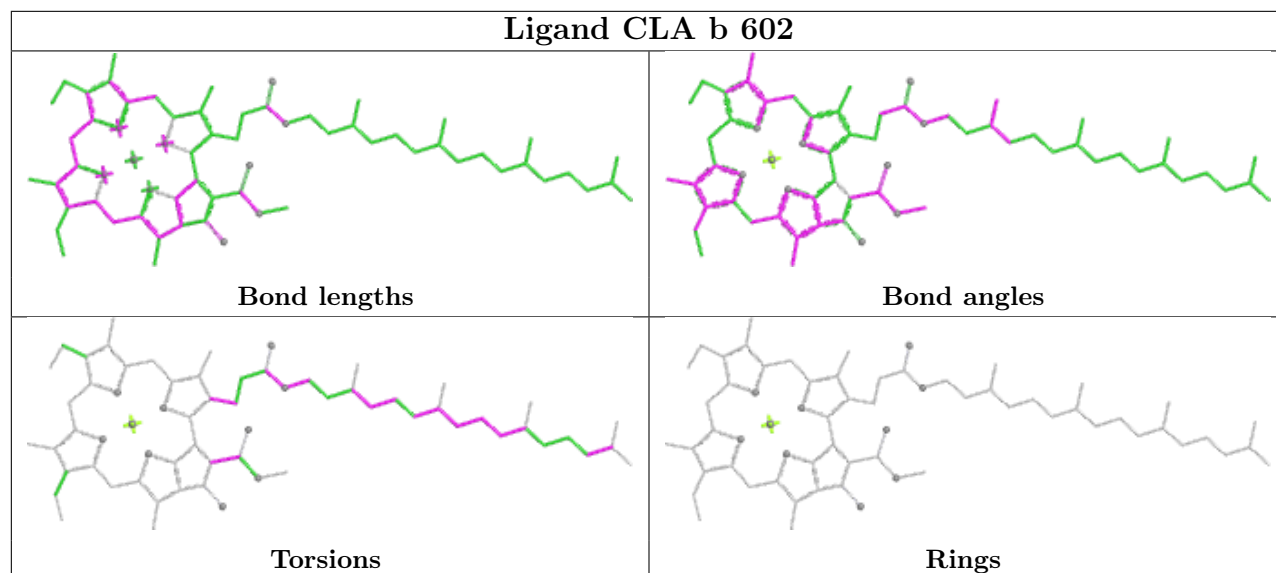
Ligand BCR h 101

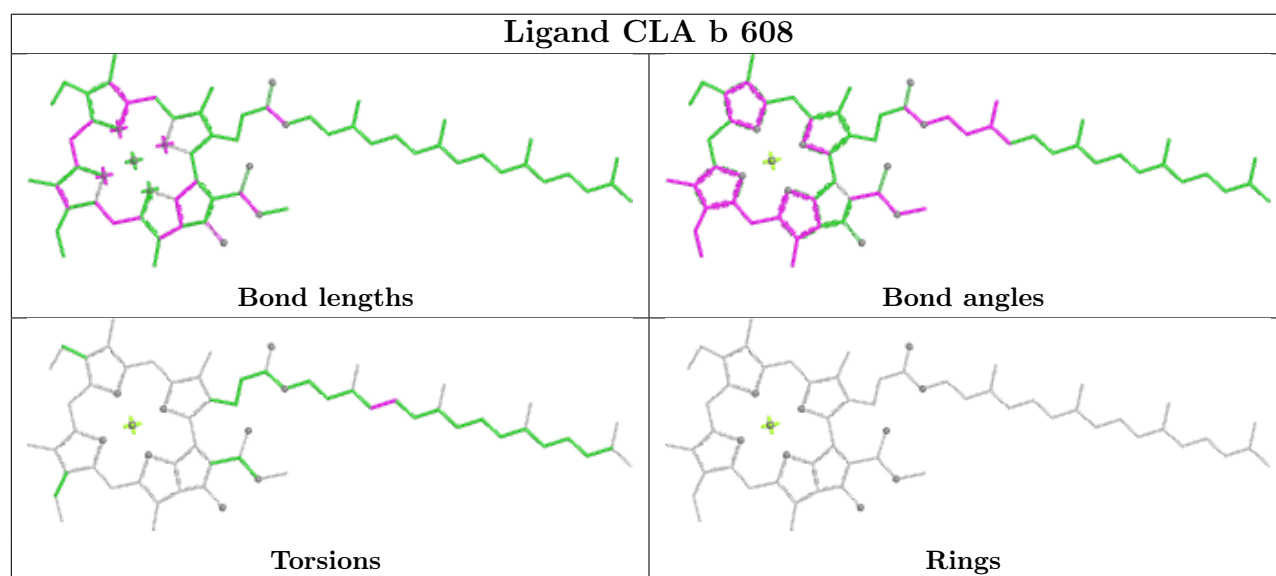
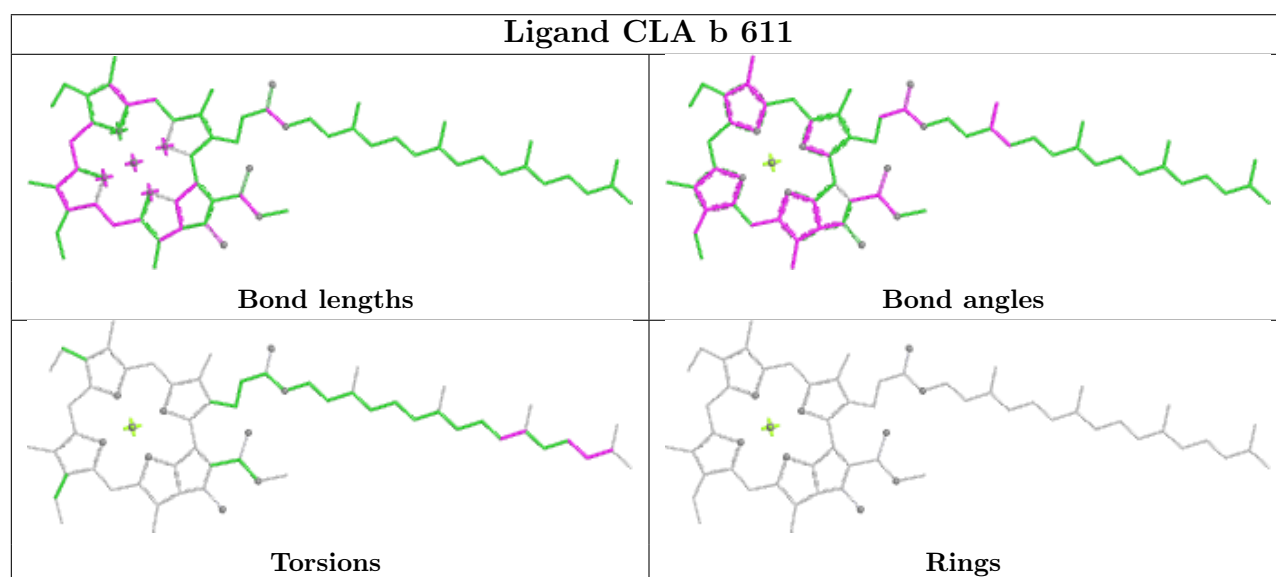
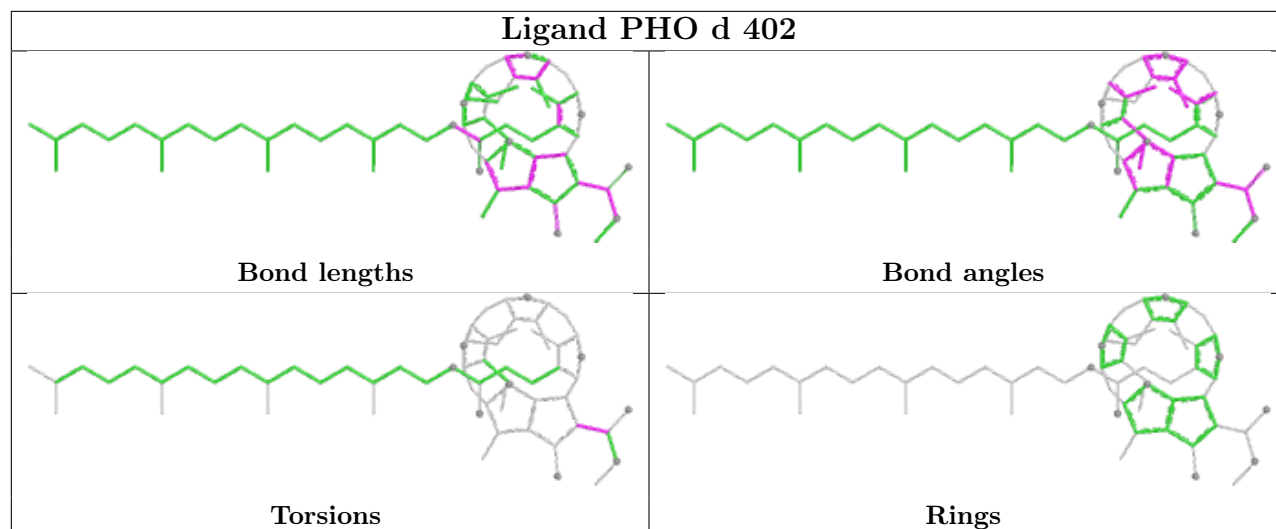


Ligand CLA C 509

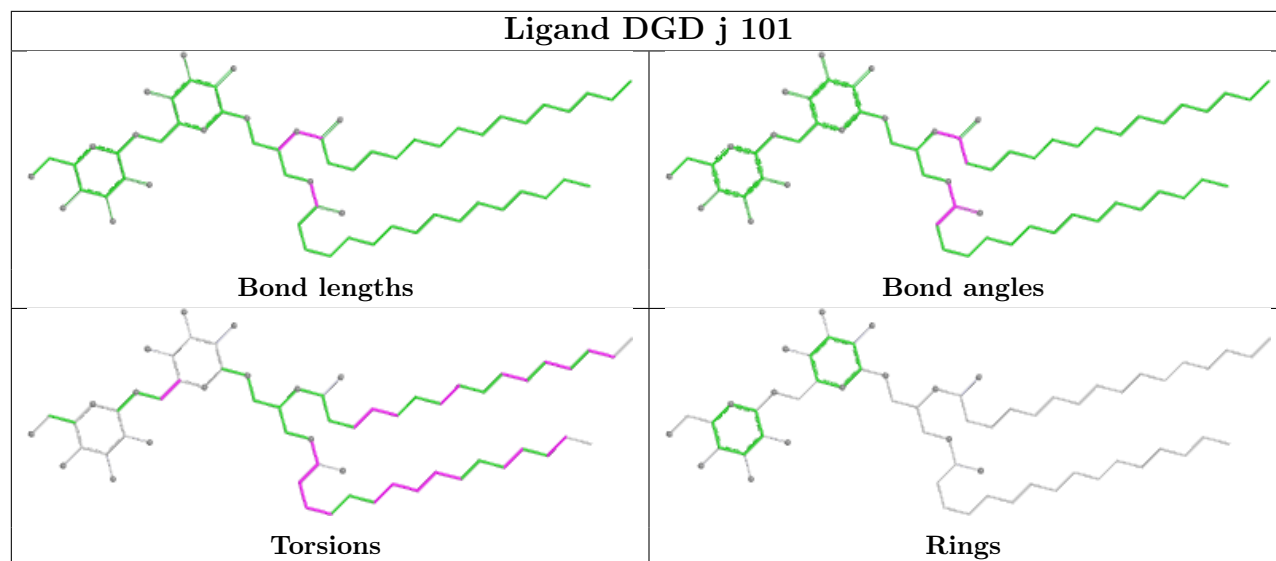


Ligand CLA b 602

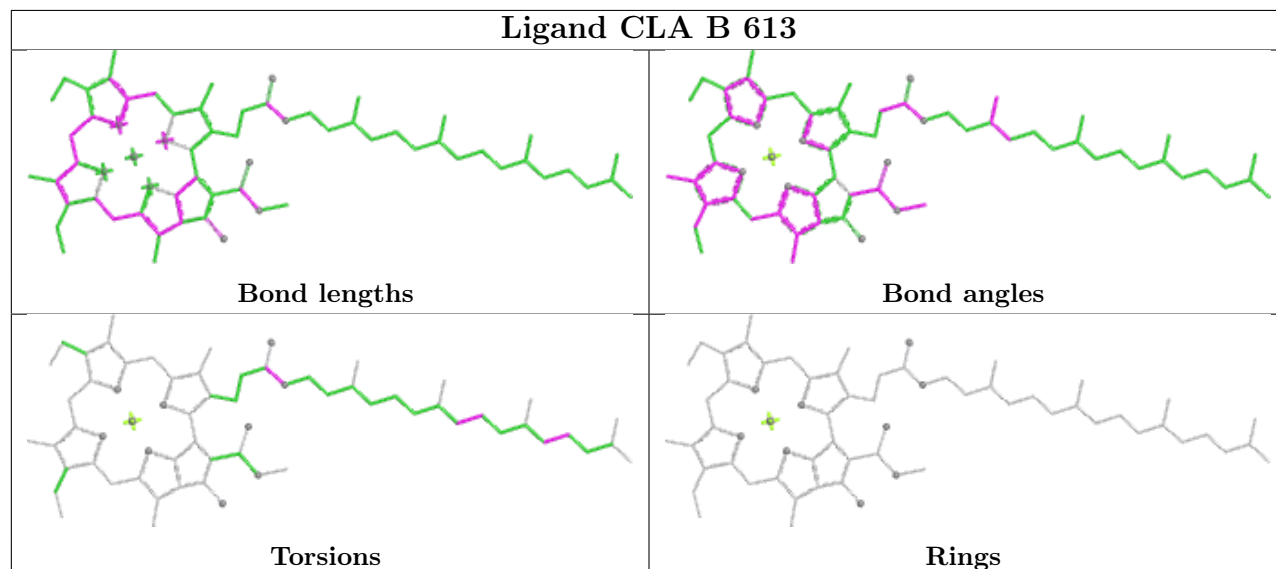




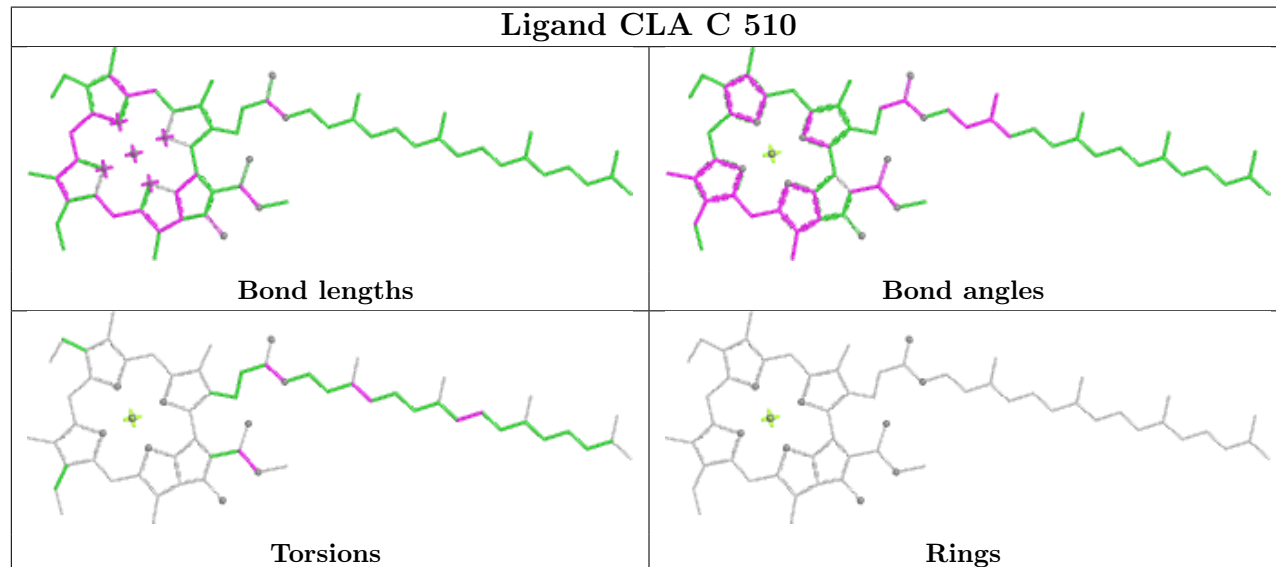
Ligand DGD j 101

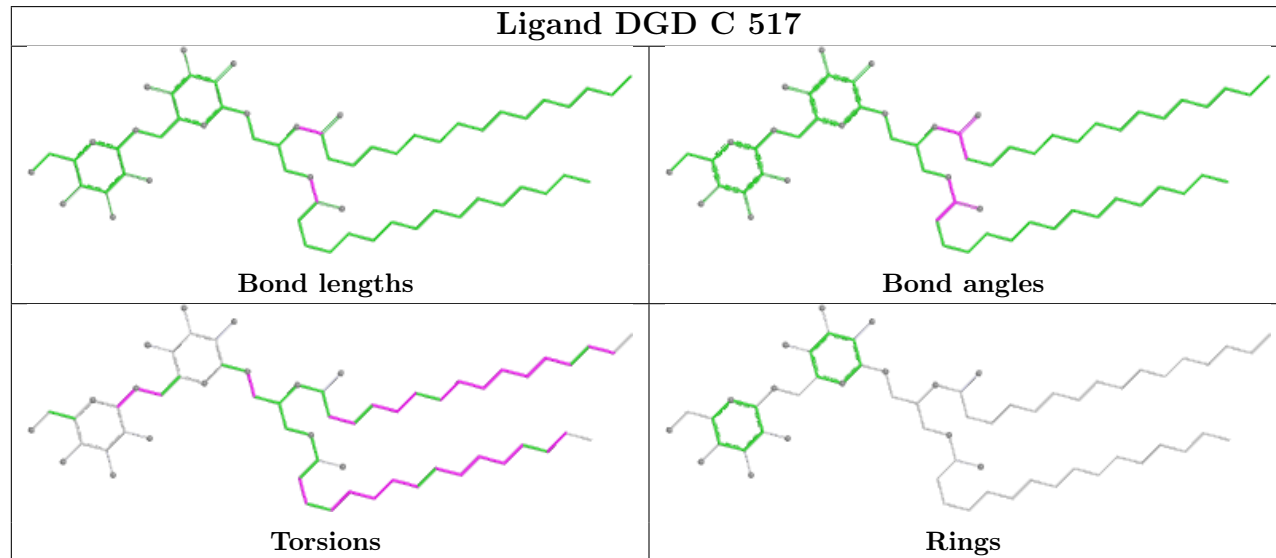
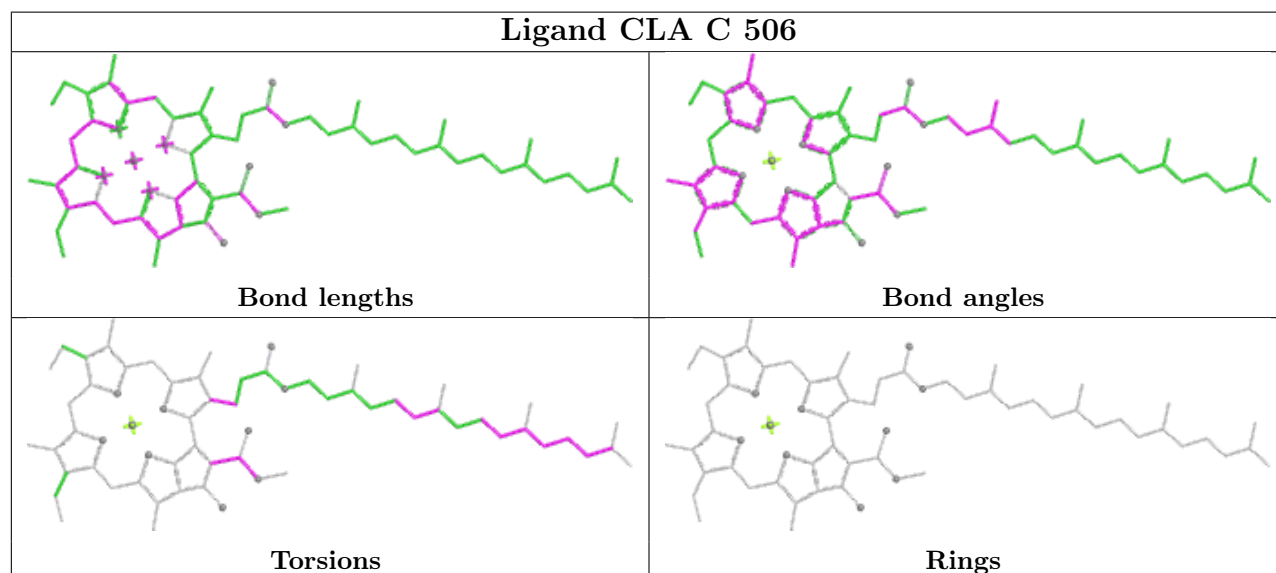
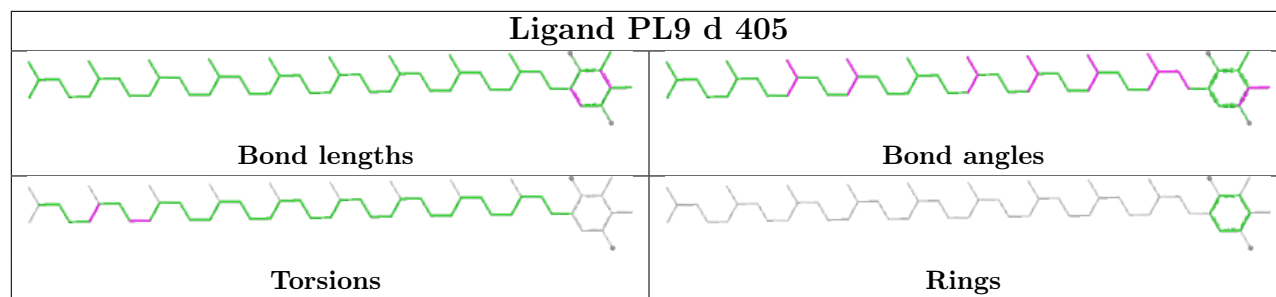


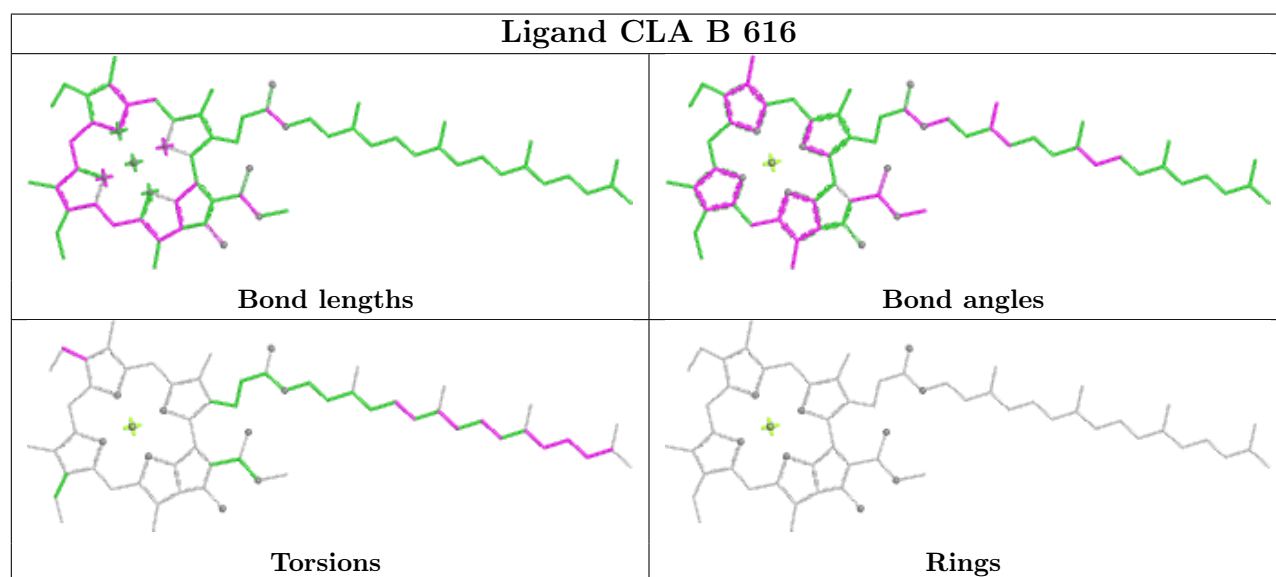
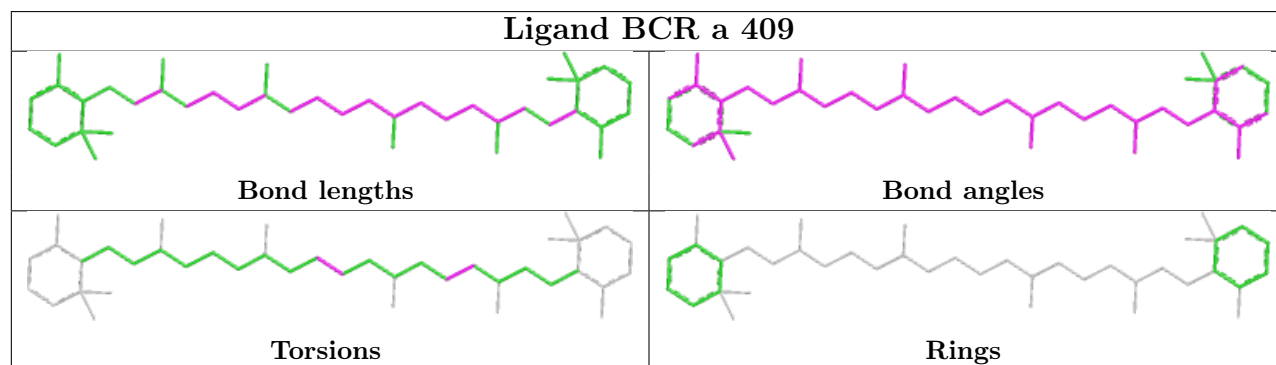
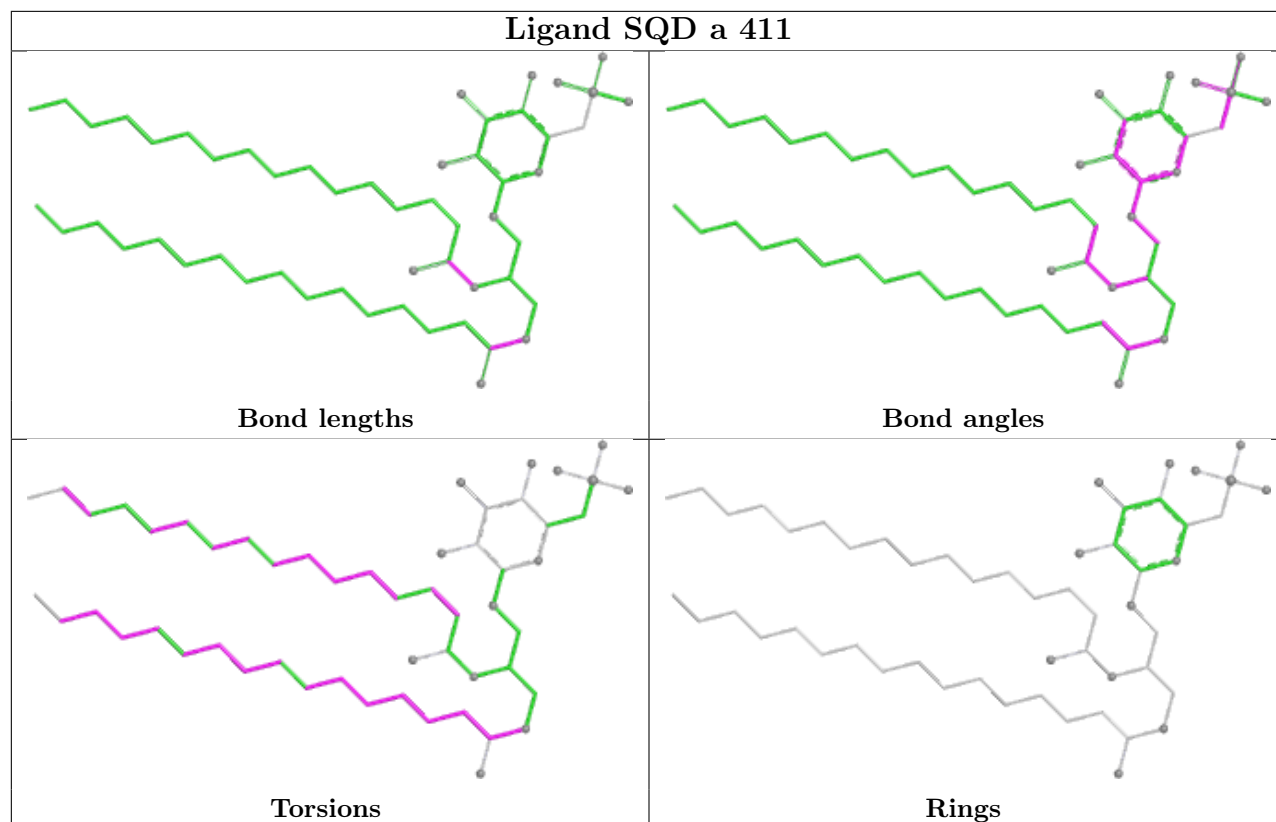
Ligand CLA B 613



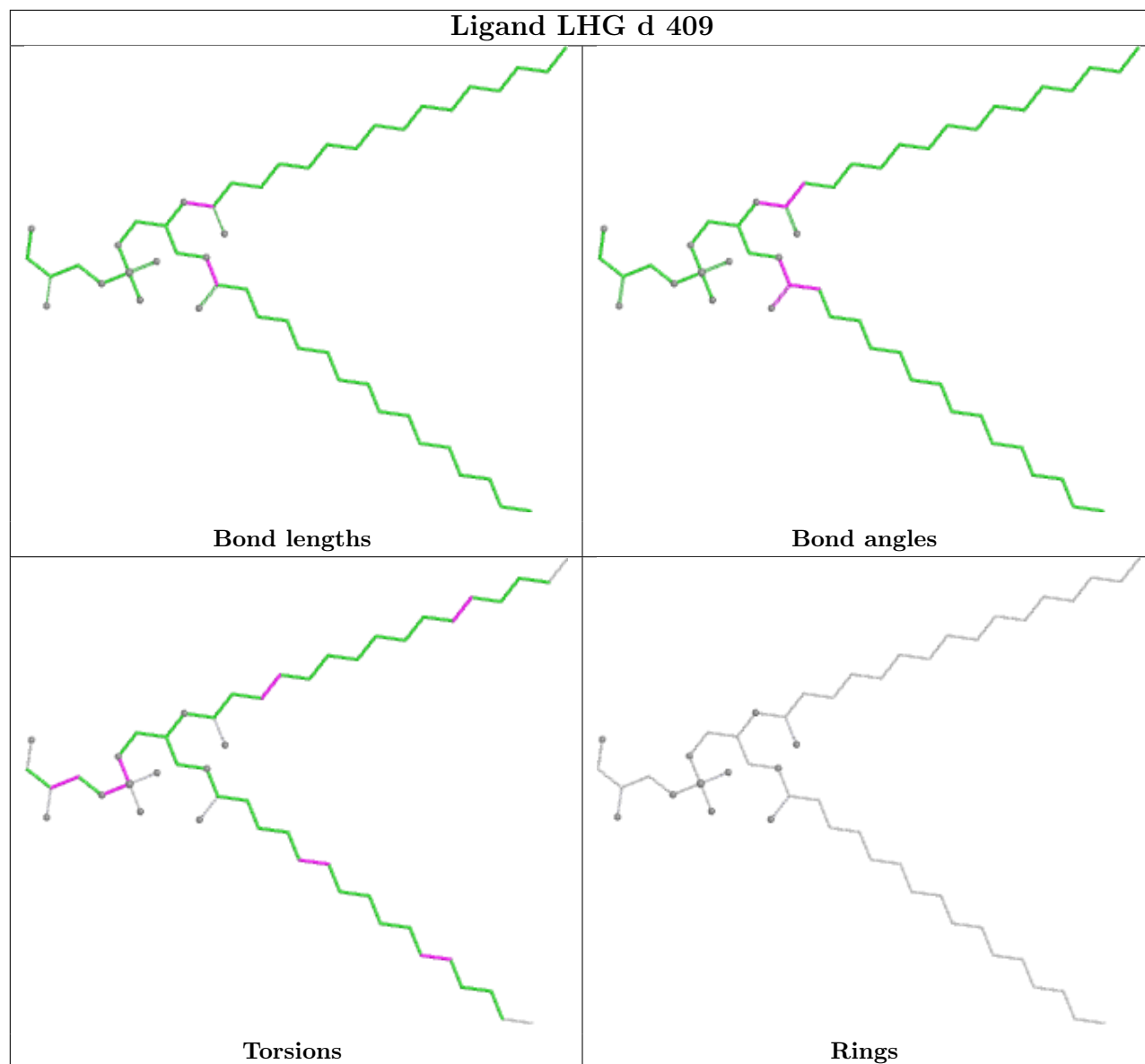
Ligand CLA C 510



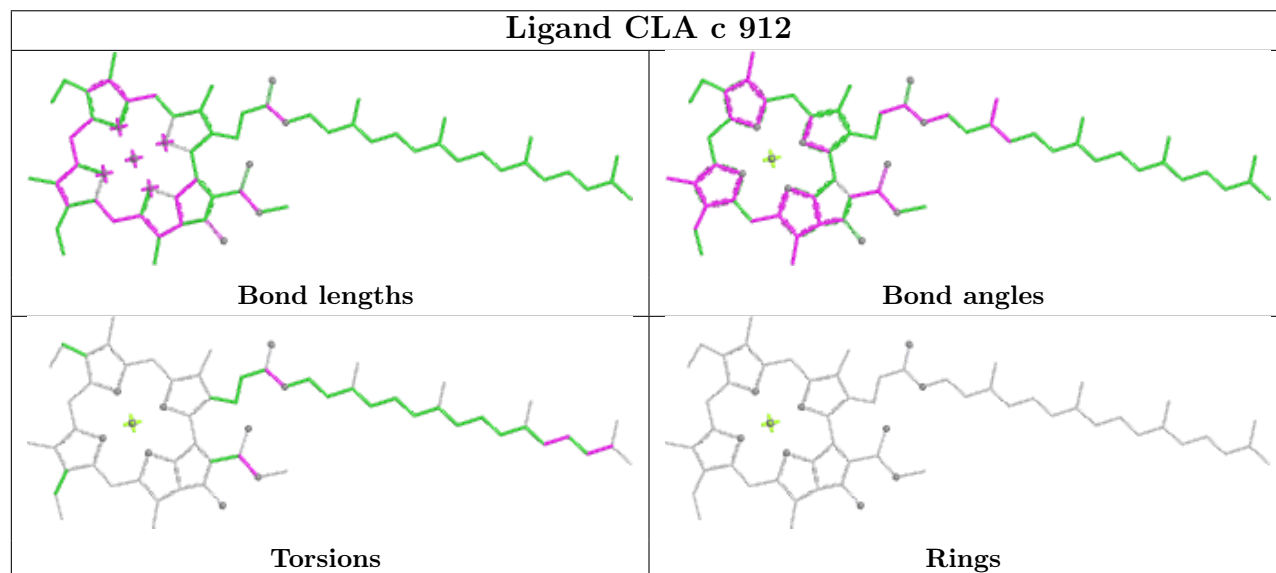


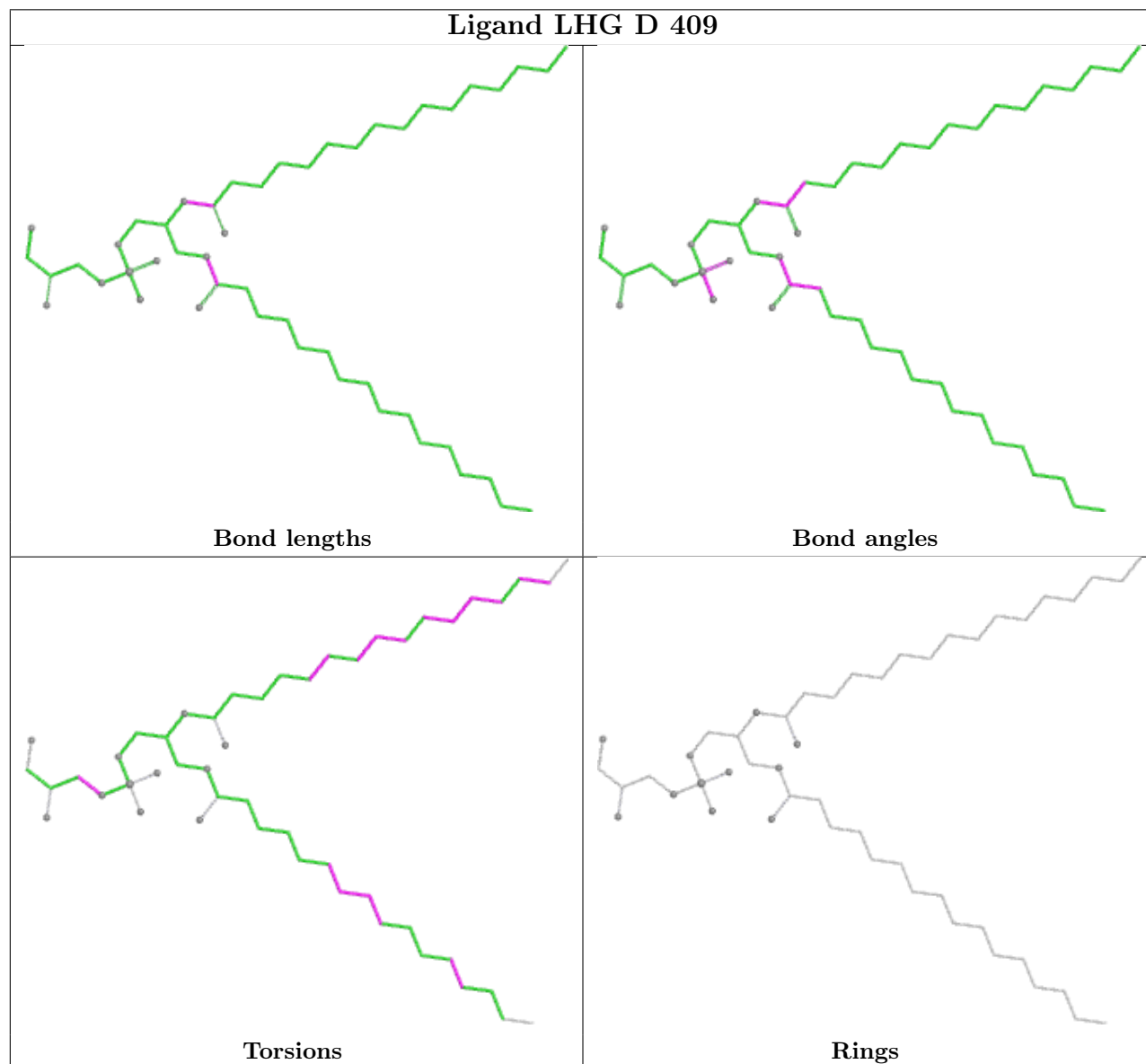
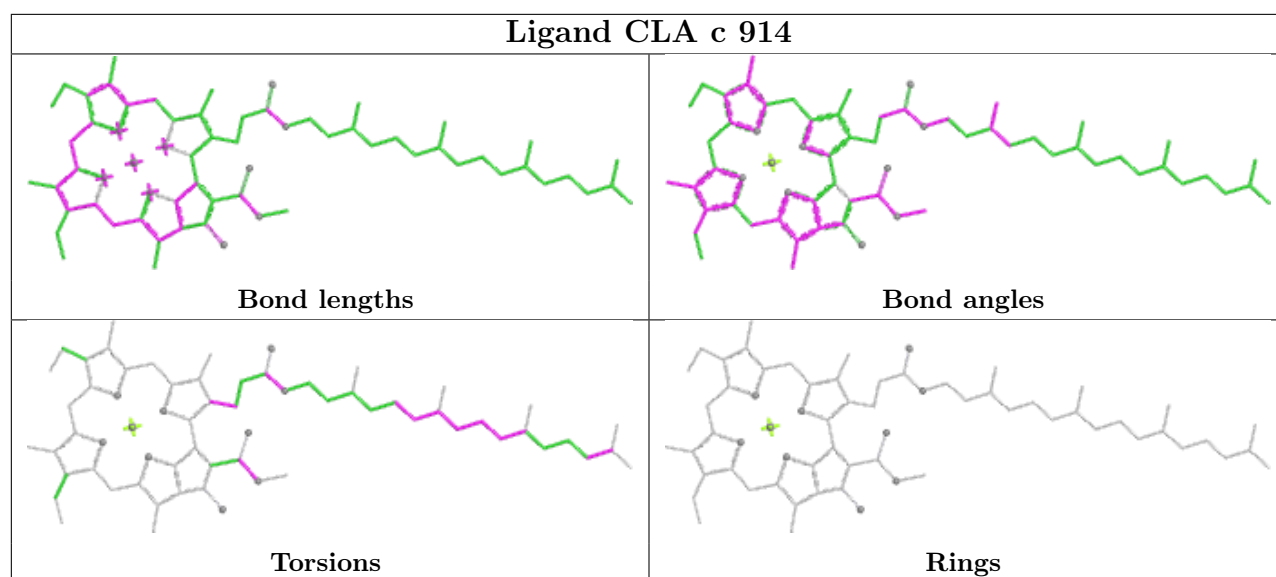


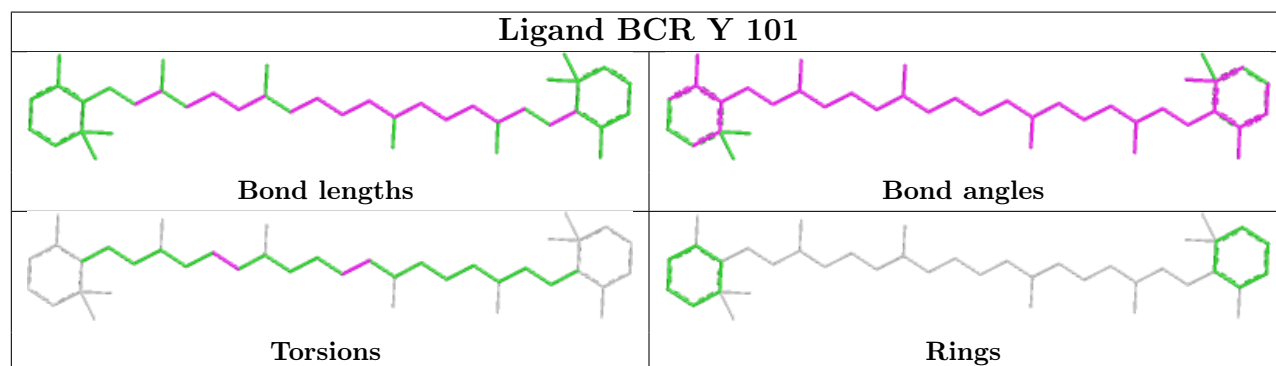
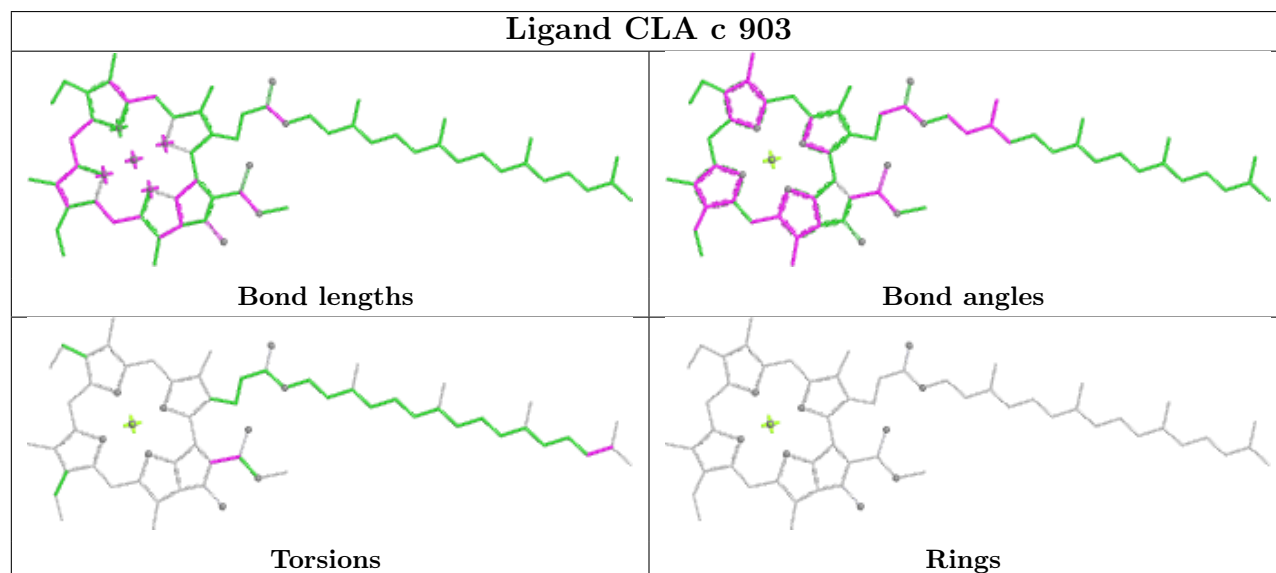
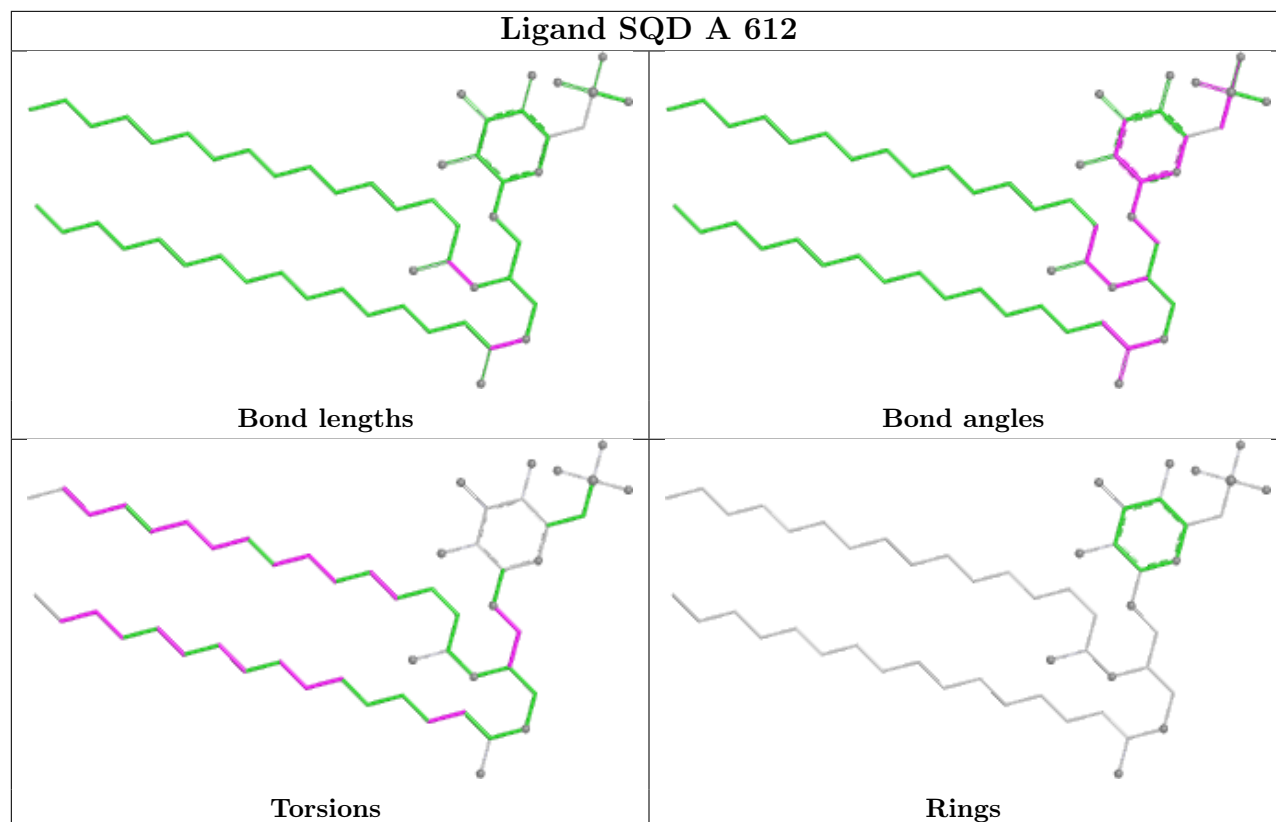
Ligand LHG d 409

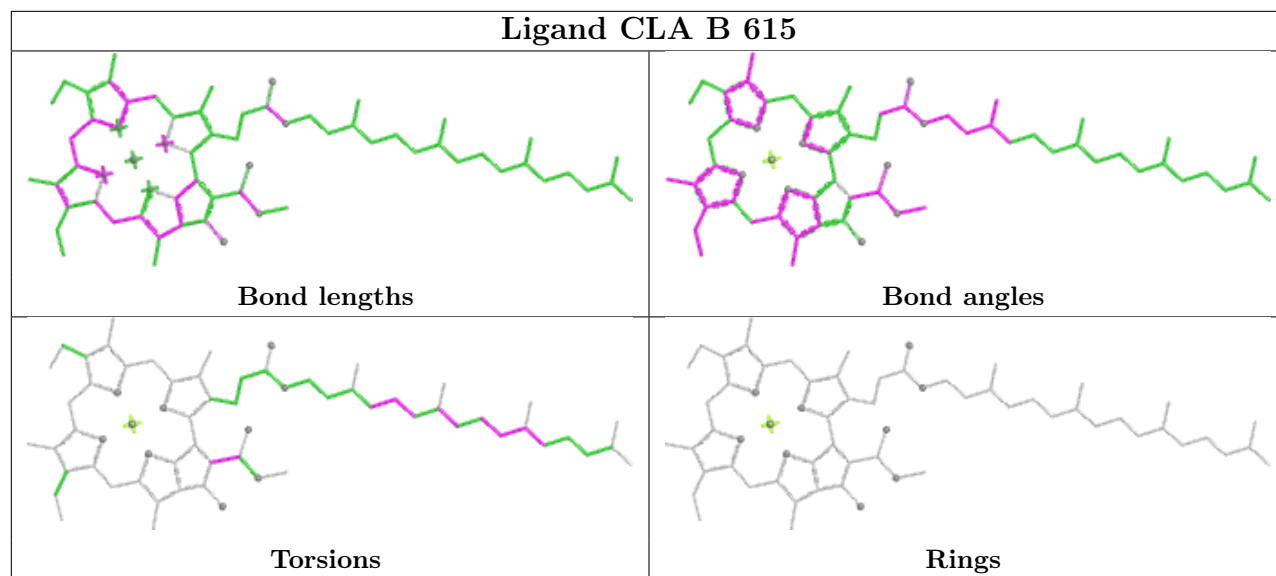


Ligand CLA c 912









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%)	-0.66	0 100 100	16, 22, 43, 53	0
1	a	334/334 (100%)	-0.70	0 100 100	19, 24, 45, 62	0
2	B	504/504 (100%)	-0.64	1 (0%) 91 83	18, 27, 49, 70	0
2	b	504/504 (100%)	-0.67	2 (0%) 88 77	20, 29, 52, 93	0
3	C	451/455 (99%)	-0.67	0 100 100	21, 31, 44, 56	0
3	c	455/455 (100%)	-0.74	1 (0%) 91 83	24, 34, 45, 59	0
4	D	342/342 (100%)	-0.63	1 (0%) 90 80	17, 23, 39, 61	0
4	d	341/342 (99%)	-0.64	1 (0%) 90 80	19, 26, 42, 59	0
5	E	81/81 (100%)	-0.66	0 100 100	27, 40, 57, 63	0
5	e	81/81 (100%)	-0.74	0 100 100	34, 45, 67, 76	0
6	F	34/34 (100%)	-0.65	0 100 100	28, 33, 58, 61	0
6	f	32/34 (94%)	-0.59	1 (3%) 51 42	30, 36, 60, 62	0
7	H	65/65 (100%)	-0.69	0 100 100	23, 34, 40, 58	0
7	h	65/65 (100%)	-0.67	0 100 100	28, 37, 48, 58	0
8	I	38/38 (100%)	-0.64	0 100 100	26, 33, 65, 68	0
8	i	38/38 (100%)	-0.91	0 100 100	29, 34, 62, 65	0
9	J	38/40 (95%)	-0.77	0 100 100	26, 37, 68, 72	0
9	j	40/40 (100%)	-0.71	0 100 100	31, 42, 76, 80	0
10	K	37/37 (100%)	-0.88	0 100 100	33, 38, 45, 47	0
10	k	37/37 (100%)	-0.59	0 100 100	38, 43, 55, 58	0
11	L	37/37 (100%)	-0.72	0 100 100	17, 22, 50, 59	0
11	l	37/37 (100%)	-0.81	0 100 100	19, 22, 55, 62	0
12	M	34/34 (100%)	-0.32	1 (2%) 53 44	21, 23, 36, 52	0
12	m	34/34 (100%)	-0.53	0 100 100	21, 25, 37, 53	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	-0.67	1 (0%) 88 77	18, 32, 55, 71	0
13	o	243/243 (100%)	-0.63	0 100 100	21, 35, 61, 72	0
14	T	30/30 (100%)	-0.46	0 100 100	19, 23, 44, 52	0
14	t	30/30 (100%)	-0.54	0 100 100	20, 24, 44, 50	0
15	U	97/97 (100%)	-0.60	0 100 100	23, 30, 48, 50	0
15	u	97/97 (100%)	-0.71	0 100 100	25, 31, 37, 47	0
16	V	137/137 (100%)	-0.71	0 100 100	23, 28, 39, 48	0
16	v	137/137 (100%)	-0.76	1 (0%) 84 71	27, 37, 51, 57	0
17	Y	29/29 (100%)	-0.76	0 100 100	42, 48, 75, 77	0
17	y	29/29 (100%)	-0.57	0 100 100	50, 56, 75, 76	0
18	X	39/39 (100%)	-0.82	0 100 100	33, 40, 66, 68	0
18	x	39/39 (100%)	-0.75	0 100 100	37, 43, 75, 77	0
19	Z	62/62 (100%)	-0.77	0 100 100	39, 48, 68, 72	0
19	z	62/62 (100%)	-0.55	0 100 100	53, 61, 82, 87	0
All	All	5267/5276 (99%)	-0.67	10 (0%) 91 83	16, 30, 56, 93	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	f	14	PRO	3.1
4	D	183	LEU	2.6
13	O	161	GLY	2.3
4	d	292	ASN	2.2
2	b	361	ALA	2.2
12	M	6	LEU	2.2
16	v	135	VAL	2.2
2	B	474	LEU	2.1
3	c	377	LEU	2.1
2	b	63	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CL	V	201	1/1	-0.02	0.10	50,50,50,50	0
30	CA	F	102	1/1	0.32	0.10	56,56,56,56	0
33	MG	j	102	1/1	0.34	0.13	34,34,34,34	0
22	CL	v	201	1/1	0.37	0.49	60,60,60,60	0
30	CA	B	601	1/1	0.47	0.09	76,76,76,76	0
30	CA	f	102	1/1	0.56	0.14	58,58,58,58	0
30	CA	b	601	1/1	0.78	0.07	77,77,77,77	0
23	BCT	a	414	4/4	0.79	0.20	34,34,35,37	0
22	CL	A	603	1/1	0.80	0.09	24,24,24,24	0
26	BCR	B	620	40/40	0.81	0.11	27,33,39,39	0
24	CLA	a	407	65/65	0.82	0.13	19,23,63,65	0
24	CLA	b	602	65/65	0.82	0.10	38,46,68,68	0
24	CLA	b	617	65/65	0.83	0.10	27,33,74,75	0
26	BCR	b	619	40/40	0.84	0.11	30,34,41,42	0
24	CLA	B	602	65/65	0.84	0.10	32,41,66,66	0
26	BCR	C	514	40/40	0.84	0.12	37,43,47,47	0
27	PL9	A	611	55/55	0.85	0.13	52,69,78,78	0
26	BCR	T	102	40/40	0.85	0.14	25,29,31,31	0
31	DGD	d	406	62/66	0.85	0.12	80,91,105,105	0
24	CLA	b	607	65/65	0.85	0.10	26,30,41,42	0
25	PHO	D	401	64/64	0.86	0.09	19,22,28,32	0
31	DGD	D	406	62/66	0.86	0.12	77,89,103,103	0
27	PL9	a	410	55/55	0.86	0.14	63,80,85,85	0
28	SQD	d	407	43/54	0.86	0.10	84,90,93,94	0
29	LHG	A	615	42/49	0.87	0.11	69,83,86,86	0
27	PL9	D	405	55/55	0.87	0.13	19,23,29,32	0
26	BCR	k	101	40/40	0.87	0.09	37,41,45,45	0
24	CLA	b	608	65/65	0.87	0.13	19,23,30,32	0
24	CLA	B	616	65/65	0.88	0.12	25,27,45,46	0
29	LHG	D	408	49/49	0.88	0.16	24,28,37,40	0
26	BCR	c	915	40/40	0.88	0.09	30,37,41,42	0
26	BCR	c	918	40/40	0.88	0.09	50,52,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	C	515	40/40	0.88	0.09	30,37,40,41	0
26	BCR	H	101	40/40	0.88	0.12	26,33,42,42	0
22	CL	A	604	1/1	0.88	0.08	21,21,21,21	0
26	BCR	a	409	40/40	0.88	0.12	21,26,29,29	0
26	BCR	b	618	40/40	0.88	0.13	24,28,39,39	0
24	CLA	C	513	65/65	0.89	0.10	39,45,64,64	0
24	CLA	a	406	65/65	0.89	0.10	18,20,28,33	0
29	LHG	a	413	42/49	0.89	0.12	95,107,110,111	0
29	LHG	d	410	49/49	0.89	0.10	28,34,66,67	0
24	CLA	B	608	65/65	0.89	0.10	17,20,32,34	0
24	CLA	C	504	65/65	0.89	0.11	25,28,54,54	0
27	PL9	d	405	55/55	0.89	0.12	19,25,29,31	0
28	SQD	A	612	54/54	0.89	0.10	49,57,66,67	0
31	DGD	C	517	62/66	0.89	0.11	23,35,62,63	0
28	SQD	A	613	54/54	0.89	0.14	50,63,68,68	0
26	BCR	A	610	40/40	0.89	0.11	22,27,32,32	0
28	SQD	I	101	54/54	0.89	0.15	57,69,84,85	0
24	CLA	B	617	65/65	0.90	0.10	22,29,77,78	0
26	BCR	T	101	40/40	0.90	0.10	25,37,44,45	0
29	LHG	b	620	49/49	0.90	0.11	24,31,46,50	0
24	CLA	D	403	65/65	0.90	0.12	24,27,65,67	0
26	BCR	B	618	40/40	0.90	0.11	23,27,28,29	0
26	BCR	B	619	40/40	0.90	0.11	21,28,40,40	0
24	CLA	B	607	65/65	0.90	0.08	24,28,40,41	0
24	CLA	C	509	65/65	0.90	0.09	29,32,46,47	0
28	SQD	a	402	54/54	0.90	0.13	51,67,75,76	0
24	CLA	c	914	65/65	0.90	0.09	46,51,73,74	0
26	BCR	f	101	40/40	0.90	0.09	30,34,48,49	0
26	BCR	h	101	40/40	0.90	0.10	29,37,45,45	0
24	CLA	D	402	65/65	0.91	0.10	13,18,34,35	0
24	CLA	b	612	65/65	0.91	0.10	20,23,37,41	0
24	CLA	b	616	65/65	0.91	0.09	27,30,45,46	0
24	CLA	B	613	65/65	0.91	0.11	20,24,30,31	0
26	BCR	k	102	40/40	0.91	0.09	33,44,47,48	0
26	BCR	D	404	40/40	0.91	0.12	25,30,48,49	0
24	CLA	c	902	65/65	0.91	0.09	30,33,41,45	0
24	CLA	C	508	65/65	0.91	0.08	25,29,54,58	0
24	CLA	d	404	65/65	0.91	0.10	26,31,67,68	0
24	CLA	A	606	65/65	0.91	0.12	15,19,25,34	0
25	PHO	a	412	64/64	0.91	0.09	20,25,30,33	0
31	DGD	C	518	62/66	0.91	0.09	22,31,52,56	0
24	CLA	C	512	65/65	0.91	0.10	37,41,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	SQD	a	411	54/54	0.91	0.10	50,60,75,76	0
31	DGD	j	101	62/66	0.91	0.09	25,34,52,55	0
22	CL	a	405	1/1	0.91	0.08	26,26,26,26	0
24	CLA	c	912	65/65	0.92	0.09	32,37,43,44	0
29	LHG	D	409	49/49	0.92	0.09	26,33,62,64	0
24	CLA	c	913	65/65	0.92	0.09	38,42,62,63	0
24	CLA	a	408	65/65	0.92	0.10	20,24,75,75	0
24	CLA	b	613	65/65	0.92	0.11	21,26,33,35	0
26	BCR	K	101	40/40	0.92	0.08	29,33,37,37	0
25	PHO	A	608	64/64	0.92	0.07	16,21,25,26	0
24	CLA	A	607	65/65	0.92	0.14	19,21,63,65	0
26	BCR	Y	101	40/40	0.92	0.08	34,38,39,39	0
22	CL	a	404	1/1	0.92	0.08	28,28,28,28	0
24	CLA	C	511	65/65	0.92	0.07	29,34,37,38	0
24	CLA	c	904	65/65	0.92	0.08	26,37,39,40	0
31	DGD	c	916	62/66	0.92	0.12	24,35,60,61	0
31	DGD	c	917	62/66	0.92	0.10	28,36,64,65	0
24	CLA	c	905	65/65	0.92	0.08	28,30,55,56	0
24	CLA	c	907	65/65	0.92	0.09	30,35,64,64	0
26	BCR	B	622	40/40	0.92	0.10	23,34,41,41	0
24	CLA	c	910	65/65	0.93	0.07	27,30,46,46	0
24	CLA	b	614	65/65	0.93	0.10	21,24,44,45	0
29	LHG	d	409	49/49	0.93	0.10	23,27,38,40	0
24	CLA	c	903	65/65	0.93	0.10	25,28,42,45	0
24	CLA	b	615	65/65	0.93	0.09	22,26,65,66	0
24	CLA	C	507	65/65	0.93	0.07	29,33,52,53	0
24	CLA	A	614	65/65	0.93	0.09	14,18,29,35	0
32	HEM	e	101	43/43	0.93	0.09	43,46,52,55	0
28	SQD	L	101	54/54	0.93	0.11	58,66,80,80	0
24	CLA	b	603	65/65	0.94	0.09	26,29,36,37	0
24	CLA	B	609	65/65	0.94	0.09	20,24,31,31	0
30	CA	c	901	1/1	0.94	0.22	46,46,46,46	0
24	CLA	B	606	65/65	0.94	0.08	19,23,34,35	0
29	LHG	D	407	49/49	0.94	0.09	29,34,41,41	0
24	CLA	C	501	65/65	0.94	0.08	29,32,44,46	0
24	CLA	d	401	65/65	0.94	0.10	17,20,27,31	0
24	CLA	C	503	65/65	0.94	0.09	27,31,35,36	0
24	CLA	B	615	65/65	0.94	0.11	20,24,60,61	0
29	LHG	d	408	49/49	0.94	0.09	29,37,41,42	0
24	CLA	C	505	65/65	0.94	0.10	28,30,44,45	0
24	CLA	c	908	65/65	0.94	0.08	28,32,50,51	0
24	CLA	c	909	65/65	0.94	0.08	27,29,57,60	0

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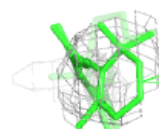
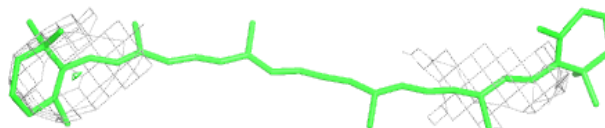
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	CA	O	301	1/1	0.95	0.04	49,49,49,49	0
25	PHO	d	402	64/64	0.95	0.10	18,22,24,25	0
24	CLA	b	605	65/65	0.95	0.08	20,25,53,55	0
24	CLA	c	911	65/65	0.95	0.07	26,30,39,40	0
30	CA	o	301	1/1	0.95	0.05	51,51,51,51	0
31	DGD	C	516	62/66	0.95	0.08	23,33,61,62	0
24	CLA	B	605	65/65	0.95	0.07	19,22,50,51	0
24	CLA	B	611	65/65	0.95	0.09	21,25,32,37	0
23	BCT	A	605	4/4	0.95	0.06	39,39,40,42	0
24	CLA	C	510	65/65	0.95	0.06	24,28,35,37	0
28	SQD	F	101	43/54	0.95	0.07	67,74,78,79	0
24	CLA	c	906	65/65	0.95	0.07	28,31,44,44	0
31	DGD	h	102	62/66	0.95	0.13	29,36,43,44	0
24	CLA	A	609	65/65	0.95	0.08	21,24,71,72	0
24	CLA	B	603	65/65	0.95	0.07	23,26,32,32	0
24	CLA	C	506	65/65	0.95	0.07	31,38,74,75	0
31	DGD	H	102	62/66	0.96	0.08	26,32,38,40	0
24	CLA	b	610	65/65	0.96	0.07	28,31,33,36	0
29	LHG	B	621	49/49	0.96	0.09	23,31,43,44	0
24	CLA	b	611	65/65	0.96	0.08	25,28,34,37	0
24	CLA	d	403	65/65	0.96	0.09	18,21,38,39	0
24	CLA	B	610	65/65	0.96	0.07	23,28,31,32	0
32	HEM	E	101	43/43	0.96	0.07	39,42,45,47	0
24	CLA	b	606	65/65	0.96	0.06	21,24,32,33	0
32	HEM	v	202	43/43	0.96	0.08	28,31,34,36	0
24	CLA	b	609	65/65	0.96	0.07	22,27,38,39	0
24	CLA	B	614	65/65	0.97	0.06	19,22,45,47	0
24	CLA	b	604	65/65	0.97	0.06	23,26,35,38	0
32	HEM	V	202	43/43	0.97	0.07	23,24,27,29	0
24	CLA	B	612	65/65	0.97	0.07	19,21,32,34	0
24	CLA	C	502	65/65	0.97	0.07	24,26,39,42	0
24	CLA	B	604	65/65	0.97	0.10	18,22,31,35	0
20	OEX	A	601	10/10	0.99	0.07	22,23,26,26	0
20	OEX	a	401	10/10	0.99	0.09	25,27,28,28	0
21	FE2	A	602	1/1	1.00	0.03	26,26,26,26	0
21	FE2	a	403	1/1	1.00	0.15	27,27,27,27	0

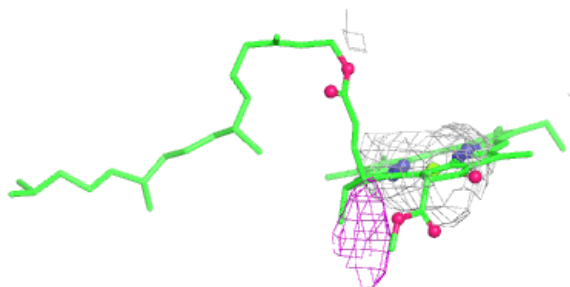
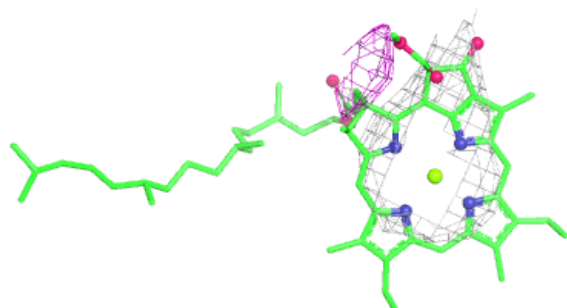
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BCR B 620:

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

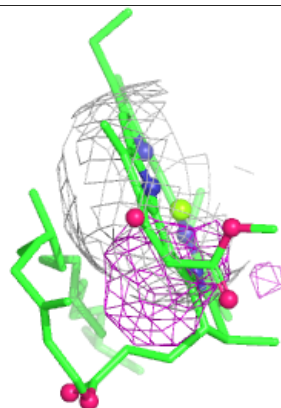
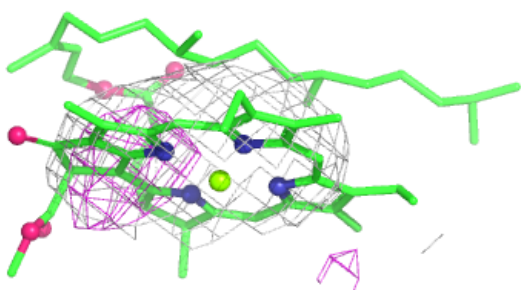
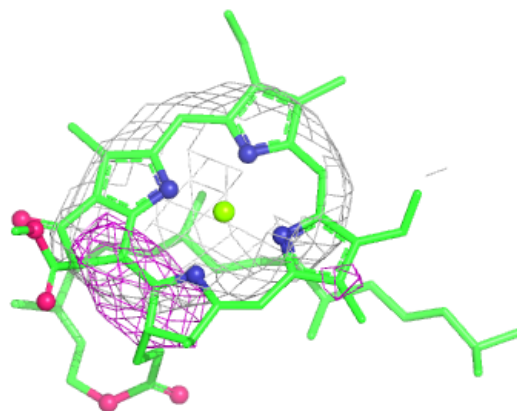
**Electron density around CLA a 407:**

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



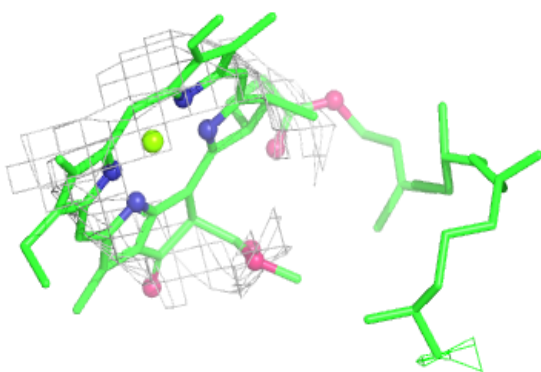
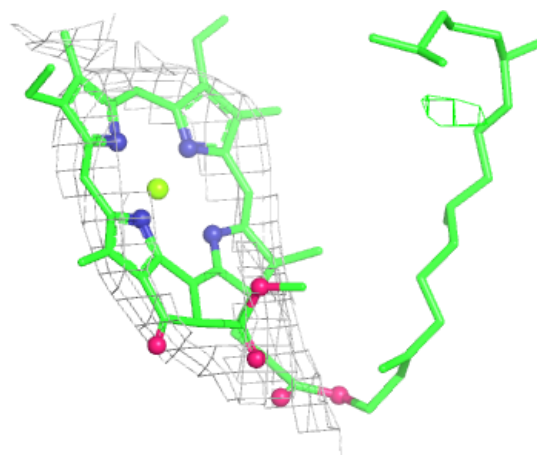
Electron density around CLA b 602:

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



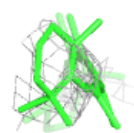
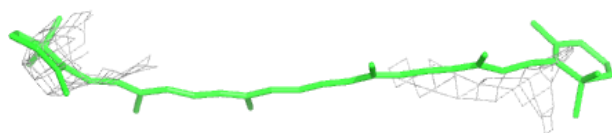
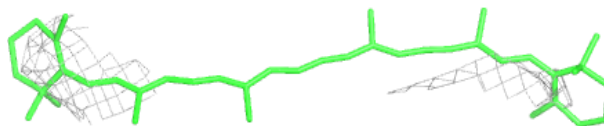
Electron density around CLA b 617:

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

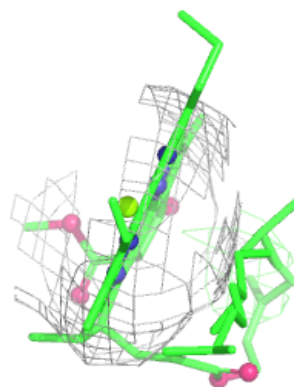
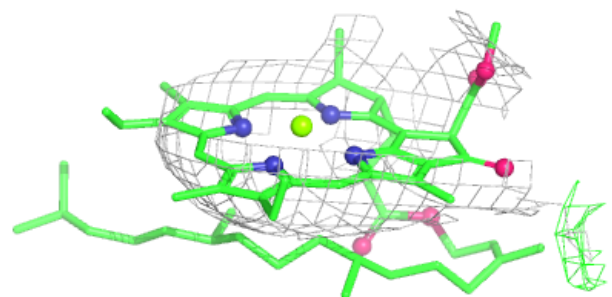
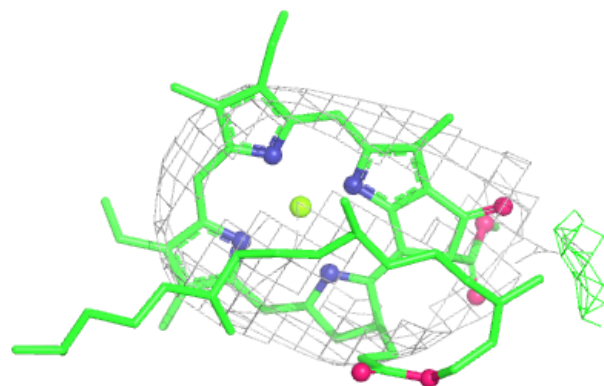


Electron density around BCR b 619:

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

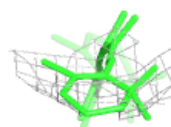
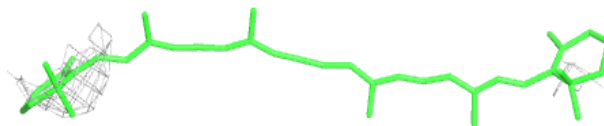
**Electron density around CLA B 602:**

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

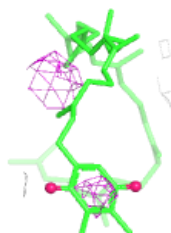
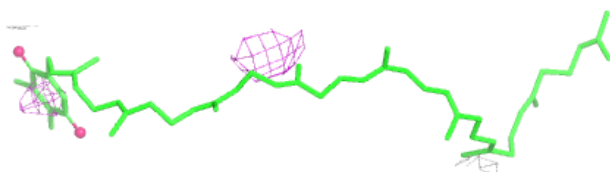
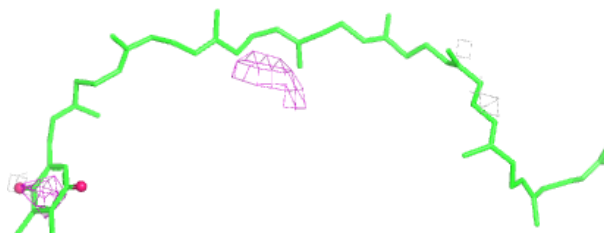


Electron density around BCR C 514:

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

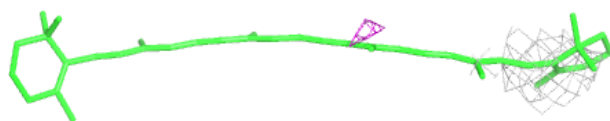
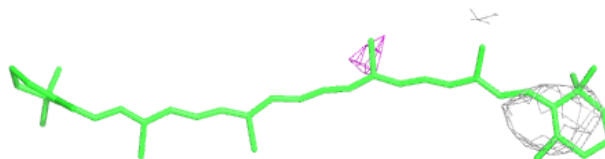
**Electron density around PL9 A 611:**

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

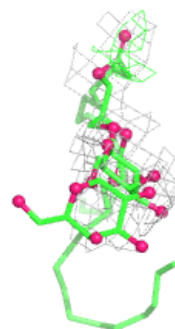
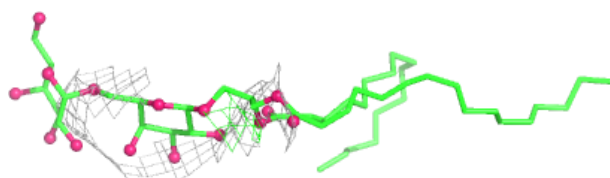


Electron density around BCR T 102:

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

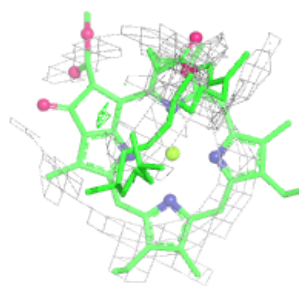
**Electron density around DGD d 406:**

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



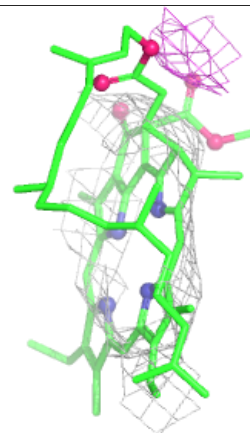
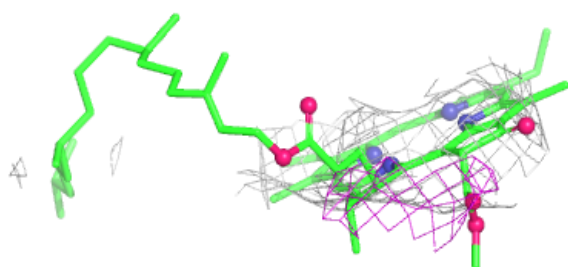
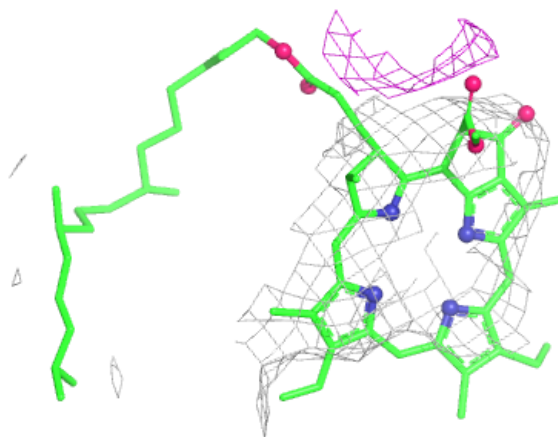
Electron density around CLA b 607:

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

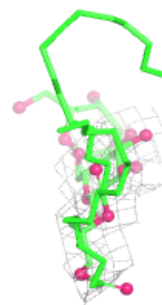
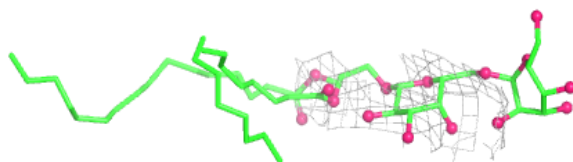
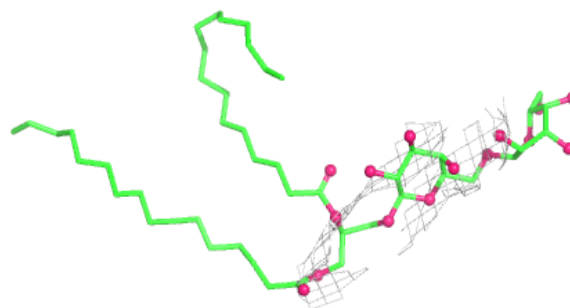


Electron density around PHO D 401:

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

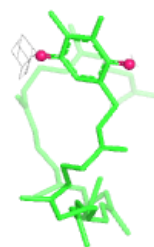
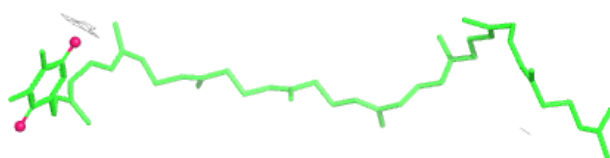
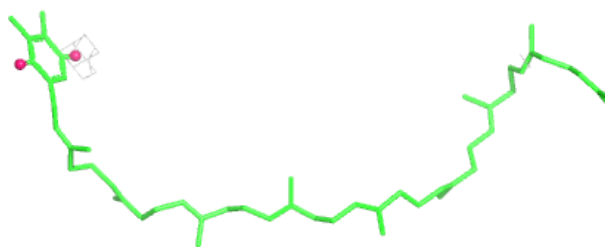
**Electron density around DGD D 406:**

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

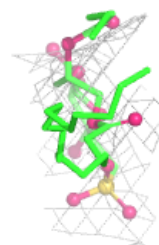
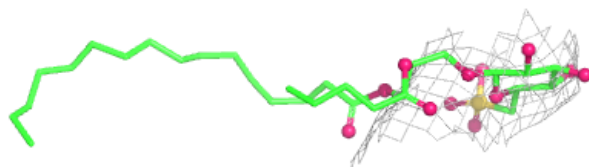
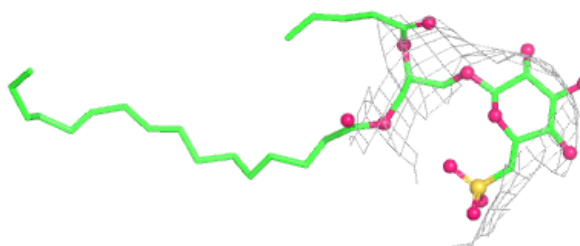


Electron density around PL9 a 410:

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

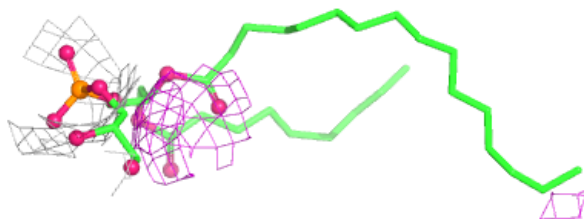
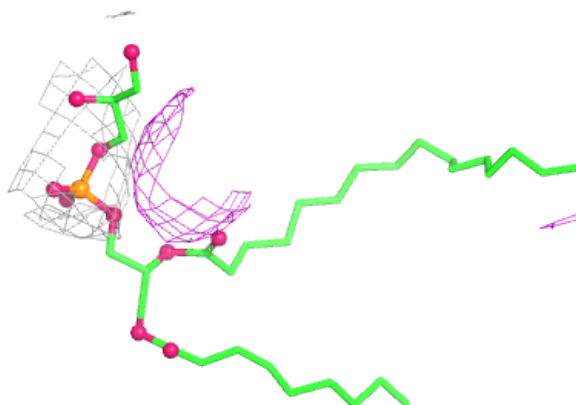
**Electron density around SQD d 407:**

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

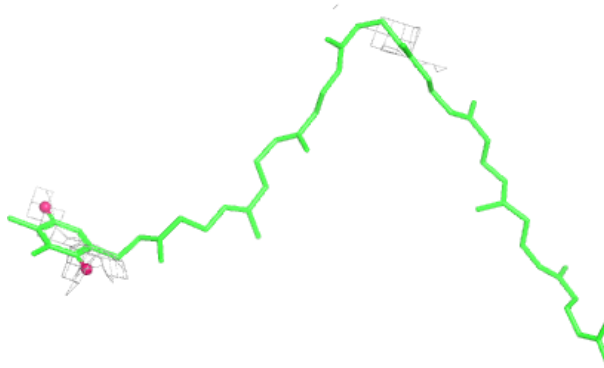


Electron density around LHG A 615:

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

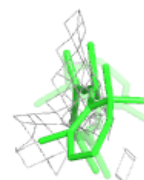
**Electron density around PL9 D 405:**

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

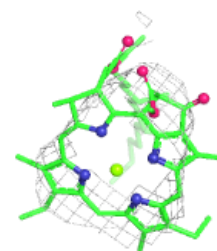
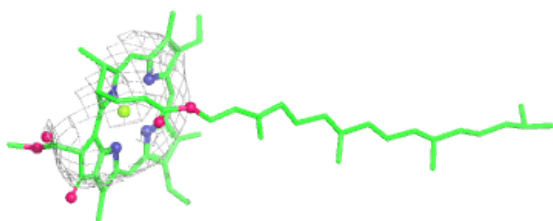
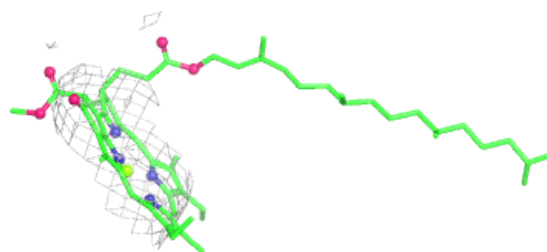


Electron density around BCR k 101:

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

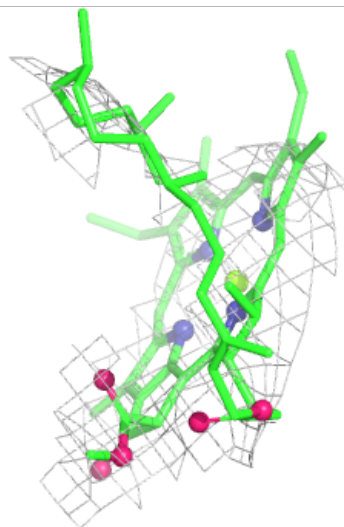
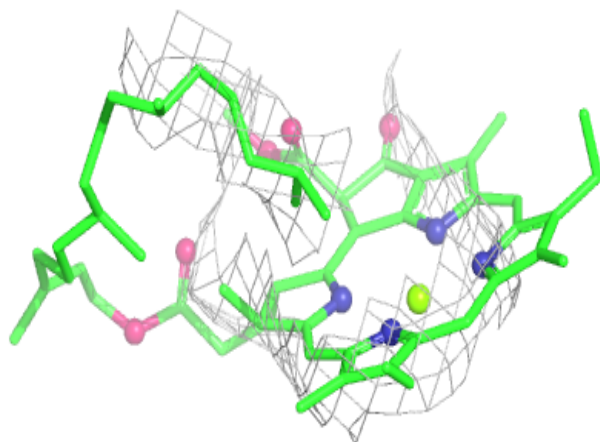
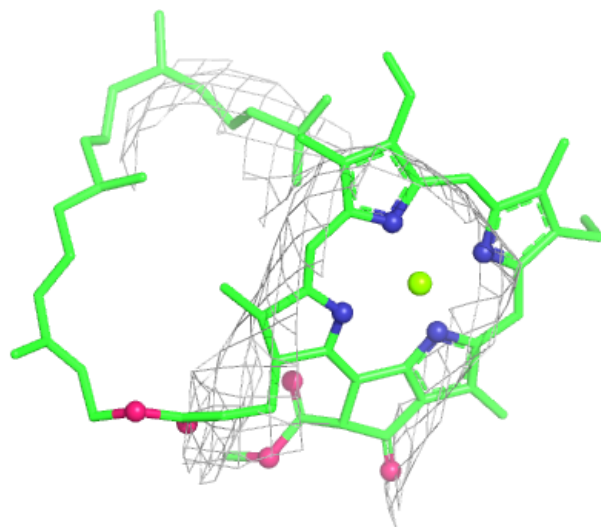
**Electron density around CLA b 608:**

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



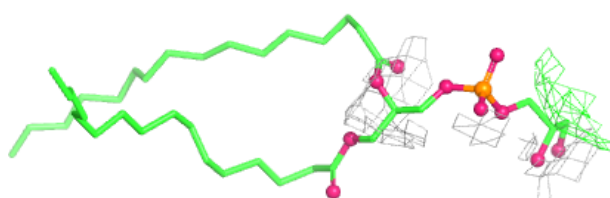
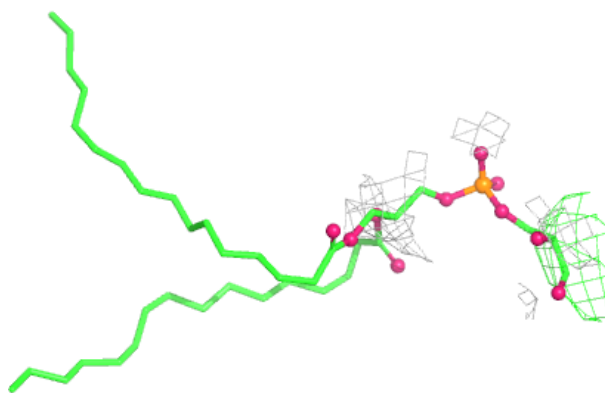
Electron density around CLA B 616:

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

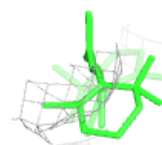
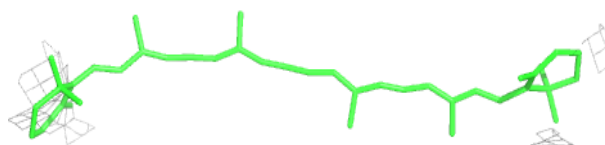


Electron density around LHG D 408:

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

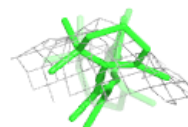
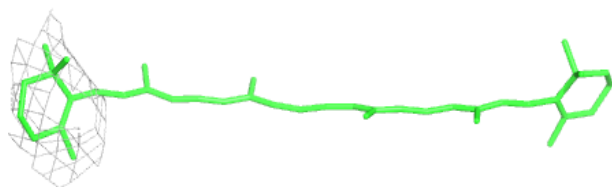
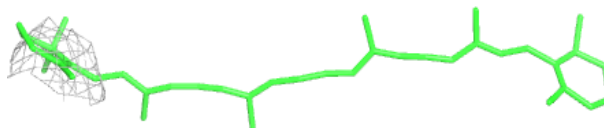
**Electron density around BCR c 915:**

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

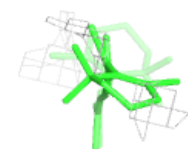
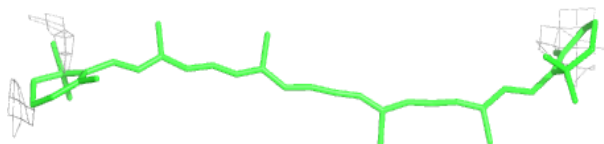


Electron density around BCR c 918:

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

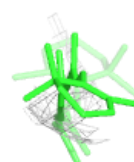
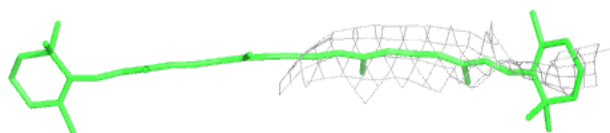
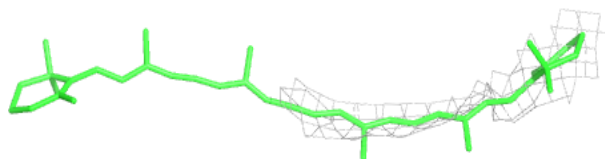
**Electron density around BCR C 515:**

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

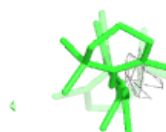
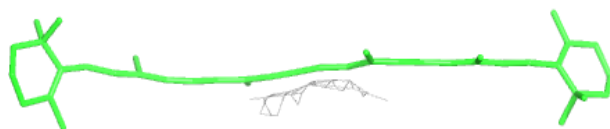
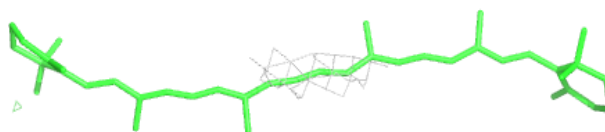


Electron density around BCR H 101:

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

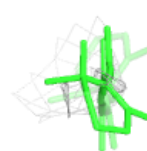
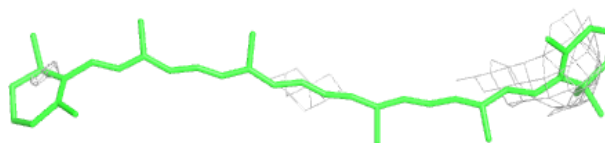
**Electron density around BCR a 409:**

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

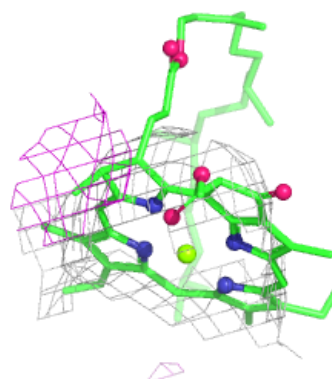
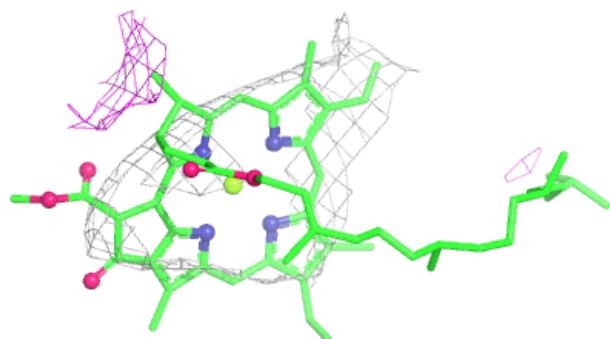
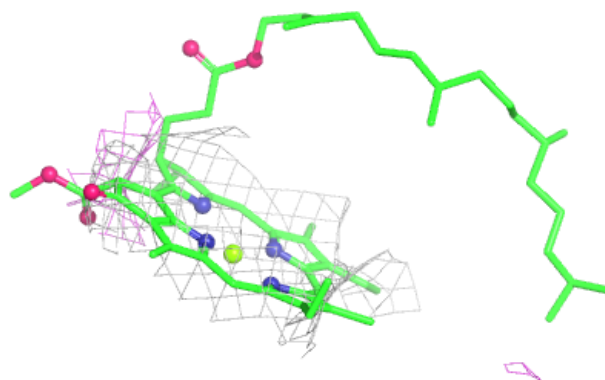


Electron density around BCR b 618:

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

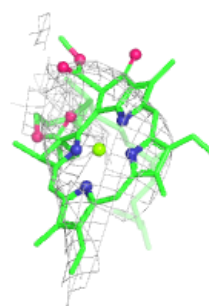
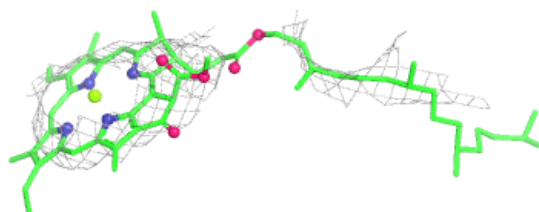
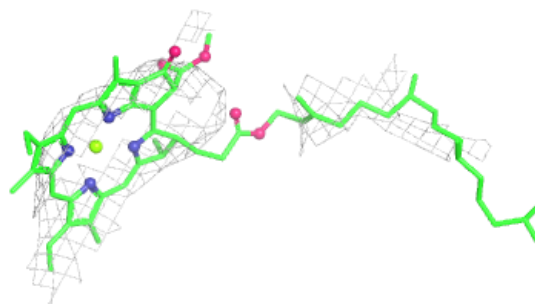
**Electron density around CLA C 513:**

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

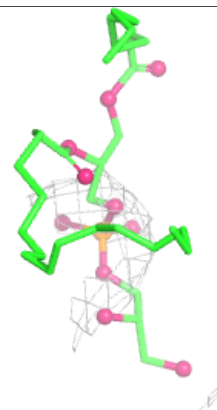
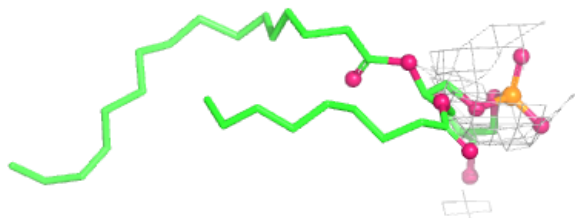
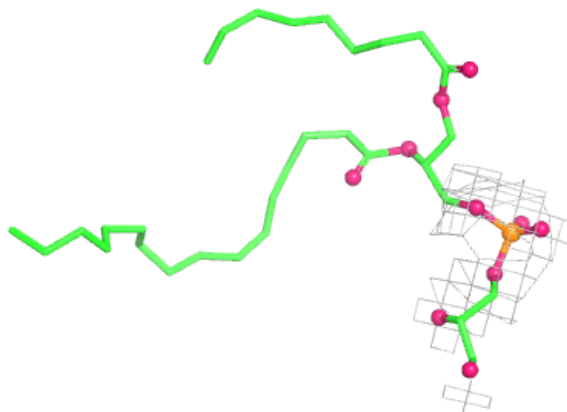


Electron density around CLA a 406:

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

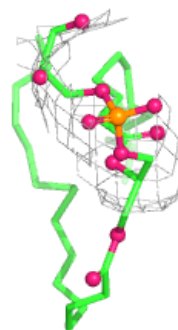
**Electron density around LHG a 413:**

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

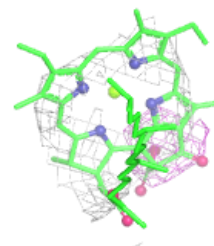
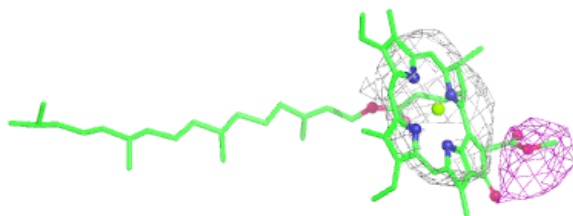
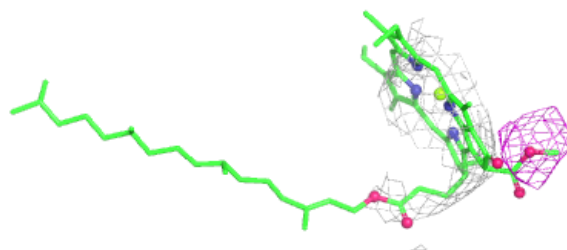


Electron density around LHG d 410:

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

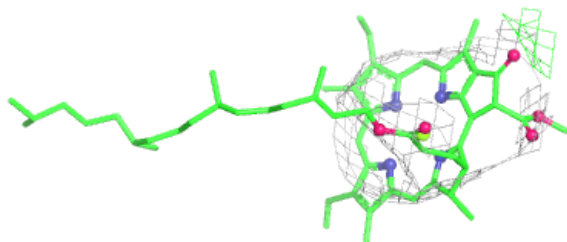
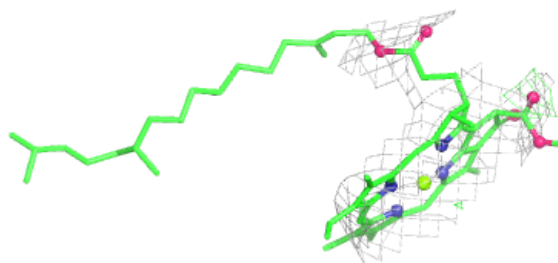
**Electron density around CLA B 608:**

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

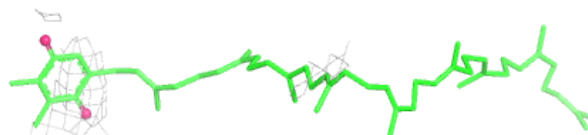
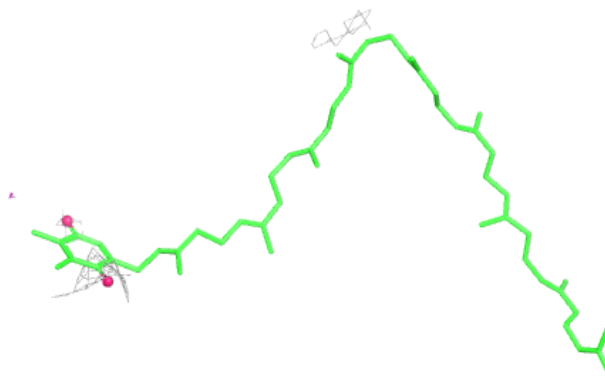


Electron density around CLA C 504:

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

**Electron density around 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)



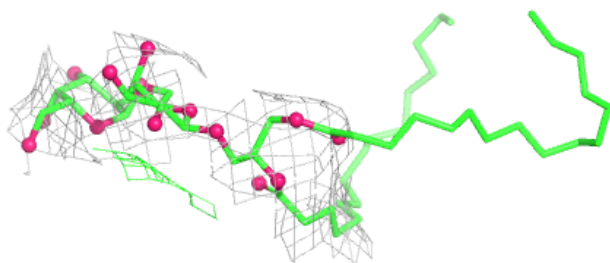
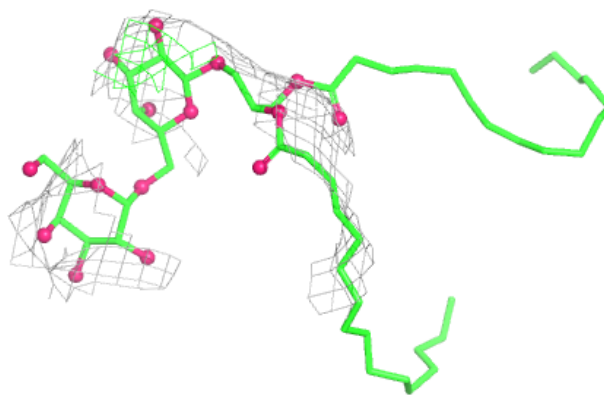
Electron density around SQD A 612:

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

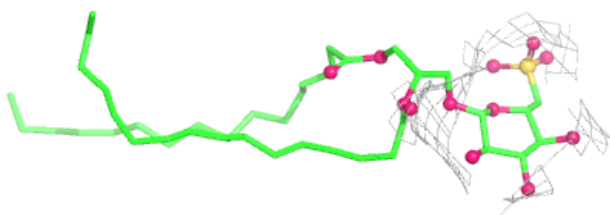
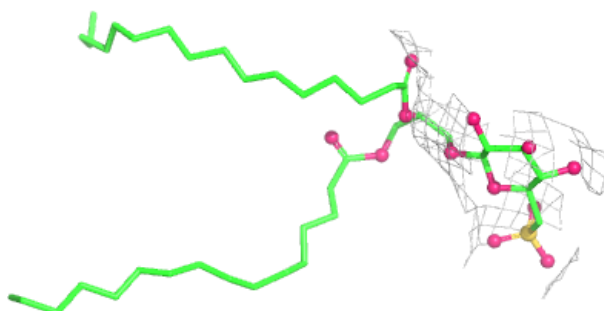


Electron density around DGD C 517:

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

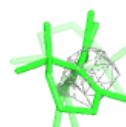
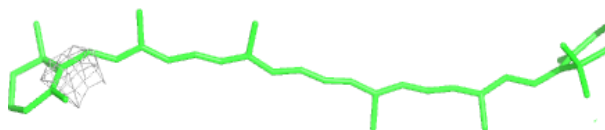
**Electron density around SQD A 613:**

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

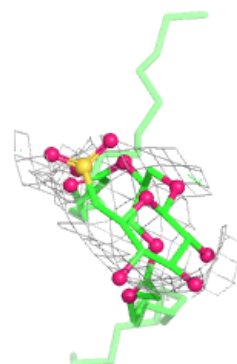
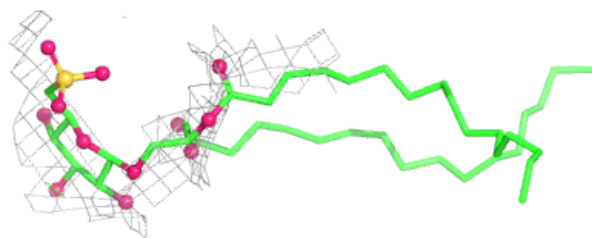
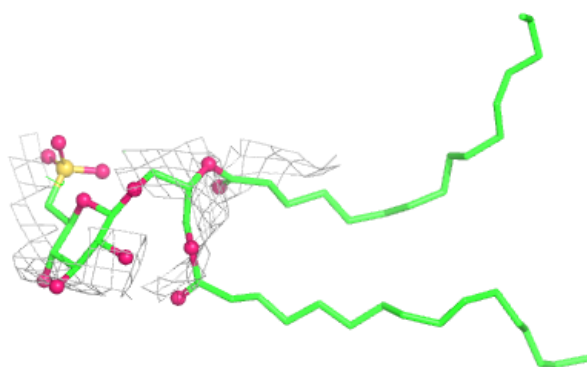


Electron density around BCR A 610:

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

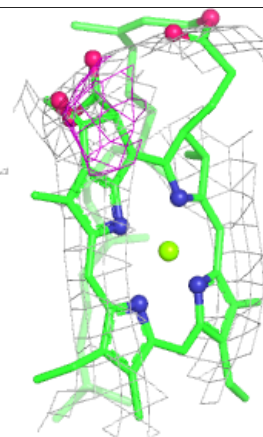
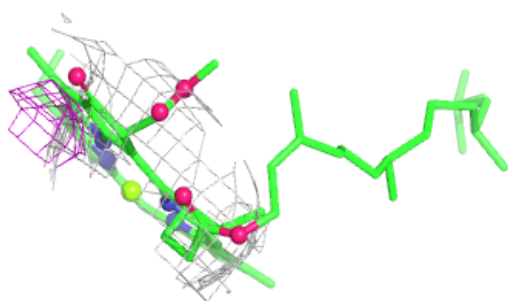
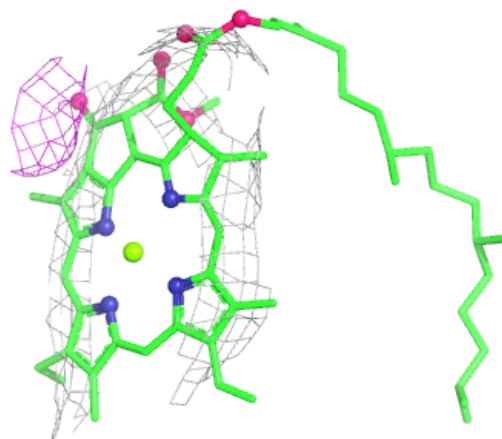
**Electron density around SQD 1 101:**

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

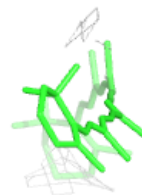
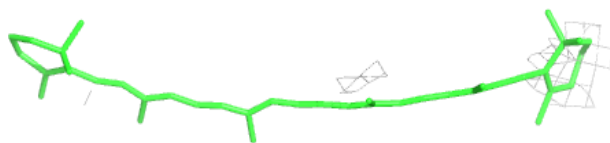
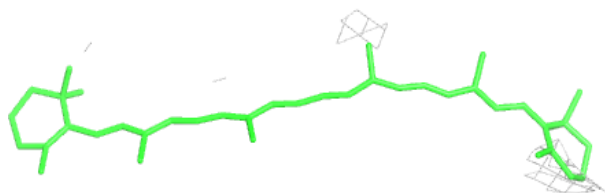


Electron density around CLA B 617:

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

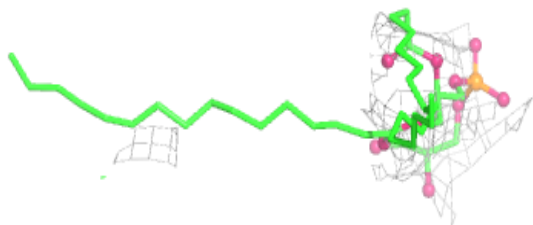
**Electron density around BCR T 101:**

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



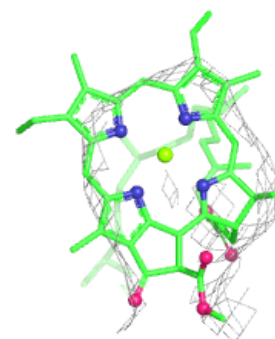
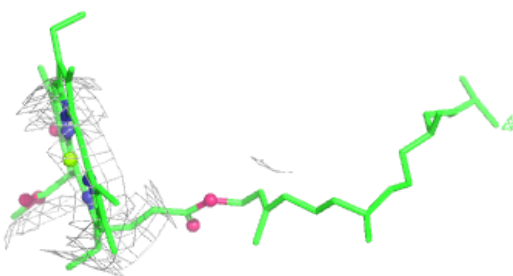
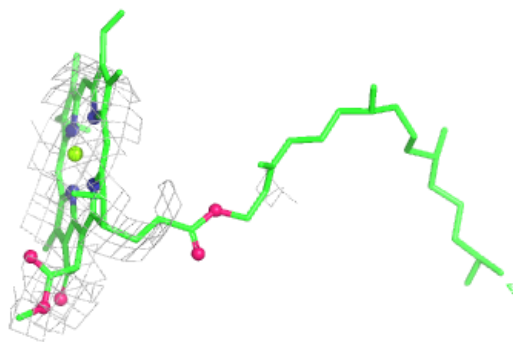
Electron density around LHG b 620:

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

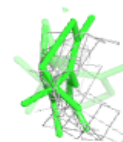
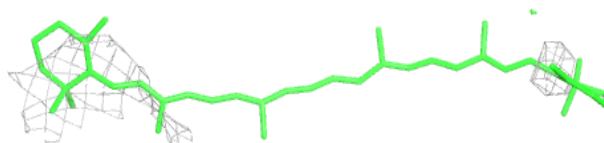


Electron density around CLA D 403:

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

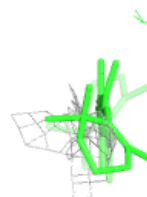
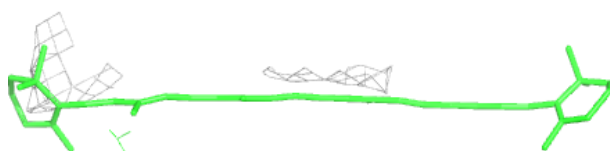
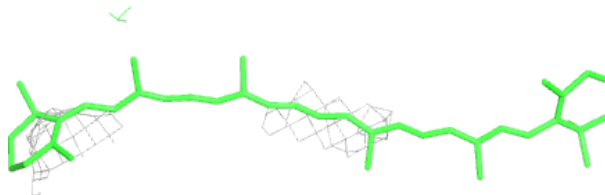
**Electron density around BCR B 618:**

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

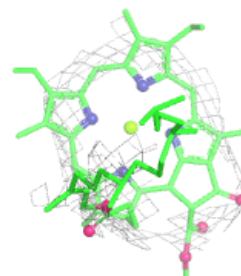
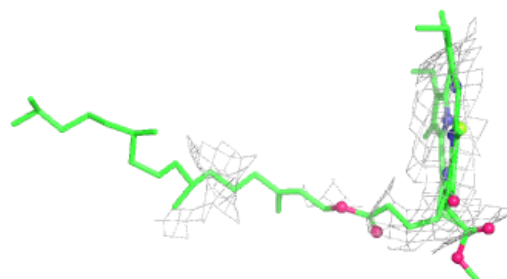


Electron density around BCR B 619:

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

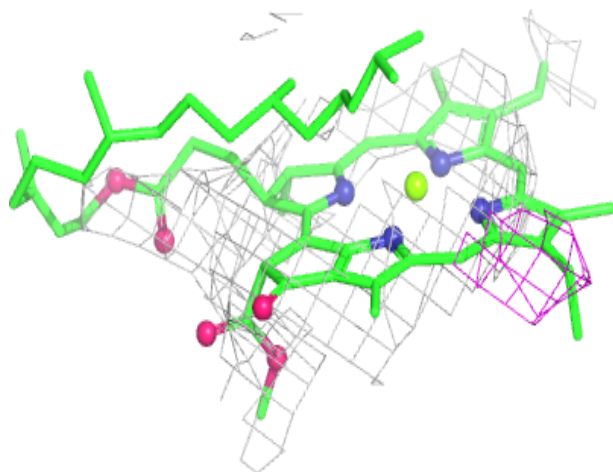
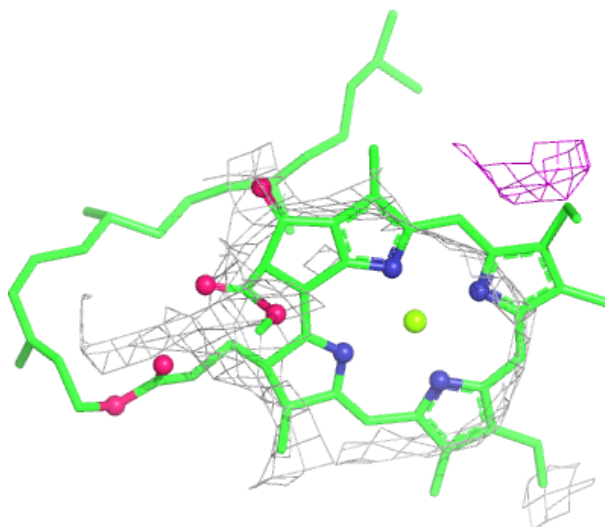
**Electron density around CLA B 607:**

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



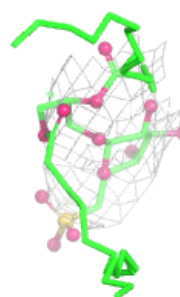
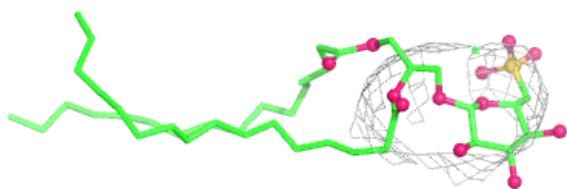
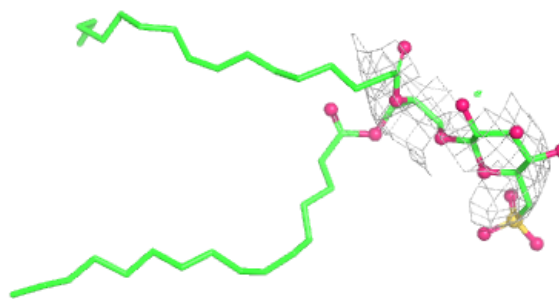
Electron density around CLA C 509:

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

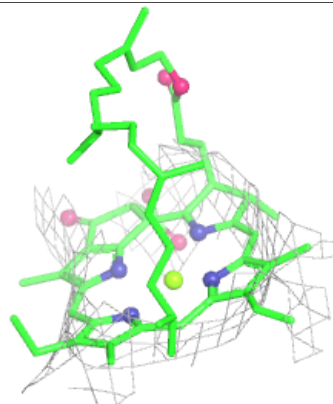
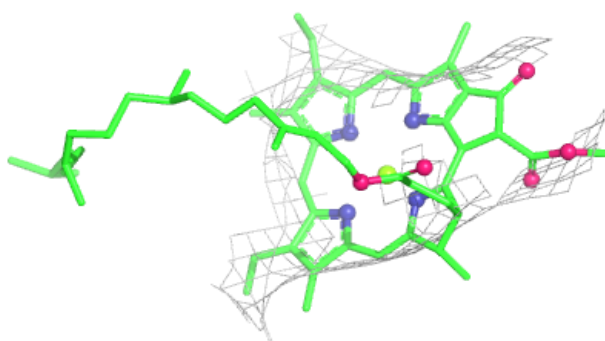
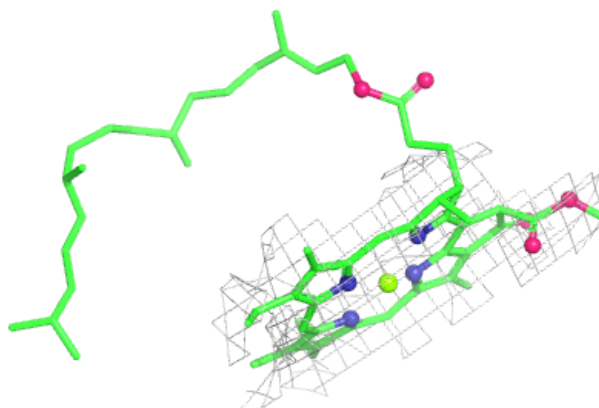


Electron density around SQD a 402:

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

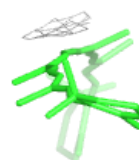
**Electron density around CLA c 914:**

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

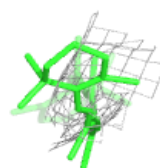
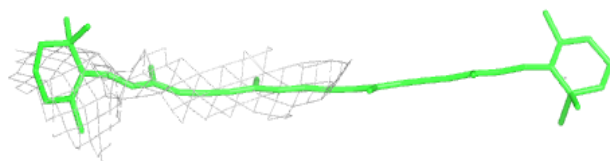
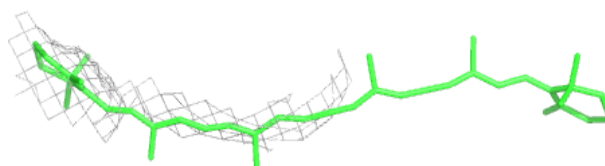


Electron density around BCR f 101:

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

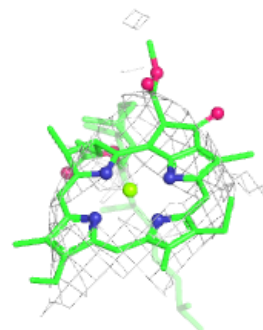
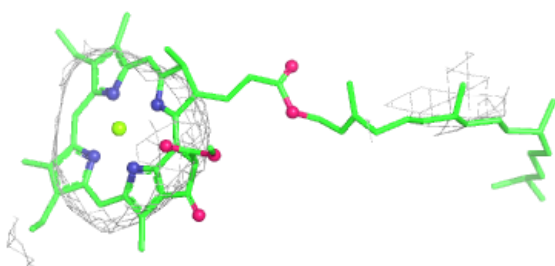
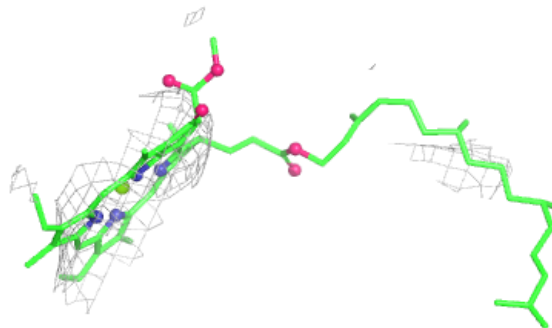
**Electron density around BCR h 101:**

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



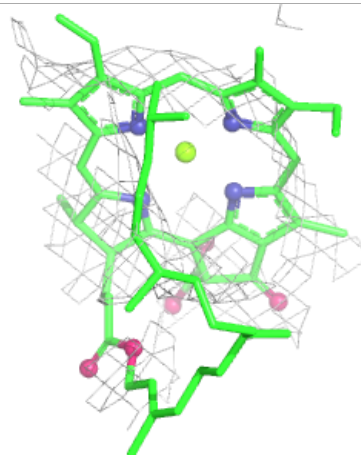
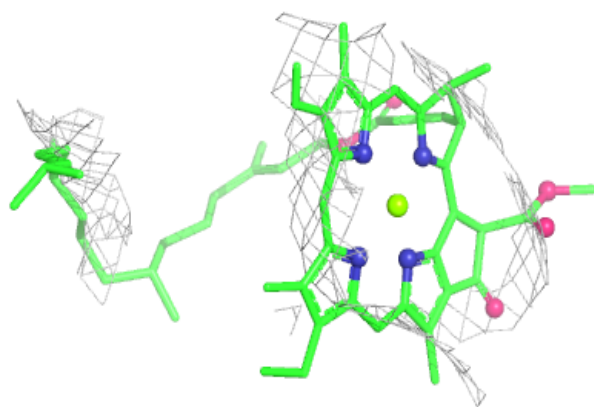
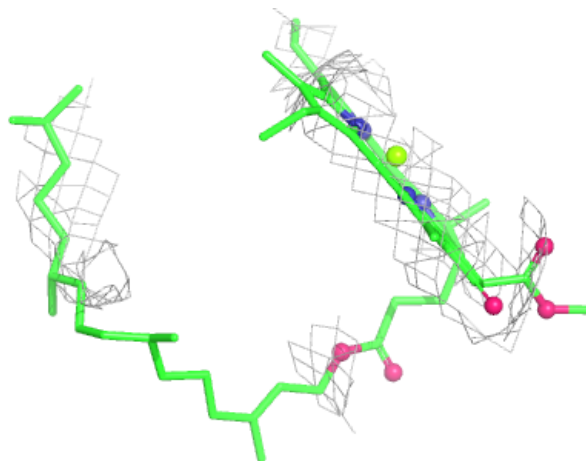
Electron density around CLA D 402:

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



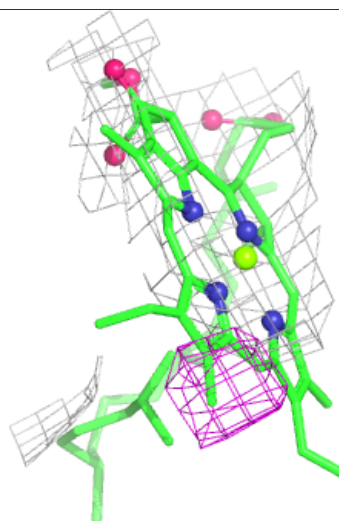
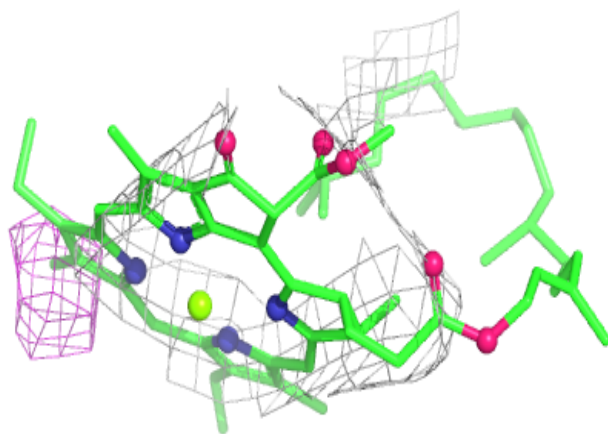
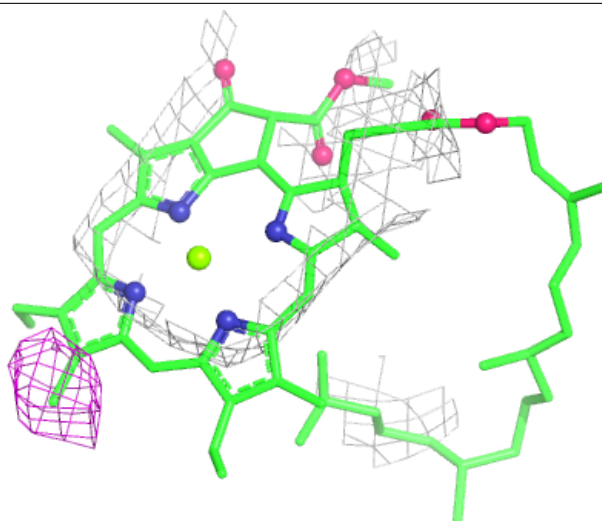
Electron density around CLA b 612:

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



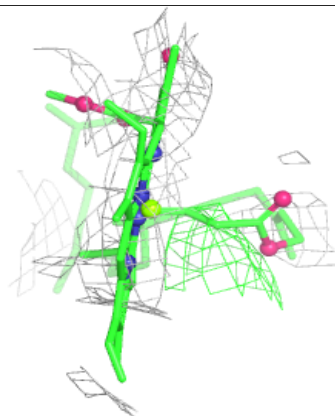
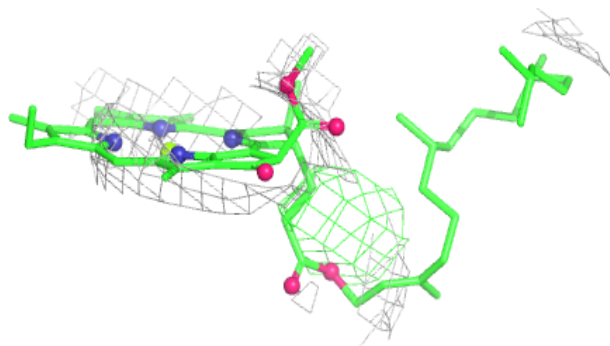
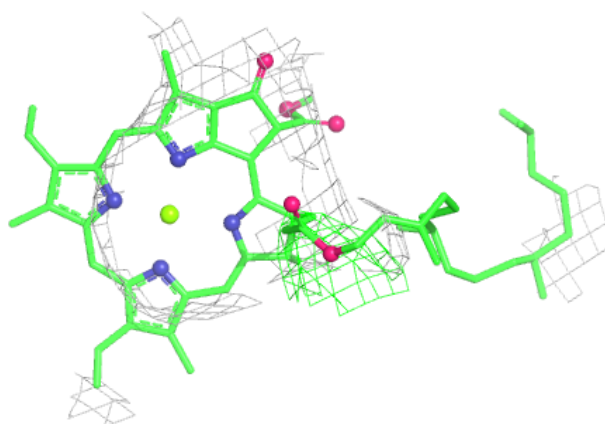
Electron density around CLA b 616:

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

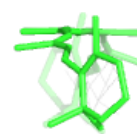
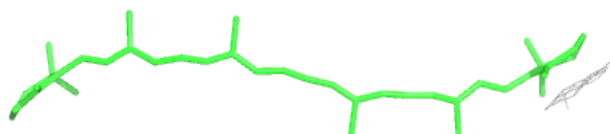
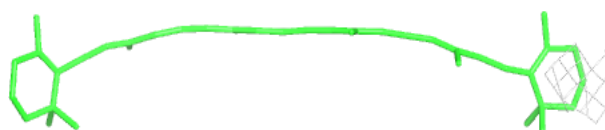


Electron density around CLA B 613:

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

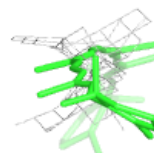
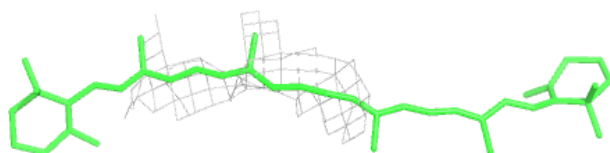
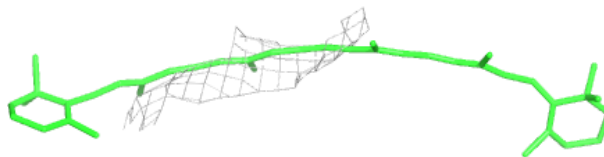
**Electron density around BCR k 102:**

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

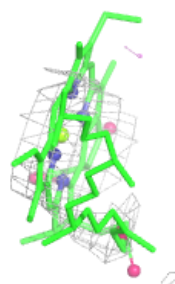
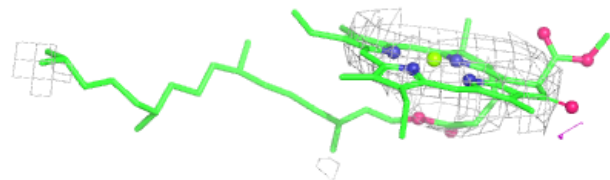
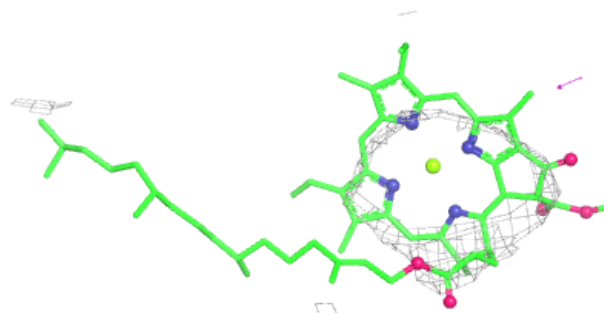


Electron density around BCR D 404:

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

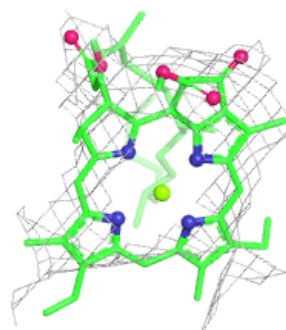
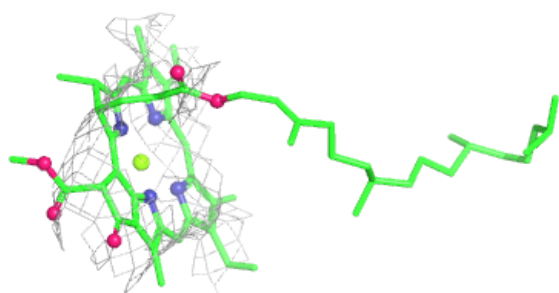
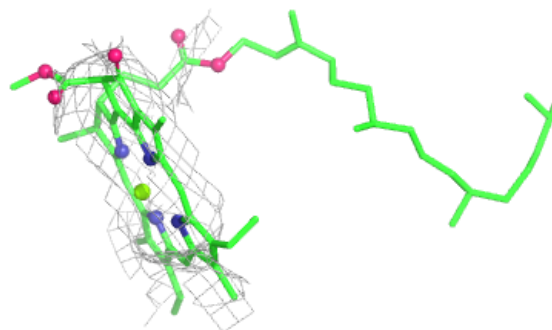
**Electron density around CLA c 902:**

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

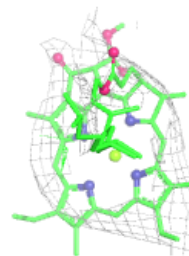
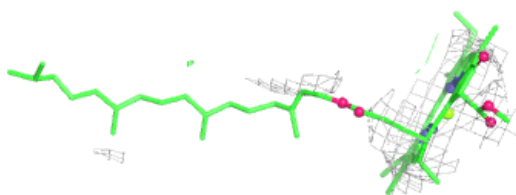
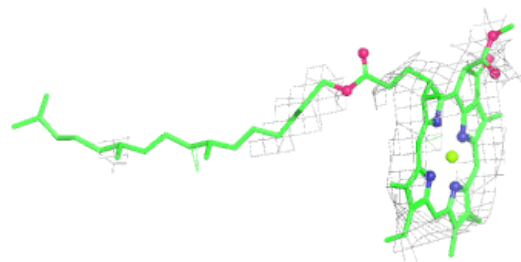


Electron density around CLA C 508:

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

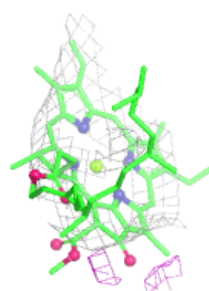
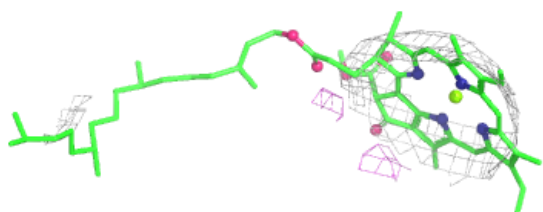
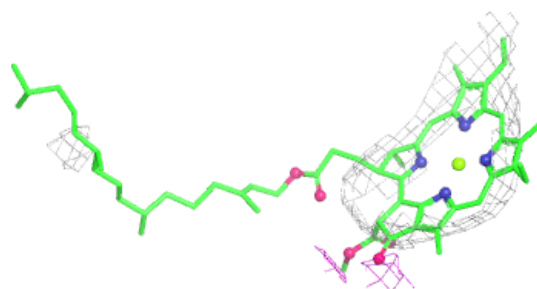
**Electron density around CLA d 404:**

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

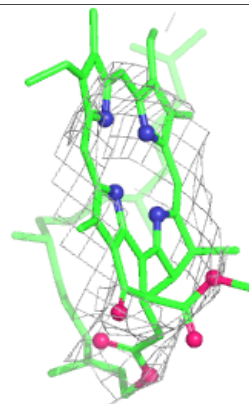
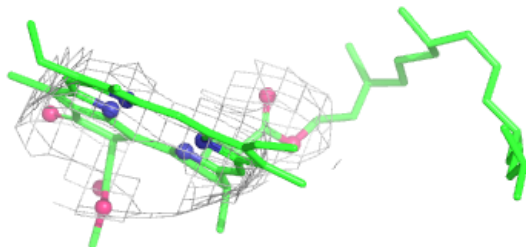
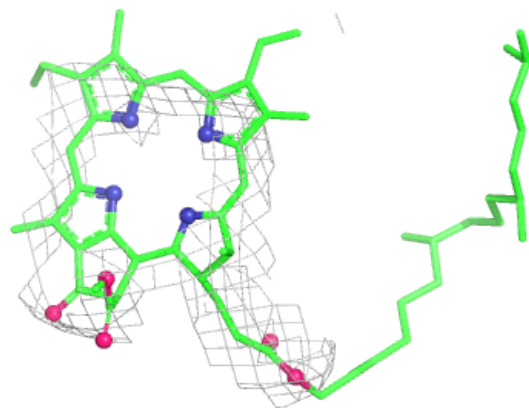


Electron density around CLA A 606:

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

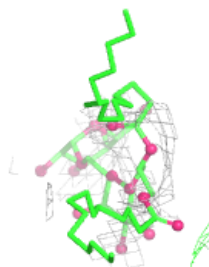
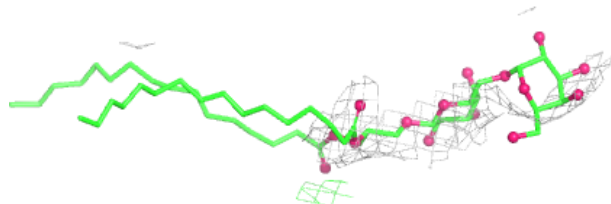
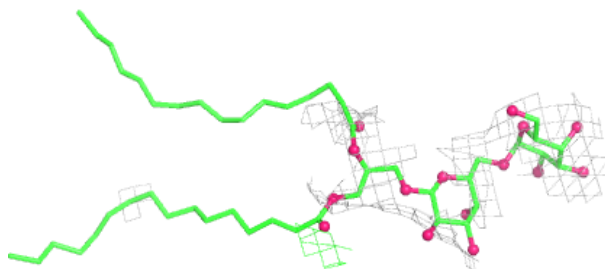
**Electron density around PHO a 412:**

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



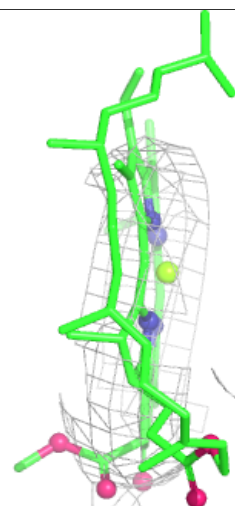
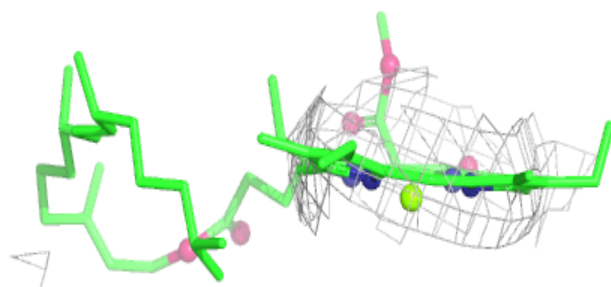
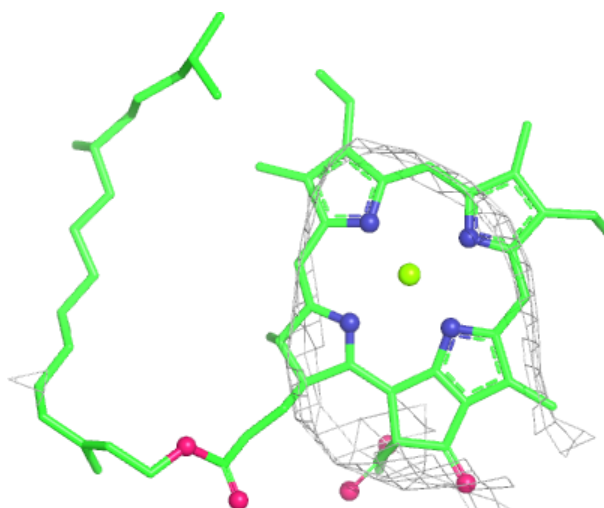
Electron density around DGD C 518:

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



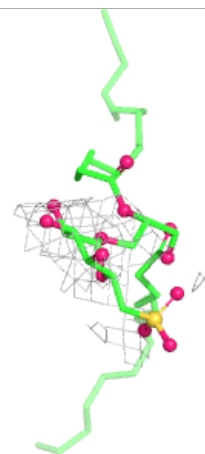
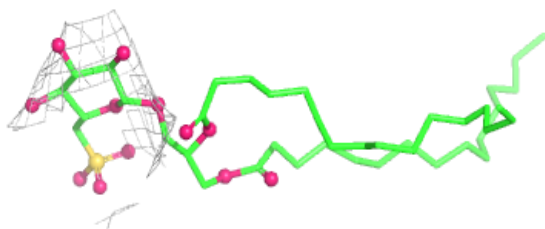
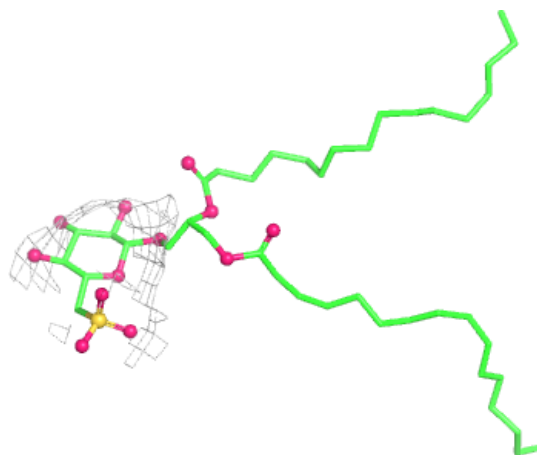
Electron density around CLA C 512:

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



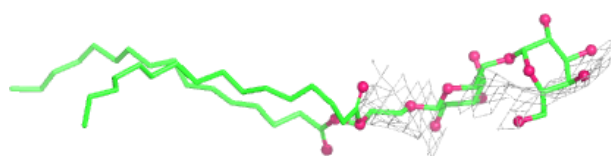
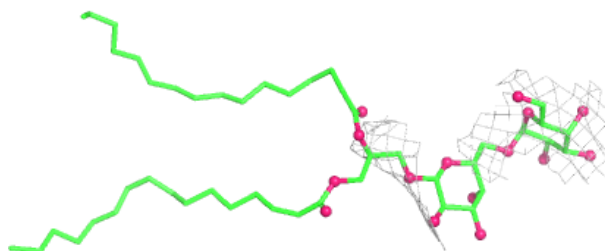
Electron density around SQD a 411:

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

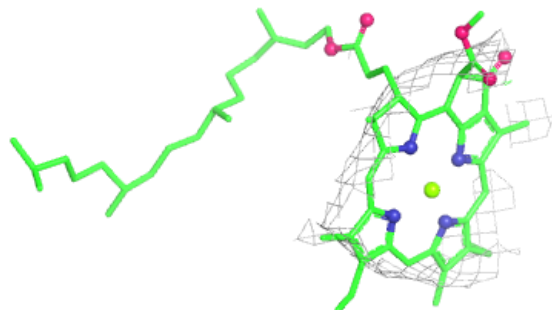


Electron density around DGD j 101:

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

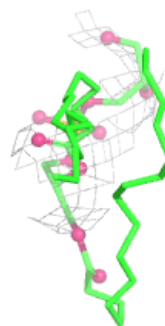
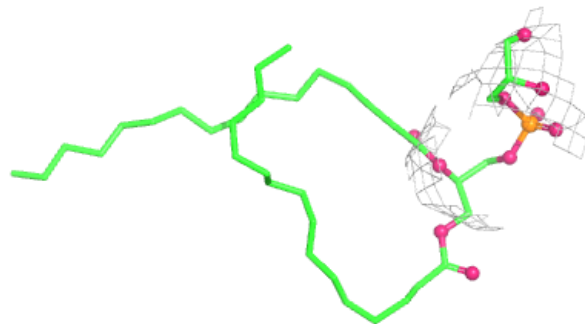
**Electron density around CLA c 912:**

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



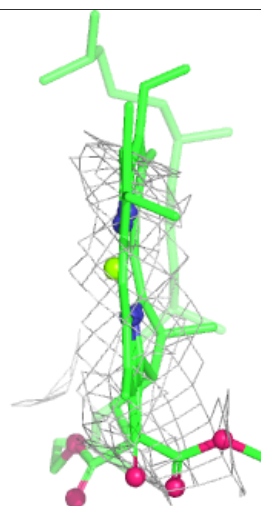
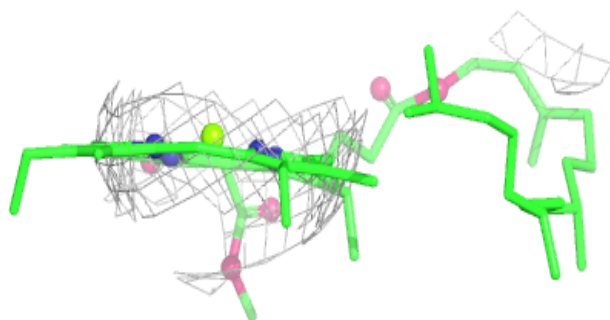
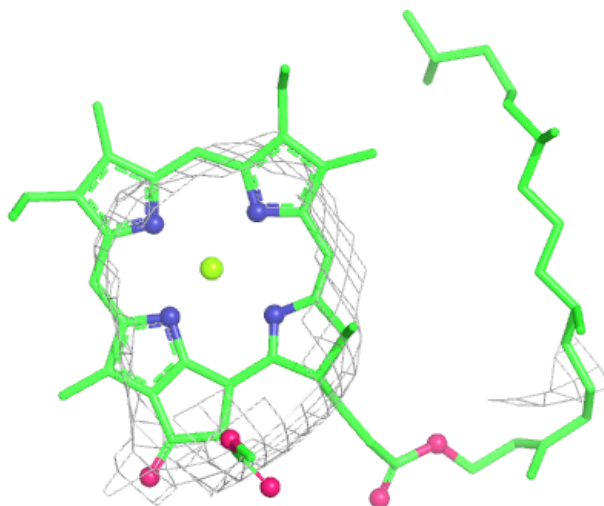
Electron density around LHG D 409:

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



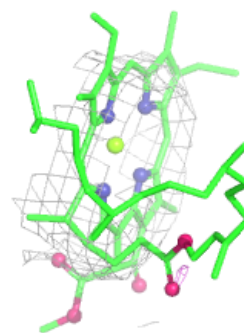
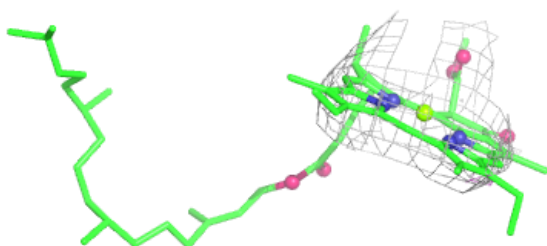
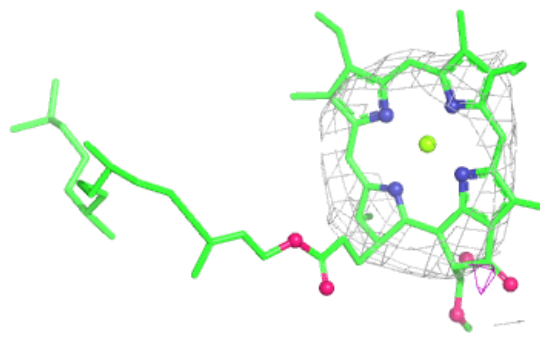
Electron density around CLA c 913:

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

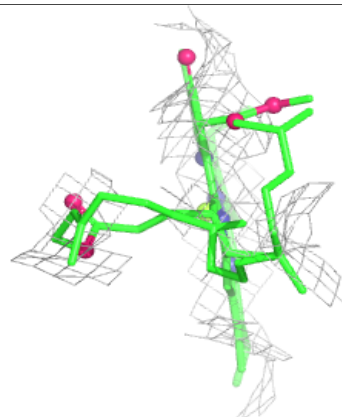
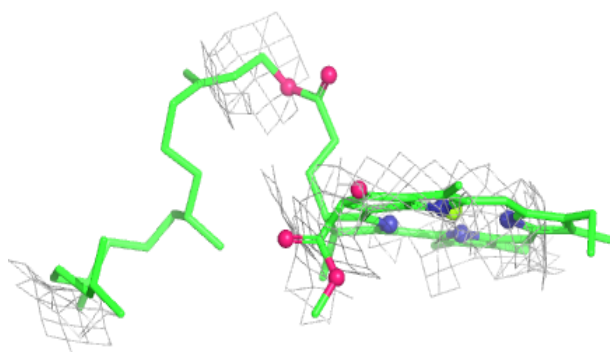
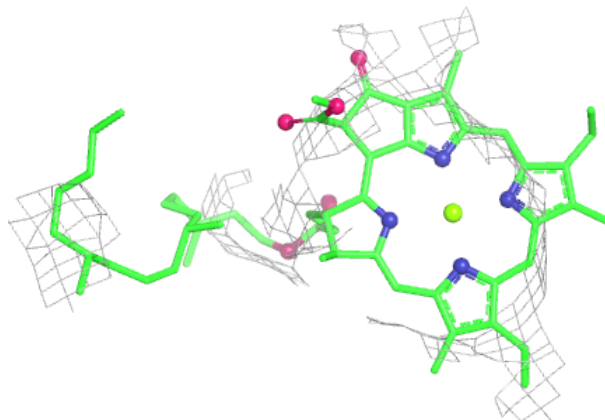


Electron density around CLA a 408:

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

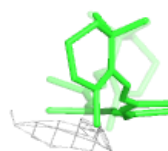
**Electron density around CLA b 613:**

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

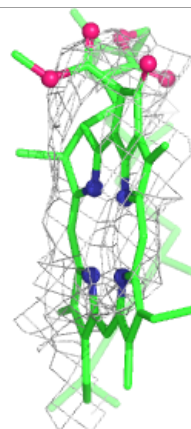
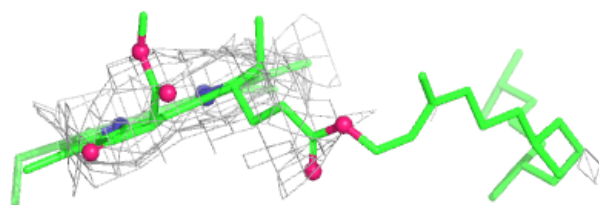
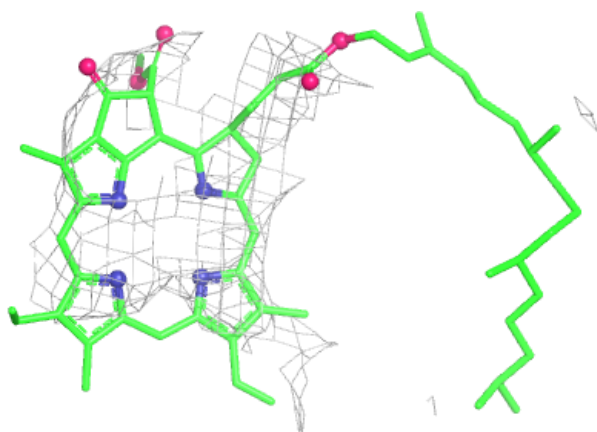


Electron density around BCR K 101:

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

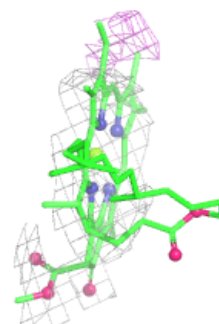
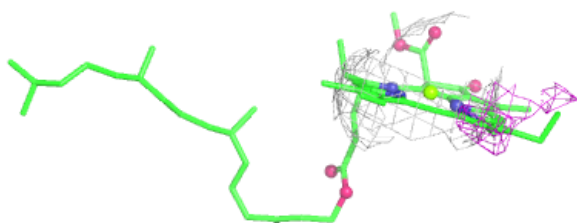
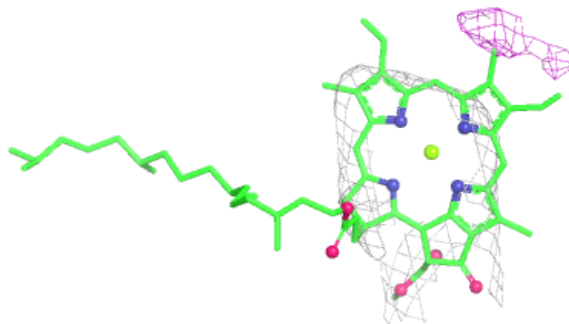
**Electron density around PHO A 608:**

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

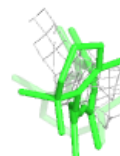
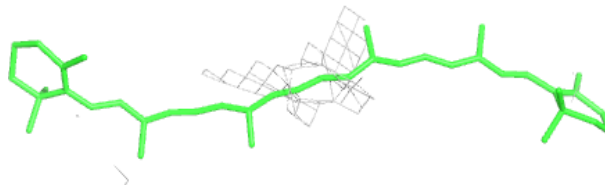


Electron density around CLA A 607:

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

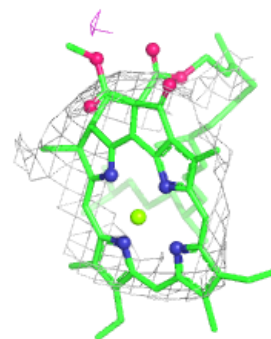
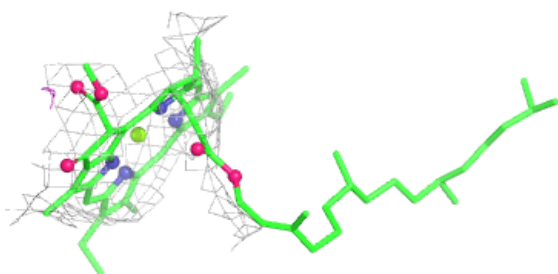
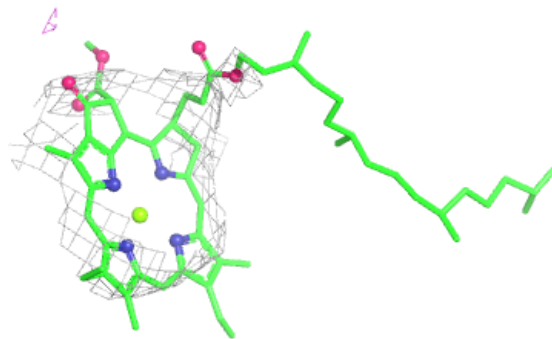
**Electron density around BCR Y 101:**

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



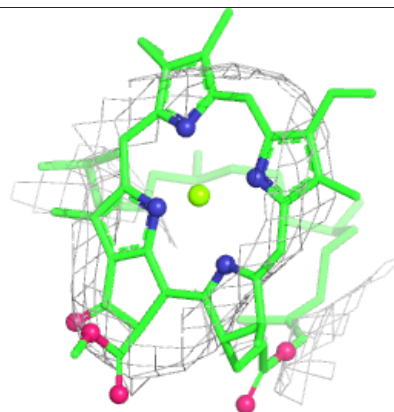
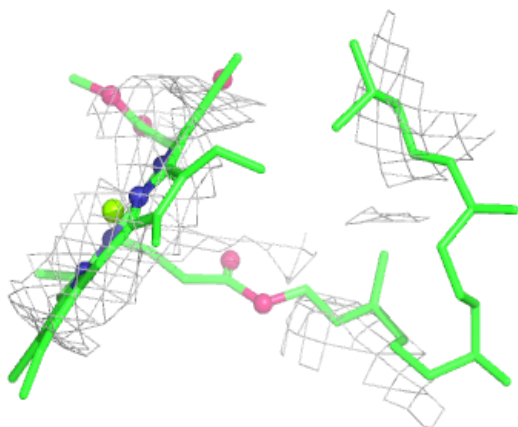
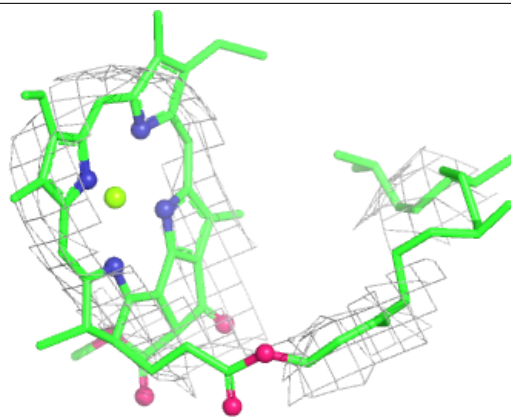
Electron density around CLA C 511:

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

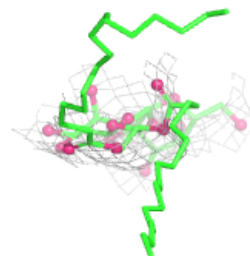
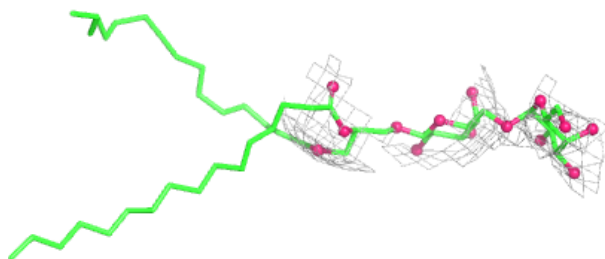


Electron density around CLA c 904:

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

**Electron density around DGD c 916:**

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

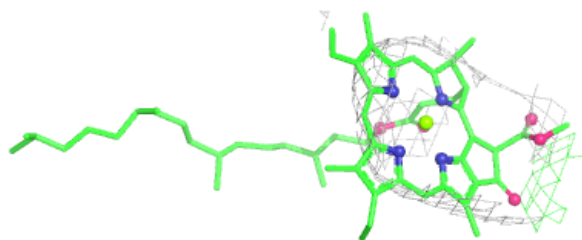
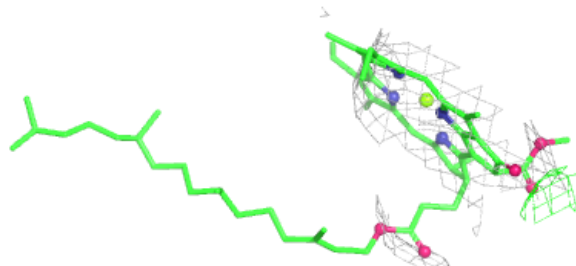


Electron density around DGD c 917:

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

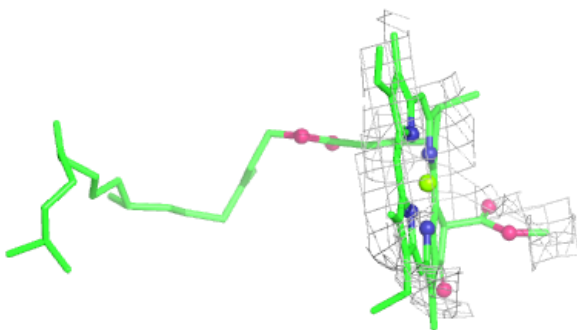
**Electron density around CLA c 905:**

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

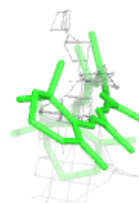
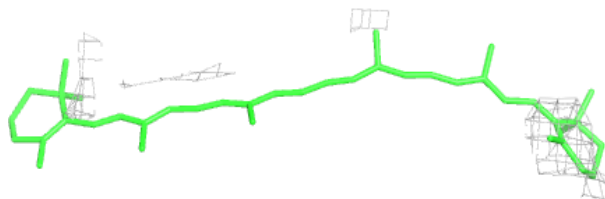


Electron density around CLA c 907:

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

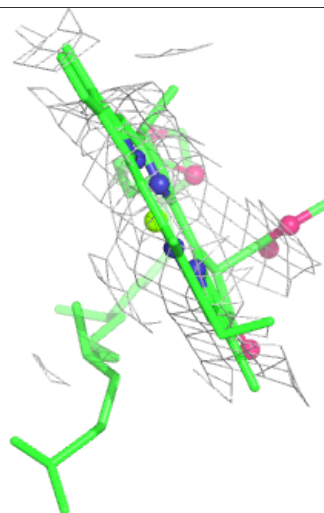
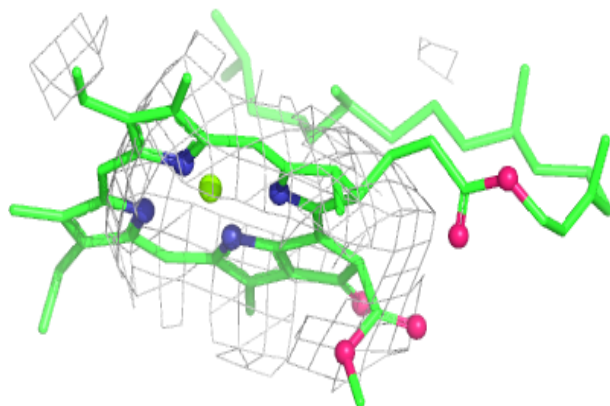
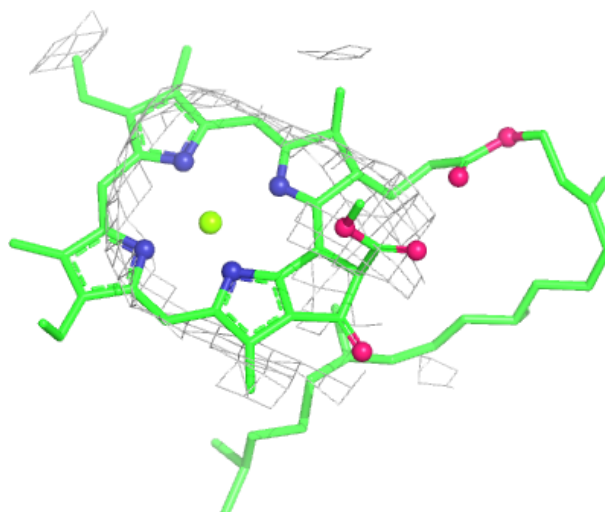
**Electron density around BCR B 622:**

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



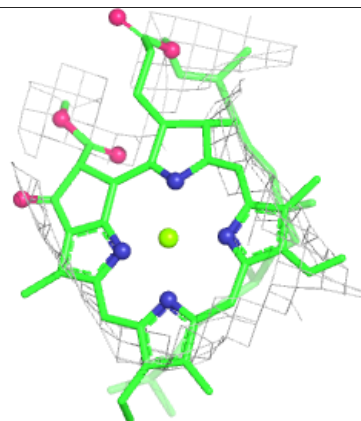
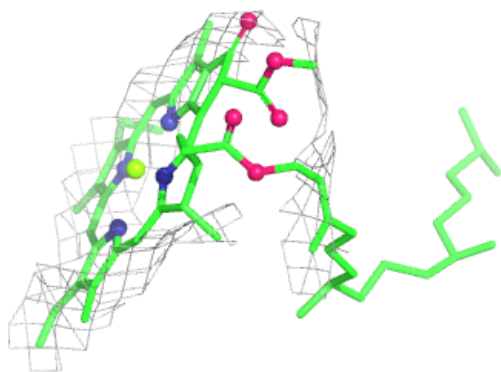
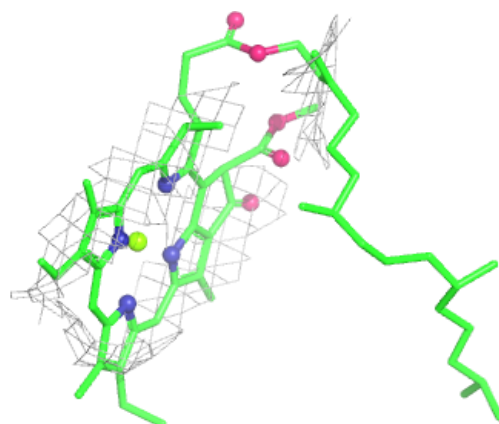
Electron density around CLA c 910:

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

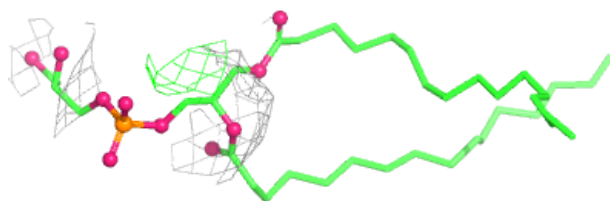
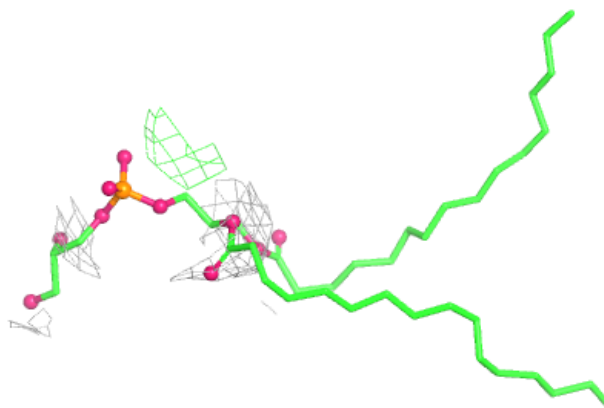


Electron density around CLA b 614:

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

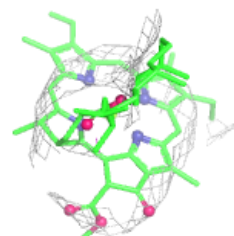
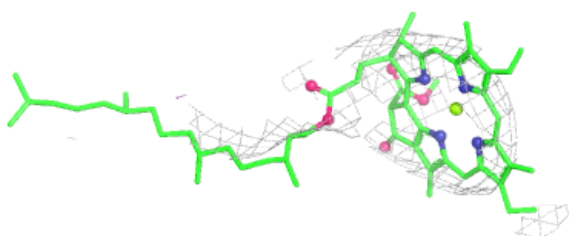
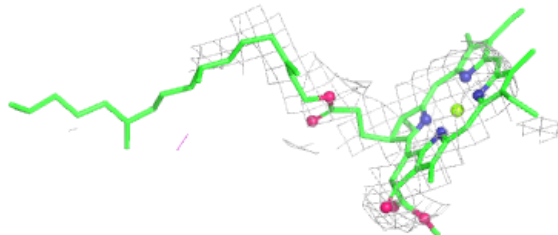
**Electron density around LHG d 409:**

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

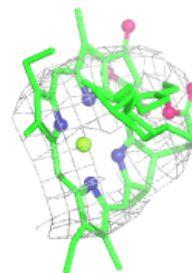
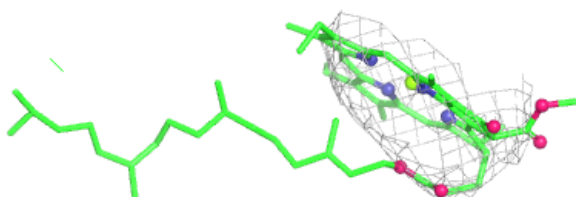
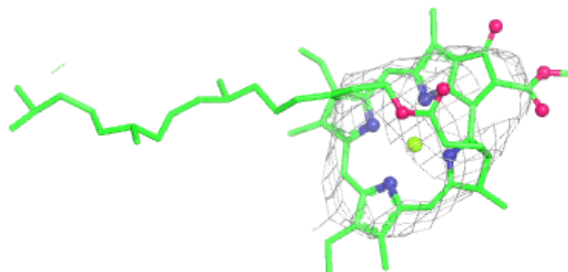


Electron density around CLA c 903:

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

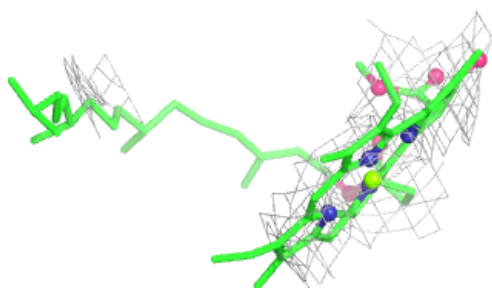
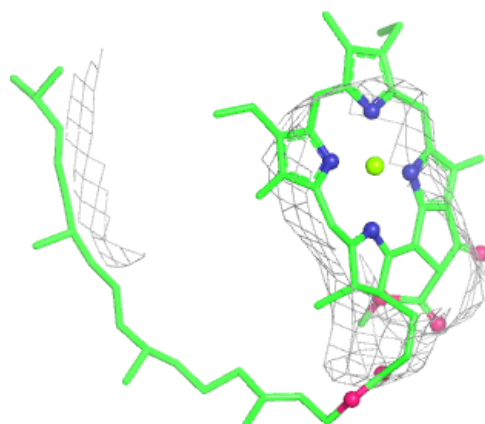
**Electron density around CLA b 615:**

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

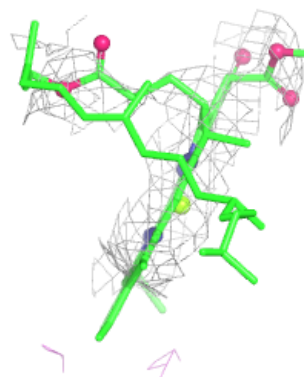
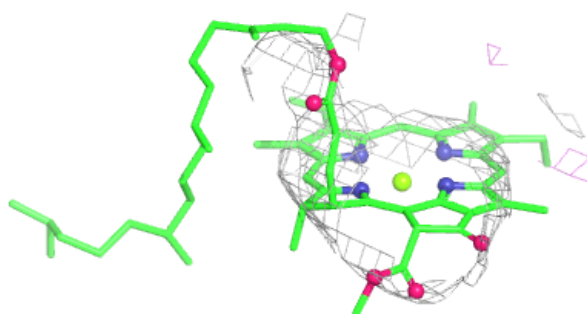
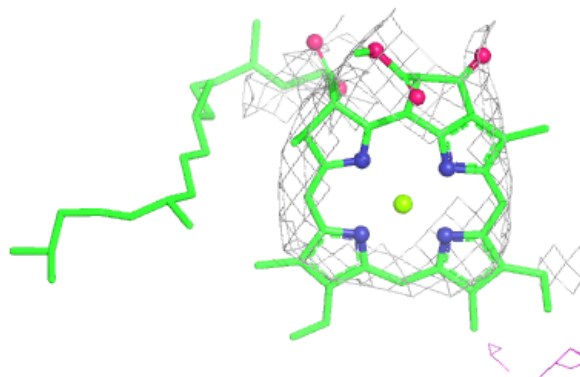


Electron density around CLA C 507:

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

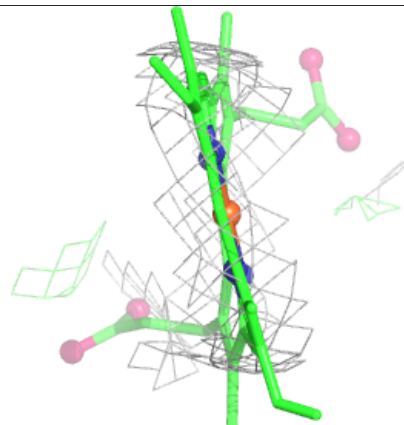
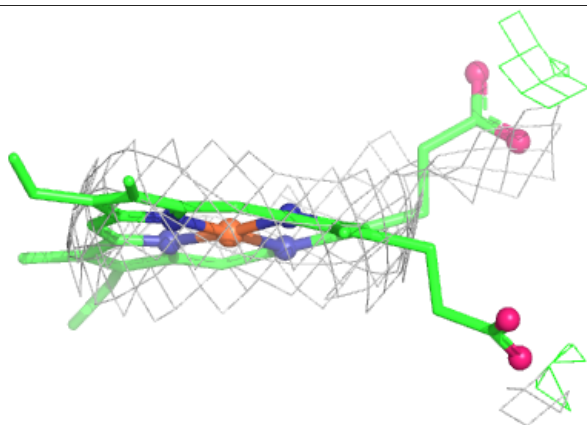
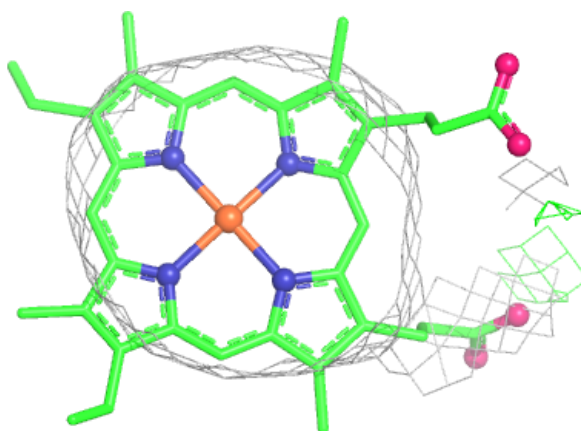
**Electron density around CLA A 614:**

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

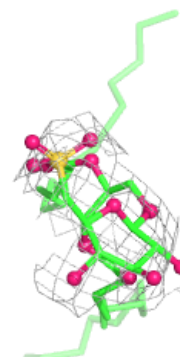
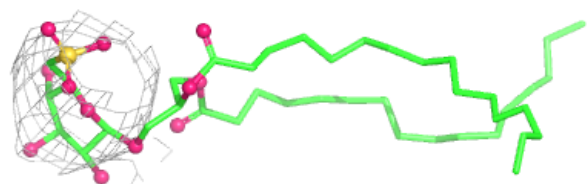
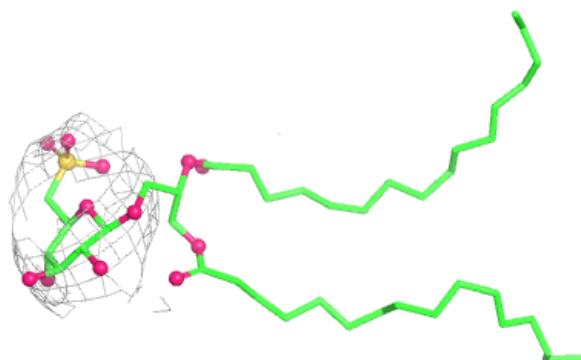


Electron density around HEM e 101:

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

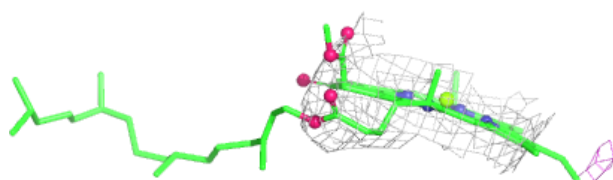
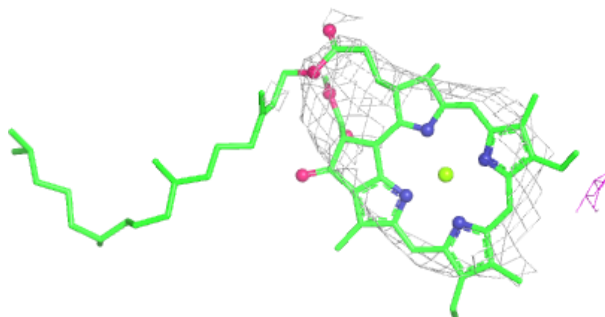
**Electron density around SQD L 101:**

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

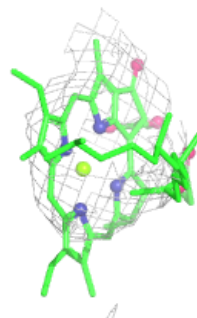
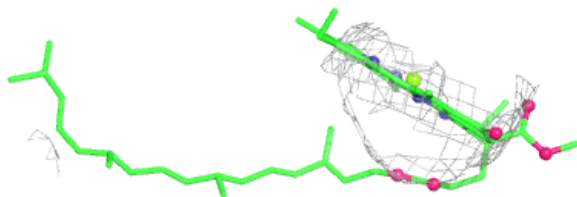


Electron density around CLA b 603:

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

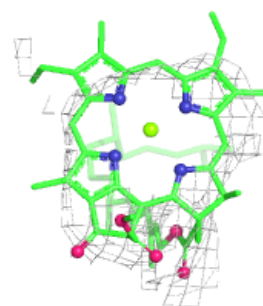
**Electron density around CLA B 609:**

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

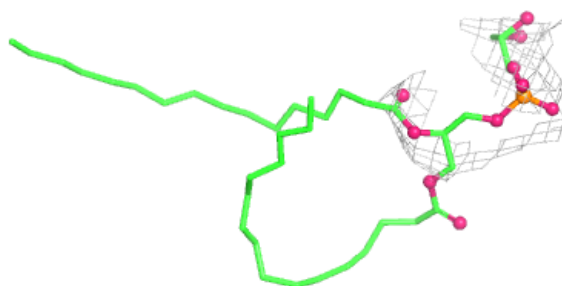


Electron density around CLA B 606:

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

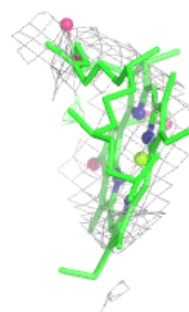
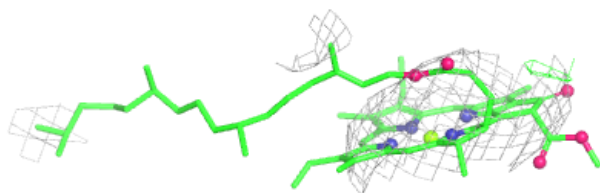
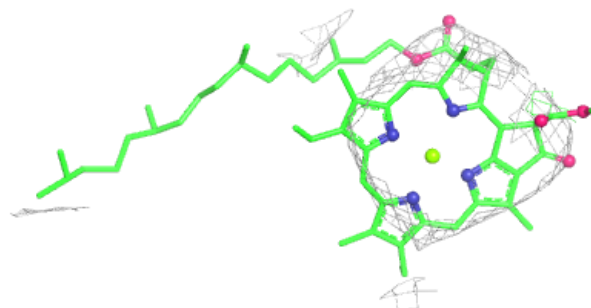
**Electron density around LHG D 407:**

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

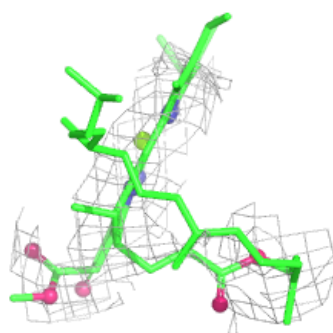
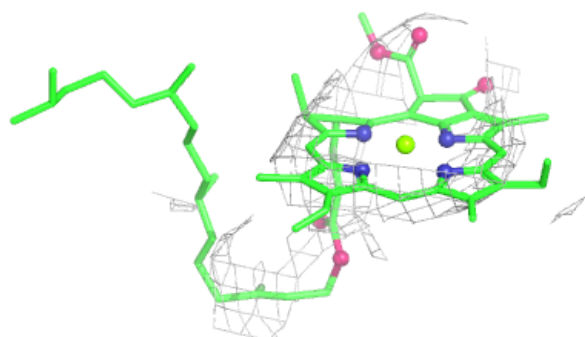
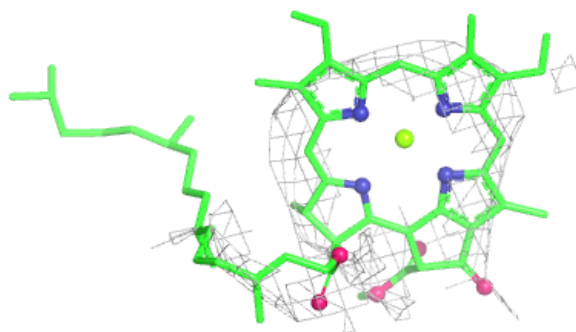


Electron density around CLA C 501:

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

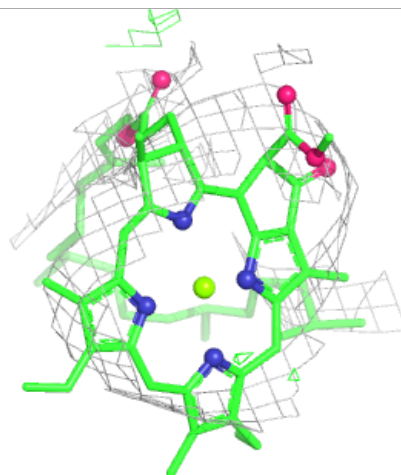
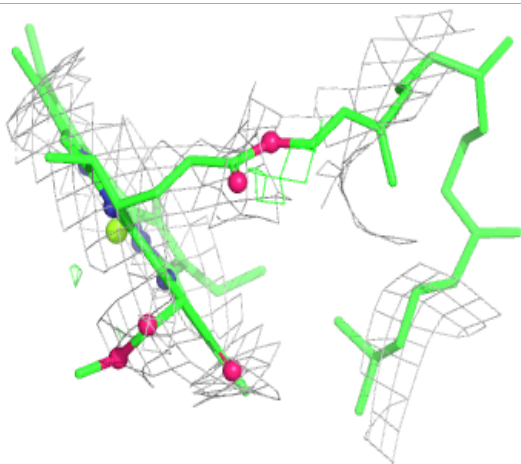
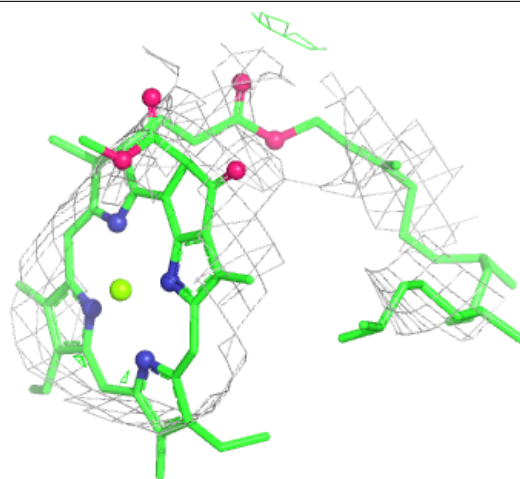
**Electron density around CLA d 401:**

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



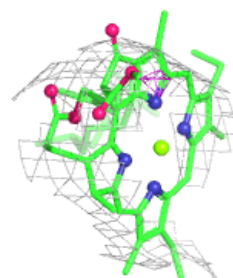
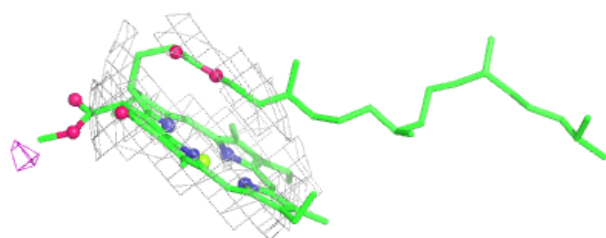
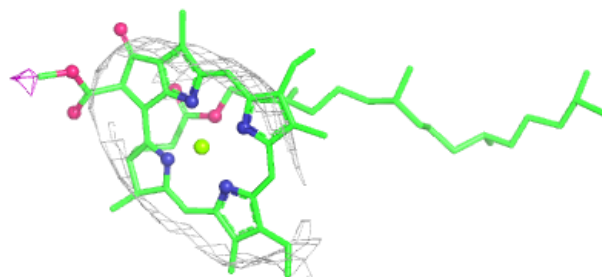
Electron density around CLA C 503:

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

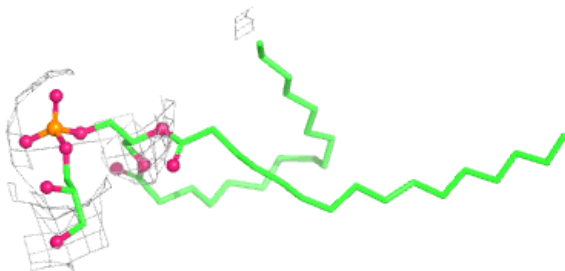


Electron density around CLA B 615:

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

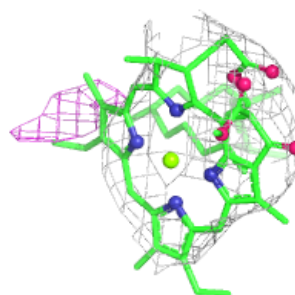
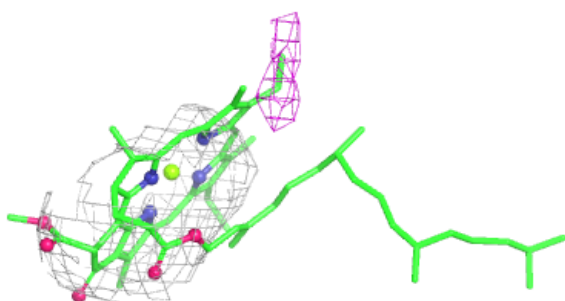
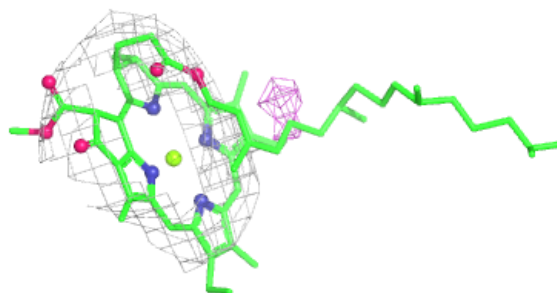
**Electron density around LHG d 408:**

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

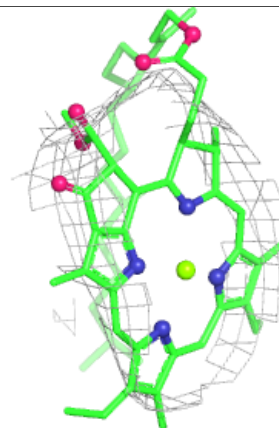
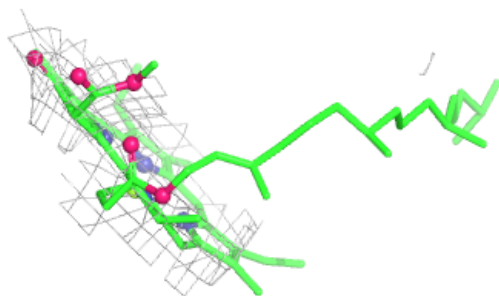
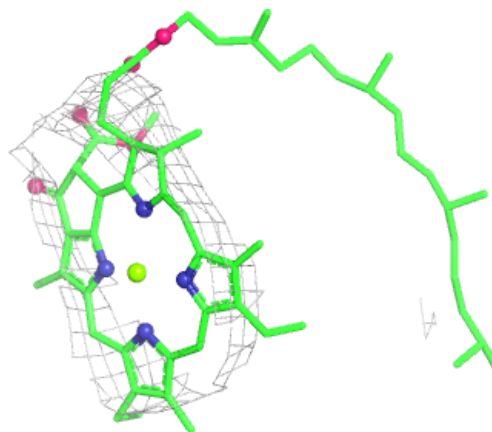


Electron density around CLA C 505:

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

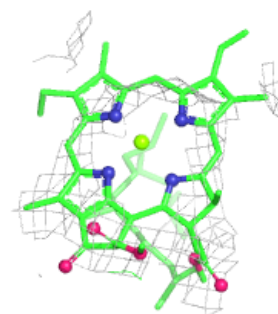
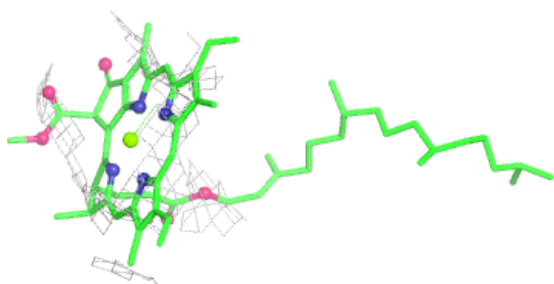
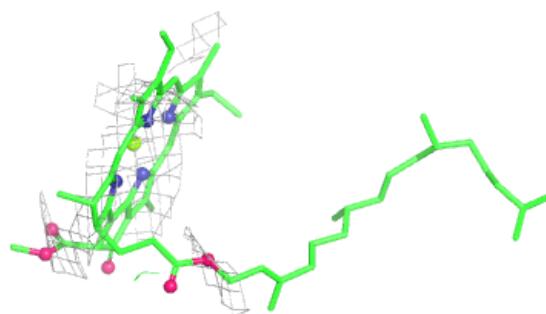
**Electron density around CLA c 908:**

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



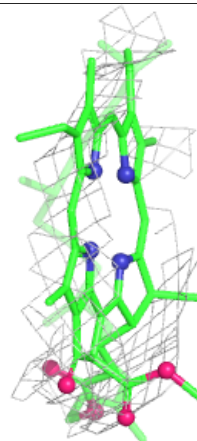
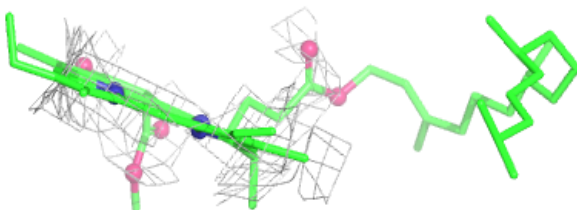
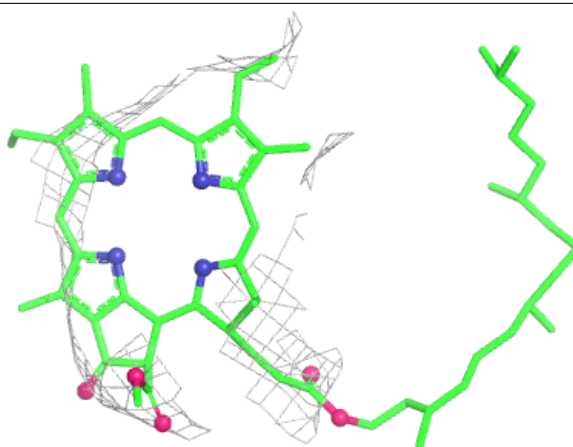
Electron density around CLA c 909:

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



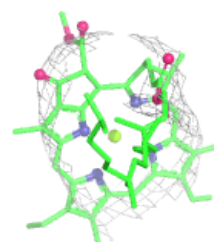
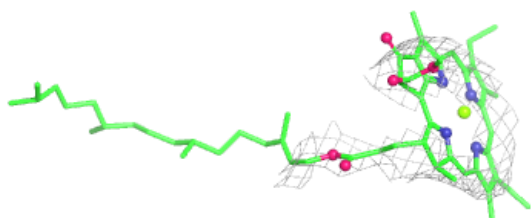
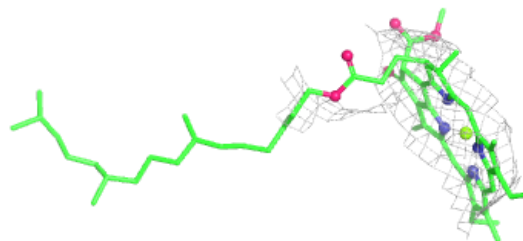
Electron density around PHO d 402:

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



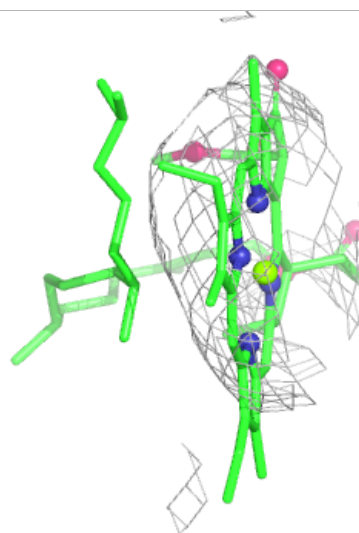
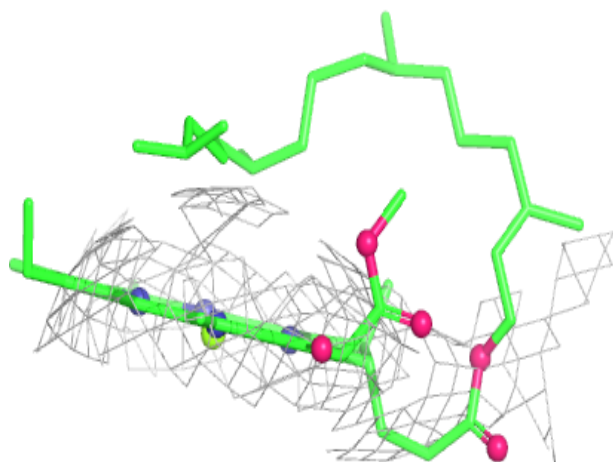
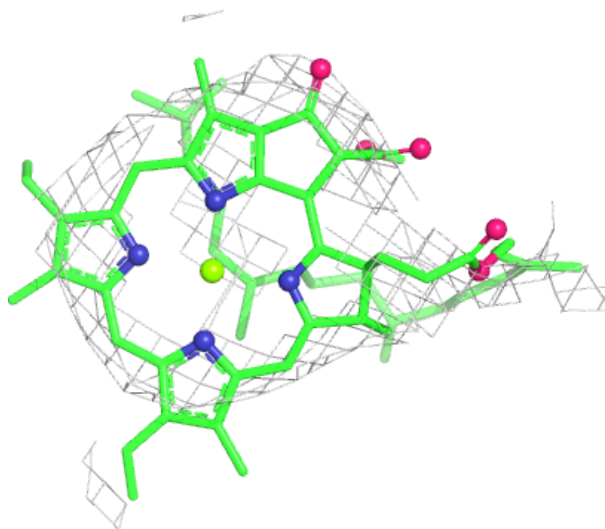
Electron density around CLA b 605:

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



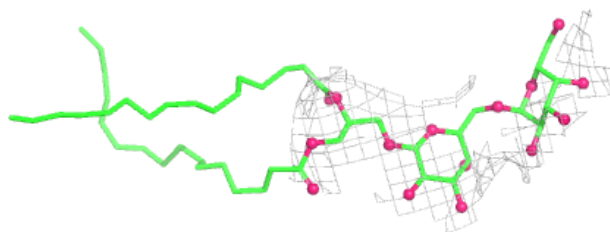
Electron density around CLA c 911:

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

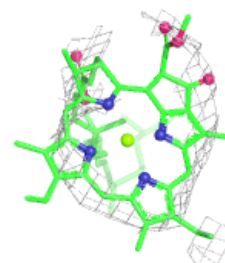
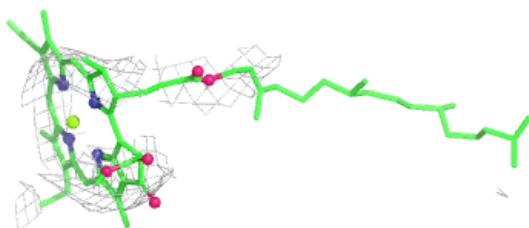
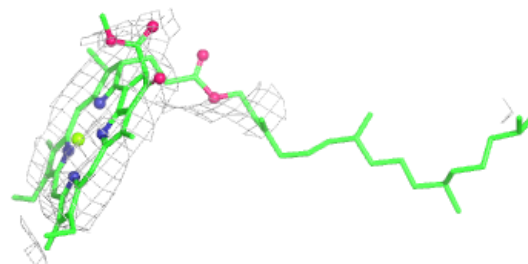


Electron density around DGD C 516:

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

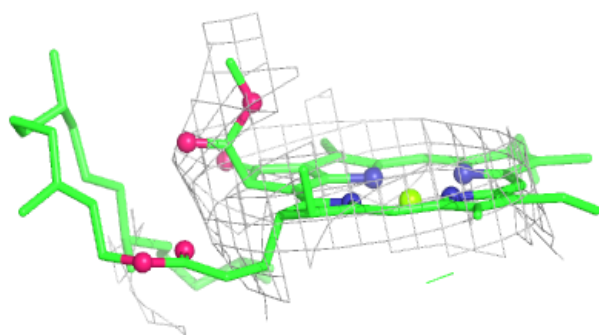
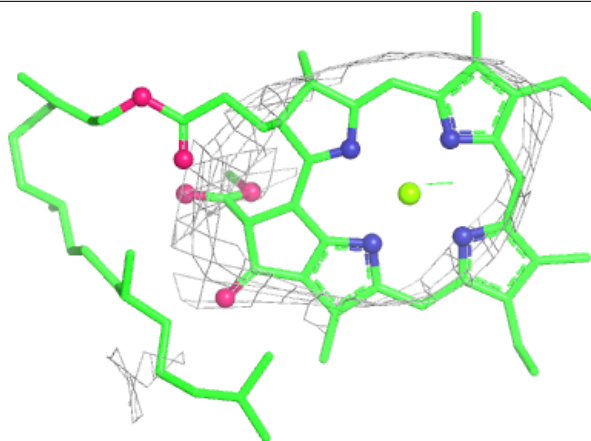
**Electron density around CLA B 605:**

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



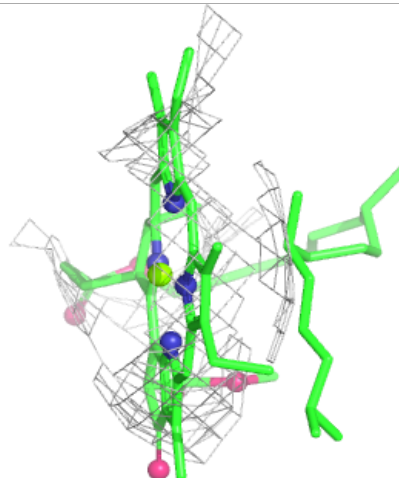
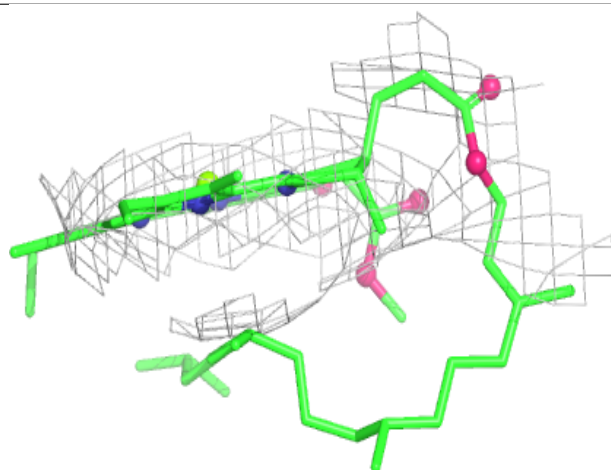
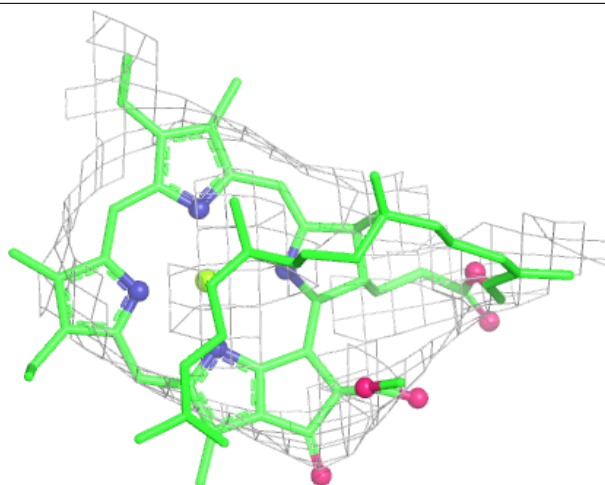
Electron density around CLA B 611:

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



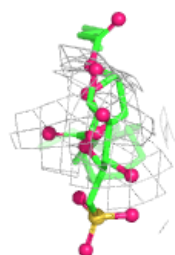
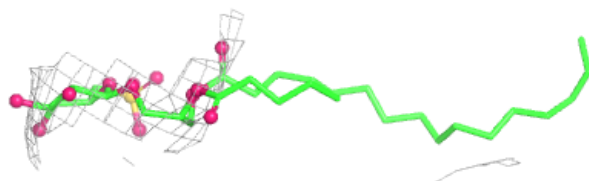
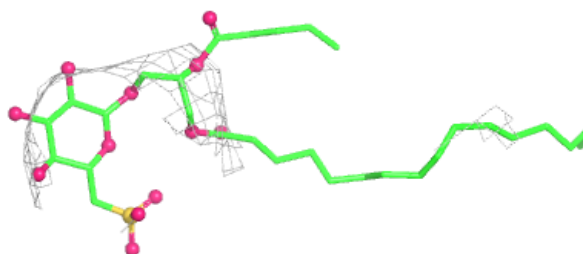
Electron density around CLA C 510:

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

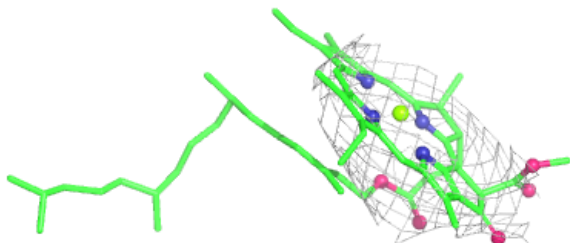
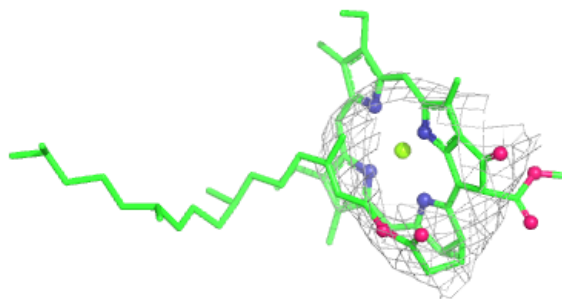


Electron density around SQD F 101:

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

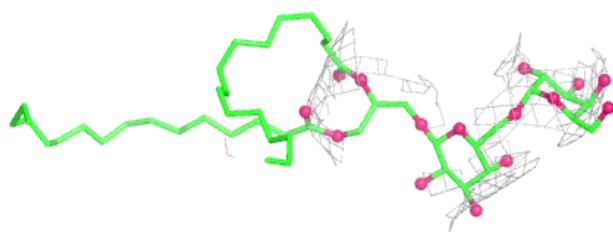
**Electron density around CLA c 906:**

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

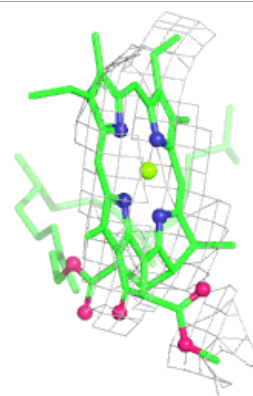
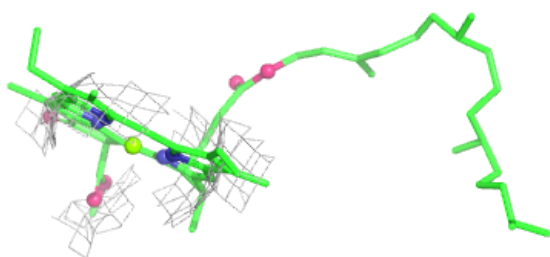
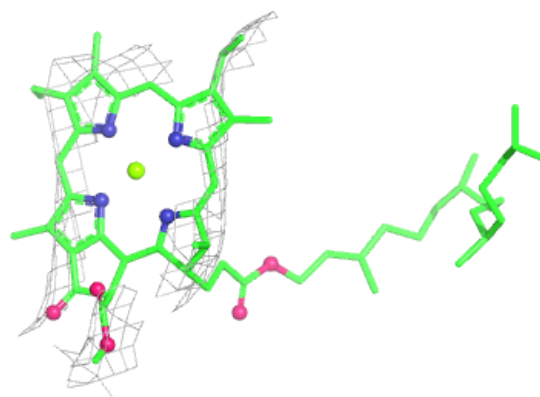


Electron density around DGD h 102:

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

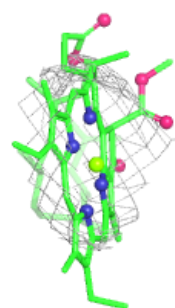
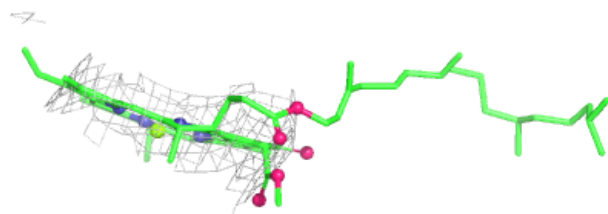
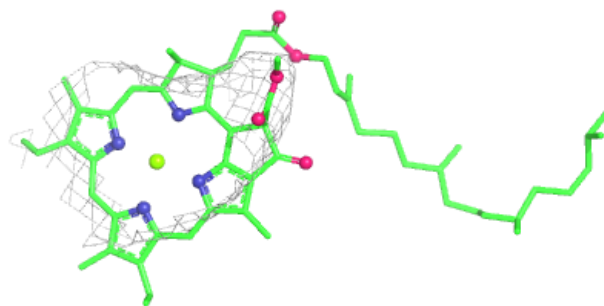
**Electron density around CLA A 609:**

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

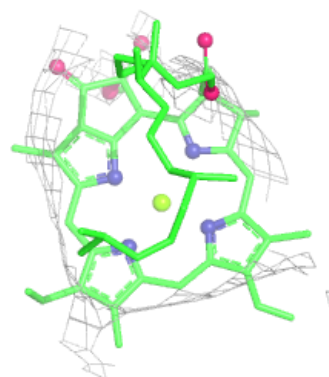
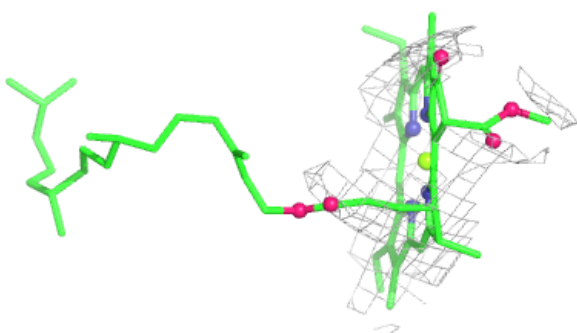
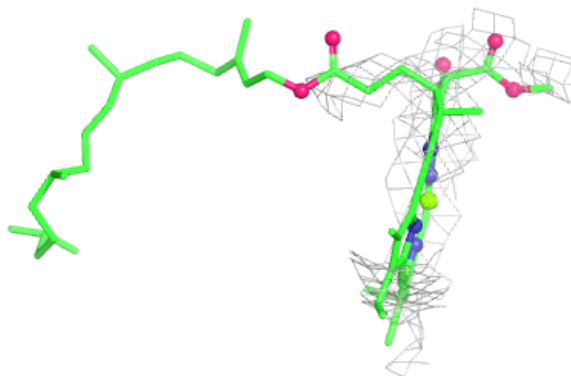


Electron density around CLA B 603:

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

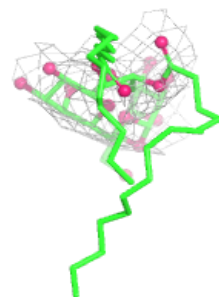
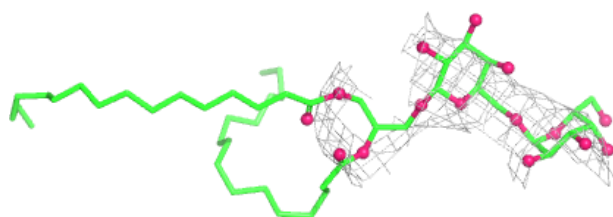
**Electron density around CLA C 506:**

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

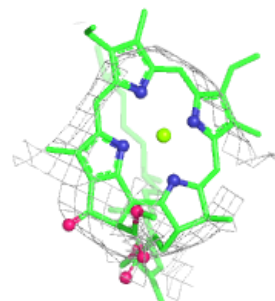
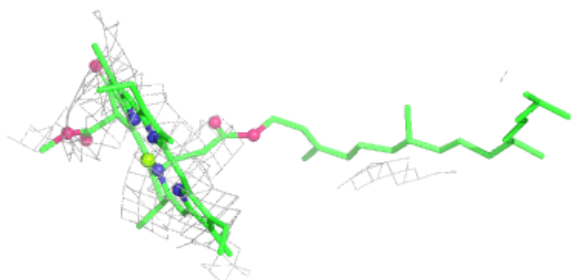
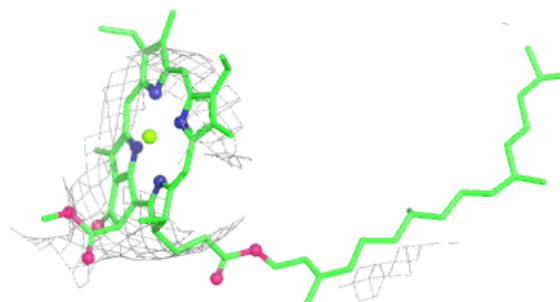


Electron density around DGD H 102:

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

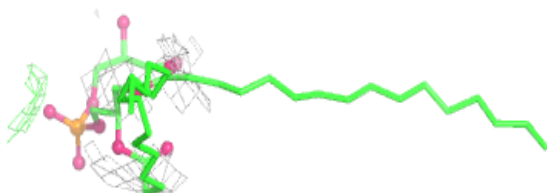
**Electron density around CLA b 610:**

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



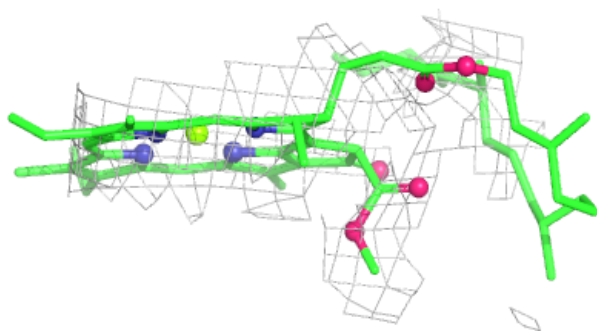
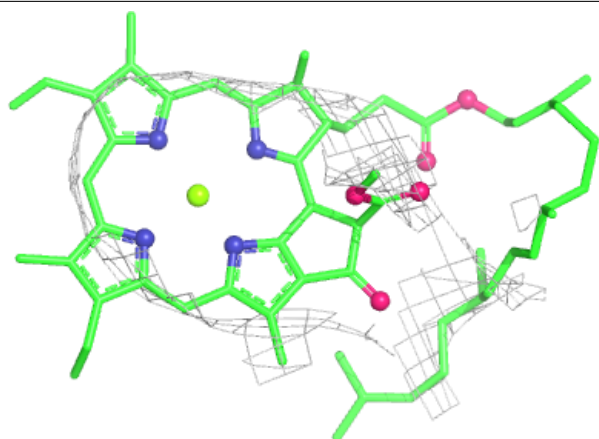
Electron density around LHG B 621:

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



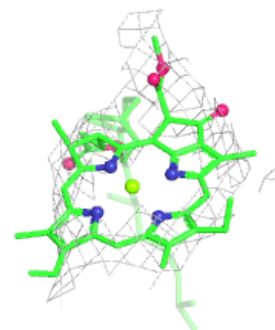
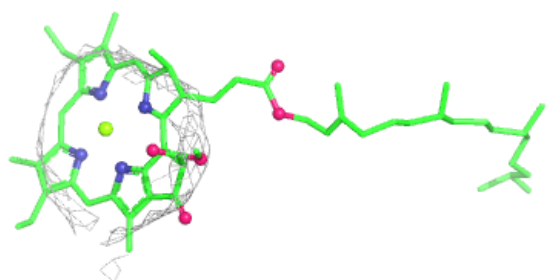
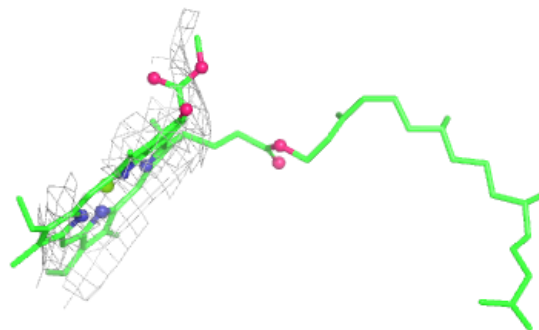
Electron density around CLA b 611:

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

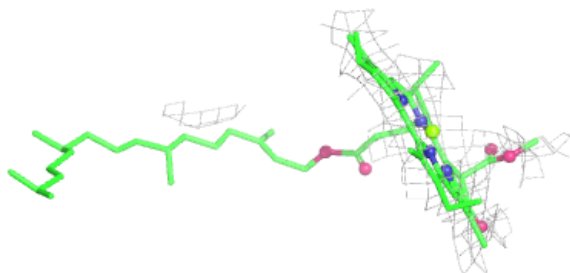
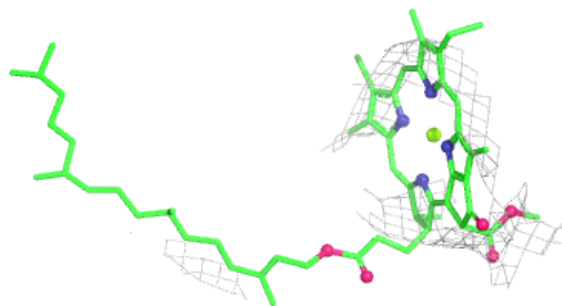


Electron density around CLA d 403:

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

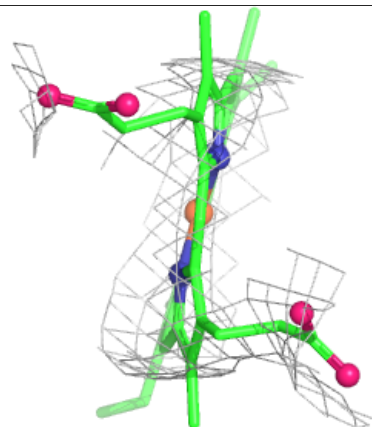
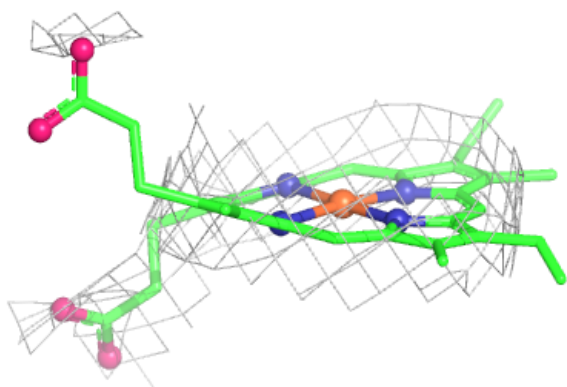
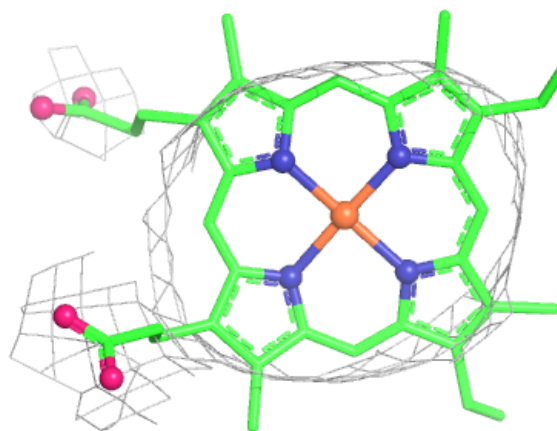
**Electron density around CLA B 610:**

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

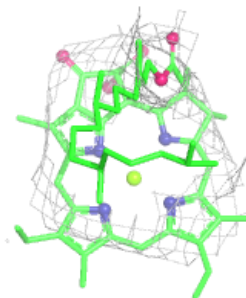
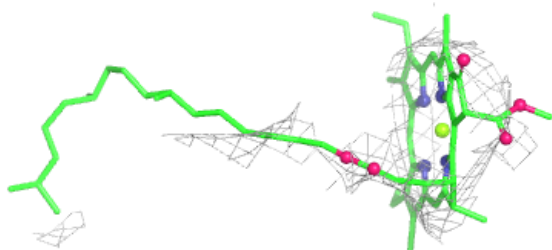
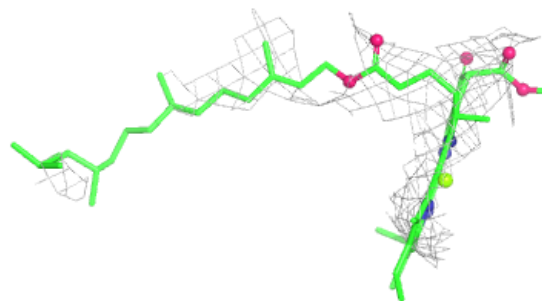


Electron density around HEM E 101:

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

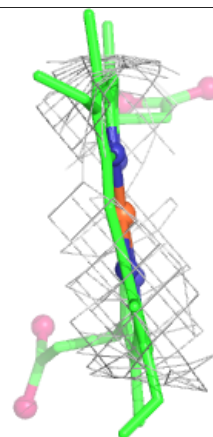
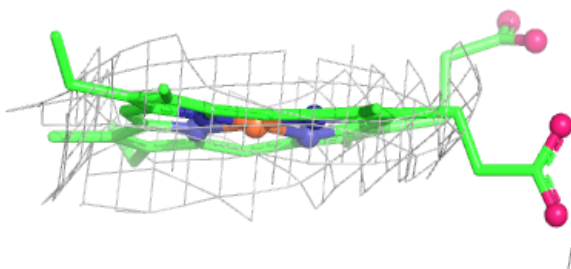
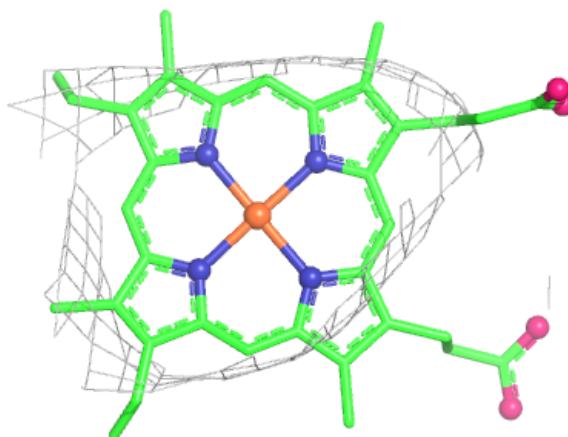
**Electron density around CLA b 606:**

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



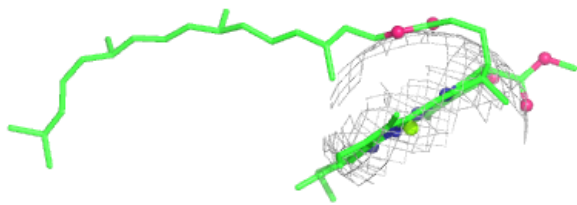
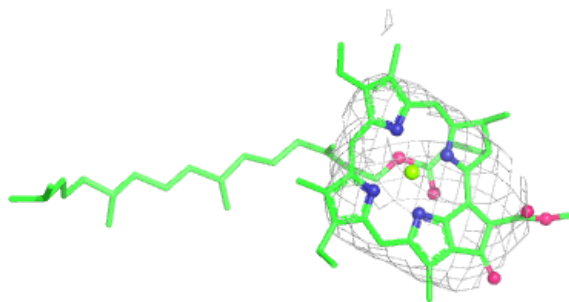
Electron density around HEM v 202:

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



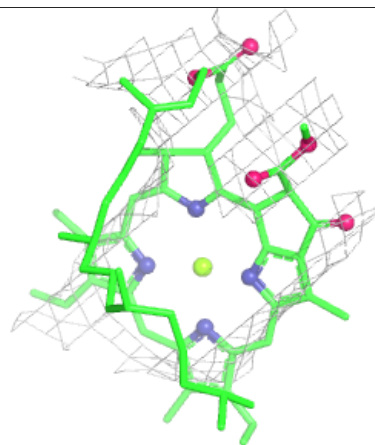
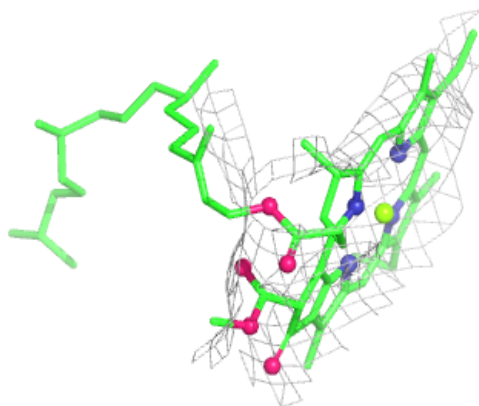
Electron density around CLA b 609:

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



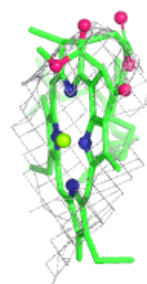
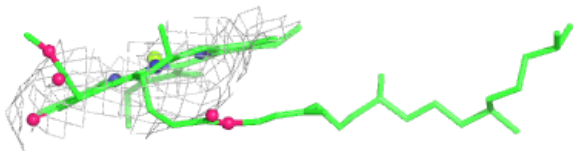
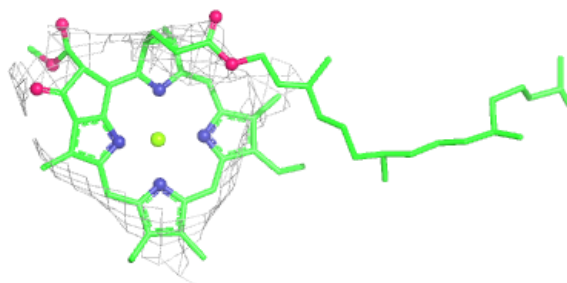
Electron density around CLA B 614:

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

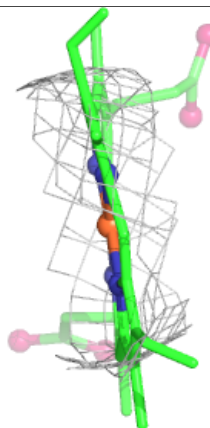
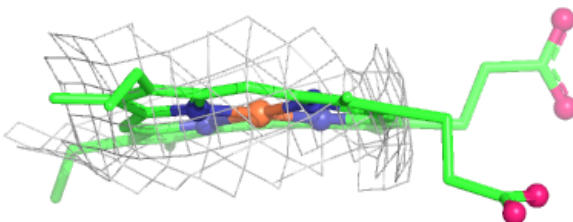
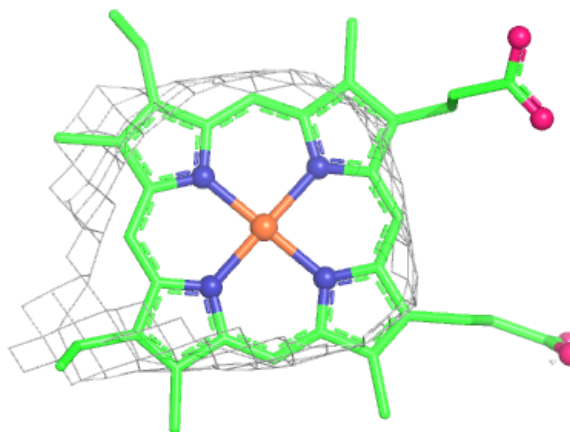


Electron density around CLA b 604:

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

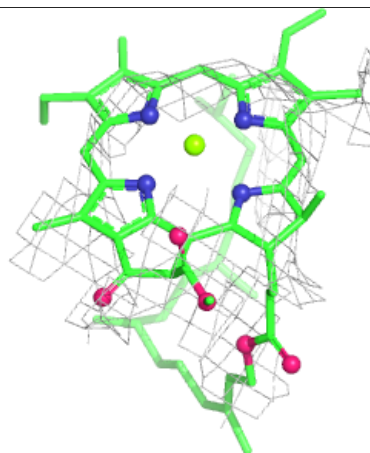
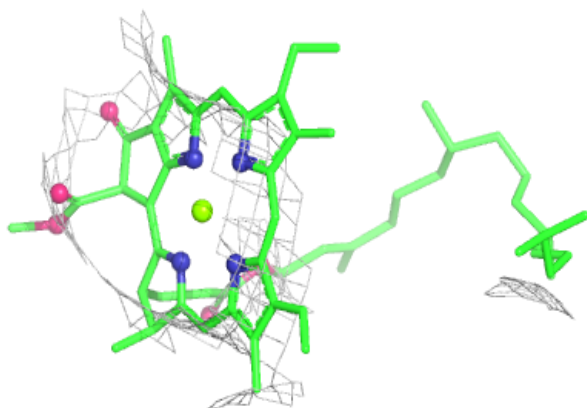
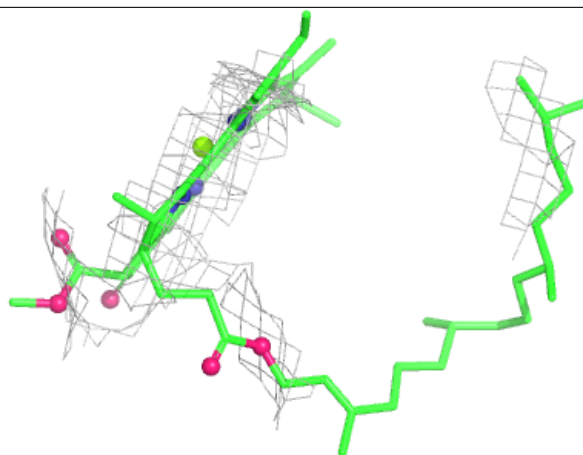
**Electron density around HEM V 202:**

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



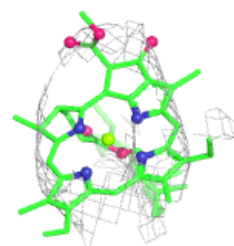
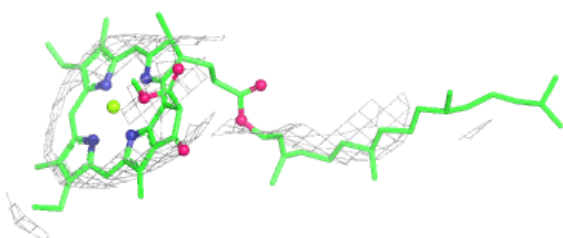
Electron density around CLA B 612:

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

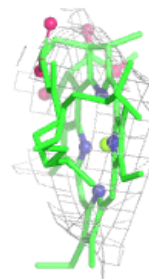
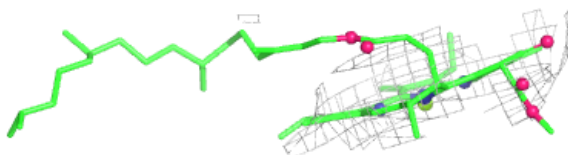
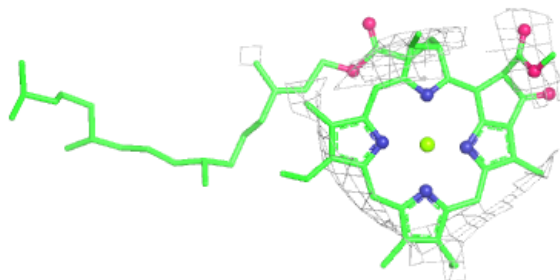


Electron density around CLA C 502:

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

**Electron density around CLA B 604:**

$2mF_o-DF_c$ (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.