



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:56 PM UTC

PDB ID : 4RVY / pdb_00004rvy
Title : Serial Time resolved crystallography of Photosystem II using a femtosecond X-ray laser. The S state after two flashes (S3)
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.; 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 : 2014-11-29
Resolution : 5.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0

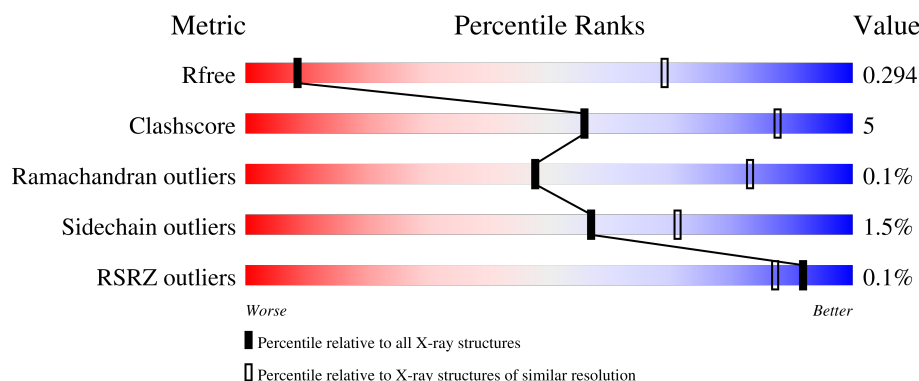
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 Å.

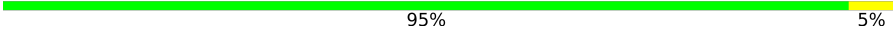
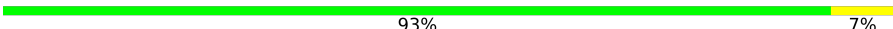
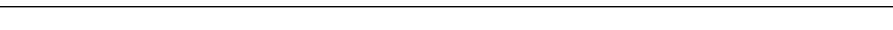
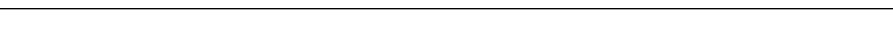
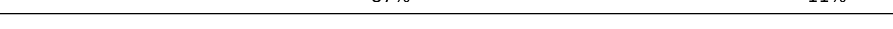
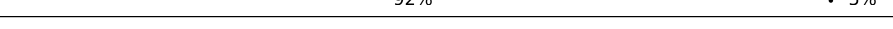
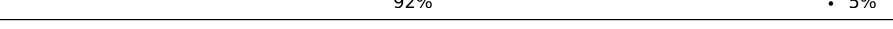
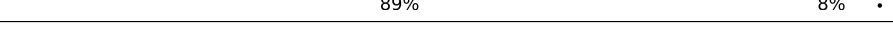
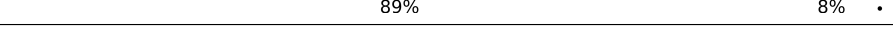
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

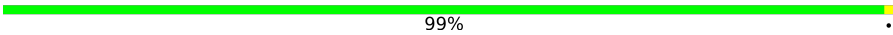
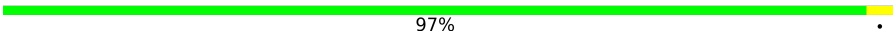
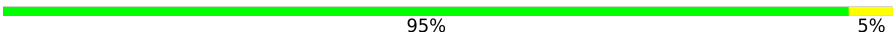
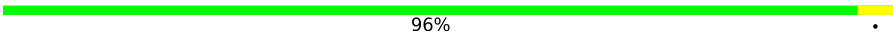
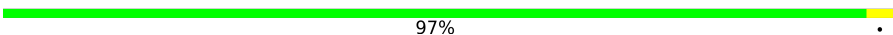
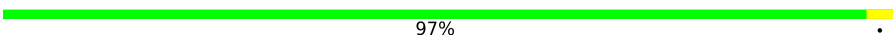
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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	 95% 5%
1	a	334	 93% 7%
2	B	504	 93% 7%
2	b	504	 92% 7%
3	C	461	 92% 6% •
3	c	461	 92% 6% •
4	D	342	 94% 6%
4	d	342	 94% 6%
5	E	81	 94% 6%
5	e	81	 94% 6%
6	F	34	 85% 12% •
6	f	34	 85% 12% •
7	H	65	 92% 6% •
7	h	65	 92% 6% •
8	I	38	 87% 11% •
8	i	38	 87% 11% •
9	J	40	 92% 5% •
9	j	40	 92% 5% •
10	K	37	 89% 8% •
10	k	37	 89% 8% •
11	L	37	 86% 11% •
11	l	37	 84% 14% •
12	M	34	 3% 74% 26%
12	m	34	 74% 26%
13	O	243	 92% 7% •
13	o	243	 91% 8% •

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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	X	39	
17	x	39	
18	Y	29	
18	y	29	
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	CLA	A	603	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	a	603	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	d	401	X	-	-	-
24	BCR	K	102	-	X	-	-
24	BCR	k	102	-	X	-	-
26	CL	u	201	-	-	-	X

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 49594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			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 CP47 reaction center 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 reaction center protein.

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	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	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	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	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	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 X protein.

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

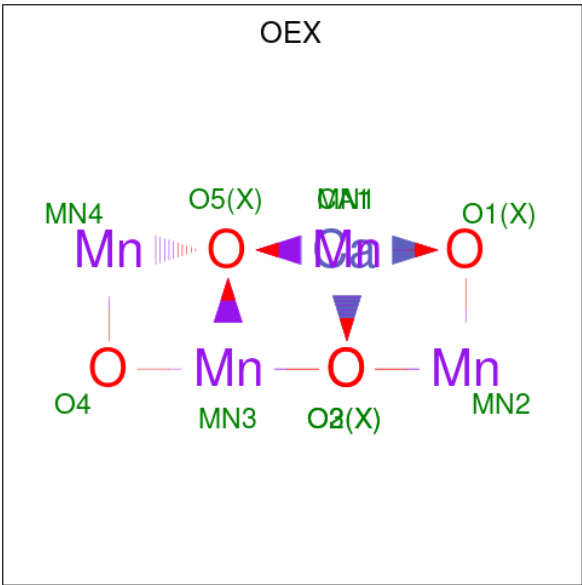
- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

- 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).

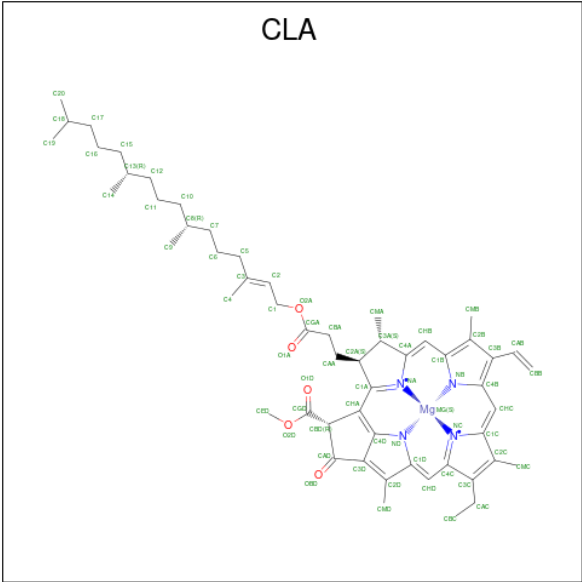


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



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

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

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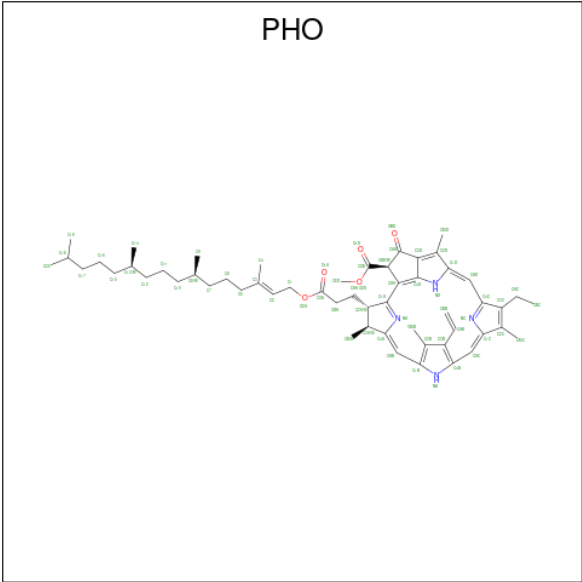
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N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

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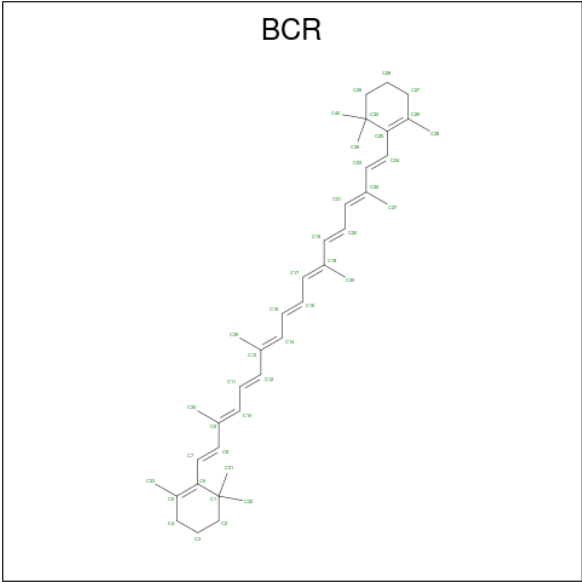
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N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

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



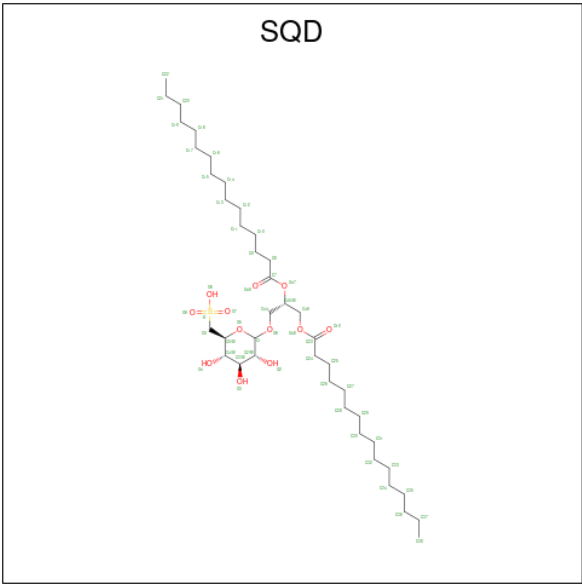
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).

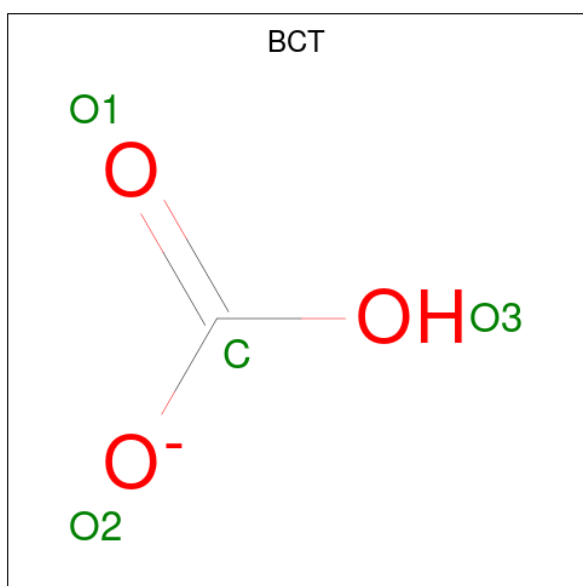


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	S	0	0
			54	41	12	1		
25	a	1	Total	C	O	S	0	0
			54	41	12	1		
25	B	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	D	1	Total	C	O	S	0	0
			43	30	12	1		
25	d	1	Total	C	O	S	0	0
			43	30	12	1		
25	L	1	Total	C	O	S	0	0
			54	41	12	1		
25	l	1	Total	C	O	S	0	0
			54	41	12	1		
25	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 26 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

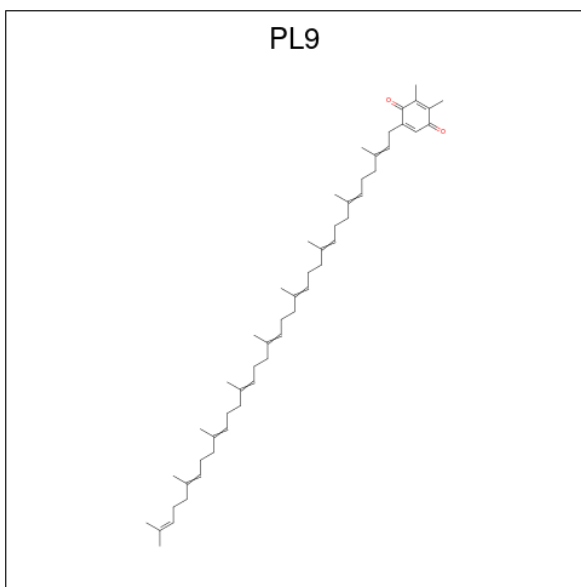
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	2	Total Cl 2 2	0	0
26	a	2	Total Cl 2 2	0	0
26	U	1	Total Cl 1 1	0	0
26	u	1	Total Cl 1 1	0	0

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



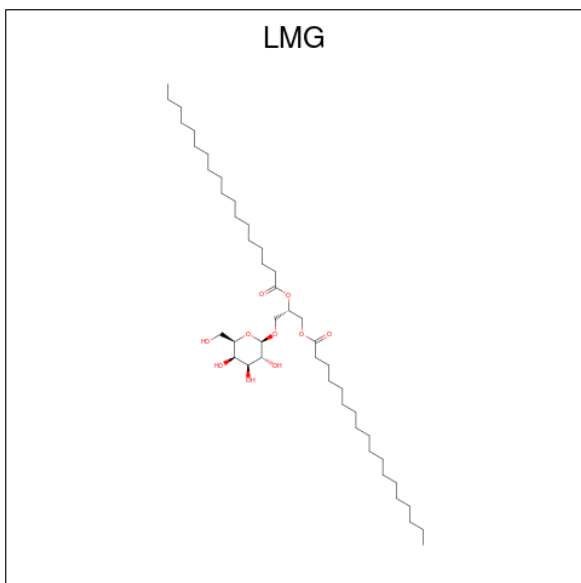
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 4 1 3	0	0
27	a	1	Total C O 4 1 3	0	0

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

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

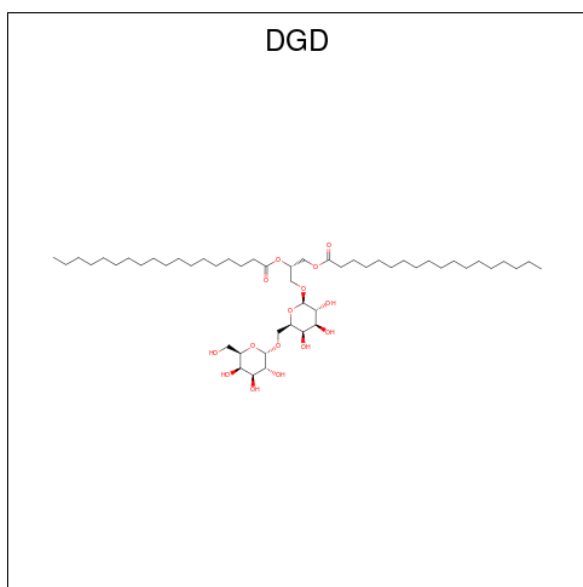


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 51 41 10	0	0
29	a	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	b	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	D	1	Total C O 51 41 10	0	0
29	d	1	Total C O 51 41 10	0	0
29	Z	1	Total C O 37 27 10	0	0
29	z	1	Total C O 37 27 10	0	0

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

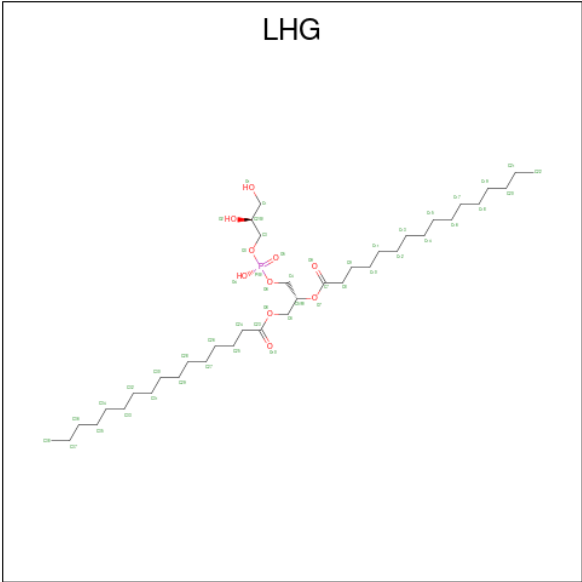
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total Ca 1 1	0	0
30	b	1	Total Ca 1 1	0	0
30	F	1	Total Ca 1 1	0	0
30	f	1	Total Ca 1 1	0	0
30	O	1	Total Ca 1 1	0	0
30	o	1	Total Ca 1 1	0	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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	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	d	1	Total	C	O	0	0
			62	47	15		
31	H	1	Total	C	O	0	0
			62	47	15		
31	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



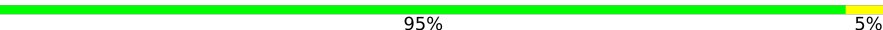
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0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

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

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1

Chain A:  95% 5%

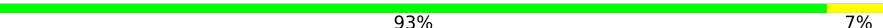


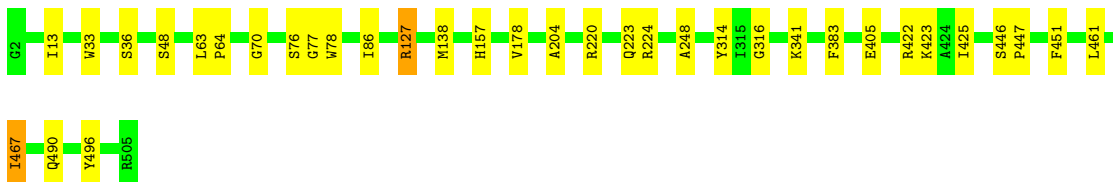
- Molecule 1: Photosystem II protein D1 1

Chain a:  93% 7%



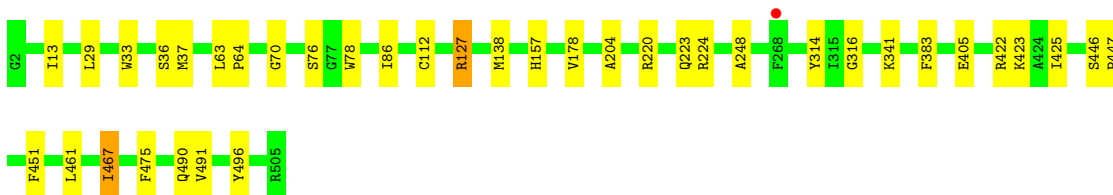
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  93% 7%



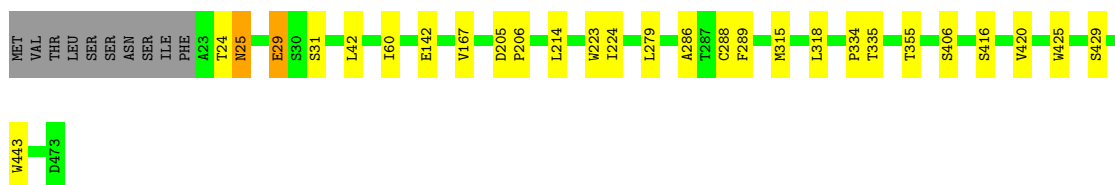
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  92% 7%



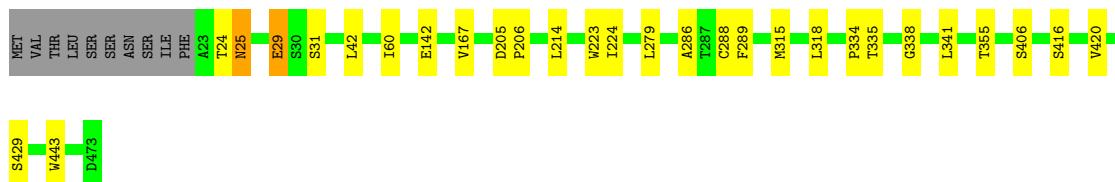
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  92% 6% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 92% 6% •



- Molecule 4: Photosystem II D2 protein

Chain D: 94% 6%



- Molecule 4: Photosystem II D2 protein

Chain d: 94% 6%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 94% 6%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 94% 6%



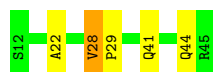
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 85% 12% •



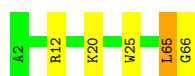
- Molecule 6: Cytochrome b559 subunit beta

Chain f: 85% 12% .



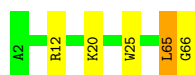
- Molecule 7: Photosystem II reaction center protein H

Chain H: 92% 6% .



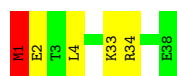
- Molecule 7: Photosystem II reaction center protein H

Chain h: 92% 6% .



- Molecule 8: Photosystem II reaction center protein I

Chain I: 87% 11% .



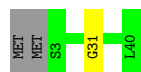
- Molecule 8: Photosystem II reaction center protein I

Chain i: 87% 11% .



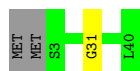
- Molecule 9: Photosystem II reaction center protein J

Chain J: 92% 5% .



- Molecule 9: Photosystem II reaction center protein J

Chain j: 92% 5% .



- Molecule 10: Photosystem II reaction center protein K

Chain K: 89% 8% .



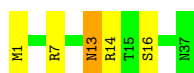
- Molecule 10: Photosystem II reaction center protein K

Chain k: 89% 8% .



- Molecule 11: Photosystem II reaction center protein L

Chain L: 86% 11% .



- Molecule 11: Photosystem II reaction center protein L

Chain l: 84% 14% .



- Molecule 12: Photosystem II reaction center protein M

Chain M: 3% 74% 26% .



- Molecule 12: Photosystem II reaction center protein M

Chain m: 74% 26% .



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 92% 7% .



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 91% 8% .



- Molecule 14: Photosystem II reaction center protein T

Chain T: 77% 20% .



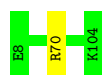
- Molecule 14: Photosystem II reaction center protein T

Chain t: 77% 20% .



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 99% .



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 97% .



- Molecule 16: Cytochrome c-550

Chain V: 95% 5% .



- Molecule 16: Cytochrome c-550

Chain v: 96% .



- Molecule 17: Photosystem II reaction center X protein

Chain X: 92% 8%



- Molecule 17: Photosystem II reaction center X protein

Chain x: 92% 8%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y: 86% 14%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y: 86% 14%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 97% 3%



- Molecule 19: Photosystem II reaction center protein Z

Chain z: 97% 3%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.61Å 228.09Å 308.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.30 – 5.50 102.30 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (102.30-5.50) 100.0 (102.30-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 5.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1336)	Depositor
R, R_{free}	0.281 , 0.291 0.289 , 0.294	Depositor DCC
R_{free} test set	1626 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	357.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 133.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	49594	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.62	0/2705	0.80	0/3689
2	B	0.58	0/4109	0.79	0/5600
2	b	0.58	0/4109	0.79	0/5600
3	C	0.55	0/3599	0.78	0/4900
3	c	0.55	0/3599	0.78	0/4900
4	D	0.61	0/2821	0.78	0/3844
4	d	0.61	0/2821	0.78	0/3844
5	E	0.55	0/681	0.81	0/928
5	e	0.55	0/681	0.81	0/928
6	F	0.69	1/284 (0.4%)	0.73	0/387
6	f	0.68	1/284 (0.4%)	0.74	0/387
7	H	0.58	0/524	0.77	0/713
7	h	0.58	0/524	0.77	0/713
8	I	2.40	2/319 (0.6%)	1.35	3/429 (0.7%)
8	i	2.40	2/319 (0.6%)	1.35	3/429 (0.7%)
9	J	0.59	0/278	0.82	0/376
9	j	0.59	0/278	0.83	0/376
10	K	0.57	0/303	0.81	0/416
10	k	0.57	0/303	0.81	0/416
11	L	0.57	0/311	0.77	0/422
11	l	0.57	0/311	0.77	0/422
12	M	0.60	0/270	0.87	0/367
12	m	0.59	0/270	0.87	0/367
13	O	0.54	0/1896	0.74	0/2571
13	o	0.54	0/1896	0.74	0/2571
14	T	0.56	0/265	0.77	0/359
14	t	0.56	0/265	0.77	0/359
15	U	0.55	0/785	0.74	0/1064
15	u	0.55	0/785	0.74	0/1064
16	V	0.57	0/1085	0.78	0/1473
16	v	0.57	0/1085	0.78	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.53	0/290	0.83	0/392
17	x	0.53	0/290	0.83	0/392
18	Y	0.57	0/216	0.83	0/289
18	y	0.57	0/216	0.83	0/289
19	Z	0.54	0/490	0.87	0/669
19	z	0.54	0/490	0.87	0/669
All	All	0.64	6/42462 (0.0%)	0.80	6/57776 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	1	1
8	i	1	1
All	All	2	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	MET	N-CA	38.97	2.20	1.46
8	I	1	MET	N-CA	38.95	2.20	1.46
8	I	1	MET	CA-C	15.19	1.84	1.52
8	i	1	MET	CA-C	15.18	1.84	1.52
6	F	28	VAL	CA-CB	5.99	1.57	1.54
6	f	28	VAL	CA-CB	5.64	1.57	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	MET	N-CA-CB	-18.88	78.41	110.50
8	I	1	MET	N-CA-CB	-18.85	78.45	110.50
8	I	1	MET	N-CA-C	-12.53	75.92	111.00
8	i	1	MET	N-CA-C	-12.52	75.94	111.00
8	I	1	MET	CB-CA-C	-6.38	97.97	110.10
8	i	1	MET	CB-CA-C	-6.38	97.97	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	I	1	MET	CA

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Mol	Chain	Res	Type	Atom
8	i	1	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	1	MET	Mainchain
8	i	1	MET	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2620	0	2517	15	0
1	a	2620	0	2517	18	0
2	B	3969	0	3828	38	0
2	b	3969	0	3828	35	0
3	C	3486	0	3407	18	0
3	c	3486	0	3407	18	0
4	D	2726	0	2627	18	0
4	d	2726	0	2627	20	0
5	E	662	0	648	3	0
5	e	662	0	648	3	0
6	F	275	0	282	3	0
6	f	275	0	282	3	0
7	H	511	0	532	4	0
7	h	511	0	532	4	0
8	I	312	0	329	16	0
8	i	312	0	329	15	0
9	J	272	0	279	1	0
9	j	272	0	279	1	0
10	K	293	0	305	5	0
10	k	293	0	305	5	0
11	L	304	0	316	8	0
11	l	304	0	316	9	0
12	M	267	0	288	43	0
12	m	267	0	287	43	0
13	O	1865	0	1838	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	o	1865	0	1838	20	0
14	T	256	0	262	7	0
14	t	256	0	262	9	0
15	U	774	0	773	0	0
15	u	774	0	773	0	7
16	V	1064	0	1073	10	7
16	v	1064	0	1073	10	0
17	X	287	0	317	3	0
17	x	287	0	317	3	0
18	Y	215	0	246	2	0
18	y	215	0	246	2	0
19	Z	479	0	516	0	0
19	z	479	0	516	0	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	195	0	216	8	0
22	B	1040	0	1152	23	0
22	C	845	0	936	23	0
22	D	195	0	216	6	0
22	a	195	0	216	7	0
22	b	1040	0	1152	19	0
22	c	845	0	936	22	0
22	d	195	0	216	6	0
23	A	128	0	148	4	0
23	a	128	0	148	4	0
24	A	40	0	48	0	0
24	B	120	0	140	6	0
24	C	80	0	93	0	0
24	D	40	0	48	3	0
24	H	40	0	46	1	0
24	K	80	0	93	1	0
24	T	80	0	95	3	0
24	a	40	0	48	1	0
24	b	80	0	92	3	0
24	c	80	0	93	0	0
24	d	40	0	48	3	0
24	h	40	0	46	0	0
24	k	80	0	93	1	0
24	t	40	0	47	7	0
25	A	54	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	54	0	78	4	0
25	D	43	0	53	0	0
25	L	54	0	34	6	0
25	a	54	0	78	2	0
25	b	108	0	112	7	0
25	d	43	0	53	0	0
25	l	108	0	59	14	0
26	A	2	0	0	0	0
26	U	1	0	0	0	0
26	a	2	0	0	0	0
26	u	1	0	0	0	0
27	A	4	0	0	0	0
27	a	4	0	0	0	0
28	A	55	0	80	8	0
28	D	55	0	80	0	0
28	a	55	0	80	8	0
28	d	55	0	80	0	0
29	A	51	0	72	3	0
29	B	51	0	72	3	0
29	C	102	0	144	1	0
29	D	51	0	72	2	0
29	Z	37	0	44	1	0
29	a	51	0	72	3	0
29	b	51	0	72	3	0
29	c	102	0	144	1	0
29	d	51	0	72	2	0
29	z	37	0	44	1	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	C	186	0	246	5	0
31	D	62	0	82	3	0
31	H	62	0	82	1	0
31	c	186	0	246	5	0
31	d	62	0	82	3	0
31	h	62	0	82	1	0
32	D	147	0	222	13	0
32	E	42	0	57	1	0
32	L	49	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	d	147	0	222	12	0
32	e	42	0	57	2	0
32	l	49	0	74	0	0
33	F	43	0	30	1	0
33	V	43	0	30	9	0
33	f	43	0	30	1	0
33	v	43	0	30	9	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	49594	0	50450	474	7

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 5.

All (474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:16:LEU:HD21	12:m:16:LEU:CD2	1.23	1.60
12:M:16:LEU:CD2	12:m:16:LEU:HD21	1.36	1.56
8:i:1:MET:C	8:i:1:MET:CA	1.84	1.49
16:V:37:CYS:SG	33:V:201:HEM:HAB	1.52	1.48
16:v:37:CYS:SG	33:v:201:HEM:HAB	1.52	1.48
8:I:1:MET:C	8:I:1:MET:CA	1.84	1.47
16:V:37:CYS:SG	33:V:201:HEM:CAB	2.02	1.47
16:v:40:CYS:SG	33:v:201:HEM:CAC	2.04	1.46
16:v:37:CYS:SG	33:v:201:HEM:CAB	2.03	1.45
16:V:40:CYS:SG	33:V:201:HEM:CAC	2.04	1.44
16:v:40:CYS:SG	33:v:201:HEM:HAC	1.57	1.44
16:V:40:CYS:SG	33:V:201:HEM:HAC	1.57	1.41
8:i:1:MET:HG2	8:i:1:MET:N	1.37	1.35
8:I:1:MET:CG	8:I:1:MET:N	1.89	1.35
8:I:1:MET:N	8:I:1:MET:HG2	1.37	1.35
8:i:1:MET:N	8:i:1:MET:CG	1.89	1.33
12:M:16:LEU:CD2	12:m:16:LEU:CD2	2.01	1.22
1:A:214:MET:HG2	28:A:613:PL9:H102	1.20	1.17
1:a:214:MET:HG2	28:a:613:PL9:H102	1.20	1.15
12:M:16:LEU:HD22	12:m:16:LEU:HD11	1.27	1.11
12:M:16:LEU:HD13	12:m:16:LEU:HD13	1.37	1.07
12:M:16:LEU:HD21	12:m:16:LEU:HD22	1.33	1.05
8:i:1:MET:CA	8:i:1:MET:N	2.20	1.04
8:I:1:MET:CA	8:I:1:MET:N	2.20	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:16:LEU:HD22	12:m:16:LEU:CD1	1.91	0.99
10:k:17:ILE:HD13	10:k:17:ILE:H	1.29	0.97
10:K:17:ILE:H	10:K:17:ILE:HD13	1.29	0.97
8:I:1:MET:HG2	8:I:1:MET:H1	0.87	0.97
12:M:20:VAL:HG11	12:m:20:VAL:CG2	1.96	0.95
8:i:1:MET:HG2	8:i:1:MET:H1	0.77	0.93
32:d:409:LHG:H132	32:d:409:LHG:H372	1.48	0.93
2:B:76:SER:OG	13:o:112:GLY:CA	2.18	0.92
32:D:409:LHG:H132	32:D:409:LHG:H372	1.48	0.91
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.35	0.91
2:b:127:ARG:HH11	2:b:127:ARG:HG3	1.35	0.90
1:a:214:MET:HG2	28:a:613:PL9:C10	2.02	0.88
1:A:214:MET:HG2	28:A:613:PL9:C10	2.02	0.88
25:l:101:SQD:H342	14:t:12:CYS:HB3	1.55	0.87
11:L:14:ARG:HD3	25:L:101:SQD:H241	1.57	0.86
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.56	0.86
22:b:615:CLA:H43	25:b:621:SQD:H121	1.58	0.85
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.56	0.85
12:M:16:LEU:HD11	12:m:16:LEU:HD22	1.57	0.83
32:d:409:LHG:H352	32:d:409:LHG:H151	1.59	0.83
32:D:409:LHG:H352	32:D:409:LHG:H151	1.59	0.82
8:I:1:MET:N	8:I:1:MET:CB	2.42	0.82
8:i:1:MET:N	8:i:1:MET:CB	2.42	0.82
12:M:20:VAL:CG2	12:m:20:VAL:HG11	2.10	0.81
12:M:16:LEU:HD22	12:m:16:LEU:HD21	1.59	0.81
8:I:1:MET:CG	8:I:1:MET:H2	1.73	0.80
8:I:1:MET:C	8:I:1:MET:CB	2.56	0.78
8:i:1:MET:N	8:i:1:MET:SD	2.43	0.78
8:i:1:MET:HE3	8:i:4:LEU:HB2	1.65	0.78
22:B:615:CLA:H43	25:l:102:SQD:H121	1.66	0.78
8:i:1:MET:C	8:i:1:MET:CB	2.56	0.78
8:I:1:MET:HE3	8:I:4:LEU:HB2	1.65	0.77
12:M:16:LEU:HD22	12:m:16:LEU:CD2	2.13	0.77
2:B:76:SER:OG	13:o:112:GLY:HA2	1.85	0.77
12:M:33:GLN:HB2	12:m:33:GLN:HB2	1.65	0.77
25:b:621:SQD:H62	11:l:7:ARG:HH21	1.48	0.76
11:L:7:ARG:HH21	25:l:102:SQD:H62	1.52	0.75
8:i:1:MET:CA	8:i:2:GLU:N	2.50	0.75
12:M:20:VAL:HG11	12:m:20:VAL:HG21	1.69	0.73
13:O:57:LYS:O	13:O:58:ASN:HB2	1.87	0.73
12:M:16:LEU:CD1	12:m:16:LEU:HD13	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:1:MET:N	8:I:1:MET:SD	2.43	0.72
32:D:409:LHG:H112	32:D:409:LHG:H382	1.72	0.72
32:d:409:LHG:H382	32:d:409:LHG:H112	1.72	0.72
12:M:16:LEU:HD21	12:m:16:LEU:HD21	0.72	0.72
13:o:57:LYS:O	13:o:58:ASN:HB2	1.87	0.72
8:I:1:MET:CA	8:I:2:GLU:N	2.50	0.72
12:M:16:LEU:CD2	12:m:16:LEU:HD22	2.03	0.71
12:M:16:LEU:CD2	12:m:16:LEU:CD1	2.69	0.71
25:B:601:SQD:H252	24:t:101:BCR:H373	1.73	0.70
12:M:16:LEU:CD1	12:m:16:LEU:HD22	2.20	0.70
2:B:77:GLY:C	13:o:111:ALA:HB1	2.17	0.70
8:I:1:MET:C	8:I:1:MET:N	2.50	0.70
8:i:1:MET:C	8:i:1:MET:N	2.50	0.70
16:V:37:CYS:SG	33:V:201:HEM:C3B	2.85	0.70
1:a:214:MET:CG	28:a:613:PL9:H102	2.12	0.69
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.75	0.69
16:v:37:CYS:SG	33:v:201:HEM:C3B	2.85	0.68
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.75	0.68
22:B:615:CLA:H18	29:B:620:LMG:H421	1.76	0.67
3:C:286:ALA:HB2	22:C:502:CLA:HMD1	1.75	0.67
12:M:31:SER:OG	12:m:28:GLN:O	2.09	0.67
1:A:214:MET:CG	28:A:613:PL9:H102	2.12	0.67
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.77	0.67
4:d:24:ARG:HD3	17:x:37:VAL:HG22	1.76	0.67
11:L:7:ARG:NH2	25:l:102:SQD:H62	2.09	0.67
22:c:509:CLA:HMB1	22:c:509:CLA:HBB1	1.76	0.67
10:k:17:ILE:HD13	10:k:17:ILE:N	2.08	0.67
25:b:621:SQD:H62	11:l:7:ARG:NH2	2.11	0.66
22:C:509:CLA:HBB1	22:C:509:CLA:HMB1	1.76	0.66
22:b:615:CLA:H18	29:b:619:LMG:H421	1.76	0.66
2:B:76:SER:OG	13:o:112:GLY:C	2.39	0.65
16:V:40:CYS:SG	33:V:201:HEM:CB C	2.81	0.65
16:v:40:CYS:SG	33:v:201:HEM:C3C	2.90	0.64
2:B:33:TRP:CD1	24:B:622:BCR:H381	2.32	0.64
22:C:506:CLA:HMC2	22:C:507:CLA:H102	1.79	0.64
22:c:506:CLA:HMC2	22:c:507:CLA:H102	1.79	0.64
11:l:14:ARG:HD3	25:l:101:SQD:H241	1.80	0.64
16:v:40:CYS:SG	33:v:201:HEM:CB C	2.81	0.63
29:z:101:LMG:O2	29:z:101:LMG:HC71	1.99	0.63
16:V:40:CYS:SG	33:V:201:HEM:C3C	2.90	0.63
29:Z:101:LMG:O2	29:Z:101:LMG:HC71	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:409:LHG:H112	32:d:409:LHG:C38	2.30	0.61
3:c:286:ALA:HB2	22:c:502:CLA:HMD2	1.80	0.61
10:K:17:ILE:HD13	10:K:17:ILE:N	2.08	0.61
25:L:101:SQD:H45	14:T:23:PHE:CD1	2.35	0.61
32:D:409:LHG:H112	32:D:409:LHG:C38	2.30	0.60
24:d:404:BCR:H383	29:d:406:LMG:H172	1.83	0.60
3:C:167:VAL:HG21	22:C:512:CLA:HBB	1.83	0.60
3:c:167:VAL:HG21	22:c:512:CLA:HBB	1.84	0.60
2:B:33:TRP:HD1	24:B:622:BCR:H381	1.66	0.60
32:d:409:LHG:H372	32:d:409:LHG:C13	2.29	0.60
22:c:510:CLA:H43	32:d:409:LHG:H383	1.84	0.60
22:a:603:CLA:HBB1	22:a:603:CLA:HMB3	1.84	0.60
22:C:510:CLA:H43	32:D:409:LHG:H383	1.84	0.59
22:B:606:CLA:C14	22:B:611:CLA:HED2	2.33	0.59
11:L:13:ASN:ND2	11:L:16:SER:H	2.01	0.59
12:M:20:VAL:HG13	12:m:20:VAL:HG13	1.83	0.59
24:D:404:BCR:H383	29:D:406:LMG:H172	1.83	0.59
22:B:611:CLA:HHC	22:B:611:CLA:HBB1	1.85	0.59
28:A:613:PL9:H502	4:D:39:PRO:HG3	1.85	0.58
28:a:613:PL9:H502	4:d:39:PRO:HG3	1.85	0.58
2:B:76:SER:O	13:o:111:ALA:HA	2.03	0.58
22:b:606:CLA:C14	22:b:611:CLA:HED2	2.33	0.58
11:l:13:ASN:ND2	11:l:16:SER:H	2.01	0.58
22:A:603:CLA:HBB1	22:A:603:CLA:HMB3	1.84	0.58
2:b:33:TRP:CD1	24:b:622:BCR:H381	2.39	0.58
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.85	0.58
25:l:101:SQD:O8	25:l:102:SQD:O8	0.60	0.58
2:B:467:ILE:HG13	4:D:126:MET:HE1	1.85	0.57
22:b:611:CLA:HHC	22:b:611:CLA:HBB1	1.85	0.57
22:b:616:CLA:H2	22:b:617:CLA:HBB2	1.87	0.57
12:M:28:GLN:HA	12:m:28:GLN:CB	2.35	0.57
22:B:616:CLA:H2	22:B:617:CLA:HBB2	1.87	0.57
32:D:409:LHG:H372	32:D:409:LHG:C13	2.29	0.56
12:M:31:SER:O	12:m:32:GLN:HG2	2.05	0.56
2:B:76:SER:OG	13:o:112:GLY:N	2.38	0.56
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.40	0.56
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.12	0.56
2:b:127:ARG:HG3	2:b:127:ARG:NH1	2.12	0.56
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.42	0.55
1:A:183:MET:HA	22:A:603:CLA:HMD1	1.89	0.55
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:1:MET:C	8:i:1:MET:SD	2.90	0.55
2:b:76:SER:OG	13:O:112:GLY:CA	2.54	0.55
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.42	0.55
3:C:279:LEU:HD22	22:C:509:CLA:HED2	1.89	0.55
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.89	0.55
3:c:279:LEU:HD22	22:c:509:CLA:HED2	1.89	0.55
8:I:1:MET:C	8:I:1:MET:SD	2.90	0.55
10:K:17:ILE:H	10:K:17:ILE:CD1	2.00	0.55
24:d:404:BCR:H313	31:d:410:DGD:HA91	1.89	0.55
16:v:37:CYS:SG	33:v:201:HEM:CBB	2.88	0.54
11:l:13:ASN:C	11:l:13:ASN:HD22	2.15	0.54
12:M:16:LEU:HD22	12:m:16:LEU:CG	2.37	0.54
1:a:183:MET:HA	22:a:603:CLA:HMD1	1.89	0.54
22:b:614:CLA:H122	29:b:619:LMG:H232	1.89	0.54
11:L:13:ASN:C	11:L:13:ASN:HD22	2.15	0.54
12:M:28:GLN:HA	12:m:28:GLN:HA	1.90	0.54
22:B:614:CLA:H122	29:B:620:LMG:H232	1.88	0.54
3:c:443:TRP:CZ2	22:c:508:CLA:HMD1	2.43	0.54
22:c:501:CLA:C4D	22:c:503:CLA:H2	2.38	0.54
7:h:65:LEU:HD12	7:h:66:GLY:H	1.73	0.54
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.89	0.53
25:b:621:SQD:C46	25:L:101:SQD:O49	2.53	0.53
7:H:65:LEU:HD12	7:H:66:GLY:H	1.73	0.53
12:M:16:LEU:CD2	12:m:16:LEU:CG	2.83	0.53
22:C:501:CLA:C4D	22:C:503:CLA:H2	2.38	0.53
24:D:404:BCR:H313	31:D:410:DGD:HA91	1.89	0.53
12:M:28:GLN:O	12:m:31:SER:OG	2.17	0.53
12:M:20:VAL:CG1	12:m:20:VAL:HG22	2.33	0.53
25:l:101:SQD:H45	14:t:23:PHE:CD1	2.44	0.53
25:b:621:SQD:H292	25:L:101:SQD:H311	1.83	0.53
25:B:601:SQD:C25	24:t:101:BCR:H373	2.39	0.53
2:b:446:SER:HB2	2:b:447:PRO:CD	2.38	0.53
3:C:443:TRP:CZ2	22:C:508:CLA:HMD1	2.43	0.52
4:D:123:ILE:HD11	31:H:102:DGD:HAE1	1.92	0.52
2:B:446:SER:HB2	2:B:447:PRO:CD	2.38	0.52
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.92	0.52
13:o:40:ILE:HG12	13:o:243:ILE:HD13	1.92	0.52
22:a:603:CLA:CBD	22:d:402:CLA:HAC2	2.40	0.52
2:B:76:SER:O	13:o:112:GLY:N	2.38	0.52
22:c:510:CLA:C4	32:d:409:LHG:H383	2.40	0.52
4:d:123:ILE:HD11	31:h:102:DGD:HAE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:614:CLA:HMB1	22:b:614:CLA:HBB1	1.91	0.52
25:l:101:SQD:O6	14:t:23:PHE:CD1	2.63	0.52
16:V:37:CYS:SG	33:V:201:HEM:CBB	2.88	0.52
1:a:84:PRO:HA	1:a:112:TYR:CG	2.45	0.52
12:M:20:VAL:CG1	12:m:20:VAL:CG2	2.81	0.52
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.45	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.51
8:I:1:MET:CE	8:I:4:LEU:HB2	2.37	0.51
2:B:248:ALA:HA	22:B:604:CLA:H42	1.92	0.51
25:B:601:SQD:H252	24:t:101:BCR:C37	2.39	0.51
2:b:37:MET:CE	24:b:622:BCR:H282	2.41	0.51
22:C:508:CLA:H92	32:D:409:LHG:H371	1.93	0.51
8:i:1:MET:CE	8:i:4:LEU:HB2	2.37	0.51
25:L:101:SQD:H342	14:T:12:CYS:HB3	1.90	0.51
22:A:603:CLA:CB D	22:D:402:CLA:HAC2	2.40	0.51
22:C:510:CLA:C4	32:D:409:LHG:H383	2.40	0.51
22:d:403:CLA:H192	17:x:15:LEU:HD11	1.93	0.51
22:c:508:CLA:H92	32:d:409:LHG:H371	1.93	0.51
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.45	0.51
28:A:613:PL9:H403	6:F:22:ALA:HB2	1.93	0.51
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.93	0.51
3:C:42:LEU:HD21	22:C:511:CLA:H2A	1.93	0.51
22:B:614:CLA:HBB1	22:B:614:CLA:HMB1	1.91	0.50
3:c:42:LEU:HD21	22:c:511:CLA:H2A	1.93	0.50
2:b:248:ALA:HA	22:b:604:CLA:H42	1.92	0.50
25:l:102:SQD:C1	25:l:102:SQD:H462	2.41	0.50
28:a:613:PL9:H403	6:f:22:ALA:HB2	1.93	0.50
29:b:619:LMG:H242	4:d:284:ILE:HD13	1.94	0.50
11:l:13:ASN:HD22	11:l:16:SER:H	1.60	0.50
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.47	0.50
2:b:76:SER:OG	13:O:112:GLY:HA2	2.12	0.50
11:L:7:ARG:HD2	25:l:102:SQD:O8	2.11	0.50
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.47	0.50
2:b:36:SER:OG	24:b:618:BCR:H362	2.12	0.49
29:B:620:LMG:H242	4:D:284:ILE:HD13	1.94	0.49
2:b:341:LYS:HA	2:b:405:GLU:HG2	1.94	0.49
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.93	0.49
22:D:402:CLA:HMB1	22:D:402:CLA:HBB1	1.94	0.49
22:D:403:CLA:H192	17:X:15:LEU:HD11	1.93	0.49
2:B:48:SER:O	13:o:57:LYS:HE3	2.13	0.49
2:B:422:ARG:O	2:B:425:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:LYS:HA	2:B:405:GLU:HG2	1.94	0.49
22:B:604:CLA:HAB	22:B:606:CLA:H171	1.95	0.49
32:D:409:LHG:H132	32:D:409:LHG:C37	2.33	0.49
5:E:82:GLN:C	5:E:84:LYS:H	2.21	0.49
3:C:60:ILE:HG22	22:C:503:CLA:HHD	1.95	0.49
2:B:36:SER:OG	24:B:619:BCR:H362	2.12	0.49
2:b:29:LEU:HD21	25:b:621:SQD:H191	1.95	0.49
22:d:402:CLA:HMB1	22:d:402:CLA:HBB1	1.94	0.49
31:c:517:DGD:HB22	29:c:519:LMG:H302	1.95	0.49
31:C:517:DGD:HB22	29:C:519:LMG:H302	1.95	0.48
18:Y:38:LEU:O	18:Y:42:ARG:HD3	2.13	0.48
32:D:409:LHG:H382	32:D:409:LHG:C11	2.42	0.48
11:L:13:ASN:HD22	11:L:16:SER:H	1.60	0.48
11:l:18:TYR:OH	25:l:101:SQD:H242	2.13	0.48
3:c:60:ILE:HG22	22:c:503:CLA:HHD	1.95	0.48
22:b:615:CLA:H171	14:T:8:PHE:CE1	2.48	0.48
18:y:38:LEU:O	18:y:42:ARG:HD3	2.13	0.48
12:M:32:GLN:HG2	12:m:31:SER:O	2.13	0.48
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.96	0.48
13:O:49:THR:OG1	13:O:236:GLN:HB2	2.14	0.48
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.96	0.47
22:b:604:CLA:HAB	22:b:606:CLA:H171	1.95	0.47
2:b:422:ARG:O	2:b:425:ILE:HG12	2.13	0.47
25:b:621:SQD:H461	25:L:101:SQD:O49	2.13	0.47
12:M:16:LEU:CG	12:m:16:LEU:HD22	2.45	0.47
13:o:49:THR:OG1	13:o:236:GLN:HB2	2.14	0.47
29:A:614:LMG:H291	3:C:214:LEU:O	2.14	0.47
22:B:615:CLA:H151	14:t:8:PHE:HE1	1.79	0.47
3:c:25:ASN:HD21	3:c:31:SER:HA	1.79	0.47
24:K:102:BCR:H24C	24:K:102:BCR:H371	1.70	0.47
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.50	0.47
3:C:29:GLU:CD	3:C:29:GLU:H	2.22	0.47
23:A:606:PHO:HHD	23:A:606:PHO:HBC2	1.97	0.47
3:c:288:CYS:SG	31:c:516:DGD:HB32	2.55	0.47
5:e:82:GLN:C	5:e:84:LYS:H	2.21	0.47
3:C:288:CYS:SG	31:C:516:DGD:HB32	2.55	0.47
4:d:272:LEU:C	4:d:272:LEU:HD23	2.40	0.47
11:l:18:TYR:OH	25:l:101:SQD:C24	2.63	0.47
25:l:101:SQD:H311	25:l:102:SQD:H341	1.29	0.47
13:O:42:ARG:O	13:O:241:ALA:HA	2.15	0.47
14:t:18:PHE:HE1	24:t:101:BCR:H381	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:200:LEU:HG	31:c:518:DGD:HAT2	1.97	0.47
2:b:112:CYS:HG	14:T:18:PHE:HZ	1.59	0.47
13:o:42:ARG:O	13:o:241:ALA:HA	2.15	0.47
23:a:606:PHO:HBC2	23:a:606:PHO:HHD	1.97	0.46
2:b:127:ARG:HH11	2:b:127:ARG:CG	2.18	0.46
3:C:25:ASN:HD21	3:C:31:SER:HA	1.79	0.46
3:c:29:GLU:CD	3:c:29:GLU:H	2.22	0.46
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.46
10:k:17:ILE:H	10:k:17:ILE:CD1	2.00	0.46
24:B:618:BCR:H24C	24:B:618:BCR:H371	1.83	0.46
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.98	0.46
32:d:409:LHG:H382	32:d:409:LHG:C11	2.42	0.46
11:L:14:ARG:HB3	14:T:25:GLU:HG2	1.97	0.46
1:A:63:ILE:HB	3:C:335:THR:HG21	1.97	0.46
3:C:429:SER:HB3	31:C:517:DGD:HBT2	1.98	0.46
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.98	0.46
4:d:27:PHE:CD1	32:e:101:LHG:HC12	2.51	0.46
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.98	0.46
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.98	0.46
4:D:272:LEU:C	4:D:272:LEU:HD23	2.40	0.46
2:b:490:GLN:HA	2:b:496:TYR:CE2	2.50	0.46
4:D:27:PHE:CD1	32:E:101:LHG:HC12	2.51	0.46
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.16	0.46
29:a:614:LMG:H291	3:c:214:LEU:O	2.14	0.46
22:C:508:CLA:HMB3	22:C:508:CLA:HBB1	1.97	0.46
22:b:617:CLA:HED2	22:b:617:CLA:H43	1.98	0.45
1:A:200:LEU:HG	31:C:518:DGD:HAT2	1.97	0.45
22:A:607:CLA:H162	22:A:607:CLA:H122	1.76	0.45
22:B:611:CLA:H152	22:B:611:CLA:OBD	2.16	0.45
22:b:611:CLA:H152	22:b:611:CLA:OBD	2.16	0.45
3:c:223:TRP:CG	3:c:224:ILE:H	2.35	0.45
11:l:14:ARG:HB3	14:t:25:GLU:HG2	1.97	0.45
24:T:102:BCR:H24C	24:T:102:BCR:H371	1.78	0.45
24:t:101:BCR:H24C	24:t:101:BCR:H371	1.78	0.45
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.51	0.45
22:c:510:CLA:HBC3	22:c:510:CLA:H192	1.99	0.45
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.51	0.45
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.16	0.45
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.81	0.45
13:o:142:PHE:HB2	13:o:199:LEU:HB2	1.98	0.45
1:a:63:ILE:HB	3:c:335:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:429:SER:HB3	31:c:517:DGD:HBT2	1.98	0.45
22:c:508:CLA:HMB3	22:c:508:CLA:HBB1	1.97	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.45
13:o:58:ASN:HA	13:o:60:ARG:HH21	1.80	0.45
13:o:180:GLU:CD	13:o:180:GLU:H	2.24	0.45
4:D:209:LEU:HD23	4:D:209:LEU:C	2.42	0.44
1:A:215:HIS:HA	28:A:613:PL9:O1	2.17	0.44
22:A:607:CLA:H192	22:C:505:CLA:H142	2.00	0.44
22:B:606:CLA:H62	22:B:606:CLA:H41	1.77	0.44
8:i:1:MET:HE3	8:i:4:LEU:CB	2.43	0.44
29:a:614:LMG:H201	29:a:614:LMG:H231	1.86	0.44
2:B:78:TRP:N	13:o:111:ALA:HB1	2.32	0.44
2:B:138:MET:HE3	22:B:616:CLA:CHD	2.47	0.44
3:c:334:PRO:HA	13:o:153:THR:OG1	2.17	0.44
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.99	0.44
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.99	0.44
22:d:403:CLA:H121	17:x:18:ALA:HB2	1.99	0.44
25:l:101:SQD:O7	25:l:102:SQD:H442	2.18	0.44
12:M:28:GLN:HG2	12:m:27:VAL:HG12	1.99	0.44
13:O:180:GLU:CD	13:O:180:GLU:H	2.24	0.44
22:B:617:CLA:HED2	22:B:617:CLA:H43	1.98	0.44
4:d:209:LEU:HD23	4:d:209:LEU:C	2.42	0.44
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.53	0.44
32:d:409:LHG:H132	32:d:409:LHG:C37	2.33	0.44
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.44
3:C:334:PRO:HA	13:O:153:THR:OG1	2.17	0.44
22:C:510:CLA:HBC3	22:C:510:CLA:H192	1.99	0.44
29:A:614:LMG:H201	29:A:614:LMG:H231	1.86	0.44
3:C:318:LEU:C	3:C:318:LEU:HD23	2.43	0.44
24:k:102:BCR:H24C	24:k:102:BCR:H371	1.70	0.44
1:a:215:HIS:HA	28:a:613:PL9:O1	2.17	0.44
22:a:607:CLA:H192	22:c:505:CLA:H142	2.00	0.44
24:a:608:BCR:H24C	24:a:608:BCR:H371	1.84	0.44
24:B:618:BCR:C38	14:t:19:PHE:HZ	2.31	0.44
3:c:205:ASP:HA	3:c:206:PRO:HD3	1.90	0.43
24:d:404:BCR:HC22	31:d:410:DGD:HA72	2.00	0.43
12:M:27:VAL:HG12	12:m:28:GLN:HG2	1.99	0.43
22:b:616:CLA:H2	22:b:617:CLA:CBB	2.48	0.43
22:C:505:CLA:HAA1	22:C:505:CLA:HBD	1.99	0.43
22:c:506:CLA:H122	22:c:506:CLA:H162	1.72	0.43
2:B:13:ILE:HG12	22:B:613:CLA:HAC2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ARG:HH11	2:B:127:ARG:CG	2.18	0.43
24:B:622:BCR:H24C	24:B:622:BCR:H371	1.89	0.43
3:c:318:LEU:C	3:c:318:LEU:HD23	2.43	0.43
22:c:509:CLA:HBB1	22:c:509:CLA:CMB	2.47	0.43
4:D:85:MET:CE	4:D:96:GLU:HG2	2.49	0.43
22:D:403:CLA:H121	17:X:18:ALA:HB2	1.99	0.43
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.53	0.43
14:T:22:PHE:HB3	24:T:102:BCR:H271	2.00	0.43
2:b:13:ILE:HG12	22:b:613:CLA:HAC2	2.00	0.43
2:b:138:MET:HE3	22:b:616:CLA:CHD	2.47	0.43
13:O:58:ASN:HA	13:O:60:ARG:NH2	2.33	0.43
22:B:616:CLA:H2	22:B:617:CLA:CBB	2.48	0.43
13:o:58:ASN:HA	13:o:60:ARG:NH2	2.33	0.43
29:A:614:LMG:H151	31:C:516:DGD:HA62	2.01	0.43
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.00	0.43
22:c:505:CLA:HBD	22:c:505:CLA:HAA1	1.99	0.43
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.52	0.43
29:a:614:LMG:H151	31:c:516:DGD:HA62	2.01	0.43
5:e:27:ILE:HG12	33:f:101:HEM:HMC3	2.01	0.43
1:A:215:HIS:ND1	28:A:613:PL9:O1	2.47	0.43
1:a:215:HIS:ND1	28:a:613:PL9:O1	2.47	0.43
3:C:205:ASP:HA	3:C:206:PRO:HD3	1.90	0.43
8:I:33:LYS:HB3	8:I:34:ARG:H	1.50	0.43
16:V:37:CYS:CB	33:V:201:HEM:HAB	2.43	0.43
22:c:501:CLA:H42	22:c:502:CLA:HMD3	2.01	0.43
4:d:85:MET:CE	4:d:96:GLU:HG2	2.49	0.43
4:d:102:THR:OG1	31:d:410:DGD:HG31	2.19	0.43
10:K:10:LYS:HD2	10:K:10:LYS:N	2.34	0.43
22:C:506:CLA:H162	22:C:506:CLA:H122	1.72	0.42
8:I:1:MET:HE3	8:I:4:LEU:CB	2.43	0.42
12:M:20:VAL:HG21	12:m:20:VAL:HG11	1.98	0.42
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.51	0.42
22:a:603:CLA:CAD	22:d:402:CLA:HAC2	2.50	0.42
8:i:33:LYS:HB3	8:i:34:ARG:H	1.50	0.42
22:B:605:CLA:H43	22:B:606:CLA:H2	2.01	0.42
24:D:404:BCR:HC22	31:D:410:DGD:HA72	2.00	0.42
12:M:20:VAL:HG13	12:m:20:VAL:CG1	2.50	0.42
16:v:37:CYS:CB	33:v:201:HEM:HAB	2.43	0.42
22:a:604:CLA:H142	29:d:406:LMG:H232	2.01	0.42
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.42
22:A:604:CLA:H142	29:D:406:LMG:H232	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:504:CLA:H201	32:D:409:LHG:H342	2.01	0.42
23:A:605:PHO:NC	23:A:605:PHO:ND	2.68	0.42
25:a:609:SQD:O10	32:d:409:LHG:H122	2.20	0.42
22:B:614:CLA:H162	22:B:614:CLA:H121	1.88	0.42
22:b:605:CLA:H43	22:b:606:CLA:H2	2.01	0.42
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	2.01	0.42
10:k:10:LYS:HD2	10:k:10:LYS:N	2.34	0.42
2:b:220:ARG:HG3	7:h:20:LYS:HD3	2.01	0.42
32:D:409:LHG:H332	32:D:409:LHG:H302	1.88	0.42
4:d:27:PHE:HD1	32:e:101:LHG:HC12	1.85	0.42
2:B:467:ILE:HG13	4:D:126:MET:CE	2.48	0.42
22:B:612:CLA:H142	32:L:102:LHG:H361	2.02	0.42
2:b:157:HIS:CD2	2:b:157:HIS:C	2.98	0.42
22:c:504:CLA:H201	32:d:409:LHG:H342	2.01	0.42
24:H:101:BCR:H24C	24:H:101:BCR:H371	1.81	0.42
13:o:59:LYS:HD2	13:o:61:GLN:CG	2.50	0.42
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.54	0.42
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.55	0.42
2:B:220:ARG:HG3	7:H:20:LYS:HD3	2.01	0.42
2:b:204:ALA:CB	22:b:603:CLA:HAB	2.50	0.42
2:b:467:ILE:HG13	4:d:126:MET:CE	2.48	0.42
12:M:28:GLN:CB	12:m:28:GLN:HA	2.49	0.42
13:O:59:LYS:HD2	13:O:61:GLN:CG	2.50	0.42
22:A:603:CLA:CAD	22:D:402:CLA:HAC2	2.50	0.41
22:C:501:CLA:H42	22:C:502:CLA:HMD1	2.02	0.41
5:E:27:ILE:HG12	33:F:101:HEM:HMC3	2.01	0.41
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.55	0.41
25:B:601:SQD:H252	24:t:101:BCR:C22	2.49	0.41
22:A:603:CLA:HBD	22:D:402:CLA:HAC2	2.02	0.41
25:A:609:SQD:O10	32:D:409:LHG:H122	2.20	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
12:M:16:LEU:HD13	12:m:16:LEU:CD1	2.27	0.41
2:B:157:HIS:C	2:B:157:HIS:CD2	2.98	0.41
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.94	0.41
2:B:451:PHE:CD2	2:B:451:PHE:C	2.98	0.41
22:B:605:CLA:H141	22:B:605:CLA:H161	1.93	0.41
22:C:502:CLA:H61	22:C:512:CLA:H42	2.03	0.41
4:D:102:THR:OG1	31:D:410:DGD:HG31	2.19	0.41
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.51	0.41
1:a:79:THR:HG22	4:d:315:TYR:HB2	2.02	0.41
1:a:278:TRP:HB3	1:a:279:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:614:CLA:H121	22:b:614:CLA:H162	1.88	0.41
22:C:509:CLA:HBB1	22:C:509:CLA:CMB	2.47	0.41
12:M:16:LEU:CD1	12:m:16:LEU:CD1	2.94	0.41
24:T:101:BCR:H24C	24:T:101:BCR:H371	1.83	0.41
23:A:606:PHO:HMA2	28:A:613:PL9:C22	2.51	0.41
2:B:204:ALA:CB	22:B:603:CLA:HAB	2.50	0.41
2:b:63:LEU:N	2:b:64:PRO:HD2	2.35	0.41
2:b:451:PHE:CD2	2:b:451:PHE:C	2.98	0.41
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.02	0.41
22:B:611:CLA:HHC	22:B:611:CLA:CBB	2.50	0.41
22:c:502:CLA:H61	22:c:512:CLA:H42	2.03	0.41
23:A:606:PHO:HBB1	23:A:606:PHO:HMB1	2.03	0.41
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.03	0.41
22:a:603:CLA:HBD	22:d:402:CLA:HAC2	2.02	0.41
23:a:606:PHO:HMA2	28:a:613:PL9:C22	2.51	0.41
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.94	0.41
3:C:425:TRP:CD1	22:C:504:CLA:HMA3	2.56	0.41
10:k:20:PRO:HB3	18:y:21:GLN:HG3	2.01	0.41
12:M:28:GLN:HA	12:m:28:GLN:CA	2.50	0.41
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.56	0.41
3:c:406:SER:HA	3:c:420:VAL:HG23	2.03	0.41
12:M:16:LEU:C	12:M:16:LEU:HD23	2.46	0.41
23:a:606:PHO:HMB1	23:a:606:PHO:HBB1	2.03	0.40
22:B:617:CLA:HBB1	22:B:617:CLA:HMB3	2.03	0.40
3:c:338:GLY:HA3	3:c:341:LEU:O	2.22	0.40
2:b:475:PHE:CD2	4:d:140:PRO:HG3	2.56	0.40
14:t:18:PHE:CE1	24:t:101:BCR:H381	2.56	0.40
2:b:78:TRP:HD1	13:O:112:GLY:HA2	1.85	0.40
22:b:617:CLA:HBB1	22:b:617:CLA:HMB3	2.03	0.40
3:C:406:SER:HA	3:C:420:VAL:HG23	2.03	0.40
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.04	0.40
1:a:249:VAL:HG12	2:b:491:VAL:CG2	2.52	0.40
2:B:127:ARG:NH1	2:B:127:ARG:CG	2.81	0.40
12:m:16:LEU:C	12:m:16:LEU:HD23	2.46	0.40
25:A:609:SQD:H291	22:C:508:CLA:H71	2.03	0.40
23:a:606:PHO:ND	23:a:606:PHO:NC	2.70	0.40
25:a:609:SQD:H291	22:c:508:CLA:H71	2.03	0.40
4:D:103:ARG:O	4:D:107:LEU:HG	2.21	0.40
4:d:103:ARG:O	4:d:107:LEU:HG	2.21	0.40
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.04	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:73:GLN:OE1	16:V:70:GLU:CD[3_544]	0.80	1.40
15:u:73:GLN:OE1	16:V:70:GLU:OE1[3_544]	1.22	0.98
15:u:73:GLN:OE1	16:V:70:GLU:OE2[3_544]	1.45	0.75
15:u:73:GLN:CD	16:V:70:GLU:OE1[3_544]	1.79	0.41
15:u:73:GLN:CD	16:V:70:GLU:CD[3_544]	1.89	0.31
15:u:73:GLN:OE1	16:V:70:GLU:CG[3_544]	1.98	0.22
15:u:60:ASP:OD2	16:V:110:LYS:CD[3_544]	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%)	328 (99%)	3 (1%)	1 (0%)	36	72
2	B	502/504 (100%)	497 (99%)	5 (1%)	0	100	100
2	b	502/504 (100%)	496 (99%)	6 (1%)	0	100	100
3	C	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	43	78
3	c	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	43	78
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (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	32/34 (94%)	32 (100%)	0	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/40 (90%)	36 (100%)	0	0	100	100
9	j	36/40 (90%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	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%)	233 (97%)	7 (3%)	1 (0%)	30	67
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	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%)	132 (98%)	3 (2%)	0	100	100
17	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
17	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
18	Y	27/29 (93%)	27 (100%)	0	0	100	100
18	y	27/29 (93%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5188/5288 (98%)	5085 (98%)	97 (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%)	269 (100%)	0	100	100
1	a	269/269 (100%)	269 (100%)	0	100	100
2	B	402/402 (100%)	398 (99%)	4 (1%)	68	77
2	b	402/402 (100%)	398 (99%)	4 (1%)	68	77
3	C	352/362 (97%)	345 (98%)	7 (2%)	48	66
3	c	352/362 (97%)	345 (98%)	7 (2%)	48	66
4	D	277/277 (100%)	275 (99%)	2 (1%)	76	80
4	d	277/277 (100%)	275 (99%)	2 (1%)	76	80
5	E	72/72 (100%)	71 (99%)	1 (1%)	59	72
5	e	72/72 (100%)	71 (99%)	1 (1%)	59	72
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	52
6	f	28/28 (100%)	27 (96%)	1 (4%)	31	52
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	51
7	h	54/54 (100%)	52 (96%)	2 (4%)	30	51
8	I	35/35 (100%)	34 (97%)	1 (3%)	37	57
8	i	35/35 (100%)	34 (97%)	1 (3%)	37	57
9	J	26/28 (93%)	26 (100%)	0	100	100
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15	36
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	36
11	L	35/35 (100%)	33 (94%)	2 (6%)	18	40
11	l	35/35 (100%)	33 (94%)	2 (6%)	18	40
12	M	31/31 (100%)	30 (97%)	1 (3%)	34	55
12	m	31/31 (100%)	30 (97%)	1 (3%)	34	55
13	O	206/206 (100%)	202 (98%)	4 (2%)	50	66
13	o	206/206 (100%)	202 (98%)	4 (2%)	50	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	27/27 (100%)	26 (96%)	1 (4%)	30	51
14	t	27/27 (100%)	26 (96%)	1 (4%)	30	51
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	78
16	v	117/117 (100%)	116 (99%)	1 (1%)	70	78
17	X	32/32 (100%)	32 (100%)	0	100	100
17	x	32/32 (100%)	32 (100%)	0	100	100
18	Y	22/22 (100%)	21 (96%)	1 (4%)	24	46
18	y	22/22 (100%)	21 (96%)	1 (4%)	24	46
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	50
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	50
All	All	4302/4326 (99%)	4236 (98%)	66 (2%)	57	71

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

Mol	Chain	Res	Type
2	B	86	ILE
2	B	127	ARG
2	B	223	GLN
2	B	467	ILE
2	b	86	ILE
2	b	127	ARG
2	b	223	GLN
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
3	c	24	THR
3	c	25	ASN
3	c	29	GLU
3	c	142	GLU
3	c	289	PHE
3	c	315	MET

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Mol	Chain	Res	Type
3	c	355	THR
4	D	11	GLU
4	D	90	LEU
4	d	11	GLU
4	d	90	LEU
5	E	71	GLU
5	e	71	GLU
6	F	44	GLN
6	f	44	GLN
7	H	12	ARG
7	H	65	LEU
7	h	12	ARG
7	h	65	LEU
8	I	1	MET
8	i	1	MET
10	K	13	GLU
10	K	17	ILE
10	k	13	GLU
10	k	17	ILE
11	L	1	MET
11	L	13	ASN
11	l	1	MET
11	l	13	ASN
12	M	9	ILE
12	m	9	ILE
13	O	61	GLN
13	O	62	GLU
13	O	181	GLU
13	O	234	LYS
13	o	61	GLN
13	o	62	GLU
13	o	181	GLU
13	o	234	LYS
14	T	25	GLU
14	t	25	GLU
15	U	70	ARG
15	u	70	ARG
16	V	30	LYS
16	v	30	LYS
18	Y	27	MET
18	y	27	MET
19	Z	4	LEU

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Mol	Chain	Res	Type
19	Z	6	GLN
19	z	4	LEU
19	z	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	261	GLN
1	A	315	ASN
1	a	75	ASN
1	a	165	GLN
1	a	261	GLN
1	a	315	ASN
2	B	14	ASN
2	B	53	ASN
2	B	223	GLN
2	B	281	GLN
2	B	374	ASN
2	B	409	GLN
2	b	53	ASN
2	b	223	GLN
2	b	281	GLN
2	b	282	GLN
2	b	331	ASN
2	b	409	GLN
3	C	25	ASN
3	C	44	ASN
3	C	373	ASN
3	C	415	ASN
3	c	25	ASN
3	c	373	ASN
4	D	83	ASN
4	D	186	GLN
4	D	255	GLN
4	D	332	GLN
4	d	83	ASN
4	d	186	GLN
4	d	255	GLN
4	d	332	GLN
5	E	74	GLN

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Mol	Chain	Res	Type
5	e	74	GLN
6	F	44	GLN
6	f	44	GLN
10	K	40	GLN
10	k	40	GLN
11	L	13	ASN
11	l	13	ASN
13	O	124	ASN
13	O	147	ASN
13	o	124	ASN
13	o	147	ASN
16	V	34	GLN
16	v	34	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	SQD	A	609	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PL9	a	613	-	55,55,55	0.72	2 (3%)	68,69,69	1.56	13 (19%)
22	CLA	D	403	-	69,73,73	2.37	19 (27%)	82,113,113	2.50	22 (26%)
27	BCT	a	612	21	3,3,3	0.51	0	2,3,3	0.65	0
25	SQD	l	101	-	52,54,54	1.00	3 (5%)	62,65,65	1.32	8 (12%)
25	SQD	d	411	-	41,43,54	1.15	3 (7%)	51,54,65	1.42	7 (13%)
32	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	0.85	2 (3%)
22	CLA	B	614	-	69,73,73	2.26	17 (24%)	82,113,113	2.47	24 (29%)
22	CLA	b	616	-	69,73,73	2.44	20 (28%)	82,113,113	2.50	21 (25%)
32	LHG	d	409	-	48,48,48	0.95	2 (4%)	51,54,54	0.91	3 (5%)
20	OEX	A	601	3,1	0,15,15	-	-	-	-	-
22	CLA	C	509	-	69,73,73	2.45	19 (27%)	82,113,113	2.60	27 (32%)
22	CLA	C	503	-	69,73,73	2.47	18 (26%)	82,113,113	2.40	21 (25%)
24	BCR	c	514	-	41,41,41	3.67	15 (36%)	56,56,56	8.55	36 (64%)
22	CLA	c	505	-	69,73,73	2.34	20 (28%)	82,113,113	2.35	21 (25%)
22	CLA	A	607	-	69,73,73	2.18	16 (23%)	82,113,113	2.55	24 (29%)
25	SQD	D	411	-	41,43,54	1.16	3 (7%)	51,54,65	1.42	7 (13%)
22	CLA	c	512	-	69,73,73	2.66	18 (26%)	82,113,113	2.42	26 (31%)
22	CLA	D	401	-	69,73,73	2.09	18 (26%)	82,113,113	2.38	27 (32%)
22	CLA	B	612	-	69,73,73	2.11	17 (24%)	82,113,113	2.51	23 (28%)
22	CLA	c	509	-	69,73,73	2.44	19 (27%)	82,113,113	2.60	27 (32%)
24	BCR	c	515	-	41,41,41	3.63	14 (34%)	56,56,56	8.32	38 (67%)
31	DGD	c	518	-	63,63,67	0.80	3 (4%)	77,77,81	0.90	3 (3%)
22	CLA	d	403	-	69,73,73	2.37	19 (27%)	82,113,113	2.51	22 (26%)
22	CLA	B	617	-	69,73,73	2.16	18 (26%)	82,113,113	2.47	26 (31%)
32	LHG	l	103	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	3 (5%)
22	CLA	B	603	-	69,73,73	2.33	20 (28%)	82,113,113	2.31	21 (25%)
20	OEX	a	601	3,1	0,15,15	-	-	-	-	-
22	CLA	C	512	-	69,73,73	2.65	18 (26%)	82,113,113	2.41	26 (31%)
22	CLA	a	607	-	69,73,73	2.18	16 (23%)	82,113,113	2.54	24 (29%)
29	LMG	a	614	-	51,51,55	0.95	2 (3%)	59,59,63	0.96	3 (5%)
22	CLA	b	606	-	69,73,73	2.31	17 (24%)	82,113,113	2.40	23 (28%)
33	HEM	f	101	6,5	50,50,50	1.98	9 (18%)	67,82,82	1.35	5 (7%)
22	CLA	C	501	-	69,73,73	2.28	18 (26%)	82,113,113	2.52	23 (28%)
31	DGD	d	410	-	63,63,67	1.00	4 (6%)	77,77,81	1.03	6 (7%)
28	PL9	d	408	-	55,55,55	0.82	2 (3%)	68,69,69	1.32	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PL9	A	613	-	55,55,55	0.72	2 (3%)	68,69,69	1.56	14 (20%)
32	LHG	L	102	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	3 (5%)
29	LMG	C	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	4 (6%)
22	CLA	B	610	-	69,73,73	2.24	19 (27%)	82,113,113	2.43	22 (26%)
31	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	3 (3%)
22	CLA	C	507	-	69,73,73	2.46	20 (28%)	82,113,113	2.60	25 (30%)
24	BCR	D	404	-	41,41,41	3.63	14 (34%)	56,56,56	7.88	40 (71%)
29	LMG	z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.32	5 (11%)
27	BCT	A	612	21	3,3,3	0.50	0	2,3,3	0.59	0
23	PHO	A	605	-	58,69,69	2.53	12 (20%)	55,99,99	2.93	11 (20%)
24	BCR	a	608	-	41,41,41	3.53	14 (34%)	56,56,56	7.78	37 (66%)
29	LMG	C	520	-	51,51,55	1.01	3 (5%)	59,59,63	0.99	2 (3%)
33	HEM	v	201	16	50,50,50	1.86	10 (20%)	67,82,82	1.28	4 (5%)
25	SQD	B	601	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
22	CLA	b	603	-	69,73,73	2.33	19 (27%)	82,113,113	2.32	21 (25%)
22	CLA	c	503	-	69,73,73	2.47	18 (26%)	82,113,113	2.39	21 (25%)
22	CLA	c	506	-	69,73,73	2.33	18 (26%)	82,113,113	2.48	24 (29%)
31	DGD	C	516	-	63,63,67	0.88	3 (4%)	77,77,81	0.98	2 (2%)
29	LMG	c	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	4 (6%)
22	CLA	A	603	-	69,73,73	2.13	17 (24%)	82,113,113	2.39	25 (30%)
22	CLA	b	612	-	69,73,73	2.10	17 (24%)	82,113,113	2.51	22 (26%)
22	CLA	C	508	-	69,73,73	2.50	21 (30%)	82,113,113	2.43	19 (23%)
31	DGD	c	517	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	4 (5%)
22	CLA	c	513	-	69,73,73	2.61	19 (27%)	82,113,113	2.43	24 (29%)
32	LHG	d	405	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	4 (7%)
22	CLA	c	504	-	69,73,73	2.36	19 (27%)	82,113,113	2.51	22 (26%)
22	CLA	c	507	-	69,73,73	2.46	20 (28%)	82,113,113	2.60	25 (30%)
29	LMG	Z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.32	5 (11%)
32	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	0.91	3 (5%)
22	CLA	B	615	-	69,73,73	2.23	20 (28%)	82,113,113	2.51	27 (32%)
22	CLA	a	604	-	69,73,73	2.28	18 (26%)	82,113,113	2.55	25 (30%)
24	BCR	C	514	-	41,41,41	3.68	15 (36%)	56,56,56	8.55	36 (64%)
31	DGD	c	516	-	63,63,67	0.88	3 (4%)	77,77,81	0.97	2 (2%)
24	BCR	k	102	-	41,41,41	3.58	14 (34%)	56,56,56	7.86	43 (76%)
22	CLA	b	608	-	69,73,73	2.26	18 (26%)	82,113,113	2.41	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	508	-	69,73,73	2.49	21 (30%)	82,113,113	2.43	19 (23%)
23	PHO	a	605	-	58,69,69	2.54	12 (20%)	55,99,99	2.95	11 (20%)
22	CLA	C	505	-	69,73,73	2.34	22 (31%)	82,113,113	2.35	21 (25%)
24	BCR	t	101	-	41,41,41	3.55	14 (34%)	56,56,56	8.52	42 (75%)
29	LMG	B	620	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
22	CLA	B	607	-	69,73,73	2.42	17 (24%)	82,113,113	2.57	27 (32%)
33	HEM	V	201	16	50,50,50	1.86	10 (20%)	67,82,82	1.29	4 (5%)
22	CLA	B	606	-	69,73,73	2.31	17 (24%)	82,113,113	2.40	24 (29%)
22	CLA	B	604	-	69,73,73	2.18	18 (26%)	82,113,113	2.53	26 (31%)
23	PHO	A	606	-	58,69,69	2.69	12 (20%)	55,99,99	2.86	15 (27%)
24	BCR	B	618	-	41,41,41	3.49	14 (34%)	56,56,56	7.56	38 (67%)
25	SQD	b	621	-	52,54,54	1.03	3 (5%)	62,65,65	1.41	9 (14%)
29	LMG	D	406	34	51,51,55	0.87	2 (3%)	59,59,63	0.79	3 (5%)
25	SQD	b	601	-	52,54,54	0.99	2 (3%)	62,65,65	1.19	6 (9%)
22	CLA	C	506	-	69,73,73	2.33	19 (27%)	82,113,113	2.48	24 (29%)
22	CLA	C	510	-	69,73,73	2.30	20 (28%)	82,113,113	2.53	26 (31%)
31	DGD	C	518	-	63,63,67	0.80	3 (4%)	77,77,81	0.90	3 (3%)
22	CLA	b	611	-	69,73,73	2.27	18 (26%)	82,113,113	2.50	24 (29%)
24	BCR	b	618	-	41,41,41	3.49	14 (34%)	56,56,56	7.83	41 (73%)
22	CLA	d	402	-	69,73,73	1.97	18 (26%)	82,113,113	2.38	24 (29%)
31	DGD	D	410	-	63,63,67	0.99	4 (6%)	77,77,81	1.04	6 (7%)
22	CLA	B	605	-	69,73,73	2.37	16 (23%)	82,113,113	2.58	26 (31%)
22	CLA	d	401	-	69,73,73	2.09	18 (26%)	82,113,113	2.38	26 (31%)
24	BCR	b	622	-	41,41,41	3.62	14 (34%)	56,56,56	7.16	39 (69%)
24	BCR	k	101	-	41,41,41	3.64	15 (36%)	56,56,56	8.11	36 (64%)
22	CLA	b	617	-	69,73,73	2.16	18 (26%)	82,113,113	2.47	26 (31%)
22	CLA	b	614	-	69,73,73	2.26	17 (24%)	82,113,113	2.47	25 (30%)
24	BCR	K	101	-	41,41,41	3.65	14 (34%)	56,56,56	8.11	36 (64%)
22	CLA	a	603	-	69,73,73	2.13	17 (24%)	82,113,113	2.39	24 (29%)
24	BCR	d	404	-	41,41,41	3.63	14 (34%)	56,56,56	7.88	40 (71%)
22	CLA	B	611	-	69,73,73	2.27	18 (26%)	82,113,113	2.50	24 (29%)
29	LMG	A	614	-	51,51,55	0.95	2 (3%)	59,59,63	0.96	3 (5%)
29	LMG	b	619	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
22	CLA	C	511	3	69,73,73	2.46	17 (24%)	82,113,113	2.60	23 (28%)
22	CLA	b	615	-	69,73,73	2.23	19 (27%)	82,113,113	2.51	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	613	-	69,73,73	2.35	19 (27%)	82,113,113	2.44	21 (25%)
24	BCR	B	619	-	41,41,41	3.49	14 (34%)	56,56,56	7.82	41 (73%)
31	DGD	h	102	-	63,63,67	0.93	3 (4%)	77,77,81	0.94	4 (5%)
22	CLA	b	605	-	69,73,73	2.37	16 (23%)	82,113,113	2.57	27 (32%)
24	BCR	h	101	-	41,41,41	3.61	14 (34%)	56,56,56	8.34	41 (73%)
33	HEM	F	101	6,5	50,50,50	1.98	9 (18%)	67,82,82	1.35	5 (7%)
22	CLA	B	608	-	69,73,73	2.26	18 (26%)	82,113,113	2.41	23 (28%)
22	CLA	b	604	-	69,73,73	2.19	18 (26%)	82,113,113	2.54	26 (31%)
22	CLA	b	607	-	69,73,73	2.42	18 (26%)	82,113,113	2.56	26 (31%)
24	BCR	B	622	-	41,41,41	3.61	14 (34%)	56,56,56	7.16	39 (69%)
22	CLA	c	511	3	69,73,73	2.46	17 (24%)	82,113,113	2.59	23 (28%)
28	PL9	D	408	-	55,55,55	0.83	1 (1%)	68,69,69	1.32	9 (13%)
32	LHG	D	405	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	4 (7%)
22	CLA	c	501	-	69,73,73	2.28	18 (26%)	82,113,113	2.53	23 (28%)
32	LHG	d	407	-	48,48,48	0.90	3 (6%)	51,54,54	0.85	2 (3%)
23	PHO	a	606	-	58,69,69	2.68	12 (20%)	55,99,99	2.85	15 (27%)
24	BCR	T	101	-	41,41,41	3.49	14 (34%)	56,56,56	7.56	38 (67%)
32	LHG	e	101	-	41,41,48	1.06	2 (4%)	44,47,54	1.08	3 (6%)
24	BCR	C	515	-	41,41,41	3.64	14 (34%)	56,56,56	8.33	38 (67%)
22	CLA	c	510	-	69,73,73	2.30	20 (28%)	82,113,113	2.53	25 (30%)
29	LMG	c	520	-	51,51,55	1.01	3 (5%)	59,59,63	0.99	2 (3%)
25	SQD	a	609	-	52,54,54	0.92	2 (3%)	62,65,65	1.49	11 (17%)
22	CLA	b	610	-	69,73,73	2.24	19 (27%)	82,113,113	2.42	22 (26%)
22	CLA	D	402	-	69,73,73	1.97	18 (26%)	82,113,113	2.38	24 (29%)
25	SQD	L	101	-	52,54,54	0.99	3 (5%)	62,65,65	1.33	8 (12%)
22	CLA	B	609	-	69,73,73	2.09	17 (24%)	82,113,113	2.45	27 (32%)
22	CLA	c	502	-	69,73,73	2.20	16 (23%)	82,113,113	2.43	21 (25%)
31	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	0.94	4 (5%)
22	CLA	C	502	-	69,73,73	2.20	16 (23%)	82,113,113	2.43	21 (25%)
24	BCR	H	101	-	41,41,41	3.61	14 (34%)	56,56,56	8.34	41 (73%)
29	LMG	d	406	34	51,51,55	0.88	2 (3%)	59,59,63	0.79	3 (5%)
22	CLA	A	604	-	69,73,73	2.28	18 (26%)	82,113,113	2.56	25 (30%)
22	CLA	B	616	-	69,73,73	2.44	20 (28%)	82,113,113	2.51	22 (26%)
22	CLA	b	602	-	69,73,73	2.55	20 (28%)	82,113,113	2.60	23 (28%)
22	CLA	C	513	-	69,73,73	2.61	19 (27%)	82,113,113	2.43	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	SQD	l	102	-	52,54,54	1.03	3 (5%)	62,65,65	1.40	9 (14%)
32	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.08	3 (6%)
22	CLA	C	504	-	69,73,73	2.36	19 (27%)	82,113,113	2.50	22 (26%)
24	BCR	A	608	-	41,41,41	3.54	14 (34%)	56,56,56	7.79	37 (66%)
24	BCR	T	102	-	41,41,41	3.55	14 (34%)	56,56,56	8.52	42 (75%)
22	CLA	B	602	-	69,73,73	2.55	21 (30%)	82,113,113	2.60	23 (28%)
22	CLA	b	613	-	69,73,73	2.36	18 (26%)	82,113,113	2.44	21 (25%)
24	BCR	K	102	-	41,41,41	3.58	14 (34%)	56,56,56	7.87	43 (76%)
22	CLA	b	609	-	69,73,73	2.09	17 (24%)	82,113,113	2.45	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
25	SQD	A	609	-	-	17/49/69/69	0/1/1/1
28	PL9	a	613	-	-	9/53/73/73	0/1/1/1
22	CLA	D	403	-	-	14/39/115/115	-
25	SQD	l	101	-	-	28/49/69/69	0/1/1/1
25	SQD	d	411	-	-	17/38/58/69	0/1/1/1
32	LHG	D	407	-	-	13/53/53/53	-
22	CLA	B	614	-	1/1/15/20	3/39/115/115	-
22	CLA	b	616	-	1/1/15/20	11/39/115/115	-
32	LHG	d	409	-	-	12/53/53/53	-
22	CLA	C	509	-	1/1/15/20	8/39/115/115	-
22	CLA	C	503	-	1/1/15/20	1/39/115/115	-
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
22	CLA	c	505	-	1/1/15/20	2/39/115/115	-
22	CLA	A	607	-	-	13/39/115/115	-
25	SQD	D	411	-	-	17/38/58/69	0/1/1/1
22	CLA	c	512	-	1/1/15/20	9/39/115/115	-
22	CLA	D	401	-	1/1/15/20	5/39/115/115	-
22	CLA	B	612	-	-	3/39/115/115	-
22	CLA	c	509	-	1/1/15/20	8/39/115/115	-
24	BCR	c	515	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	c	518	-	-	16/51/91/95	0/2/2/2
22	CLA	d	403	-	-	14/39/115/115	-
22	CLA	B	617	-	1/1/15/20	15/39/115/115	-
32	LHG	l	103	-	-	17/53/53/53	-
22	CLA	B	603	-	1/1/15/20	0/39/115/115	-
22	CLA	C	512	-	1/1/15/20	9/39/115/115	-
22	CLA	a	607	-	-	13/39/115/115	-
29	LMG	a	614	-	-	31/46/66/70	0/1/1/1
22	CLA	b	606	-	1/1/15/20	5/39/115/115	-
33	HEM	f	101	6,5	-	4/14/54/54	-
22	CLA	C	501	-	-	9/39/115/115	-
31	DGD	d	410	-	-	33/51/91/95	0/2/2/2
28	PL9	d	408	-	-	1/53/73/73	0/1/1/1
28	PL9	A	613	-	-	9/53/73/73	0/1/1/1
32	LHG	L	102	-	-	17/53/53/53	-
29	LMG	C	519	-	-	22/46/66/70	0/1/1/1
22	CLA	B	610	-	1/1/15/20	0/39/115/115	-
31	DGD	C	517	-	-	24/51/91/95	0/2/2/2
22	CLA	C	507	-	1/1/15/20	11/39/115/115	-
24	BCR	D	404	-	-	6/29/63/63	0/2/2/2
29	LMG	z	101	-	-	18/31/51/70	0/1/1/1
23	PHO	A	605	-	-	2/37/103/103	0/5/6/6
24	BCR	a	608	-	-	4/29/63/63	0/2/2/2
29	LMG	C	520	-	-	26/46/66/70	0/1/1/1
33	HEM	v	201	16	-	6/14/54/54	-
25	SQD	B	601	-	-	23/49/69/69	0/1/1/1
22	CLA	b	603	-	1/1/15/20	0/39/115/115	-
22	CLA	c	503	-	1/1/15/20	1/39/115/115	-
22	CLA	c	506	-	1/1/15/20	15/39/115/115	-
31	DGD	C	516	-	-	24/51/91/95	0/2/2/2
29	LMG	c	519	-	-	22/46/66/70	0/1/1/1
22	CLA	A	603	-	1/1/15/20	3/39/115/115	-
22	CLA	b	612	-	-	3/39/115/115	-
22	CLA	C	508	-	-	5/39/115/115	-
31	DGD	c	517	-	-	24/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	513	-	-	9/39/115/115	-
32	LHG	d	405	-	-	13/53/53/53	-
22	CLA	c	504	-	1/1/15/20	9/39/115/115	-
22	CLA	c	507	-	1/1/15/20	11/39/115/115	-
29	LMG	Z	101	-	-	18/31/51/70	0/1/1/1
32	LHG	D	409	-	-	12/53/53/53	-
22	CLA	B	615	-	1/1/15/20	10/39/115/115	-
22	CLA	a	604	-	-	7/39/115/115	-
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
31	DGD	c	516	-	-	24/51/91/95	0/2/2/2
24	BCR	k	102	-	-	10/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/15/20	2/39/115/115	-
22	CLA	c	508	-	-	5/39/115/115	-
23	PHO	a	605	-	-	2/37/103/103	0/5/6/6
22	CLA	C	505	-	1/1/15/20	2/39/115/115	-
24	BCR	t	101	-	-	1/29/63/63	0/2/2/2
29	LMG	B	620	-	-	19/46/66/70	0/1/1/1
22	CLA	B	607	-	-	7/39/115/115	-
33	HEM	V	201	16	-	6/14/54/54	-
22	CLA	B	606	-	1/1/15/20	5/39/115/115	-
22	CLA	B	604	-	1/1/15/20	5/39/115/115	-
23	PHO	A	606	-	-	4/37/103/103	0/5/6/6
24	BCR	B	618	-	-	5/29/63/63	0/2/2/2
25	SQD	b	621	-	-	29/49/69/69	0/1/1/1
29	LMG	D	406	34	-	16/46/66/70	0/1/1/1
25	SQD	b	601	-	-	23/49/69/69	0/1/1/1
22	CLA	C	506	-	1/1/15/20	15/39/115/115	-
22	CLA	C	510	-	1/1/15/20	6/39/115/115	-
31	DGD	C	518	-	-	16/51/91/95	0/2/2/2
22	CLA	b	611	-	1/1/15/20	7/39/115/115	-
24	BCR	b	618	-	-	4/29/63/63	0/2/2/2
22	CLA	d	402	-	-	2/39/115/115	-
31	DGD	D	410	-	-	33/51/91/95	0/2/2/2
22	CLA	B	605	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	401	-	1/1/15/20	5/39/115/115	-
24	BCR	b	622	-	-	1/29/63/63	0/2/2/2
24	BCR	k	101	-	-	2/29/63/63	0/2/2/2
22	CLA	b	617	-	1/1/15/20	15/39/115/115	-
22	CLA	b	614	-	1/1/15/20	3/39/115/115	-
24	BCR	K	101	-	-	2/29/63/63	0/2/2/2
22	CLA	a	603	-	1/1/15/20	3/39/115/115	-
24	BCR	d	404	-	-	6/29/63/63	0/2/2/2
22	CLA	B	611	-	1/1/15/20	7/39/115/115	-
29	LMG	A	614	-	-	31/46/66/70	0/1/1/1
29	LMG	b	619	-	-	19/46/66/70	0/1/1/1
22	CLA	C	511	3	-	0/39/115/115	-
22	CLA	b	615	-	1/1/15/20	10/39/115/115	-
22	CLA	B	613	-	1/1/15/20	3/39/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
31	DGD	h	102	-	-	15/51/91/95	0/2/2/2
22	CLA	b	605	-	1/1/15/20	4/39/115/115	-
24	BCR	h	101	-	-	8/29/63/63	0/2/2/2
33	HEM	F	101	6,5	-	4/14/54/54	-
22	CLA	B	608	-	1/1/15/20	2/39/115/115	-
22	CLA	b	604	-	1/1/15/20	5/39/115/115	-
22	CLA	b	607	-	-	7/39/115/115	-
24	BCR	B	622	-	-	1/29/63/63	0/2/2/2
22	CLA	c	511	3	-	0/39/115/115	-
28	PL9	D	408	-	-	1/53/73/73	0/1/1/1
32	LHG	D	405	-	-	13/53/53/53	-
22	CLA	c	501	-	-	9/39/115/115	-
32	LHG	d	407	-	-	13/53/53/53	-
23	PHO	a	606	-	-	4/37/103/103	0/5/6/6
24	BCR	T	101	-	-	5/29/63/63	0/2/2/2
32	LHG	e	101	-	-	24/46/46/53	-
24	BCR	C	515	-	-	4/29/63/63	0/2/2/2
22	CLA	c	510	-	1/1/15/20	6/39/115/115	-
29	LMG	c	520	-	-	26/46/66/70	0/1/1/1
25	SQD	a	609	-	-	17/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	610	-	1/1/15/20	0/39/115/115	-
22	CLA	D	402	-	-	2/39/115/115	-
25	SQD	L	101	-	-	28/49/69/69	0/1/1/1
22	CLA	B	609	-	-	1/39/115/115	-
22	CLA	c	502	-	-	7/39/115/115	-
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
22	CLA	C	502	-	-	7/39/115/115	-
24	BCR	H	101	-	-	8/29/63/63	0/2/2/2
29	LMG	d	406	34	-	16/46/66/70	0/1/1/1
22	CLA	A	604	-	-	7/39/115/115	-
22	CLA	B	616	-	1/1/15/20	11/39/115/115	-
22	CLA	b	602	-	1/1/15/20	18/39/115/115	-
22	CLA	C	513	-	-	9/39/115/115	-
25	SQD	l	102	-	-	29/49/69/69	0/1/1/1
32	LHG	E	101	-	-	24/46/46/53	-
22	CLA	C	504	-	1/1/15/20	9/39/115/115	-
24	BCR	A	608	-	-	4/29/63/63	0/2/2/2
24	BCR	T	102	-	-	1/29/63/63	0/2/2/2
22	CLA	B	602	-	1/1/15/20	18/39/115/115	-
22	CLA	b	613	-	1/1/15/20	3/39/115/115	-
24	BCR	K	102	-	-	10/29/63/63	0/2/2/2
22	CLA	b	609	-	-	1/39/115/115	-

All (1792) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	MG-NA	14.10	2.39	2.06
22	C	512	CLA	MG-NA	14.10	2.39	2.06
22	b	605	CLA	MG-NA	12.06	2.34	2.06
22	B	605	CLA	MG-NA	12.06	2.34	2.06
22	B	616	CLA	MG-NA	11.81	2.34	2.06
22	b	616	CLA	MG-NA	11.80	2.34	2.06
22	C	513	CLA	MG-NA	11.59	2.33	2.06
22	c	513	CLA	MG-NA	11.57	2.33	2.06
22	C	507	CLA	MG-NA	11.44	2.33	2.06
22	c	507	CLA	MG-NA	11.42	2.33	2.06
22	c	511	CLA	MG-NA	11.40	2.33	2.06
22	C	511	CLA	MG-NA	11.39	2.33	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	MG-NA	11.18	2.32	2.06
22	B	607	CLA	MG-NA	11.18	2.32	2.06
22	C	503	CLA	MG-NC	11.11	2.32	2.06
22	c	503	CLA	MG-NC	11.09	2.32	2.06
22	b	613	CLA	MG-NA	10.98	2.32	2.06
22	B	613	CLA	MG-NA	10.97	2.32	2.06
22	a	604	CLA	MG-NA	10.93	2.32	2.06
22	A	604	CLA	MG-NA	10.89	2.32	2.06
22	C	509	CLA	MG-NA	10.35	2.30	2.06
22	c	509	CLA	MG-NA	10.34	2.30	2.06
22	b	602	CLA	MG-NA	10.30	2.30	2.06
22	B	602	CLA	MG-NA	10.27	2.30	2.06
22	C	508	CLA	MG-NA	10.17	2.30	2.06
22	c	508	CLA	MG-NA	10.13	2.30	2.06
22	b	614	CLA	MG-NA	9.88	2.29	2.06
22	B	614	CLA	MG-NA	9.87	2.29	2.06
22	c	506	CLA	MG-NA	9.75	2.29	2.06
22	C	506	CLA	MG-NA	9.74	2.29	2.06
22	B	606	CLA	MG-NA	9.71	2.29	2.06
22	b	606	CLA	MG-NA	9.67	2.29	2.06
23	A	606	PHO	C1D-C2D	9.52	1.50	1.39
23	a	606	PHO	C1D-C2D	9.50	1.49	1.39
22	d	403	CLA	MG-NA	9.35	2.28	2.06
22	D	403	CLA	MG-NA	9.34	2.28	2.06
22	C	505	CLA	MG-NA	9.33	2.28	2.06
22	c	505	CLA	MG-NA	9.33	2.28	2.06
22	b	603	CLA	MG-NA	9.27	2.28	2.06
22	B	603	CLA	MG-NA	9.23	2.28	2.06
23	A	605	PHO	C1B-C2B	9.21	1.49	1.39
23	a	605	PHO	C1B-C2B	9.21	1.49	1.39
22	c	501	CLA	MG-NA	9.15	2.28	2.06
22	C	501	CLA	MG-NA	9.14	2.28	2.06
22	B	608	CLA	MG-NA	9.10	2.27	2.06
22	b	608	CLA	MG-NA	9.07	2.27	2.06
23	a	605	PHO	C1D-C2D	9.05	1.49	1.39
23	A	605	PHO	C1D-C2D	9.04	1.49	1.39
22	c	510	CLA	MG-NA	9.03	2.27	2.06
22	C	510	CLA	MG-NA	9.00	2.27	2.06
23	a	606	PHO	C1B-C2B	8.90	1.49	1.39
23	A	606	PHO	C1B-C2B	8.87	1.49	1.39
24	C	514	BCR	C8-C9	-8.85	1.27	1.46
24	c	514	BCR	C8-C9	-8.81	1.27	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	BCR	C8-C9	-8.78	1.27	1.46
24	C	514	BCR	C12-C13	-8.77	1.27	1.46
24	K	102	BCR	C8-C9	-8.76	1.27	1.46
24	k	102	BCR	C8-C9	-8.75	1.27	1.46
22	B	612	CLA	MG-NA	8.75	2.27	2.06
24	D	404	BCR	C8-C9	-8.75	1.27	1.46
24	c	514	BCR	C12-C13	-8.74	1.27	1.46
24	h	101	BCR	C19-C18	-8.72	1.27	1.46
24	H	101	BCR	C19-C18	-8.70	1.27	1.46
22	b	612	CLA	MG-NA	8.70	2.26	2.06
24	k	101	BCR	C19-C18	-8.69	1.27	1.46
24	B	622	BCR	C8-C9	-8.69	1.27	1.46
24	b	622	BCR	C8-C9	-8.68	1.27	1.46
24	c	515	BCR	C8-C9	-8.67	1.27	1.46
24	C	515	BCR	C8-C9	-8.64	1.27	1.46
24	K	101	BCR	C19-C18	-8.64	1.27	1.46
24	K	101	BCR	C8-C9	-8.63	1.27	1.46
24	T	102	BCR	C8-C9	-8.61	1.27	1.46
24	k	101	BCR	C8-C9	-8.59	1.27	1.46
24	t	101	BCR	C8-C9	-8.59	1.27	1.46
24	b	622	BCR	C12-C13	-8.57	1.27	1.46
24	c	515	BCR	C19-C18	-8.54	1.27	1.46
24	B	622	BCR	C12-C13	-8.54	1.27	1.46
24	D	404	BCR	C19-C18	-8.54	1.27	1.46
24	C	514	BCR	C19-C18	-8.52	1.27	1.46
24	d	404	BCR	C19-C18	-8.52	1.27	1.46
24	K	101	BCR	C12-C13	-8.51	1.27	1.46
24	t	101	BCR	C12-C13	-8.51	1.27	1.46
24	c	514	BCR	C19-C18	-8.50	1.27	1.46
24	B	618	BCR	C8-C9	-8.50	1.27	1.46
24	k	101	BCR	C12-C13	-8.50	1.27	1.46
24	T	101	BCR	C8-C9	-8.50	1.27	1.46
24	C	515	BCR	C12-C13	-8.49	1.27	1.46
24	C	515	BCR	C19-C18	-8.49	1.27	1.46
22	B	604	CLA	MG-NA	8.48	2.26	2.06
24	H	101	BCR	C12-C13	-8.47	1.27	1.46
24	T	102	BCR	C12-C13	-8.47	1.27	1.46
24	H	101	BCR	C8-C9	-8.47	1.27	1.46
24	h	101	BCR	C8-C9	-8.46	1.27	1.46
22	b	604	CLA	MG-NA	8.45	2.26	2.06
24	c	515	BCR	C12-C13	-8.45	1.27	1.46
24	h	101	BCR	C12-C13	-8.44	1.27	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	619	BCR	C8-C9	-8.43	1.27	1.46
24	b	618	BCR	C8-C9	-8.42	1.27	1.46
24	k	102	BCR	C19-C18	-8.42	1.27	1.46
24	K	102	BCR	C19-C18	-8.42	1.27	1.46
24	a	608	BCR	C8-C9	-8.41	1.28	1.46
24	A	608	BCR	C8-C9	-8.39	1.28	1.46
24	b	622	BCR	C19-C18	-8.38	1.28	1.46
24	B	622	BCR	C19-C18	-8.37	1.28	1.46
24	d	404	BCR	C12-C13	-8.36	1.28	1.46
24	B	619	BCR	C19-C18	-8.35	1.28	1.46
24	D	404	BCR	C12-C13	-8.34	1.28	1.46
24	b	618	BCR	C19-C18	-8.33	1.28	1.46
24	k	102	BCR	C12-C13	-8.31	1.28	1.46
24	B	618	BCR	C12-C13	-8.31	1.28	1.46
24	T	101	BCR	C12-C13	-8.31	1.28	1.46
24	K	102	BCR	C12-C13	-8.29	1.28	1.46
24	A	608	BCR	C12-C13	-8.27	1.28	1.46
24	a	608	BCR	C12-C13	-8.24	1.28	1.46
24	A	608	BCR	C19-C18	-8.24	1.28	1.46
24	b	618	BCR	C12-C13	-8.20	1.28	1.46
24	t	101	BCR	C19-C18	-8.20	1.28	1.46
24	a	608	BCR	C19-C18	-8.18	1.28	1.46
24	B	619	BCR	C12-C13	-8.18	1.28	1.46
24	T	102	BCR	C19-C18	-8.16	1.28	1.46
22	c	502	CLA	MG-NA	8.15	2.25	2.06
22	C	502	CLA	MG-NA	8.13	2.25	2.06
24	B	618	BCR	C19-C18	-8.10	1.28	1.46
24	T	101	BCR	C19-C18	-8.05	1.28	1.46
22	c	504	CLA	MG-NC	7.98	2.25	2.06
22	C	504	CLA	MG-NC	7.97	2.25	2.06
33	F	101	HEM	C3D-C2D	7.67	1.53	1.36
33	f	101	HEM	C3D-C2D	7.66	1.53	1.36
24	d	404	BCR	C20-C21	-7.50	1.19	1.43
24	k	101	BCR	C20-C21	-7.48	1.20	1.43
24	D	404	BCR	C20-C21	-7.47	1.20	1.43
24	K	101	BCR	C20-C21	-7.46	1.20	1.43
24	C	514	BCR	C20-C21	-7.46	1.20	1.43
24	h	101	BCR	C20-C21	-7.46	1.20	1.43
24	c	514	BCR	C20-C21	-7.45	1.20	1.43
24	H	101	BCR	C20-C21	-7.44	1.20	1.43
24	c	514	BCR	C16-C17	-7.42	1.20	1.43
24	c	515	BCR	C16-C17	-7.42	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	BCR	C16-C17	-7.41	1.20	1.43
22	B	611	CLA	MG-NA	7.40	2.23	2.06
24	K	101	BCR	C16-C17	-7.40	1.20	1.43
24	C	515	BCR	C16-C17	-7.39	1.20	1.43
22	b	611	CLA	MG-NA	7.39	2.23	2.06
24	C	515	BCR	C20-C21	-7.38	1.20	1.43
24	c	515	BCR	C20-C21	-7.37	1.20	1.43
24	k	101	BCR	C16-C17	-7.36	1.20	1.43
24	k	102	BCR	C20-C21	-7.34	1.20	1.43
24	K	102	BCR	C20-C21	-7.33	1.20	1.43
24	d	404	BCR	C16-C17	-7.30	1.20	1.43
24	D	404	BCR	C16-C17	-7.29	1.20	1.43
24	H	101	BCR	C16-C17	-7.29	1.20	1.43
24	B	622	BCR	C16-C17	-7.29	1.20	1.43
24	b	622	BCR	C16-C17	-7.28	1.20	1.43
24	h	101	BCR	C16-C17	-7.28	1.20	1.43
24	A	608	BCR	C20-C21	-7.28	1.20	1.43
24	b	622	BCR	C20-C21	-7.28	1.20	1.43
33	V	201	HEM	C3D-C2D	7.26	1.52	1.36
24	a	608	BCR	C20-C21	-7.26	1.20	1.43
24	B	622	BCR	C20-C21	-7.25	1.20	1.43
24	t	101	BCR	C16-C17	-7.24	1.20	1.43
24	b	618	BCR	C20-C21	-7.24	1.20	1.43
24	T	102	BCR	C16-C17	-7.24	1.20	1.43
33	v	201	HEM	C3D-C2D	7.22	1.52	1.36
24	B	619	BCR	C20-C21	-7.21	1.20	1.43
24	A	608	BCR	C16-C17	-7.21	1.20	1.43
24	K	102	BCR	C16-C17	-7.20	1.20	1.43
22	a	603	CLA	MG-NA	7.20	2.23	2.06
24	k	102	BCR	C16-C17	-7.20	1.20	1.43
24	a	608	BCR	C16-C17	-7.20	1.20	1.43
24	t	101	BCR	C20-C21	-7.18	1.20	1.43
24	T	102	BCR	C20-C21	-7.17	1.21	1.43
22	A	603	CLA	MG-NA	7.17	2.23	2.06
24	B	618	BCR	C20-C21	-7.15	1.21	1.43
24	T	101	BCR	C20-C21	-7.12	1.21	1.43
24	T	101	BCR	C16-C17	-7.06	1.21	1.43
24	B	618	BCR	C16-C17	-7.05	1.21	1.43
24	B	619	BCR	C16-C17	-7.04	1.21	1.43
24	b	618	BCR	C16-C17	-7.04	1.21	1.43
22	b	615	CLA	MG-NC	7.02	2.22	2.06
22	B	615	CLA	MG-NC	7.01	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	MG-NC	6.97	2.22	2.06
22	b	602	CLA	MG-NC	6.92	2.22	2.06
22	C	504	CLA	MG-NA	6.86	2.22	2.06
22	c	504	CLA	MG-NA	6.85	2.22	2.06
22	c	513	CLA	MG-NC	6.77	2.22	2.06
22	C	513	CLA	MG-NC	6.76	2.22	2.06
22	b	617	CLA	MG-NA	6.68	2.22	2.06
22	B	617	CLA	MG-NA	6.67	2.22	2.06
23	A	606	PHO	C3B-C4B	6.57	1.48	1.41
22	B	610	CLA	MG-NA	6.55	2.21	2.06
22	b	610	CLA	MG-NA	6.54	2.21	2.06
23	a	606	PHO	C3B-C4B	6.52	1.48	1.41
22	b	615	CLA	MG-NA	6.39	2.21	2.06
22	B	615	CLA	MG-NA	6.39	2.21	2.06
22	b	610	CLA	MG-NC	6.37	2.21	2.06
22	B	610	CLA	MG-NC	6.31	2.21	2.06
22	b	609	CLA	MG-NA	6.27	2.21	2.06
22	B	609	CLA	MG-NA	6.26	2.21	2.06
22	B	611	CLA	MG-NC	6.08	2.20	2.06
22	b	611	CLA	MG-NC	6.08	2.20	2.06
22	a	607	CLA	MG-NC	6.03	2.20	2.06
22	A	607	CLA	MG-NC	6.02	2.20	2.06
22	d	403	CLA	MG-NC	6.00	2.20	2.06
22	D	403	CLA	MG-NC	5.98	2.20	2.06
22	D	401	CLA	MG-NA	5.98	2.20	2.06
24	B	622	BCR	C16-C15	-5.98	1.19	1.36
24	b	622	BCR	C16-C15	-5.97	1.19	1.36
24	c	514	BCR	C16-C15	-5.97	1.19	1.36
22	d	401	CLA	MG-NA	5.96	2.20	2.06
24	C	514	BCR	C16-C15	-5.94	1.20	1.36
23	A	606	PHO	C3B-C2B	5.93	1.48	1.40
23	a	606	PHO	C3B-C2B	5.92	1.48	1.40
24	C	515	BCR	C16-C15	-5.86	1.20	1.36
24	k	101	BCR	C16-C15	-5.86	1.20	1.36
24	c	515	BCR	C16-C15	-5.85	1.20	1.36
24	K	101	BCR	C16-C15	-5.85	1.20	1.36
22	D	401	CLA	MG-NC	5.77	2.20	2.06
22	d	401	CLA	MG-NC	5.77	2.20	2.06
24	a	608	BCR	C16-C15	-5.77	1.20	1.36
24	h	101	BCR	C16-C15	-5.76	1.20	1.36
24	B	618	BCR	C16-C15	-5.74	1.20	1.36
24	H	101	BCR	C16-C15	-5.74	1.20	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	608	BCR	C16-C15	-5.74	1.20	1.36
24	T	101	BCR	C16-C15	-5.73	1.20	1.36
24	D	404	BCR	C16-C15	-5.73	1.20	1.36
24	d	404	BCR	C16-C15	-5.72	1.20	1.36
24	k	102	BCR	C16-C15	-5.72	1.20	1.36
24	K	102	BCR	C16-C15	-5.71	1.20	1.36
24	T	102	BCR	C16-C15	-5.71	1.20	1.36
24	c	514	BCR	C11-C12	-5.70	1.19	1.34
24	t	101	BCR	C16-C15	-5.69	1.20	1.36
24	k	101	BCR	C11-C12	-5.69	1.19	1.34
22	A	607	CLA	MG-NA	5.69	2.19	2.06
24	C	514	BCR	C11-C12	-5.67	1.19	1.34
22	a	607	CLA	MG-NA	5.67	2.19	2.06
22	c	503	CLA	MG-NA	5.67	2.19	2.06
22	C	503	CLA	MG-NA	5.66	2.19	2.06
24	a	608	BCR	C20-C19	-5.66	1.19	1.34
24	K	101	BCR	C11-C12	-5.66	1.19	1.34
24	C	515	BCR	C20-C19	-5.65	1.19	1.34
24	D	404	BCR	C20-C19	-5.62	1.20	1.34
23	A	606	PHO	C4D-CHA	5.62	1.47	1.39
24	c	515	BCR	C20-C19	-5.62	1.20	1.34
24	A	608	BCR	C20-C19	-5.62	1.20	1.34
24	K	101	BCR	C20-C19	-5.61	1.20	1.34
24	T	102	BCR	C11-C12	-5.60	1.20	1.34
24	h	101	BCR	C20-C19	-5.58	1.20	1.34
24	H	101	BCR	C20-C19	-5.58	1.20	1.34
24	b	622	BCR	C11-C12	-5.57	1.20	1.34
24	t	101	BCR	C11-C12	-5.57	1.20	1.34
23	a	606	PHO	C4D-CHA	5.57	1.47	1.39
24	k	101	BCR	C20-C19	-5.57	1.20	1.34
24	d	404	BCR	C20-C19	-5.56	1.20	1.34
24	B	622	BCR	C11-C12	-5.56	1.20	1.34
24	c	514	BCR	C20-C19	-5.56	1.20	1.34
24	C	514	BCR	C20-C19	-5.55	1.20	1.34
24	D	404	BCR	C11-C12	-5.54	1.20	1.34
24	d	404	BCR	C11-C12	-5.54	1.20	1.34
23	a	605	PHO	C3B-C4B	5.52	1.47	1.41
23	A	605	PHO	C3B-C2B	5.50	1.47	1.40
24	B	622	BCR	C20-C19	-5.49	1.20	1.34
23	A	605	PHO	C3B-C4B	5.49	1.47	1.41
24	c	515	BCR	C11-C12	-5.48	1.20	1.34
24	b	622	BCR	C20-C19	-5.47	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	605	PHO	C3B-C2B	5.46	1.47	1.40
24	h	101	BCR	C11-C12	-5.46	1.20	1.34
24	K	102	BCR	C20-C19	-5.45	1.20	1.34
24	K	102	BCR	C11-C12	-5.44	1.20	1.34
24	C	515	BCR	C11-C12	-5.44	1.20	1.34
24	H	101	BCR	C11-C12	-5.44	1.20	1.34
24	k	102	BCR	C20-C19	-5.44	1.20	1.34
24	k	102	BCR	C11-C12	-5.42	1.20	1.34
22	c	508	CLA	C3C-C2C	5.42	1.48	1.36
24	T	102	BCR	C20-C19	-5.41	1.20	1.34
22	B	606	CLA	MG-NC	5.39	2.19	2.06
24	t	101	BCR	C20-C19	-5.38	1.20	1.34
22	b	606	CLA	MG-NC	5.38	2.19	2.06
22	C	508	CLA	C3C-C2C	5.38	1.48	1.36
22	b	603	CLA	C3C-C2C	5.38	1.48	1.36
24	B	619	BCR	C16-C15	-5.35	1.21	1.36
22	c	512	CLA	C3C-C2C	5.34	1.48	1.36
22	C	513	CLA	C3C-C2C	5.34	1.48	1.36
22	B	603	CLA	C3C-C2C	5.33	1.48	1.36
24	b	618	BCR	C16-C15	-5.33	1.21	1.36
24	b	618	BCR	C20-C19	-5.32	1.20	1.34
22	C	512	CLA	C3C-C2C	5.32	1.48	1.36
24	B	619	BCR	C20-C19	-5.31	1.20	1.34
24	b	618	BCR	C11-C12	-5.30	1.20	1.34
22	c	513	CLA	C3C-C2C	5.30	1.48	1.36
24	B	619	BCR	C11-C12	-5.30	1.20	1.34
22	b	603	CLA	CHC-C1C	5.29	1.49	1.38
24	B	618	BCR	C11-C12	-5.27	1.20	1.34
22	C	503	CLA	C3C-C2C	5.26	1.48	1.36
22	B	617	CLA	MG-NC	5.26	2.18	2.06
24	a	608	BCR	C11-C12	-5.26	1.21	1.34
22	B	603	CLA	CHC-C1C	5.25	1.49	1.38
24	T	101	BCR	C11-C12	-5.24	1.21	1.34
22	b	617	CLA	MG-NC	5.23	2.18	2.06
24	A	608	BCR	C11-C12	-5.23	1.21	1.34
22	B	602	CLA	O2D-CGD	5.23	1.46	1.33
24	C	514	BCR	C11-C10	-5.23	1.27	1.43
22	b	602	CLA	O2D-CGD	5.22	1.46	1.33
23	a	605	PHO	C4D-CHA	5.22	1.47	1.39
22	c	503	CLA	C3C-C2C	5.21	1.48	1.36
24	c	514	BCR	C11-C10	-5.20	1.27	1.43
22	b	616	CLA	C3C-C2C	5.19	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	C3C-C2C	5.18	1.48	1.36
22	B	616	CLA	C3C-C2C	5.18	1.47	1.36
22	C	509	CLA	MG-NB	-5.18	1.95	2.05
22	B	613	CLA	CHC-C1C	5.17	1.48	1.38
22	b	602	CLA	C3C-C2C	5.17	1.47	1.36
22	b	613	CLA	CHC-C1C	5.16	1.48	1.38
22	A	603	CLA	C3C-C2C	5.16	1.47	1.36
22	C	507	CLA	C3C-C2C	5.16	1.47	1.36
22	C	502	CLA	CHC-C1C	5.16	1.48	1.38
22	B	602	CLA	C3C-C2C	5.15	1.47	1.36
22	c	509	CLA	MG-NB	-5.15	1.95	2.05
22	c	502	CLA	CHC-C1C	5.15	1.48	1.38
24	H	101	BCR	C11-C10	-5.15	1.27	1.43
24	h	101	BCR	C11-C10	-5.14	1.27	1.43
23	A	605	PHO	C4D-CHA	5.14	1.47	1.39
24	d	404	BCR	C11-C10	-5.13	1.27	1.43
24	D	404	BCR	C11-C10	-5.13	1.27	1.43
22	B	607	CLA	C3C-C2C	5.13	1.47	1.36
22	B	606	CLA	C3C-C2C	5.13	1.47	1.36
24	C	515	BCR	C11-C10	-5.12	1.27	1.43
22	C	513	CLA	O2D-CGD	5.11	1.45	1.33
22	c	512	CLA	CHC-C1C	5.11	1.48	1.38
22	B	611	CLA	C3C-C2C	5.10	1.47	1.36
22	a	603	CLA	C3C-C2C	5.10	1.47	1.36
22	b	607	CLA	C3C-C2C	5.09	1.47	1.36
22	c	509	CLA	O2D-CGD	5.09	1.45	1.33
24	c	515	BCR	C11-C10	-5.09	1.27	1.43
22	c	513	CLA	O2D-CGD	5.09	1.45	1.33
22	b	606	CLA	C3C-C2C	5.09	1.47	1.36
22	C	512	CLA	CHC-C1C	5.08	1.48	1.38
22	c	513	CLA	CHC-C1C	5.08	1.48	1.38
22	c	506	CLA	O2D-CGD	5.08	1.45	1.33
22	C	513	CLA	CHC-C1C	5.08	1.48	1.38
22	C	509	CLA	O2D-CGD	5.08	1.45	1.33
22	c	503	CLA	CHC-C1C	5.07	1.48	1.38
22	b	611	CLA	C3C-C2C	5.07	1.47	1.36
22	C	511	CLA	O2D-CGD	5.07	1.45	1.33
22	C	503	CLA	CHC-C1C	5.07	1.48	1.38
24	T	101	BCR	C20-C19	-5.06	1.21	1.34
24	b	622	BCR	C11-C10	-5.06	1.27	1.43
22	c	507	CLA	O2D-CGD	5.06	1.45	1.33
22	b	602	CLA	CHC-C1C	5.06	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	622	BCR	C11-C10	-5.06	1.27	1.43
22	c	511	CLA	O2D-CGD	5.06	1.45	1.33
22	C	506	CLA	O2D-CGD	5.06	1.45	1.33
22	c	508	CLA	O2D-CGD	5.05	1.45	1.33
24	K	101	BCR	C11-C10	-5.05	1.27	1.43
22	C	508	CLA	MG-NB	5.05	2.15	2.05
24	C	514	BCR	C15-C14	-5.05	1.27	1.43
22	d	403	CLA	C3C-C2C	5.05	1.47	1.36
22	C	505	CLA	C3C-C2C	5.05	1.47	1.36
22	c	505	CLA	C3C-C2C	5.05	1.47	1.36
22	D	403	CLA	C3C-C2C	5.05	1.47	1.36
24	k	101	BCR	C11-C10	-5.04	1.27	1.43
24	c	514	BCR	C15-C14	-5.03	1.27	1.43
22	C	508	CLA	O2D-CGD	5.02	1.45	1.33
24	B	618	BCR	C20-C19	-5.02	1.21	1.34
22	A	607	CLA	C3C-C2C	5.02	1.47	1.36
22	c	508	CLA	MG-NB	5.02	2.15	2.05
22	C	508	CLA	MG-NC	5.01	2.18	2.06
22	B	602	CLA	CHC-C1C	5.01	1.48	1.38
22	c	508	CLA	MG-NC	5.01	2.18	2.06
22	b	609	CLA	C3C-C2C	5.01	1.47	1.36
22	C	507	CLA	O2D-CGD	5.00	1.45	1.33
24	B	622	BCR	C15-C14	-5.00	1.27	1.43
24	A	608	BCR	C11-C10	-5.00	1.27	1.43
22	B	609	CLA	C3C-C2C	5.00	1.47	1.36
24	C	515	BCR	C15-C14	-5.00	1.27	1.43
22	c	510	CLA	C3C-C2C	5.00	1.47	1.36
22	C	506	CLA	C3C-C2C	5.00	1.47	1.36
22	C	510	CLA	C3C-C2C	5.00	1.47	1.36
24	b	622	BCR	C15-C14	-4.99	1.27	1.43
22	C	507	CLA	CHC-C1C	4.99	1.48	1.38
22	C	501	CLA	CHC-C1C	4.99	1.48	1.38
22	B	609	CLA	O2D-CGD	4.99	1.45	1.33
22	C	512	CLA	O2D-CGD	4.99	1.45	1.33
24	a	608	BCR	C11-C10	-4.99	1.27	1.43
24	H	101	BCR	C15-C14	-4.99	1.27	1.43
22	c	501	CLA	CHC-C1C	4.98	1.48	1.38
22	a	607	CLA	C3C-C2C	4.98	1.47	1.36
24	c	515	BCR	C15-C14	-4.98	1.27	1.43
22	c	507	CLA	CHC-C1C	4.98	1.48	1.38
22	C	511	CLA	C3C-C2C	4.98	1.47	1.36
22	c	512	CLA	O2D-CGD	4.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	CHC-C1C	4.98	1.48	1.38
22	b	609	CLA	O2D-CGD	4.98	1.45	1.33
24	h	101	BCR	C15-C14	-4.97	1.27	1.43
24	k	102	BCR	C11-C10	-4.97	1.27	1.43
22	c	506	CLA	C3C-C2C	4.97	1.47	1.36
24	K	102	BCR	C11-C10	-4.97	1.27	1.43
22	b	606	CLA	CHC-C1C	4.96	1.48	1.38
22	B	608	CLA	C3C-C2C	4.96	1.47	1.36
24	B	622	BCR	C23-C22	-4.95	1.35	1.46
24	C	515	BCR	C23-C22	-4.95	1.35	1.46
23	A	606	PHO	OBD-CAD	4.95	1.28	1.22
22	C	502	CLA	O2D-CGD	4.95	1.45	1.33
22	c	506	CLA	CHC-C1C	4.95	1.48	1.38
22	b	608	CLA	MG-NC	4.95	2.18	2.06
22	c	511	CLA	C3C-C2C	4.94	1.47	1.36
24	T	102	BCR	C11-C10	-4.94	1.27	1.43
24	T	101	BCR	C11-C10	-4.94	1.27	1.43
24	b	622	BCR	C23-C22	-4.94	1.35	1.46
22	C	506	CLA	CHC-C1C	4.94	1.48	1.38
24	k	101	BCR	C15-C14	-4.94	1.27	1.43
24	K	101	BCR	C15-C14	-4.93	1.27	1.43
22	b	607	CLA	CHC-C1C	4.93	1.48	1.38
22	B	607	CLA	O2D-CGD	4.93	1.45	1.33
22	b	608	CLA	C3C-C2C	4.93	1.47	1.36
22	c	505	CLA	O2D-CGD	4.93	1.45	1.33
22	b	614	CLA	C3C-C2C	4.93	1.47	1.36
22	c	509	CLA	C3C-C2C	4.93	1.47	1.36
24	d	404	BCR	C15-C14	-4.93	1.27	1.43
24	t	101	BCR	C11-C10	-4.93	1.27	1.43
24	B	618	BCR	C11-C10	-4.93	1.27	1.43
24	D	404	BCR	C15-C14	-4.93	1.27	1.43
24	t	101	BCR	C15-C14	-4.92	1.27	1.43
24	T	102	BCR	C15-C14	-4.92	1.27	1.43
22	c	502	CLA	O2D-CGD	4.91	1.45	1.33
23	a	606	PHO	OBD-CAD	4.91	1.28	1.22
22	C	505	CLA	CHC-C1C	4.91	1.48	1.38
23	A	606	PHO	O2D-CGD	4.91	1.45	1.33
22	b	617	CLA	C3C-C2C	4.91	1.47	1.36
24	c	515	BCR	C23-C22	-4.90	1.35	1.46
22	B	607	CLA	CHC-C1C	4.90	1.48	1.38
22	C	509	CLA	C3C-C2C	4.90	1.47	1.36
22	B	614	CLA	C3C-C2C	4.90	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	606	PHO	O2D-CGD	4.90	1.45	1.33
22	C	505	CLA	O2D-CGD	4.90	1.45	1.33
22	b	607	CLA	O2D-CGD	4.89	1.45	1.33
22	B	608	CLA	MG-NC	4.89	2.17	2.06
24	k	102	BCR	C15-C14	-4.89	1.28	1.43
22	A	607	CLA	CHC-C1C	4.89	1.48	1.38
22	C	501	CLA	C3C-C2C	4.88	1.47	1.36
22	B	610	CLA	C3C-C2C	4.88	1.47	1.36
22	b	610	CLA	C3C-C2C	4.88	1.47	1.36
22	C	504	CLA	C3C-C2C	4.88	1.47	1.36
22	B	614	CLA	CHC-C1C	4.88	1.48	1.38
33	F	101	HEM	FE-NC	4.88	2.11	1.95
22	B	611	CLA	CHC-C1C	4.88	1.48	1.38
22	B	617	CLA	C3C-C2C	4.87	1.47	1.36
22	d	403	CLA	CHC-C1C	4.87	1.48	1.38
24	K	102	BCR	C15-C14	-4.87	1.28	1.43
22	c	505	CLA	CHC-C1C	4.87	1.48	1.38
22	C	509	CLA	CHD-C1D	4.87	1.47	1.38
33	f	101	HEM	FE-NC	4.87	2.11	1.95
22	d	402	CLA	C3C-C2C	4.87	1.47	1.36
22	b	611	CLA	CHC-C1C	4.86	1.48	1.38
22	c	510	CLA	O2D-CGD	4.85	1.45	1.33
22	D	402	CLA	C3C-C2C	4.85	1.47	1.36
22	c	501	CLA	C3C-C2C	4.85	1.47	1.36
22	B	605	CLA	C3C-C2C	4.84	1.47	1.36
22	c	509	CLA	CHD-C1D	4.84	1.47	1.38
24	A	608	BCR	C15-C14	-4.84	1.28	1.43
22	a	607	CLA	CHC-C1C	4.84	1.48	1.38
23	A	606	PHO	C3D-C4D	-4.84	1.34	1.41
22	C	510	CLA	O2D-CGD	4.84	1.45	1.33
22	c	504	CLA	C3C-C2C	4.84	1.47	1.36
24	D	404	BCR	C23-C22	-4.84	1.35	1.46
22	c	508	CLA	CHC-C1C	4.84	1.48	1.38
33	v	201	HEM	FE-ND	4.84	2.09	1.94
24	d	404	BCR	C23-C22	-4.84	1.35	1.46
22	b	614	CLA	CHC-C1C	4.83	1.48	1.38
22	C	508	CLA	CHC-C1C	4.83	1.48	1.38
24	B	619	BCR	C11-C10	-4.83	1.28	1.43
22	d	401	CLA	C3C-C2C	4.83	1.47	1.36
33	V	201	HEM	FE-ND	4.83	2.09	1.94
22	b	615	CLA	C3C-C2C	4.83	1.47	1.36
22	D	401	CLA	C3C-C2C	4.83	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	BCR	C11-C10	-4.83	1.28	1.43
22	B	606	CLA	O2D-CGD	4.83	1.45	1.33
33	F	101	HEM	FE-ND	4.82	2.09	1.94
22	B	616	CLA	O2D-CGD	4.82	1.45	1.33
22	b	606	CLA	O2D-CGD	4.82	1.45	1.33
22	c	502	CLA	C3C-C2C	4.82	1.47	1.36
24	a	608	BCR	C15-C14	-4.82	1.28	1.43
22	D	403	CLA	CHC-C1C	4.82	1.48	1.38
22	B	604	CLA	O2D-CGD	4.82	1.45	1.33
22	B	617	CLA	O2D-CGD	4.81	1.45	1.33
22	B	615	CLA	C3C-C2C	4.81	1.47	1.36
33	f	101	HEM	FE-ND	4.81	2.09	1.94
22	A	603	CLA	O2D-CGD	4.81	1.45	1.33
22	b	605	CLA	C3C-C2C	4.81	1.47	1.36
22	a	603	CLA	O2D-CGD	4.80	1.45	1.33
22	C	502	CLA	C3C-C2C	4.80	1.47	1.36
22	b	617	CLA	O2D-CGD	4.80	1.45	1.33
24	K	101	BCR	C23-C22	-4.80	1.35	1.46
22	b	616	CLA	O2D-CGD	4.80	1.45	1.33
22	b	604	CLA	O2D-CGD	4.80	1.45	1.33
24	T	101	BCR	C23-C22	-4.79	1.35	1.46
22	b	615	CLA	CHC-C1C	4.79	1.48	1.38
22	b	602	CLA	O2A-CGA	4.79	1.47	1.33
24	B	618	BCR	C23-C22	-4.79	1.35	1.46
22	B	602	CLA	O2A-CGA	4.79	1.47	1.33
22	B	615	CLA	CHC-C1C	4.78	1.48	1.38
24	K	102	BCR	C23-C22	-4.78	1.35	1.46
24	k	101	BCR	C23-C22	-4.77	1.35	1.46
22	b	617	CLA	CHC-C1C	4.77	1.48	1.38
22	b	613	CLA	C3C-C2C	4.77	1.47	1.36
23	a	606	PHO	C3D-C4D	-4.77	1.34	1.41
24	C	514	BCR	C23-C22	-4.77	1.35	1.46
24	H	101	BCR	C23-C22	-4.76	1.35	1.46
24	k	102	BCR	C23-C22	-4.76	1.35	1.46
22	B	613	CLA	O2D-CGD	4.76	1.44	1.33
22	B	611	CLA	CHD-C1D	4.75	1.47	1.38
22	B	613	CLA	C3C-C2C	4.75	1.47	1.36
24	c	514	BCR	C23-C22	-4.75	1.35	1.46
22	b	613	CLA	O2D-CGD	4.75	1.44	1.33
22	b	611	CLA	CHD-C1D	4.74	1.47	1.38
22	b	610	CLA	CHC-C1C	4.74	1.48	1.38
22	B	617	CLA	CHC-C1C	4.74	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	CHD-C1D	4.74	1.47	1.38
22	B	616	CLA	CHC-C1C	4.74	1.48	1.38
22	D	402	CLA	MG-NA	4.74	2.17	2.06
22	C	513	CLA	CHD-C1D	4.73	1.47	1.38
22	C	503	CLA	O2D-CGD	4.73	1.44	1.33
22	c	503	CLA	O2D-CGD	4.73	1.44	1.33
22	A	604	CLA	C3C-C2C	4.73	1.47	1.36
22	B	608	CLA	O2D-CGD	4.73	1.44	1.33
22	b	608	CLA	O2D-CGD	4.72	1.44	1.33
22	b	616	CLA	CHC-C1C	4.72	1.47	1.38
22	c	511	CLA	CHC-C1C	4.72	1.47	1.38
22	c	511	CLA	MG-NC	4.72	2.17	2.06
22	B	615	CLA	O2D-CGD	4.72	1.44	1.33
22	B	610	CLA	CHC-C1C	4.72	1.47	1.38
22	d	402	CLA	MG-NA	4.72	2.17	2.06
24	h	101	BCR	C23-C22	-4.71	1.35	1.46
22	c	505	CLA	CHD-C1D	4.71	1.47	1.38
22	A	603	CLA	CHC-C1C	4.71	1.47	1.38
22	b	615	CLA	O2D-CGD	4.71	1.44	1.33
22	a	603	CLA	CHC-C1C	4.70	1.47	1.38
22	C	511	CLA	MG-NC	4.70	2.17	2.06
22	a	604	CLA	C3C-C2C	4.69	1.46	1.36
22	C	511	CLA	CHC-C1C	4.68	1.47	1.38
22	C	509	CLA	CHC-C1C	4.68	1.47	1.38
22	b	609	CLA	MG-NC	4.68	2.17	2.06
22	b	604	CLA	C3C-C2C	4.68	1.46	1.36
22	C	505	CLA	CHD-C1D	4.68	1.47	1.38
22	B	604	CLA	C3C-C2C	4.68	1.46	1.36
24	B	619	BCR	C15-C14	-4.68	1.28	1.43
22	c	509	CLA	CHC-C1C	4.67	1.47	1.38
22	c	501	CLA	CHD-C1D	4.67	1.47	1.38
22	c	504	CLA	O2D-CGD	4.67	1.44	1.33
24	b	618	BCR	C15-C14	-4.67	1.28	1.43
22	B	609	CLA	MG-NC	4.67	2.17	2.06
22	A	604	CLA	O2D-CGD	4.67	1.44	1.33
22	C	504	CLA	O2D-CGD	4.67	1.44	1.33
22	D	401	CLA	O2D-CGD	4.67	1.44	1.33
22	B	608	CLA	CHC-C1C	4.66	1.47	1.38
22	D	403	CLA	O2D-CGD	4.66	1.44	1.33
22	C	507	CLA	CHD-C1D	4.66	1.47	1.38
22	a	607	CLA	C3D-C4D	-4.66	1.33	1.44
22	c	507	CLA	CHD-C1D	4.65	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	607	CLA	C3D-C4D	-4.65	1.33	1.44
24	B	618	BCR	C15-C14	-4.65	1.28	1.43
24	T	101	BCR	C15-C14	-4.64	1.28	1.43
22	c	512	CLA	CHD-C1D	4.64	1.47	1.38
22	d	403	CLA	O2D-CGD	4.64	1.44	1.33
22	C	512	CLA	CHD-C1D	4.64	1.47	1.38
22	B	612	CLA	C3C-C2C	4.63	1.46	1.36
23	a	605	PHO	C3D-C4D	-4.63	1.34	1.41
22	B	615	CLA	CHD-C1D	4.63	1.47	1.38
22	a	604	CLA	O2D-CGD	4.63	1.44	1.33
22	b	612	CLA	C3C-C2C	4.62	1.46	1.36
22	d	401	CLA	O2D-CGD	4.61	1.44	1.33
22	D	403	CLA	CHB-C1B	4.61	1.49	1.39
22	C	501	CLA	CHD-C1D	4.61	1.47	1.38
22	b	608	CLA	CHC-C1C	4.60	1.47	1.38
23	A	605	PHO	C3D-C4D	-4.59	1.35	1.41
22	d	403	CLA	CHB-C1B	4.59	1.49	1.39
24	b	618	BCR	C23-C22	-4.59	1.36	1.46
22	B	607	CLA	CHD-C1D	4.59	1.47	1.38
29	b	619	LMG	O8-C28	4.58	1.46	1.33
22	b	604	CLA	CHC-C1C	4.58	1.47	1.38
22	c	501	CLA	O2D-CGD	4.58	1.44	1.33
22	B	608	CLA	CHB-C1B	4.58	1.49	1.39
22	C	501	CLA	O2D-CGD	4.58	1.44	1.33
22	b	615	CLA	CHD-C1D	4.58	1.47	1.38
22	b	608	CLA	CHB-C1B	4.57	1.49	1.39
24	B	619	BCR	C23-C22	-4.57	1.36	1.46
22	C	504	CLA	CHC-C1C	4.57	1.47	1.38
23	a	605	PHO	O2D-CGD	4.57	1.44	1.33
25	D	411	SQD	O48-C23	4.56	1.46	1.33
29	B	620	LMG	O8-C28	4.56	1.46	1.33
22	c	504	CLA	CHC-C1C	4.56	1.47	1.38
22	b	605	CLA	CHD-C1D	4.55	1.47	1.38
22	c	506	CLA	CHB-C1B	4.55	1.49	1.39
22	B	611	CLA	O2D-CGD	4.55	1.44	1.33
23	A	605	PHO	O2D-CGD	4.55	1.44	1.33
22	b	611	CLA	O2D-CGD	4.55	1.44	1.33
22	B	606	CLA	CHB-C1B	4.54	1.49	1.39
22	b	614	CLA	CHB-C1B	4.54	1.49	1.39
22	b	602	CLA	CHD-C1D	4.53	1.47	1.38
22	c	510	CLA	CHB-C1B	4.53	1.49	1.39
22	b	607	CLA	CHD-C1D	4.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	410	DGD	O1G-C1A	4.53	1.46	1.33
22	C	510	CLA	CHB-C1B	4.52	1.49	1.39
22	b	614	CLA	O2D-CGD	4.52	1.44	1.33
22	C	506	CLA	CHB-C1B	4.52	1.49	1.39
25	d	411	SQD	O48-C23	4.52	1.46	1.33
22	b	606	CLA	CHB-C1B	4.52	1.49	1.39
29	C	520	LMG	O7-C10	4.52	1.47	1.34
29	c	520	LMG	O7-C10	4.52	1.47	1.34
24	T	102	BCR	C23-C22	-4.52	1.36	1.46
24	t	101	BCR	C23-C22	-4.52	1.36	1.46
22	B	603	CLA	CHB-C1B	4.51	1.49	1.39
22	B	604	CLA	CHC-C1C	4.51	1.47	1.38
22	B	614	CLA	CHB-C1B	4.51	1.49	1.39
22	C	511	CLA	CHB-C1B	4.51	1.49	1.39
22	B	614	CLA	O2D-CGD	4.51	1.44	1.33
31	d	410	DGD	O1G-C1A	4.51	1.46	1.33
25	b	601	SQD	O48-C23	4.51	1.46	1.33
22	b	603	CLA	CHB-C1B	4.50	1.49	1.39
32	e	101	LHG	O8-C23	4.50	1.46	1.33
22	B	607	CLA	MG-NC	4.50	2.17	2.06
22	B	605	CLA	CHD-C1D	4.50	1.47	1.38
22	c	511	CLA	CHB-C1B	4.49	1.49	1.39
25	B	601	SQD	O48-C23	4.49	1.46	1.33
22	b	607	CLA	MG-NC	4.49	2.16	2.06
25	D	411	SQD	O47-C7	4.49	1.47	1.34
22	c	504	CLA	CHD-C1D	4.49	1.47	1.38
22	B	602	CLA	CHD-C1D	4.48	1.47	1.38
31	D	410	DGD	O2G-C1B	4.48	1.46	1.34
22	C	504	CLA	CHD-C1D	4.48	1.47	1.38
25	d	411	SQD	O47-C7	4.48	1.46	1.34
22	b	610	CLA	O2D-CGD	4.48	1.44	1.33
22	c	513	CLA	CHB-C1B	4.48	1.49	1.39
22	B	612	CLA	O2D-CGD	4.48	1.44	1.33
32	E	101	LHG	O8-C23	4.48	1.46	1.33
22	b	612	CLA	O2D-CGD	4.48	1.44	1.33
22	C	513	CLA	CHB-C1B	4.47	1.49	1.39
22	c	512	CLA	CHB-C1B	4.47	1.49	1.39
22	B	610	CLA	O2D-CGD	4.47	1.44	1.33
31	d	410	DGD	O2G-C1B	4.47	1.46	1.34
24	a	608	BCR	C23-C22	-4.46	1.36	1.46
22	B	615	CLA	CHB-C1B	4.46	1.49	1.39
22	c	504	CLA	CHB-C1B	4.45	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	CHB-C1B	4.45	1.49	1.39
25	l	102	SQD	O48-C23	4.45	1.46	1.33
22	C	512	CLA	CHB-C1B	4.45	1.49	1.39
22	B	602	CLA	CHC-C4B	4.44	1.49	1.39
22	A	607	CLA	CHB-C1B	4.44	1.49	1.39
22	b	615	CLA	CHB-C1B	4.44	1.49	1.39
22	D	403	CLA	CHD-C1D	4.44	1.47	1.38
22	C	506	CLA	CHD-C1D	4.44	1.47	1.38
22	b	607	CLA	CHB-C1B	4.44	1.49	1.39
22	C	504	CLA	CHB-C1B	4.44	1.49	1.39
22	c	508	CLA	CHB-C1B	4.44	1.49	1.39
22	c	508	CLA	CHD-C1D	4.44	1.47	1.38
22	B	611	CLA	C3D-C4D	-4.44	1.34	1.44
22	c	506	CLA	CHD-C1D	4.43	1.47	1.38
22	C	508	CLA	CHB-C1B	4.43	1.49	1.39
22	B	603	CLA	CHD-C1D	4.43	1.47	1.38
22	C	502	CLA	MG-NC	4.43	2.16	2.06
22	c	507	CLA	CHB-C1B	4.43	1.49	1.39
25	b	621	SQD	O48-C23	4.43	1.46	1.33
22	a	607	CLA	CHB-C1B	4.43	1.49	1.39
22	C	507	CLA	CHB-C1B	4.42	1.49	1.39
24	A	608	BCR	C23-C22	-4.42	1.36	1.46
22	c	510	CLA	C3D-C4D	-4.42	1.34	1.44
22	b	602	CLA	CHC-C4B	4.42	1.49	1.39
25	l	102	SQD	O47-C7	4.42	1.46	1.34
22	C	510	CLA	C3D-C4D	-4.42	1.34	1.44
22	B	603	CLA	O2D-CGD	4.42	1.44	1.33
22	b	605	CLA	O2D-CGD	4.41	1.44	1.33
22	B	605	CLA	O2D-CGD	4.41	1.44	1.33
22	C	508	CLA	CHD-C1D	4.41	1.47	1.38
22	c	502	CLA	MG-NC	4.41	2.16	2.06
22	B	607	CLA	CHB-C1B	4.41	1.49	1.39
22	d	403	CLA	C3D-C4D	-4.40	1.34	1.44
22	b	611	CLA	C3D-C4D	-4.40	1.34	1.44
22	d	403	CLA	CHD-C1D	4.40	1.47	1.38
25	b	621	SQD	O47-C7	4.40	1.46	1.34
22	B	604	CLA	CHD-C1D	4.40	1.47	1.38
22	D	403	CLA	C3D-C4D	-4.39	1.34	1.44
22	c	505	CLA	CHB-C1B	4.39	1.49	1.39
22	b	603	CLA	O2D-CGD	4.39	1.44	1.33
22	b	604	CLA	CHD-C1D	4.39	1.47	1.38
22	b	603	CLA	CHD-C1D	4.38	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	520	LMG	O8-C28	4.38	1.46	1.33
25	l	101	SQD	O47-C7	4.38	1.46	1.34
22	B	616	CLA	CHD-C1D	4.37	1.46	1.38
22	B	608	CLA	CHD-C1D	4.37	1.46	1.38
33	f	101	HEM	FE-NA	4.37	2.09	1.95
22	C	510	CLA	CHD-C1D	4.36	1.46	1.38
33	F	101	HEM	FE-NA	4.36	2.09	1.95
22	c	511	CLA	CHD-C1D	4.36	1.46	1.38
25	L	101	SQD	O47-C7	4.36	1.46	1.34
22	c	506	CLA	O2A-CGA	4.36	1.46	1.33
22	b	608	CLA	CHD-C1D	4.36	1.46	1.38
29	c	520	LMG	O8-C28	4.34	1.46	1.33
22	B	605	CLA	CHB-C1B	4.34	1.49	1.39
22	C	510	CLA	CHC-C1C	4.34	1.47	1.38
22	c	504	CLA	CHD-C4C	4.34	1.49	1.39
22	c	510	CLA	CHC-C1C	4.33	1.47	1.38
22	C	506	CLA	O2A-CGA	4.33	1.46	1.33
22	b	609	CLA	CHD-C1D	4.33	1.46	1.38
22	b	616	CLA	CHD-C1D	4.33	1.46	1.38
22	b	604	CLA	CHB-C1B	4.33	1.49	1.39
22	B	609	CLA	CHD-C1D	4.31	1.46	1.38
22	A	604	CLA	CHD-C1D	4.31	1.46	1.38
22	A	604	CLA	CHC-C1C	4.31	1.47	1.38
22	a	604	CLA	CHD-C1D	4.31	1.46	1.38
22	C	511	CLA	CHD-C1D	4.31	1.46	1.38
22	b	605	CLA	CHB-C1B	4.30	1.49	1.39
22	a	607	CLA	O2D-CGD	4.30	1.43	1.33
22	B	604	CLA	CHB-C1B	4.30	1.49	1.39
22	b	605	CLA	CHC-C1C	4.30	1.47	1.38
22	a	604	CLA	CHC-C1C	4.30	1.47	1.38
22	A	607	CLA	O2D-CGD	4.30	1.43	1.33
22	c	510	CLA	CHD-C1D	4.30	1.46	1.38
22	C	503	CLA	CHD-C1D	4.30	1.46	1.38
22	B	612	CLA	CHC-C1C	4.29	1.47	1.38
29	z	101	LMG	O7-C10	4.29	1.46	1.34
22	c	503	CLA	CHD-C1D	4.29	1.46	1.38
22	c	505	CLA	C3D-C4D	-4.29	1.34	1.44
22	b	612	CLA	CHC-C1C	4.29	1.47	1.38
22	D	401	CLA	O2A-CGA	4.28	1.45	1.33
29	c	519	LMG	O8-C28	4.28	1.45	1.33
22	B	605	CLA	CHC-C1C	4.28	1.47	1.38
25	b	601	SQD	O47-C7	4.28	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	SQD	O47-C7	4.28	1.46	1.34
22	C	512	CLA	C3D-C4D	-4.28	1.34	1.44
22	C	504	CLA	CHD-C4C	4.28	1.48	1.39
22	b	608	CLA	C3D-C4D	-4.27	1.34	1.44
22	C	505	CLA	C3D-C4D	-4.27	1.34	1.44
22	C	509	CLA	O2A-CGA	4.27	1.45	1.33
29	Z	101	LMG	O7-C10	4.27	1.46	1.34
22	b	617	CLA	O2A-CGA	4.27	1.45	1.33
22	B	610	CLA	CHB-C1B	4.27	1.49	1.39
29	C	519	LMG	O8-C28	4.26	1.45	1.33
22	B	608	CLA	C3D-C4D	-4.26	1.34	1.44
22	b	613	CLA	CHB-C1B	4.26	1.49	1.39
22	c	512	CLA	O2A-CGA	4.26	1.45	1.33
22	C	513	CLA	CHC-C4B	4.26	1.49	1.39
22	c	509	CLA	O2A-CGA	4.26	1.45	1.33
22	b	610	CLA	CHB-C1B	4.26	1.49	1.39
22	c	513	CLA	CHC-C4B	4.26	1.49	1.39
22	B	617	CLA	O2A-CGA	4.25	1.45	1.33
22	C	506	CLA	C3D-C4D	-4.25	1.34	1.44
29	c	519	LMG	O7-C10	4.25	1.46	1.34
22	c	512	CLA	C3D-C4D	-4.25	1.34	1.44
32	E	101	LHG	O7-C7	4.25	1.46	1.34
22	b	606	CLA	CHD-C1D	4.25	1.46	1.38
22	A	607	CLA	CHD-C1D	4.25	1.46	1.38
29	A	614	LMG	O7-C10	4.25	1.46	1.34
22	B	613	CLA	CHB-C1B	4.25	1.48	1.39
22	C	513	CLA	C3D-C4D	-4.24	1.34	1.44
22	C	504	CLA	C3D-C4D	-4.24	1.34	1.44
22	c	506	CLA	C3D-C4D	-4.24	1.34	1.44
29	a	614	LMG	O7-C10	4.24	1.46	1.34
22	c	504	CLA	C3D-C4D	-4.24	1.34	1.44
22	C	507	CLA	O2A-CGA	4.24	1.45	1.33
29	A	614	LMG	O8-C28	4.24	1.45	1.33
22	C	502	CLA	CHD-C1D	4.24	1.46	1.38
22	c	507	CLA	O2A-CGA	4.24	1.45	1.33
23	A	606	PHO	C3D-C2D	4.23	1.46	1.39
32	e	101	LHG	O7-C7	4.23	1.46	1.34
29	a	614	LMG	O8-C28	4.23	1.45	1.33
22	c	513	CLA	C3D-C4D	-4.23	1.34	1.44
22	C	511	CLA	C3D-C4D	-4.22	1.34	1.44
22	c	502	CLA	CHD-C1D	4.22	1.46	1.38
22	d	401	CLA	O2A-CGA	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	C3D-C4D	-4.22	1.34	1.44
29	C	519	LMG	O7-C10	4.22	1.46	1.34
22	C	512	CLA	O2A-CGA	4.22	1.45	1.33
22	a	607	CLA	CHD-C1D	4.22	1.46	1.38
22	B	610	CLA	CHD-C1D	4.21	1.46	1.38
22	C	507	CLA	C3D-C4D	-4.21	1.34	1.44
22	b	609	CLA	C3D-C4D	-4.21	1.34	1.44
22	B	605	CLA	C3D-C4D	-4.20	1.34	1.44
22	c	501	CLA	CHB-C1B	4.20	1.48	1.39
23	a	606	PHO	C3D-C2D	4.20	1.46	1.39
22	C	503	CLA	CHC-C4B	4.20	1.48	1.39
22	D	402	CLA	O2D-CGD	4.20	1.43	1.33
22	a	607	CLA	O2A-CGA	4.20	1.45	1.33
22	C	503	CLA	O2A-CGA	4.20	1.45	1.33
22	b	610	CLA	CHD-C1D	4.19	1.46	1.38
22	c	501	CLA	C3D-C4D	-4.19	1.34	1.44
22	c	511	CLA	C3D-C4D	-4.19	1.34	1.44
22	B	606	CLA	CHD-C1D	4.19	1.46	1.38
22	c	507	CLA	C3D-C4D	-4.18	1.34	1.44
22	c	503	CLA	CHC-C4B	4.18	1.48	1.39
22	c	509	CLA	C3D-C4D	-4.18	1.34	1.44
22	c	513	CLA	O2A-CGA	4.18	1.45	1.33
22	b	609	CLA	CHC-C1C	4.18	1.46	1.38
22	b	605	CLA	C3D-C4D	-4.18	1.34	1.44
22	c	503	CLA	O2A-CGA	4.18	1.45	1.33
22	b	602	CLA	C3D-C4D	-4.18	1.34	1.44
22	C	501	CLA	CHB-C1B	4.17	1.48	1.39
22	C	509	CLA	C3D-C4D	-4.17	1.34	1.44
22	A	607	CLA	O2A-CGA	4.17	1.45	1.33
22	D	401	CLA	CHC-C1C	4.17	1.46	1.38
22	C	513	CLA	O2A-CGA	4.17	1.45	1.33
22	d	402	CLA	O2D-CGD	4.17	1.43	1.33
22	d	403	CLA	O2A-CGA	4.16	1.45	1.33
22	b	616	CLA	CHB-C1B	4.16	1.48	1.39
22	C	502	CLA	C3D-C4D	-4.16	1.34	1.44
22	d	401	CLA	CHC-C1C	4.16	1.46	1.38
22	B	616	CLA	CHB-C1B	4.16	1.48	1.39
22	c	503	CLA	C3D-C4D	-4.16	1.34	1.44
22	b	604	CLA	C3D-C4D	-4.16	1.34	1.44
22	C	503	CLA	C3D-C4D	-4.16	1.34	1.44
22	C	501	CLA	C3D-C4D	-4.15	1.34	1.44
22	b	616	CLA	O2A-CGA	4.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	511	CLA	O2A-CGA	4.15	1.45	1.33
22	B	602	CLA	C3D-C4D	-4.15	1.34	1.44
22	B	609	CLA	CHC-C1C	4.15	1.46	1.38
22	b	614	CLA	C3D-C4D	-4.14	1.34	1.44
22	c	505	CLA	CHC-C4B	4.14	1.48	1.39
22	D	402	CLA	CHC-C1C	4.14	1.46	1.38
22	D	403	CLA	O2A-CGA	4.14	1.45	1.33
22	c	501	CLA	CHD-C4C	4.14	1.48	1.39
22	B	616	CLA	O2A-CGA	4.14	1.45	1.33
22	B	614	CLA	C3D-C4D	-4.14	1.34	1.44
22	C	511	CLA	O2A-CGA	4.13	1.45	1.33
22	c	502	CLA	C3D-C4D	-4.13	1.34	1.44
25	A	609	SQD	O47-C7	4.13	1.46	1.34
32	d	409	LHG	O8-C23	4.13	1.45	1.33
22	a	603	CLA	CHB-C1B	4.13	1.48	1.39
32	D	409	LHG	O8-C23	4.13	1.45	1.33
22	C	512	CLA	CHD-C4C	4.13	1.48	1.39
25	a	609	SQD	O47-C7	4.13	1.45	1.34
22	B	604	CLA	C3D-C4D	-4.13	1.34	1.44
22	C	505	CLA	CHC-C4B	4.13	1.48	1.39
25	L	101	SQD	O48-C23	4.13	1.45	1.33
22	d	402	CLA	CHC-C1C	4.13	1.46	1.38
22	c	512	CLA	CHD-C4C	4.13	1.48	1.39
22	C	508	CLA	C3D-C4D	-4.13	1.34	1.44
22	C	502	CLA	CHB-C1B	4.13	1.48	1.39
22	C	509	CLA	MG-NC	4.13	2.16	2.06
22	A	603	CLA	CHB-C1B	4.12	1.48	1.39
22	B	617	CLA	CHB-C1B	4.12	1.48	1.39
22	C	503	CLA	CHB-C1B	4.12	1.48	1.39
22	c	509	CLA	MG-NC	4.12	2.16	2.06
22	B	610	CLA	C3D-C4D	-4.12	1.34	1.44
22	C	501	CLA	CHC-C4B	4.12	1.48	1.39
22	b	603	CLA	CHC-C4B	4.12	1.48	1.39
22	b	617	CLA	CHB-C1B	4.12	1.48	1.39
22	c	502	CLA	CHB-C1B	4.12	1.48	1.39
22	B	603	CLA	CHC-C4B	4.12	1.48	1.39
22	B	611	CLA	CHB-C1B	4.12	1.48	1.39
22	b	611	CLA	CHB-C1B	4.12	1.48	1.39
22	b	610	CLA	O2A-CGA	4.11	1.45	1.33
25	l	101	SQD	O48-C23	4.11	1.45	1.33
22	C	501	CLA	CHD-C4C	4.11	1.48	1.39
22	A	604	CLA	C3D-C4D	-4.11	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	517	DGD	O1G-C1A	4.10	1.45	1.33
22	c	503	CLA	CHB-C1B	4.10	1.48	1.39
31	c	517	DGD	O1G-C1A	4.10	1.45	1.33
22	c	508	CLA	C3D-C4D	-4.10	1.35	1.44
22	C	502	CLA	O2A-CGA	4.09	1.45	1.33
22	B	610	CLA	O2A-CGA	4.09	1.45	1.33
22	b	610	CLA	C3D-C4D	-4.09	1.35	1.44
22	b	607	CLA	C3D-C4D	-4.08	1.35	1.44
22	a	604	CLA	C3D-C4D	-4.08	1.35	1.44
22	B	615	CLA	C3D-C4D	-4.08	1.35	1.44
22	B	607	CLA	C3D-C4D	-4.08	1.35	1.44
22	c	501	CLA	CHC-C4B	4.07	1.48	1.39
22	C	501	CLA	O2A-CGA	4.07	1.45	1.33
22	c	509	CLA	CHB-C1B	4.07	1.48	1.39
22	b	607	CLA	O2A-CGA	4.07	1.45	1.33
22	b	615	CLA	O2A-CGA	4.07	1.45	1.33
22	C	509	CLA	CHB-C1B	4.07	1.48	1.39
22	c	502	CLA	O2A-CGA	4.07	1.45	1.33
22	B	607	CLA	O2A-CGA	4.07	1.45	1.33
22	d	402	CLA	MG-NC	4.07	2.15	2.06
22	D	402	CLA	MG-NC	4.06	2.15	2.06
22	c	507	CLA	CHC-C4B	4.06	1.48	1.39
22	c	501	CLA	O2A-CGA	4.06	1.45	1.33
22	b	615	CLA	C3D-C4D	-4.06	1.35	1.44
22	C	507	CLA	CHC-C4B	4.05	1.48	1.39
22	B	602	CLA	CHB-C1B	4.05	1.48	1.39
22	B	615	CLA	O2A-CGA	4.05	1.45	1.33
32	L	102	LHG	O8-C23	4.04	1.45	1.33
22	b	602	CLA	MG-NB	4.03	2.13	2.05
22	b	613	CLA	C3D-C4D	-4.03	1.35	1.44
22	B	613	CLA	C3D-C4D	-4.03	1.35	1.44
22	a	607	CLA	CHC-C4B	4.03	1.48	1.39
32	l	103	LHG	O8-C23	4.03	1.45	1.33
22	b	602	CLA	CHB-C1B	4.03	1.48	1.39
22	b	604	CLA	O2A-CGA	4.03	1.45	1.33
22	a	603	CLA	CHD-C1D	4.03	1.46	1.38
22	C	501	CLA	MG-NC	4.03	2.15	2.06
22	B	602	CLA	MG-NB	4.03	2.13	2.05
22	C	508	CLA	O2A-CGA	4.03	1.45	1.33
25	A	609	SQD	O48-C23	4.02	1.45	1.33
22	c	510	CLA	MG-ND	-4.02	1.97	2.05
22	C	504	CLA	O2A-CGA	4.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	CHD-C4C	4.02	1.48	1.39
22	A	607	CLA	CHC-C4B	4.01	1.48	1.39
22	b	608	CLA	CHD-C4C	4.01	1.48	1.39
22	b	612	CLA	C3D-C4D	-4.01	1.35	1.44
22	C	510	CLA	MG-ND	-4.01	1.97	2.05
22	c	508	CLA	O2A-CGA	4.01	1.45	1.33
22	B	612	CLA	C3D-C4D	-4.01	1.35	1.44
22	C	509	CLA	OBD-CAD	4.01	1.29	1.22
25	a	609	SQD	O48-C23	4.01	1.45	1.33
22	c	501	CLA	MG-NC	4.00	2.15	2.06
22	c	509	CLA	OBD-CAD	4.00	1.29	1.22
23	a	605	PHO	OBD-CAD	4.00	1.27	1.22
22	b	613	CLA	CHD-C4C	4.00	1.48	1.39
31	h	102	DGD	O1G-C1A	4.00	1.45	1.33
22	c	504	CLA	O2A-CGA	4.00	1.45	1.33
23	A	605	PHO	OBD-CAD	3.99	1.27	1.22
32	d	405	LHG	O8-C23	3.99	1.45	1.33
22	B	608	CLA	CHD-C4C	3.99	1.48	1.39
22	C	506	CLA	CHD-C4C	3.99	1.48	1.39
22	B	613	CLA	CHD-C1D	3.99	1.46	1.38
22	B	604	CLA	O2A-CGA	3.98	1.45	1.33
22	b	611	CLA	CHC-C4B	3.98	1.48	1.39
22	c	510	CLA	O2A-CGA	3.98	1.45	1.33
32	D	405	LHG	O8-C23	3.98	1.45	1.33
31	H	102	DGD	O1G-C1A	3.98	1.45	1.33
31	c	516	DGD	O2G-C1B	3.98	1.45	1.34
29	b	619	LMG	O7-C10	3.97	1.45	1.34
22	A	607	CLA	OBD-CAD	3.97	1.29	1.22
22	B	603	CLA	MG-NC	3.97	2.15	2.06
32	d	407	LHG	O8-C23	3.97	1.44	1.33
22	A	603	CLA	CHD-C1D	3.97	1.46	1.38
22	b	612	CLA	CHD-C1D	3.96	1.46	1.38
22	b	603	CLA	MG-NC	3.96	2.15	2.06
22	B	612	CLA	CHB-C1B	3.96	1.48	1.39
22	C	510	CLA	O2A-CGA	3.96	1.44	1.33
22	A	603	CLA	C3D-C4D	-3.96	1.35	1.44
22	D	402	CLA	O2A-CGA	3.96	1.44	1.33
31	C	516	DGD	O2G-C1B	3.96	1.45	1.34
22	c	506	CLA	CHC-C4B	3.96	1.48	1.39
22	d	402	CLA	O2A-CGA	3.96	1.44	1.33
22	C	512	CLA	CHC-C4B	3.95	1.48	1.39
22	b	612	CLA	CHB-C1B	3.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	CHC-C4B	3.95	1.48	1.39
32	D	407	LHG	O8-C23	3.95	1.44	1.33
22	C	506	CLA	CHC-C4B	3.95	1.48	1.39
22	C	505	CLA	CHD-C4C	3.95	1.48	1.39
22	a	603	CLA	C3D-C4D	-3.95	1.35	1.44
22	B	603	CLA	CHD-C4C	3.95	1.48	1.39
22	c	503	CLA	CHD-C4C	3.95	1.48	1.39
23	a	605	PHO	O2A-CGA	3.95	1.44	1.33
22	b	613	CLA	CHD-C1D	3.95	1.46	1.38
22	B	602	CLA	CHD-C4C	3.95	1.48	1.39
22	c	507	CLA	CHD-C4C	3.95	1.48	1.39
22	B	611	CLA	CHC-C4B	3.94	1.48	1.39
31	C	518	DGD	O1G-C1A	3.94	1.44	1.33
22	c	506	CLA	CHD-C4C	3.94	1.48	1.39
22	B	612	CLA	CHD-C1D	3.94	1.46	1.38
22	c	505	CLA	CHD-C4C	3.94	1.48	1.39
22	d	403	CLA	CHD-C4C	3.94	1.48	1.39
22	a	603	CLA	CHC-C4B	3.94	1.48	1.39
29	D	406	LMG	O7-C10	3.94	1.45	1.34
29	B	620	LMG	O7-C10	3.94	1.45	1.34
22	b	607	CLA	CHD-C4C	3.94	1.48	1.39
22	d	403	CLA	CHC-C4B	3.94	1.48	1.39
22	a	607	CLA	OBD-CAD	3.94	1.29	1.22
22	b	603	CLA	CHD-C4C	3.93	1.48	1.39
31	c	518	DGD	O1G-C1A	3.93	1.44	1.33
22	b	602	CLA	CHD-C4C	3.93	1.48	1.39
22	b	617	CLA	C3D-C4D	-3.93	1.35	1.44
22	B	616	CLA	CHD-C4C	3.93	1.48	1.39
22	B	607	CLA	CHC-C4B	3.93	1.48	1.39
22	C	503	CLA	CHD-C4C	3.93	1.48	1.39
29	d	406	LMG	O7-C10	3.93	1.45	1.34
22	b	609	CLA	O2A-CGA	3.93	1.44	1.33
23	A	605	PHO	O2A-CGA	3.93	1.44	1.33
22	b	613	CLA	CHC-C4B	3.93	1.48	1.39
22	c	512	CLA	CHC-C4B	3.93	1.48	1.39
22	c	510	CLA	OBD-CAD	3.93	1.29	1.22
32	D	409	LHG	O7-C7	3.93	1.45	1.34
22	B	603	CLA	C3D-C4D	-3.92	1.35	1.44
22	b	603	CLA	C3D-C4D	-3.92	1.35	1.44
22	D	403	CLA	CHC-C4B	3.92	1.48	1.39
22	A	603	CLA	CHC-C4B	3.92	1.48	1.39
32	d	409	LHG	O7-C7	3.92	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	CHD-C4C	3.92	1.48	1.39
22	B	609	CLA	O2A-CGA	3.92	1.44	1.33
31	c	516	DGD	O1G-C1A	3.92	1.44	1.33
22	B	613	CLA	CHC-C4B	3.91	1.48	1.39
22	B	607	CLA	CHD-C4C	3.91	1.48	1.39
22	C	508	CLA	CHC-C4B	3.91	1.48	1.39
22	c	508	CLA	CHC-C4B	3.91	1.48	1.39
22	c	511	CLA	CHD-C4C	3.91	1.48	1.39
22	D	403	CLA	CHD-C4C	3.90	1.48	1.39
22	b	616	CLA	CHD-C4C	3.90	1.48	1.39
22	C	511	CLA	CHD-C4C	3.89	1.48	1.39
22	C	510	CLA	OBD-CAD	3.89	1.29	1.22
22	B	617	CLA	C3D-C4D	-3.89	1.35	1.44
31	C	516	DGD	O1G-C1A	3.89	1.44	1.33
22	c	505	CLA	O2A-CGA	3.89	1.44	1.33
22	B	611	CLA	O2A-CGA	3.88	1.44	1.33
22	c	513	CLA	CHD-C4C	3.88	1.48	1.39
22	C	510	CLA	CHD-C4C	3.87	1.48	1.39
22	b	609	CLA	CHB-C1B	3.87	1.48	1.39
22	C	513	CLA	CHD-C4C	3.87	1.48	1.39
31	H	102	DGD	O2G-C1B	3.87	1.45	1.34
31	h	102	DGD	O2G-C1B	3.87	1.45	1.34
22	C	505	CLA	O2A-CGA	3.86	1.44	1.33
22	B	609	CLA	CHB-C1B	3.86	1.48	1.39
22	b	611	CLA	O2A-CGA	3.86	1.44	1.33
22	A	603	CLA	CHD-C4C	3.85	1.48	1.39
22	c	510	CLA	CHD-C4C	3.85	1.48	1.39
22	d	402	CLA	OBD-CAD	3.85	1.29	1.22
22	B	617	CLA	CHD-C1D	3.85	1.45	1.38
22	a	604	CLA	O2A-CGA	3.84	1.44	1.33
22	D	401	CLA	CHC-C4B	3.83	1.48	1.39
22	d	401	CLA	CHC-C4B	3.83	1.48	1.39
22	B	610	CLA	CHC-C4B	3.83	1.48	1.39
22	a	603	CLA	OBD-CAD	3.83	1.29	1.22
22	B	617	CLA	CHC-C4B	3.83	1.48	1.39
22	b	606	CLA	C3D-C4D	-3.83	1.35	1.44
32	l	103	LHG	O7-C7	3.83	1.45	1.34
22	C	511	CLA	CHC-C4B	3.82	1.48	1.39
22	b	617	CLA	CHD-C1D	3.82	1.45	1.38
32	L	102	LHG	O7-C7	3.82	1.45	1.34
22	b	614	CLA	CHC-C4B	3.82	1.48	1.39
22	B	614	CLA	CHC-C4B	3.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	CHD-C4C	3.82	1.47	1.39
22	b	610	CLA	CHC-C4B	3.81	1.48	1.39
22	B	606	CLA	C3D-C4D	-3.81	1.35	1.44
22	a	603	CLA	CHD-C4C	3.81	1.47	1.39
22	D	402	CLA	OBD-CAD	3.81	1.29	1.22
22	C	502	CLA	CHC-C4B	3.81	1.48	1.39
22	B	617	CLA	OBD-CAD	3.81	1.29	1.22
22	b	614	CLA	CHD-C4C	3.81	1.47	1.39
22	B	605	CLA	O2A-CGA	3.81	1.44	1.33
22	d	401	CLA	CHB-C1B	3.80	1.47	1.39
22	b	617	CLA	OBD-CAD	3.79	1.29	1.22
32	d	407	LHG	O7-C7	3.79	1.45	1.34
22	b	605	CLA	O2A-CGA	3.79	1.44	1.33
22	c	511	CLA	CHC-C4B	3.79	1.47	1.39
22	C	508	CLA	CHD-C4C	3.79	1.47	1.39
22	C	508	CLA	MG-ND	-3.79	1.98	2.05
22	A	604	CLA	O2A-CGA	3.79	1.44	1.33
32	D	407	LHG	O7-C7	3.78	1.45	1.34
33	V	201	HEM	FE-NB	3.78	2.06	1.94
22	c	508	CLA	CHD-C4C	3.78	1.47	1.39
22	b	604	CLA	OBD-CAD	3.78	1.29	1.22
22	D	401	CLA	OBD-CAD	3.78	1.29	1.22
22	c	502	CLA	CHC-C4B	3.78	1.47	1.39
22	A	603	CLA	OBD-CAD	3.78	1.29	1.22
22	D	401	CLA	CHB-C1B	3.78	1.47	1.39
23	a	605	PHO	C3D-C2D	3.78	1.46	1.39
22	B	614	CLA	CHD-C4C	3.77	1.47	1.39
22	d	401	CLA	OBD-CAD	3.77	1.29	1.22
22	b	617	CLA	CHC-C4B	3.77	1.47	1.39
22	C	509	CLA	CHD-C4C	3.76	1.47	1.39
33	v	201	HEM	FE-NB	3.76	2.06	1.94
22	B	606	CLA	CHC-C4B	3.76	1.47	1.39
22	B	616	CLA	C3D-C4D	-3.76	1.35	1.44
31	c	517	DGD	O2G-C1B	3.76	1.44	1.34
22	d	402	CLA	CHC-C4B	3.76	1.47	1.39
22	B	614	CLA	CHD-C1D	3.76	1.45	1.38
22	B	609	CLA	CHD-C4C	3.75	1.47	1.39
22	b	606	CLA	CHC-C4B	3.75	1.47	1.39
22	b	606	CLA	O2A-CGA	3.75	1.44	1.33
22	A	604	CLA	CHD-C4C	3.75	1.47	1.39
22	B	605	CLA	CHD-C4C	3.75	1.47	1.39
22	b	612	CLA	CHC-C4B	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	402	CLA	CHC-C4B	3.74	1.47	1.39
23	A	606	PHO	O2A-CGA	3.74	1.44	1.33
22	B	604	CLA	OBD-CAD	3.74	1.28	1.22
23	a	606	PHO	O2A-CGA	3.74	1.44	1.33
31	C	517	DGD	O2G-C1B	3.74	1.44	1.34
22	b	616	CLA	C3D-C4D	-3.74	1.35	1.44
22	B	603	CLA	OBD-CAD	3.73	1.28	1.22
22	b	603	CLA	OBD-CAD	3.73	1.28	1.22
22	B	606	CLA	O2A-CGA	3.73	1.44	1.33
22	B	614	CLA	O2A-CGA	3.73	1.44	1.33
22	D	401	CLA	C3D-C4D	-3.73	1.35	1.44
22	c	511	CLA	OBD-CAD	3.73	1.28	1.22
22	d	401	CLA	C3D-C4D	-3.73	1.35	1.44
22	C	511	CLA	OBD-CAD	3.72	1.28	1.22
23	A	605	PHO	C3D-C2D	3.72	1.46	1.39
22	a	604	CLA	CHD-C4C	3.72	1.47	1.39
22	a	604	CLA	CHB-C1B	3.72	1.47	1.39
22	c	513	CLA	OBD-CAD	3.72	1.28	1.22
22	b	609	CLA	CHD-C4C	3.72	1.47	1.39
22	B	613	CLA	O2A-CGA	3.72	1.44	1.33
29	d	406	LMG	O8-C28	3.71	1.44	1.33
22	b	614	CLA	O2A-CGA	3.71	1.44	1.33
29	D	406	LMG	O8-C28	3.71	1.44	1.33
22	b	605	CLA	CHD-C4C	3.71	1.47	1.39
22	c	508	CLA	MG-ND	-3.71	1.98	2.05
22	b	614	CLA	CHD-C1D	3.71	1.45	1.38
22	b	607	CLA	OBD-CAD	3.70	1.28	1.22
22	B	612	CLA	CHC-C4B	3.70	1.47	1.39
22	b	613	CLA	O2A-CGA	3.70	1.44	1.33
22	B	616	CLA	CHC-C4B	3.70	1.47	1.39
22	d	402	CLA	CHB-C1B	3.70	1.47	1.39
22	b	616	CLA	CHC-C4B	3.70	1.47	1.39
22	C	513	CLA	OBD-CAD	3.69	1.28	1.22
22	b	611	CLA	CHD-C4C	3.69	1.47	1.39
22	B	616	CLA	MG-NC	3.69	2.15	2.06
22	b	616	CLA	MG-NC	3.69	2.15	2.06
22	B	611	CLA	CHD-C4C	3.69	1.47	1.39
22	D	402	CLA	CHB-C1B	3.68	1.47	1.39
22	A	604	CLA	CHB-C1B	3.68	1.47	1.39
22	B	607	CLA	OBD-CAD	3.67	1.28	1.22
22	c	509	CLA	CHC-C4B	3.67	1.47	1.39
24	c	515	BCR	C21-C22	-3.67	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	604	CLA	OBD-CAD	3.66	1.28	1.22
22	a	607	CLA	CHD-C4C	3.66	1.47	1.39
22	c	513	CLA	MG-ND	-3.66	1.98	2.05
24	k	101	BCR	C21-C22	-3.65	1.27	1.35
22	b	615	CLA	CHD-C4C	3.65	1.47	1.39
22	A	607	CLA	CHD-C4C	3.65	1.47	1.39
22	C	509	CLA	CHC-C4B	3.65	1.47	1.39
22	B	615	CLA	CHD-C4C	3.64	1.47	1.39
24	K	101	BCR	C21-C22	-3.63	1.27	1.35
24	C	515	BCR	C21-C22	-3.63	1.27	1.35
22	b	604	CLA	CHC-C4B	3.63	1.47	1.39
22	C	504	CLA	OBD-CAD	3.62	1.28	1.22
22	B	604	CLA	CHC-C4B	3.62	1.47	1.39
22	c	510	CLA	CHC-C4B	3.62	1.47	1.39
22	d	402	CLA	C3D-C4D	-3.61	1.36	1.44
22	c	502	CLA	OBD-CAD	3.61	1.28	1.22
22	A	604	CLA	OBD-CAD	3.61	1.28	1.22
22	a	603	CLA	MG-ND	-3.60	1.98	2.05
24	D	404	BCR	C21-C22	-3.60	1.27	1.35
24	h	101	BCR	C21-C22	-3.60	1.27	1.35
24	d	404	BCR	C21-C22	-3.60	1.27	1.35
22	C	513	CLA	MG-ND	-3.60	1.98	2.05
22	B	602	CLA	OBD-CAD	3.59	1.28	1.22
24	H	101	BCR	C21-C22	-3.59	1.27	1.35
22	D	402	CLA	C3D-C4D	-3.59	1.36	1.44
22	C	512	CLA	MG-NC	3.59	2.14	2.06
24	B	622	BCR	C21-C22	-3.59	1.27	1.35
22	b	604	CLA	CHD-C4C	3.59	1.47	1.39
22	C	510	CLA	CHC-C4B	3.59	1.47	1.39
22	b	602	CLA	OBD-CAD	3.59	1.28	1.22
22	b	610	CLA	OBD-CAD	3.58	1.28	1.22
24	k	102	BCR	C21-C22	-3.58	1.27	1.35
24	K	102	BCR	C21-C22	-3.58	1.27	1.35
22	c	512	CLA	MG-NC	3.58	2.14	2.06
24	C	514	BCR	C17-C18	-3.58	1.27	1.35
22	c	501	CLA	OBD-CAD	3.58	1.28	1.22
22	c	504	CLA	OBD-CAD	3.58	1.28	1.22
24	c	514	BCR	C17-C18	-3.57	1.27	1.35
22	d	401	CLA	CHD-C1D	3.57	1.45	1.38
22	A	603	CLA	MG-ND	-3.56	1.98	2.05
22	d	402	CLA	CHD-C1D	3.56	1.45	1.38
24	b	622	BCR	C21-C22	-3.56	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	OBD-CAD	3.56	1.28	1.22
22	C	501	CLA	OBD-CAD	3.55	1.28	1.22
22	C	502	CLA	OBD-CAD	3.55	1.28	1.22
24	K	101	BCR	C17-C18	-3.55	1.27	1.35
22	c	507	CLA	OBD-CAD	3.55	1.28	1.22
24	k	101	BCR	C17-C18	-3.55	1.27	1.35
22	D	401	CLA	CHD-C1D	3.55	1.45	1.38
22	A	603	CLA	O2A-CGA	3.55	1.43	1.33
22	B	608	CLA	CHC-C4B	3.55	1.47	1.39
22	B	604	CLA	CHD-C4C	3.55	1.47	1.39
22	b	608	CLA	CHC-C4B	3.54	1.47	1.39
22	B	617	CLA	CHD-C4C	3.54	1.47	1.39
22	C	506	CLA	OBD-CAD	3.53	1.28	1.22
22	B	610	CLA	OBD-CAD	3.53	1.28	1.22
22	D	402	CLA	CHD-C1D	3.53	1.45	1.38
22	b	617	CLA	CHD-C4C	3.53	1.47	1.39
22	b	616	CLA	OBD-CAD	3.53	1.28	1.22
24	c	514	BCR	C21-C22	-3.53	1.27	1.35
22	C	507	CLA	OBD-CAD	3.53	1.28	1.22
22	C	508	CLA	OBD-CAD	3.52	1.28	1.22
24	C	514	BCR	C21-C22	-3.52	1.27	1.35
22	a	603	CLA	O2A-CGA	3.52	1.43	1.33
22	c	504	CLA	CHC-C4B	3.52	1.47	1.39
24	B	619	BCR	C21-C22	-3.52	1.27	1.35
22	C	505	CLA	OBD-CAD	3.51	1.28	1.22
22	b	611	CLA	OBD-CAD	3.50	1.28	1.22
22	d	401	CLA	CHD-C4C	3.50	1.47	1.39
22	b	612	CLA	MG-NC	3.50	2.14	2.06
22	c	506	CLA	OBD-CAD	3.50	1.28	1.22
24	b	618	BCR	C21-C22	-3.50	1.27	1.35
22	B	610	CLA	CHD-C4C	3.50	1.47	1.39
24	A	608	BCR	C17-C18	-3.50	1.27	1.35
22	B	615	CLA	CHC-C4B	3.50	1.47	1.39
22	c	508	CLA	OBD-CAD	3.50	1.28	1.22
22	c	502	CLA	CHD-C4C	3.49	1.47	1.39
22	d	403	CLA	OBD-CAD	3.49	1.28	1.22
22	b	613	CLA	OBD-CAD	3.49	1.28	1.22
22	C	502	CLA	CHD-C4C	3.49	1.47	1.39
22	B	612	CLA	CHD-C4C	3.49	1.47	1.39
22	B	616	CLA	OBD-CAD	3.49	1.28	1.22
22	B	611	CLA	OBD-CAD	3.49	1.28	1.22
22	B	612	CLA	MG-NC	3.49	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	608	BCR	C17-C18	-3.48	1.27	1.35
22	D	401	CLA	CHD-C4C	3.48	1.47	1.39
22	b	615	CLA	CHC-C4B	3.48	1.47	1.39
22	C	504	CLA	CHC-C4B	3.48	1.47	1.39
22	B	612	CLA	O2A-CGA	3.47	1.43	1.33
22	D	403	CLA	OBD-CAD	3.47	1.28	1.22
22	B	603	CLA	O2A-CGA	3.46	1.43	1.33
22	b	612	CLA	O2A-CGA	3.46	1.43	1.33
22	B	613	CLA	OBD-CAD	3.46	1.28	1.22
22	b	603	CLA	O2A-CGA	3.46	1.43	1.33
22	b	612	CLA	CHD-C4C	3.45	1.47	1.39
22	b	610	CLA	CHD-C4C	3.45	1.47	1.39
24	C	515	BCR	C17-C18	-3.45	1.27	1.35
24	T	102	BCR	C21-C22	-3.44	1.27	1.35
24	d	404	BCR	C17-C18	-3.44	1.27	1.35
24	t	101	BCR	C21-C22	-3.44	1.27	1.35
24	D	404	BCR	C17-C18	-3.43	1.27	1.35
24	b	622	BCR	C17-C18	-3.43	1.27	1.35
24	B	622	BCR	C17-C18	-3.43	1.27	1.35
22	b	606	CLA	OBD-CAD	3.42	1.28	1.22
22	C	505	CLA	MG-NC	3.42	2.14	2.06
22	b	605	CLA	CHC-C4B	3.42	1.47	1.39
22	B	605	CLA	CHC-C4B	3.42	1.47	1.39
22	d	402	CLA	CHD-C4C	3.41	1.47	1.39
22	D	402	CLA	CHD-C4C	3.41	1.47	1.39
24	c	515	BCR	C17-C18	-3.41	1.27	1.35
22	c	505	CLA	MG-NC	3.40	2.14	2.06
31	c	518	DGD	O2G-C1B	3.39	1.43	1.34
22	B	606	CLA	OBD-CAD	3.39	1.28	1.22
24	T	101	BCR	C21-C22	-3.39	1.28	1.35
24	H	101	BCR	C17-C18	-3.39	1.28	1.35
22	b	615	CLA	OBD-CAD	3.39	1.28	1.22
24	K	102	BCR	C17-C18	-3.38	1.28	1.35
24	k	102	BCR	C17-C18	-3.38	1.28	1.35
24	h	101	BCR	C17-C18	-3.38	1.28	1.35
22	b	609	CLA	OBD-CAD	3.38	1.28	1.22
31	C	518	DGD	O2G-C1B	3.38	1.43	1.34
22	B	606	CLA	CHD-C4C	3.37	1.46	1.39
24	A	608	BCR	C21-C22	-3.37	1.28	1.35
22	b	603	CLA	C1B-C2B	3.37	1.51	1.43
22	B	608	CLA	OBD-CAD	3.37	1.28	1.22
22	B	603	CLA	C1B-C2B	3.36	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	OBD-CAD	3.36	1.28	1.22
22	B	609	CLA	OBD-CAD	3.35	1.28	1.22
22	C	512	CLA	OBD-CAD	3.35	1.28	1.22
24	a	608	BCR	C21-C22	-3.35	1.28	1.35
22	B	615	CLA	OBD-CAD	3.35	1.28	1.22
24	B	618	BCR	C21-C22	-3.34	1.28	1.35
22	B	616	CLA	C1B-C2B	3.34	1.51	1.43
22	b	616	CLA	C1B-C2B	3.34	1.51	1.43
22	c	512	CLA	OBD-CAD	3.33	1.28	1.22
22	b	606	CLA	CHD-C4C	3.32	1.46	1.39
22	B	614	CLA	MG-NC	3.32	2.14	2.06
22	b	609	CLA	CHC-C4B	3.31	1.46	1.39
22	b	608	CLA	O2A-CGA	3.31	1.43	1.33
22	B	608	CLA	O2A-CGA	3.30	1.43	1.33
22	B	609	CLA	CHC-C4B	3.30	1.46	1.39
22	A	604	CLA	CHC-C4B	3.30	1.46	1.39
33	v	201	HEM	CAB-C3B	3.29	1.56	1.47
22	C	506	CLA	MG-NC	3.29	2.14	2.06
22	c	506	CLA	MG-NC	3.28	2.14	2.06
23	A	606	PHO	C3A-C2A	-3.28	1.51	1.54
22	a	604	CLA	CHC-C4B	3.28	1.46	1.39
22	b	614	CLA	MG-NC	3.28	2.14	2.06
22	b	610	CLA	MG-NB	3.28	2.12	2.05
24	T	102	BCR	C17-C18	-3.27	1.28	1.35
33	V	201	HEM	CAB-C3B	3.27	1.56	1.47
23	a	606	PHO	C3A-C2A	-3.27	1.51	1.54
22	B	610	CLA	MG-NB	3.27	2.12	2.05
22	B	614	CLA	OBD-CAD	3.26	1.28	1.22
24	t	101	BCR	C17-C18	-3.26	1.28	1.35
22	b	614	CLA	OBD-CAD	3.26	1.28	1.22
22	B	605	CLA	C1B-C2B	3.22	1.50	1.43
22	b	612	CLA	OBD-CAD	3.22	1.28	1.22
22	B	612	CLA	OBD-CAD	3.21	1.28	1.22
22	b	605	CLA	C1B-C2B	3.20	1.50	1.43
24	T	101	BCR	C17-C18	-3.19	1.28	1.35
22	c	508	CLA	C3D-C2D	3.18	1.47	1.39
32	D	405	LHG	O7-C7	3.18	1.43	1.34
24	B	618	BCR	C17-C18	-3.18	1.28	1.35
32	d	405	LHG	O7-C7	3.15	1.43	1.34
33	V	201	HEM	CAC-C3C	3.15	1.55	1.47
33	v	201	HEM	CAC-C3C	3.14	1.55	1.47
22	A	603	CLA	MG-NC	3.14	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	C3D-C2D	3.14	1.47	1.39
22	C	504	CLA	MG-NB	3.13	2.12	2.05
22	B	603	CLA	C3D-C2D	3.12	1.47	1.39
22	c	504	CLA	MG-NB	3.11	2.11	2.05
22	C	511	CLA	C1B-C2B	3.10	1.50	1.43
33	f	101	HEM	CAB-C3B	3.10	1.55	1.47
22	b	603	CLA	C3D-C2D	3.10	1.47	1.39
22	a	603	CLA	MG-NC	3.10	2.13	2.06
22	c	511	CLA	C1B-C2B	3.09	1.50	1.43
33	F	101	HEM	CAB-C3B	3.09	1.55	1.47
22	c	505	CLA	C1B-C2B	3.08	1.50	1.43
22	B	604	CLA	MG-NC	3.08	2.13	2.06
22	B	617	CLA	C3D-C2D	3.07	1.47	1.39
22	c	513	CLA	C3D-C2D	3.07	1.47	1.39
22	C	505	CLA	C1B-C2B	3.06	1.50	1.43
22	b	603	CLA	MG-NB	3.06	2.11	2.05
24	b	618	BCR	C17-C18	-3.06	1.28	1.35
22	b	604	CLA	MG-NC	3.06	2.13	2.06
22	b	617	CLA	C3D-C2D	3.06	1.47	1.39
22	B	610	CLA	C1B-C2B	3.06	1.50	1.43
22	C	513	CLA	C3D-C2D	3.06	1.47	1.39
24	B	619	BCR	C17-C18	-3.05	1.28	1.35
22	B	604	CLA	C3D-C2D	3.05	1.47	1.39
22	C	511	CLA	C3D-C2D	3.05	1.47	1.39
22	B	603	CLA	MG-NB	3.04	2.11	2.05
22	b	604	CLA	C3D-C2D	3.04	1.47	1.39
22	c	504	CLA	C3D-C2D	3.04	1.47	1.39
22	C	510	CLA	MG-NB	3.04	2.11	2.05
22	b	610	CLA	C1B-C2B	3.03	1.50	1.43
22	c	511	CLA	C3D-C2D	3.03	1.47	1.39
22	C	504	CLA	C3D-C2D	3.02	1.47	1.39
22	C	512	CLA	C3D-C2D	3.01	1.47	1.39
22	c	510	CLA	MG-NB	3.01	2.11	2.05
22	d	403	CLA	C1B-C2B	3.00	1.50	1.43
22	c	503	CLA	OBD-CAD	3.00	1.27	1.22
22	D	403	CLA	C1B-C2B	3.00	1.50	1.43
22	B	611	CLA	C3D-C2D	3.00	1.47	1.39
22	C	503	CLA	OBD-CAD	2.99	1.27	1.22
22	b	611	CLA	C3D-C2D	2.99	1.47	1.39
22	c	512	CLA	C3D-C2D	2.99	1.47	1.39
33	F	101	HEM	FE-NB	2.99	2.04	1.94
22	b	611	CLA	MG-ND	-2.99	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	CLA	C3D-C2D	2.98	1.47	1.39
22	B	604	CLA	C1B-C2B	2.98	1.50	1.43
22	b	604	CLA	C1B-C2B	2.98	1.50	1.43
33	f	101	HEM	FE-NB	2.98	2.04	1.94
22	c	504	CLA	MG-ND	-2.98	1.99	2.05
22	a	604	CLA	C3D-C2D	2.97	1.47	1.39
22	c	501	CLA	C3D-C2D	2.97	1.47	1.39
22	D	402	CLA	C3D-C2D	2.97	1.47	1.39
22	B	614	CLA	C3D-C2D	2.96	1.47	1.39
22	c	507	CLA	C4D-CHA	2.96	1.48	1.38
22	b	614	CLA	C3D-C2D	2.96	1.47	1.39
33	V	201	HEM	FE-NA	2.96	2.04	1.95
22	B	611	CLA	MG-ND	-2.96	1.99	2.05
22	d	402	CLA	C3D-C2D	2.96	1.47	1.39
22	C	507	CLA	C4D-CHA	2.96	1.48	1.38
22	b	605	CLA	OBD-CAD	2.96	1.27	1.22
33	v	201	HEM	FE-NA	2.95	2.04	1.95
22	D	401	CLA	C1B-C2B	2.95	1.50	1.43
22	A	604	CLA	C1B-C2B	2.95	1.50	1.43
22	a	604	CLA	C1B-C2B	2.95	1.50	1.43
22	A	604	CLA	C3D-C2D	2.95	1.47	1.39
22	C	507	CLA	C1B-C2B	2.95	1.50	1.43
22	C	504	CLA	MG-ND	-2.94	2.00	2.05
22	B	613	CLA	C4B-NB	-2.94	1.34	1.37
33	F	101	HEM	CAC-C3C	2.94	1.55	1.47
22	b	613	CLA	C4B-NB	-2.94	1.34	1.37
22	D	402	CLA	C1B-C2B	2.94	1.50	1.43
22	d	401	CLA	C1B-C2B	2.94	1.50	1.43
22	C	501	CLA	C1B-C2B	2.93	1.50	1.43
22	C	511	CLA	C4D-CHA	2.92	1.48	1.38
22	c	511	CLA	C4D-CHA	2.92	1.48	1.38
33	f	101	HEM	CAC-C3C	2.92	1.55	1.47
22	B	610	CLA	C3D-C2D	2.92	1.46	1.39
22	B	609	CLA	C3D-C2D	2.92	1.46	1.39
22	b	609	CLA	C3D-C2D	2.91	1.46	1.39
22	B	605	CLA	OBD-CAD	2.91	1.27	1.22
28	A	613	PL9	C6-C5	2.91	1.49	1.35
28	a	613	PL9	C6-C5	2.91	1.49	1.35
22	c	507	CLA	C1B-C2B	2.91	1.50	1.43
22	b	615	CLA	C1B-C2B	2.91	1.50	1.43
22	c	501	CLA	C1B-C2B	2.91	1.49	1.43
22	d	402	CLA	C1B-C2B	2.90	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	C3D-C2D	2.90	1.46	1.39
22	b	610	CLA	C3D-C2D	2.89	1.46	1.39
22	B	616	CLA	C3D-C2D	2.89	1.46	1.39
22	b	606	CLA	C3D-C2D	2.89	1.46	1.39
22	b	616	CLA	C3D-C2D	2.89	1.46	1.39
22	c	512	CLA	C1B-C2B	2.89	1.49	1.43
22	d	403	CLA	C3D-C2D	2.89	1.46	1.39
22	C	512	CLA	C1B-C2B	2.88	1.49	1.43
22	C	503	CLA	C1B-C2B	2.88	1.49	1.43
22	b	602	CLA	C4D-CHA	2.88	1.48	1.38
22	B	606	CLA	C1B-C2B	2.88	1.49	1.43
22	B	615	CLA	C1B-C2B	2.87	1.49	1.43
22	B	606	CLA	C3D-C2D	2.87	1.46	1.39
22	B	602	CLA	C4D-CHA	2.87	1.48	1.38
22	c	503	CLA	C1B-C2B	2.87	1.49	1.43
22	b	609	CLA	MG-NB	-2.86	2.00	2.05
23	a	605	PHO	CBD-CGD	-2.85	1.48	1.52
28	d	408	PL9	C6-C5	2.85	1.49	1.35
28	D	408	PL9	C6-C5	2.85	1.49	1.35
22	c	503	CLA	C4D-CHA	2.85	1.48	1.38
22	B	609	CLA	MG-NB	-2.85	2.00	2.05
22	c	501	CLA	C4D-CHA	2.84	1.48	1.38
22	C	501	CLA	C4D-CHA	2.84	1.48	1.38
22	C	513	CLA	C4D-CHA	2.84	1.48	1.38
22	C	503	CLA	C4D-CHA	2.84	1.48	1.38
22	c	510	CLA	C3D-C2D	2.84	1.46	1.39
22	C	510	CLA	C3D-C2D	2.84	1.46	1.39
22	b	606	CLA	C1B-C2B	2.84	1.49	1.43
22	C	512	CLA	C4D-CHA	2.83	1.48	1.38
22	c	505	CLA	C3D-C2D	2.83	1.46	1.39
22	c	512	CLA	C4D-CHA	2.83	1.48	1.38
22	B	608	CLA	C3D-C2D	2.82	1.46	1.39
22	a	603	CLA	C3D-C2D	2.82	1.46	1.39
22	C	509	CLA	C1B-C2B	2.82	1.49	1.43
22	B	615	CLA	C3D-C2D	2.82	1.46	1.39
22	C	507	CLA	C3D-C2D	2.82	1.46	1.39
22	c	502	CLA	C3D-C2D	2.82	1.46	1.39
22	C	505	CLA	C3D-C2D	2.82	1.46	1.39
22	c	507	CLA	C3D-C2D	2.82	1.46	1.39
22	b	615	CLA	C3D-C2D	2.81	1.46	1.39
22	b	608	CLA	C3D-C2D	2.81	1.46	1.39
22	c	509	CLA	C1B-C2B	2.81	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	C1B-C2B	2.81	1.49	1.43
22	c	513	CLA	C4D-CHA	2.81	1.48	1.38
22	C	507	CLA	MG-NC	2.81	2.12	2.06
22	b	607	CLA	C1B-C2B	2.81	1.49	1.43
22	C	505	CLA	MG-ND	-2.81	2.00	2.05
22	C	502	CLA	C3D-C2D	2.81	1.46	1.39
22	c	507	CLA	MG-NC	2.80	2.12	2.06
22	d	402	CLA	C4B-NB	-2.80	1.34	1.37
23	A	605	PHO	CBD-CGD	-2.80	1.49	1.52
22	C	504	CLA	C4D-CHA	2.80	1.48	1.38
22	A	603	CLA	C3D-C2D	2.80	1.46	1.39
22	c	504	CLA	C4D-CHA	2.80	1.48	1.38
22	A	607	CLA	C3D-C2D	2.80	1.46	1.39
22	b	613	CLA	C3D-C2D	2.79	1.46	1.39
22	c	509	CLA	C3D-C2D	2.79	1.46	1.39
22	c	506	CLA	C3D-C2D	2.79	1.46	1.39
22	a	607	CLA	C1B-C2B	2.79	1.49	1.43
22	D	402	CLA	C4B-NB	-2.79	1.34	1.37
22	C	506	CLA	C3D-C2D	2.78	1.46	1.39
22	B	611	CLA	C1B-C2B	2.78	1.49	1.43
22	C	509	CLA	C3D-C2D	2.78	1.46	1.39
22	c	509	CLA	C4D-CHA	2.78	1.47	1.38
22	a	607	CLA	C3D-C2D	2.77	1.46	1.39
22	A	607	CLA	C1B-C2B	2.77	1.49	1.43
22	B	613	CLA	C3D-C2D	2.77	1.46	1.39
22	C	509	CLA	C4D-CHA	2.76	1.47	1.38
22	b	605	CLA	C4D-CHA	2.76	1.47	1.38
22	D	403	CLA	MG-NB	-2.76	2.00	2.05
22	c	505	CLA	MG-ND	-2.75	2.00	2.05
22	C	513	CLA	C1B-C2B	2.75	1.49	1.43
22	c	504	CLA	C1B-C2B	2.75	1.49	1.43
29	z	101	LMG	O8-C28	2.75	1.46	1.33
22	c	513	CLA	C1B-C2B	2.75	1.49	1.43
22	B	607	CLA	C3D-C2D	2.74	1.46	1.39
22	B	605	CLA	C4D-CHA	2.74	1.47	1.38
22	b	611	CLA	C1B-C2B	2.74	1.49	1.43
29	Z	101	LMG	O8-C28	2.74	1.46	1.33
22	d	403	CLA	MG-NB	-2.72	2.00	2.05
22	b	613	CLA	C1B-C2B	2.72	1.49	1.43
31	H	102	DGD	O5D-C1E	2.72	1.44	1.40
22	C	503	CLA	C3D-C2D	2.72	1.46	1.39
22	C	504	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	C3D-C2D	2.71	1.46	1.39
22	b	612	CLA	C3D-C2D	2.71	1.46	1.39
22	b	614	CLA	C1B-C2B	2.71	1.49	1.43
22	b	611	CLA	C4D-CHA	2.71	1.47	1.38
22	b	614	CLA	C4D-CHA	2.70	1.47	1.38
22	B	612	CLA	C3D-C2D	2.70	1.46	1.39
22	B	614	CLA	C4D-CHA	2.70	1.47	1.38
22	C	503	CLA	C1C-C2C	2.69	1.50	1.44
31	h	102	DGD	O5D-C1E	2.69	1.44	1.40
22	c	503	CLA	C3D-C2D	2.69	1.46	1.39
22	a	604	CLA	C4B-NB	-2.69	1.34	1.37
22	c	506	CLA	C4D-CHA	2.69	1.47	1.38
22	c	506	CLA	C1B-C2B	2.69	1.49	1.43
22	B	613	CLA	C1B-C2B	2.69	1.49	1.43
22	B	611	CLA	C4D-CHA	2.69	1.47	1.38
24	k	102	BCR	C24-C25	-2.69	1.35	1.45
24	c	515	BCR	C24-C25	-2.68	1.35	1.45
22	B	614	CLA	C1B-C2B	2.68	1.49	1.43
24	K	102	BCR	C24-C25	-2.68	1.35	1.45
22	C	510	CLA	C1B-C2B	2.68	1.49	1.43
22	B	617	CLA	C1B-C2B	2.68	1.49	1.43
22	b	617	CLA	C1B-C2B	2.68	1.49	1.43
22	c	510	CLA	C1B-C2B	2.67	1.49	1.43
22	C	506	CLA	C4D-CHA	2.67	1.47	1.38
22	C	506	CLA	C1B-C2B	2.67	1.49	1.43
22	A	604	CLA	C4B-NB	-2.67	1.34	1.37
22	C	505	CLA	MG-NB	2.66	2.11	2.05
22	c	503	CLA	C1C-C2C	2.66	1.49	1.44
22	b	607	CLA	C4D-CHA	2.66	1.47	1.38
22	c	505	CLA	C4D-CHA	2.66	1.47	1.38
24	C	515	BCR	C24-C25	-2.65	1.36	1.45
22	c	511	CLA	MG-NB	-2.65	2.00	2.05
22	C	505	CLA	C4D-CHA	2.65	1.47	1.38
24	c	514	BCR	C24-C25	-2.65	1.36	1.45
22	a	607	CLA	MG-NB	-2.65	2.00	2.05
22	A	607	CLA	MG-NB	-2.65	2.00	2.05
22	B	602	CLA	C3D-C2D	2.65	1.46	1.39
22	B	607	CLA	C4D-CHA	2.65	1.47	1.38
24	h	101	BCR	C24-C25	-2.65	1.36	1.45
24	H	101	BCR	C24-C25	-2.64	1.36	1.45
22	C	502	CLA	C4D-CHA	2.64	1.47	1.38
22	b	616	CLA	C4D-CHA	2.64	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	C3D-C2D	2.64	1.46	1.39
24	C	514	BCR	C24-C25	-2.64	1.36	1.45
22	B	615	CLA	C1C-NC	-2.64	1.33	1.37
22	C	511	CLA	MG-NB	-2.63	2.00	2.05
22	c	502	CLA	C4D-CHA	2.63	1.47	1.38
22	B	616	CLA	C4D-CHA	2.63	1.47	1.38
22	b	603	CLA	C4D-CHA	2.63	1.47	1.38
22	B	602	CLA	C1B-C2B	2.62	1.49	1.43
22	b	602	CLA	C1B-C2B	2.62	1.49	1.43
24	k	101	BCR	C24-C25	-2.62	1.36	1.45
22	b	602	CLA	C1D-C2D	2.62	1.50	1.45
22	B	617	CLA	C4D-CHA	2.61	1.47	1.38
22	c	505	CLA	MG-NB	2.61	2.11	2.05
22	b	617	CLA	C4D-CHA	2.61	1.47	1.38
24	K	101	BCR	C24-C25	-2.61	1.36	1.45
22	B	602	CLA	C1D-C2D	2.61	1.50	1.45
22	c	510	CLA	C4D-CHA	2.61	1.47	1.38
22	C	508	CLA	C4D-CHA	2.61	1.47	1.38
22	B	610	CLA	C4D-CHA	2.61	1.47	1.38
22	A	607	CLA	C4D-CHA	2.61	1.47	1.38
22	b	615	CLA	C1C-NC	-2.60	1.33	1.37
22	B	603	CLA	C4D-CHA	2.60	1.47	1.38
22	b	610	CLA	C4D-CHA	2.60	1.47	1.38
22	B	609	CLA	C4D-CHA	2.60	1.47	1.38
22	c	508	CLA	C4D-CHA	2.60	1.47	1.38
22	a	604	CLA	C4D-CHA	2.60	1.47	1.38
24	t	101	BCR	C24-C25	-2.59	1.36	1.45
22	c	508	CLA	C1B-C2B	2.59	1.49	1.43
22	b	602	CLA	C1C-C2C	2.59	1.49	1.44
22	d	403	CLA	C4D-CHA	2.59	1.47	1.38
22	b	609	CLA	C4D-CHA	2.59	1.47	1.38
22	A	604	CLA	C4D-CHA	2.59	1.47	1.38
22	B	617	CLA	C4B-NB	-2.59	1.34	1.37
22	C	502	CLA	C1B-C2B	2.59	1.49	1.43
22	B	602	CLA	C1C-C2C	2.59	1.49	1.44
22	d	401	CLA	C3D-C2D	2.59	1.46	1.39
22	D	401	CLA	C3D-C2D	2.59	1.46	1.39
22	C	508	CLA	C1B-C2B	2.58	1.49	1.43
24	B	618	BCR	C24-C25	-2.58	1.36	1.45
24	T	101	BCR	C24-C25	-2.58	1.36	1.45
22	a	607	CLA	C4D-CHA	2.58	1.47	1.38
22	C	510	CLA	C4D-CHA	2.58	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	C4D-CHA	2.58	1.47	1.38
22	b	605	CLA	C3D-C2D	2.57	1.46	1.39
22	D	401	CLA	MG-ND	-2.57	2.00	2.05
22	B	605	CLA	C3D-C2D	2.56	1.46	1.39
22	d	401	CLA	MG-ND	-2.56	2.00	2.05
24	T	102	BCR	C24-C25	-2.56	1.36	1.45
22	c	507	CLA	C1C-C2C	2.56	1.49	1.44
22	c	502	CLA	C1B-C2B	2.56	1.49	1.43
22	b	617	CLA	C4B-NB	-2.56	1.34	1.37
22	b	608	CLA	C1B-C2B	2.55	1.49	1.43
22	A	603	CLA	C1B-C2B	2.55	1.49	1.43
22	d	401	CLA	C4D-CHA	2.55	1.47	1.38
24	D	404	BCR	C24-C25	-2.55	1.36	1.45
22	b	606	CLA	C4D-CHA	2.55	1.47	1.38
22	B	615	CLA	C4D-CHA	2.55	1.47	1.38
24	d	404	BCR	C24-C25	-2.54	1.36	1.45
22	c	507	CLA	MG-NB	-2.54	2.00	2.05
22	b	615	CLA	C4D-CHA	2.54	1.47	1.38
22	B	606	CLA	C4D-CHA	2.53	1.47	1.38
22	D	401	CLA	C4D-CHA	2.53	1.47	1.38
22	d	402	CLA	C4D-CHA	2.53	1.47	1.38
22	a	603	CLA	C1B-C2B	2.53	1.49	1.43
22	b	607	CLA	C1D-C2D	2.53	1.50	1.45
22	C	507	CLA	MG-NB	-2.53	2.00	2.05
22	B	608	CLA	C1B-C2B	2.53	1.49	1.43
22	C	504	CLA	C4B-NB	-2.53	1.34	1.37
22	A	604	CLA	MG-NB	-2.52	2.00	2.05
22	b	612	CLA	C1B-C2B	2.52	1.49	1.43
22	c	504	CLA	C4B-NB	-2.52	1.34	1.37
22	C	507	CLA	C1C-C2C	2.52	1.49	1.44
22	a	603	CLA	C4D-CHA	2.52	1.47	1.38
24	a	608	BCR	C24-C25	-2.52	1.36	1.45
22	D	402	CLA	C4D-CHA	2.52	1.47	1.38
24	A	608	BCR	C24-C25	-2.52	1.36	1.45
22	B	607	CLA	C1D-C2D	2.51	1.50	1.45
22	B	608	CLA	C1B-NB	-2.51	1.34	1.37
22	C	509	CLA	C4B-NB	-2.50	1.34	1.37
22	a	604	CLA	MG-NB	-2.49	2.00	2.05
24	b	622	BCR	C24-C25	-2.49	1.36	1.45
22	A	603	CLA	C4D-CHA	2.49	1.46	1.38
22	B	612	CLA	C4D-CHA	2.49	1.46	1.38
22	b	612	CLA	C4D-CHA	2.49	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	v	201	HEM	CMA-C3A	2.48	1.55	1.50
22	b	603	CLA	C1D-C2D	2.48	1.50	1.45
22	B	612	CLA	C1B-C2B	2.48	1.48	1.43
22	B	610	CLA	MG-ND	-2.46	2.00	2.05
24	B	622	BCR	C24-C25	-2.46	1.36	1.45
22	c	513	CLA	C1C-C2C	2.46	1.49	1.44
33	V	201	HEM	CMA-C3A	2.45	1.55	1.50
22	C	512	CLA	C1C-C2C	2.45	1.49	1.44
22	B	613	CLA	C4D-CHA	2.45	1.46	1.38
22	C	501	CLA	C1D-C2D	2.45	1.50	1.45
33	v	201	HEM	CMB-C2B	2.44	1.55	1.50
22	b	608	CLA	C1B-NB	-2.44	1.34	1.37
22	b	610	CLA	MG-ND	-2.44	2.00	2.05
22	C	510	CLA	C4B-NB	-2.44	1.34	1.37
22	b	613	CLA	C4D-CHA	2.44	1.46	1.38
22	b	608	CLA	C4D-CHA	2.44	1.46	1.38
22	c	509	CLA	C4B-NB	-2.44	1.34	1.37
22	c	510	CLA	C4B-NB	-2.44	1.34	1.37
22	B	608	CLA	C4D-CHA	2.44	1.46	1.38
22	c	501	CLA	C1D-C2D	2.43	1.50	1.45
22	B	603	CLA	C1D-C2D	2.43	1.50	1.45
22	c	512	CLA	C1C-C2C	2.42	1.49	1.44
22	C	513	CLA	C1C-C2C	2.42	1.49	1.44
22	C	506	CLA	MG-ND	-2.42	2.01	2.05
33	V	201	HEM	FE-NC	2.42	2.03	1.95
33	v	201	HEM	FE-NC	2.41	2.03	1.95
22	c	506	CLA	MG-ND	-2.40	2.01	2.05
22	C	513	CLA	C1D-C2D	2.40	1.50	1.45
22	c	513	CLA	C1D-C2D	2.40	1.50	1.45
33	V	201	HEM	CMB-C2B	2.39	1.55	1.50
33	F	101	HEM	CMA-C3A	2.38	1.55	1.50
24	b	618	BCR	C24-C25	-2.38	1.36	1.45
22	B	610	CLA	C4B-NB	-2.38	1.34	1.37
28	a	613	PL9	C2-C3	2.37	1.40	1.34
24	B	619	BCR	C24-C25	-2.37	1.37	1.45
33	V	201	HEM	CMC-C2C	2.36	1.55	1.50
22	b	610	CLA	C4B-NB	-2.35	1.34	1.37
22	b	604	CLA	C4D-CHA	2.35	1.46	1.38
22	C	503	CLA	C1D-C2D	2.35	1.50	1.45
22	C	508	CLA	C4C-C3C	2.35	1.49	1.45
22	B	604	CLA	C4D-CHA	2.35	1.46	1.38
22	c	506	CLA	C1D-C2D	2.34	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	613	PL9	C2-C3	2.34	1.40	1.34
22	C	506	CLA	C1D-C2D	2.34	1.50	1.45
22	c	508	CLA	C4C-C3C	2.33	1.49	1.45
33	v	201	HEM	CMC-C2C	2.33	1.55	1.50
22	c	503	CLA	C1D-C2D	2.31	1.49	1.45
33	f	101	HEM	CMA-C3A	2.31	1.55	1.50
22	b	615	CLA	C1B-NB	-2.31	1.34	1.37
22	A	604	CLA	C1D-C2D	2.30	1.49	1.45
22	c	501	CLA	C1C-C2C	2.30	1.49	1.44
22	b	613	CLA	C1B-NB	-2.29	1.34	1.37
22	D	402	CLA	C1D-C2D	2.29	1.49	1.45
22	B	613	CLA	C1B-NB	-2.29	1.34	1.37
22	C	510	CLA	MG-NC	2.29	2.11	2.06
29	Z	101	LMG	O1-C1	2.29	1.44	1.40
22	C	502	CLA	C4B-NB	-2.28	1.34	1.37
22	c	510	CLA	C1D-C2D	2.28	1.49	1.45
22	b	609	CLA	C1B-C2B	2.28	1.48	1.43
22	C	501	CLA	C1C-C2C	2.27	1.49	1.44
22	a	604	CLA	C1D-C2D	2.27	1.49	1.45
33	F	101	HEM	CMB-C2B	2.27	1.55	1.50
29	z	101	LMG	O1-C1	2.27	1.44	1.40
31	d	410	DGD	O5D-C1E	2.27	1.44	1.40
22	C	504	CLA	C1D-C2D	2.27	1.49	1.45
22	b	610	CLA	C1D-C2D	2.27	1.49	1.45
22	c	502	CLA	C4B-NB	-2.26	1.34	1.37
22	B	609	CLA	C1B-C2B	2.25	1.48	1.43
22	C	507	CLA	C3B-C2B	2.25	1.48	1.41
22	c	507	CLA	C3B-C2B	2.25	1.48	1.41
22	c	504	CLA	C1D-C2D	2.25	1.49	1.45
22	d	402	CLA	C1D-C2D	2.24	1.49	1.45
22	B	608	CLA	C1D-C2D	2.24	1.49	1.45
22	C	505	CLA	C1C-C2C	2.24	1.49	1.44
22	C	506	CLA	C1C-C2C	2.24	1.49	1.44
22	b	602	CLA	MG-ND	-2.24	2.01	2.05
22	d	403	CLA	C1C-C2C	2.24	1.49	1.44
22	B	616	CLA	C4B-NB	-2.24	1.34	1.37
33	f	101	HEM	CMB-C2B	2.23	1.55	1.50
22	c	506	CLA	C1C-C2C	2.23	1.49	1.44
22	D	403	CLA	C1C-C2C	2.23	1.49	1.44
22	b	608	CLA	C1D-C2D	2.23	1.49	1.45
22	C	510	CLA	C1D-C2D	2.23	1.49	1.45
22	B	615	CLA	C1B-NB	-2.23	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	510	CLA	MG-NC	2.23	2.11	2.06
31	C	518	DGD	O2G-C2G	-2.23	1.41	1.46
22	b	616	CLA	C4B-NB	-2.23	1.34	1.37
22	c	505	CLA	C1C-C2C	2.23	1.49	1.44
22	C	509	CLA	C1D-C2D	2.23	1.49	1.45
22	b	616	CLA	C1B-NB	-2.23	1.34	1.37
22	C	512	CLA	C4C-C3C	2.23	1.48	1.45
22	c	512	CLA	C4C-C3C	2.22	1.48	1.45
31	c	518	DGD	O2G-C2G	-2.22	1.41	1.46
22	B	613	CLA	MG-NB	2.22	2.10	2.05
22	b	613	CLA	MG-NB	2.22	2.10	2.05
22	B	603	CLA	C1C-C2C	2.21	1.49	1.44
22	B	602	CLA	MG-ND	-2.21	2.01	2.05
29	c	520	LMG	O1-C1	2.21	1.43	1.40
22	B	607	CLA	C1C-C2C	2.21	1.49	1.44
22	B	616	CLA	C1B-NB	-2.21	1.35	1.37
22	C	507	CLA	C4B-NB	-2.21	1.35	1.37
22	b	607	CLA	C1C-C2C	2.21	1.49	1.44
22	B	610	CLA	C1D-C2D	2.21	1.49	1.45
22	c	505	CLA	C4C-C3C	2.20	1.48	1.45
31	D	410	DGD	O5D-C1E	2.20	1.43	1.40
22	B	614	CLA	C1C-C2C	2.20	1.49	1.44
22	c	509	CLA	C4C-C3C	2.20	1.48	1.45
22	b	614	CLA	C1C-C2C	2.20	1.49	1.44
22	d	403	CLA	C4C-C3C	2.20	1.48	1.45
22	C	509	CLA	C4C-C3C	2.20	1.48	1.45
25	l	101	SQD	O6-C1	2.19	1.43	1.40
22	D	403	CLA	C4C-C3C	2.19	1.48	1.45
31	d	410	DGD	O3G-C1D	2.18	1.43	1.40
22	c	509	CLA	C1D-C2D	2.18	1.49	1.45
22	C	507	CLA	C1D-C2D	2.18	1.49	1.45
29	C	520	LMG	O1-C1	2.18	1.43	1.40
22	B	611	CLA	C1C-NC	-2.17	1.34	1.37
22	c	507	CLA	C1D-C2D	2.17	1.49	1.45
22	D	401	CLA	C1D-ND	-2.17	1.35	1.37
22	C	510	CLA	C1C-C2C	2.17	1.48	1.44
22	b	604	CLA	C1C-NC	-2.17	1.34	1.37
22	b	603	CLA	C1C-C2C	2.17	1.48	1.44
22	c	510	CLA	C1C-C2C	2.17	1.48	1.44
25	l	102	SQD	O6-C1	2.17	1.43	1.40
22	A	604	CLA	C1B-NB	-2.17	1.35	1.37
22	b	611	CLA	C3B-C4B	2.16	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	C4B-NB	-2.16	1.35	1.37
22	D	401	CLA	C4C-C3C	2.16	1.48	1.45
22	d	401	CLA	C1D-ND	-2.15	1.35	1.37
22	c	513	CLA	C3B-C2B	2.15	1.48	1.41
22	b	608	CLA	C1D-ND	-2.15	1.35	1.37
22	B	611	CLA	C3B-C4B	2.15	1.49	1.42
22	a	604	CLA	C1B-NB	-2.15	1.35	1.37
25	b	621	SQD	O6-C1	2.15	1.43	1.40
22	C	513	CLA	C3B-C2B	2.14	1.48	1.41
22	b	611	CLA	C1C-NC	-2.14	1.34	1.37
23	A	606	PHO	CBD-CGD	-2.14	1.49	1.52
22	b	615	CLA	C1D-C2D	2.14	1.49	1.45
22	B	605	CLA	C1D-C2D	2.14	1.49	1.45
22	C	505	CLA	C4C-C3C	2.14	1.48	1.45
22	b	605	CLA	MG-NC	2.14	2.11	2.06
22	D	402	CLA	C1D-ND	-2.14	1.35	1.37
22	b	605	CLA	C1D-C2D	2.13	1.49	1.45
25	L	101	SQD	O6-C1	2.13	1.43	1.40
22	C	511	CLA	C1C-C2C	2.13	1.48	1.44
22	c	507	CLA	C4B-NB	-2.13	1.35	1.37
22	B	605	CLA	MG-NC	2.13	2.11	2.06
22	B	604	CLA	C1C-NC	-2.13	1.34	1.37
22	B	616	CLA	C1C-C2C	2.13	1.48	1.44
22	b	616	CLA	C1C-C2C	2.12	1.48	1.44
22	b	615	CLA	C4B-NB	-2.12	1.35	1.37
23	A	605	PHO	C3A-C2A	-2.12	1.52	1.54
22	c	508	CLA	C1D-C2D	2.12	1.49	1.45
22	d	401	CLA	C4C-C3C	2.12	1.48	1.45
24	c	514	BCR	C8-C7	-2.11	1.26	1.33
22	d	402	CLA	C1D-ND	-2.11	1.35	1.37
31	D	410	DGD	O3G-C1D	2.11	1.43	1.40
22	c	511	CLA	C1C-C2C	2.11	1.48	1.44
23	a	606	PHO	CBD-CGD	-2.10	1.49	1.52
22	b	616	CLA	C1D-C2D	2.10	1.49	1.45
22	B	615	CLA	C1D-C2D	2.10	1.49	1.45
24	C	514	BCR	C8-C7	-2.09	1.26	1.33
22	b	603	CLA	C3B-C2B	2.09	1.48	1.41
22	b	609	CLA	C4B-NB	-2.09	1.35	1.37
22	B	603	CLA	C3B-C2B	2.09	1.48	1.41
22	C	508	CLA	C1D-C2D	2.08	1.49	1.45
22	B	608	CLA	C1D-ND	-2.08	1.35	1.37
22	C	506	CLA	C4B-NB	-2.08	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	C1C-C2C	2.08	1.48	1.44
22	C	512	CLA	C1D-C2D	2.08	1.49	1.45
22	C	501	CLA	C4B-NB	-2.08	1.35	1.37
23	a	605	PHO	C3A-C2A	-2.08	1.52	1.54
22	B	616	CLA	C1D-C2D	2.08	1.49	1.45
22	A	603	CLA	C1B-NB	-2.08	1.35	1.37
22	c	512	CLA	C1D-C2D	2.07	1.49	1.45
22	B	616	CLA	C4C-C3C	2.07	1.48	1.45
22	B	602	CLA	C3B-C4B	2.07	1.48	1.42
22	B	609	CLA	C4B-NB	-2.07	1.35	1.37
22	d	403	CLA	C1C-NC	-2.07	1.34	1.37
22	B	606	CLA	MG-ND	-2.07	2.01	2.05
31	c	516	DGD	O5D-C1E	2.06	1.43	1.40
22	b	616	CLA	C4C-C3C	2.06	1.48	1.45
22	b	617	CLA	C3B-C2B	2.06	1.48	1.41
22	c	505	CLA	C1B-NB	-2.06	1.35	1.37
22	B	602	CLA	C4C-C3C	2.06	1.48	1.45
22	b	602	CLA	C3B-C4B	2.06	1.48	1.42
22	C	505	CLA	C4B-NB	-2.05	1.35	1.37
22	b	613	CLA	C1D-C2D	2.05	1.49	1.45
22	B	613	CLA	C1D-C2D	2.05	1.49	1.45
22	c	508	CLA	C1C-C2C	2.05	1.48	1.44
25	D	411	SQD	O6-C1	2.05	1.43	1.40
22	B	604	CLA	C1D-C2D	2.05	1.49	1.45
22	a	603	CLA	C1B-NB	-2.05	1.35	1.37
22	c	508	CLA	C3B-C2B	2.05	1.48	1.41
32	D	407	LHG	O7-C5	-2.04	1.41	1.46
22	B	613	CLA	C1D-ND	-2.04	1.35	1.37
22	C	505	CLA	C1B-NB	-2.04	1.35	1.37
22	C	508	CLA	C1C-C2C	2.04	1.48	1.44
22	b	614	CLA	MG-ND	2.04	2.09	2.05
31	C	516	DGD	O5D-C1E	2.04	1.43	1.40
22	b	604	CLA	C1C-C2C	2.04	1.48	1.44
22	B	612	CLA	C1D-C2D	2.04	1.49	1.45
22	B	617	CLA	C3B-C2B	2.04	1.48	1.41
22	c	503	CLA	C3B-C2B	2.03	1.48	1.41
22	B	614	CLA	MG-ND	2.03	2.09	2.05
22	b	617	CLA	MG-NB	2.03	2.09	2.05
22	c	501	CLA	C4B-NB	-2.03	1.35	1.37
22	C	503	CLA	C3B-C2B	2.03	1.48	1.41
22	b	606	CLA	C3B-C4B	2.03	1.48	1.42
22	b	612	CLA	MG-ND	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	407	LHG	O7-C5	-2.03	1.41	1.46
22	b	607	CLA	C4C-C3C	2.03	1.48	1.45
22	C	508	CLA	C3B-C2B	2.02	1.48	1.41
22	b	604	CLA	C1D-C2D	2.02	1.49	1.45
22	B	606	CLA	C3B-C4B	2.02	1.48	1.42
22	D	403	CLA	C1C-NC	-2.02	1.34	1.37
22	b	612	CLA	C1D-C2D	2.01	1.49	1.45
22	B	612	CLA	MG-ND	-2.01	2.01	2.05
25	d	411	SQD	O6-C1	2.01	1.43	1.40
22	B	603	CLA	C3B-C4B	2.01	1.48	1.42
24	k	101	BCR	C8-C7	-2.01	1.27	1.33
22	B	617	CLA	MG-NB	2.01	2.09	2.05
22	B	615	CLA	C1C-C2C	2.01	1.48	1.44
22	b	606	CLA	MG-ND	-2.00	2.01	2.05
28	d	408	PL9	C2-C3	2.00	1.39	1.34
22	C	505	CLA	C1D-C2D	2.00	1.49	1.45

All (2832) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	BCR	C20-C21-C22	27.41	165.72	127.28
24	h	101	BCR	C20-C21-C22	27.40	165.71	127.28
24	T	102	BCR	C20-C21-C22	27.09	165.27	127.28
24	t	101	BCR	C20-C21-C22	27.07	165.24	127.28
24	c	514	BCR	C15-C16-C17	26.84	178.43	123.52
24	C	514	BCR	C15-C16-C17	26.79	178.33	123.52
24	C	515	BCR	C20-C21-C22	26.21	164.04	127.28
24	c	515	BCR	C20-C21-C22	26.15	163.95	127.28
24	K	101	BCR	C20-C21-C22	26.05	163.81	127.28
24	k	101	BCR	C20-C21-C22	26.02	163.77	127.28
24	t	101	BCR	C16-C17-C18	25.91	163.61	127.28
24	T	102	BCR	C16-C17-C18	25.90	163.60	127.28
24	a	608	BCR	C20-C21-C22	25.62	163.21	127.28
24	A	608	BCR	C20-C21-C22	25.62	163.21	127.28
24	c	514	BCR	C16-C17-C18	25.55	163.11	127.28
24	C	514	BCR	C16-C17-C18	25.53	163.08	127.28
24	t	101	BCR	C15-C16-C17	25.37	175.44	123.52
24	T	102	BCR	C15-C16-C17	25.36	175.40	123.52
24	h	101	BCR	C15-C16-C17	25.32	175.33	123.52
24	H	101	BCR	C15-C16-C17	25.32	175.32	123.52
24	T	101	BCR	C16-C17-C18	24.65	161.85	127.28
24	B	618	BCR	C16-C17-C18	24.64	161.83	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	101	BCR	C16-C17-C18	23.77	160.61	127.28
24	K	101	BCR	C16-C17-C18	23.75	160.59	127.28
24	C	515	BCR	C15-C16-C17	23.71	172.04	123.52
24	c	515	BCR	C15-C16-C17	23.68	171.97	123.52
24	C	514	BCR	C20-C21-C22	23.50	160.23	127.28
24	c	514	BCR	C20-C21-C22	23.48	160.21	127.28
24	D	404	BCR	C15-C16-C17	23.23	171.05	123.52
24	d	404	BCR	C15-C16-C17	23.21	171.02	123.52
24	d	404	BCR	C20-C21-C22	22.91	159.41	127.28
24	D	404	BCR	C20-C21-C22	22.89	159.38	127.28
24	d	404	BCR	C16-C17-C18	22.73	159.16	127.28
24	D	404	BCR	C16-C17-C18	22.73	159.15	127.28
24	k	102	BCR	C15-C16-C17	22.39	169.34	123.52
24	K	102	BCR	C15-C16-C17	22.37	169.28	123.52
24	b	618	BCR	C20-C21-C22	22.33	158.60	127.28
24	B	619	BCR	C20-C21-C22	22.33	158.59	127.28
24	A	608	BCR	C16-C17-C18	21.95	158.06	127.28
24	a	608	BCR	C16-C17-C18	21.92	158.03	127.28
24	C	515	BCR	C16-C15-C14	21.81	168.15	123.52
24	c	515	BCR	C16-C15-C14	21.79	168.10	123.52
24	K	102	BCR	C20-C21-C22	21.37	157.25	127.28
24	k	102	BCR	C20-C21-C22	21.32	157.18	127.28
24	B	622	BCR	C15-C16-C17	21.18	166.85	123.52
24	b	622	BCR	C15-C16-C17	21.15	166.79	123.52
24	B	619	BCR	C16-C17-C18	21.01	156.75	127.28
24	b	618	BCR	C16-C17-C18	21.01	156.74	127.28
24	C	515	BCR	C16-C17-C18	21.00	156.73	127.28
24	c	515	BCR	C16-C17-C18	21.00	156.72	127.28
24	h	101	BCR	C16-C17-C18	20.92	156.61	127.28
24	H	101	BCR	C16-C17-C18	20.90	156.59	127.28
24	c	514	BCR	C16-C15-C14	20.73	165.94	123.52
24	C	514	BCR	C16-C15-C14	20.72	165.91	123.52
24	K	101	BCR	C15-C16-C17	20.71	165.89	123.52
24	k	101	BCR	C15-C16-C17	20.71	165.89	123.52
24	B	622	BCR	C16-C15-C14	20.36	165.18	123.52
24	b	622	BCR	C16-C15-C14	20.34	165.14	123.52
24	D	404	BCR	C16-C15-C14	20.18	164.82	123.52
24	d	404	BCR	C16-C15-C14	20.18	164.81	123.52
24	T	101	BCR	C15-C16-C17	19.72	163.86	123.52
24	B	618	BCR	C15-C16-C17	19.67	163.77	123.52
24	k	102	BCR	C16-C15-C14	19.23	162.86	123.52
24	K	102	BCR	C16-C15-C14	19.20	162.80	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	BCR	C16-C17-C18	19.09	154.04	127.28
24	k	102	BCR	C16-C17-C18	19.07	154.02	127.28
24	T	102	BCR	C16-C15-C14	18.41	161.18	123.52
24	t	101	BCR	C16-C15-C14	18.39	161.15	123.52
24	B	618	BCR	C20-C21-C22	18.39	153.07	127.28
24	T	101	BCR	C20-C21-C22	18.39	153.07	127.28
24	C	514	BCR	C21-C20-C19	18.25	176.07	123.20
24	c	514	BCR	C21-C20-C19	18.23	176.01	123.20
24	A	608	BCR	C15-C16-C17	18.14	160.63	123.52
24	a	608	BCR	C15-C16-C17	18.12	160.60	123.52
24	B	622	BCR	C16-C17-C18	17.57	151.91	127.28
24	C	515	BCR	C21-C20-C19	17.55	174.06	123.20
24	c	515	BCR	C21-C20-C19	17.55	174.04	123.20
24	b	622	BCR	C16-C17-C18	17.55	151.88	127.28
24	k	101	BCR	C16-C15-C14	16.56	157.39	123.52
24	K	101	BCR	C16-C15-C14	16.55	157.37	123.52
24	h	101	BCR	C21-C20-C19	16.12	169.92	123.20
24	H	101	BCR	C21-C20-C19	16.12	169.92	123.20
24	H	101	BCR	C16-C15-C14	16.11	156.47	123.52
24	h	101	BCR	C16-C15-C14	16.08	156.42	123.52
24	b	618	BCR	C15-C16-C17	16.04	156.33	123.52
24	B	619	BCR	C15-C16-C17	16.03	156.31	123.52
24	b	618	BCR	C16-C15-C14	15.86	155.97	123.52
24	B	619	BCR	C16-C15-C14	15.85	155.96	123.52
24	K	101	BCR	C21-C20-C19	15.75	168.84	123.20
24	k	101	BCR	C21-C20-C19	15.75	168.83	123.20
24	b	618	BCR	C21-C20-C19	15.74	168.82	123.20
24	B	619	BCR	C21-C20-C19	15.73	168.76	123.20
24	B	618	BCR	C19-C18-C17	15.06	142.69	119.01
24	T	101	BCR	C19-C18-C17	15.03	142.66	119.01
24	K	102	BCR	C21-C20-C19	14.79	166.04	123.20
24	k	102	BCR	C21-C20-C19	14.78	166.03	123.20
24	c	515	BCR	C11-C10-C9	14.75	147.97	127.28
24	C	515	BCR	C11-C10-C9	14.74	147.96	127.28
24	a	608	BCR	C16-C15-C14	14.62	153.43	123.52
24	A	608	BCR	C16-C15-C14	14.61	153.41	123.52
24	K	102	BCR	C15-C14-C13	14.43	147.51	127.28
24	k	102	BCR	C15-C14-C13	14.43	147.51	127.28
24	T	102	BCR	C21-C20-C19	14.36	164.81	123.20
24	t	101	BCR	C21-C20-C19	14.34	164.76	123.20
24	b	622	BCR	C20-C21-C22	14.26	147.27	127.28
24	B	622	BCR	C20-C21-C22	14.25	147.26	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	101	BCR	C16-C15-C14	14.11	152.40	123.52
24	H	101	BCR	C11-C10-C9	14.09	147.04	127.28
24	B	618	BCR	C16-C15-C14	14.09	152.35	123.52
24	h	101	BCR	C11-C10-C9	14.09	147.04	127.28
24	b	618	BCR	C19-C18-C17	13.98	141.00	119.01
24	B	619	BCR	C19-C18-C17	13.98	140.99	119.01
24	B	619	BCR	C15-C14-C13	13.82	146.66	127.28
24	b	618	BCR	C15-C14-C13	13.81	146.65	127.28
24	A	608	BCR	C21-C20-C19	13.70	162.90	123.20
24	a	608	BCR	C21-C20-C19	13.68	162.84	123.20
24	d	404	BCR	C21-C20-C19	13.65	162.76	123.20
24	D	404	BCR	C21-C20-C19	13.65	162.75	123.20
24	B	619	BCR	C11-C10-C9	13.58	146.32	127.28
24	b	618	BCR	C11-C10-C9	13.56	146.29	127.28
24	k	101	BCR	C11-C10-C9	13.27	145.89	127.28
24	K	101	BCR	C11-C10-C9	13.26	145.88	127.28
24	C	514	BCR	C20-C19-C18	13.02	162.05	126.36
24	c	514	BCR	C20-C19-C18	13.01	162.03	126.36
24	T	102	BCR	C19-C18-C17	12.88	139.28	119.01
24	T	102	BCR	C11-C10-C9	12.86	145.32	127.28
24	c	514	BCR	C10-C11-C12	12.86	160.46	123.20
24	C	514	BCR	C10-C11-C12	12.85	160.44	123.20
24	t	101	BCR	C19-C18-C17	12.84	139.20	119.01
24	t	101	BCR	C11-C10-C9	12.78	145.20	127.28
24	C	515	BCR	C20-C19-C18	12.68	161.13	126.36
24	b	622	BCR	C10-C11-C12	12.68	159.94	123.20
24	B	622	BCR	C10-C11-C12	12.66	159.90	123.20
24	c	515	BCR	C20-C19-C18	12.66	161.08	126.36
24	k	102	BCR	C20-C19-C18	12.57	160.84	126.36
24	K	102	BCR	C20-C19-C18	12.55	160.78	126.36
24	b	622	BCR	C11-C10-C9	12.52	144.84	127.28
24	B	622	BCR	C11-C10-C9	12.51	144.82	127.28
24	K	101	BCR	C19-C18-C17	12.34	138.41	119.01
24	k	101	BCR	C19-C18-C17	12.29	138.34	119.01
24	A	608	BCR	C19-C18-C17	12.12	138.07	119.01
24	a	608	BCR	C19-C18-C17	12.09	138.03	119.01
24	B	618	BCR	C21-C20-C19	12.09	158.22	123.20
24	T	101	BCR	C21-C20-C19	12.07	158.19	123.20
24	k	102	BCR	C19-C18-C17	11.90	137.73	119.01
24	K	102	BCR	C19-C18-C17	11.90	137.73	119.01
24	b	622	BCR	C11-C12-C13	11.88	158.93	126.36
24	B	622	BCR	C11-C12-C13	11.85	158.86	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	BCR	C15-C14-C13	11.75	143.76	127.28
24	h	101	BCR	C15-C14-C13	11.73	143.73	127.28
24	C	515	BCR	C15-C14-C13	11.73	143.73	127.28
24	c	515	BCR	C15-C14-C13	11.73	143.72	127.28
22	C	507	CLA	C4A-NA-C1A	11.70	112.02	106.68
22	c	511	CLA	C4A-NA-C1A	11.68	112.01	106.68
24	k	102	BCR	C10-C11-C12	11.64	156.93	123.20
24	K	102	BCR	C10-C11-C12	11.63	156.90	123.20
24	A	608	BCR	C11-C10-C9	11.63	143.59	127.28
22	C	511	CLA	C4A-NA-C1A	11.62	111.98	106.68
24	k	102	BCR	C11-C12-C13	11.61	158.21	126.36
24	K	102	BCR	C11-C12-C13	11.60	158.18	126.36
24	k	101	BCR	C15-C14-C13	11.59	143.54	127.28
24	a	608	BCR	C11-C10-C9	11.59	143.54	127.28
22	c	507	CLA	C4A-NA-C1A	11.58	111.96	106.68
24	K	101	BCR	C15-C14-C13	11.57	143.51	127.28
24	K	101	BCR	C20-C19-C18	11.46	157.79	126.36
24	k	101	BCR	C20-C19-C18	11.44	157.72	126.36
24	T	101	BCR	C12-C13-C14	11.39	136.92	119.01
24	B	618	BCR	C12-C13-C14	11.36	136.88	119.01
24	B	618	BCR	C11-C10-C9	11.25	143.05	127.28
24	T	101	BCR	C11-C10-C9	11.23	143.03	127.28
24	H	101	BCR	C20-C19-C18	11.19	157.04	126.36
24	h	101	BCR	C20-C19-C18	11.18	157.02	126.36
24	b	622	BCR	C20-C19-C18	11.04	156.64	126.36
24	B	622	BCR	C20-C19-C18	11.03	156.61	126.36
24	B	618	BCR	C20-C19-C18	11.02	156.58	126.36
24	T	101	BCR	C20-C19-C18	11.01	156.55	126.36
24	a	608	BCR	C15-C14-C13	11.01	142.71	127.28
24	b	618	BCR	C20-C19-C18	10.99	156.50	126.36
24	A	608	BCR	C15-C14-C13	10.98	142.68	127.28
24	b	622	BCR	C21-C20-C19	10.97	155.00	123.20
24	B	619	BCR	C20-C19-C18	10.97	156.44	126.36
24	B	622	BCR	C21-C20-C19	10.96	154.94	123.20
24	T	102	BCR	C10-C11-C12	10.95	154.93	123.20
24	t	101	BCR	C10-C11-C12	10.93	154.86	123.20
24	c	515	BCR	C10-C11-C12	10.92	154.85	123.20
24	C	515	BCR	C10-C11-C12	10.91	154.81	123.20
24	c	514	BCR	C11-C12-C13	10.87	156.18	126.36
24	C	514	BCR	C11-C12-C13	10.87	156.18	126.36
22	B	605	CLA	C4A-NA-C1A	10.85	111.63	106.68
24	a	608	BCR	C23-C22-C21	10.79	135.99	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	BCR	C15-C14-C13	10.79	142.41	127.28
24	A	608	BCR	C23-C22-C21	10.78	135.96	119.01
24	D	404	BCR	C15-C14-C13	10.76	142.36	127.28
22	b	605	CLA	C4A-NA-C1A	10.75	111.58	106.68
24	D	404	BCR	C11-C10-C9	10.60	142.15	127.28
24	d	404	BCR	C11-C10-C9	10.57	142.10	127.28
24	T	102	BCR	C15-C14-C13	10.55	142.07	127.28
24	a	608	BCR	C12-C13-C14	10.55	135.60	119.01
24	A	608	BCR	C12-C13-C14	10.54	135.59	119.01
24	t	101	BCR	C15-C14-C13	10.49	141.99	127.28
23	a	605	PHO	C3B-C4B-NB	10.49	114.30	107.46
23	A	605	PHO	C3B-C4B-NB	10.47	114.29	107.46
24	H	101	BCR	C19-C18-C17	10.42	135.40	119.01
24	h	101	BCR	C19-C18-C17	10.42	135.40	119.01
24	T	102	BCR	C11-C12-C13	10.38	154.83	126.36
24	t	101	BCR	C11-C12-C13	10.38	154.81	126.36
24	A	608	BCR	C10-C11-C12	10.37	153.24	123.20
24	a	608	BCR	C10-C11-C12	10.36	153.22	123.20
22	B	616	CLA	C4A-NA-C1A	10.32	111.39	106.68
22	b	616	CLA	C4A-NA-C1A	10.31	111.38	106.68
24	c	514	BCR	C19-C18-C17	10.26	135.15	119.01
24	C	514	BCR	C19-C18-C17	10.24	135.11	119.01
24	h	101	BCR	C10-C11-C12	10.23	152.83	123.20
24	H	101	BCR	C10-C11-C12	10.21	152.78	123.20
22	b	602	CLA	C4A-NA-C1A	10.09	111.28	106.68
22	B	602	CLA	C4A-NA-C1A	10.08	111.28	106.68
22	C	513	CLA	C4A-NA-C1A	10.06	111.27	106.68
24	B	622	BCR	C15-C14-C13	10.03	141.34	127.28
24	b	622	BCR	C15-C14-C13	10.02	141.34	127.28
24	a	608	BCR	C11-C12-C13	10.01	153.80	126.36
24	A	608	BCR	C11-C12-C13	10.00	153.78	126.36
24	C	514	BCR	C7-C8-C9	9.97	140.99	126.23
22	c	513	CLA	C4A-NA-C1A	9.95	111.22	106.68
22	c	504	CLA	C4A-NA-C1A	9.92	111.20	106.68
24	c	514	BCR	C7-C8-C9	9.91	140.90	126.23
24	C	514	BCR	C15-C14-C13	9.90	141.16	127.28
24	c	514	BCR	C15-C14-C13	9.89	141.15	127.28
22	C	509	CLA	C4A-NA-C1A	9.85	111.17	106.68
22	C	504	CLA	C4A-NA-C1A	9.84	111.17	106.68
22	c	509	CLA	C4A-NA-C1A	9.81	111.15	106.68
24	D	404	BCR	C20-C19-C18	9.78	153.17	126.36
24	d	404	BCR	C20-C19-C18	9.78	153.17	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	BCR	C11-C12-C13	9.66	152.85	126.36
24	D	404	BCR	C11-C12-C13	9.64	152.80	126.36
24	T	101	BCR	C11-C12-C13	9.64	152.78	126.36
24	B	618	BCR	C11-C12-C13	9.63	152.77	126.36
24	T	102	BCR	C20-C19-C18	9.61	152.73	126.36
22	b	613	CLA	C4A-NA-C1A	9.61	111.06	106.68
22	c	506	CLA	C4A-NA-C1A	9.61	111.06	106.68
24	t	101	BCR	C20-C19-C18	9.59	152.66	126.36
22	C	506	CLA	C4A-NA-C1A	9.54	111.03	106.68
22	B	613	CLA	C4A-NA-C1A	9.52	111.02	106.68
24	K	102	BCR	C7-C8-C9	9.51	140.31	126.23
24	h	101	BCR	C11-C12-C13	9.51	152.44	126.36
24	k	102	BCR	C7-C8-C9	9.50	140.29	126.23
24	H	101	BCR	C11-C12-C13	9.50	152.42	126.36
24	T	102	BCR	C7-C8-C9	9.49	140.28	126.23
24	t	101	BCR	C7-C8-C9	9.49	140.28	126.23
24	B	622	BCR	C19-C18-C17	9.49	133.93	119.01
24	b	622	BCR	C19-C18-C17	9.49	133.93	119.01
22	C	505	CLA	C4A-NA-C1A	9.48	111.01	106.68
24	D	404	BCR	C30-C25-C26	-9.40	109.80	122.64
24	d	404	BCR	C30-C25-C26	-9.38	109.82	122.64
23	a	605	PHO	C2D-C1D-ND	9.38	116.21	109.43
22	d	403	CLA	C4A-NA-C1A	9.36	110.95	106.68
22	C	510	CLA	C4A-NA-C1A	9.36	110.95	106.68
24	K	102	BCR	C12-C13-C14	9.34	133.71	119.01
22	c	505	CLA	C4A-NA-C1A	9.33	110.94	106.68
24	k	102	BCR	C12-C13-C14	9.33	133.69	119.01
24	c	515	BCR	C19-C18-C17	9.33	133.68	119.01
22	c	510	CLA	C4A-NA-C1A	9.33	110.94	106.68
24	C	515	BCR	C19-C18-C17	9.33	133.68	119.01
23	A	605	PHO	C2D-C1D-ND	9.31	116.16	109.43
24	T	101	BCR	C10-C11-C12	9.30	150.14	123.20
24	C	515	BCR	C12-C13-C14	9.29	133.63	119.01
24	B	618	BCR	C10-C11-C12	9.29	150.12	123.20
22	D	403	CLA	C4A-NA-C1A	9.29	110.92	106.68
24	c	515	BCR	C12-C13-C14	9.27	133.59	119.01
24	b	618	BCR	C12-C13-C14	9.24	133.54	119.01
22	B	610	CLA	C4A-NA-C1A	9.24	110.89	106.68
24	D	404	BCR	C19-C18-C17	9.23	133.53	119.01
24	d	404	BCR	C19-C18-C17	9.23	133.53	119.01
24	B	619	BCR	C12-C13-C14	9.23	133.52	119.01
24	H	101	BCR	C12-C13-C14	9.19	133.46	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	101	BCR	C12-C13-C14	9.18	133.44	119.01
22	c	512	CLA	C4A-NA-C1A	9.16	110.86	106.68
22	b	610	CLA	C4A-NA-C1A	9.14	110.85	106.68
22	B	612	CLA	C4A-NA-C1A	9.14	110.85	106.68
22	C	512	CLA	C4A-NA-C1A	9.12	110.84	106.68
24	K	102	BCR	C11-C10-C9	9.10	140.04	127.28
24	T	102	BCR	C36-C18-C17	-9.10	108.08	122.82
23	a	606	PHO	C3B-C4B-NB	9.09	113.39	107.46
24	t	101	BCR	C36-C18-C17	-9.09	108.09	122.82
24	k	102	BCR	C11-C10-C9	9.09	140.02	127.28
24	B	622	BCR	C7-C8-C9	9.08	139.67	126.23
22	b	612	CLA	C4A-NA-C1A	9.07	110.82	106.68
24	B	619	BCR	C36-C18-C19	-9.07	104.24	118.09
24	b	622	BCR	C7-C8-C9	9.06	139.64	126.23
24	b	618	BCR	C36-C18-C19	-9.06	104.25	118.09
23	A	606	PHO	C3B-C4B-NB	9.04	113.35	107.46
22	B	614	CLA	C4A-NA-C1A	8.98	110.78	106.68
22	b	614	CLA	C4A-NA-C1A	8.93	110.75	106.68
22	C	508	CLA	C4A-NA-C1A	8.91	110.74	106.68
22	B	607	CLA	C4A-NA-C1A	8.88	110.73	106.68
22	C	503	CLA	C4A-NA-C1A	8.88	110.73	106.68
24	b	618	BCR	C24-C23-C22	8.86	139.34	126.23
24	D	404	BCR	C29-C30-C25	8.85	123.29	110.44
22	c	501	CLA	C4A-NA-C1A	8.83	110.71	106.68
22	c	503	CLA	C4A-NA-C1A	8.83	110.71	106.68
24	B	619	BCR	C24-C23-C22	8.82	139.28	126.23
24	d	404	BCR	C29-C30-C25	8.82	123.25	110.44
22	c	508	CLA	C4A-NA-C1A	8.81	110.70	106.68
22	C	501	CLA	C4A-NA-C1A	8.80	110.69	106.68
22	b	607	CLA	C4A-NA-C1A	8.78	110.69	106.68
24	A	608	BCR	C20-C19-C18	8.78	150.43	126.36
24	C	515	BCR	C11-C12-C13	8.76	150.40	126.36
22	A	607	CLA	C1D-ND-C4D	-8.76	100.16	106.31
24	a	608	BCR	C20-C19-C18	8.76	150.38	126.36
24	c	515	BCR	C11-C12-C13	8.74	150.34	126.36
24	b	618	BCR	C23-C22-C21	8.70	132.69	119.01
22	a	607	CLA	C1D-ND-C4D	-8.69	100.21	106.31
24	B	619	BCR	C23-C22-C21	8.68	132.67	119.01
22	B	611	CLA	C4A-NA-C1A	8.62	110.61	106.68
22	b	611	CLA	C4A-NA-C1A	8.60	110.60	106.68
24	k	101	BCR	C11-C12-C13	8.57	149.87	126.36
24	K	101	BCR	C11-C12-C13	8.56	149.85	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	101	BCR	C23-C22-C21	8.55	132.46	119.01
24	T	102	BCR	C23-C22-C21	8.52	132.41	119.01
24	d	404	BCR	C32-C1-C6	8.50	123.58	110.24
24	D	404	BCR	C32-C1-C6	8.50	123.58	110.24
24	H	101	BCR	C23-C22-C21	8.49	132.36	119.01
24	h	101	BCR	C23-C22-C21	8.49	132.36	119.01
24	T	101	BCR	C15-C14-C13	8.47	139.15	127.28
24	k	101	BCR	C10-C11-C12	8.47	147.73	123.20
24	B	618	BCR	C15-C14-C13	8.46	139.15	127.28
24	K	101	BCR	C10-C11-C12	8.45	147.69	123.20
22	B	617	CLA	C4A-NA-C1A	8.43	110.52	106.68
24	B	619	BCR	C10-C11-C12	8.41	147.56	123.20
24	b	618	BCR	C10-C11-C12	8.40	147.54	123.20
23	A	606	PHO	C2D-C1D-ND	8.40	115.50	109.43
22	b	617	CLA	C4A-NA-C1A	8.38	110.50	106.68
24	C	514	BCR	C11-C10-C9	8.38	139.02	127.28
24	a	608	BCR	C37-C22-C21	-8.37	109.26	122.82
24	c	514	BCR	C11-C10-C9	8.36	139.01	127.28
23	a	606	PHO	C2D-C1D-ND	8.34	115.46	109.43
24	A	608	BCR	C37-C22-C21	-8.34	109.31	122.82
24	a	608	BCR	C27-C26-C25	8.28	133.90	122.70
24	A	608	BCR	C27-C26-C25	8.24	133.84	122.70
23	a	606	PHO	C2B-C1B-NB	8.22	115.37	109.43
23	A	606	PHO	C2B-C1B-NB	8.21	115.37	109.43
24	A	608	BCR	C7-C8-C9	8.15	138.29	126.23
24	K	102	BCR	C23-C22-C21	8.12	131.79	119.01
24	k	102	BCR	C23-C22-C21	8.12	131.78	119.01
22	B	602	CLA	CMD-C2D-C1D	8.11	139.01	124.73
22	B	606	CLA	C4A-NA-C1A	8.09	110.37	106.68
22	b	602	CLA	CMD-C2D-C1D	8.09	138.97	124.73
24	a	608	BCR	C7-C8-C9	8.06	138.16	126.23
22	A	607	CLA	C4A-NA-C1A	8.02	110.34	106.68
22	a	607	CLA	C4A-NA-C1A	8.02	110.34	106.68
22	b	606	CLA	C4A-NA-C1A	8.02	110.34	106.68
24	B	619	BCR	C7-C8-C9	8.02	138.10	126.23
22	b	615	CLA	C4A-NA-C1A	8.01	110.33	106.68
24	b	618	BCR	C7-C8-C9	8.01	138.08	126.23
22	B	607	CLA	CMD-C2D-C1D	8.00	138.82	124.73
24	h	101	BCR	C7-C8-C9	7.99	138.06	126.23
24	H	101	BCR	C7-C8-C9	7.98	138.04	126.23
22	B	611	CLA	C1D-ND-C4D	-7.98	100.72	106.31
22	B	615	CLA	C4A-NA-C1A	7.97	110.32	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	C1D-ND-C4D	-7.97	100.72	106.31
22	b	607	CLA	CMD-C2D-C1D	7.97	138.76	124.73
22	B	608	CLA	C4A-NA-C1A	7.95	110.31	106.68
24	T	101	BCR	C35-C13-C12	-7.94	105.96	118.09
22	c	502	CLA	C4A-NA-C1A	7.92	110.29	106.68
24	B	618	BCR	C35-C13-C12	-7.92	105.99	118.09
22	b	604	CLA	C1D-ND-C4D	-7.91	100.76	106.31
22	a	603	CLA	C1D-ND-C4D	-7.89	100.78	106.31
22	C	502	CLA	C4A-NA-C1A	7.88	110.27	106.68
22	B	604	CLA	C1D-ND-C4D	-7.88	100.79	106.31
22	b	608	CLA	C4A-NA-C1A	7.86	110.27	106.68
22	A	603	CLA	C1D-ND-C4D	-7.82	100.83	106.31
24	k	101	BCR	C33-C5-C6	7.80	132.99	124.48
22	B	604	CLA	C4A-NA-C1A	7.80	110.24	106.68
24	k	101	BCR	C7-C8-C9	7.78	137.74	126.23
24	d	404	BCR	C12-C13-C14	7.77	131.23	119.01
24	K	101	BCR	C33-C5-C6	7.76	132.95	124.48
24	d	404	BCR	C10-C11-C12	7.75	145.65	123.20
22	B	609	CLA	C1D-ND-C4D	-7.75	100.88	106.31
24	D	404	BCR	C12-C13-C14	7.75	131.20	119.01
22	b	604	CLA	C4A-NA-C1A	7.74	110.21	106.68
24	K	101	BCR	C7-C8-C9	7.74	137.68	126.23
24	D	404	BCR	C10-C11-C12	7.74	145.61	123.20
22	b	609	CLA	C1D-ND-C4D	-7.70	100.91	106.31
22	C	508	CLA	C1D-ND-C4D	-7.69	100.92	106.31
22	A	604	CLA	C4A-NA-C1A	7.68	110.19	106.68
24	k	101	BCR	C33-C5-C4	-7.67	97.25	113.60
24	b	622	BCR	C33-C5-C6	7.66	132.84	124.48
22	D	403	CLA	C1D-ND-C4D	-7.66	100.94	106.31
22	C	503	CLA	CMD-C2D-C1D	7.66	138.21	124.73
22	d	403	CLA	C1D-ND-C4D	-7.66	100.94	106.31
24	K	101	BCR	C33-C5-C4	-7.66	97.27	113.60
24	B	618	BCR	C8-C9-C10	7.66	131.05	119.01
22	a	604	CLA	C4A-NA-C1A	7.65	110.17	106.68
24	B	622	BCR	C33-C5-C6	7.64	132.82	124.48
22	c	503	CLA	CMD-C2D-C1D	7.63	138.16	124.73
24	T	101	BCR	C8-C9-C10	7.63	131.00	119.01
22	c	508	CLA	C1D-ND-C4D	-7.59	100.99	106.31
22	b	603	CLA	C4A-NA-C1A	7.58	110.14	106.68
22	c	507	CLA	CMD-C2D-C1D	7.58	138.07	124.73
23	a	605	PHO	C2B-C1B-NB	7.57	114.90	109.43
22	C	507	CLA	CMD-C2D-C1D	7.57	138.06	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	CMD-C2D-C1D	7.57	138.06	124.73
22	C	510	CLA	CMD-C2D-C1D	7.55	138.03	124.73
23	A	605	PHO	C2B-C1B-NB	7.55	114.89	109.43
24	B	618	BCR	C36-C18-C19	-7.55	106.56	118.09
22	C	509	CLA	CMD-C2D-C1D	7.55	138.02	124.73
22	c	509	CLA	CMD-C2D-C1D	7.54	138.01	124.73
24	T	101	BCR	C36-C18-C19	-7.54	106.57	118.09
24	b	618	BCR	C30-C25-C26	-7.47	112.43	122.64
24	B	619	BCR	C30-C25-C26	-7.47	112.43	122.64
22	c	506	CLA	CMD-C2D-C1D	7.46	137.86	124.73
22	B	603	CLA	C4A-NA-C1A	7.45	110.08	106.68
22	B	614	CLA	CMD-C2D-C1D	7.45	137.84	124.73
24	B	618	BCR	C36-C18-C17	-7.45	110.75	122.82
22	c	501	CLA	CMD-C2D-C1D	7.45	137.84	124.73
24	T	101	BCR	C36-C18-C17	-7.43	110.77	122.82
22	b	614	CLA	CMD-C2D-C1D	7.43	137.81	124.73
22	C	501	CLA	CMD-C2D-C1D	7.42	137.79	124.73
22	B	615	CLA	C1D-ND-C4D	-7.41	101.11	106.31
22	C	506	CLA	CMD-C2D-C1D	7.41	137.77	124.73
22	b	615	CLA	C1D-ND-C4D	-7.37	101.14	106.31
22	c	510	CLA	C1D-ND-C4D	-7.30	101.19	106.31
22	C	510	CLA	C1D-ND-C4D	-7.28	101.20	106.31
22	B	606	CLA	C1D-ND-C4D	-7.26	101.22	106.31
22	b	606	CLA	C1D-ND-C4D	-7.21	101.25	106.31
24	k	101	BCR	C12-C13-C14	7.21	130.35	119.01
22	b	605	CLA	CMD-C2D-C1D	7.21	137.42	124.73
22	B	605	CLA	CMD-C2D-C1D	7.20	137.41	124.73
24	K	101	BCR	C12-C13-C14	7.19	130.31	119.01
24	B	622	BCR	C8-C7-C6	7.14	146.06	127.00
23	a	605	PHO	O2D-CGD-CBD	7.14	118.79	110.95
22	B	607	CLA	C1D-ND-C4D	-7.13	101.31	106.31
24	b	622	BCR	C8-C7-C6	7.13	146.04	127.00
24	T	101	BCR	C24-C23-C22	7.12	136.77	126.23
23	A	605	PHO	O2D-CGD-CBD	7.12	118.77	110.95
22	b	607	CLA	C1D-ND-C4D	-7.10	101.33	106.31
22	D	403	CLA	CMD-C2D-C1D	7.09	137.21	124.73
22	d	403	CLA	CMD-C2D-C1D	7.09	137.21	124.73
24	T	102	BCR	C12-C13-C14	7.07	130.14	119.01
24	B	618	BCR	C24-C23-C22	7.07	136.70	126.23
24	H	101	BCR	C36-C18-C19	-7.07	107.29	118.09
24	h	101	BCR	C36-C18-C19	-7.07	107.29	118.09
24	K	101	BCR	C36-C18-C19	-7.07	107.29	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	504	CLA	CMD-C2D-C1D	7.07	137.17	124.73
24	A	608	BCR	C36-C18-C17	-7.06	111.38	122.82
22	C	504	CLA	CMD-C2D-C1D	7.06	137.16	124.73
22	C	502	CLA	C1D-ND-C4D	-7.06	101.36	106.31
24	t	101	BCR	C12-C13-C14	7.05	130.10	119.01
24	a	608	BCR	C36-C18-C17	-7.03	111.43	122.82
22	b	612	CLA	C1D-ND-C4D	-7.01	101.39	106.31
22	B	612	CLA	C1D-ND-C4D	-7.00	101.40	106.31
22	C	509	CLA	C1D-ND-C4D	-7.00	101.40	106.31
24	k	101	BCR	C36-C18-C19	-6.99	107.41	118.09
22	c	509	CLA	C1D-ND-C4D	-6.99	101.41	106.31
22	c	502	CLA	C1D-ND-C4D	-6.98	101.42	106.31
22	C	502	CLA	CMD-C2D-C1D	6.95	136.97	124.73
22	A	604	CLA	C1D-ND-C4D	-6.95	101.44	106.31
22	b	617	CLA	C1D-ND-C4D	-6.95	101.44	106.31
22	c	502	CLA	CMD-C2D-C1D	6.94	136.95	124.73
24	k	101	BCR	C29-C30-C25	6.94	120.51	110.44
24	K	101	BCR	C29-C30-C25	6.94	120.51	110.44
24	b	622	BCR	C12-C13-C14	6.93	129.91	119.01
24	B	622	BCR	C12-C13-C14	6.92	129.89	119.01
22	a	604	CLA	C1D-ND-C4D	-6.90	101.47	106.31
22	B	617	CLA	C1D-ND-C4D	-6.90	101.47	106.31
23	A	606	PHO	O2D-CGD-CBD	6.86	118.48	110.95
24	k	102	BCR	C36-C18-C19	-6.85	107.62	118.09
23	a	606	PHO	O2D-CGD-CBD	6.84	118.47	110.95
22	B	611	CLA	CMD-C2D-C1D	6.82	136.74	124.73
22	b	611	CLA	CMD-C2D-C1D	6.82	136.73	124.73
24	K	102	BCR	C36-C18-C19	-6.81	107.68	118.09
22	a	604	CLA	CMD-C2D-C1D	6.79	136.69	124.73
24	C	515	BCR	C24-C23-C22	6.75	136.22	126.23
22	b	602	CLA	C1D-ND-C4D	-6.75	101.58	106.31
22	A	604	CLA	CMD-C2D-C1D	6.75	136.61	124.73
22	c	505	CLA	CMD-C2D-C1D	6.75	136.61	124.73
22	B	608	CLA	C1D-ND-C4D	-6.74	101.58	106.31
22	c	513	CLA	CMD-C2D-C1D	6.74	136.59	124.73
22	C	505	CLA	CMD-C2D-C1D	6.73	136.59	124.73
22	B	614	CLA	C1D-ND-C4D	-6.73	101.59	106.31
22	b	614	CLA	C1D-ND-C4D	-6.73	101.59	106.31
22	C	513	CLA	CMD-C2D-C1D	6.72	136.56	124.73
23	a	605	PHO	C4D-ND-C1D	-6.71	100.83	108.87
24	a	608	BCR	C35-C13-C14	-6.71	111.95	122.82
24	A	608	BCR	C35-C13-C14	-6.71	111.95	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	BCR	C33-C5-C6	6.70	131.80	124.48
24	c	515	BCR	C24-C23-C22	6.70	136.15	126.23
22	B	602	CLA	C1D-ND-C4D	-6.70	101.61	106.31
22	b	608	CLA	C1D-ND-C4D	-6.70	101.61	106.31
24	C	514	BCR	C38-C26-C27	-6.69	99.32	113.60
23	A	605	PHO	C4D-ND-C1D	-6.69	100.86	108.87
22	C	512	CLA	CMD-C2D-C1D	6.68	136.49	124.73
22	c	512	CLA	CMD-C2D-C1D	6.68	136.49	124.73
24	c	514	BCR	C38-C26-C27	-6.67	99.37	113.60
22	C	511	CLA	C1D-ND-C4D	-6.66	101.64	106.31
22	B	613	CLA	C1D-ND-C4D	-6.66	101.64	106.31
22	b	613	CLA	C1D-ND-C4D	-6.66	101.64	106.31
22	B	603	CLA	CMD-C2D-C1D	6.64	136.41	124.73
24	C	514	BCR	C33-C5-C6	6.63	131.72	124.48
23	a	605	PHO	C3D-C4D-ND	6.62	116.20	107.71
22	c	511	CLA	C1D-ND-C4D	-6.62	101.67	106.31
22	b	603	CLA	CMD-C2D-C1D	6.61	136.36	124.73
24	h	101	BCR	C32-C1-C6	6.60	120.60	110.24
24	H	101	BCR	C32-C1-C6	6.60	120.59	110.24
22	c	511	CLA	CMD-C2D-C1D	6.58	136.32	124.73
22	C	511	CLA	CMD-C2D-C1D	6.58	136.32	124.73
23	A	605	PHO	C3D-C4D-ND	6.58	116.14	107.71
23	A	606	PHO	C3D-C4D-ND	6.58	116.14	107.71
24	B	619	BCR	C23-C24-C25	6.57	144.56	127.00
24	b	618	BCR	C23-C24-C25	6.57	144.55	127.00
23	a	606	PHO	C3D-C4D-ND	6.54	116.09	107.71
24	K	102	BCR	C8-C7-C6	6.53	144.44	127.00
24	k	102	BCR	C8-C7-C6	6.51	144.40	127.00
24	T	101	BCR	C23-C22-C21	6.50	129.23	119.01
22	B	610	CLA	CMD-C2D-C1D	6.49	136.16	124.73
24	H	101	BCR	C8-C9-C10	6.48	129.20	119.01
22	d	402	CLA	C2C-C1C-NC	6.48	116.78	109.98
24	h	101	BCR	C8-C9-C10	6.47	129.18	119.01
22	D	402	CLA	C2C-C1C-NC	6.47	116.77	109.98
24	C	515	BCR	C23-C22-C21	6.46	129.18	119.01
22	B	616	CLA	CMD-C2D-C1D	6.46	136.10	124.73
24	B	618	BCR	C23-C22-C21	6.45	129.16	119.01
22	b	616	CLA	CMD-C2D-C1D	6.45	136.08	124.73
22	b	610	CLA	CMD-C2D-C1D	6.45	136.08	124.73
22	c	506	CLA	C1D-ND-C4D	-6.44	101.79	106.31
24	B	619	BCR	C11-C12-C13	6.44	144.01	126.36
24	b	618	BCR	C11-C12-C13	6.44	144.01	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	BCR	C37-C22-C21	-6.43	112.40	122.82
22	D	401	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	a	603	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	C	506	CLA	C1D-ND-C4D	-6.42	101.81	106.31
22	B	615	CLA	CMD-C2D-C1D	6.42	136.03	124.73
22	B	610	CLA	C1D-ND-C4D	-6.41	101.81	106.31
24	c	515	BCR	C23-C22-C21	6.41	129.09	119.01
22	b	615	CLA	CMD-C2D-C1D	6.40	135.99	124.73
24	h	101	BCR	C37-C22-C21	-6.39	112.47	122.82
22	B	616	CLA	C1D-ND-C4D	-6.38	101.83	106.31
22	b	610	CLA	C1D-ND-C4D	-6.38	101.84	106.31
22	d	401	CLA	CMD-C2D-C1D	6.37	135.94	124.73
22	D	401	CLA	CMD-C2D-C1D	6.35	135.91	124.73
22	A	607	CLA	CMD-C2D-C1D	6.35	135.90	124.73
23	A	606	PHO	C4D-ND-C1D	-6.33	101.29	108.87
22	A	603	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	b	616	CLA	C1D-ND-C4D	-6.32	101.88	106.31
22	c	508	CLA	CMD-C2D-C1D	6.32	135.85	124.73
22	a	607	CLA	CMD-C2D-C1D	6.31	135.85	124.73
22	b	612	CLA	CMD-C2D-C1D	6.31	135.83	124.73
22	b	605	CLA	C1D-ND-C4D	-6.31	101.89	106.31
22	B	612	CLA	CMD-C2D-C1D	6.30	135.82	124.73
22	C	508	CLA	CMD-C2D-C1D	6.29	135.81	124.73
23	a	606	PHO	C4D-ND-C1D	-6.29	101.34	108.87
22	d	401	CLA	C1D-ND-C4D	-6.29	101.90	106.31
22	d	401	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	D	401	CLA	C1D-ND-C4D	-6.26	101.92	106.31
22	B	605	CLA	C1D-ND-C4D	-6.26	101.92	106.31
24	C	514	BCR	C24-C23-C22	6.25	135.48	126.23
24	C	515	BCR	C31-C1-C6	6.24	120.03	110.24
22	c	504	CLA	C1D-ND-C4D	-6.23	101.94	106.31
24	c	514	BCR	C24-C23-C22	6.22	135.44	126.23
24	B	622	BCR	C24-C23-C22	6.22	135.44	126.23
24	c	515	BCR	C31-C1-C6	6.21	119.98	110.24
22	b	604	CLA	CMD-C2D-C1D	6.21	135.66	124.73
22	C	513	CLA	C1D-ND-C4D	-6.20	101.96	106.31
22	c	513	CLA	C1D-ND-C4D	-6.20	101.96	106.31
24	K	101	BCR	C37-C22-C21	-6.20	112.78	122.82
24	b	622	BCR	C24-C23-C22	6.19	135.39	126.23
22	B	604	CLA	CMD-C2D-C1D	6.18	135.60	124.73
22	d	401	CLA	C2D-C1D-ND	6.17	116.23	110.13
24	a	608	BCR	C38-C26-C27	-6.16	100.45	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	401	CLA	C2D-C1D-ND	6.16	116.22	110.13
24	B	618	BCR	C7-C8-C9	6.16	135.35	126.23
24	A	608	BCR	C38-C26-C27	-6.15	100.48	113.60
24	k	101	BCR	C37-C22-C21	-6.15	112.85	122.82
22	C	504	CLA	C1D-ND-C4D	-6.15	102.00	106.31
24	T	101	BCR	C7-C8-C9	6.13	135.30	126.23
22	B	617	CLA	CMD-C2D-C1D	6.12	135.50	124.73
24	C	514	BCR	C38-C26-C25	6.11	131.15	124.48
22	c	501	CLA	O2D-CGD-CBD	6.11	121.90	111.23
22	C	501	CLA	O2D-CGD-CBD	6.10	121.89	111.23
22	a	604	CLA	C2C-C1C-NC	6.09	116.38	109.98
24	B	622	BCR	C36-C18-C17	-6.09	112.95	122.82
24	b	622	BCR	C36-C18-C17	-6.09	112.95	122.82
22	A	604	CLA	C2C-C1C-NC	6.08	116.37	109.98
24	A	608	BCR	C8-C9-C10	6.08	128.57	119.01
22	c	512	CLA	C1D-ND-C4D	-6.08	102.05	106.31
22	C	512	CLA	C1D-ND-C4D	-6.07	102.06	106.31
22	b	617	CLA	CMD-C2D-C1D	6.07	135.41	124.73
24	c	514	BCR	C38-C26-C25	6.06	131.10	124.48
24	B	619	BCR	C29-C30-C25	6.05	119.23	110.44
22	B	603	CLA	C1D-ND-C4D	-6.05	102.07	106.31
24	H	101	BCR	C30-C25-C26	-6.05	114.37	122.64
24	B	619	BCR	C8-C9-C10	6.05	128.53	119.01
24	b	618	BCR	C29-C30-C25	6.05	119.23	110.44
22	B	605	CLA	C2C-C1C-NC	6.05	116.33	109.98
22	b	603	CLA	C1D-ND-C4D	-6.05	102.07	106.31
24	T	102	BCR	C8-C9-C10	6.04	128.51	119.01
24	C	514	BCR	C8-C7-C6	6.03	143.11	127.00
22	b	605	CLA	C2C-C1C-NC	6.03	116.31	109.98
24	a	608	BCR	C8-C9-C10	6.03	128.49	119.01
24	b	618	BCR	C8-C9-C10	6.02	128.48	119.01
24	c	514	BCR	C8-C7-C6	6.01	143.05	127.00
24	h	101	BCR	C30-C25-C26	-6.01	114.43	122.64
24	t	101	BCR	C8-C9-C10	6.00	128.44	119.01
22	b	609	CLA	C2C-C1C-NC	5.99	116.28	109.98
22	B	609	CLA	C2C-C1C-NC	5.99	116.28	109.98
22	b	608	CLA	CMD-C2D-C1D	5.98	135.26	124.73
22	b	613	CLA	CMD-C2D-C1D	5.97	135.24	124.73
22	B	608	CLA	CMD-C2D-C1D	5.97	135.24	124.73
22	B	613	CLA	CMD-C2D-C1D	5.96	135.22	124.73
22	a	603	CLA	C2D-C1D-ND	5.95	116.02	110.13
22	B	614	CLA	C2D-C1D-ND	5.95	116.01	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	607	CLA	C2D-C1D-ND	5.94	116.00	110.13
22	A	603	CLA	C2D-C1D-ND	5.93	115.99	110.13
24	c	515	BCR	C7-C8-C9	5.92	134.99	126.23
22	c	501	CLA	C1D-ND-C4D	-5.91	102.16	106.31
22	b	614	CLA	C2D-C1D-ND	5.91	115.97	110.13
24	C	515	BCR	C7-C8-C9	5.91	134.97	126.23
24	k	101	BCR	C30-C25-C26	-5.90	114.57	122.64
24	K	101	BCR	C30-C25-C26	-5.89	114.59	122.64
22	a	607	CLA	C2D-C1D-ND	5.87	115.94	110.13
24	b	622	BCR	C2-C1-C6	5.86	118.96	110.44
24	B	622	BCR	C2-C1-C6	5.86	118.95	110.44
22	B	617	CLA	C2D-C1D-ND	5.86	115.93	110.13
22	C	501	CLA	C1D-ND-C4D	-5.84	102.21	106.31
24	c	514	BCR	C36-C18-C17	-5.84	113.36	122.82
24	C	514	BCR	C36-C18-C17	-5.83	113.38	122.82
22	d	402	CLA	C2D-C1D-ND	5.82	115.89	110.13
22	b	617	CLA	C2D-C1D-ND	5.80	115.87	110.13
22	D	402	CLA	C2D-C1D-ND	5.80	115.86	110.13
22	b	606	CLA	CMD-C2D-C1D	5.77	134.89	124.73
22	D	402	CLA	C3D-C2D-C1D	-5.77	97.96	105.83
22	d	402	CLA	C3D-C2D-C1D	-5.77	97.96	105.83
22	d	402	CLA	CMD-C2D-C1D	5.76	134.88	124.73
22	C	503	CLA	C1D-ND-C4D	-5.76	102.27	106.31
22	D	402	CLA	CMD-C2D-C1D	5.76	134.87	124.73
22	b	612	CLA	C2D-C1D-ND	5.75	115.82	110.13
22	B	602	CLA	O2D-CGD-CBD	5.75	121.28	111.23
22	B	606	CLA	CMD-C2D-C1D	5.75	134.85	124.73
22	c	503	CLA	C1D-ND-C4D	-5.75	102.28	106.31
22	B	612	CLA	C2D-C1D-ND	5.75	115.81	110.13
22	b	602	CLA	O2D-CGD-CBD	5.74	121.27	111.23
24	c	514	BCR	C29-C30-C25	5.73	118.76	110.44
24	C	514	BCR	C29-C30-C25	5.72	118.75	110.44
22	b	606	CLA	C2D-C1D-ND	5.72	115.78	110.13
22	d	402	CLA	C1D-ND-C4D	-5.68	102.33	106.31
24	K	101	BCR	C24-C23-C22	5.66	134.61	126.23
22	B	606	CLA	C2D-C1D-ND	5.66	115.73	110.13
24	C	514	BCR	C12-C13-C14	5.66	127.91	119.01
22	B	614	CLA	C3D-C2D-C1D	-5.65	98.12	105.83
24	c	514	BCR	C12-C13-C14	5.64	127.88	119.01
24	k	101	BCR	C24-C23-C22	5.64	134.58	126.23
24	B	618	BCR	C34-C9-C10	-5.64	113.69	122.82
22	B	609	CLA	C2D-C1D-ND	5.63	115.70	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	C3D-C2D-C1D	-5.63	98.15	105.83
22	b	609	CLA	C2D-C1D-ND	5.63	115.69	110.13
22	c	507	CLA	C1D-ND-C4D	-5.63	102.36	106.31
24	T	101	BCR	C34-C9-C10	-5.62	113.71	122.82
24	D	404	BCR	C23-C22-C21	5.61	127.84	119.01
22	B	616	CLA	C2D-C1D-ND	5.61	115.68	110.13
22	b	611	CLA	C2D-C1D-ND	5.61	115.68	110.13
24	d	404	BCR	C23-C22-C21	5.61	127.83	119.01
22	D	402	CLA	C1D-ND-C4D	-5.60	102.39	106.31
22	C	507	CLA	C1D-ND-C4D	-5.60	102.39	106.31
24	h	101	BCR	C33-C5-C6	5.59	130.58	124.48
22	b	604	CLA	C2C-C1C-NC	5.59	115.85	109.98
24	k	101	BCR	C8-C7-C6	5.58	141.91	127.00
22	B	611	CLA	C2D-C1D-ND	5.58	115.65	110.13
33	V	201	HEM	C4D-ND-C1D	5.57	111.80	105.21
24	K	101	BCR	C8-C7-C6	5.57	141.87	127.00
22	b	616	CLA	C2D-C1D-ND	5.55	115.61	110.13
24	K	102	BCR	C37-C22-C21	-5.54	113.83	122.82
22	D	401	CLA	C3D-C2D-C1D	-5.54	98.27	105.83
33	v	201	HEM	C4D-ND-C1D	5.54	111.77	105.21
24	k	102	BCR	C37-C22-C21	-5.53	113.85	122.82
22	d	401	CLA	C3D-C2D-C1D	-5.53	98.28	105.83
24	c	515	BCR	C8-C7-C6	5.53	141.77	127.00
24	H	101	BCR	C33-C5-C6	5.53	130.52	124.48
22	B	609	CLA	CMD-C2D-C1D	5.52	134.45	124.73
24	C	515	BCR	C8-C7-C6	5.51	141.72	127.00
22	b	609	CLA	CMD-C2D-C1D	5.50	134.42	124.73
22	B	604	CLA	C2C-C1C-NC	5.50	115.75	109.98
24	a	608	BCR	C30-C25-C26	-5.49	115.13	122.64
24	A	608	BCR	C30-C25-C26	-5.49	115.13	122.64
24	K	102	BCR	C23-C24-C25	5.49	141.66	127.00
24	k	102	BCR	C23-C24-C25	5.49	141.65	127.00
22	b	604	CLA	C2D-C1D-ND	5.47	115.54	110.13
22	A	603	CLA	CMD-C2D-C1D	5.47	134.36	124.73
22	D	403	CLA	C2D-C1D-ND	5.47	115.54	110.13
22	a	603	CLA	CMD-C2D-C1D	5.46	134.35	124.73
22	B	615	CLA	C2D-C1D-ND	5.46	115.53	110.13
22	C	502	CLA	C2D-C1D-ND	5.44	115.51	110.13
22	d	403	CLA	C2D-C1D-ND	5.44	115.51	110.13
22	B	604	CLA	C2D-C1D-ND	5.43	115.50	110.13
24	H	101	BCR	C29-C30-C25	5.43	118.33	110.44
24	H	101	BCR	C35-C13-C12	-5.42	109.81	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	613	CLA	C2D-C1D-ND	5.42	115.49	110.13
22	c	505	CLA	C1D-ND-C4D	-5.42	102.51	106.31
22	b	615	CLA	C2D-C1D-ND	5.41	115.48	110.13
22	b	613	CLA	C2D-C1D-ND	5.41	115.48	110.13
24	h	101	BCR	C35-C13-C12	-5.41	109.82	118.09
24	t	101	BCR	C37-C22-C23	-5.41	109.83	118.09
22	a	607	CLA	C2C-C1C-NC	5.41	115.66	109.98
22	C	507	CLA	C3B-C2B-C1B	-5.39	100.81	107.17
22	C	505	CLA	C1D-ND-C4D	-5.39	102.53	106.31
22	A	607	CLA	C2C-C1C-NC	5.39	115.64	109.98
22	c	502	CLA	C2D-C1D-ND	5.38	115.45	110.13
22	c	509	CLA	C2C-C1C-NC	5.38	115.64	109.98
22	C	511	CLA	C2D-C1D-ND	5.38	115.45	110.13
22	b	608	CLA	C2D-C1D-ND	5.38	115.45	110.13
24	h	101	BCR	C29-C30-C25	5.38	118.25	110.44
22	c	511	CLA	C2D-C1D-ND	5.38	115.45	110.13
22	B	610	CLA	C2C-C1C-NC	5.38	115.63	109.98
24	C	515	BCR	C35-C13-C12	-5.38	109.88	118.09
22	C	509	CLA	C2C-C1C-NC	5.37	115.62	109.98
22	c	507	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
22	B	608	CLA	C2D-C1D-ND	5.37	115.44	110.13
22	b	610	CLA	C2C-C1C-NC	5.36	115.61	109.98
22	c	509	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
24	c	515	BCR	C35-C13-C12	-5.36	109.90	118.09
24	T	102	BCR	C37-C22-C23	-5.36	109.90	118.09
22	b	609	CLA	C2B-C1B-NB	5.35	115.88	110.33
22	B	612	CLA	C2C-C1C-NC	5.35	115.60	109.98
24	a	608	BCR	C24-C23-C22	5.34	134.14	126.23
22	C	504	CLA	C2C-C1C-NC	5.34	115.59	109.98
22	c	508	CLA	C2D-C1D-ND	5.34	115.41	110.13
22	C	508	CLA	C2D-C1D-ND	5.33	115.41	110.13
24	T	101	BCR	C2-C1-C6	5.33	118.18	110.44
22	B	609	CLA	C2B-C1B-NB	5.32	115.85	110.33
22	b	612	CLA	C2C-C1C-NC	5.32	115.57	109.98
24	c	515	BCR	C29-C30-C25	5.32	118.17	110.44
24	A	608	BCR	C24-C23-C22	5.32	134.11	126.23
22	c	504	CLA	C2C-C1C-NC	5.32	115.57	109.98
24	B	618	BCR	C2-C1-C6	5.32	118.16	110.44
22	C	509	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
24	C	515	BCR	C29-C30-C25	5.31	118.15	110.44
22	B	616	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
22	b	616	CLA	C3B-C2B-C1B	-5.30	100.92	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	F	101	HEM	C4D-ND-C1D	5.30	111.49	105.21
22	D	401	CLA	C2C-C1C-NC	5.30	115.55	109.98
22	d	401	CLA	C2C-C1C-NC	5.30	115.55	109.98
24	B	619	BCR	C40-C30-C25	5.30	118.55	110.24
22	B	608	CLA	C2C-C1C-NC	5.29	115.54	109.98
24	k	101	BCR	C36-C18-C17	-5.29	114.24	122.82
24	b	618	BCR	C40-C30-C25	5.28	118.53	110.24
24	b	618	BCR	C38-C26-C27	-5.28	102.34	113.60
24	d	404	BCR	C39-C30-C29	-5.28	88.70	108.95
24	B	619	BCR	C38-C26-C27	-5.27	102.35	113.60
24	D	404	BCR	C39-C30-C29	-5.27	88.71	108.95
24	K	102	BCR	C8-C9-C10	5.26	127.29	119.01
24	k	102	BCR	C8-C9-C10	5.26	127.28	119.01
24	K	101	BCR	C36-C18-C17	-5.26	114.29	122.82
33	f	101	HEM	C4D-ND-C1D	5.26	111.44	105.21
22	B	612	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
24	D	404	BCR	C24-C23-C22	5.25	134.00	126.23
22	B	616	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
22	b	612	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
24	k	101	BCR	C8-C9-C10	5.25	127.26	119.01
24	h	101	BCR	C33-C5-C4	-5.24	102.42	113.60
22	b	608	CLA	C2C-C1C-NC	5.24	115.48	109.98
22	C	512	CLA	O2D-CGD-CBD	5.24	120.39	111.23
22	b	616	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
24	K	101	BCR	C4-C5-C6	5.24	129.78	122.70
24	H	101	BCR	C33-C5-C4	-5.23	102.44	113.60
24	K	101	BCR	C8-C9-C10	5.23	127.24	119.01
22	c	512	CLA	O2D-CGD-CBD	5.23	120.37	111.23
24	c	514	BCR	C2-C1-C6	5.22	118.02	110.44
22	d	402	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
24	k	101	BCR	C4-C5-C6	5.22	129.76	122.70
22	D	402	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
22	c	506	CLA	O2D-CGD-CBD	5.22	120.35	111.23
22	C	506	CLA	O2D-CGD-CBD	5.22	120.35	111.23
22	A	603	CLA	C2B-C1B-NB	5.21	115.72	110.33
24	d	404	BCR	C24-C23-C22	5.20	133.93	126.23
22	A	604	CLA	C2D-C1D-ND	5.20	115.28	110.13
22	a	604	CLA	C2D-C1D-ND	5.20	115.27	110.13
22	a	603	CLA	C2B-C1B-NB	5.20	115.72	110.33
22	B	603	CLA	C2D-C1D-ND	5.20	115.27	110.13
22	C	510	CLA	C2D-C1D-ND	5.19	115.26	110.13
24	D	404	BCR	C8-C7-C6	5.19	140.87	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	404	BCR	C4-C5-C6	5.19	129.72	122.70
24	C	514	BCR	C2-C1-C6	5.19	117.97	110.44
24	d	404	BCR	C8-C7-C6	5.19	140.85	127.00
22	c	501	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
22	c	513	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
22	b	614	CLA	C2C-C1C-NC	5.18	115.42	109.98
22	b	615	CLA	C2C-C1C-NC	5.18	115.42	109.98
22	B	615	CLA	C2C-C1C-NC	5.17	115.42	109.98
22	c	510	CLA	C2D-C1D-ND	5.17	115.24	110.13
24	d	404	BCR	C4-C5-C6	5.17	129.69	122.70
22	C	501	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
24	C	515	BCR	C36-C18-C19	-5.16	110.20	118.09
22	c	510	CLA	C2C-C1C-NC	5.16	115.40	109.98
22	C	507	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
22	C	513	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
22	b	603	CLA	C2D-C1D-ND	5.16	115.23	110.13
22	B	614	CLA	C2C-C1C-NC	5.15	115.40	109.98
22	b	602	CLA	C2D-C1D-ND	5.15	115.23	110.13
22	c	507	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
22	B	607	CLA	C2D-C1D-ND	5.14	115.21	110.13
24	c	515	BCR	C36-C18-C19	-5.13	110.25	118.09
22	B	602	CLA	C2D-C1D-ND	5.13	115.20	110.13
22	C	510	CLA	C2C-C1C-NC	5.12	115.36	109.98
22	a	604	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
22	C	503	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
22	B	610	CLA	C2D-C1D-ND	5.12	115.19	110.13
22	A	604	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
22	C	506	CLA	C2C-C1C-NC	5.11	115.34	109.98
22	A	607	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
24	b	618	BCR	C27-C26-C25	5.09	129.58	122.70
24	H	101	BCR	C34-C9-C10	-5.09	114.58	122.82
22	c	506	CLA	C2C-C1C-NC	5.09	115.32	109.98
22	b	607	CLA	C2D-C1D-ND	5.08	115.15	110.13
22	a	607	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
22	c	503	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
22	b	617	CLA	C3B-C2B-C1B	-5.08	101.19	107.17
24	K	102	BCR	C36-C18-C17	-5.07	114.59	122.82
22	b	610	CLA	C2D-C1D-ND	5.07	115.15	110.13
24	B	619	BCR	C27-C26-C25	5.07	129.56	122.70
24	t	101	BCR	C24-C23-C22	5.06	133.73	126.23
24	B	618	BCR	C38-C26-C27	-5.06	102.81	113.60
24	h	101	BCR	C34-C9-C10	-5.06	114.62	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	617	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
22	B	602	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
24	K	101	BCR	C23-C22-C21	5.05	126.96	119.01
22	A	604	CLA	C2B-C1B-NB	5.05	115.57	110.33
24	C	514	BCR	C27-C26-C25	5.05	129.53	122.70
22	a	604	CLA	C2B-C1B-NB	5.05	115.56	110.33
24	c	514	BCR	C27-C26-C25	5.05	129.53	122.70
24	k	102	BCR	C36-C18-C17	-5.04	114.65	122.82
24	T	101	BCR	C38-C26-C27	-5.04	102.86	113.60
22	B	617	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
22	b	602	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
24	k	101	BCR	C23-C22-C21	5.03	126.93	119.01
22	b	617	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
22	B	603	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
22	B	602	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
22	b	602	CLA	C3B-C2B-C1B	-5.03	101.25	107.17
22	D	403	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
22	C	503	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
24	T	102	BCR	C24-C23-C22	5.01	133.65	126.23
22	b	603	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
22	C	506	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
22	C	511	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
22	c	506	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
22	B	604	CLA	O2D-CGD-CBD	5.00	119.98	111.23
22	b	609	CLA	C4A-NA-C1A	5.00	108.96	106.68
24	D	404	BCR	C8-C9-C10	5.00	126.87	119.01
22	A	604	CLA	C3B-C4B-NB	5.00	114.99	110.53
24	B	619	BCR	C37-C22-C21	-4.99	114.73	122.82
22	c	503	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
22	c	501	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
22	C	504	CLA	O2D-CGD-CBD	4.99	119.95	111.23
22	d	403	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
22	b	604	CLA	O2D-CGD-CBD	4.98	119.94	111.23
24	b	618	BCR	C37-C22-C21	-4.98	114.74	122.82
22	A	603	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
22	c	504	CLA	O2D-CGD-CBD	4.98	119.94	111.23
22	c	511	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
24	K	101	BCR	C23-C24-C25	4.98	140.29	127.00
24	b	618	BCR	C36-C18-C17	-4.98	114.75	122.82
22	b	608	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
24	k	101	BCR	C23-C24-C25	4.97	140.28	127.00
24	B	619	BCR	C36-C18-C17	-4.97	114.77	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	604	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
22	C	502	CLA	C3D-C2D-C1D	-4.97	99.06	105.83
24	C	515	BCR	C38-C26-C25	4.96	129.90	124.48
24	d	404	BCR	C8-C9-C10	4.96	126.80	119.01
22	a	603	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
24	D	404	BCR	C7-C8-C9	4.96	133.57	126.23
22	a	604	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
24	c	515	BCR	C38-C26-C25	4.95	129.89	124.48
22	c	506	CLA	C2D-C1D-ND	4.95	115.03	110.13
22	B	608	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
24	B	619	BCR	C35-C13-C14	-4.95	114.80	122.82
22	C	501	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
24	d	404	BCR	C7-C8-C9	4.95	133.56	126.23
22	A	604	CLA	O2D-CGD-CBD	4.95	119.88	111.23
22	A	604	CLA	C1C-C2C-C3C	-4.95	101.78	106.98
22	c	502	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
22	a	604	CLA	C3B-C4B-NB	4.94	114.94	110.53
22	C	502	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
22	C	501	CLA	C2C-C1C-NC	4.94	115.17	109.98
22	D	402	CLA	C4A-NA-C1A	4.94	108.93	106.68
22	B	615	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
24	a	608	BCR	C36-C18-C19	-4.94	110.54	118.09
22	B	613	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
24	b	618	BCR	C35-C13-C14	-4.94	114.82	122.82
22	A	603	CLA	C2C-C1C-NC	4.94	115.17	109.98
22	a	604	CLA	O2D-CGD-CBD	4.94	119.86	111.23
24	A	608	BCR	C36-C18-C19	-4.93	110.55	118.09
22	B	609	CLA	C4A-NA-C1A	4.93	108.93	106.68
22	a	603	CLA	C2C-C1C-NC	4.93	115.16	109.98
22	A	603	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
22	c	512	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
22	c	510	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
22	B	611	CLA	C2B-C1B-NB	4.93	115.44	110.33
22	C	506	CLA	C2D-C1D-ND	4.93	115.00	110.13
22	b	609	CLA	O2D-CGD-CBD	4.93	119.84	111.23
22	c	502	CLA	C3B-C2B-C1B	-4.92	101.36	107.17
22	c	505	CLA	C3B-C2B-C1B	-4.92	101.36	107.17
22	b	615	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
22	C	510	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
22	a	604	CLA	C1C-C2C-C3C	-4.92	101.81	106.98
22	c	504	CLA	C2D-C1D-ND	4.92	114.99	110.13
22	b	611	CLA	C2B-C1B-NB	4.91	115.42	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	501	CLA	C2C-C1C-NC	4.91	115.14	109.98
22	b	613	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
22	B	609	CLA	O2D-CGD-CBD	4.91	119.82	111.23
22	B	606	CLA	C2C-C1C-NC	4.91	115.14	109.98
22	a	603	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
22	C	505	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
22	b	609	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
22	C	512	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
22	B	607	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
22	b	606	CLA	C2C-C1C-NC	4.90	115.13	109.98
22	C	511	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
22	D	402	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
22	A	607	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
22	B	611	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
22	b	611	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
22	b	607	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
22	B	609	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
22	a	607	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
22	B	606	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
24	t	101	BCR	C33-C5-C4	-4.88	103.19	113.60
22	b	613	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	B	619	BCR	C2-C1-C6	4.87	117.52	110.44
24	T	102	BCR	C33-C5-C4	-4.87	103.22	113.60
22	b	605	CLA	C2D-C1D-ND	4.87	114.94	110.13
22	d	402	CLA	C4A-NA-C1A	4.87	108.90	106.68
22	d	402	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
22	B	613	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
22	c	511	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
22	B	615	CLA	C2B-C1B-NB	4.86	115.37	110.33
24	b	618	BCR	C2-C1-C6	4.86	117.50	110.44
22	c	507	CLA	C2D-C1D-ND	4.86	114.93	110.13
22	b	613	CLA	O2D-CGD-CBD	4.85	119.71	111.23
22	b	607	CLA	C2C-C1C-NC	4.85	115.08	109.98
22	c	504	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
22	c	512	CLA	C2D-C1D-ND	4.85	114.92	110.13
22	c	505	CLA	C2C-C1C-NC	4.85	115.07	109.98
22	C	504	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
22	b	606	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
22	B	610	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
22	B	607	CLA	C2C-C1C-NC	4.84	115.07	109.98
22	C	509	CLA	C2D-C1D-ND	4.84	114.92	110.13
22	C	507	CLA	C2D-C1D-ND	4.84	114.92	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	C2C-C1C-NC	4.84	115.06	109.98
22	C	504	CLA	C2D-C1D-ND	4.84	114.91	110.13
24	k	102	BCR	C35-C13-C12	-4.84	110.70	118.09
22	b	610	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
22	D	403	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
22	b	615	CLA	C2B-C1B-NB	4.83	115.34	110.33
24	K	102	BCR	C35-C13-C12	-4.83	110.71	118.09
22	B	613	CLA	O2D-CGD-CBD	4.83	119.68	111.23
22	B	605	CLA	C2D-C1D-ND	4.83	114.91	110.13
25	A	609	SQD	O6-C1-C2	4.83	115.61	108.27
22	c	508	CLA	C2C-C1C-NC	4.83	115.05	109.98
22	C	512	CLA	C2D-C1D-ND	4.82	114.90	110.13
22	c	509	CLA	C2D-C1D-ND	4.82	114.90	110.13
22	C	509	CLA	O2D-CGD-CBD	4.82	119.66	111.23
22	d	403	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
22	B	615	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
25	a	609	SQD	O6-C1-C2	4.82	115.59	108.27
22	C	511	CLA	C2C-C1C-NC	4.82	115.04	109.98
22	c	512	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
22	C	512	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
22	c	502	CLA	C2C-C1C-NC	4.81	115.03	109.98
22	C	502	CLA	C2C-C1C-NC	4.81	115.03	109.98
22	c	511	CLA	C2C-C1C-NC	4.81	115.03	109.98
22	b	613	CLA	C2C-C1C-NC	4.81	115.03	109.98
22	B	605	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
22	b	615	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
22	b	605	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
22	c	509	CLA	O2D-CGD-CBD	4.80	119.62	111.23
22	B	616	CLA	C2C-C1C-NC	4.79	115.02	109.98
22	A	607	CLA	C2B-C1B-NB	4.79	115.30	110.33
22	C	508	CLA	C2C-C1C-NC	4.79	115.01	109.98
22	a	607	CLA	C2B-C1B-NB	4.78	115.28	110.33
22	B	613	CLA	C2C-C1C-NC	4.77	115.00	109.98
22	b	606	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
22	B	611	CLA	C2C-C1C-NC	4.76	114.98	109.98
22	b	611	CLA	C2C-C1C-NC	4.76	114.98	109.98
22	b	609	CLA	C3B-C4B-NB	4.75	114.77	110.53
25	L	101	SQD	O6-C1-C2	4.75	115.49	108.27
24	c	514	BCR	C35-C13-C12	-4.75	110.83	118.09
22	B	602	CLA	C2B-C1B-NB	4.75	115.25	110.33
22	b	615	CLA	O2D-CGD-CBD	4.75	119.53	111.23
22	b	616	CLA	C2C-C1C-NC	4.75	114.97	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	BCR	C35-C13-C12	-4.75	110.84	118.09
22	C	503	CLA	C2D-C1D-ND	4.75	114.82	110.13
22	B	615	CLA	O2D-CGD-CBD	4.74	119.52	111.23
22	b	612	CLA	C3C-C4C-NC	4.74	116.50	110.43
22	B	612	CLA	C3C-C4C-NC	4.74	116.50	110.43
22	c	501	CLA	C2D-C1D-ND	4.74	114.81	110.13
22	c	509	CLA	C2B-C1B-NB	4.73	115.24	110.33
22	c	503	CLA	C2D-C1D-ND	4.73	114.81	110.13
22	b	604	CLA	C1C-C2C-C3C	-4.72	102.01	106.98
22	B	611	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
22	B	609	CLA	C3B-C4B-NB	4.72	114.74	110.53
22	d	403	CLA	C2C-C1C-NC	4.72	114.94	109.98
22	B	610	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
22	B	606	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
22	b	617	CLA	C2C-C1C-NC	4.71	114.92	109.98
22	b	612	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
22	B	604	CLA	C1C-C2C-C3C	-4.71	102.03	106.98
25	l	101	SQD	O6-C1-C2	4.70	115.42	108.27
24	t	101	BCR	C8-C7-C6	4.70	139.56	127.00
22	b	602	CLA	C2B-C1B-NB	4.70	115.20	110.33
24	T	102	BCR	C8-C7-C6	4.70	139.55	127.00
22	b	611	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
22	D	403	CLA	C2C-C1C-NC	4.68	114.90	109.98
29	z	101	LMG	O7-C10-C11	4.68	121.60	111.48
29	Z	101	LMG	O7-C10-C11	4.68	121.60	111.48
22	C	509	CLA	C2B-C1B-NB	4.68	115.18	110.33
24	t	101	BCR	C29-C30-C25	4.68	117.23	110.44
22	c	502	CLA	C2B-C1B-NB	4.67	115.17	110.33
22	C	508	CLA	O2D-CGD-CBD	4.67	119.40	111.23
22	B	612	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
24	T	102	BCR	C34-C9-C8	-4.67	110.96	118.09
22	c	510	CLA	C3B-C2B-C1B	-4.67	101.67	107.17
24	T	102	BCR	C29-C30-C25	4.66	117.21	110.44
22	d	401	CLA	C3C-C4C-NC	4.66	116.40	110.43
22	C	507	CLA	C2C-C1C-NC	4.66	114.88	109.98
22	C	510	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
24	t	101	BCR	C34-C9-C8	-4.66	110.98	118.09
22	C	501	CLA	C2D-C1D-ND	4.65	114.73	110.13
22	c	508	CLA	O2D-CGD-CBD	4.65	119.36	111.23
22	C	502	CLA	C2B-C1B-NB	4.65	115.15	110.33
24	B	622	BCR	C23-C22-C21	4.65	126.32	119.01
22	b	610	CLA	C3B-C2B-C1B	-4.65	101.69	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	607	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
22	c	513	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
22	B	605	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
22	b	607	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
24	D	404	BCR	C23-C24-C25	4.63	139.37	127.00
22	C	513	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	b	605	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
22	B	605	CLA	C3C-C4C-NC	4.63	116.36	110.43
24	d	404	BCR	C35-C13-C12	-4.63	111.02	118.09
22	B	603	CLA	C3B-C2B-C1B	-4.63	101.72	107.17
22	B	610	CLA	O2D-CGD-CBD	4.62	119.31	111.23
24	d	404	BCR	C23-C24-C25	4.62	139.35	127.00
22	b	610	CLA	O2D-CGD-CBD	4.62	119.31	111.23
22	D	401	CLA	C3C-C4C-NC	4.62	116.35	110.43
22	B	609	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
22	B	604	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
24	D	404	BCR	C36-C18-C17	-4.62	115.33	122.82
24	D	404	BCR	C35-C13-C12	-4.62	111.03	118.09
22	B	617	CLA	C2C-C1C-NC	4.62	114.83	109.98
22	b	603	CLA	C3B-C2B-C1B	-4.62	101.73	107.17
24	b	622	BCR	C23-C22-C21	4.61	126.27	119.01
22	B	606	CLA	C3C-C4C-NC	4.61	116.34	110.43
22	c	504	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
22	b	609	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
22	B	608	CLA	C3B-C4B-NB	4.61	114.64	110.53
22	b	604	CLA	C3B-C4B-NB	4.61	114.64	110.53
22	b	604	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
22	c	513	CLA	C2D-C1D-ND	4.60	114.68	110.13
24	T	101	BCR	C37-C22-C23	-4.60	111.06	118.09
24	d	404	BCR	C36-C18-C17	-4.60	115.36	122.82
22	B	604	CLA	C3B-C4B-NB	4.60	114.63	110.53
22	c	507	CLA	C2C-C1C-NC	4.59	114.81	109.98
22	c	505	CLA	O2D-CGD-CBD	4.59	119.25	111.23
22	C	505	CLA	O2D-CGD-CBD	4.58	119.24	111.23
22	c	505	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
22	b	606	CLA	C3C-C4C-NC	4.58	116.30	110.43
24	d	404	BCR	C36-C18-C19	-4.57	111.10	118.09
22	b	604	CLA	C2B-C1B-NB	4.57	115.07	110.33
22	B	604	CLA	C2B-C1B-NB	4.57	115.07	110.33
22	C	513	CLA	C2D-C1D-ND	4.57	114.65	110.13
22	b	616	CLA	C2B-C1B-NB	4.57	115.06	110.33
24	B	618	BCR	C37-C22-C23	-4.57	111.11	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C3B-C2B-C1B	-4.57	101.79	107.17
22	C	504	CLA	C1C-C2C-C3C	-4.56	102.18	106.98
22	C	503	CLA	C2C-C1C-NC	4.56	114.77	109.98
22	b	608	CLA	C3B-C4B-NB	4.56	114.60	110.53
22	b	605	CLA	C3C-C4C-NC	4.56	116.27	110.43
24	D	404	BCR	C36-C18-C19	-4.55	111.13	118.09
22	B	616	CLA	C2B-C1B-NB	4.55	115.05	110.33
24	c	514	BCR	C32-C1-C6	4.55	117.38	110.24
22	c	503	CLA	C2C-C1C-NC	4.55	114.76	109.98
22	C	505	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
22	B	608	CLA	C2B-C1B-NB	4.55	115.04	110.33
22	b	608	CLA	C2B-C1B-NB	4.54	115.04	110.33
24	b	618	BCR	C8-C7-C6	4.54	139.13	127.00
24	C	514	BCR	C32-C1-C6	4.54	117.36	110.24
24	B	619	BCR	C8-C7-C6	4.54	139.13	127.00
22	c	508	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
22	D	402	CLA	O2D-CGD-CBD	4.53	119.15	111.23
22	B	612	CLA	C2B-C1B-NB	4.53	115.02	110.33
22	b	612	CLA	C2B-C1B-NB	4.53	115.02	110.33
24	c	514	BCR	C30-C25-C26	-4.52	116.45	122.64
31	d	410	DGD	O2G-C1B-C2B	4.52	121.27	111.48
24	K	101	BCR	C1-C6-C5	-4.52	116.46	122.64
24	k	101	BCR	C1-C6-C5	-4.52	116.47	122.64
22	b	617	CLA	C3C-C4C-NC	4.52	116.22	110.43
22	D	401	CLA	C3B-C2B-C1B	-4.52	101.85	107.17
31	D	410	DGD	O2G-C1B-C2B	4.51	121.25	111.48
24	c	514	BCR	C33-C5-C4	-4.51	103.97	113.60
22	C	508	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
22	d	402	CLA	O2D-CGD-CBD	4.51	119.11	111.23
22	c	504	CLA	C1C-C2C-C3C	-4.51	102.24	106.98
24	C	514	BCR	C33-C5-C4	-4.50	103.99	113.60
22	B	617	CLA	C3C-C4C-NC	4.50	116.20	110.43
22	C	509	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	C	514	BCR	C30-C25-C26	-4.50	116.49	122.64
22	d	401	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
24	C	515	BCR	C37-C22-C21	-4.49	115.54	122.82
24	t	101	BCR	C2-C1-C6	4.49	116.96	110.44
24	c	515	BCR	C38-C26-C27	-4.48	104.03	113.60
24	C	515	BCR	C38-C26-C27	-4.48	104.04	113.60
22	c	509	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
24	T	101	BCR	C30-C25-C26	-4.48	116.51	122.64
22	C	507	CLA	O2D-CGD-CBD	4.48	119.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
22	c	511	CLA	C2B-C1B-NB	4.47	114.97	110.33
24	T	102	BCR	C2-C1-C6	4.47	116.93	110.44
24	K	102	BCR	C35-C13-C14	-4.46	115.59	122.82
22	C	511	CLA	C2B-C1B-NB	4.46	114.95	110.33
22	c	507	CLA	O2D-CGD-CBD	4.46	119.03	111.23
22	c	506	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
22	C	508	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
24	B	618	BCR	C30-C25-C26	-4.45	116.55	122.64
22	B	609	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
24	k	102	BCR	C35-C13-C14	-4.45	115.61	122.82
22	c	513	CLA	O2D-CGD-CBD	4.45	119.00	111.23
22	D	403	CLA	C2B-C1B-NB	4.44	114.93	110.33
22	C	513	CLA	O2D-CGD-CBD	4.44	118.99	111.23
22	b	609	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
24	B	618	BCR	C29-C30-C25	4.43	116.88	110.44
22	c	501	CLA	O2D-CGD-O1D	-4.43	115.22	123.85
22	d	403	CLA	C2B-C1B-NB	4.43	114.92	110.33
24	t	101	BCR	C23-C24-C25	4.43	138.83	127.00
22	b	602	CLA	C2C-C1C-NC	4.43	114.63	109.98
22	C	501	CLA	O2D-CGD-O1D	-4.43	115.23	123.85
24	T	101	BCR	C29-C30-C25	4.43	116.87	110.44
24	T	102	BCR	C23-C24-C25	4.42	138.80	127.00
25	b	621	SQD	O6-C1-C2	4.42	114.98	108.27
24	B	622	BCR	C33-C5-C4	-4.42	104.18	113.60
24	b	622	BCR	C33-C5-C4	-4.41	104.19	113.60
24	c	515	BCR	C37-C22-C21	-4.41	115.67	122.82
24	C	514	BCR	C23-C24-C25	4.41	138.78	127.00
22	b	614	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
22	C	513	CLA	C2B-C1B-NB	4.41	114.90	110.33
24	B	622	BCR	C38-C26-C27	-4.41	104.20	113.60
22	B	602	CLA	C2C-C1C-NC	4.40	114.61	109.98
22	C	506	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
22	c	513	CLA	C2B-C1B-NB	4.40	114.89	110.33
22	c	505	CLA	C2D-C1D-ND	4.40	114.48	110.13
24	c	514	BCR	C23-C24-C25	4.39	138.73	127.00
24	D	404	BCR	C34-C9-C10	-4.39	115.70	122.82
22	b	604	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	b	622	BCR	C38-C26-C27	-4.39	104.24	113.60
22	B	604	CLA	C3D-C4D-ND	4.39	117.12	109.99
24	d	404	BCR	C34-C9-C10	-4.38	115.72	122.82
22	B	614	CLA	C3B-C2B-C1B	-4.38	102.01	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	617	CLA	C2B-C1B-NB	4.38	114.87	110.33
22	B	604	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
25	l	102	SQD	O6-C1-C2	4.38	114.92	108.27
22	b	604	CLA	C3D-C4D-ND	4.37	117.10	109.99
24	k	101	BCR	C34-C9-C10	-4.37	115.74	122.82
24	K	101	BCR	C34-C9-C10	-4.36	115.75	122.82
22	C	505	CLA	C2D-C1D-ND	4.36	114.44	110.13
24	B	619	BCR	C33-C5-C6	4.36	129.24	124.48
22	B	616	CLA	C3C-C4C-NC	4.36	116.01	110.43
22	B	617	CLA	C2B-C1B-NB	4.35	114.84	110.33
22	c	501	CLA	C2B-C1B-NB	4.35	114.84	110.33
22	C	508	CLA	C3D-C4D-ND	4.35	117.06	109.99
22	b	616	CLA	C3C-C4C-NC	4.35	116.00	110.43
22	B	612	CLA	O2D-CGD-CBD	4.35	118.83	111.23
24	b	618	BCR	C33-C5-C6	4.34	129.22	124.48
22	C	503	CLA	C2B-C1B-NB	4.34	114.82	110.33
25	A	609	SQD	O47-C7-C8	4.34	120.86	111.48
25	a	609	SQD	O47-C7-C8	4.34	120.86	111.48
24	T	102	BCR	C30-C25-C26	-4.34	116.71	122.64
24	h	101	BCR	C8-C7-C6	4.34	138.58	127.00
22	D	402	CLA	C3C-C4C-NC	4.33	115.98	110.43
22	b	612	CLA	O2D-CGD-CBD	4.33	118.81	111.23
24	t	101	BCR	C30-C25-C26	-4.33	116.72	122.64
33	F	101	HEM	CBD-CAD-C3D	-4.33	100.56	112.53
22	c	509	CLA	C1C-C2C-C3C	-4.33	102.42	106.98
22	c	508	CLA	C3D-C4D-ND	4.33	117.02	109.99
22	A	607	CLA	C1C-C2C-C3C	-4.33	102.43	106.98
22	c	512	CLA	C2C-C1C-NC	4.32	114.52	109.98
24	H	101	BCR	C8-C7-C6	4.32	138.54	127.00
24	c	514	BCR	C36-C18-C19	-4.32	111.49	118.09
33	f	101	HEM	CBD-CAD-C3D	-4.32	100.60	112.53
22	a	607	CLA	C1C-C2C-C3C	-4.31	102.44	106.98
22	d	402	CLA	C3C-C4C-NC	4.31	115.95	110.43
22	b	605	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
22	c	503	CLA	C2B-C1B-NB	4.31	114.80	110.33
22	B	608	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
24	C	514	BCR	C36-C18-C19	-4.31	111.51	118.09
22	c	510	CLA	C2B-C1B-NB	4.30	114.79	110.33
24	b	622	BCR	C27-C26-C25	4.30	128.51	122.70
22	B	605	CLA	C3B-C2B-C1B	-4.30	102.11	107.17
22	d	402	CLA	C2B-C1B-NB	4.29	114.78	110.33
22	b	603	CLA	C2C-C1C-NC	4.29	114.49	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	402	CLA	C2B-C1B-NB	4.29	114.77	110.33
24	h	101	BCR	C28-C27-C26	4.29	121.70	114.06
22	C	509	CLA	C1C-C2C-C3C	-4.28	102.47	106.98
25	d	411	SQD	O6-C1-C2	4.28	114.78	108.27
22	b	614	CLA	C1C-C2C-C3C	-4.28	102.48	106.98
24	B	622	BCR	C27-C26-C25	4.28	128.49	122.70
22	C	512	CLA	C2C-C1C-NC	4.28	114.48	109.98
22	C	510	CLA	C2B-C1B-NB	4.28	114.76	110.33
22	B	614	CLA	C1C-C2C-C3C	-4.28	102.48	106.98
25	D	411	SQD	O6-C1-C2	4.28	114.77	108.27
24	H	101	BCR	C28-C27-C26	4.28	121.68	114.06
24	B	618	BCR	C38-C26-C25	4.28	129.15	124.48
22	B	606	CLA	C2B-C1B-NB	4.27	114.75	110.33
22	C	501	CLA	C2B-C1B-NB	4.27	114.75	110.33
31	C	516	DGD	O2G-C1B-C2B	4.27	120.71	111.48
22	b	606	CLA	C2B-C1B-NB	4.26	114.75	110.33
24	a	608	BCR	C23-C24-C25	4.26	138.38	127.00
22	b	607	CLA	O2D-CGD-O1D	-4.26	115.56	123.85
22	A	607	CLA	O2D-CGD-CBD	4.26	118.67	111.23
22	B	603	CLA	C2C-C1C-NC	4.25	114.45	109.98
22	B	607	CLA	O2D-CGD-O1D	-4.25	115.58	123.85
22	b	608	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
24	A	608	BCR	C23-C24-C25	4.25	138.34	127.00
22	c	511	CLA	O2D-CGD-CBD	4.24	118.65	111.23
31	c	516	DGD	O2G-C1B-C2B	4.24	120.66	111.48
24	T	101	BCR	C38-C26-C25	4.24	129.11	124.48
22	B	607	CLA	CHD-C1D-ND	-4.24	118.83	124.80
24	B	619	BCR	C33-C5-C4	-4.23	104.58	113.60
22	b	607	CLA	CHD-C1D-ND	-4.22	118.86	124.80
24	b	618	BCR	C35-C13-C12	-4.22	111.64	118.09
22	C	511	CLA	O2D-CGD-CBD	4.22	118.61	111.23
22	a	607	CLA	O2D-CGD-CBD	4.22	118.60	111.23
24	t	101	BCR	C33-C5-C6	4.21	129.08	124.48
22	c	507	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	b	618	BCR	C33-C5-C4	-4.21	104.62	113.60
22	C	506	CLA	C3C-C4C-NC	4.21	115.82	110.43
24	k	101	BCR	C35-C13-C14	-4.21	116.00	122.82
22	C	508	CLA	C2B-C1B-NB	4.21	114.69	110.33
22	C	507	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	K	101	BCR	C35-C13-C14	-4.20	116.01	122.82
24	b	622	BCR	C30-C25-C26	-4.20	116.89	122.64
24	B	619	BCR	C35-C13-C12	-4.20	111.67	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	C2B-C1B-NB	4.20	114.68	110.33
22	C	513	CLA	C2C-C1C-NC	4.20	114.39	109.98
22	b	604	CLA	C3C-C4C-NC	4.19	115.80	110.43
22	c	504	CLA	CHD-C1D-ND	-4.19	118.90	124.80
22	c	501	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
22	C	501	CLA	C1C-C2C-C3C	-4.18	102.58	106.98
22	C	504	CLA	CHD-C1D-ND	-4.18	118.92	124.80
24	D	404	BCR	C33-C5-C4	-4.18	104.68	113.60
22	B	604	CLA	C3C-C4C-NC	4.17	115.78	110.43
22	c	506	CLA	C3C-C4C-NC	4.17	115.78	110.43
22	B	609	CLA	C3C-C4C-NC	4.17	115.77	110.43
24	c	515	BCR	C36-C18-C17	-4.17	116.06	122.82
22	a	603	CLA	C3B-C4B-NB	4.17	114.25	110.53
22	c	510	CLA	C3B-C4B-NB	4.17	114.25	110.53
22	A	607	CLA	C3D-C4D-ND	4.17	116.76	109.99
22	c	513	CLA	C2C-C1C-NC	4.17	114.36	109.98
22	C	501	CLA	CHD-C1D-ND	-4.16	118.94	124.80
22	B	613	CLA	C3C-C4C-NC	4.16	115.76	110.43
24	T	102	BCR	C33-C5-C6	4.16	129.02	124.48
22	c	501	CLA	CHD-C1D-ND	-4.16	118.95	124.80
22	c	502	CLA	O2D-CGD-CBD	4.15	118.49	111.23
24	B	622	BCR	C30-C25-C26	-4.15	116.96	122.64
22	C	510	CLA	C3B-C4B-NB	4.15	114.23	110.53
22	C	502	CLA	O2D-CGD-CBD	4.15	118.48	111.23
22	c	504	CLA	C2B-C1B-NB	4.15	114.63	110.33
24	T	101	BCR	C23-C24-C25	4.15	138.08	127.00
24	B	618	BCR	C23-C24-C25	4.15	138.07	127.00
22	c	507	CLA	C1C-C2C-C3C	-4.14	102.62	106.98
22	A	603	CLA	C3C-C4C-NC	4.14	115.73	110.43
22	b	613	CLA	C3C-C4C-NC	4.14	115.73	110.43
24	d	404	BCR	C33-C5-C4	-4.14	104.78	113.60
22	a	607	CLA	C3D-C4D-ND	4.14	116.71	109.99
22	c	503	CLA	CHD-C1D-ND	-4.13	118.98	124.80
24	C	515	BCR	C36-C18-C17	-4.13	116.12	122.82
22	A	603	CLA	C3B-C4B-NB	4.13	114.22	110.53
22	c	512	CLA	C2B-C1B-NB	4.13	114.61	110.33
22	C	507	CLA	C1C-C2C-C3C	-4.12	102.64	106.98
22	b	609	CLA	C3C-C4C-NC	4.12	115.71	110.43
22	B	610	CLA	C3C-C4C-NC	4.12	115.70	110.43
22	b	602	CLA	CHD-C1D-ND	-4.11	119.02	124.80
22	C	503	CLA	CHD-C1D-ND	-4.11	119.02	124.80
22	C	504	CLA	C2B-C1B-NB	4.11	114.58	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	603	CLA	C3C-C4C-NC	4.11	115.69	110.43
22	C	512	CLA	C2B-C1B-NB	4.09	114.57	110.33
22	B	611	CLA	C3C-C4C-NC	4.09	115.67	110.43
24	C	515	BCR	C2-C1-C6	4.09	116.38	110.44
22	c	502	CLA	C3C-C4C-NC	4.08	115.66	110.43
24	k	102	BCR	C30-C25-C26	-4.08	117.06	122.64
22	b	614	CLA	C2B-C1B-NB	4.08	114.56	110.33
22	B	602	CLA	CHD-C1D-ND	-4.08	119.07	124.80
22	b	611	CLA	C3C-C4C-NC	4.07	115.65	110.43
24	C	515	BCR	C31-C1-C2	-4.07	93.32	108.95
24	c	515	BCR	C31-C1-C2	-4.07	93.32	108.95
24	c	515	BCR	C2-C1-C6	4.07	116.35	110.44
22	B	609	CLA	C3D-C4D-ND	4.07	116.60	109.99
22	C	511	CLA	C3C-C4C-NC	4.07	115.64	110.43
22	c	511	CLA	C3C-C4C-NC	4.07	115.64	110.43
24	C	514	BCR	C23-C22-C21	4.06	125.40	119.01
22	B	617	CLA	O2D-CGD-CBD	4.06	118.33	111.23
22	C	510	CLA	CHD-C1D-ND	-4.06	119.09	124.80
24	K	102	BCR	C30-C25-C26	-4.06	117.09	122.64
22	c	510	CLA	CHD-C1D-ND	-4.06	119.09	124.80
24	c	514	BCR	C23-C22-C21	4.05	125.39	119.01
22	b	603	CLA	O2D-CGD-CBD	4.05	118.31	111.23
22	C	502	CLA	C3C-C4C-NC	4.05	115.62	110.43
22	b	609	CLA	C3D-C4D-ND	4.05	116.56	109.99
24	c	514	BCR	C32-C1-C2	-4.04	93.42	108.95
24	B	619	BCR	C40-C30-C29	-4.04	93.43	108.95
22	B	614	CLA	C2B-C1B-NB	4.04	114.52	110.33
24	b	618	BCR	C40-C30-C29	-4.04	93.44	108.95
24	C	514	BCR	C32-C1-C2	-4.04	93.45	108.95
22	b	610	CLA	C3C-C4C-NC	4.03	115.60	110.43
24	B	618	BCR	C8-C7-C6	4.03	137.77	127.00
22	B	603	CLA	O2D-CGD-CBD	4.03	118.28	111.23
22	d	403	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
22	b	617	CLA	O2D-CGD-CBD	4.03	118.27	111.23
22	A	604	CLA	C3C-C4C-NC	4.02	115.58	110.43
22	C	503	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
22	b	607	CLA	C2B-C1B-NB	4.01	114.49	110.33
22	b	602	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
24	T	101	BCR	C8-C7-C6	4.01	137.71	127.00
22	D	403	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
22	B	607	CLA	C2B-C1B-NB	4.00	114.47	110.33
22	c	510	CLA	C3D-C4D-ND	4.00	116.49	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	607	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
22	a	604	CLA	C3C-C4C-NC	4.00	115.55	110.43
22	b	614	CLA	C3C-C4C-NC	4.00	115.55	110.43
22	B	602	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
22	c	509	CLA	C3C-C4C-NC	3.99	115.54	110.43
22	C	506	CLA	C1C-C2C-C3C	-3.98	102.80	106.98
22	c	503	CLA	C1C-C2C-C3C	-3.97	102.80	106.98
32	E	101	LHG	O7-C7-C8	3.97	120.07	111.48
22	B	614	CLA	CHD-C1D-ND	-3.97	119.22	124.80
22	c	510	CLA	C1C-C2C-C3C	-3.97	102.81	106.98
32	e	101	LHG	O7-C7-C8	3.97	120.06	111.48
22	C	510	CLA	C3D-C4D-ND	3.97	116.43	109.99
22	c	505	CLA	C3C-C4C-NC	3.96	115.51	110.43
22	b	607	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
22	C	505	CLA	C3C-C4C-NC	3.96	115.50	110.43
22	b	614	CLA	CHD-C1D-ND	-3.96	119.23	124.80
22	C	503	CLA	C3C-C4C-NC	3.96	115.50	110.43
22	b	608	CLA	C3B-C2B-C1B	-3.96	102.50	107.17
25	b	621	SQD	O47-C7-C8	3.95	120.03	111.48
22	C	509	CLA	C3C-C4C-NC	3.95	115.50	110.43
22	B	614	CLA	C3C-C4C-NC	3.95	115.49	110.43
22	d	402	CLA	C3B-C4B-NB	3.95	114.06	110.53
22	c	503	CLA	C3C-C4C-NC	3.95	115.49	110.43
24	B	618	BCR	C27-C26-C25	3.95	128.04	122.70
24	C	515	BCR	C8-C9-C10	3.95	125.22	119.01
22	C	507	CLA	CHD-C1D-ND	-3.94	119.25	124.80
22	b	613	CLA	CHD-C1D-ND	-3.94	119.25	124.80
25	l	102	SQD	O47-C7-C8	3.94	120.01	111.48
22	B	613	CLA	CHD-C1D-ND	-3.94	119.26	124.80
22	c	513	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
24	T	101	BCR	C27-C26-C25	3.94	128.03	122.70
22	c	507	CLA	CHD-C1D-ND	-3.93	119.27	124.80
22	B	608	CLA	C3B-C2B-C1B	-3.93	102.53	107.17
24	B	622	BCR	C8-C9-C10	3.93	125.19	119.01
22	A	607	CLA	C3B-C4B-NB	3.93	114.04	110.53
24	b	622	BCR	C8-C9-C10	3.93	125.19	119.01
22	C	513	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
22	C	511	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
22	D	402	CLA	C3B-C4B-NB	3.92	114.03	110.53
29	z	101	LMG	O1-C1-C2	3.92	114.22	108.27
22	a	607	CLA	C3B-C4B-NB	3.92	114.03	110.53
22	b	606	CLA	O2D-CGD-CBD	3.92	118.08	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	515	BCR	C8-C9-C10	3.91	125.17	119.01
22	C	510	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
22	c	506	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
22	d	403	CLA	C3D-C4D-ND	3.91	116.34	109.99
22	D	403	CLA	C3D-C4D-ND	3.91	116.34	109.99
22	b	610	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
22	B	606	CLA	O2D-CGD-CBD	3.91	118.06	111.23
29	B	620	LMG	O7-C10-C11	3.90	119.93	111.48
22	c	508	CLA	C3C-C4C-NC	3.90	115.43	110.43
22	c	503	CLA	O2D-CGD-CBD	3.90	118.05	111.23
24	C	515	BCR	C35-C13-C14	-3.90	116.50	122.82
24	K	102	BCR	C2-C1-C6	3.90	116.11	110.44
22	B	610	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
22	c	511	CLA	C1C-C2C-C3C	-3.89	102.88	106.98
24	c	515	BCR	C35-C13-C14	-3.89	116.51	122.82
29	b	619	LMG	O7-C10-C11	3.89	119.91	111.48
24	k	101	BCR	C27-C26-C25	3.89	127.95	122.70
22	a	604	CLA	C3D-C4D-ND	3.88	116.30	109.99
29	Z	101	LMG	O1-C1-C2	3.88	114.17	108.27
22	A	604	CLA	C3D-C4D-ND	3.88	116.29	109.99
22	C	510	CLA	O2D-CGD-CBD	3.88	118.01	111.23
24	k	102	BCR	C2-C1-C6	3.88	116.07	110.44
22	d	401	CLA	C2B-C1B-NB	3.88	114.35	110.33
24	d	404	BCR	C38-C26-C27	-3.88	105.33	113.60
22	C	503	CLA	O2D-CGD-CBD	3.88	118.00	111.23
22	C	508	CLA	C3C-C4C-NC	3.87	115.39	110.43
24	D	404	BCR	C38-C26-C27	-3.87	105.34	113.60
22	b	615	CLA	C3D-C4D-ND	3.87	116.28	109.99
22	B	615	CLA	C3D-C4D-ND	3.87	116.28	109.99
22	b	617	CLA	CHD-C1D-ND	-3.87	119.36	124.80
22	c	510	CLA	O2D-CGD-CBD	3.87	117.99	111.23
24	K	101	BCR	C27-C26-C25	3.87	127.93	122.70
22	c	508	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
22	b	615	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
22	b	607	CLA	C3C-C4C-NC	3.86	115.38	110.43
22	B	617	CLA	CHD-C1D-ND	-3.86	119.37	124.80
22	D	401	CLA	C2B-C1B-NB	3.86	114.33	110.33
22	B	615	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
29	C	520	LMG	O7-C10-C11	3.85	119.81	111.48
22	B	607	CLA	C3C-C4C-NC	3.85	115.36	110.43
22	c	504	CLA	C3B-C4B-NB	3.84	113.96	110.53
22	A	603	CLA	C1C-C2C-C3C	-3.84	102.94	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	BCR	C32-C1-C6	3.83	116.25	110.24
22	b	605	CLA	C3B-C4B-NB	3.83	113.95	110.53
22	B	606	CLA	C4-C3-C5	3.83	121.87	115.23
22	B	603	CLA	C3C-C4C-NC	3.83	115.33	110.43
24	c	515	BCR	C33-C5-C6	3.83	128.66	124.48
22	B	604	CLA	CHD-C1D-ND	-3.82	119.42	124.80
24	C	515	BCR	C33-C5-C6	3.82	128.66	124.48
22	c	505	CLA	C2B-C1B-NB	3.82	114.29	110.33
22	b	606	CLA	C4-C3-C5	3.82	121.86	115.23
29	c	520	LMG	O7-C10-C11	3.82	119.74	111.48
22	b	604	CLA	CHD-C1D-ND	-3.82	119.43	124.80
22	C	510	CLA	C3C-C4C-NC	3.81	115.31	110.43
22	B	610	CLA	C2B-C1B-NB	3.81	114.28	110.33
22	a	603	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
22	C	508	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
22	C	505	CLA	C2B-C1B-NB	3.81	114.28	110.33
22	B	605	CLA	C3B-C4B-NB	3.81	113.93	110.53
22	C	511	CLA	C3B-C4B-NB	3.81	113.93	110.53
24	k	102	BCR	C32-C1-C6	3.81	116.21	110.24
22	a	603	CLA	C3D-C4D-ND	3.80	116.17	109.99
29	C	519	LMG	O7-C10-C11	3.80	119.71	111.48
22	c	510	CLA	C3C-C4C-NC	3.80	115.30	110.43
22	c	512	CLA	C3C-C4C-NC	3.80	115.29	110.43
22	B	607	CLA	O2D-CGD-CBD	3.80	117.86	111.23
22	b	611	CLA	C3D-C4D-ND	3.79	116.15	109.99
22	c	509	CLA	C3B-C4B-NB	3.79	113.92	110.53
22	b	607	CLA	O2D-CGD-CBD	3.79	117.85	111.23
22	b	602	CLA	C3C-C4C-NC	3.79	115.28	110.43
22	b	603	CLA	C3C-C4C-NC	3.79	115.28	110.43
22	B	611	CLA	C3D-C4D-ND	3.78	116.14	109.99
22	C	509	CLA	C3B-C4B-NB	3.78	113.90	110.53
24	b	622	BCR	C35-C13-C14	-3.78	116.70	122.82
22	B	616	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
29	c	519	LMG	O7-C10-C11	3.77	119.64	111.48
24	H	101	BCR	C23-C24-C25	3.77	137.07	127.00
22	B	608	CLA	C3D-C4D-ND	3.77	116.11	109.99
24	K	101	BCR	C38-C26-C27	-3.77	105.56	113.60
24	h	101	BCR	C23-C24-C25	3.77	137.06	127.00
24	k	101	BCR	C38-C26-C27	-3.77	105.57	113.60
22	c	506	CLA	CHD-C1D-ND	-3.76	119.50	124.80
22	C	506	CLA	CHD-C1D-ND	-3.76	119.51	124.80
22	C	512	CLA	C3C-C4C-NC	3.76	115.25	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	C3C-C4C-NC	3.76	115.25	110.43
22	A	603	CLA	C3D-C4D-ND	3.76	116.10	109.99
22	B	613	CLA	C2B-C1B-NB	3.76	114.22	110.33
24	B	622	BCR	C35-C13-C14	-3.76	116.73	122.82
22	B	606	CLA	C3D-C4D-ND	3.76	116.09	109.99
24	H	101	BCR	C35-C13-C14	-3.75	116.73	122.82
24	h	101	BCR	C35-C13-C14	-3.75	116.73	122.82
22	A	607	CLA	C3C-C4C-NC	3.75	115.24	110.43
22	b	610	CLA	C2B-C1B-NB	3.75	114.22	110.33
22	b	608	CLA	C3D-C4D-ND	3.75	116.08	109.99
22	C	504	CLA	C3B-C4B-NB	3.75	113.87	110.53
22	b	613	CLA	C3D-C4D-ND	3.75	116.08	109.99
22	c	511	CLA	C3B-C4B-NB	3.74	113.87	110.53
22	b	616	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
24	h	101	BCR	C24-C23-C22	3.74	131.77	126.23
24	T	102	BCR	C4-C5-C6	3.74	127.76	122.70
22	b	606	CLA	C3D-C4D-ND	3.74	116.07	109.99
25	l	101	SQD	O47-C7-C8	3.74	119.57	111.48
25	l	102	SQD	C3-C4-C5	3.74	117.01	110.23
22	B	602	CLA	C3C-C4C-NC	3.74	115.22	110.43
25	b	621	SQD	C3-C4-C5	3.74	117.01	110.23
22	B	607	CLA	C3D-C4D-ND	3.74	116.06	109.99
25	D	411	SQD	O47-C7-C8	3.73	119.56	111.48
24	T	102	BCR	C27-C26-C25	3.73	127.75	122.70
22	b	613	CLA	C2B-C1B-NB	3.73	114.20	110.33
22	B	610	CLA	C3D-C4D-ND	3.73	116.05	109.99
24	t	101	BCR	C27-C26-C25	3.73	127.75	122.70
22	B	613	CLA	C3D-C4D-ND	3.73	116.05	109.99
25	d	411	SQD	O47-C7-C8	3.73	119.55	111.48
22	b	610	CLA	C3D-C4D-ND	3.73	116.05	109.99
24	D	404	BCR	C27-C26-C25	3.73	127.74	122.70
22	a	607	CLA	C3C-C4C-NC	3.73	115.20	110.43
22	B	615	CLA	C3C-C4C-NC	3.73	115.20	110.43
25	L	101	SQD	O47-C7-C8	3.73	119.54	111.48
24	d	404	BCR	C27-C26-C25	3.72	127.74	122.70
22	b	611	CLA	O2D-CGD-CBD	3.72	117.74	111.23
22	c	508	CLA	C3B-C4B-NB	3.72	113.85	110.53
24	t	101	BCR	C4-C5-C6	3.72	127.73	122.70
22	b	615	CLA	C3C-C4C-NC	3.72	115.20	110.43
24	H	101	BCR	C24-C23-C22	3.72	131.74	126.23
22	b	607	CLA	C3D-C4D-ND	3.72	116.03	109.99
24	C	515	BCR	C33-C5-C4	-3.72	105.67	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	517	DGD	O2G-C1B-C2B	3.72	119.52	111.48
22	c	513	CLA	C3C-C4C-NC	3.72	115.19	110.43
24	c	515	BCR	C33-C5-C4	-3.72	105.67	113.60
22	B	611	CLA	O2D-CGD-CBD	3.71	117.72	111.23
22	d	401	CLA	C3B-C4B-NB	3.71	113.84	110.53
22	b	605	CLA	O2D-CGD-CBD	3.70	117.71	111.23
22	d	401	CLA	CHD-C1D-ND	-3.70	119.59	124.80
22	D	401	CLA	CHD-C1D-ND	-3.70	119.59	124.80
22	C	508	CLA	C3B-C4B-NB	3.70	113.83	110.53
22	D	401	CLA	C3B-C4B-NB	3.70	113.83	110.53
28	D	408	PL9	C40-C39-C41	3.70	121.64	115.23
22	C	512	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
22	c	512	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
31	c	517	DGD	O2G-C1B-C2B	3.69	119.47	111.48
22	B	605	CLA	O2D-CGD-CBD	3.69	117.68	111.23
24	a	608	BCR	C35-C13-C12	-3.69	112.45	118.09
22	B	603	CLA	CHD-C1D-ND	-3.69	119.61	124.80
24	A	608	BCR	C35-C13-C12	-3.69	112.46	118.09
22	B	612	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
22	d	403	CLA	C3C-C4C-NC	3.67	115.13	110.43
22	c	509	CLA	C3D-C4D-ND	3.67	115.95	109.99
22	B	603	CLA	C2B-C1B-NB	3.67	114.13	110.33
28	d	408	PL9	C40-C39-C41	3.66	121.58	115.23
22	b	603	CLA	CHD-C1D-ND	-3.66	119.65	124.80
22	B	610	CLA	C3B-C4B-NB	3.66	113.79	110.53
22	d	403	CLA	C3B-C4B-NB	3.65	113.79	110.53
22	C	509	CLA	C3D-C4D-ND	3.65	115.92	109.99
22	b	612	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
22	b	610	CLA	C3B-C4B-NB	3.64	113.78	110.53
24	b	618	BCR	C37-C22-C23	-3.64	112.53	118.09
22	C	505	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
22	b	603	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
22	D	403	CLA	C3C-C4C-NC	3.64	115.09	110.43
22	C	502	CLA	C3D-C4D-ND	3.64	115.90	109.99
22	c	502	CLA	C3D-C4D-ND	3.63	115.89	109.99
24	H	101	BCR	C27-C26-C25	3.63	127.61	122.70
22	B	615	CLA	C3B-C4B-NB	3.63	113.77	110.53
22	c	505	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
22	D	403	CLA	C3B-C4B-NB	3.63	113.77	110.53
22	B	612	CLA	C3D-C4D-ND	3.63	115.89	109.99
22	b	603	CLA	C2B-C1B-NB	3.63	114.09	110.33
22	C	502	CLA	C1C-C2C-C3C	-3.63	103.17	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	C3C-C4C-NC	3.63	115.08	110.43
24	h	101	BCR	C38-C26-C27	-3.62	105.87	113.60
22	b	612	CLA	C3D-C4D-ND	3.62	115.87	109.99
24	B	619	BCR	C37-C22-C23	-3.62	112.56	118.09
24	H	101	BCR	C38-C26-C27	-3.62	105.88	113.60
24	D	404	BCR	C1-C6-C5	-3.62	117.69	122.64
24	K	101	BCR	C2-C1-C6	3.62	115.69	110.44
22	b	615	CLA	C3B-C4B-NB	3.62	113.76	110.53
24	h	101	BCR	C27-C26-C25	3.61	127.58	122.70
24	k	101	BCR	C2-C1-C6	3.61	115.68	110.44
24	D	404	BCR	C32-C1-C2	-3.60	95.11	108.95
22	c	502	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
24	d	404	BCR	C1-C6-C5	-3.60	117.72	122.64
22	b	614	CLA	C3B-C4B-NB	3.60	113.74	110.53
22	B	603	CLA	C1C-C2C-C3C	-3.60	103.20	106.98
24	d	404	BCR	C32-C1-C2	-3.60	95.15	108.95
22	B	614	CLA	C3B-C4B-NB	3.59	113.74	110.53
28	a	613	PL9	C20-C19-C21	3.59	121.45	115.23
22	B	611	CLA	C1C-C2C-C3C	-3.58	103.22	106.98
22	b	617	CLA	C3D-C4D-ND	3.58	115.80	109.99
22	C	507	CLA	C3C-C4C-NC	3.57	115.00	110.43
22	b	611	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
24	A	608	BCR	C34-C9-C8	-3.57	112.64	118.09
24	T	102	BCR	C36-C18-C19	-3.56	112.64	118.09
28	A	613	PL9	C20-C19-C21	3.56	121.41	115.23
24	k	102	BCR	C24-C23-C22	3.56	131.50	126.23
24	K	102	BCR	C24-C23-C22	3.56	131.50	126.23
22	b	603	CLA	C3D-C4D-ND	3.56	115.77	109.99
22	B	617	CLA	C3D-C4D-ND	3.55	115.76	109.99
22	B	604	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
22	b	616	CLA	C3B-C4B-NB	3.55	113.70	110.53
25	A	609	SQD	O9-S-C6	3.55	112.06	106.76
22	b	606	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
25	a	609	SQD	O9-S-C6	3.54	112.05	106.76
22	b	611	CLA	C3B-C4B-NB	3.54	113.69	110.53
22	B	603	CLA	C3D-C4D-ND	3.54	115.73	109.99
22	B	613	CLA	CAC-C3C-C4C	3.54	129.39	124.79
22	B	611	CLA	C3B-C4B-NB	3.53	113.69	110.53
24	a	608	BCR	C34-C9-C8	-3.52	112.70	118.09
22	b	612	CLA	C3B-C4B-NB	3.52	113.68	110.53
24	T	102	BCR	C35-C13-C14	-3.52	117.11	122.82
24	T	101	BCR	C35-C13-C14	-3.52	117.11	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	101	BCR	C36-C18-C19	-3.52	112.71	118.09
22	c	504	CLA	C3D-C4D-ND	3.52	115.71	109.99
22	b	613	CLA	CAC-C3C-C4C	3.52	129.37	124.79
24	C	515	BCR	C40-C30-C25	3.52	115.76	110.24
24	k	102	BCR	C38-C26-C27	-3.51	106.10	113.60
22	B	606	CLA	C1C-C2C-C3C	-3.51	103.28	106.98
22	b	617	CLA	C4C-C3C-C2C	-3.51	101.78	106.89
24	B	618	BCR	C35-C13-C14	-3.51	117.13	122.82
22	B	608	CLA	CHD-C1D-ND	-3.51	119.86	124.80
22	b	612	CLA	CHD-C1D-ND	-3.51	119.86	124.80
24	K	102	BCR	C38-C26-C27	-3.51	106.12	113.60
24	c	515	BCR	C40-C30-C25	3.51	115.74	110.24
22	B	608	CLA	C3C-C4C-NC	3.50	114.92	110.43
22	C	504	CLA	C3D-C4D-ND	3.50	115.68	109.99
24	t	101	BCR	C35-C13-C14	-3.50	117.14	122.82
22	b	608	CLA	CHD-C1D-ND	-3.50	119.88	124.80
33	V	201	HEM	CBD-CAD-C3D	-3.50	102.86	112.53
22	B	617	CLA	C4C-C3C-C2C	-3.50	101.80	106.89
33	v	201	HEM	CBD-CAD-C3D	-3.49	102.87	112.53
22	a	607	CLA	C4-C3-C5	3.49	121.29	115.23
24	T	102	BCR	C35-C13-C12	-3.49	112.75	118.09
22	c	501	CLA	C3C-C4C-NC	3.49	114.90	110.43
24	t	101	BCR	C35-C13-C12	-3.49	112.76	118.09
22	B	612	CLA	CHD-C1D-ND	-3.49	119.90	124.80
22	B	605	CLA	C2B-C1B-NB	3.48	113.94	110.33
22	b	604	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
22	d	401	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
22	A	607	CLA	C4-C3-C5	3.47	121.26	115.23
22	C	501	CLA	C3C-C4C-NC	3.47	114.88	110.43
22	b	605	CLA	CED-O2D-CGD	3.47	123.78	115.92
22	B	605	CLA	CED-O2D-CGD	3.46	123.77	115.92
22	b	608	CLA	C3C-C4C-NC	3.46	114.86	110.43
22	D	401	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
22	B	616	CLA	C3B-C4B-NB	3.46	113.62	110.53
22	b	605	CLA	C2B-C1B-NB	3.46	113.92	110.33
22	C	511	CLA	C1-O2A-CGA	3.46	125.03	116.65
22	B	606	CLA	C4C-C3C-C2C	-3.46	101.86	106.89
32	d	405	LHG	O8-C23-C24	3.45	122.36	111.83
32	D	405	LHG	O8-C23-C24	3.45	122.36	111.83
22	A	604	CLA	CHD-C1D-ND	-3.44	119.96	124.80
22	b	614	CLA	C3D-C4D-ND	3.44	115.58	109.99
22	d	402	CLA	CHD-C1D-ND	-3.43	119.97	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	402	CLA	CHD-C1D-ND	-3.43	119.97	124.80
22	c	511	CLA	C1-O2A-CGA	3.43	124.95	116.65
22	B	614	CLA	C3D-C4D-ND	3.42	115.55	109.99
22	b	606	CLA	C4C-C3C-C2C	-3.41	101.92	106.89
22	a	604	CLA	CHD-C1D-ND	-3.41	120.00	124.80
22	C	513	CLA	C3D-C4D-ND	3.40	115.52	109.99
22	d	401	CLA	C4C-C3C-C2C	-3.40	101.94	106.89
24	K	102	BCR	C31-C1-C6	3.40	115.57	110.24
24	h	101	BCR	C36-C18-C17	-3.40	117.31	122.82
24	H	101	BCR	C36-C18-C17	-3.40	117.31	122.82
24	k	102	BCR	C31-C1-C6	3.39	115.56	110.24
22	c	506	CLA	C2B-C1B-NB	3.39	113.84	110.33
22	B	612	CLA	C3B-C4B-NB	3.39	113.56	110.53
22	c	513	CLA	C3D-C4D-ND	3.39	115.50	109.99
22	d	402	CLA	C3D-C4D-ND	3.39	115.49	109.99
22	D	401	CLA	C4C-C3C-C2C	-3.39	101.96	106.89
25	B	601	SQD	O47-C7-C8	3.39	118.80	111.48
22	c	505	CLA	C3D-C4D-ND	3.38	115.49	109.99
24	A	608	BCR	C30-C25-C24	3.38	124.83	115.65
24	T	102	BCR	C37-C22-C21	-3.38	117.34	122.82
22	b	615	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
25	b	601	SQD	O47-C7-C8	3.38	118.79	111.48
24	T	101	BCR	C32-C1-C6	3.37	115.53	110.24
22	C	505	CLA	C3D-C4D-ND	3.37	115.47	109.99
24	t	101	BCR	C37-C22-C21	-3.37	117.36	122.82
22	D	402	CLA	CBC-CAC-C3C	-3.37	103.29	112.42
22	c	502	CLA	CAC-C3C-C4C	3.37	129.17	124.79
24	a	608	BCR	C30-C25-C24	3.36	124.78	115.65
22	c	505	CLA	CHD-C1D-ND	-3.36	120.08	124.80
22	b	617	CLA	CAC-C3C-C4C	3.36	129.16	124.79
22	b	615	CLA	C4-C3-C5	3.36	121.06	115.23
22	C	502	CLA	CAC-C3C-C4C	3.35	129.16	124.79
22	D	402	CLA	C3D-C4D-ND	3.35	115.44	109.99
24	B	618	BCR	C32-C1-C6	3.35	115.50	110.24
22	B	615	CLA	C4-C3-C5	3.35	121.05	115.23
22	B	615	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
22	B	613	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
22	d	402	CLA	CBC-CAC-C3C	-3.35	103.34	112.42
22	D	403	CLA	CHD-C1D-ND	-3.35	120.09	124.80
22	d	403	CLA	CHD-C1D-ND	-3.35	120.09	124.80
22	B	617	CLA	CAC-C3C-C4C	3.35	129.15	124.79
22	B	611	CLA	C4C-C3C-C2C	-3.35	102.02	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	BCR	C33-C5-C4	-3.34	106.47	113.60
22	C	506	CLA	C2B-C1B-NB	3.34	113.79	110.33
22	C	508	CLA	CHD-C1D-ND	-3.34	120.10	124.80
22	C	505	CLA	CHD-C1D-ND	-3.34	120.11	124.80
22	b	613	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
24	k	102	BCR	C33-C5-C4	-3.33	106.49	113.60
22	D	401	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
22	C	511	CLA	C3D-C4D-ND	3.33	115.40	109.99
22	b	611	CLA	C4C-C3C-C2C	-3.33	102.05	106.89
22	c	508	CLA	CHD-C1D-ND	-3.32	120.12	124.80
22	d	403	CLA	O2D-CGD-CBD	3.32	117.04	111.23
22	C	502	CLA	CHD-C1D-ND	-3.32	120.13	124.80
22	c	511	CLA	C3D-C4D-ND	3.32	115.38	109.99
22	A	604	CLA	CAC-C3C-C4C	3.32	129.10	124.79
22	c	502	CLA	CHD-C1D-ND	-3.32	120.14	124.80
22	c	506	CLA	C3D-C4D-ND	3.31	115.37	109.99
24	A	608	BCR	C40-C30-C25	3.31	115.44	110.24
22	d	401	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
22	B	617	CLA	C3B-C4B-NB	3.31	113.49	110.53
24	B	619	BCR	C34-C9-C8	-3.31	113.04	118.09
22	b	609	CLA	CHD-C1D-ND	-3.30	120.15	124.80
24	a	608	BCR	C40-C30-C25	3.30	115.42	110.24
24	b	618	BCR	C34-C9-C8	-3.30	113.04	118.09
22	C	506	CLA	C3D-C4D-ND	3.30	115.35	109.99
24	K	102	BCR	C27-C26-C25	3.30	127.16	122.70
22	B	609	CLA	CHD-C1D-ND	-3.30	120.17	124.80
22	D	403	CLA	O2D-CGD-CBD	3.29	116.99	111.23
22	B	610	CLA	CAC-C3C-C4C	3.29	129.07	124.79
24	B	619	BCR	C38-C26-C25	3.29	128.08	124.48
24	k	102	BCR	C27-C26-C25	3.29	127.15	122.70
22	C	501	CLA	C3D-C4D-ND	3.29	115.33	109.99
22	C	512	CLA	C3D-C4D-ND	3.29	115.33	109.99
29	a	614	LMG	O7-C10-C11	3.29	118.59	111.48
22	D	401	CLA	O2D-CGD-CBD	3.29	116.98	111.23
22	d	401	CLA	O2D-CGD-CBD	3.29	116.98	111.23
22	B	610	CLA	CHD-C1D-ND	-3.29	120.18	124.80
24	b	618	BCR	C38-C26-C25	3.29	128.07	124.48
22	c	501	CLA	C3D-C4D-ND	3.29	115.33	109.99
29	A	614	LMG	O7-C10-C11	3.28	118.58	111.48
22	b	610	CLA	CHD-C1D-ND	-3.28	120.19	124.80
22	c	512	CLA	C3D-C4D-ND	3.28	115.32	109.99
25	A	609	SQD	C1-C2-C3	-3.28	103.11	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	609	SQD	C1-C2-C3	-3.28	103.12	110.01
22	a	604	CLA	CAC-C3C-C4C	3.27	129.05	124.79
22	b	610	CLA	CAC-C3C-C4C	3.27	129.05	124.79
22	A	607	CLA	CHD-C1D-ND	-3.27	120.20	124.80
22	b	616	CLA	C4C-C3C-C2C	-3.27	102.14	106.89
22	B	616	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
24	B	622	BCR	C34-C9-C8	-3.26	113.10	118.09
22	B	616	CLA	CHD-C1D-ND	-3.26	120.21	124.80
24	B	622	BCR	C36-C18-C19	-3.26	113.11	118.09
24	b	622	BCR	C36-C18-C19	-3.25	113.12	118.09
22	b	616	CLA	CHD-C1D-ND	-3.25	120.23	124.80
24	b	622	BCR	C34-C9-C8	-3.25	113.13	118.09
24	d	404	BCR	C37-C22-C21	-3.24	117.56	122.82
22	C	512	CLA	C4-C3-C5	3.24	120.86	115.23
22	b	605	CLA	C3D-C4D-ND	3.24	115.25	109.99
22	b	604	CLA	CMC-C2C-C1C	3.24	130.10	125.03
22	C	508	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
22	a	607	CLA	CHD-C1D-ND	-3.24	120.25	124.80
22	b	617	CLA	C3B-C4B-NB	3.24	113.42	110.53
22	B	615	CLA	CHD-C1D-ND	-3.24	120.25	124.80
22	d	401	CLA	C3D-C4D-ND	3.24	115.25	109.99
22	c	508	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
22	c	512	CLA	C4-C3-C5	3.22	120.82	115.23
22	B	608	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
22	B	612	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
22	B	616	CLA	O2D-CGD-CBD	3.22	116.86	111.23
22	b	612	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
25	b	621	SQD	O7-S-C6	3.21	111.56	106.76
24	D	404	BCR	C37-C22-C21	-3.21	117.61	122.82
22	C	507	CLA	CBC-CAC-C3C	-3.21	103.71	112.42
22	D	401	CLA	C3D-C4D-ND	3.21	115.21	109.99
22	c	507	CLA	CBC-CAC-C3C	-3.21	103.72	112.42
24	H	101	BCR	C4-C5-C6	3.21	127.04	122.70
22	b	602	CLA	C3D-C4D-ND	3.21	115.20	109.99
22	c	513	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
22	C	502	CLA	C3B-C4B-NB	3.21	113.39	110.53
22	b	615	CLA	CHD-C1D-ND	-3.20	120.29	124.80
25	b	601	SQD	O6-C1-C2	3.20	113.14	108.27
23	a	606	PHO	C1-C2-C3	-3.20	120.95	126.20
23	A	606	PHO	C1-C2-C3	-3.20	120.95	126.20
22	B	605	CLA	C3D-C4D-ND	3.20	115.18	109.99
22	c	502	CLA	C3B-C4B-NB	3.20	113.38	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	601	SQD	O6-C1-C2	3.20	113.13	108.27
22	B	613	CLA	C4-C3-C5	3.19	120.77	115.23
22	B	602	CLA	C3D-C4D-ND	3.19	115.17	109.99
32	D	409	LHG	O7-C7-C8	3.19	118.38	111.48
22	b	616	CLA	O2D-CGD-CBD	3.19	116.80	111.23
25	l	102	SQD	O7-S-C6	3.19	111.51	106.76
22	b	608	CLA	CED-O2D-CGD	3.19	123.14	115.92
22	B	604	CLA	CMC-C2C-C1C	3.18	130.01	125.03
22	B	608	CLA	CED-O2D-CGD	3.18	123.14	115.92
24	h	101	BCR	C4-C5-C6	3.18	127.00	122.70
22	C	513	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
22	b	613	CLA	C4-C3-C5	3.16	120.72	115.23
32	d	409	LHG	O7-C7-C8	3.16	118.32	111.48
22	B	608	CLA	C1-C2-C3	-3.16	121.02	126.20
22	b	608	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
22	b	608	CLA	CBC-CAC-C3C	-3.16	103.85	112.42
24	T	102	BCR	C30-C25-C24	3.16	124.22	115.65
22	B	608	CLA	CBC-CAC-C3C	-3.16	103.86	112.42
24	t	101	BCR	C30-C25-C24	3.16	124.22	115.65
22	b	613	CLA	C4C-C3C-C2C	-3.16	102.30	106.89
22	b	608	CLA	C1-C2-C3	-3.15	121.03	126.20
22	A	603	CLA	O2D-CGD-CBD	3.15	116.74	111.23
24	a	608	BCR	C33-C5-C4	-3.15	106.89	113.60
24	c	514	BCR	C37-C22-C21	-3.14	117.73	122.82
22	a	603	CLA	O2D-CGD-CBD	3.14	116.72	111.23
22	c	502	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
22	c	511	CLA	CMB-C2B-C1B	3.14	130.20	125.42
24	d	404	BCR	C3-C2-C1	3.14	125.54	114.43
24	A	608	BCR	C33-C5-C4	-3.14	106.91	113.60
24	a	608	BCR	C33-C5-C6	3.14	127.91	124.48
22	B	613	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
22	C	511	CLA	CMB-C2B-C1B	3.13	130.19	125.42
23	a	606	PHO	C4-C3-C5	3.13	120.66	115.23
24	C	514	BCR	C37-C22-C21	-3.13	117.75	122.82
24	d	404	BCR	C35-C13-C14	-3.13	117.75	122.82
24	c	515	BCR	C30-C25-C26	-3.13	118.36	122.64
22	b	607	CLA	C3B-C4B-NB	3.13	113.32	110.53
24	A	608	BCR	C8-C7-C6	3.12	135.34	127.00
24	D	404	BCR	C3-C2-C1	3.12	125.48	114.43
24	C	515	BCR	C30-C25-C26	-3.12	118.37	122.64
22	c	504	CLA	C3C-C4C-NC	3.12	114.42	110.43
24	D	404	BCR	C35-C13-C14	-3.12	117.76	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C3C-C4C-NC	3.11	114.42	110.43
32	L	102	LHG	O7-C7-C8	3.11	118.21	111.48
31	C	518	DGD	O3G-C3G-C2G	-3.11	103.25	110.82
22	B	612	CLA	C1-C2-C3	-3.11	121.11	126.20
32	l	103	LHG	O7-C7-C8	3.11	118.20	111.48
22	b	612	CLA	C1-C2-C3	-3.10	121.11	126.20
22	C	502	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
22	B	607	CLA	C3B-C4B-NB	3.10	113.30	110.53
32	E	101	LHG	O8-C23-C24	3.10	121.28	111.83
24	A	608	BCR	C33-C5-C6	3.10	127.86	124.48
24	a	608	BCR	C8-C7-C6	3.10	135.27	127.00
22	c	509	CLA	CMB-C2B-C1B	3.10	130.13	125.42
22	B	602	CLA	O2A-CGA-CBA	3.09	121.27	111.83
23	A	606	PHO	C4-C3-C5	3.09	120.60	115.23
31	c	518	DGD	O3G-C3G-C2G	-3.09	103.30	110.82
22	b	603	CLA	C4-C3-C5	3.09	120.59	115.23
22	c	511	CLA	C4C-C3C-C2C	-3.08	102.40	106.89
22	b	602	CLA	O2A-CGA-CBA	3.08	121.23	111.83
22	c	506	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
32	e	101	LHG	O8-C23-C24	3.08	121.23	111.83
24	B	622	BCR	C35-C13-C12	-3.08	113.38	118.09
22	b	606	CLA	CMB-C2B-C1B	3.08	130.11	125.42
24	C	515	BCR	C34-C9-C8	-3.08	113.38	118.09
22	C	511	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
24	c	515	BCR	C34-C9-C8	-3.07	113.39	118.09
22	C	506	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
24	A	608	BCR	C31-C1-C6	3.07	115.06	110.24
24	K	102	BCR	C40-C30-C25	3.07	115.06	110.24
24	b	622	BCR	C35-C13-C12	-3.07	113.40	118.09
22	B	603	CLA	C4-C3-C5	3.07	120.56	115.23
22	B	610	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
24	k	102	BCR	C40-C30-C25	3.07	115.05	110.24
25	d	411	SQD	O48-C23-C24	3.07	121.18	111.83
22	C	513	CLA	CHD-C1D-ND	-3.06	120.49	124.80
25	L	101	SQD	O7-S-C6	3.06	111.33	106.76
24	a	608	BCR	C31-C1-C6	3.06	115.04	110.24
22	B	606	CLA	CMB-C2B-C1B	3.06	130.08	125.42
22	b	615	CLA	CAC-C3C-C4C	3.06	128.77	124.79
22	B	617	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
22	B	615	CLA	CAC-C3C-C4C	3.06	128.77	124.79
25	B	601	SQD	O48-C23-C24	3.05	121.15	111.83
22	c	513	CLA	CHD-C1D-ND	-3.05	120.51	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	CMB-C2B-C1B	3.05	130.07	125.42
25	D	411	SQD	O48-C23-C24	3.05	121.14	111.83
22	b	616	CLA	C3D-C4D-ND	3.05	114.94	109.99
32	D	405	LHG	O8-C23-O10	-3.05	116.00	123.63
22	A	604	CLA	C4-C3-C5	3.05	120.52	115.23
22	C	509	CLA	CHD-C1D-ND	-3.05	120.52	124.80
25	b	601	SQD	O48-C23-C24	3.05	121.12	111.83
22	b	617	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
24	b	618	BCR	C1-C6-C5	-3.04	118.48	122.64
22	a	604	CLA	C4-C3-C5	3.04	120.51	115.23
22	B	616	CLA	C3D-C4D-ND	3.04	114.93	109.99
32	d	405	LHG	O8-C23-O10	-3.04	116.02	123.63
25	l	101	SQD	O7-S-C6	3.04	111.29	106.76
29	c	519	LMG	O8-C28-C29	3.04	121.09	111.83
22	b	610	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
22	c	509	CLA	CHD-C1D-ND	-3.03	120.53	124.80
22	c	506	CLA	C4-C3-C5	3.03	120.49	115.23
24	B	619	BCR	C1-C6-C5	-3.03	118.49	122.64
29	C	519	LMG	O8-C28-C29	3.03	121.07	111.83
22	C	506	CLA	C4-C3-C5	3.03	120.48	115.23
28	A	613	PL9	C32-C33-C34	-3.02	120.71	127.62
22	C	507	CLA	C4-C3-C5	3.02	120.47	115.23
28	a	613	PL9	C32-C33-C34	-3.01	120.73	127.62
22	c	507	CLA	C4-C3-C5	3.01	120.45	115.23
22	A	604	CLA	CMC-C2C-C1C	3.01	129.73	125.03
22	B	603	CLA	C4C-C3C-C2C	-3.01	102.52	106.89
31	h	102	DGD	O1G-C1A-C2A	3.00	120.97	111.83
22	b	603	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
22	b	617	CLA	C1C-C2C-C3C	-2.99	103.83	106.98
24	H	101	BCR	C32-C1-C31	-2.99	100.06	108.63
22	C	503	CLA	C3D-C4D-ND	2.99	114.85	109.99
24	t	101	BCR	C39-C30-C25	2.99	114.93	110.24
24	h	101	BCR	C32-C1-C31	-2.99	100.07	108.63
22	C	504	CLA	CAC-C3C-C4C	2.99	128.68	124.79
31	H	102	DGD	O1G-C1A-C2A	2.99	120.95	111.83
22	B	615	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
22	C	513	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
22	c	512	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
22	b	616	CLA	CMB-C2B-C1B	2.98	129.96	125.42
22	a	604	CLA	CMC-C2C-C1C	2.98	129.69	125.03
22	c	505	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
22	b	615	CLA	C4C-C3C-C2C	-2.98	102.56	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	618	BCR	C39-C30-C25	2.98	114.91	110.24
22	B	617	CLA	C1C-C2C-C3C	-2.98	103.85	106.98
22	c	504	CLA	CAC-C3C-C4C	2.98	128.66	124.79
22	B	616	CLA	CMB-C2B-C1B	2.98	129.95	125.42
22	C	505	CLA	CAC-C3C-C4C	2.97	128.66	124.79
22	c	505	CLA	CAC-C3C-C4C	2.97	128.66	124.79
22	c	503	CLA	C3D-C4D-ND	2.97	114.81	109.99
22	B	615	CLA	CBC-CAC-C3C	-2.97	104.37	112.42
22	b	615	CLA	CBC-CAC-C3C	-2.97	104.37	112.42
22	B	612	CLA	CMC-C2C-C1C	2.97	129.67	125.03
22	C	505	CLA	C4C-C3C-C2C	-2.97	102.58	106.89
22	b	604	CLA	C4-C3-C5	2.96	120.37	115.23
22	C	504	CLA	C4-C3-C5	2.96	120.37	115.23
22	C	512	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
22	B	609	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	b	605	CLA	CMB-C2B-C1B	2.95	129.92	125.42
24	T	102	BCR	C39-C30-C25	2.95	114.87	110.24
22	c	504	CLA	C4-C3-C5	2.95	120.35	115.23
22	b	605	CLA	CHD-C1D-ND	-2.95	120.65	124.80
23	a	605	PHO	C4B-NB-C1B	-2.95	104.52	108.82
22	b	612	CLA	CMC-C2C-C1C	2.95	129.64	125.03
22	B	604	CLA	C4-C3-C5	2.94	120.34	115.23
22	B	605	CLA	CMB-C2B-C1B	2.94	129.90	125.42
22	b	609	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	b	603	CLA	C3B-C4B-NB	2.94	113.15	110.53
22	c	513	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
31	H	102	DGD	O2G-C1B-C2B	2.94	117.84	111.48
24	h	101	BCR	C39-C30-C29	-2.94	97.68	108.95
23	A	605	PHO	C4B-NB-C1B	-2.94	104.54	108.82
24	b	622	BCR	C29-C30-C25	2.93	114.70	110.44
24	H	101	BCR	C39-C30-C29	-2.93	97.69	108.95
31	h	102	DGD	O2G-C1B-C2B	2.93	117.82	111.48
23	a	606	PHO	CMB-C2B-C3B	2.93	130.54	124.68
22	d	403	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
25	A	609	SQD	C45-O47-C7	-2.93	110.80	117.80
22	C	501	CLA	C3B-C4B-NB	2.92	113.14	110.53
22	c	504	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	B	605	CLA	CHD-C1D-ND	-2.92	120.69	124.80
24	B	622	BCR	C29-C30-C25	2.92	114.68	110.44
31	h	102	DGD	O1G-C1A-O1A	-2.92	116.33	123.63
22	c	501	CLA	CMB-C2B-C1B	2.92	129.86	125.42
28	a	613	PL9	C7-C3-C4	2.92	119.31	116.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	609	SQD	C45-O47-C7	-2.91	110.82	117.80
24	T	101	BCR	C39-C30-C25	2.91	114.81	110.24
22	C	504	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
22	C	505	CLA	CMC-C2C-C1C	2.91	129.58	125.03
22	B	611	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
24	k	101	BCR	C35-C13-C12	-2.91	113.65	118.09
22	D	403	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
22	c	505	CLA	CMC-C2C-C1C	2.90	129.57	125.03
22	C	511	CLA	CHD-C1D-ND	-2.90	120.72	124.80
23	A	606	PHO	CMB-C2B-C3B	2.90	130.49	124.68
22	c	503	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
22	b	608	CLA	O2D-CGD-CBD	2.90	116.30	111.23
31	H	102	DGD	O1G-C1A-O1A	-2.90	116.38	123.63
22	c	501	CLA	C3B-C4B-NB	2.90	113.12	110.53
22	B	607	CLA	O1D-CGD-CBD	-2.90	118.80	124.52
22	A	603	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
22	C	503	CLA	C4C-C3C-C2C	-2.90	102.68	106.89
24	C	514	BCR	C39-C30-C29	-2.90	97.83	108.95
28	A	613	PL9	C30-C29-C31	2.90	120.25	115.23
22	c	511	CLA	CHD-C1D-ND	-2.90	120.73	124.80
22	C	501	CLA	CMB-C2B-C1B	2.89	129.83	125.42
24	K	102	BCR	C31-C1-C2	-2.89	97.84	108.95
22	b	607	CLA	O1D-CGD-CBD	-2.89	118.81	124.52
22	b	611	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	c	514	BCR	C39-C30-C29	-2.89	97.85	108.95
23	A	605	PHO	O1D-CGD-CBD	-2.89	120.34	124.72
22	c	506	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	k	102	BCR	C31-C1-C2	-2.89	97.85	108.95
24	D	404	BCR	C2-C1-C6	2.89	114.64	110.44
22	c	509	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
22	B	608	CLA	O2D-CGD-CBD	2.89	116.28	111.23
24	K	101	BCR	C35-C13-C12	-2.89	113.68	118.09
22	C	509	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
22	B	611	CLA	CHD-C1D-ND	-2.88	120.75	124.80
22	B	603	CLA	C3B-C4B-NB	2.88	113.10	110.53
22	c	512	CLA	CHD-C1D-ND	-2.87	120.76	124.80
23	a	605	PHO	O1D-CGD-CBD	-2.87	120.37	124.72
22	b	607	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
22	a	603	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
28	a	613	PL9	C30-C29-C31	2.87	120.20	115.23
22	C	506	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
22	b	611	CLA	CHD-C1D-ND	-2.86	120.78	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	622	BCR	C1-C6-C5	-2.85	118.74	122.64
22	b	609	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
22	C	512	CLA	CHD-C1D-ND	-2.85	120.79	124.80
24	d	404	BCR	C2-C1-C6	2.85	114.58	110.44
24	k	102	BCR	C29-C30-C25	2.85	114.57	110.44
22	B	607	CLA	C4-C3-C5	2.84	120.17	115.23
28	A	613	PL9	C7-C3-C4	2.84	119.25	116.91
22	B	609	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
25	b	601	SQD	O9-S-C6	2.84	111.00	106.76
22	B	607	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
28	a	613	PL9	C25-C24-C26	2.84	120.15	115.23
22	B	605	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
25	l	101	SQD	C1-O5-C5	-2.83	108.18	113.72
25	l	101	SQD	O48-C23-C24	2.83	120.47	111.83
22	b	607	CLA	C4-C3-C5	2.83	120.14	115.23
29	B	620	LMG	O8-C28-C29	2.83	120.47	111.83
22	B	603	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
25	l	102	SQD	O48-C23-C24	2.83	120.46	111.83
25	B	601	SQD	O9-S-C6	2.83	110.98	106.76
25	L	101	SQD	O48-C23-C24	2.83	120.46	111.83
24	b	622	BCR	C1-C6-C5	-2.83	118.77	122.64
24	B	622	BCR	C23-C24-C25	2.82	134.54	127.00
24	b	622	BCR	C23-C24-C25	2.82	134.53	127.00
24	k	102	BCR	C37-C22-C23	-2.82	113.78	118.09
25	b	621	SQD	O48-C23-C24	2.82	120.42	111.83
22	C	512	CLA	C1-C2-C3	-2.82	121.58	126.20
24	K	102	BCR	C37-C22-C23	-2.81	113.79	118.09
22	c	502	CLA	CMB-C2B-C1B	2.81	129.70	125.42
24	b	618	BCR	C1-C6-C7	2.81	123.28	115.65
22	D	402	CLA	C4-C3-C5	2.81	120.11	115.23
24	C	515	BCR	C23-C24-C25	2.81	134.51	127.00
28	A	613	PL9	C15-C14-C16	2.81	120.11	115.23
29	b	619	LMG	O8-C28-C29	2.81	120.40	111.83
22	C	510	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
22	C	502	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	c	507	CLA	C3D-C4D-ND	2.81	114.55	109.99
28	d	408	PL9	C53-C6-C1	2.80	121.02	115.28
28	A	613	PL9	C25-C24-C26	2.80	120.10	115.23
22	A	603	CLA	CAC-C3C-C4C	2.80	128.44	124.79
28	a	613	PL9	C15-C14-C16	2.80	120.09	115.23
22	d	401	CLA	CAC-C3C-C4C	2.80	128.43	124.79
24	K	102	BCR	C29-C30-C25	2.80	114.51	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
22	D	402	CLA	CAC-C3C-C4C	2.80	128.43	124.79
22	d	402	CLA	CAC-C3C-C4C	2.80	128.43	124.79
25	L	101	SQD	C1-O5-C5	-2.80	108.26	113.72
24	B	619	BCR	C1-C6-C7	2.80	123.24	115.65
22	c	502	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
22	b	605	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
22	b	608	CLA	C4-C3-C5	2.79	120.08	115.23
22	b	614	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
22	d	402	CLA	C4-C3-C5	2.79	120.08	115.23
22	C	507	CLA	C3D-C4D-ND	2.79	114.52	109.99
24	B	618	BCR	C4-C5-C6	2.79	126.47	122.70
24	c	515	BCR	C23-C24-C25	2.79	134.45	127.00
28	D	408	PL9	C53-C6-C1	2.79	120.98	115.28
22	B	609	CLA	O2A-CGA-CBA	2.79	120.33	111.83
22	C	502	CLA	CMB-C2B-C1B	2.79	129.66	125.42
22	B	608	CLA	C4-C3-C5	2.78	120.06	115.23
22	b	613	CLA	C3B-C4B-NB	2.78	113.01	110.53
24	T	101	BCR	C4-C5-C6	2.78	126.46	122.70
22	B	602	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
24	A	608	BCR	C29-C30-C25	2.78	114.48	110.44
22	c	512	CLA	C1-C2-C3	-2.78	121.64	126.20
22	b	609	CLA	O2A-CGA-CBA	2.78	120.30	111.83
22	b	613	CLA	CED-O2D-CGD	2.78	122.21	115.92
23	a	606	PHO	O1D-CGD-CBD	-2.77	120.52	124.72
22	B	602	CLA	CMC-C2C-C1C	2.77	129.37	125.03
33	V	201	HEM	C1B-NB-C4B	2.77	108.49	105.21
22	c	510	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
22	B	613	CLA	C3B-C4B-NB	2.76	113.00	110.53
22	b	602	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
24	k	101	BCR	C39-C30-C29	-2.76	98.34	108.95
22	a	603	CLA	CAC-C3C-C4C	2.76	128.38	124.79
22	B	611	CLA	O2A-CGA-CBA	2.76	120.25	111.83
24	a	608	BCR	C29-C30-C25	2.76	114.45	110.44
23	A	606	PHO	O1D-CGD-CBD	-2.76	120.54	124.72
24	K	101	BCR	C39-C30-C29	-2.76	98.35	108.95
22	b	602	CLA	CMC-C2C-C1C	2.76	129.34	125.03
22	B	613	CLA	CED-O2D-CGD	2.76	122.17	115.92
22	b	607	CLA	CMB-C2B-C1B	2.76	129.62	125.42
22	B	614	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
22	b	602	CLA	C4D-C3D-CAD	2.76	111.10	108.11
22	b	611	CLA	O2A-CGA-CBA	2.76	120.24	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	CMB-C2B-C1B	2.76	129.62	125.42
22	B	617	CLA	O2A-CGA-CBA	2.76	120.24	111.83
22	B	607	CLA	CMB-C2B-C1B	2.76	129.61	125.42
24	B	618	BCR	C39-C30-C29	-2.75	98.40	108.95
22	a	604	CLA	CBC-CAC-C3C	-2.75	104.97	112.42
22	D	401	CLA	CAC-C3C-C4C	2.75	128.36	124.79
24	T	101	BCR	C39-C30-C29	-2.74	98.42	108.95
22	B	612	CLA	CAC-C3C-C4C	2.73	128.35	124.79
22	b	605	CLA	C4-C3-C5	2.73	119.97	115.23
22	A	604	CLA	CBC-CAC-C3C	-2.73	105.02	112.42
22	C	504	CLA	C1-O2A-CGA	2.73	123.26	116.65
22	b	617	CLA	O2A-CGA-CBA	2.73	120.15	111.83
33	v	201	HEM	C1B-NB-C4B	2.72	108.43	105.21
22	c	504	CLA	C1-O2A-CGA	2.72	123.25	116.65
22	b	602	CLA	CMB-C2B-C1B	2.72	129.57	125.42
28	a	613	PL9	C35-C34-C36	2.72	119.95	115.23
22	B	602	CLA	C4D-C3D-CAD	2.72	111.06	108.11
28	a	613	PL9	C53-C6-C1	2.72	120.85	115.28
22	c	501	CLA	CAC-C3C-C4C	2.72	128.33	124.79
24	C	514	BCR	C39-C30-C25	2.71	114.50	110.24
22	C	510	CLA	CHD-C4C-C3C	-2.71	120.82	124.77
22	C	505	CLA	C3B-C4B-NB	2.71	112.95	110.53
28	A	613	PL9	C53-C6-C1	2.71	120.83	115.28
22	b	612	CLA	CAC-C3C-C4C	2.71	128.31	124.79
31	D	410	DGD	O5D-C1E-C2E	2.71	112.38	108.27
28	A	613	PL9	C35-C34-C36	2.71	119.92	115.23
24	B	619	BCR	C34-C9-C10	-2.70	118.44	122.82
22	C	501	CLA	CAC-C3C-C4C	2.70	128.31	124.79
22	B	614	CLA	O2D-CGD-CBD	2.70	115.95	111.23
22	C	508	CLA	C4-C3-C5	2.70	119.92	115.23
22	C	511	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
22	a	603	CLA	CHD-C1D-ND	-2.70	121.01	124.80
22	B	605	CLA	C4-C3-C5	2.69	119.91	115.23
24	c	514	BCR	C39-C30-C25	2.69	114.47	110.24
22	b	614	CLA	O2D-CGD-CBD	2.69	115.94	111.23
22	c	511	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
22	c	507	CLA	C3B-C4B-NB	2.69	112.93	110.53
22	B	609	CLA	CAC-C3C-C4C	2.69	128.29	124.79
22	b	606	CLA	CHD-C1D-ND	-2.69	121.02	124.80
22	A	607	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
22	B	615	CLA	CMB-C2B-C1B	2.69	129.51	125.42
22	c	510	CLA	CHD-C4C-C3C	-2.69	120.86	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	C4-C3-C5	2.68	119.89	115.23
31	d	410	DGD	O1G-C1A-C2A	2.68	120.01	111.83
22	c	505	CLA	C3B-C4B-NB	2.68	112.92	110.53
22	d	403	CLA	CAC-C3C-C4C	2.68	128.28	124.79
31	D	410	DGD	O1G-C1A-C2A	2.68	120.01	111.83
24	b	618	BCR	C34-C9-C10	-2.68	118.47	122.82
28	A	613	PL9	C37-C38-C39	-2.68	121.49	127.62
31	d	410	DGD	O5D-C1E-C2E	2.68	112.34	108.27
22	B	610	CLA	C1-C2-C3	-2.68	121.81	126.20
28	a	613	PL9	C40-C39-C41	2.68	119.88	115.23
22	b	607	CLA	C1-C2-C3	-2.68	121.81	126.20
31	c	518	DGD	O1G-C1A-C2A	2.67	119.99	111.83
22	a	607	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
31	C	518	DGD	O1G-C1A-C2A	2.67	119.98	111.83
22	b	609	CLA	O1D-CGD-CBD	-2.67	119.25	124.52
23	a	606	PHO	C4B-NB-C1B	-2.67	104.93	108.82
22	B	607	CLA	C1-C2-C3	-2.67	121.83	126.20
28	a	613	PL9	C37-C38-C39	-2.67	121.52	127.62
25	l	102	SQD	C4-C3-C2	2.66	115.51	110.83
24	k	102	BCR	C34-C9-C8	-2.66	114.02	118.09
25	a	609	SQD	O8-S-C6	2.66	111.12	105.97
22	B	606	CLA	CHD-C1D-ND	-2.66	121.05	124.80
24	K	102	BCR	C33-C5-C6	2.66	127.39	124.48
22	A	603	CLA	CHD-C1D-ND	-2.66	121.06	124.80
22	C	507	CLA	C3B-C4B-NB	2.66	112.91	110.53
28	A	613	PL9	C40-C39-C41	2.66	119.84	115.23
22	b	615	CLA	CMB-C2B-C1B	2.66	129.46	125.42
22	c	501	CLA	C1-O2A-CGA	2.66	123.08	116.65
22	b	609	CLA	CAC-C3C-C4C	2.65	128.24	124.79
22	B	610	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
25	D	411	SQD	O7-S-C6	2.65	110.72	106.76
25	b	621	SQD	C4-C3-C2	2.65	115.48	110.83
22	b	610	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
22	B	612	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
22	D	403	CLA	CAC-C3C-C4C	2.65	128.23	124.79
23	A	606	PHO	C4B-NB-C1B	-2.65	104.96	108.82
22	d	401	CLA	C4-C3-C5	2.64	119.82	115.23
25	d	411	SQD	O7-S-C6	2.64	110.70	106.76
22	b	610	CLA	C1-C2-C3	-2.64	121.87	126.20
24	t	101	BCR	C40-C30-C39	-2.64	101.07	108.63
22	b	604	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
22	C	501	CLA	C1-O2A-CGA	2.64	123.05	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	609	SQD	O8-S-C6	2.64	111.07	105.97
24	K	102	BCR	C34-C9-C8	-2.64	114.05	118.09
22	b	612	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
22	c	509	CLA	CAC-C3C-C4C	2.64	128.22	124.79
22	A	607	CLA	CMB-C2B-C1B	2.64	129.44	125.42
24	D	404	BCR	C30-C25-C24	2.64	122.80	115.65
22	b	608	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
24	d	404	BCR	C30-C25-C24	2.64	122.80	115.65
23	A	605	PHO	CMB-C2B-C3B	2.64	129.95	124.68
24	T	102	BCR	C40-C30-C39	-2.63	101.09	108.63
24	k	102	BCR	C33-C5-C6	2.63	127.36	124.48
22	B	609	CLA	O1D-CGD-CBD	-2.63	119.33	124.52
22	B	608	CLA	C4C-C3C-C2C	-2.63	103.07	106.89
22	d	403	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
22	d	403	CLA	CED-O2D-CGD	2.62	121.87	115.92
24	h	101	BCR	C29-C28-C27	-2.62	105.51	111.28
23	a	605	PHO	CMB-C2B-C3B	2.62	129.92	124.68
22	B	604	CLA	C4C-C3C-C2C	-2.62	103.08	106.89
24	B	622	BCR	C37-C22-C23	-2.62	114.08	118.09
22	c	510	CLA	CMC-C2C-C1C	2.62	129.13	125.03
22	B	612	CLA	CHD-C4C-C3C	-2.61	120.96	124.77
22	C	507	CLA	O1D-CGD-CBD	-2.61	119.36	124.52
22	D	401	CLA	C4-C3-C5	2.61	119.76	115.23
24	h	101	BCR	C39-C30-C25	2.61	114.34	110.24
22	D	403	CLA	CED-O2D-CGD	2.61	121.84	115.92
22	C	507	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
22	C	503	CLA	C4-C3-C5	2.61	119.76	115.23
22	D	403	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
22	b	612	CLA	CHD-C4C-C3C	-2.61	120.97	124.77
22	C	512	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
24	H	101	BCR	C39-C30-C25	2.61	114.33	110.24
22	c	507	CLA	C4C-C3C-C2C	-2.61	103.10	106.89
22	a	607	CLA	CMB-C2B-C1B	2.61	129.39	125.42
31	c	517	DGD	O2G-C1B-O1B	-2.60	117.62	123.70
31	C	517	DGD	O2G-C1B-O1B	-2.60	117.62	123.70
22	c	509	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
24	b	622	BCR	C37-C22-C23	-2.60	114.11	118.09
22	a	603	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
24	H	101	BCR	C29-C28-C27	-2.60	105.56	111.28
22	C	509	CLA	CAC-C3C-C4C	2.60	128.17	124.79
22	c	503	CLA	C4-C3-C5	2.60	119.74	115.23
22	A	603	CLA	O2D-CGD-O1D	-2.60	118.79	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	411	SQD	O9-S-C6	2.60	110.64	106.76
25	d	411	SQD	O9-S-C6	2.60	110.63	106.76
24	C	515	BCR	C1-C6-C5	-2.60	119.09	122.64
24	B	618	BCR	C2-C3-C4	2.60	116.99	111.28
22	A	607	CLA	CAC-C3C-C4C	2.59	128.17	124.79
22	C	506	CLA	CAC-C3C-C4C	2.59	128.17	124.79
22	c	507	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
22	C	512	CLA	C3B-C4B-NB	2.59	112.84	110.53
22	c	513	CLA	CMC-C2C-C1C	2.59	129.08	125.03
22	A	607	CLA	CED-O2D-CGD	2.59	121.79	115.92
22	c	509	CLA	C4D-C3D-CAD	2.59	110.92	108.11
25	a	609	SQD	C44-O6-C1	-2.59	108.25	113.80
24	c	515	BCR	C1-C6-C5	-2.59	119.10	122.64
24	B	622	BCR	C38-C26-C25	2.59	127.31	124.48
25	A	609	SQD	C44-O6-C1	-2.59	108.25	113.80
22	C	510	CLA	CMC-C2C-C1C	2.58	129.07	125.03
22	C	513	CLA	CMC-C2C-C1C	2.58	129.07	125.03
22	C	509	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
22	a	607	CLA	CED-O2D-CGD	2.58	121.77	115.92
22	C	501	CLA	CBC-CAC-C3C	-2.58	105.43	112.42
22	B	603	CLA	C1-C2-C3	-2.58	121.97	126.20
22	c	501	CLA	CBC-CAC-C3C	-2.58	105.43	112.42
24	T	101	BCR	C2-C3-C4	2.58	116.95	111.28
22	c	512	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
22	c	511	CLA	C4-C3-C5	2.58	119.70	115.23
22	b	603	CLA	C1-C2-C3	-2.57	121.98	126.20
29	c	520	LMG	O8-C28-C29	2.57	119.67	111.83
22	c	502	CLA	C4-C3-C5	2.57	119.68	115.23
29	C	520	LMG	O8-C28-C29	2.57	119.66	111.83
24	K	102	BCR	C34-C9-C10	-2.57	118.66	122.82
22	C	503	CLA	C3B-C4B-NB	2.57	112.82	110.53
22	C	511	CLA	C4-C3-C5	2.56	119.68	115.23
31	C	516	DGD	O3G-C3G-C2G	-2.56	104.59	110.82
29	a	614	LMG	O1-C1-C2	2.56	112.16	108.27
22	C	502	CLA	C4-C3-C5	2.56	119.67	115.23
22	c	512	CLA	C3B-C4B-NB	2.56	112.81	110.53
22	c	506	CLA	CAC-C3C-C4C	2.56	128.12	124.79
22	b	616	CLA	C4-C3-C5	2.56	119.67	115.23
22	b	611	CLA	CMB-C2B-C1B	2.56	129.31	125.42
24	k	102	BCR	C4-C5-C6	2.56	126.16	122.70
24	T	102	BCR	C31-C1-C6	2.56	114.25	110.24
24	B	618	BCR	C1-C6-C5	-2.55	119.14	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	C4-C3-C5	2.55	119.66	115.23
24	B	619	BCR	C4-C5-C6	2.55	126.15	122.70
31	c	516	DGD	O3G-C3G-C2G	-2.55	104.61	110.82
22	C	509	CLA	C4D-C3D-CAD	2.55	110.88	108.11
24	h	101	BCR	C30-C25-C24	2.55	122.57	115.65
22	a	607	CLA	CAC-C3C-C4C	2.55	128.11	124.79
24	T	101	BCR	C1-C6-C5	-2.55	119.15	122.64
24	H	101	BCR	C30-C25-C24	2.55	122.57	115.65
22	B	606	CLA	C3B-C4B-NB	2.55	112.80	110.53
24	K	102	BCR	C4-C5-C6	2.55	126.15	122.70
25	a	609	SQD	C1-O5-C5	-2.55	108.75	113.72
22	B	611	CLA	CMB-C2B-C1B	2.55	129.30	125.42
22	c	509	CLA	O2A-CGA-CBA	2.55	119.59	111.83
24	t	101	BCR	C1-C6-C5	-2.54	119.16	122.64
22	b	614	CLA	CHD-C4C-C3C	-2.54	121.06	124.77
24	k	102	BCR	C34-C9-C10	-2.54	118.70	122.82
22	C	501	CLA	CMC-C2C-C1C	2.54	129.00	125.03
22	C	509	CLA	O2A-CGA-CBA	2.54	119.58	111.83
24	b	618	BCR	C4-C5-C6	2.54	126.13	122.70
24	b	622	BCR	C38-C26-C25	2.54	127.25	124.48
24	T	102	BCR	C1-C6-C5	-2.54	119.17	122.64
29	A	614	LMG	O1-C1-C2	2.53	112.12	108.27
22	d	401	CLA	CHD-C4C-C3C	-2.53	121.08	124.77
22	C	512	CLA	O2A-CGA-CBA	2.52	119.53	111.83
22	c	503	CLA	C3B-C4B-NB	2.52	112.78	110.53
22	b	614	CLA	C4-C3-C5	2.52	119.61	115.23
25	A	609	SQD	C1-O5-C5	-2.52	108.80	113.72
22	B	614	CLA	CHD-C4C-C3C	-2.52	121.10	124.77
22	B	602	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
22	b	613	CLA	CMC-C2C-C1C	2.51	128.96	125.03
24	B	622	BCR	C37-C22-C21	-2.51	118.74	122.82
22	B	614	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
32	D	405	LHG	O7-C7-C8	2.51	116.92	111.48
22	D	401	CLA	CHD-C4C-C3C	-2.51	121.11	124.77
22	b	614	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
24	t	101	BCR	C31-C1-C6	2.51	114.18	110.24
24	B	622	BCR	C40-C30-C25	2.51	114.17	110.24
24	b	622	BCR	C40-C30-C25	2.50	114.17	110.24
22	B	614	CLA	C4-C3-C5	2.50	119.57	115.23
22	c	501	CLA	CMC-C2C-C1C	2.50	128.94	125.03
22	B	617	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
24	B	622	BCR	C1-C6-C7	2.50	122.42	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	O2A-CGA-CBA	2.50	119.45	111.83
22	b	602	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
24	b	622	BCR	C1-C6-C7	2.49	122.42	115.65
24	b	622	BCR	C37-C22-C21	-2.49	118.78	122.82
22	b	615	CLA	C1-O2A-CGA	2.49	122.68	116.65
22	C	501	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
24	c	515	BCR	C27-C26-C25	2.49	126.07	122.70
28	d	408	PL9	C7-C3-C4	2.49	118.96	116.91
32	d	405	LHG	O7-C7-C8	2.49	116.87	111.48
22	b	617	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
22	B	615	CLA	C1-O2A-CGA	2.49	122.67	116.65
28	a	613	PL9	C10-C9-C11	2.49	119.55	115.23
24	C	515	BCR	C27-C26-C25	2.49	126.06	122.70
22	A	604	CLA	C4B-C3B-C2B	-2.49	104.21	107.30
22	D	403	CLA	C4-C3-C5	2.48	119.54	115.23
28	D	408	PL9	C7-C3-C4	2.48	118.95	116.91
22	b	611	CLA	C4-C3-C5	2.48	119.54	115.23
24	A	608	BCR	C34-C9-C10	-2.48	118.80	122.82
22	D	401	CLA	CMC-C2C-C1C	2.48	128.91	125.03
22	c	513	CLA	C3B-C4B-NB	2.48	112.74	110.53
24	a	608	BCR	C34-C9-C10	-2.48	118.80	122.82
29	D	406	LMG	O8-C28-O10	-2.48	117.44	123.63
22	B	611	CLA	C4-C3-C5	2.47	119.52	115.23
22	c	501	CLA	C4C-C3C-C2C	-2.47	103.29	106.89
29	d	406	LMG	O8-C28-O10	-2.47	117.44	123.63
28	A	613	PL9	C10-C9-C11	2.47	119.52	115.23
22	C	507	CLA	CMB-C2B-C1B	2.47	129.18	125.42
22	b	606	CLA	C3B-C4B-NB	2.47	112.74	110.53
22	c	507	CLA	CMB-C2B-C1B	2.47	129.18	125.42
22	C	512	CLA	CED-O2D-CGD	2.47	121.52	115.92
22	B	602	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
22	d	401	CLA	CMC-C2C-C1C	2.47	128.89	125.03
22	a	607	CLA	CMC-C2C-C1C	2.47	128.89	125.03
23	A	606	PHO	CED-O2D-CGD	2.47	121.51	115.92
23	a	605	PHO	CBC-CAC-C3C	-2.46	109.34	112.87
22	B	610	CLA	CMB-C2B-C1B	2.46	129.17	125.42
22	B	607	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
22	c	512	CLA	CED-O2D-CGD	2.46	121.50	115.92
22	B	607	CLA	O2A-CGA-CBA	2.46	119.34	111.83
22	b	607	CLA	O2A-CGA-CBA	2.46	119.34	111.83
23	A	605	PHO	CMA-C3A-C4A	-2.46	109.31	114.61
22	C	513	CLA	O2A-CGA-CBA	2.46	119.34	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	604	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
22	B	613	CLA	CMC-C2C-C1C	2.46	128.88	125.03
22	A	607	CLA	CMC-C2C-C1C	2.46	128.88	125.03
22	c	513	CLA	O2A-CGA-CBA	2.46	119.33	111.83
22	C	503	CLA	CMC-C2C-C1C	2.46	128.88	125.03
22	C	510	CLA	CAC-C3C-C4C	2.46	127.99	124.79
24	B	622	BCR	C32-C1-C6	2.46	114.09	110.24
22	d	403	CLA	C4-C3-C5	2.45	119.49	115.23
22	a	604	CLA	C4B-C3B-C2B	-2.45	104.25	107.30
23	a	605	PHO	CMA-C3A-C4A	-2.45	109.32	114.61
23	a	606	PHO	CED-O2D-CGD	2.45	121.48	115.92
22	a	604	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
22	C	513	CLA	C3B-C4B-NB	2.45	112.72	110.53
22	C	513	CLA	CAC-C3C-C4C	2.45	127.98	124.79
22	b	602	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
22	C	506	CLA	C3B-C4B-NB	2.45	112.72	110.53
22	b	607	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
29	B	620	LMG	O7-C10-O9	-2.45	117.99	123.70
22	B	612	CLA	CMB-C2B-C1B	2.45	129.14	125.42
24	T	102	BCR	C32-C1-C2	-2.44	99.57	108.95
24	K	102	BCR	C1-C6-C5	-2.44	119.30	122.64
22	b	610	CLA	CMB-C2B-C1B	2.44	129.14	125.42
22	D	401	CLA	CHB-C1B-C2B	-2.44	120.35	127.43
22	c	510	CLA	CAC-C3C-C4C	2.44	127.96	124.79
24	t	101	BCR	C32-C1-C2	-2.44	99.60	108.95
22	b	606	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
22	b	602	CLA	C3B-C4B-NB	2.44	112.70	110.53
24	k	102	BCR	C1-C6-C5	-2.44	119.31	122.64
22	b	604	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
22	c	503	CLA	CMC-C2C-C1C	2.43	128.84	125.03
22	c	506	CLA	C3B-C4B-NB	2.43	112.70	110.53
22	d	401	CLA	CHB-C1B-C2B	-2.43	120.37	127.43
24	T	101	BCR	C37-C22-C21	-2.43	118.88	122.82
23	A	605	PHO	CBC-CAC-C3C	-2.43	109.39	112.87
22	b	617	CLA	C1-O2A-CGA	2.43	122.53	116.65
24	B	622	BCR	C3-C4-C5	2.43	118.38	114.06
24	b	622	BCR	C3-C4-C5	2.43	118.38	114.06
22	b	612	CLA	CMB-C2B-C1B	2.43	129.11	125.42
24	B	618	BCR	C37-C22-C21	-2.43	118.89	122.82
22	B	617	CLA	C1-O2A-CGA	2.43	122.52	116.65
22	C	511	CLA	CAC-C3C-C4C	2.43	127.94	124.79
22	C	505	CLA	CED-O2D-CGD	2.42	121.42	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	410	DGD	O6D-C5D-C6D	2.42	111.50	106.69
22	c	511	CLA	CAC-C3C-C4C	2.42	127.94	124.79
22	B	606	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
24	b	622	BCR	C32-C1-C6	2.42	114.04	110.24
22	d	402	CLA	CHC-C1C-C2C	-2.42	120.06	126.95
22	c	505	CLA	CED-O2D-CGD	2.42	121.41	115.92
23	A	606	PHO	O2D-CGD-O1D	-2.42	119.14	123.85
24	k	101	BCR	C30-C25-C24	2.42	122.22	115.65
22	b	602	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
29	b	619	LMG	O7-C10-O9	-2.42	118.05	123.70
24	h	101	BCR	C28-C29-C30	2.42	122.99	114.43
22	C	512	CLA	C1-O2A-CGA	2.42	122.50	116.65
22	c	512	CLA	CAC-C3C-C4C	2.42	127.93	124.79
22	B	604	CLA	C4B-C3B-C2B	-2.41	104.30	107.30
24	H	101	BCR	C28-C29-C30	2.41	122.97	114.43
22	D	402	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
22	B	602	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
24	K	101	BCR	C30-C25-C24	2.41	122.18	115.65
22	B	614	CLA	C1-C2-C3	-2.41	122.25	126.20
22	B	614	CLA	CBC-CAC-C3C	-2.41	105.89	112.42
22	b	614	CLA	CBC-CAC-C3C	-2.41	105.89	112.42
22	b	614	CLA	O2A-CGA-CBA	2.41	119.17	111.83
22	c	502	CLA	CMC-C2C-C1C	2.41	128.79	125.03
22	c	513	CLA	CAC-C3C-C4C	2.41	127.92	124.79
22	B	614	CLA	O2A-CGA-CBA	2.40	119.16	111.83
22	b	609	CLA	C4B-C3B-C2B	-2.40	104.32	107.30
28	d	408	PL9	C7-C3-C2	-2.40	120.56	123.39
29	a	614	LMG	O8-C28-C29	2.40	119.15	111.83
22	b	614	CLA	C1-C2-C3	-2.40	122.27	126.20
22	C	504	CLA	C4B-C3B-C2B	-2.40	104.32	107.30
23	a	606	PHO	O2D-CGD-O1D	-2.40	119.18	123.85
28	D	408	PL9	C7-C3-C2	-2.39	120.57	123.39
22	C	513	CLA	C4-C3-C5	2.39	119.38	115.23
22	C	512	CLA	CAC-C3C-C4C	2.39	127.90	124.79
22	c	504	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
22	C	502	CLA	CMC-C2C-C1C	2.39	128.77	125.03
22	A	604	CLA	C4C-C3C-C2C	-2.39	103.41	106.89
22	B	602	CLA	C3B-C4B-NB	2.39	112.66	110.53
22	B	609	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
22	C	507	CLA	CMC-C2C-C1C	2.39	128.77	125.03
31	d	410	DGD	O6D-C5D-C6D	2.39	111.43	106.69
29	A	614	LMG	O8-C28-C29	2.38	119.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	C4B-C3B-C2B	-2.38	104.34	107.30
22	C	513	CLA	C4D-C3D-CAD	2.38	110.69	108.11
22	B	612	CLA	CBC-CAC-C3C	-2.38	105.97	112.42
22	a	604	CLA	C4C-C3C-C2C	-2.38	103.43	106.89
22	b	604	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
22	c	508	CLA	C4B-C3B-C2B	-2.38	104.34	107.30
22	d	402	CLA	CHD-C4C-C3C	-2.38	121.31	124.77
22	D	402	CLA	CHD-C4C-C3C	-2.38	121.31	124.77
22	c	513	CLA	C4-C3-C5	2.38	119.35	115.23
22	c	510	CLA	C4B-C3B-C2B	-2.38	104.35	107.30
22	C	510	CLA	C4B-C3B-C2B	-2.37	104.35	107.30
22	B	604	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
22	c	507	CLA	CMC-C2C-C1C	2.37	128.74	125.03
22	B	610	CLA	CED-O2D-CGD	2.37	121.28	115.92
22	b	610	CLA	CED-O2D-CGD	2.37	121.28	115.92
22	c	512	CLA	C1-O2A-CGA	2.37	122.38	116.65
24	c	514	BCR	C3-C4-C5	2.36	118.27	114.06
33	f	101	HEM	CMD-C2D-C1D	2.36	128.73	125.03
22	b	612	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
32	d	407	LHG	O8-C23-C24	2.36	119.03	111.83
32	D	407	LHG	O8-C23-C24	2.36	119.03	111.83
28	d	408	PL9	C27-C28-C29	-2.36	122.22	127.62
31	d	410	DGD	O6E-C5E-C6E	2.36	112.29	106.44
22	c	509	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
24	C	514	BCR	C3-C4-C5	2.36	118.26	114.06
22	D	403	CLA	CMB-C2B-C1B	2.36	129.01	125.42
31	D	410	DGD	O6E-C5E-C6E	2.36	112.28	106.44
33	F	101	HEM	CMD-C2D-C1D	2.36	128.72	125.03
22	C	509	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
22	c	504	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
24	A	608	BCR	C37-C22-C23	-2.35	114.49	118.09
24	D	404	BCR	C37-C22-C23	-2.35	114.49	118.09
28	D	408	PL9	C27-C28-C29	-2.35	122.24	127.62
22	C	510	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
22	C	504	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
22	c	513	CLA	CHD-C4C-NC	-2.35	120.59	124.23
22	d	403	CLA	CMB-C2B-C1B	2.35	128.99	125.42
22	D	402	CLA	C4C-C3C-C2C	-2.34	103.48	106.89
22	d	402	CLA	C4C-C3C-C2C	-2.34	103.48	106.89
22	C	504	CLA	CMC-C2C-C1C	2.34	128.69	125.03
22	a	607	CLA	O2A-CGA-CBA	2.34	118.97	111.83
22	A	607	CLA	C1-O2A-CGA	2.34	122.32	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	607	CLA	C1-O2A-CGA	2.34	122.31	116.65
22	C	513	CLA	CHD-C4C-NC	-2.34	120.61	124.23
24	b	618	BCR	C29-C28-C27	-2.34	106.14	111.28
28	a	613	PL9	C45-C44-C46	2.33	119.28	115.23
24	a	608	BCR	C37-C22-C23	-2.33	114.52	118.09
22	B	611	CLA	CHB-C4A-NA	2.33	127.76	124.40
22	b	611	CLA	CHB-C4A-NA	2.33	127.76	124.40
22	B	605	CLA	CAC-C3C-C4C	2.33	127.82	124.79
22	c	513	CLA	C4D-C3D-CAD	2.33	110.63	108.11
22	A	607	CLA	O2A-CGA-CBA	2.33	118.93	111.83
22	b	615	CLA	CMC-C2C-C1C	2.33	128.67	125.03
22	C	506	CLA	CMC-C2C-C1C	2.33	128.67	125.03
31	D	410	DGD	O2G-C1B-O1B	-2.33	118.27	123.70
28	A	613	PL9	C45-C44-C46	2.32	119.26	115.23
31	d	410	DGD	O2G-C1B-O1B	-2.32	118.28	123.70
24	d	404	BCR	C37-C22-C23	-2.32	114.55	118.09
22	b	603	CLA	C1-O2A-CGA	2.32	122.25	116.65
25	a	609	SQD	O48-C23-C24	2.32	118.89	111.83
29	Z	101	LMG	O7-C10-O9	-2.31	118.30	123.70
22	c	508	CLA	CAC-C3C-C4C	2.31	127.80	124.79
29	z	101	LMG	O7-C10-O9	-2.31	118.30	123.70
22	c	510	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
24	B	619	BCR	C29-C28-C27	-2.31	106.19	111.28
22	c	510	CLA	O2A-CGA-CBA	2.31	118.88	111.83
22	B	603	CLA	C1-O2A-CGA	2.31	122.25	116.65
25	A	609	SQD	O48-C23-C24	2.31	118.88	111.83
22	b	605	CLA	O2A-CGA-CBA	2.31	118.88	111.83
24	k	101	BCR	C28-C27-C26	2.31	118.17	114.06
24	K	101	BCR	C28-C27-C26	2.31	118.17	114.06
22	d	402	CLA	CMC-C2C-C1C	2.31	128.64	125.03
28	D	408	PL9	C35-C34-C36	2.30	119.23	115.23
22	C	510	CLA	O2A-CGA-CBA	2.30	118.86	111.83
22	c	506	CLA	CMC-C2C-C1C	2.30	128.63	125.03
22	B	605	CLA	O2A-CGA-CBA	2.30	118.86	111.83
22	b	603	CLA	CED-O2D-CGD	2.30	121.14	115.92
22	B	603	CLA	CED-O2D-CGD	2.30	121.14	115.92
22	c	501	CLA	C1-C2-C3	-2.30	122.43	126.20
22	c	504	CLA	CMC-C2C-C1C	2.30	128.63	125.03
22	B	615	CLA	CMC-C2C-C1C	2.30	128.62	125.03
22	C	509	CLA	CHD-C4C-NC	-2.30	120.67	124.23
22	b	606	CLA	CED-O2D-CGD	2.30	121.12	115.92
22	D	402	CLA	CMC-C2C-C1C	2.30	128.62	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	CAC-C3C-C4C	2.29	127.77	124.79
22	B	606	CLA	CED-O2D-CGD	2.29	121.12	115.92
28	d	408	PL9	C35-C34-C36	2.29	119.21	115.23
22	b	606	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
24	c	515	BCR	C37-C22-C23	-2.28	114.60	118.09
28	d	408	PL9	C7-C8-C9	-2.28	122.90	126.83
22	B	606	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
33	f	101	HEM	C3B-C2B-C1B	2.28	108.12	106.41
22	b	613	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
29	c	519	LMG	O8-C28-O10	-2.28	117.93	123.63
28	D	408	PL9	C7-C8-C9	-2.28	122.91	126.83
24	C	515	BCR	C37-C22-C23	-2.28	114.61	118.09
22	c	509	CLA	CHD-C4C-NC	-2.28	120.70	124.23
22	b	611	CLA	CAC-C3C-C4C	2.28	127.75	124.79
22	B	613	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
22	B	611	CLA	CAC-C3C-C4C	2.27	127.75	124.79
24	c	514	BCR	C40-C30-C29	-2.27	100.22	108.95
22	C	507	CLA	O2A-CGA-CBA	2.27	118.77	111.83
22	c	507	CLA	O2A-CGA-CBA	2.27	118.77	111.83
22	B	616	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
22	B	616	CLA	C1-O2A-CGA	2.27	122.15	116.65
32	D	409	LHG	O4-P-O5	2.27	123.00	112.44
22	C	501	CLA	C1-C2-C3	-2.27	122.48	126.20
29	C	519	LMG	O8-C28-O10	-2.27	117.96	123.63
22	A	603	CLA	C4-C3-C5	2.27	119.16	115.23
24	C	514	BCR	C40-C30-C29	-2.27	100.25	108.95
22	b	616	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
22	A	603	CLA	CMB-C2B-C3B	2.26	131.87	126.55
24	K	102	BCR	C1-C6-C7	2.26	121.78	115.65
25	l	102	SQD	O9-S-C6	2.26	110.13	106.76
22	B	607	CLA	C4D-C3D-CAD	2.26	110.56	108.11
32	d	409	LHG	O4-P-O5	2.26	122.95	112.44
33	F	101	HEM	C3B-C2B-C1B	2.26	108.11	106.41
22	b	608	CLA	C1-O2A-CGA	2.26	122.11	116.65
22	C	508	CLA	CAC-C3C-C4C	2.26	127.73	124.79
25	d	411	SQD	O48-C23-O10	-2.26	117.99	123.63
24	k	102	BCR	C1-C6-C7	2.25	121.77	115.65
22	b	616	CLA	C1-O2A-CGA	2.25	122.10	116.65
25	B	601	SQD	C3-C4-C5	2.25	114.32	110.23
25	b	621	SQD	O9-S-C6	2.25	110.12	106.76
32	E	101	LHG	O8-C23-O10	-2.25	118.00	123.63
22	A	604	CLA	C1-O2A-CGA	2.25	122.09	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	CMB-C2B-C1B	2.24	128.84	125.42
25	D	411	SQD	O48-C23-O10	-2.24	118.01	123.63
28	d	408	PL9	C10-C9-C11	2.24	119.12	115.23
22	b	616	CLA	CED-O2D-CGD	2.24	121.00	115.92
24	d	404	BCR	C38-C26-C25	2.24	126.93	124.48
22	a	603	CLA	CMB-C2B-C3B	2.24	131.82	126.55
22	C	505	CLA	CMB-C2B-C1B	2.24	128.83	125.42
22	B	608	CLA	C1-O2A-CGA	2.24	122.07	116.65
25	b	601	SQD	C3-C4-C5	2.24	114.29	110.23
25	A	609	SQD	O48-C23-O10	-2.24	118.03	123.63
22	B	616	CLA	CED-O2D-CGD	2.24	120.99	115.92
28	D	408	PL9	C10-C9-C11	2.24	119.11	115.23
22	d	401	CLA	O2A-CGA-CBA	2.23	118.65	111.83
24	D	404	BCR	C38-C26-C25	2.23	126.92	124.48
22	B	607	CLA	C1-O2A-CGA	2.23	122.05	116.65
24	A	608	BCR	C2-C1-C6	2.23	113.68	110.44
22	D	401	CLA	O2A-CGA-CBA	2.23	118.63	111.83
32	e	101	LHG	O8-C23-O10	-2.23	118.06	123.63
22	b	607	CLA	C4D-C3D-CAD	2.23	110.53	108.11
22	D	401	CLA	CED-O2D-CGD	2.23	120.97	115.92
22	d	401	CLA	CED-O2D-CGD	2.23	120.96	115.92
25	a	609	SQD	O48-C23-O10	-2.22	118.06	123.63
22	b	617	CLA	CED-O2D-CGD	2.22	120.96	115.92
22	a	603	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
22	A	604	CLA	CED-O2D-CGD	2.22	120.95	115.92
22	C	507	CLA	CED-O2D-CGD	2.22	120.95	115.92
22	a	604	CLA	C1-O2A-CGA	2.22	122.03	116.65
22	b	607	CLA	C1-O2A-CGA	2.22	122.02	116.65
22	b	605	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
22	a	603	CLA	C4-C3-C5	2.22	119.08	115.23
22	b	609	CLA	C11-C12-C13	-2.22	108.60	115.97
22	b	613	CLA	O2A-CGA-CBA	2.21	118.59	111.83
22	b	609	CLA	C4-C3-C5	2.21	119.07	115.23
22	B	617	CLA	CED-O2D-CGD	2.21	120.94	115.92
32	d	405	LHG	O4-P-O5	2.21	122.74	112.44
22	A	603	CLA	CMC-C2C-C1C	2.21	128.49	125.03
29	d	406	LMG	O7-C10-C11	2.21	116.27	111.48
22	a	604	CLA	CED-O2D-CGD	2.21	120.93	115.92
24	a	608	BCR	C2-C1-C6	2.21	113.65	110.44
22	B	609	CLA	C11-C12-C13	-2.21	108.62	115.97
32	D	405	LHG	O4-P-O5	2.21	122.72	112.44
22	B	605	CLA	O2D-CGD-O1D	-2.21	119.55	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	406	LMG	O7-C10-C11	2.21	116.26	111.48
22	c	502	CLA	CHD-C4C-C3C	-2.21	121.56	124.77
22	C	505	CLA	C1-O2A-CGA	2.21	121.99	116.65
22	B	605	CLA	C4B-C3B-C2B	-2.21	104.56	107.30
22	B	609	CLA	C4-C3-C5	2.20	119.06	115.23
22	c	510	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
22	c	505	CLA	C1-O2A-CGA	2.20	121.99	116.65
22	B	613	CLA	O2A-CGA-CBA	2.20	118.55	111.83
22	C	503	CLA	C4D-CHA-C1A	2.20	123.87	121.24
24	c	514	BCR	C2-C3-C4	2.20	116.12	111.28
25	l	102	SQD	O47-C7-O49	-2.20	118.56	123.70
22	a	603	CLA	O2A-CGA-CBA	2.20	118.54	111.83
24	C	515	BCR	C4-C5-C6	2.20	125.68	122.70
24	a	608	BCR	C28-C27-C26	-2.20	110.13	114.06
22	c	507	CLA	CED-O2D-CGD	2.20	120.91	115.92
22	a	603	CLA	C1D-CHD-C4C	-2.20	121.34	126.02
32	D	409	LHG	O8-C23-C24	2.20	118.54	111.83
24	C	514	BCR	C2-C3-C4	2.20	116.11	111.28
23	A	606	PHO	CAC-C3C-C4C	2.20	129.68	124.03
23	a	606	PHO	CAC-C3C-C4C	2.20	129.68	124.03
22	A	603	CLA	C1D-CHD-C4C	-2.20	121.35	126.02
22	B	615	CLA	CED-O2D-CGD	2.20	120.89	115.92
22	C	502	CLA	CHD-C4C-C3C	-2.20	121.57	124.77
25	l	102	SQD	O5-C1-C2	-2.20	105.86	110.37
32	d	409	LHG	O8-C23-C24	2.19	118.53	111.83
24	c	515	BCR	C4-C5-C6	2.19	125.67	122.70
22	A	603	CLA	O2A-CGA-CBA	2.19	118.51	111.83
22	b	615	CLA	CED-O2D-CGD	2.19	120.88	115.92
22	b	617	CLA	CMB-C2B-C1B	2.19	128.75	125.42
22	b	605	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
24	A	608	BCR	C28-C27-C26	-2.19	110.16	114.06
24	T	102	BCR	C3-C2-C1	2.19	122.17	114.43
24	B	618	BCR	C33-C5-C4	-2.19	108.94	113.60
22	B	605	CLA	CHD-C4C-NC	-2.19	120.84	124.23
22	B	604	CLA	O2A-CGA-CBA	2.18	118.50	111.83
24	t	101	BCR	C3-C2-C1	2.18	122.16	114.43
22	A	603	CLA	C4B-C3B-C2B	-2.18	104.59	107.30
31	H	102	DGD	O6E-C5E-C6E	2.18	111.85	106.44
24	b	618	BCR	C28-C29-C30	2.18	122.15	114.43
24	B	619	BCR	C28-C29-C30	2.18	122.15	114.43
22	C	510	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
22	b	617	CLA	CBC-CAC-C3C	-2.18	106.51	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	603	CLA	CMC-C2C-C1C	2.18	128.44	125.03
25	b	621	SQD	O5-C1-C2	-2.18	105.89	110.37
24	T	101	BCR	C33-C5-C4	-2.18	108.95	113.60
25	b	621	SQD	O47-C7-O49	-2.18	118.61	123.70
22	c	503	CLA	C4D-CHA-C1A	2.18	123.84	121.24
31	h	102	DGD	O6E-C5E-C6E	2.18	111.83	106.44
22	C	511	CLA	CED-O2D-CGD	2.18	120.85	115.92
22	c	511	CLA	CED-O2D-CGD	2.18	120.85	115.92
22	B	617	CLA	CHD-C4C-C3C	-2.17	121.60	124.77
29	c	519	LMG	O1-C7-C8	-2.17	105.53	110.82
22	D	401	CLA	CAA-CBA-CGA	-2.17	107.03	113.21
29	C	519	LMG	O1-C7-C8	-2.17	105.53	110.82
28	d	408	PL9	C2-C1-C6	2.17	121.58	119.00
22	b	604	CLA	O2A-CGA-CBA	2.17	118.46	111.83
22	b	609	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
22	B	617	CLA	CMB-C2B-C1B	2.17	128.72	125.42
22	c	509	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
22	b	614	CLA	CMC-C2C-C1C	2.17	128.42	125.03
22	d	401	CLA	CAA-CBA-CGA	-2.17	107.06	113.21
22	b	610	CLA	CBC-CAC-C3C	-2.16	106.56	112.42
24	D	404	BCR	C24-C25-C26	2.16	126.53	121.56
22	b	617	CLA	CHD-C4C-C3C	-2.16	121.62	124.77
22	B	610	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
24	d	404	BCR	C24-C25-C26	2.16	126.53	121.56
22	C	509	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
22	b	605	CLA	CHD-C4C-NC	-2.16	120.89	124.23
22	A	607	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
22	d	402	CLA	CMB-C2B-C1B	2.16	128.70	125.42
22	B	617	CLA	CBC-CAC-C3C	-2.16	106.58	112.42
22	D	402	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
22	c	509	CLA	C1-O2A-CGA	2.15	121.86	116.65
22	B	617	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	C	509	CLA	C1-O2A-CGA	2.15	121.86	116.65
22	B	609	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	b	609	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
22	D	402	CLA	CMB-C2B-C1B	2.15	128.69	125.42
22	b	611	CLA	C4B-C3B-C2B	-2.15	104.63	107.30
22	c	512	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
22	B	602	CLA	C1-O2A-CGA	2.15	121.85	116.65
22	d	402	CLA	C4B-C3B-C2B	-2.15	104.63	107.30
22	c	506	CLA	CMB-C2B-C1B	2.14	128.68	125.42
22	B	611	CLA	O2A-CGA-O1A	-2.14	118.27	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	617	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
28	D	408	PL9	C2-C1-C6	2.14	121.54	119.00
31	c	518	DGD	O1G-C1A-O1A	-2.14	118.27	123.63
22	C	501	CLA	C4-C3-C5	2.14	118.94	115.23
24	T	102	BCR	C40-C30-C25	2.14	113.60	110.24
22	b	602	CLA	C1-O2A-CGA	2.14	121.83	116.65
22	B	609	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
22	B	614	CLA	CMC-C2C-C1C	2.14	128.38	125.03
22	b	614	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
32	d	407	LHG	O7-C7-C8	2.14	116.11	111.48
22	b	606	CLA	CHD-C4C-C3C	-2.14	121.66	124.77
22	b	605	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
22	a	607	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
22	d	402	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
22	c	501	CLA	C4-C3-C5	2.14	118.94	115.23
22	b	609	CLA	CHC-C1C-C2C	-2.14	120.88	126.95
22	B	605	CLA	CHB-C1B-NB	-2.13	120.85	124.05
22	B	614	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
22	b	605	CLA	CHB-C1B-NB	-2.13	120.85	124.05
22	b	611	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
32	D	407	LHG	O7-C7-C8	2.13	116.09	111.48
22	B	605	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
22	C	503	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
24	b	622	BCR	C2-C3-C4	2.13	115.96	111.28
22	C	512	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
24	t	101	BCR	C40-C30-C25	2.13	113.58	110.24
24	h	101	BCR	C40-C30-C29	-2.13	100.78	108.95
22	c	503	CLA	CED-O2D-CGD	2.13	120.74	115.92
31	C	518	DGD	O1G-C1A-O1A	-2.13	118.31	123.63
24	H	101	BCR	C40-C30-C29	-2.13	100.78	108.95
22	c	503	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
22	B	605	CLA	CMC-C2C-C1C	2.12	128.35	125.03
24	B	622	BCR	C2-C3-C4	2.12	115.95	111.28
25	A	609	SQD	O5-C1-C2	-2.12	106.01	110.37
22	B	609	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
22	C	508	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
22	B	606	CLA	CHD-C4C-C3C	-2.12	121.68	124.77
22	C	503	CLA	CED-O2D-CGD	2.12	120.72	115.92
25	a	609	SQD	O5-C1-C2	-2.12	106.02	110.37
22	c	508	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
22	b	615	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
29	Z	101	LMG	C9-O8-C28	2.12	122.30	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	615	CLA	C4B-C3B-C2B	-2.12	104.67	107.30
22	C	504	CLA	C7-C6-C5	-2.12	107.62	113.26
22	b	615	CLA	C4B-C3B-C2B	-2.11	104.67	107.30
22	b	606	CLA	CAC-C3C-C4C	2.11	127.54	124.79
22	c	510	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
22	D	402	CLA	C4B-C3B-C2B	-2.11	104.67	107.30
22	c	507	CLA	C1-O2A-CGA	2.11	121.76	116.65
22	C	506	CLA	O2A-CGA-CBA	2.11	118.27	111.83
22	b	604	CLA	CAC-C3C-C4C	2.11	127.53	124.79
22	c	505	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
24	t	101	BCR	C1-C6-C7	2.11	121.37	115.65
24	k	102	BCR	C30-C25-C24	2.11	121.37	115.65
22	C	510	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
22	B	604	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
22	C	507	CLA	C1-O2A-CGA	2.11	121.75	116.65
22	c	507	CLA	CHB-C1B-NB	-2.11	120.89	124.05
22	C	506	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
22	D	403	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
24	K	102	BCR	C30-C25-C24	2.11	121.36	115.65
22	b	604	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
22	c	504	CLA	C7-C6-C5	-2.10	107.65	113.26
29	z	101	LMG	C9-O8-C28	2.10	122.27	117.08
22	C	505	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
24	H	101	BCR	C1-C6-C5	-2.10	119.76	122.64
22	B	606	CLA	CAC-C3C-C4C	2.10	127.52	124.79
22	d	401	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
22	C	507	CLA	CHB-C1B-NB	-2.10	120.90	124.05
22	B	611	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
22	c	506	CLA	O2A-CGA-CBA	2.10	118.24	111.83
22	C	506	CLA	CMB-C2B-C1B	2.10	128.61	125.42
22	D	401	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
22	B	604	CLA	CAC-C3C-C4C	2.10	127.52	124.79
22	A	604	CLA	CHC-C1C-C2C	-2.10	120.99	126.95
25	L	101	SQD	O8-S-C6	2.09	110.01	105.97
22	d	403	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
33	v	201	HEM	C1D-C2D-C3D	-2.09	104.78	106.98
22	c	506	CLA	C1-C2-C3	-2.09	122.77	126.20
22	B	615	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
32	l	103	LHG	O4-P-O5	2.09	122.17	112.44
22	C	503	CLA	CMB-C2B-C3B	2.09	131.47	126.55
24	T	102	BCR	C1-C6-C7	2.09	121.32	115.65
22	b	605	CLA	CMC-C2C-C1C	2.09	128.30	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	BCR	C29-C28-C27	-2.09	106.69	111.28
32	L	102	LHG	O4-P-O5	2.09	122.16	112.44
22	C	506	CLA	C1-C2-C3	-2.09	122.78	126.20
22	B	614	CLA	C4B-C3B-C2B	-2.09	104.71	107.30
25	l	101	SQD	O8-S-C6	2.09	110.00	105.97
22	B	604	CLA	C4D-C3D-CAD	2.09	110.37	108.11
24	k	102	BCR	C29-C28-C27	-2.08	106.70	111.28
22	b	615	CLA	O2A-CGA-CBA	2.08	118.18	111.83
22	b	606	CLA	C1-C2-C3	-2.08	122.79	126.20
22	a	604	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
24	h	101	BCR	C1-C6-C5	-2.08	119.80	122.64
22	b	603	CLA	O2A-CGA-CBA	2.08	118.17	111.83
22	C	513	CLA	CMB-C2B-C1B	2.08	128.58	125.42
22	c	506	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
31	c	517	DGD	O1G-C1A-C2A	2.08	118.17	111.83
22	c	512	CLA	CMB-C2B-C1B	2.08	128.58	125.42
22	b	614	CLA	C4B-C3B-C2B	-2.08	104.72	107.30
22	D	401	CLA	C4D-CHA-C1A	2.08	123.72	121.24
22	c	512	CLA	CMC-C2C-C1C	2.08	128.28	125.03
22	b	617	CLA	C4-C3-C5	2.07	118.83	115.23
33	F	101	HEM	C1B-NB-C4B	2.07	107.66	105.21
22	C	509	CLA	C1-C2-C3	-2.07	122.80	126.20
22	b	604	CLA	CHD-C4C-C3C	-2.07	121.75	124.77
22	b	615	CLA	C1-C2-C3	-2.07	122.81	126.20
24	k	102	BCR	C38-C26-C25	2.07	126.74	124.48
31	C	517	DGD	O1G-C1A-C2A	2.07	118.15	111.83
22	B	603	CLA	O2A-CGA-CBA	2.07	118.14	111.83
22	B	615	CLA	C1-C2-C3	-2.07	122.81	126.20
22	B	604	CLA	CHD-C4C-C3C	-2.07	121.76	124.77
33	V	201	HEM	C1D-C2D-C3D	-2.07	104.81	106.98
22	C	511	CLA	CMC-C2C-C1C	2.07	128.26	125.03
22	b	604	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
22	B	615	CLA	O2A-CGA-CBA	2.06	118.13	111.83
22	B	606	CLA	C1-C2-C3	-2.06	122.81	126.20
25	d	411	SQD	C3-C4-C5	2.06	113.97	110.23
22	c	509	CLA	CHC-C1C-C2C	-2.06	121.08	126.95
22	B	617	CLA	C4-C3-C5	2.06	118.81	115.23
22	A	607	CLA	CHB-C4A-NA	2.06	127.37	124.40
22	A	603	CLA	CHC-C1C-C2C	-2.06	121.09	126.95
32	L	102	LHG	O7-C7-O9	-2.06	118.89	123.70
22	c	513	CLA	CMB-C2B-C1B	2.06	128.55	125.42
22	c	503	CLA	CMB-C2B-C3B	2.06	131.39	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	604	CLA	C4D-C3D-CAD	2.06	110.34	108.11
22	C	511	CLA	C4D-C3D-CAD	2.06	110.34	108.11
22	C	512	CLA	C4D-C3D-CAD	2.06	110.34	108.11
22	a	607	CLA	CHB-C4A-NA	2.05	127.36	124.40
22	C	509	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
25	l	101	SQD	O47-C7-O49	-2.05	118.91	123.70
22	d	401	CLA	C4D-CHA-C1A	2.05	123.69	121.24
22	a	603	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
24	K	102	BCR	C38-C26-C25	2.05	126.72	124.48
22	C	506	CLA	C4D-C3D-CAD	2.05	110.33	108.11
22	c	511	CLA	C4D-C3D-CAD	2.05	110.33	108.11
22	C	512	CLA	CMC-C2C-C1C	2.05	128.24	125.03
22	b	609	CLA	C11-C10-C8	-2.05	109.16	115.97
22	a	604	CLA	CMB-C2B-C3B	2.05	131.37	126.55
32	l	103	LHG	O7-C7-O9	-2.05	118.92	123.70
22	c	509	CLA	C4-C3-C5	2.05	118.78	115.23
22	A	604	CLA	CMB-C2B-C3B	2.05	131.36	126.55
22	b	607	CLA	CAC-C3C-C4C	2.04	127.45	124.79
22	b	605	CLA	C4D-C3D-CAD	2.04	110.33	108.11
22	b	608	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
22	B	616	CLA	C11-C10-C8	-2.04	109.18	115.97
25	D	411	SQD	C3-C4-C5	2.04	113.93	110.23
33	f	101	HEM	C1B-NB-C4B	2.04	107.62	105.21
25	L	101	SQD	O47-C7-O49	-2.04	118.94	123.70
22	C	509	CLA	C4-C3-C5	2.04	118.77	115.23
25	b	601	SQD	O5-C1-C2	-2.04	106.18	110.37
22	C	512	CLA	CMB-C2B-C1B	2.04	128.52	125.42
29	Z	101	LMG	O8-C28-C29	2.04	121.03	112.38
29	z	101	LMG	O8-C28-C29	2.04	121.03	112.38
22	B	609	CLA	C11-C10-C8	-2.04	109.19	115.97
22	B	607	CLA	CAC-C3C-C4C	2.03	127.44	124.79
22	c	511	CLA	CMC-C2C-C1C	2.03	128.21	125.03
22	c	509	CLA	C1-C2-C3	-2.03	122.86	126.20
22	B	611	CLA	CAA-CBA-CGA	-2.03	107.43	113.21
22	c	512	CLA	C4D-C3D-CAD	2.03	110.31	108.11
25	B	601	SQD	O5-C1-C2	-2.03	106.19	110.37
23	a	606	PHO	CMA-C3A-C4A	-2.03	110.24	114.61
29	D	406	LMG	O8-C28-C29	2.03	118.02	111.83
22	b	614	CLA	CMB-C2B-C1B	2.03	128.50	125.42
29	d	406	LMG	O8-C28-C29	2.03	118.01	111.83
22	b	611	CLA	CAA-CBA-CGA	-2.03	107.45	113.21
22	C	513	CLA	CHC-C1C-NC	-2.03	121.26	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	101	SQD	C4-C3-C2	2.03	114.39	110.83
22	b	609	CLA	CMC-C2C-C1C	2.03	128.20	125.03
22	b	616	CLA	C11-C10-C8	-2.02	109.24	115.97
22	c	510	CLA	C1-C2-C3	-2.02	122.88	126.20
22	D	401	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
22	C	510	CLA	C1-C2-C3	-2.02	122.89	126.20
22	B	608	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
22	D	403	CLA	O2A-CGA-CBA	2.02	118.00	111.83
22	c	513	CLA	CED-O2D-CGD	2.02	120.50	115.92
23	A	606	PHO	CMA-C3A-C4A	-2.02	110.26	114.61
22	B	604	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
22	c	506	CLA	C4D-C3D-CAD	2.02	110.30	108.11
22	c	507	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
31	c	517	DGD	O1G-C1A-O1A	-2.01	118.59	123.63
22	B	606	CLA	CMC-C2C-C1C	2.01	128.18	125.03
22	B	616	CLA	CMC-C2C-C1C	2.01	128.18	125.03
22	d	403	CLA	O2A-CGA-CBA	2.01	117.97	111.83
22	B	607	CLA	CMC-C2C-C1C	2.01	128.18	125.03
22	B	610	CLA	CMC-C2C-C1C	2.01	128.18	125.03
24	t	101	BCR	C31-C1-C2	-2.01	101.23	108.95
28	A	613	PL9	C17-C18-C19	-2.01	123.02	127.62
25	l	101	SQD	C4-C3-C2	2.01	114.36	110.83
28	A	613	PL9	C51-C49-C50	2.01	119.21	114.59
22	B	607	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
22	B	609	CLA	CMC-C2C-C1C	2.01	128.17	125.03
22	B	612	CLA	C1D-CHD-C4C	-2.01	121.75	126.02
22	B	608	CLA	CHB-C4A-NA	2.01	127.30	124.40
22	C	510	CLA	C4-C3-C5	2.01	118.71	115.23
24	T	102	BCR	C31-C1-C2	-2.00	101.25	108.95
22	C	513	CLA	CED-O2D-CGD	2.00	120.46	115.92
22	A	603	CLA	C7-C6-C5	-2.00	107.92	113.26
22	C	507	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
22	b	607	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
22	b	610	CLA	CMC-C2C-C1C	2.00	128.16	125.03
22	c	510	CLA	C4-C3-C5	2.00	118.70	115.23
22	b	608	CLA	CHB-C4A-NA	2.00	127.29	124.40
28	a	613	PL9	C51-C49-C50	2.00	119.19	114.59
22	C	510	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (46) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom

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

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Mol	Chain	Res	Type	Atom
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	512	CLA	ND
22	D	401	CLA	ND
22	d	401	CLA	ND

All (1484) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	B	617	CLA	CHA-CBD-CGD-O1D
22	b	602	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	CAD-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	b	617	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O1D
24	B	618	BCR	C10-C11-C12-C13
24	B	618	BCR	C11-C12-C13-C14
24	C	514	BCR	C14-C15-C16-C17
24	C	514	BCR	C18-C19-C20-C21
24	C	515	BCR	C14-C15-C16-C17
24	C	515	BCR	C18-C19-C20-C21
24	c	514	BCR	C14-C15-C16-C17
24	c	514	BCR	C18-C19-C20-C21
24	c	515	BCR	C14-C15-C16-C17
24	c	515	BCR	C18-C19-C20-C21
24	D	404	BCR	C14-C15-C16-C17
24	D	404	BCR	C22-C23-C24-C25
24	D	404	BCR	C23-C24-C25-C26
24	d	404	BCR	C14-C15-C16-C17
24	d	404	BCR	C22-C23-C24-C25
24	d	404	BCR	C23-C24-C25-C26
24	H	101	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	H	101	BCR	C18-C19-C20-C21
24	h	101	BCR	C10-C11-C12-C13
24	h	101	BCR	C18-C19-C20-C21
24	K	102	BCR	C10-C11-C12-C13
24	K	102	BCR	C17-C18-C19-C20
24	K	102	BCR	C18-C19-C20-C21
24	k	102	BCR	C10-C11-C12-C13
24	k	102	BCR	C17-C18-C19-C20
24	k	102	BCR	C18-C19-C20-C21
24	T	101	BCR	C10-C11-C12-C13
24	T	101	BCR	C11-C12-C13-C14
25	B	601	SQD	O6-C44-C45-O47
25	b	601	SQD	O6-C44-C45-O47
25	b	621	SQD	O5-C1-O6-C44
25	b	621	SQD	C8-C7-O47-C45
25	b	621	SQD	O5-C5-C6-S
25	L	101	SQD	C8-C7-O47-C45
25	L	101	SQD	O5-C5-C6-S
25	l	101	SQD	C8-C7-O47-C45
25	l	101	SQD	O5-C5-C6-S
25	l	102	SQD	O5-C1-O6-C44
25	l	102	SQD	C8-C7-O47-C45
25	l	102	SQD	O5-C5-C6-S
28	A	613	PL9	C18-C19-C21-C22
28	A	613	PL9	C20-C19-C21-C22
28	a	613	PL9	C18-C19-C21-C22
28	a	613	PL9	C20-C19-C21-C22
29	Z	101	LMG	O6-C1-O1-C7
29	Z	101	LMG	O1-C7-C8-O7
29	Z	101	LMG	O9-C10-O7-C8
29	z	101	LMG	O6-C1-O1-C7
29	z	101	LMG	O1-C7-C8-O7
29	z	101	LMG	O9-C10-O7-C8
31	D	410	DGD	C2B-C1B-O2G-C2G
31	D	410	DGD	C2D-C1D-O3G-C3G
31	d	410	DGD	C2B-C1B-O2G-C2G
31	d	410	DGD	C2D-C1D-O3G-C3G
32	D	407	LHG	O1-C1-C2-C3
32	D	407	LHG	O2-C2-C3-O3
32	D	407	LHG	C3-O3-P-O5
32	D	407	LHG	C3-O3-P-O6
32	D	407	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
32	d	407	LHG	O1-C1-C2-C3
32	d	407	LHG	O2-C2-C3-O3
32	d	407	LHG	C3-O3-P-O5
32	d	407	LHG	C3-O3-P-O6
32	d	407	LHG	C4-O6-P-O4
32	E	101	LHG	O9-C7-O7-C5
32	E	101	LHG	C8-C7-O7-C5
32	e	101	LHG	O9-C7-O7-C5
32	e	101	LHG	C8-C7-O7-C5
32	L	102	LHG	C4-O6-P-O3
32	L	102	LHG	C4-O6-P-O4
32	L	102	LHG	C4-O6-P-O5
32	l	103	LHG	C4-O6-P-O3
32	l	103	LHG	C4-O6-P-O4
32	l	103	LHG	C4-O6-P-O5
33	v	201	HEM	C2B-C3B-CAB-CBB
29	Z	101	LMG	C29-C28-O8-C9
29	z	101	LMG	C29-C28-O8-C9
25	D	411	SQD	O10-C23-O48-C46
25	d	411	SQD	O10-C23-O48-C46
32	E	101	LHG	O10-C23-O8-C6
32	e	101	LHG	O10-C23-O8-C6
25	D	411	SQD	C24-C23-O48-C46
25	d	411	SQD	C24-C23-O48-C46
32	E	101	LHG	C24-C23-O8-C6
32	e	101	LHG	C24-C23-O8-C6
29	Z	101	LMG	O10-C28-O8-C9
29	z	101	LMG	O10-C28-O8-C9
25	b	621	SQD	O49-C7-O47-C45
25	l	102	SQD	O49-C7-O47-C45
31	D	410	DGD	O1B-C1B-O2G-C2G
31	d	410	DGD	O1B-C1B-O2G-C2G
22	B	615	CLA	C3-C5-C6-C7
22	b	615	CLA	C3-C5-C6-C7
22	B	617	CLA	CBA-CGA-O2A-C1
22	b	617	CLA	CBA-CGA-O2A-C1
22	C	513	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CBD-CGD-O2D-CED
29	Z	101	LMG	C11-C10-O7-C8
29	z	101	LMG	C11-C10-O7-C8
22	B	606	CLA	C4-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C2-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
22	C	513	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	C3-C5-C6-C7
22	b	602	CLA	C3-C5-C6-C7
24	D	404	BCR	C15-C16-C17-C18
24	d	404	BCR	C15-C16-C17-C18
25	L	101	SQD	O49-C7-O47-C45
25	l	101	SQD	O49-C7-O47-C45
22	B	617	CLA	O1A-CGA-O2A-C1
22	b	617	CLA	O1A-CGA-O2A-C1
31	D	410	DGD	O6E-C5E-C6E-O5E
31	d	410	DGD	O6E-C5E-C6E-O5E
28	A	613	PL9	C9-C11-C12-C13
28	A	613	PL9	C14-C16-C17-C18
28	A	613	PL9	C19-C21-C22-C23
28	A	613	PL9	C24-C26-C27-C28
28	a	613	PL9	C9-C11-C12-C13
28	a	613	PL9	C14-C16-C17-C18
28	a	613	PL9	C19-C21-C22-C23
28	a	613	PL9	C24-C26-C27-C28
25	D	411	SQD	O5-C1-O6-C44
25	d	411	SQD	O5-C1-O6-C44
31	D	410	DGD	O6E-C1E-O5D-C6D
31	d	410	DGD	O6E-C1E-O5D-C6D
22	C	508	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
29	C	520	LMG	O6-C5-C6-O5
29	c	520	LMG	O6-C5-C6-O5
24	C	515	BCR	C15-C16-C17-C18
24	c	515	BCR	C15-C16-C17-C18
32	D	407	LHG	C1-C2-C3-O3
32	d	407	LHG	C1-C2-C3-O3
25	L	101	SQD	C24-C23-O48-C46
25	l	101	SQD	C24-C23-O48-C46
22	B	602	CLA	C11-C10-C8-C9
22	b	602	CLA	C11-C10-C8-C9
22	C	501	CLA	C11-C12-C13-C14
22	C	502	CLA	C14-C13-C15-C16
22	C	504	CLA	C11-C12-C13-C14
22	C	509	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	C11-C12-C13-C14
22	c	502	CLA	C14-C13-C15-C16
22	c	504	CLA	C11-C12-C13-C14
22	c	509	CLA	C6-C7-C8-C9
29	C	520	LMG	C4-C5-C6-O5
29	c	520	LMG	C4-C5-C6-O5
25	D	411	SQD	C2-C1-O6-C44
25	d	411	SQD	C2-C1-O6-C44
31	D	410	DGD	C2E-C1E-O5D-C6D
31	d	410	DGD	C2E-C1E-O5D-C6D
24	B	618	BCR	C11-C12-C13-C35
24	K	102	BCR	C36-C18-C19-C20
24	k	102	BCR	C36-C18-C19-C20
24	T	101	BCR	C11-C12-C13-C35
25	L	101	SQD	O10-C23-O48-C46
25	l	101	SQD	O10-C23-O48-C46
31	D	410	DGD	C1A-C2A-C3A-C4A
31	d	410	DGD	C1A-C2A-C3A-C4A
32	D	407	LHG	O1-C1-C2-O2
32	d	407	LHG	O1-C1-C2-O2
29	C	519	LMG	C28-C29-C30-C31
29	c	519	LMG	C28-C29-C30-C31
24	C	514	BCR	C19-C20-C21-C22
24	c	514	BCR	C19-C20-C21-C22
31	D	410	DGD	C4E-C5E-C6E-O5E
31	d	410	DGD	C4E-C5E-C6E-O5E
29	C	520	LMG	C28-C29-C30-C31
29	c	520	LMG	C28-C29-C30-C31
32	D	405	LHG	C23-C24-C25-C26
32	d	405	LHG	C23-C24-C25-C26
22	A	607	CLA	C10-C11-C12-C13
22	a	607	CLA	C10-C11-C12-C13
22	B	616	CLA	C5-C6-C7-C8
22	b	616	CLA	C5-C6-C7-C8
22	A	607	CLA	C13-C15-C16-C17
22	a	607	CLA	C13-C15-C16-C17
22	B	602	CLA	C10-C11-C12-C13
22	B	615	CLA	C5-C6-C7-C8
22	b	602	CLA	C10-C11-C12-C13
22	b	615	CLA	C5-C6-C7-C8
25	B	601	SQD	C23-C24-C25-C26
25	b	601	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
31	C	517	DGD	C1B-C2B-C3B-C4B
31	c	517	DGD	C1B-C2B-C3B-C4B
31	D	410	DGD	C1B-C2B-C3B-C4B
31	d	410	DGD	C1B-C2B-C3B-C4B
32	E	101	LHG	C7-C8-C9-C10
32	e	101	LHG	C7-C8-C9-C10
31	D	410	DGD	O6D-C1D-O3G-C3G
31	d	410	DGD	O6D-C1D-O3G-C3G
22	B	607	CLA	C13-C15-C16-C17
22	B	615	CLA	C10-C11-C12-C13
22	b	607	CLA	C13-C15-C16-C17
22	b	615	CLA	C10-C11-C12-C13
22	C	509	CLA	C8-C10-C11-C12
22	c	509	CLA	C8-C10-C11-C12
29	A	614	LMG	C28-C29-C30-C31
29	a	614	LMG	C28-C29-C30-C31
22	c	506	CLA	C5-C6-C7-C8
22	C	506	CLA	C5-C6-C7-C8
22	D	403	CLA	C8-C10-C11-C12
22	d	403	CLA	C8-C10-C11-C12
25	b	621	SQD	C7-C8-C9-C10
25	l	102	SQD	C7-C8-C9-C10
22	A	604	CLA	C13-C15-C16-C17
22	a	604	CLA	C13-C15-C16-C17
22	B	607	CLA	C15-C16-C17-C18
22	b	607	CLA	C15-C16-C17-C18
22	D	403	CLA	C10-C11-C12-C13
22	d	403	CLA	C10-C11-C12-C13
24	C	514	BCR	C15-C16-C17-C18
24	c	514	BCR	C15-C16-C17-C18
22	B	607	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
22	C	509	CLA	C13-C15-C16-C17
22	c	509	CLA	C13-C15-C16-C17
22	A	607	CLA	C15-C16-C17-C18
22	a	607	CLA	C15-C16-C17-C18
22	B	612	CLA	C15-C16-C17-C18
22	b	612	CLA	C15-C16-C17-C18
22	B	617	CLA	C10-C11-C12-C13
22	b	617	CLA	C10-C11-C12-C13
22	C	501	CLA	C15-C16-C17-C18
22	C	506	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	C15-C16-C17-C18
22	c	506	CLA	C10-C11-C12-C13
22	A	604	CLA	C16-C17-C18-C20
22	a	604	CLA	C16-C17-C18-C20
24	B	619	BCR	C20-C21-C22-C37
24	b	618	BCR	C20-C21-C22-C37
24	C	515	BCR	C20-C21-C22-C37
24	c	515	BCR	C20-C21-C22-C37
24	H	101	BCR	C20-C21-C22-C37
24	h	101	BCR	C20-C21-C22-C37
24	K	102	BCR	C7-C8-C9-C34
24	k	102	BCR	C7-C8-C9-C34
24	T	102	BCR	C37-C22-C23-C24
24	t	101	BCR	C37-C22-C23-C24
32	D	405	LHG	O1-C1-C2-C3
32	d	405	LHG	O1-C1-C2-C3
25	L	101	SQD	C46-C45-O47-C7
25	l	101	SQD	C46-C45-O47-C7
22	C	506	CLA	C16-C17-C18-C19
22	c	506	CLA	C16-C17-C18-C19
24	B	619	BCR	C20-C21-C22-C23
24	b	618	BCR	C20-C21-C22-C23
24	C	514	BCR	C20-C21-C22-C23
24	c	514	BCR	C20-C21-C22-C23
24	H	101	BCR	C20-C21-C22-C23
24	h	101	BCR	C20-C21-C22-C23
24	K	102	BCR	C20-C21-C22-C23
24	k	102	BCR	C20-C21-C22-C23
29	A	614	LMG	C11-C10-O7-C8
29	a	614	LMG	C11-C10-O7-C8
22	B	614	CLA	C15-C16-C17-C18
22	b	614	CLA	C15-C16-C17-C18
22	B	617	CLA	C2-C1-O2A-CGA
22	b	617	CLA	C2-C1-O2A-CGA
22	D	403	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C19
25	A	609	SQD	C11-C12-C13-C14
25	a	609	SQD	C11-C12-C13-C14
25	b	601	SQD	C15-C16-C17-C18
25	L	101	SQD	C15-C16-C17-C18
25	l	101	SQD	C15-C16-C17-C18
29	B	620	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	C	520	LMG	C29-C30-C31-C32
29	c	520	LMG	C29-C30-C31-C32
31	C	516	DGD	C4B-C5B-C6B-C7B
31	c	516	DGD	C4B-C5B-C6B-C7B
31	c	518	DGD	C9B-CAB-CBB-CCB
31	D	410	DGD	C7B-C8B-C9B-CAB
31	d	410	DGD	C7B-C8B-C9B-CAB
25	D	411	SQD	C29-C30-C31-C32
25	D	411	SQD	C34-C35-C36-C37
25	d	411	SQD	C34-C35-C36-C37
29	b	619	LMG	C32-C33-C34-C35
29	D	406	LMG	C14-C15-C16-C17
29	d	406	LMG	C14-C15-C16-C17
29	Z	101	LMG	C19-C20-C21-C22
29	z	101	LMG	C19-C20-C21-C22
31	C	518	DGD	C9B-CAB-CBB-CCB
31	D	410	DGD	CCA-CDA-CEA-CFA
31	d	410	DGD	CCA-CDA-CEA-CFA
31	C	517	DGD	C1A-C2A-C3A-C4A
25	B	601	SQD	C15-C16-C17-C18
25	d	411	SQD	C29-C30-C31-C32
25	L	101	SQD	C10-C11-C12-C13
25	l	101	SQD	C10-C11-C12-C13
29	D	406	LMG	C16-C17-C18-C19
29	d	406	LMG	C16-C17-C18-C19
32	E	101	LHG	C14-C15-C16-C17
32	E	101	LHG	C24-C25-C26-C27
32	e	101	LHG	C14-C15-C16-C17
32	e	101	LHG	C24-C25-C26-C27
25	A	609	SQD	C15-C16-C17-C18
25	A	609	SQD	C28-C29-C30-C31
25	a	609	SQD	C15-C16-C17-C18
25	a	609	SQD	C28-C29-C30-C31
25	D	411	SQD	C26-C27-C28-C29
25	d	411	SQD	C26-C27-C28-C29
25	L	101	SQD	C11-C10-C9-C8
25	l	101	SQD	C11-C10-C9-C8
29	A	614	LMG	C13-C14-C15-C16
29	a	614	LMG	C13-C14-C15-C16
29	C	520	LMG	C30-C31-C32-C33
29	c	520	LMG	C30-C31-C32-C33
29	Z	101	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	z	101	LMG	C12-C13-C14-C15
32	L	102	LHG	C12-C13-C14-C15
32	l	103	LHG	C12-C13-C14-C15
25	A	609	SQD	C12-C13-C14-C15
25	a	609	SQD	C12-C13-C14-C15
29	A	614	LMG	C12-C13-C14-C15
29	a	614	LMG	C12-C13-C14-C15
29	C	519	LMG	C15-C16-C17-C18
29	c	519	LMG	C15-C16-C17-C18
31	C	517	DGD	C9A-CAA-CBA-CCA
29	Z	101	LMG	C10-C11-C12-C13
29	z	101	LMG	C10-C11-C12-C13
31	c	517	DGD	C1A-C2A-C3A-C4A
31	c	517	DGD	C9A-CAA-CBA-CCA
31	D	410	DGD	C2A-C3A-C4A-C5A
31	d	410	DGD	C2A-C3A-C4A-C5A
22	B	617	CLA	C8-C10-C11-C12
22	b	617	CLA	C8-C10-C11-C12
29	C	520	LMG	C11-C10-O7-C8
29	c	520	LMG	C11-C10-O7-C8
29	C	519	LMG	C17-C18-C19-C20
31	C	516	DGD	O6D-C5D-C6D-O5D
29	c	519	LMG	C17-C18-C19-C20
29	A	614	LMG	C34-C35-C36-C37
29	a	614	LMG	C34-C35-C36-C37
29	B	620	LMG	C31-C32-C33-C34
29	b	619	LMG	C31-C32-C33-C34
31	D	410	DGD	C9B-CAB-CBB-CCB
31	d	410	DGD	C9B-CAB-CBB-CCB
25	L	101	SQD	C24-C25-C26-C27
25	l	101	SQD	C24-C25-C26-C27
32	D	405	LHG	C32-C33-C34-C35
32	d	405	LHG	C32-C33-C34-C35
22	c	506	CLA	O1D-CGD-O2D-CED
24	H	101	BCR	C15-C16-C17-C18
31	c	516	DGD	O6D-C5D-C6D-O5D
25	A	609	SQD	C16-C17-C18-C19
25	L	101	SQD	C27-C28-C29-C30
29	D	406	LMG	C19-C20-C21-C22
29	d	406	LMG	C19-C20-C21-C22
31	C	516	DGD	C6A-C7A-C8A-C9A
31	D	410	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	O1D-CGD-O2D-CED
25	B	601	SQD	C24-C23-O48-C46
25	b	601	SQD	C24-C23-O48-C46
25	a	609	SQD	C16-C17-C18-C19
25	B	601	SQD	C16-C17-C18-C19
25	b	601	SQD	C16-C17-C18-C19
25	L	101	SQD	C12-C13-C14-C15
25	L	101	SQD	C18-C19-C20-C21
25	l	101	SQD	C12-C13-C14-C15
25	l	101	SQD	C17-C18-C19-C20
25	l	101	SQD	C27-C28-C29-C30
25	l	102	SQD	C11-C10-C9-C8
31	C	516	DGD	C5B-C6B-C7B-C8B
31	C	517	DGD	C6B-C7B-C8B-C9B
31	C	517	DGD	C9B-CAB-CBB-CCB
31	C	517	DGD	CBB-CCB-CDB-CEB
31	c	516	DGD	C6A-C7A-C8A-C9A
31	c	516	DGD	C5B-C6B-C7B-C8B
31	c	517	DGD	C6B-C7B-C8B-C9B
31	c	517	DGD	CBB-CCB-CDB-CEB
32	D	405	LHG	C29-C30-C31-C32
32	d	405	LHG	C29-C30-C31-C32
29	C	519	LMG	C10-C11-C12-C13
29	c	519	LMG	C10-C11-C12-C13
25	B	601	SQD	C26-C27-C28-C29
25	b	601	SQD	C26-C27-C28-C29
25	b	621	SQD	C11-C10-C9-C8
25	b	621	SQD	C24-C25-C26-C27
25	L	101	SQD	C17-C18-C19-C20
25	l	101	SQD	C18-C19-C20-C21
25	l	102	SQD	C24-C25-C26-C27
29	A	614	LMG	C36-C37-C38-C39
29	C	519	LMG	C32-C33-C34-C35
29	c	519	LMG	C32-C33-C34-C35
31	C	516	DGD	C4A-C5A-C6A-C7A
31	C	517	DGD	CAA-CBA-CCA-CDA
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	410	DGD	C8B-C9B-CAB-CBB
31	d	410	DGD	CBA-CCA-CDA-CEA
31	d	410	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	A	609	SQD	C9-C10-C11-C12
25	a	609	SQD	C9-C10-C11-C12
25	l	102	SQD	C31-C32-C33-C34
29	A	614	LMG	C31-C32-C33-C34
29	a	614	LMG	C31-C32-C33-C34
29	a	614	LMG	C36-C37-C38-C39
29	C	520	LMG	C31-C32-C33-C34
29	c	520	LMG	C31-C32-C33-C34
25	b	621	SQD	C31-C32-C33-C34
25	D	411	SQD	C24-C25-C26-C27
25	d	411	SQD	C24-C25-C26-C27
29	D	406	LMG	C30-C31-C32-C33
25	D	411	SQD	C31-C32-C33-C34
25	d	411	SQD	C31-C32-C33-C34
29	A	614	LMG	C15-C16-C17-C18
29	a	614	LMG	C15-C16-C17-C18
29	d	406	LMG	C30-C31-C32-C33
31	C	517	DGD	C3A-C4A-C5A-C6A
31	C	518	DGD	C2A-C3A-C4A-C5A
31	c	517	DGD	C3A-C4A-C5A-C6A
31	c	518	DGD	C2A-C3A-C4A-C5A
22	C	507	CLA	C16-C17-C18-C19
22	c	507	CLA	C16-C17-C18-C19
25	b	621	SQD	C10-C11-C12-C13
25	b	621	SQD	C34-C35-C36-C37
25	l	102	SQD	C10-C11-C12-C13
25	l	102	SQD	C34-C35-C36-C37
29	b	619	LMG	C15-C16-C17-C18
29	D	406	LMG	C36-C37-C38-C39
29	d	406	LMG	C36-C37-C38-C39
25	D	411	SQD	C8-C7-O47-C45
25	d	411	SQD	C8-C7-O47-C45
22	b	605	CLA	C13-C15-C16-C17
29	A	614	LMG	C29-C30-C31-C32
29	a	614	LMG	C29-C30-C31-C32
29	D	406	LMG	C39-C40-C41-C42
29	d	406	LMG	C39-C40-C41-C42
32	e	101	LHG	C26-C27-C28-C29
29	B	620	LMG	C15-C16-C17-C18
32	E	101	LHG	C25-C26-C27-C28
32	e	101	LHG	C25-C26-C27-C28
22	B	605	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	h	102	DGD	C7A-C8A-C9A-CAA
32	E	101	LHG	C26-C27-C28-C29
23	A	606	PHO	C2C-C3C-CAC-CBC
23	a	606	PHO	C2C-C3C-CAC-CBC
28	A	613	PL9	C4-C3-C7-C8
28	a	613	PL9	C4-C3-C7-C8
25	L	101	SQD	C29-C30-C31-C32
25	l	101	SQD	C29-C30-C31-C32
29	a	614	LMG	C14-C15-C16-C17
31	D	410	DGD	CCB-CDB-CEB-CFB
31	d	410	DGD	CCB-CDB-CEB-CFB
29	A	614	LMG	O9-C10-O7-C8
29	a	614	LMG	O9-C10-O7-C8
29	C	520	LMG	O9-C10-O7-C8
29	c	520	LMG	O9-C10-O7-C8
25	l	102	SQD	C11-C12-C13-C14
29	b	619	LMG	C17-C18-C19-C20
31	c	516	DGD	CAB-CBB-CCB-CDB
31	H	102	DGD	C7A-C8A-C9A-CAA
32	L	102	LHG	C13-C14-C15-C16
24	K	101	BCR	C10-C11-C12-C13
24	k	101	BCR	C10-C11-C12-C13
25	b	621	SQD	C11-C12-C13-C14
29	A	614	LMG	C14-C15-C16-C17
29	A	614	LMG	C18-C19-C20-C21
29	a	614	LMG	C18-C19-C20-C21
29	B	620	LMG	C17-C18-C19-C20
29	D	406	LMG	C12-C13-C14-C15
29	d	406	LMG	C12-C13-C14-C15
31	C	516	DGD	CAB-CBB-CCB-CDB
32	D	407	LHG	C16-C17-C18-C19
32	l	103	LHG	C13-C14-C15-C16
32	d	407	LHG	C16-C17-C18-C19
29	Z	101	LMG	C15-C16-C17-C18
29	z	101	LMG	C15-C16-C17-C18
32	E	101	LHG	C18-C19-C20-C21
32	e	101	LHG	C18-C19-C20-C21
24	K	102	BCR	C6-C7-C8-C9
24	k	102	BCR	C6-C7-C8-C9
25	L	101	SQD	C14-C15-C16-C17
25	l	101	SQD	C14-C15-C16-C17
31	C	517	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
31	c	517	DGD	CAB-CBB-CCB-CDB
31	H	102	DGD	CBA-CCA-CDA-CEA
31	h	102	DGD	CBA-CCA-CDA-CEA
25	L	101	SQD	C32-C33-C34-C35
25	l	101	SQD	C32-C33-C34-C35
32	L	102	LHG	C11-C12-C13-C14
32	l	103	LHG	C11-C12-C13-C14
24	h	101	BCR	C15-C16-C17-C18
32	D	409	LHG	C29-C30-C31-C32
32	d	409	LHG	C29-C30-C31-C32
32	d	407	LHG	C32-C33-C34-C35
22	C	506	CLA	C13-C15-C16-C17
22	c	506	CLA	C13-C15-C16-C17
29	C	519	LMG	C39-C40-C41-C42
29	c	519	LMG	C39-C40-C41-C42
32	D	407	LHG	C32-C33-C34-C35
25	B	601	SQD	C28-C29-C30-C31
29	C	520	LMG	C8-C7-O1-C1
29	c	520	LMG	C8-C7-O1-C1
25	b	601	SQD	C28-C29-C30-C31
22	C	506	CLA	C16-C17-C18-C20
22	D	403	CLA	C16-C17-C18-C20
22	d	403	CLA	C16-C17-C18-C20
29	B	620	LMG	C37-C38-C39-C40
29	b	619	LMG	C37-C38-C39-C40
29	Z	101	LMG	C16-C17-C18-C19
29	z	101	LMG	C16-C17-C18-C19
33	V	201	HEM	C2B-C3B-CAB-CBB
33	v	201	HEM	C2C-C3C-CAC-CBC
29	D	406	LMG	C15-C16-C17-C18
29	D	406	LMG	C20-C21-C22-C23
29	d	406	LMG	C15-C16-C17-C18
29	d	406	LMG	C20-C21-C22-C23
31	h	102	DGD	C9B-CAB-CBB-CCB
31	H	102	DGD	C9B-CAB-CBB-CCB
32	E	101	LHG	C13-C14-C15-C16
32	e	101	LHG	C13-C14-C15-C16
31	C	517	DGD	C3B-C4B-C5B-C6B
31	C	518	DGD	C6B-C7B-C8B-C9B
31	c	517	DGD	C3B-C4B-C5B-C6B
31	c	518	DGD	C6B-C7B-C8B-C9B
22	C	504	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	c	504	CLA	C13-C15-C16-C17
31	c	516	DGD	C8B-C9B-CAB-CBB
25	L	101	SQD	C7-C8-C9-C10
25	l	101	SQD	C7-C8-C9-C10
25	b	621	SQD	C29-C30-C31-C32
25	l	102	SQD	C29-C30-C31-C32
29	B	620	LMG	C34-C35-C36-C37
29	b	619	LMG	C34-C35-C36-C37
31	C	516	DGD	C8B-C9B-CAB-CBB
33	V	201	HEM	C4B-C3B-CAB-CBB
33	v	201	HEM	C4B-C3B-CAB-CBB
22	C	507	CLA	C16-C17-C18-C20
22	c	506	CLA	C16-C17-C18-C20
22	c	507	CLA	C16-C17-C18-C20
25	B	601	SQD	O10-C23-O48-C46
25	b	601	SQD	O10-C23-O48-C46
25	b	621	SQD	C18-C19-C20-C21
25	l	102	SQD	C18-C19-C20-C21
25	L	101	SQD	C16-C17-C18-C19
25	L	101	SQD	C28-C29-C30-C31
25	l	101	SQD	C16-C17-C18-C19
25	l	101	SQD	C28-C29-C30-C31
22	C	501	CLA	C13-C15-C16-C17
22	c	501	CLA	C13-C15-C16-C17
32	D	405	LHG	C24-C25-C26-C27
32	d	405	LHG	C24-C25-C26-C27
25	D	411	SQD	C30-C31-C32-C33
25	d	411	SQD	C30-C31-C32-C33
32	D	409	LHG	C15-C16-C17-C18
32	d	409	LHG	C15-C16-C17-C18
22	A	604	CLA	C16-C17-C18-C19
22	a	604	CLA	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C20
25	a	609	SQD	C30-C31-C32-C33
31	C	517	DGD	C4A-C5A-C6A-C7A
31	c	517	DGD	C4A-C5A-C6A-C7A
25	A	609	SQD	C32-C33-C34-C35
25	a	609	SQD	C32-C33-C34-C35
25	D	411	SQD	O49-C7-O47-C45
25	d	411	SQD	O49-C7-O47-C45
25	A	609	SQD	C30-C31-C32-C33
29	D	406	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	d	406	LMG	C13-C14-C15-C16
31	C	516	DGD	C3B-C4B-C5B-C6B
31	c	516	DGD	C3B-C4B-C5B-C6B
22	C	507	CLA	C5-C6-C7-C8
22	c	507	CLA	C5-C6-C7-C8
29	C	519	LMG	C34-C35-C36-C37
29	A	614	LMG	C17-C18-C19-C20
29	C	519	LMG	C29-C30-C31-C32
29	c	519	LMG	C29-C30-C31-C32
29	c	519	LMG	C34-C35-C36-C37
22	A	607	CLA	C16-C17-C18-C19
22	a	607	CLA	C16-C17-C18-C19
22	B	605	CLA	C16-C17-C18-C20
29	a	614	LMG	C17-C18-C19-C20
31	C	518	DGD	CBA-CCA-CDA-CEA
31	c	518	DGD	CBA-CCA-CDA-CEA
32	e	101	LHG	C27-C28-C29-C30
32	E	101	LHG	C27-C28-C29-C30
25	b	621	SQD	C32-C33-C34-C35
25	l	102	SQD	C32-C33-C34-C35
22	B	602	CLA	C11-C10-C8-C7
22	B	617	CLA	C11-C12-C13-C15
22	b	602	CLA	C11-C10-C8-C7
22	b	617	CLA	C11-C12-C13-C15
22	C	506	CLA	C11-C12-C13-C15
22	C	508	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C10-C8-C7
22	D	403	CLA	C11-C10-C8-C7
22	d	403	CLA	C11-C10-C8-C7
32	D	409	LHG	C10-C11-C12-C13
32	d	409	LHG	C10-C11-C12-C13
25	A	609	SQD	C34-C35-C36-C37
22	D	403	CLA	C13-C15-C16-C17
25	D	411	SQD	C23-C24-C25-C26
25	d	411	SQD	C23-C24-C25-C26
32	L	102	LHG	C7-C8-C9-C10
32	l	103	LHG	C7-C8-C9-C10
25	a	609	SQD	C34-C35-C36-C37
22	d	403	CLA	C13-C15-C16-C17
22	C	501	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C12-C13-C14
22	D	403	CLA	C11-C10-C8-C9
22	d	403	CLA	C11-C10-C8-C9
29	C	519	LMG	C21-C22-C23-C24
29	c	519	LMG	C21-C22-C23-C24
29	A	614	LMG	C21-C22-C23-C24
29	a	614	LMG	C21-C22-C23-C24
22	C	512	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
25	l	102	SQD	C27-C28-C29-C30
25	b	621	SQD	C27-C28-C29-C30
25	B	601	SQD	O6-C44-C45-C46
25	b	601	SQD	O6-C44-C45-C46
29	A	614	LMG	C7-C8-C9-O8
29	a	614	LMG	C7-C8-C9-O8
29	Z	101	LMG	O1-C7-C8-C9
29	z	101	LMG	O1-C7-C8-C9
29	C	519	LMG	C16-C17-C18-C19
29	c	519	LMG	C16-C17-C18-C19
31	H	102	DGD	C9A-CAA-CBA-CCA
31	h	102	DGD	C9A-CAA-CBA-CCA
29	D	406	LMG	O6-C5-C6-O5
29	d	406	LMG	O6-C5-C6-O5
29	C	519	LMG	C38-C39-C40-C41
29	c	519	LMG	C38-C39-C40-C41
32	E	101	LHG	C15-C16-C17-C18
29	D	406	LMG	C35-C36-C37-C38
29	d	406	LMG	C35-C36-C37-C38
32	e	101	LHG	C15-C16-C17-C18
23	A	606	PHO	O1D-CGD-O2D-CED
23	a	606	PHO	O1D-CGD-O2D-CED
31	C	516	DGD	O6E-C5E-C6E-O5E
31	c	516	DGD	O6E-C5E-C6E-O5E
31	C	516	DGD	C8A-C9A-CAA-CBA
31	D	410	DGD	C3A-C4A-C5A-C6A
31	d	410	DGD	C3A-C4A-C5A-C6A
31	c	516	DGD	C8A-C9A-CAA-CBA
22	C	509	CLA	C10-C11-C12-C13
22	c	509	CLA	C10-C11-C12-C13
22	a	607	CLA	C16-C17-C18-C20
25	b	621	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	D	410	DGD	C9A-CAA-CBA-CCA
31	d	410	DGD	C9A-CAA-CBA-CCA
22	c	512	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	C13-C15-C16-C17
22	b	613	CLA	C13-C15-C16-C17
25	l	102	SQD	C13-C14-C15-C16
29	b	619	LMG	C38-C39-C40-C41
22	C	507	CLA	C2A-CAA-CBA-CGA
29	B	620	LMG	C38-C39-C40-C41
31	C	518	DGD	C6A-C7A-C8A-C9A
31	c	518	DGD	C6A-C7A-C8A-C9A
31	D	410	DGD	C4B-C5B-C6B-C7B
31	d	410	DGD	C4B-C5B-C6B-C7B
22	A	607	CLA	C5-C6-C7-C8
22	a	607	CLA	C5-C6-C7-C8
29	B	620	LMG	C14-C15-C16-C17
29	b	619	LMG	C14-C15-C16-C17
22	C	512	CLA	O1A-CGA-O2A-C1
25	b	601	SQD	C18-C19-C20-C21
25	B	601	SQD	C18-C19-C20-C21
29	C	519	LMG	C20-C21-C22-C23
29	c	519	LMG	C20-C21-C22-C23
29	B	620	LMG	C18-C19-C20-C21
29	b	619	LMG	C18-C19-C20-C21
31	H	102	DGD	CBB-CCB-CDB-CEB
31	h	102	DGD	CBB-CCB-CDB-CEB
22	A	607	CLA	C16-C17-C18-C20
22	B	605	CLA	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C19
22	B	607	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
25	b	621	SQD	C24-C23-O48-C46
25	l	102	SQD	C24-C23-O48-C46
29	C	519	LMG	C29-C28-O8-C9
29	c	519	LMG	C29-C28-O8-C9
29	C	520	LMG	C18-C19-C20-C21
29	Z	101	LMG	C13-C14-C15-C16
29	c	520	LMG	C18-C19-C20-C21
29	z	101	LMG	C13-C14-C15-C16
22	B	617	CLA	C16-C17-C18-C20
22	b	617	CLA	C16-C17-C18-C20
25	A	609	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	a	609	SQD	C27-C28-C29-C30
31	C	516	DGD	C7B-C8B-C9B-CAB
31	c	516	DGD	C7B-C8B-C9B-CAB
31	d	410	DGD	CAA-CBA-CCA-CDA
25	D	411	SQD	C35-C36-C37-C38
25	d	411	SQD	C35-C36-C37-C38
25	b	621	SQD	C28-C29-C30-C31
25	l	102	SQD	C28-C29-C30-C31
29	B	620	LMG	C16-C17-C18-C19
29	b	619	LMG	C16-C17-C18-C19
31	C	517	DGD	C8B-C9B-CAB-CBB
31	c	517	DGD	C8B-C9B-CAB-CBB
31	D	410	DGD	CAA-CBA-CCA-CDA
32	l	103	LHG	C32-C33-C34-C35
32	E	101	LHG	C11-C10-C9-C8
32	e	101	LHG	C11-C10-C9-C8
32	L	102	LHG	C32-C33-C34-C35
29	Z	101	LMG	C4-C5-C6-O5
22	c	507	CLA	C2A-CAA-CBA-CGA
25	B	601	SQD	C19-C20-C21-C22
25	b	601	SQD	C19-C20-C21-C22
25	b	621	SQD	C35-C36-C37-C38
29	D	406	LMG	C38-C39-C40-C41
29	d	406	LMG	C38-C39-C40-C41
25	A	609	SQD	C35-C36-C37-C38
25	a	609	SQD	C35-C36-C37-C38
25	l	102	SQD	C35-C36-C37-C38
29	C	520	LMG	C17-C18-C19-C20
29	c	520	LMG	C17-C18-C19-C20
22	B	602	CLA	CBA-CGA-O2A-C1
22	b	602	CLA	CBA-CGA-O2A-C1
29	z	101	LMG	C4-C5-C6-O5
22	C	512	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C20
25	L	101	SQD	C19-C20-C21-C22
25	l	101	SQD	C19-C20-C21-C22
25	a	609	SQD	C14-C15-C16-C17
25	A	609	SQD	C14-C15-C16-C17
31	C	516	DGD	C6B-C7B-C8B-C9B
22	B	615	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C14-C13-C15-C16
22	B	617	CLA	C11-C12-C13-C14
22	b	615	CLA	C11-C12-C13-C14
22	b	615	CLA	C14-C13-C15-C16
22	b	617	CLA	C11-C12-C13-C14
22	C	507	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	c	508	CLA	C11-C10-C8-C9
31	D	410	DGD	C5A-C6A-C7A-C8A
31	d	410	DGD	C6A-C7A-C8A-C9A
22	D	401	CLA	C4B-C3B-CAB-CBB
22	d	401	CLA	C4B-C3B-CAB-CBB
31	c	516	DGD	C6B-C7B-C8B-C9B
31	D	410	DGD	C6A-C7A-C8A-C9A
31	d	410	DGD	C5A-C6A-C7A-C8A
32	D	405	LHG	C27-C28-C29-C30
32	d	405	LHG	C27-C28-C29-C30
29	c	520	LMG	C15-C16-C17-C18
31	C	517	DGD	C7B-C8B-C9B-CAB
31	c	517	DGD	C7B-C8B-C9B-CAB
29	Z	101	LMG	C2-C1-O1-C7
29	z	101	LMG	C2-C1-O1-C7
22	B	609	CLA	C13-C15-C16-C17
29	A	614	LMG	C32-C33-C34-C35
29	a	614	LMG	C32-C33-C34-C35
31	C	516	DGD	CAA-CBA-CCA-CDA
31	c	516	DGD	CAA-CBA-CCA-CDA
31	H	102	DGD	C6B-C7B-C8B-C9B
31	h	102	DGD	C6B-C7B-C8B-C9B
31	H	102	DGD	CDB-CEB-CFB-CGB
31	h	102	DGD	CDB-CEB-CFB-CGB
31	C	516	DGD	C4D-C5D-C6D-O5D
31	c	516	DGD	C4D-C5D-C6D-O5D
32	e	101	LHG	C19-C20-C21-C22
29	C	520	LMG	C15-C16-C17-C18
22	A	607	CLA	C11-C10-C8-C7
22	a	607	CLA	C11-C10-C8-C7
22	B	602	CLA	C6-C7-C8-C10
22	B	615	CLA	C11-C12-C13-C15
22	b	602	CLA	C6-C7-C8-C10
22	b	615	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	C	501	CLA	C11-C12-C13-C15
22	C	501	CLA	C12-C13-C15-C16
22	C	512	CLA	C11-C10-C8-C7
22	C	513	CLA	C6-C7-C8-C10
22	c	501	CLA	C11-C12-C13-C15
22	c	501	CLA	C12-C13-C15-C16
22	c	512	CLA	C11-C10-C8-C7
22	c	513	CLA	C6-C7-C8-C10
22	D	403	CLA	C6-C7-C8-C10
22	d	403	CLA	C6-C7-C8-C10
22	b	609	CLA	C13-C15-C16-C17
29	C	520	LMG	C40-C41-C42-C43
29	c	520	LMG	C40-C41-C42-C43
31	C	517	DGD	CDB-CEB-CFB-CGB
31	c	517	DGD	CDB-CEB-CFB-CGB
32	E	101	LHG	C19-C20-C21-C22
29	A	614	LMG	C22-C23-C24-C25
29	a	614	LMG	C22-C23-C24-C25
25	B	601	SQD	O5-C1-O6-C44
25	b	601	SQD	O5-C1-O6-C44
25	A	609	SQD	C19-C20-C21-C22
25	a	609	SQD	C19-C20-C21-C22
24	K	102	BCR	C19-C20-C21-C22
24	k	102	BCR	C19-C20-C21-C22
29	C	519	LMG	O10-C28-O8-C9
29	c	519	LMG	O10-C28-O8-C9
29	c	519	LMG	C11-C12-C13-C14
31	C	516	DGD	C5A-C6A-C7A-C8A
31	c	516	DGD	C5A-C6A-C7A-C8A
25	B	601	SQD	C25-C26-C27-C28
25	b	601	SQD	C25-C26-C27-C28
29	C	519	LMG	C11-C12-C13-C14
32	d	405	LHG	C25-C26-C27-C28
22	b	616	CLA	C13-C15-C16-C17
25	b	621	SQD	C44-C45-C46-O48
25	L	101	SQD	C44-C45-C46-O48
25	l	101	SQD	C44-C45-C46-O48
25	l	102	SQD	C44-C45-C46-O48
31	D	410	DGD	O1G-C1G-C2G-C3G
31	d	410	DGD	O1G-C1G-C2G-C3G
25	L	101	SQD	C35-C36-C37-C38
25	l	101	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	D	405	LHG	C25-C26-C27-C28
22	B	602	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C20
25	B	601	SQD	C31-C32-C33-C34
25	b	601	SQD	C31-C32-C33-C34
31	c	518	DGD	C8B-C9B-CAB-CBB
31	C	518	DGD	C8B-C9B-CAB-CBB
22	B	616	CLA	C13-C15-C16-C17
22	B	616	CLA	C10-C11-C12-C13
24	B	618	BCR	C1-C6-C7-C8
24	T	101	BCR	C1-C6-C7-C8
22	b	616	CLA	C10-C11-C12-C13
22	c	508	CLA	C5-C6-C7-C8
22	C	508	CLA	C5-C6-C7-C8
25	B	601	SQD	C32-C33-C34-C35
25	b	601	SQD	C32-C33-C34-C35
32	D	409	LHG	C12-C13-C14-C15
32	d	409	LHG	C12-C13-C14-C15
31	c	518	DGD	C3B-C4B-C5B-C6B
22	B	617	CLA	C16-C17-C18-C19
22	C	501	CLA	C16-C17-C18-C19
22	C	502	CLA	C16-C17-C18-C20
22	c	501	CLA	C16-C17-C18-C19
22	c	502	CLA	C16-C17-C18-C20
22	b	602	CLA	CAA-CBA-CGA-O2A
25	b	621	SQD	O47-C45-C46-O48
25	L	101	SQD	O47-C45-C46-O48
25	l	101	SQD	O47-C45-C46-O48
25	l	102	SQD	O47-C45-C46-O48
29	A	614	LMG	O7-C8-C9-O8
29	a	614	LMG	O7-C8-C9-O8
31	C	518	DGD	C3B-C4B-C5B-C6B
25	B	601	SQD	C35-C36-C37-C38
25	b	601	SQD	C35-C36-C37-C38
25	l	102	SQD	O10-C23-O48-C46
31	d	410	DGD	CAB-CBB-CCB-CDB
24	D	404	BCR	C18-C19-C20-C21
24	d	404	BCR	C18-C19-C20-C21
22	B	602	CLA	CAA-CBA-CGA-O2A
31	D	410	DGD	CAB-CBB-CCB-CDB
22	b	617	CLA	C16-C17-C18-C19
31	D	410	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
31	d	410	DGD	C5B-C6B-C7B-C8B
25	b	621	SQD	O10-C23-O48-C46
22	B	612	CLA	C14-C13-C15-C16
22	b	612	CLA	C14-C13-C15-C16
22	D	403	CLA	C6-C7-C8-C9
22	d	403	CLA	C6-C7-C8-C9
29	A	614	LMG	C33-C34-C35-C36
29	a	614	LMG	C33-C34-C35-C36
24	A	608	BCR	C14-C15-C16-C17
24	a	608	BCR	C14-C15-C16-C17
29	A	614	LMG	C39-C40-C41-C42
29	a	614	LMG	C39-C40-C41-C42
22	d	402	CLA	C2C-C3C-CAC-CBC
22	D	402	CLA	C2C-C3C-CAC-CBC
24	B	619	BCR	C19-C20-C21-C22
24	b	618	BCR	C19-C20-C21-C22
22	C	510	CLA	C2-C3-C5-C6
22	c	510	CLA	C2-C3-C5-C6
22	B	604	CLA	C16-C17-C18-C19
22	b	604	CLA	C16-C17-C18-C19
22	C	501	CLA	C16-C17-C18-C20
25	L	101	SQD	C30-C31-C32-C33
25	l	101	SQD	C30-C31-C32-C33
22	B	602	CLA	C15-C16-C17-C18
22	B	607	CLA	C8-C10-C11-C12
22	b	602	CLA	C15-C16-C17-C18
22	b	607	CLA	C8-C10-C11-C12
32	L	102	LHG	C33-C34-C35-C36
22	B	602	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C19
22	c	501	CLA	C16-C17-C18-C20
32	l	103	LHG	C33-C34-C35-C36
22	C	502	CLA	C15-C16-C17-C18
22	c	502	CLA	C15-C16-C17-C18
29	D	406	LMG	C17-C18-C19-C20
29	d	406	LMG	C17-C18-C19-C20
32	D	409	LHG	C13-C14-C15-C16
32	l	103	LHG	C14-C15-C16-C17
22	B	612	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C7
22	B	617	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C12-C13-C15-C16
22	b	615	CLA	C12-C13-C15-C16
22	b	616	CLA	C11-C10-C8-C7
22	b	617	CLA	C12-C13-C15-C16
22	C	504	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	c	504	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
32	d	409	LHG	C13-C14-C15-C16
32	L	102	LHG	C14-C15-C16-C17
24	K	102	BCR	C7-C8-C9-C10
24	k	102	BCR	C7-C8-C9-C10
31	C	517	DGD	C2G-C3G-O3G-C1D
31	C	517	DGD	C5D-C6D-O5D-C1E
31	c	517	DGD	C2G-C3G-O3G-C1D
31	c	517	DGD	C5D-C6D-O5D-C1E
25	l	102	SQD	C16-C17-C18-C19
22	C	508	CLA	O1D-CGD-O2D-CED
31	H	102	DGD	CCB-CDB-CEB-CFB
32	d	405	LHG	C13-C14-C15-C16
32	L	102	LHG	C34-C35-C36-C37
22	B	602	CLA	O1A-CGA-O2A-C1
22	b	602	CLA	O1A-CGA-O2A-C1
33	F	101	HEM	C2C-C3C-CAC-CBC
33	f	101	HEM	C2C-C3C-CAC-CBC
33	V	201	HEM	C2C-C3C-CAC-CBC
25	b	621	SQD	C16-C17-C18-C19
32	D	405	LHG	C13-C14-C15-C16
32	l	103	LHG	C34-C35-C36-C37
31	h	102	DGD	CCB-CDB-CEB-CFB
22	D	401	CLA	C2C-C3C-CAC-CBC
22	c	508	CLA	O1D-CGD-O2D-CED
22	d	401	CLA	C2C-C3C-CAC-CBC
31	c	517	DGD	C8A-C9A-CAA-CBA
31	C	517	DGD	C8A-C9A-CAA-CBA
29	B	620	LMG	C33-C34-C35-C36
29	b	619	LMG	C33-C34-C35-C36
32	E	101	LHG	O6-C4-C5-O7
32	e	101	LHG	O6-C4-C5-O7
29	b	619	LMG	C30-C31-C32-C33
29	A	614	LMG	O6-C1-O1-C7
29	a	614	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
29	C	520	LMG	C7-C8-C9-O8
29	c	520	LMG	C7-C8-C9-O8
29	B	620	LMG	C30-C31-C32-C33
29	C	519	LMG	C14-C15-C16-C17
29	c	519	LMG	C14-C15-C16-C17
22	C	510	CLA	C4-C3-C5-C6
22	c	510	CLA	C4-C3-C5-C6
29	C	520	LMG	C38-C39-C40-C41
29	c	520	LMG	C38-C39-C40-C41
32	D	405	LHG	C15-C16-C17-C18
32	d	405	LHG	C15-C16-C17-C18
29	A	614	LMG	O1-C7-C8-O7
29	a	614	LMG	O1-C7-C8-O7
22	B	617	CLA	C14-C13-C15-C16
22	b	617	CLA	C14-C13-C15-C16
32	D	409	LHG	C16-C17-C18-C19
31	C	518	DGD	C4A-C5A-C6A-C7A
32	D	409	LHG	C17-C18-C19-C20
32	d	409	LHG	C16-C17-C18-C19
32	d	409	LHG	C17-C18-C19-C20
31	c	518	DGD	C4A-C5A-C6A-C7A
22	C	503	CLA	C8-C10-C11-C12
22	c	503	CLA	C8-C10-C11-C12
29	a	614	LMG	C38-C39-C40-C41
32	l	103	LHG	C24-C25-C26-C27
25	B	601	SQD	C24-C25-C26-C27
25	b	601	SQD	C24-C25-C26-C27
29	A	614	LMG	C38-C39-C40-C41
32	D	407	LHG	C11-C10-C9-C8
32	d	407	LHG	C11-C10-C9-C8
32	L	102	LHG	C24-C25-C26-C27
25	B	601	SQD	C2-C1-O6-C44
25	b	601	SQD	C2-C1-O6-C44
29	A	614	LMG	C2-C1-O1-C7
29	a	614	LMG	C2-C1-O1-C7
31	H	102	DGD	CCA-CDA-CEA-CFA
31	h	102	DGD	CCA-CDA-CEA-CFA
22	b	605	CLA	C3-C5-C6-C7
25	D	411	SQD	C11-C10-C9-C8
25	d	411	SQD	C11-C10-C9-C8
25	B	601	SQD	C29-C30-C31-C32
25	b	601	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
22	B	611	CLA	C16-C17-C18-C19
22	b	611	CLA	C16-C17-C18-C19
22	B	614	CLA	C13-C15-C16-C17
22	b	614	CLA	C13-C15-C16-C17
25	B	601	SQD	C27-C28-C29-C30
22	B	605	CLA	C3-C5-C6-C7
22	C	510	CLA	O1D-CGD-O2D-CED
25	b	601	SQD	C27-C28-C29-C30
22	c	510	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
22	D	403	CLA	O1D-CGD-O2D-CED
22	d	403	CLA	O1D-CGD-O2D-CED
29	C	519	LMG	C19-C20-C21-C22
29	c	519	LMG	C19-C20-C21-C22
31	c	517	DGD	C5A-C6A-C7A-C8A
31	C	517	DGD	C5A-C6A-C7A-C8A
31	H	102	DGD	C5B-C6B-C7B-C8B
32	D	409	LHG	C27-C28-C29-C30
32	d	409	LHG	C27-C28-C29-C30
31	h	102	DGD	C5B-C6B-C7B-C8B
22	A	604	CLA	C11-C10-C8-C7
22	a	604	CLA	C11-C10-C8-C7
22	B	616	CLA	C12-C13-C15-C16
22	b	616	CLA	C12-C13-C15-C16
22	C	506	CLA	C6-C7-C8-C10
22	C	509	CLA	C6-C7-C8-C10
22	c	506	CLA	C6-C7-C8-C10
22	c	509	CLA	C6-C7-C8-C10
22	D	403	CLA	C12-C13-C15-C16
22	d	403	CLA	C11-C12-C13-C15
22	d	403	CLA	C12-C13-C15-C16
29	c	520	LMG	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C20
31	D	410	DGD	CDB-CEB-CFB-CGB
31	d	410	DGD	CDB-CEB-CFB-CGB
29	C	520	LMG	C16-C17-C18-C19
31	c	517	DGD	CBA-CCA-CDA-CEA
32	E	101	LHG	C10-C11-C12-C13
31	C	518	DGD	C9A-CAA-CBA-CCA
32	e	101	LHG	C10-C11-C12-C13
31	C	517	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
31	c	518	DGD	C9A-CAA-CBA-CCA
32	D	407	LHG	C26-C27-C28-C29
32	d	407	LHG	C26-C27-C28-C29
32	L	102	LHG	C31-C32-C33-C34
32	l	103	LHG	C31-C32-C33-C34
22	B	616	CLA	C16-C17-C18-C20
22	b	611	CLA	C8-C10-C11-C12
29	c	519	LMG	C12-C13-C14-C15
25	b	601	SQD	C9-C10-C11-C12
22	A	604	CLA	C11-C10-C8-C9
22	a	604	CLA	C11-C10-C8-C9
22	C	504	CLA	C14-C13-C15-C16
22	C	512	CLA	C11-C10-C8-C9
22	c	504	CLA	C14-C13-C15-C16
22	c	512	CLA	C11-C10-C8-C9
25	B	601	SQD	C9-C10-C11-C12
29	C	519	LMG	C12-C13-C14-C15
22	B	611	CLA	C8-C10-C11-C12
22	a	607	CLA	O1D-CGD-O2D-CED
31	D	410	DGD	O1G-C1G-C2G-O2G
31	d	410	DGD	O1G-C1G-C2G-O2G
32	E	101	LHG	O7-C5-C6-O8
32	e	101	LHG	O7-C5-C6-O8
22	A	607	CLA	O1D-CGD-O2D-CED
31	d	410	DGD	CBB-CCB-CDB-CEB
25	D	411	SQD	C28-C29-C30-C31
25	d	411	SQD	C28-C29-C30-C31
29	C	520	LMG	C33-C34-C35-C36
31	D	410	DGD	CBB-CCB-CDB-CEB
29	A	614	LMG	O1-C7-C8-C9
29	a	614	LMG	O1-C7-C8-C9
29	c	520	LMG	C33-C34-C35-C36
22	C	513	CLA	C3-C5-C6-C7
22	c	513	CLA	C3-C5-C6-C7
22	B	608	CLA	CAD-CBD-CGD-O2D
22	b	608	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
29	B	620	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	b	619	LMG	C10-C11-C12-C13
29	C	520	LMG	C10-C11-C12-C13
31	c	517	DGD	CDA-CEA-CFA-CGA
29	a	614	LMG	O10-C28-O8-C9
31	C	517	DGD	CDA-CEA-CFA-CGA
29	z	101	LMG	C17-C18-C19-C20
25	b	621	SQD	C19-C20-C21-C22
25	l	102	SQD	C19-C20-C21-C22
22	B	602	CLA	CAD-CBD-CGD-O1D
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	611	CLA	CHA-CBD-CGD-O1D
22	b	602	CLA	CAD-CBD-CGD-O1D
22	b	606	CLA	CAD-CBD-CGD-O1D
22	b	611	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
32	D	407	LHG	C3-O3-P-O4
32	d	407	LHG	C3-O3-P-O4
29	Z	101	LMG	C17-C18-C19-C20
29	c	520	LMG	C10-C11-C12-C13
29	A	614	LMG	O10-C28-O8-C9
31	C	516	DGD	CBA-CCA-CDA-CEA
24	D	404	BCR	C23-C24-C25-C30
24	d	404	BCR	C23-C24-C25-C30
31	c	516	DGD	CBA-CCA-CDA-CEA
24	A	608	BCR	C36-C18-C19-C20
24	a	608	BCR	C36-C18-C19-C20
32	D	409	LHG	C2-C3-O3-P
32	d	409	LHG	C2-C3-O3-P
25	L	101	SQD	C13-C14-C15-C16
32	D	405	LHG	C33-C34-C35-C36
32	d	405	LHG	C33-C34-C35-C36
29	C	519	LMG	C13-C14-C15-C16
29	c	519	LMG	C13-C14-C15-C16
32	L	102	LHG	C26-C27-C28-C29
32	l	103	LHG	C26-C27-C28-C29
25	l	101	SQD	C13-C14-C15-C16
25	A	609	SQD	C23-C24-C25-C26
29	B	620	LMG	O9-C10-O7-C8
31	c	516	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
31	h	102	DGD	CDA-CEA-CFA-CGA
25	b	621	SQD	C46-C45-O47-C7
25	l	102	SQD	C46-C45-O47-C7
23	A	605	PHO	C4-C3-C5-C6
31	C	516	DGD	CDA-CEA-CFA-CGA
31	H	102	DGD	CDA-CEA-CFA-CGA
25	a	609	SQD	C23-C24-C25-C26
22	B	611	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
22	C	512	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C19
29	z	101	LMG	C14-C15-C16-C17
29	Z	101	LMG	C14-C15-C16-C17
22	A	607	CLA	C11-C10-C8-C9
22	a	607	CLA	C11-C10-C8-C9
22	B	616	CLA	C11-C10-C8-C9
22	B	617	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	b	617	CLA	C6-C7-C8-C9
22	C	513	CLA	C6-C7-C8-C9
22	c	513	CLA	C6-C7-C8-C9
22	B	617	CLA	C6-C7-C8-C10
22	b	617	CLA	C6-C7-C8-C10
22	C	506	CLA	C12-C13-C15-C16
22	c	506	CLA	C12-C13-C15-C16
22	D	403	CLA	C11-C12-C13-C15
29	b	619	LMG	O9-C10-O7-C8
22	C	502	CLA	C16-C17-C18-C19
22	c	502	CLA	C16-C17-C18-C19
32	L	102	LHG	C25-C26-C27-C28
29	B	620	LMG	C28-C29-C30-C31
31	C	517	DGD	C2E-C1E-O5D-C6D
31	c	517	DGD	C2E-C1E-O5D-C6D
23	a	605	PHO	C4-C3-C5-C6
29	b	619	LMG	C28-C29-C30-C31
23	A	605	PHO	C2-C3-C5-C6
23	a	605	PHO	C2-C3-C5-C6
29	a	614	LMG	C30-C31-C32-C33
32	l	103	LHG	C25-C26-C27-C28
22	B	616	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C19
29	A	614	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	O2G-C1B-C2B-C3B
31	h	102	DGD	O2G-C1B-C2B-C3B
25	b	621	SQD	C14-C15-C16-C17
25	l	102	SQD	C14-C15-C16-C17
29	B	620	LMG	C11-C10-O7-C8
29	b	619	LMG	C11-C10-O7-C8
29	A	614	LMG	C29-C28-O8-C9
29	a	614	LMG	C29-C28-O8-C9
31	C	516	DGD	C1B-C2B-C3B-C4B
31	c	516	DGD	C1B-C2B-C3B-C4B
29	C	520	LMG	C39-C40-C41-C42
29	c	520	LMG	C39-C40-C41-C42
22	B	602	CLA	C6-C7-C8-C9
22	B	616	CLA	C14-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C9
22	b	616	CLA	C14-C13-C15-C16
22	C	506	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
29	d	406	LMG	C32-C33-C34-C35
32	l	103	LHG	C11-C10-C9-C8
29	D	406	LMG	C32-C33-C34-C35
32	L	102	LHG	C11-C10-C9-C8
29	C	520	LMG	C29-C28-O8-C9
29	c	520	LMG	C29-C28-O8-C9
24	K	101	BCR	C15-C16-C17-C18
24	k	101	BCR	C15-C16-C17-C18
33	F	101	HEM	C4C-C3C-CAC-CBC
33	f	101	HEM	C4C-C3C-CAC-CBC
33	V	201	HEM	C4C-C3C-CAC-CBC
33	v	201	HEM	C4C-C3C-CAC-CBC
22	A	607	CLA	C12-C13-C15-C16
22	a	607	CLA	C12-C13-C15-C16
29	C	520	LMG	O10-C28-O8-C9
29	c	520	LMG	O10-C28-O8-C9
31	C	518	DGD	C7A-C8A-C9A-CAA
31	c	518	DGD	C7A-C8A-C9A-CAA
22	C	512	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C20
22	C	510	CLA	O1A-CGA-O2A-C1
22	c	510	CLA	O1A-CGA-O2A-C1
29	C	520	LMG	O1-C7-C8-O7
29	c	520	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
29	C	519	LMG	C30-C31-C32-C33
29	c	519	LMG	C30-C31-C32-C33
22	c	510	CLA	C8-C10-C11-C12
29	D	406	LMG	C34-C35-C36-C37
22	A	603	CLA	C2C-C3C-CAC-CBC
22	C	510	CLA	C8-C10-C11-C12
22	a	603	CLA	C2C-C3C-CAC-CBC
29	d	406	LMG	C34-C35-C36-C37
22	D	401	CLA	C2-C1-O2A-CGA
22	d	401	CLA	C2-C1-O2A-CGA
24	B	622	BCR	C13-C14-C15-C16
29	Z	101	LMG	O6-C5-C6-O5
29	z	101	LMG	O6-C5-C6-O5
22	B	611	CLA	C13-C15-C16-C17
22	b	611	CLA	C13-C15-C16-C17
32	E	101	LHG	C17-C18-C19-C20
32	e	101	LHG	C17-C18-C19-C20
28	A	613	PL9	C2-C3-C7-C8
28	a	613	PL9	C2-C3-C7-C8
28	D	408	PL9	C39-C41-C42-C43
28	d	408	PL9	C39-C41-C42-C43
31	C	518	DGD	CAB-CBB-CCB-CDB
22	B	611	CLA	C14-C13-C15-C16
22	b	611	CLA	C14-C13-C15-C16
31	C	517	DGD	C4B-C5B-C6B-C7B
31	c	518	DGD	CAB-CBB-CCB-CDB
25	B	601	SQD	C10-C11-C12-C13
25	b	601	SQD	C10-C11-C12-C13
31	c	517	DGD	C4B-C5B-C6B-C7B
31	c	516	DGD	C2B-C3B-C4B-C5B
31	C	516	DGD	C2B-C3B-C4B-C5B
24	b	622	BCR	C13-C14-C15-C16
22	B	606	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
22	C	513	CLA	C16-C17-C18-C19
22	c	513	CLA	C16-C17-C18-C19
32	E	101	LHG	C9-C10-C11-C12
32	e	101	LHG	C9-C10-C11-C12
24	B	618	BCR	C5-C6-C7-C8
24	H	101	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C26
24	T	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	CBA-CGA-O2A-C1
31	c	516	DGD	CBB-CCB-CDB-CEB
31	C	516	DGD	CBB-CCB-CDB-CEB
32	D	409	LHG	C28-C29-C30-C31
33	F	101	HEM	CAD-CBD-CGD-O1D
33	f	101	HEM	CAD-CBD-CGD-O1D
22	C	513	CLA	C4-C3-C5-C6
22	c	513	CLA	C4-C3-C5-C6
32	d	409	LHG	C28-C29-C30-C31
22	c	510	CLA	CBA-CGA-O2A-C1
22	B	617	CLA	C13-C15-C16-C17
22	B	611	CLA	C12-C13-C15-C16
22	b	611	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C7
22	c	502	CLA	C12-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C7
29	C	520	LMG	C36-C37-C38-C39
29	c	520	LMG	C36-C37-C38-C39
22	b	617	CLA	C13-C15-C16-C17
25	A	609	SQD	O6-C44-C45-O47
25	a	609	SQD	O6-C44-C45-O47
31	H	102	DGD	O1G-C1G-C2G-O2G
31	h	102	DGD	O1G-C1G-C2G-O2G
29	B	620	LMG	C36-C37-C38-C39
29	b	619	LMG	C36-C37-C38-C39
33	V	201	HEM	CAD-CBD-CGD-O2D
33	v	201	HEM	CAD-CBD-CGD-O2D
22	C	507	CLA	C4-C3-C5-C6
22	c	507	CLA	C4-C3-C5-C6
24	A	608	BCR	C17-C18-C19-C20
24	a	608	BCR	C17-C18-C19-C20
31	H	102	DGD	CAA-CBA-CCA-CDA
31	h	102	DGD	CAA-CBA-CCA-CDA
22	A	604	CLA	C6-C7-C8-C9
22	a	604	CLA	C6-C7-C8-C9
29	C	519	LMG	C22-C23-C24-C25
29	c	519	LMG	C22-C23-C24-C25
33	v	201	HEM	CAD-CBD-CGD-O1D
33	f	101	HEM	CAD-CBD-CGD-O2D
33	V	201	HEM	CAD-CBD-CGD-O1D
31	H	102	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
31	h	102	DGD	O1G-C1G-C2G-C3G
33	F	101	HEM	CAD-CBD-CGD-O2D
22	C	501	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
22	b	616	CLA	C4B-C3B-CAB-CBB
23	A	606	PHO	CHA-CBD-CGD-O1D
23	a	606	PHO	CHA-CBD-CGD-O1D
32	E	101	LHG	O6-C4-C5-C6
32	e	101	LHG	O6-C4-C5-C6
22	a	607	CLA	C4-C3-C5-C6
31	C	516	DGD	O6E-C1E-O5D-C6D
31	c	516	DGD	O6E-C1E-O5D-C6D
31	c	517	DGD	O6E-C1E-O5D-C6D
29	C	520	LMG	C19-C20-C21-C22
32	D	405	LHG	C31-C32-C33-C34
29	c	520	LMG	C19-C20-C21-C22
32	d	405	LHG	C31-C32-C33-C34
22	B	604	CLA	C6-C7-C8-C9
22	b	604	CLA	C6-C7-C8-C9
22	b	604	CLA	C13-C15-C16-C17
25	D	411	SQD	C45-C44-O6-C1
25	d	411	SQD	C45-C44-O6-C1
31	D	410	DGD	C2G-C3G-O3G-C1D
31	d	410	DGD	C2G-C3G-O3G-C1D
22	B	604	CLA	C13-C15-C16-C17
22	C	509	CLA	C2-C1-O2A-CGA
22	c	509	CLA	C2-C1-O2A-CGA
31	C	518	DGD	O1A-C1A-O1G-C1G
31	c	518	DGD	O1A-C1A-O1G-C1G
31	C	518	DGD	C2A-C1A-O1G-C1G
31	c	518	DGD	C2A-C1A-O1G-C1G
24	A	608	BCR	C18-C19-C20-C21
24	a	608	BCR	C18-C19-C20-C21
22	B	602	CLA	CAA-CBA-CGA-O1A
22	b	602	CLA	CAA-CBA-CGA-O1A
29	b	619	LMG	C35-C36-C37-C38
29	C	519	LMG	C31-C32-C33-C34
29	B	620	LMG	C35-C36-C37-C38
29	c	519	LMG	C31-C32-C33-C34
22	A	607	CLA	C4-C3-C5-C6
32	D	407	LHG	C13-C14-C15-C16
22	B	607	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C16-C17-C18-C20
32	d	407	LHG	C13-C14-C15-C16
31	C	517	DGD	O6E-C1E-O5D-C6D
32	E	101	LHG	C4-C5-C6-O8
32	e	101	LHG	C4-C5-C6-O8
25	l	102	SQD	C33-C34-C35-C36
25	b	621	SQD	C33-C34-C35-C36
24	h	101	BCR	C9-C10-C11-C12
22	C	512	CLA	CAA-CBA-CGA-O2A
25	l	102	SQD	C17-C18-C19-C20
25	b	621	SQD	C17-C18-C19-C20
31	D	410	DGD	O2G-C2G-C3G-O3G
31	d	410	DGD	O2G-C2G-C3G-O3G
24	B	619	BCR	C14-C15-C16-C17
24	b	618	BCR	C14-C15-C16-C17
22	B	607	CLA	C11-C12-C13-C14
22	b	607	CLA	C11-C12-C13-C14
31	C	518	DGD	O6D-C5D-C6D-O5D
31	c	518	DGD	O6D-C5D-C6D-O5D
22	c	512	CLA	CAA-CBA-CGA-O2A
22	a	607	CLA	O1A-CGA-O2A-C1
22	D	402	CLA	C4C-C3C-CAC-CBC
22	A	607	CLA	O1A-CGA-O2A-C1
22	A	604	CLA	C6-C7-C8-C10
22	a	604	CLA	C6-C7-C8-C10
22	B	604	CLA	C6-C7-C8-C10
22	B	615	CLA	C11-C10-C8-C7
22	b	604	CLA	C6-C7-C8-C10
22	b	615	CLA	C11-C10-C8-C7
22	C	504	CLA	C11-C12-C13-C15
22	c	504	CLA	C11-C12-C13-C15
22	D	401	CLA	C12-C13-C15-C16
22	d	401	CLA	C12-C13-C15-C16
22	d	402	CLA	C4C-C3C-CAC-CBC
22	B	608	CLA	C2B-C3B-CAB-CBB
22	B	614	CLA	C2B-C3B-CAB-CBB
22	b	608	CLA	C2B-C3B-CAB-CBB
22	b	614	CLA	C2B-C3B-CAB-CBB
22	D	401	CLA	C2B-C3B-CAB-CBB
22	d	401	CLA	C2B-C3B-CAB-CBB
24	H	101	BCR	C23-C24-C25-C30
24	h	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
29	B	620	LMG	C12-C13-C14-C15
29	b	619	LMG	C12-C13-C14-C15
29	A	614	LMG	O8-C28-C29-C30
29	a	614	LMG	O8-C28-C29-C30
32	D	405	LHG	C34-C35-C36-C37
32	d	405	LHG	C34-C35-C36-C37
25	l	101	SQD	O48-C23-C24-C25
32	e	101	LHG	O7-C7-C8-C9
24	H	101	BCR	C9-C10-C11-C12
22	C	513	CLA	C16-C17-C18-C20
22	c	513	CLA	C16-C17-C18-C20
25	L	101	SQD	O48-C23-C24-C25
32	E	101	LHG	O7-C7-C8-C9
25	A	609	SQD	C18-C19-C20-C21
25	a	609	SQD	C18-C19-C20-C21
22	B	606	CLA	C13-C15-C16-C17
22	b	606	CLA	C13-C15-C16-C17
22	D	403	CLA	C11-C12-C13-C14
22	d	403	CLA	C11-C12-C13-C14
22	B	602	CLA	C4B-C3B-CAB-CBB
22	B	616	CLA	C4B-C3B-CAB-CBB
22	b	602	CLA	C4B-C3B-CAB-CBB
32	D	409	LHG	C33-C34-C35-C36
32	d	409	LHG	C33-C34-C35-C36
31	D	410	DGD	O1G-C1A-C2A-C3A
29	C	520	LMG	O7-C8-C9-O8
29	c	520	LMG	O7-C8-C9-O8
24	K	102	BCR	C9-C10-C11-C12
24	k	102	BCR	C9-C10-C11-C12
31	C	518	DGD	O1G-C1A-C2A-C3A
31	c	518	DGD	O1G-C1A-C2A-C3A
31	d	410	DGD	O1G-C1A-C2A-C3A
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C12-C13-C15
22	c	505	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C12-C13-C15
25	b	601	SQD	C11-C12-C13-C14
25	B	601	SQD	C11-C12-C13-C14
22	a	603	CLA	C4C-C3C-CAC-CBC
32	D	409	LHG	C19-C20-C21-C22
32	d	409	LHG	C19-C20-C21-C22
22	A	603	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	b	621	SQD	C45-C46-O48-C23
25	l	102	SQD	C45-C46-O48-C23
29	C	520	LMG	C32-C33-C34-C35
29	c	520	LMG	C32-C33-C34-C35
28	A	613	PL9	C26-C27-C28-C29
28	a	613	PL9	C26-C27-C28-C29
22	c	512	CLA	CAA-CBA-CGA-O1A
22	A	607	CLA	CBA-CGA-O2A-C1
22	a	607	CLA	CBA-CGA-O2A-C1
22	C	504	CLA	C11-C10-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	506	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C10-C8-C9
22	c	505	CLA	C14-C13-C15-C16
22	c	506	CLA	C14-C13-C15-C16
22	c	513	CLA	C11-C12-C13-C14
22	D	403	CLA	C14-C13-C15-C16
22	d	403	CLA	C14-C13-C15-C16
22	C	512	CLA	CAA-CBA-CGA-O1A
32	L	102	LHG	C5-C6-O8-C23
32	l	103	LHG	C5-C6-O8-C23
22	C	507	CLA	C2-C3-C5-C6
22	c	507	CLA	C2-C3-C5-C6
22	B	613	CLA	O1A-CGA-O2A-C1
22	b	613	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	C8-C10-C11-C12
22	b	613	CLA	C8-C10-C11-C12
22	b	616	CLA	C15-C16-C17-C18
31	C	518	DGD	O1A-C1A-C2A-C3A
31	D	410	DGD	O1A-C1A-C2A-C3A
31	d	410	DGD	O1A-C1A-C2A-C3A
22	B	616	CLA	C15-C16-C17-C18
25	A	609	SQD	C45-C44-O6-C1
25	a	609	SQD	C45-C44-O6-C1
31	C	516	DGD	C5D-C6D-O5D-C1E
31	c	516	DGD	C5D-C6D-O5D-C1E
25	L	101	SQD	O10-C23-C24-C25
25	l	101	SQD	O10-C23-C24-C25
31	c	518	DGD	O1A-C1A-C2A-C3A
32	D	405	LHG	C11-C10-C9-C8
32	d	405	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C15-C16-C17-C18
22	c	506	CLA	C15-C16-C17-C18
29	A	614	LMG	O10-C28-C29-C30
32	E	101	LHG	O9-C7-C8-C9
32	e	101	LHG	O9-C7-C8-C9
22	A	603	CLA	CAD-CBD-CGD-O2D
22	a	603	CLA	CAD-CBD-CGD-O2D
22	c	504	CLA	CAD-CBD-CGD-O2D
23	A	606	PHO	CAD-CBD-CGD-O2D
23	a	606	PHO	CAD-CBD-CGD-O2D
29	a	614	LMG	O10-C28-C29-C30
31	C	517	DGD	C6A-C7A-C8A-C9A
31	c	516	DGD	C3A-C4A-C5A-C6A
31	c	517	DGD	C6A-C7A-C8A-C9A
22	B	602	CLA	C2-C1-O2A-CGA
22	b	602	CLA	C2-C1-O2A-CGA
31	C	516	DGD	C3A-C4A-C5A-C6A
31	C	516	DGD	C9A-CAA-CBA-CCA
31	c	516	DGD	C9A-CAA-CBA-CCA
22	B	602	CLA	C8-C10-C11-C12
22	b	602	CLA	C8-C10-C11-C12
29	a	614	LMG	C35-C36-C37-C38
29	A	614	LMG	C35-C36-C37-C38

There are no ring outliers.

110 monomers are involved in 241 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	609	SQD	2	0
28	a	613	PL9	8	0
22	D	403	CLA	2	0
25	l	101	SQD	9	0
22	B	614	CLA	3	0
22	b	616	CLA	3	0
32	d	409	LHG	12	0
22	C	509	CLA	3	0
22	C	503	CLA	2	0
22	c	505	CLA	2	0
22	A	607	CLA	2	0
22	c	512	CLA	2	0
22	B	612	CLA	1	0
22	c	509	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	518	DGD	1	0
22	d	403	CLA	2	0
22	B	617	CLA	4	0
22	B	603	CLA	1	0
22	C	512	CLA	2	0
22	a	607	CLA	1	0
29	a	614	LMG	3	0
22	b	606	CLA	3	0
33	f	101	HEM	1	0
22	C	501	CLA	2	0
31	d	410	DGD	3	0
28	A	613	PL9	8	0
32	L	102	LHG	1	0
29	C	519	LMG	1	0
31	C	517	DGD	2	0
22	C	507	CLA	1	0
24	D	404	BCR	3	0
29	z	101	LMG	1	0
23	A	605	PHO	1	0
24	a	608	BCR	1	0
33	v	201	HEM	9	0
25	B	601	SQD	4	0
22	b	603	CLA	1	0
22	c	503	CLA	2	0
22	c	506	CLA	2	0
31	C	516	DGD	2	0
29	c	519	LMG	1	0
22	A	603	CLA	5	0
22	C	508	CLA	4	0
31	c	517	DGD	2	0
22	c	504	CLA	1	0
22	c	507	CLA	1	0
29	Z	101	LMG	1	0
32	D	409	LHG	13	0
22	B	615	CLA	3	0
22	a	604	CLA	1	0
31	c	516	DGD	2	0
24	k	102	BCR	1	0
22	c	508	CLA	4	0
22	C	505	CLA	2	0
24	t	101	BCR	7	0
29	B	620	LMG	3	0

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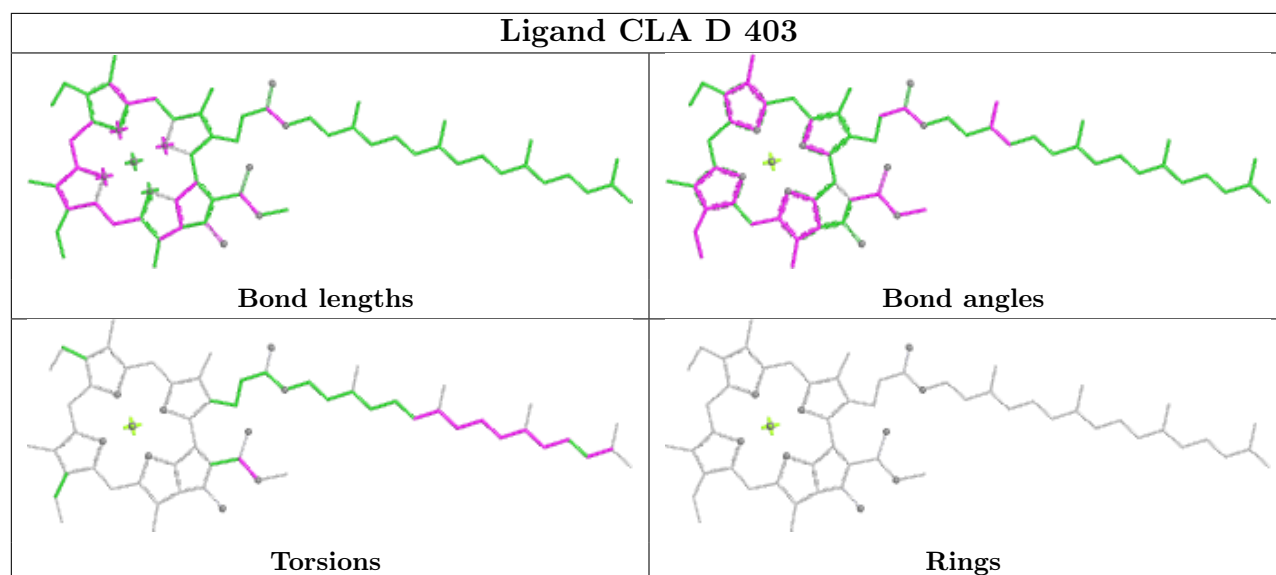
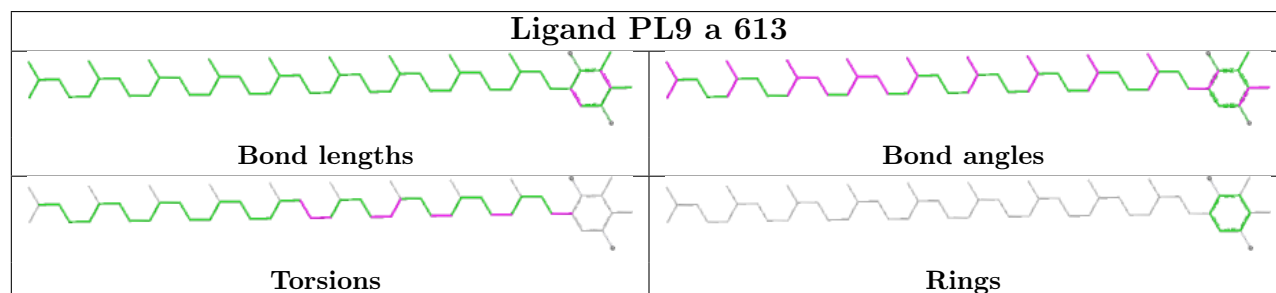
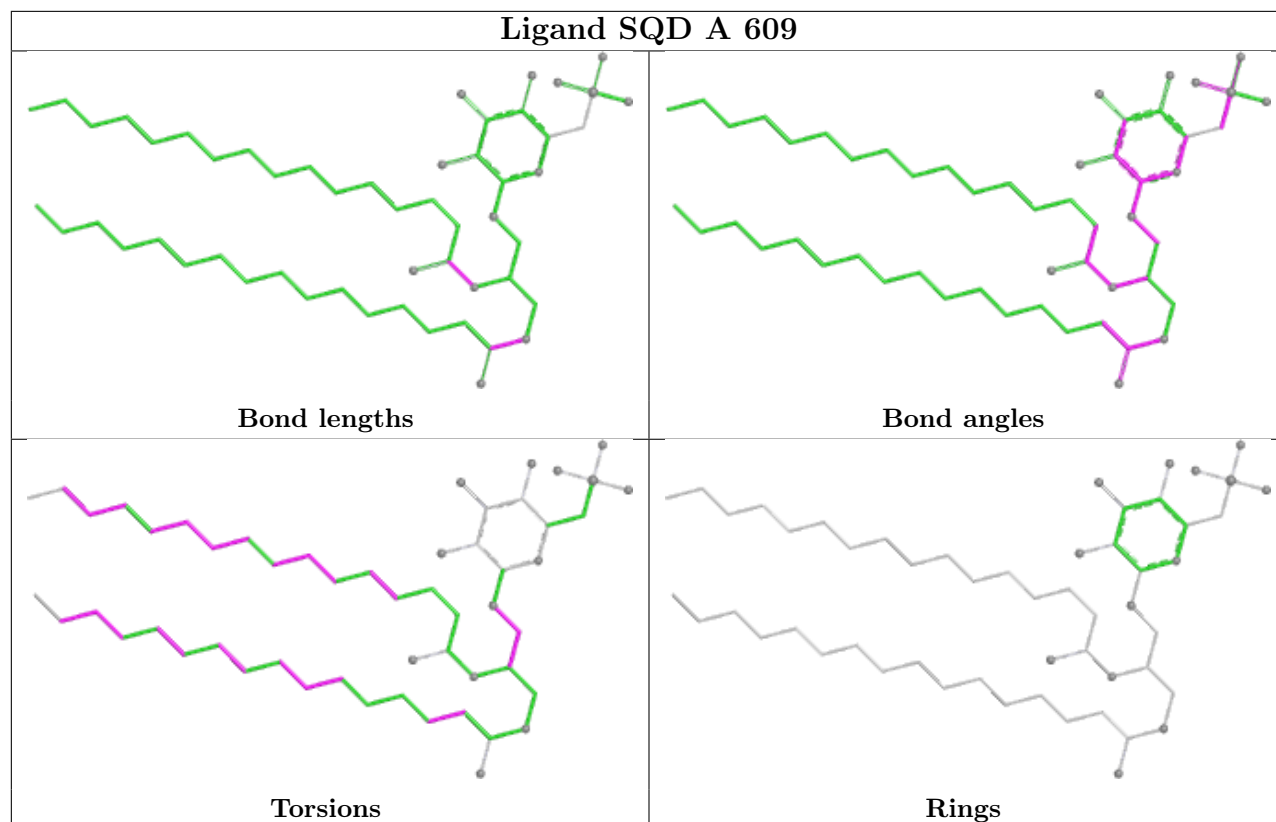
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	V	201	HEM	9	0
22	B	606	CLA	4	0
22	B	604	CLA	2	0
23	A	606	PHO	3	0
24	B	618	BCR	2	0
25	b	621	SQD	7	0
29	D	406	LMG	2	0
22	C	506	CLA	2	0
22	C	510	CLA	3	0
31	C	518	DGD	1	0
22	b	611	CLA	3	0
24	b	618	BCR	1	0
22	d	402	CLA	4	0
31	D	410	DGD	3	0
22	B	605	CLA	2	0
24	b	622	BCR	2	0
22	b	617	CLA	4	0
22	b	614	CLA	3	0
22	a	603	CLA	5	0
24	d	404	BCR	3	0
22	B	611	CLA	4	0
29	A	614	LMG	3	0
29	b	619	LMG	3	0
22	C	511	CLA	1	0
22	b	615	CLA	3	0
22	B	613	CLA	1	0
24	B	619	BCR	1	0
31	h	102	DGD	1	0
22	b	605	CLA	1	0
33	F	101	HEM	1	0
22	b	604	CLA	2	0
24	B	622	BCR	3	0
22	c	511	CLA	1	0
22	c	501	CLA	2	0
23	a	606	PHO	4	0
24	T	101	BCR	1	0
32	e	101	LHG	2	0
22	c	510	CLA	3	0
25	a	609	SQD	2	0
22	D	402	CLA	4	0
25	L	101	SQD	6	0
22	c	502	CLA	3	0

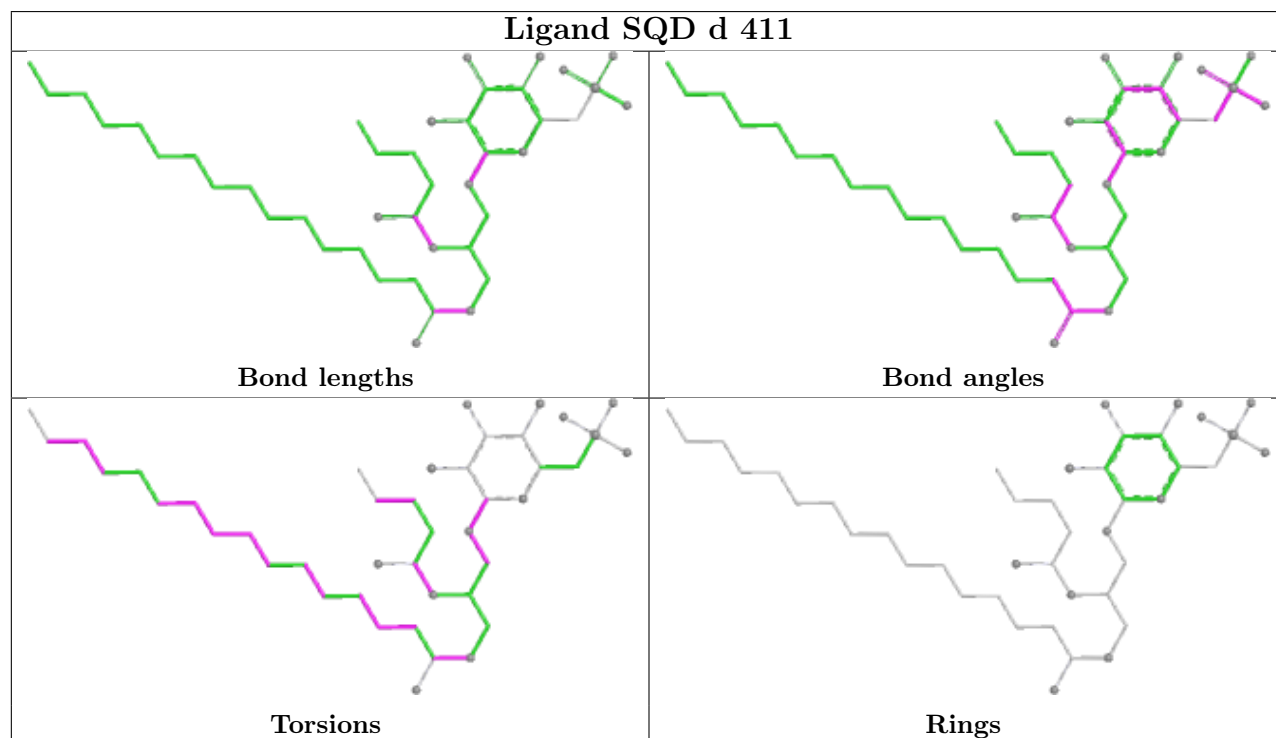
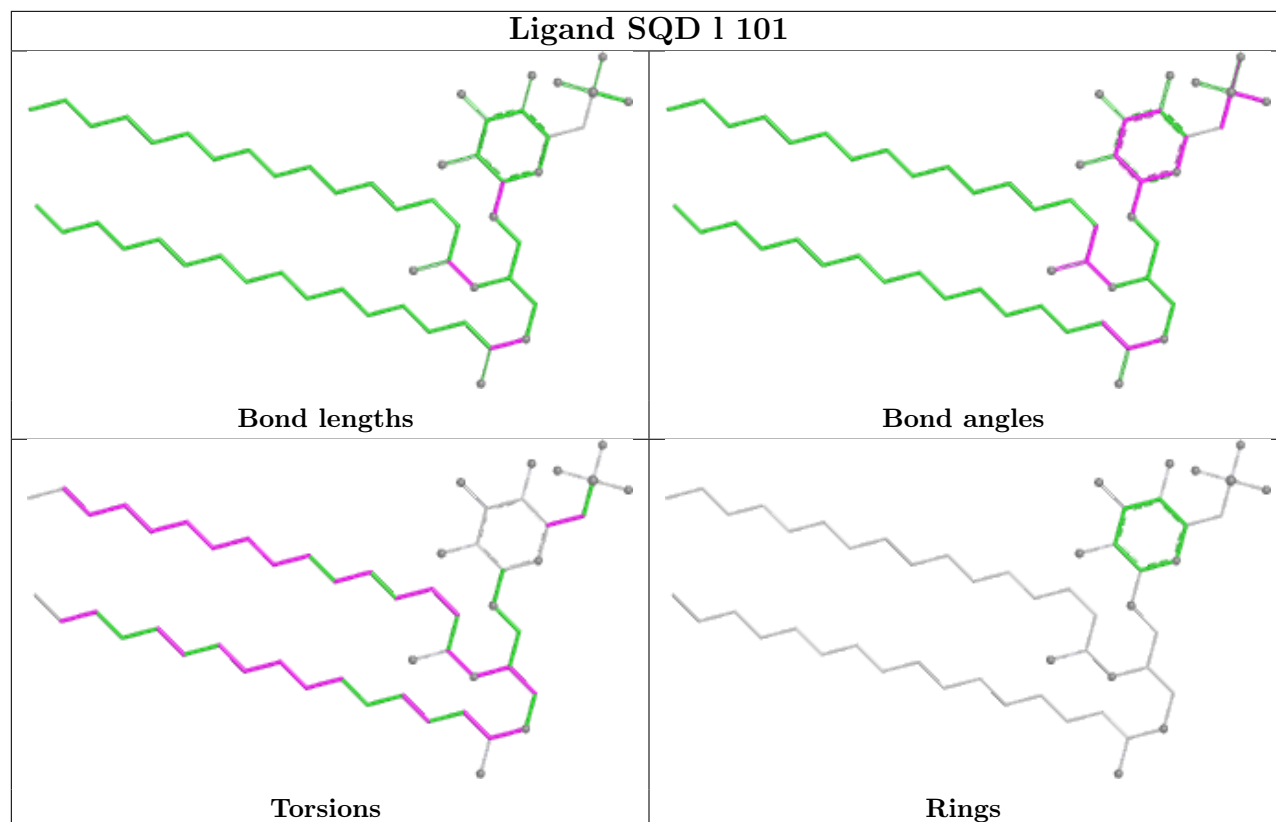
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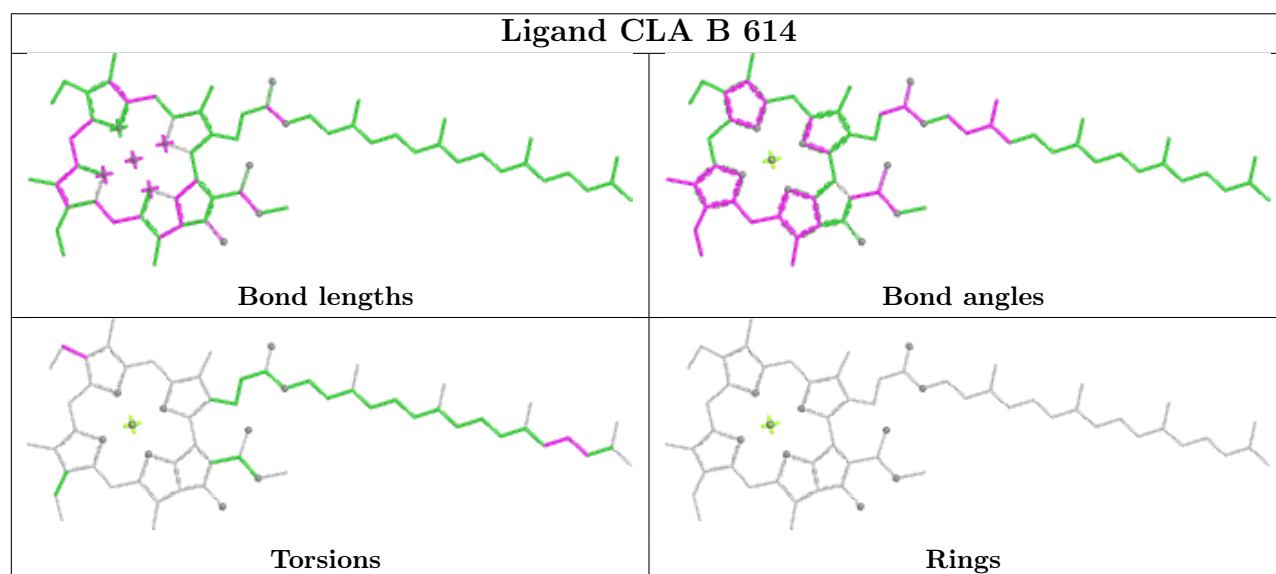
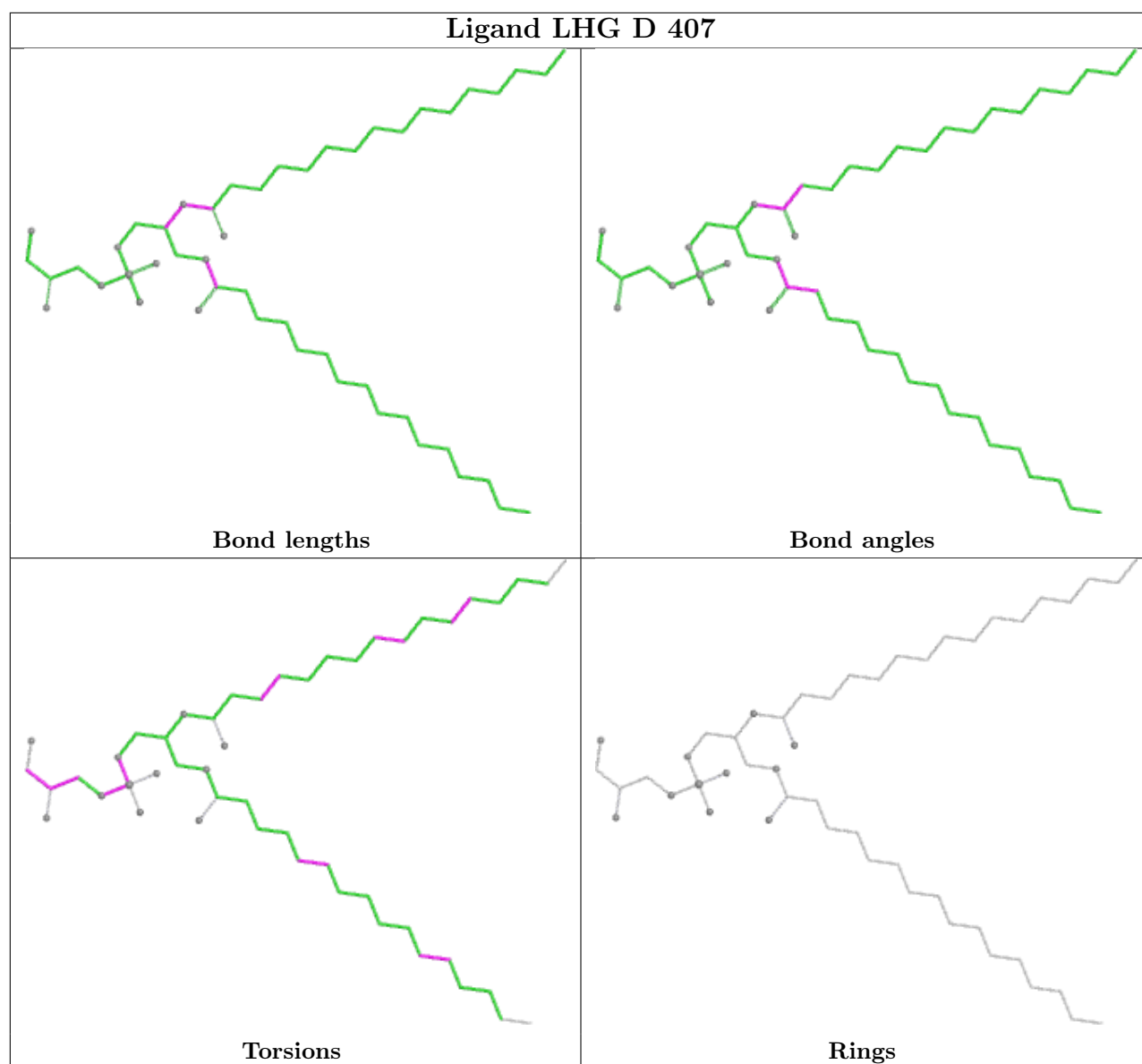
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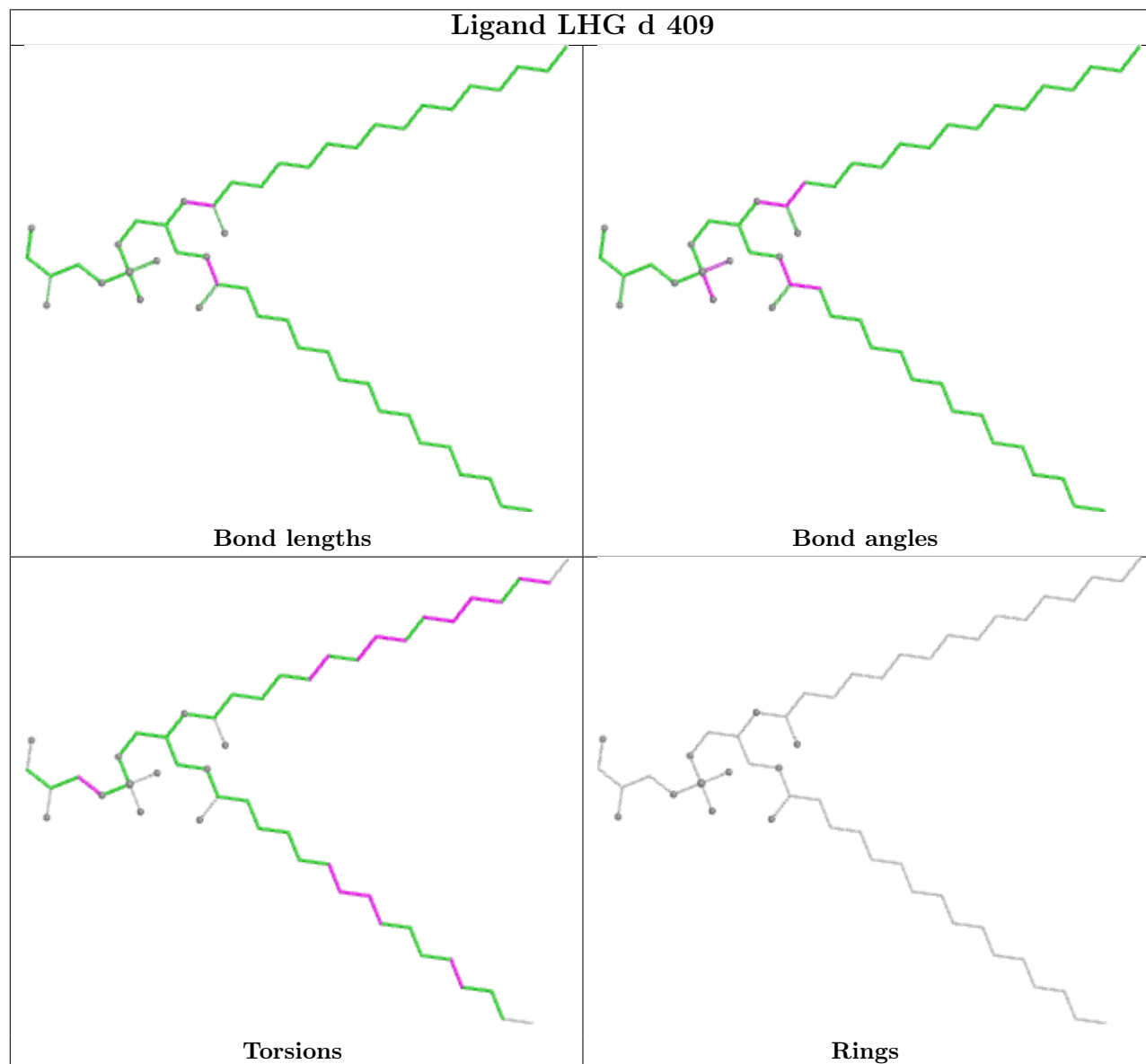
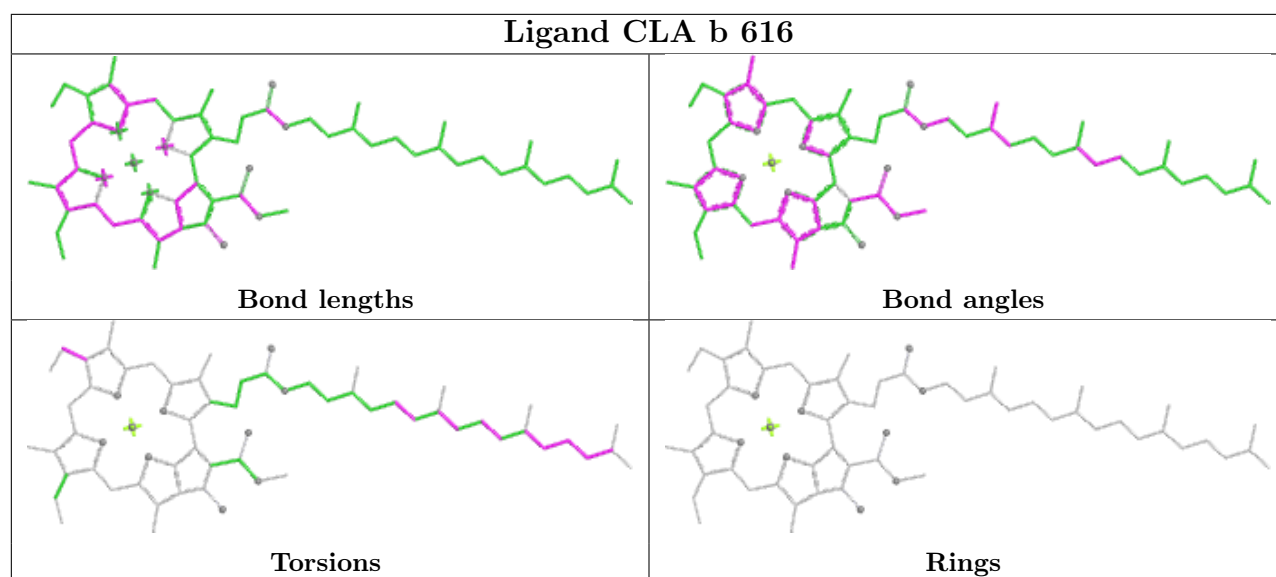
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	H	102	DGD	1	0
22	C	502	CLA	3	0
24	H	101	BCR	1	0
29	d	406	LMG	2	0
22	A	604	CLA	1	0
22	B	616	CLA	3	0
25	l	102	SQD	8	0
32	E	101	LHG	1	0
22	C	504	CLA	2	0
24	T	102	BCR	2	0
22	b	613	CLA	1	0
24	K	102	BCR	1	0

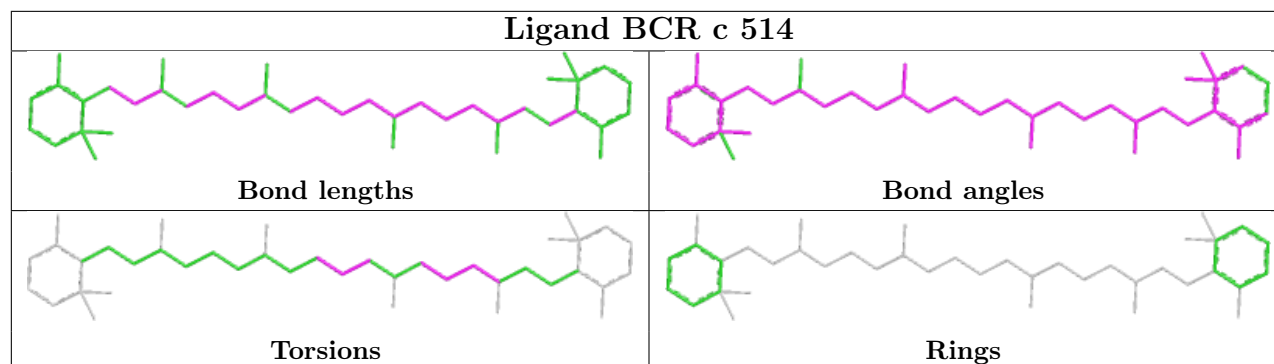
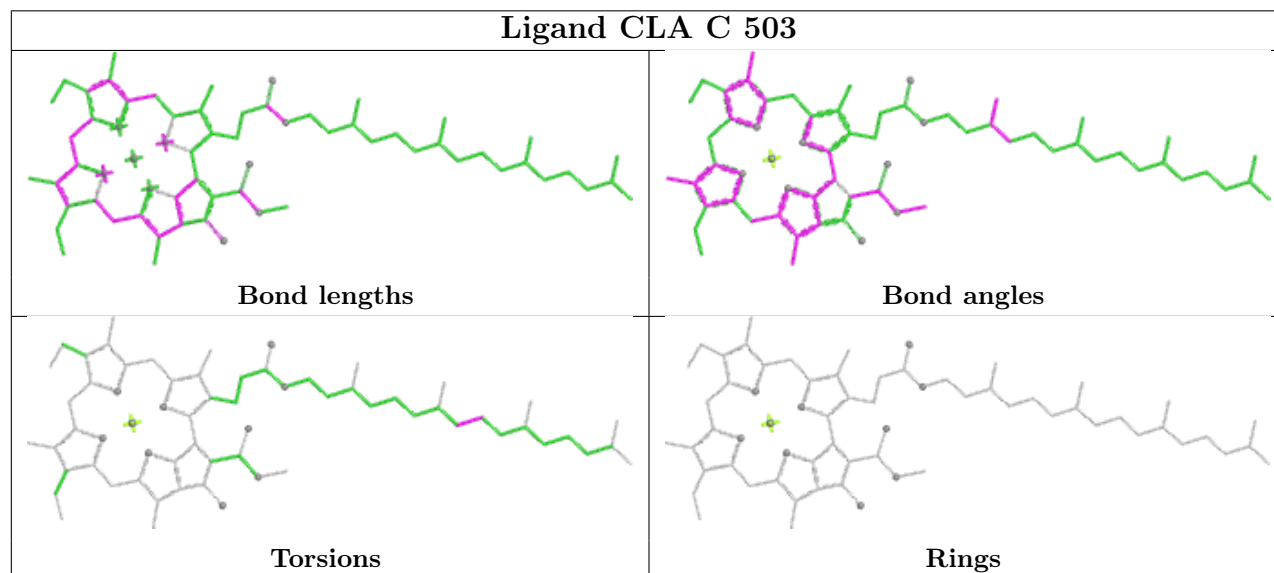
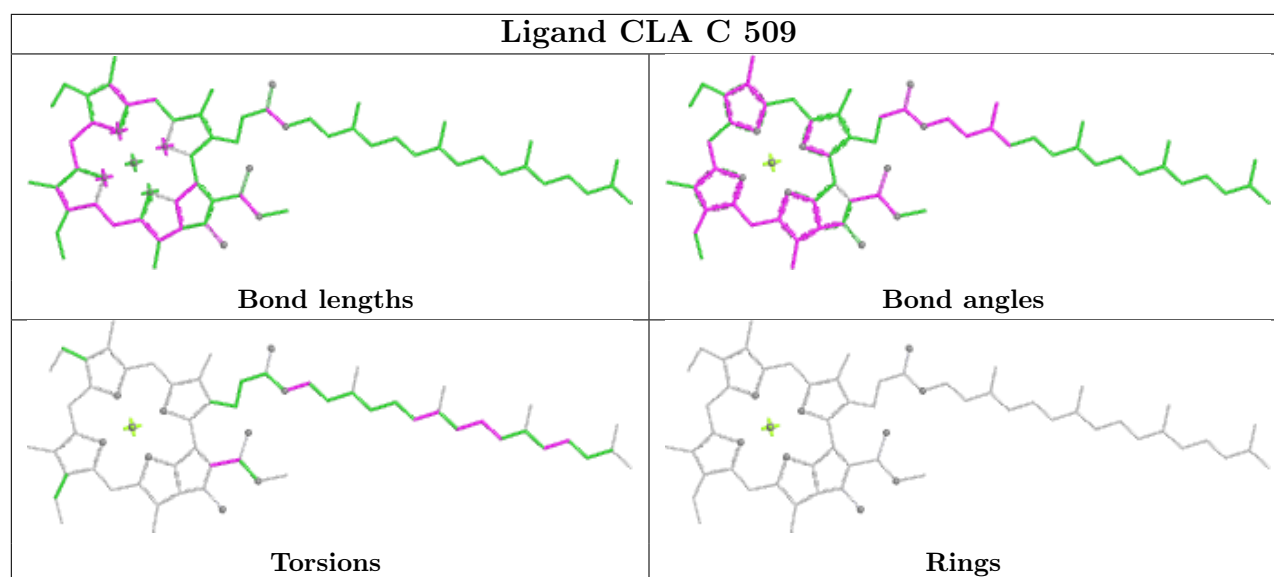
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



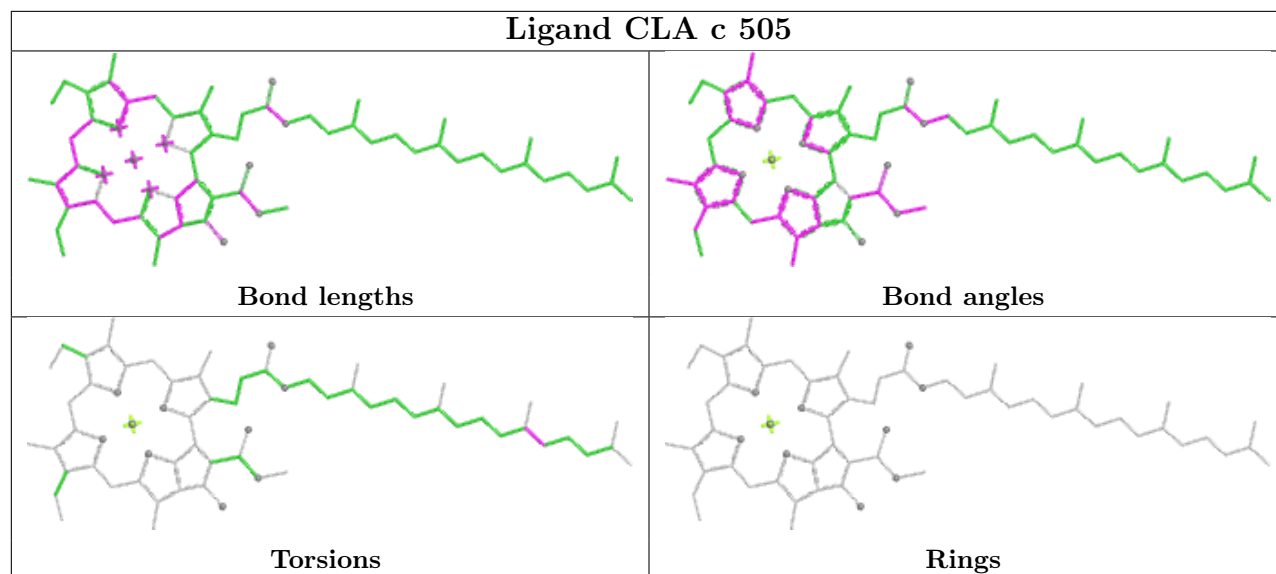




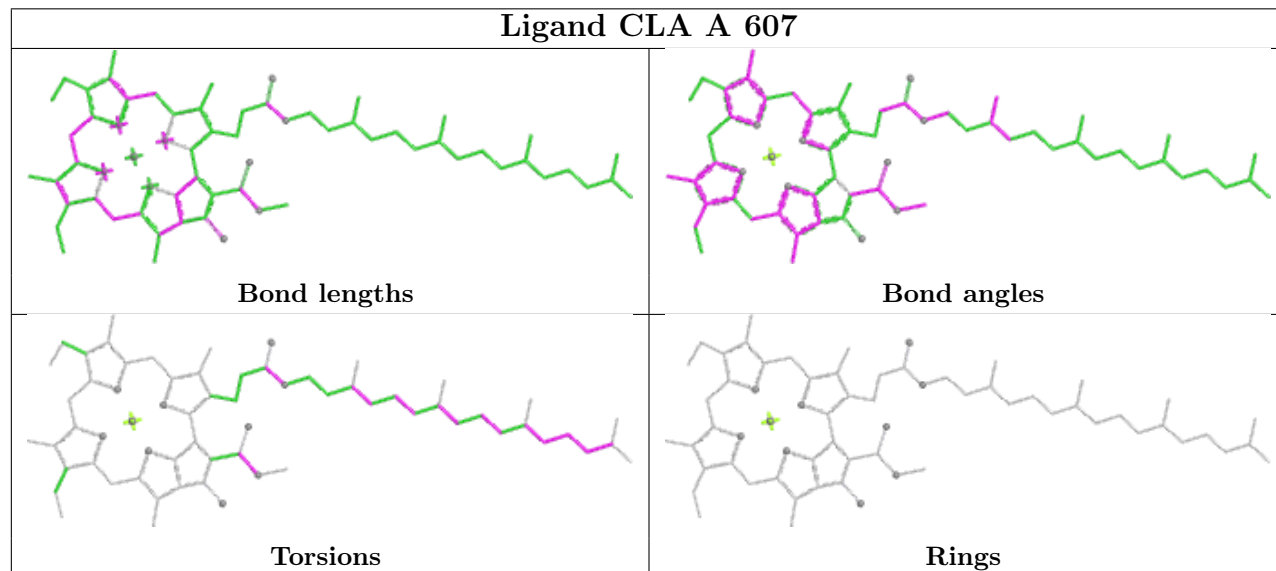


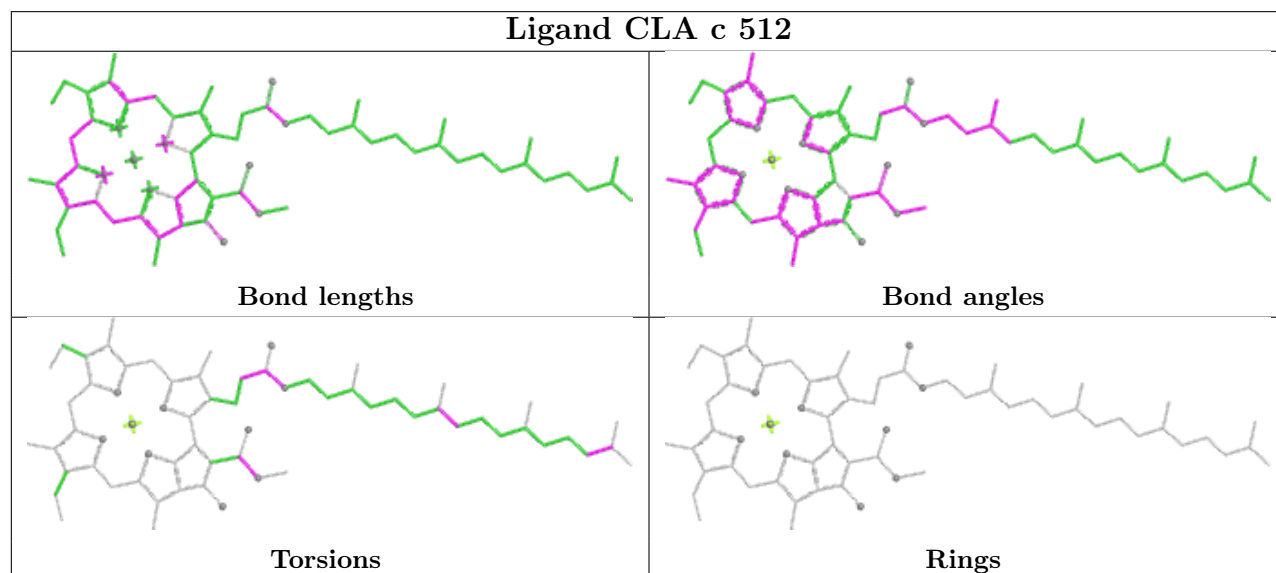
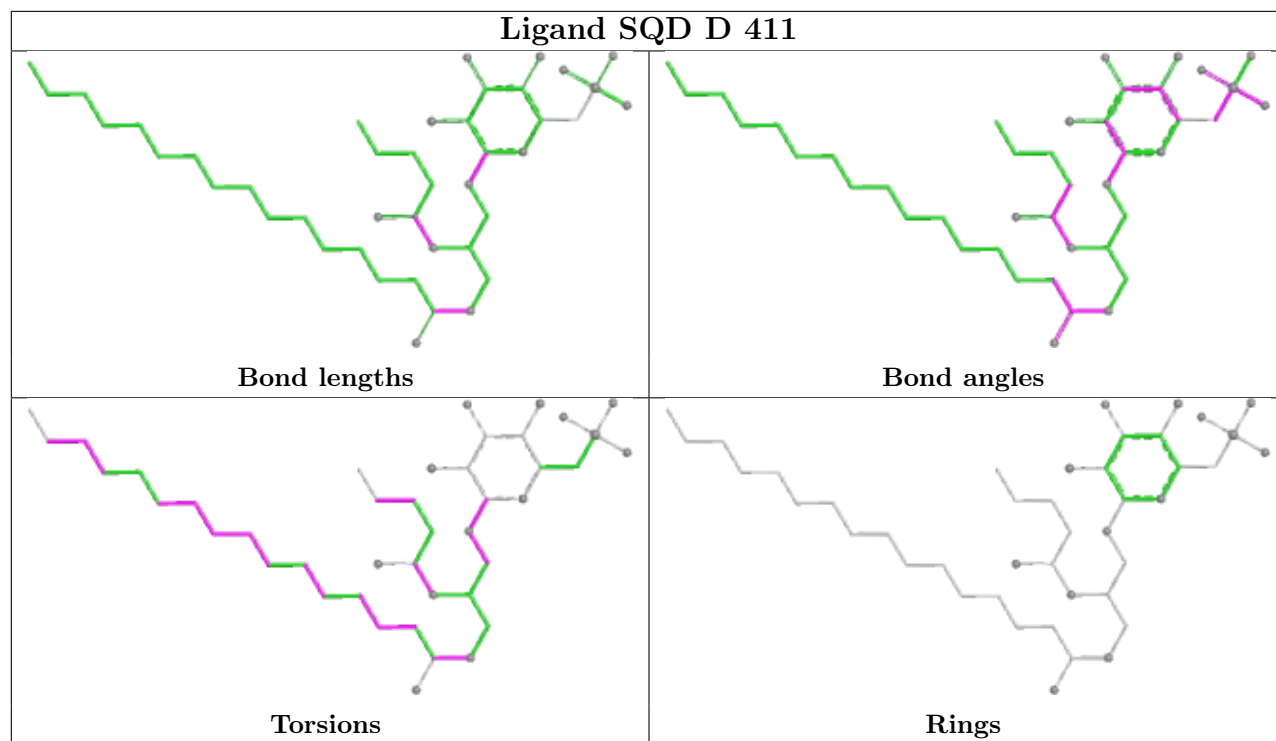


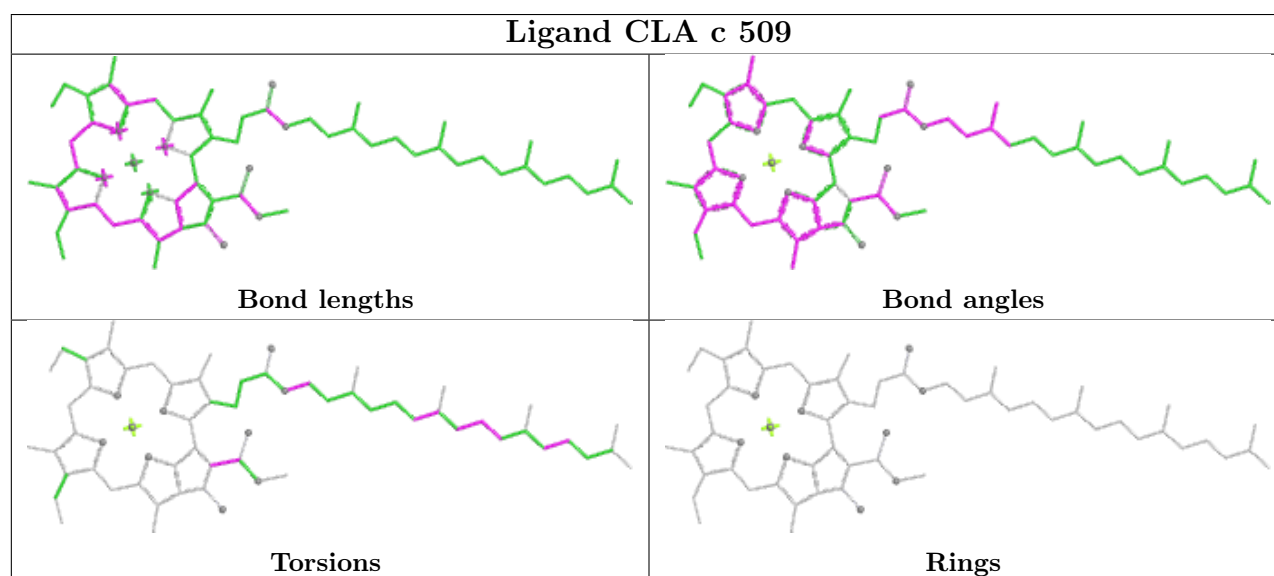
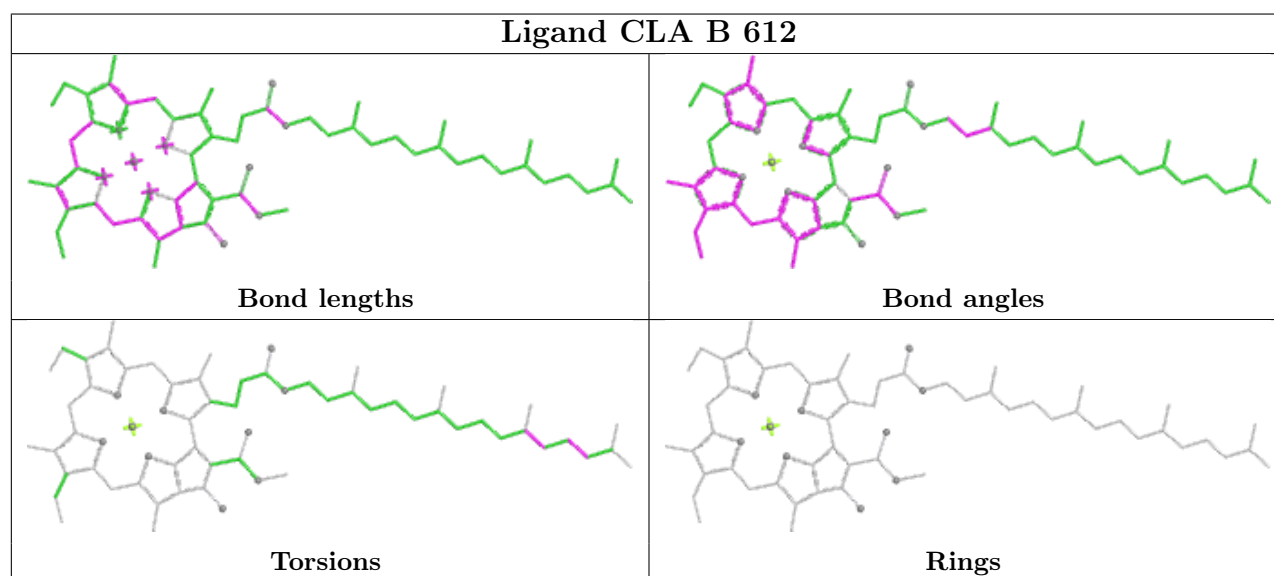
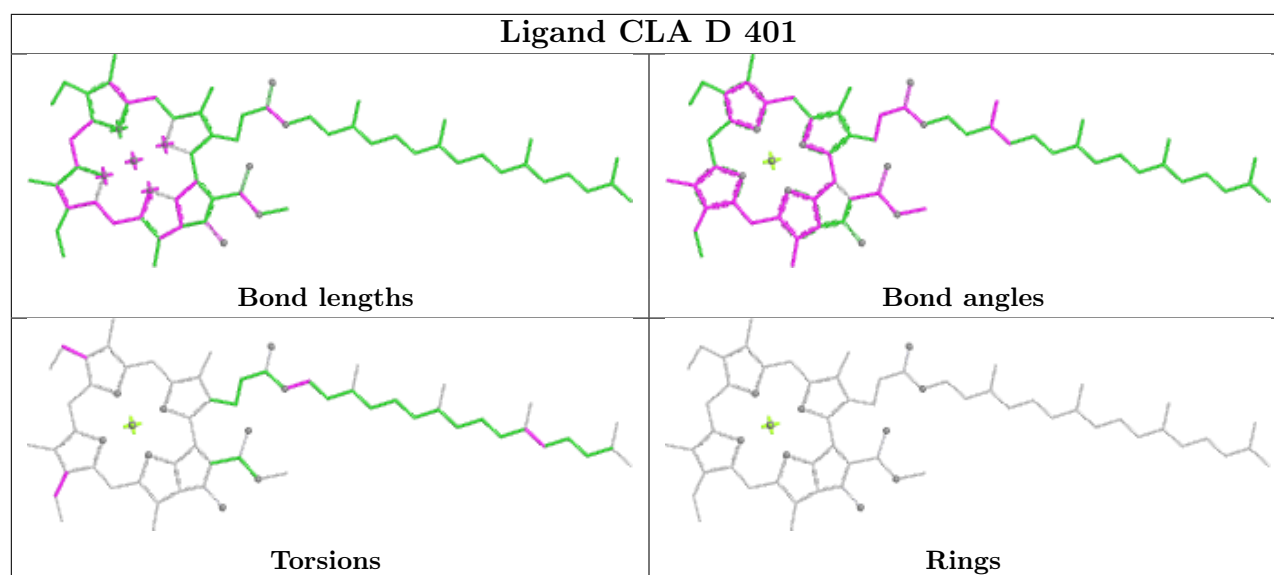
Ligand CLA c 505

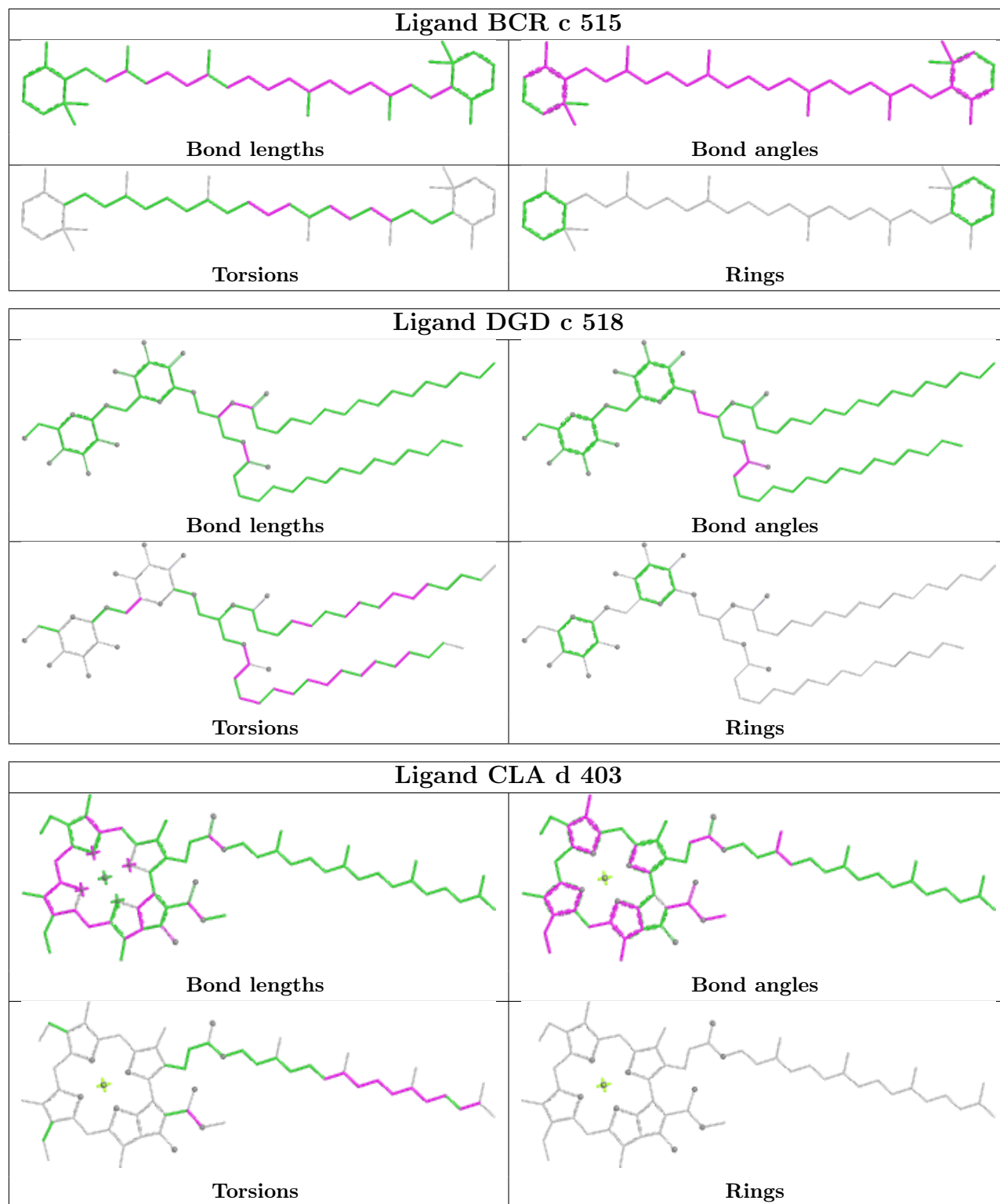


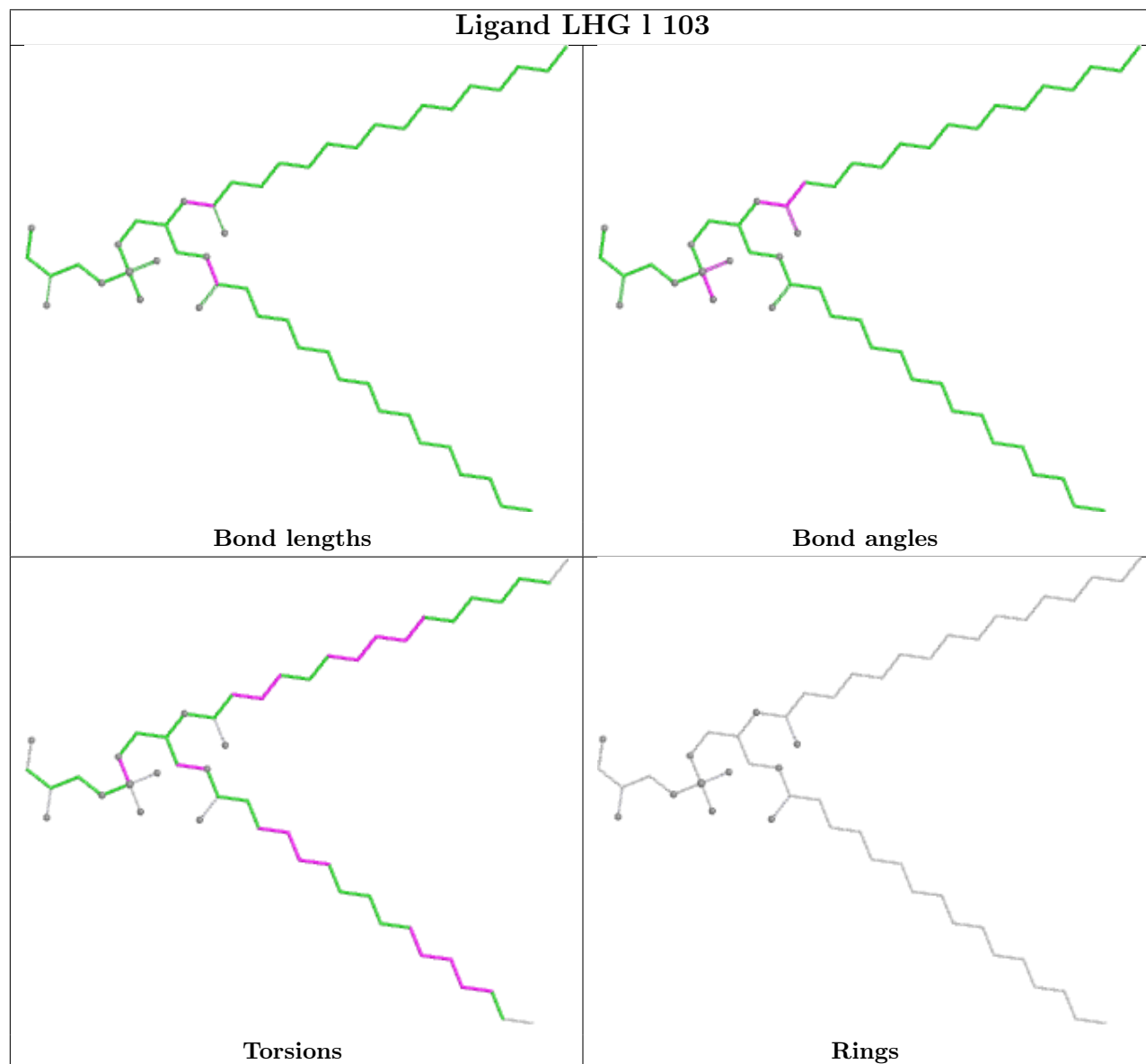
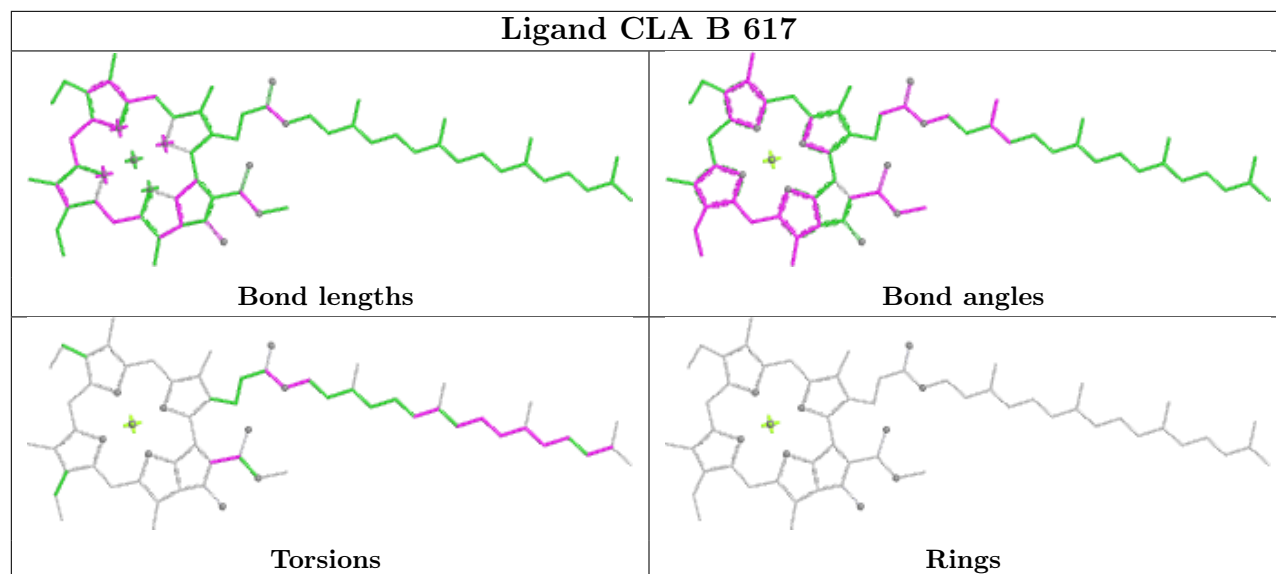
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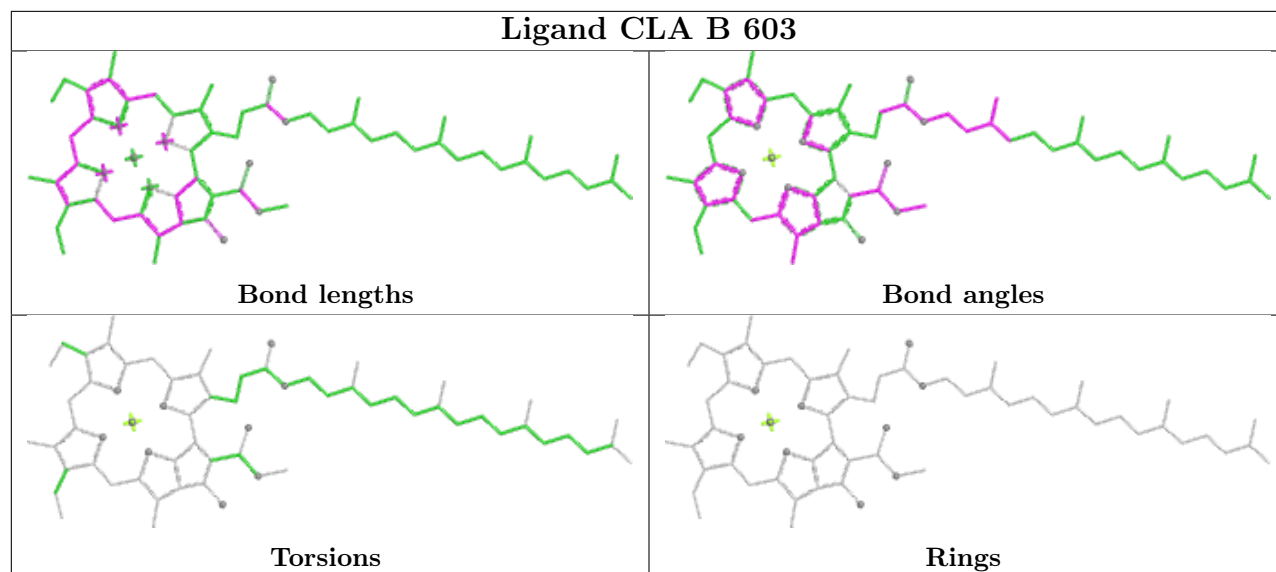




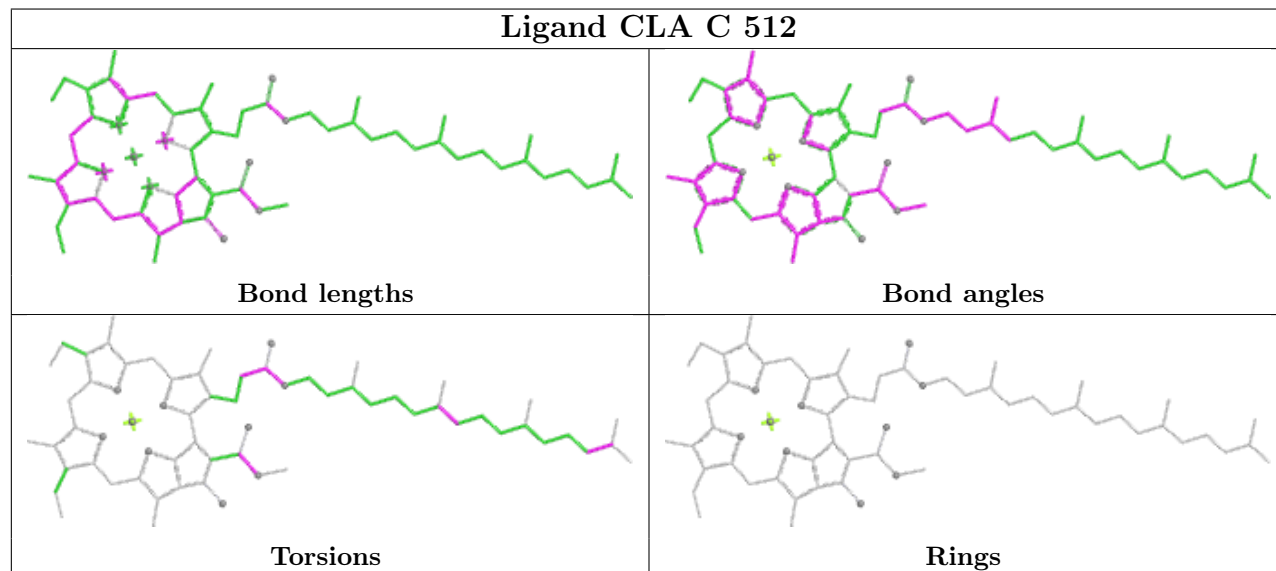




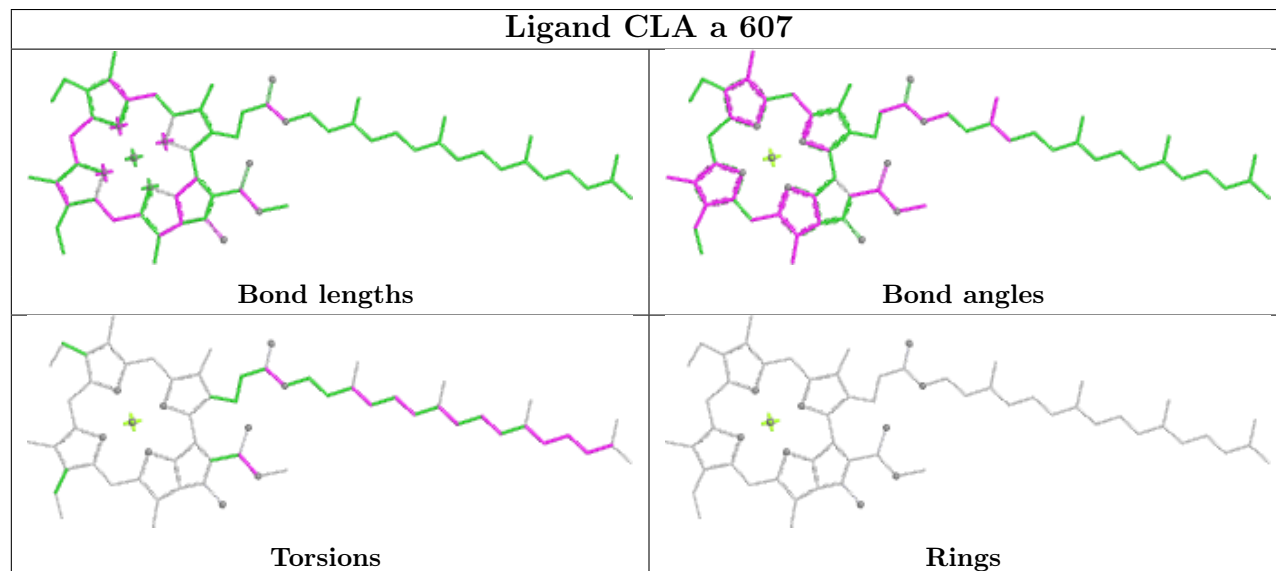
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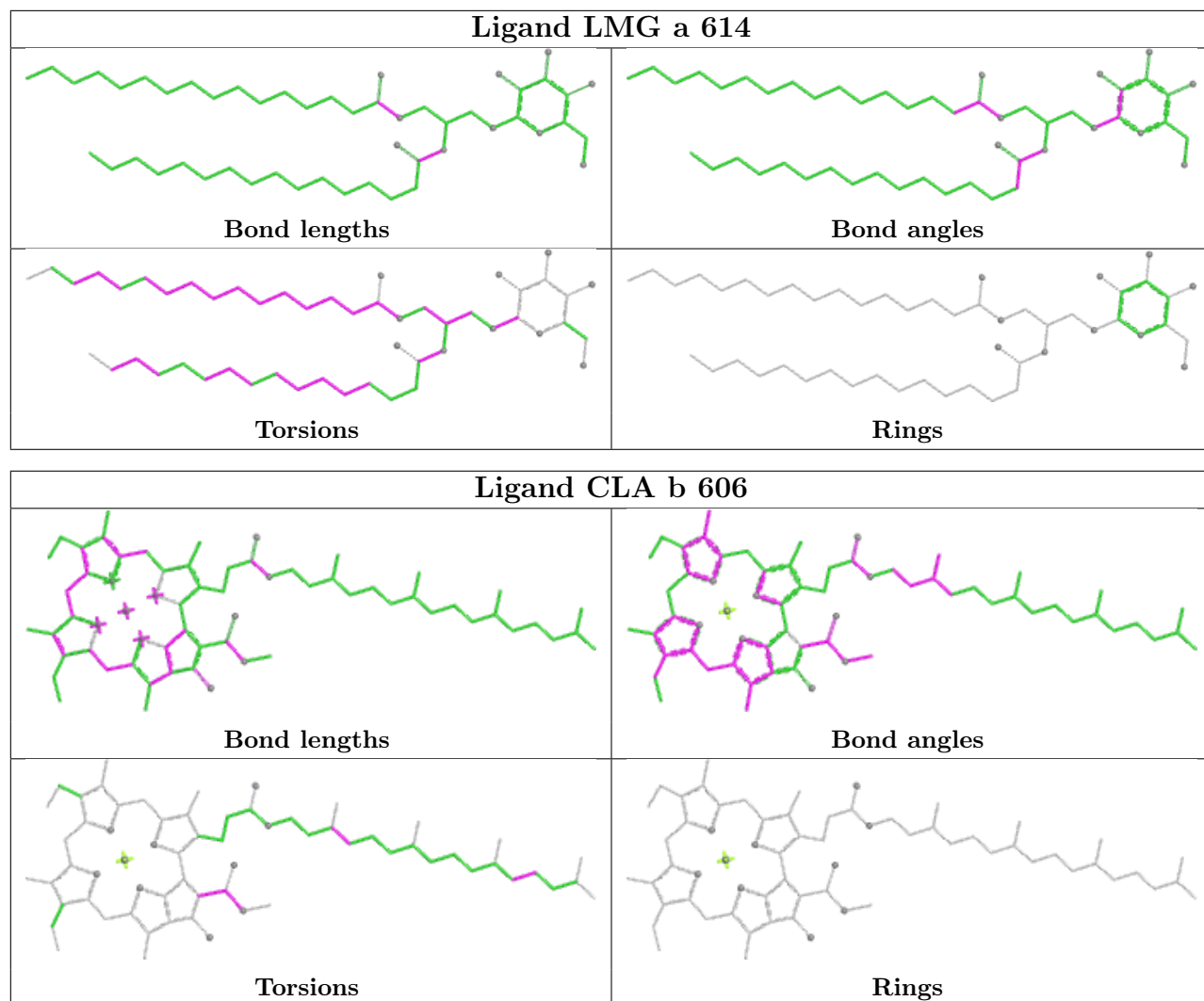


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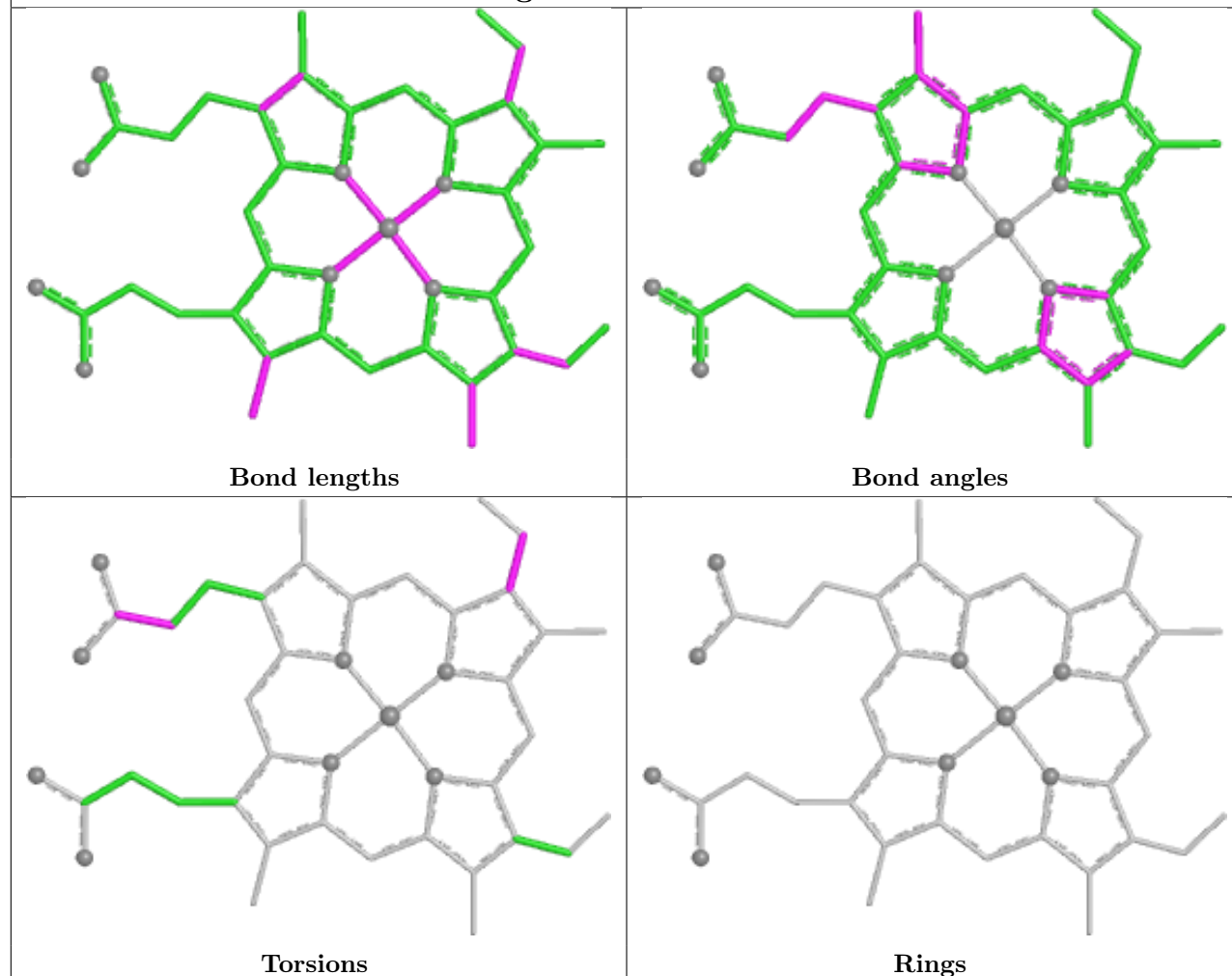


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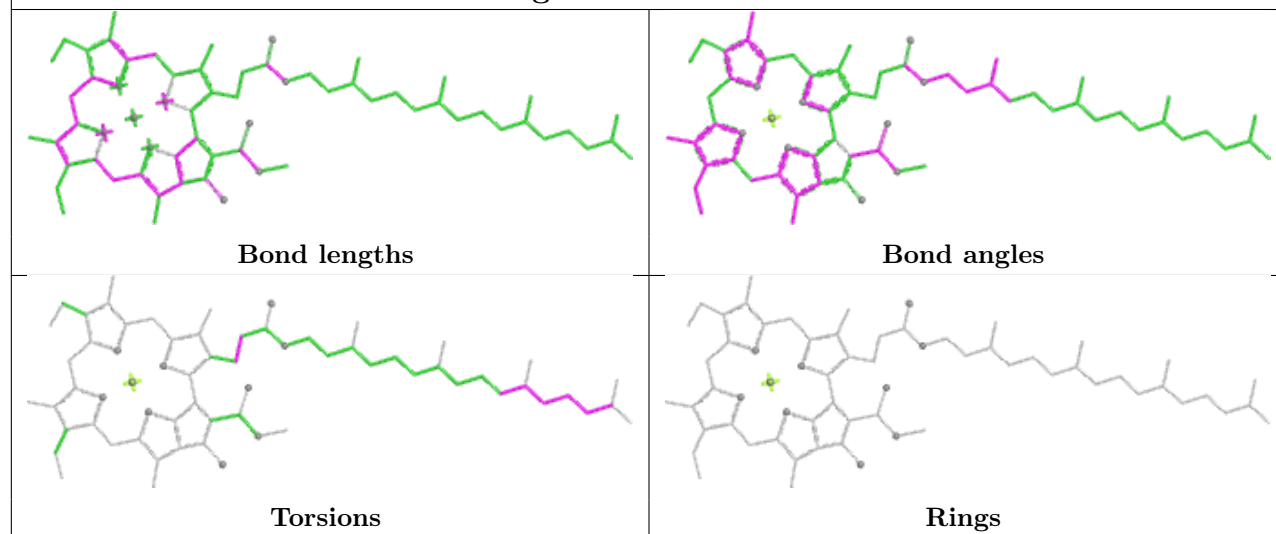


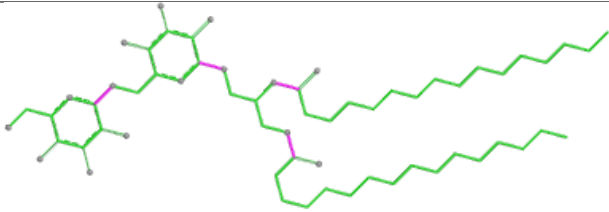
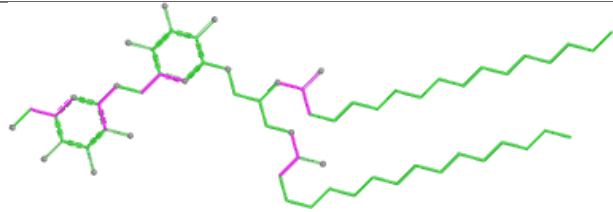
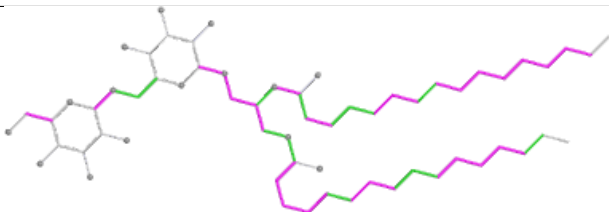
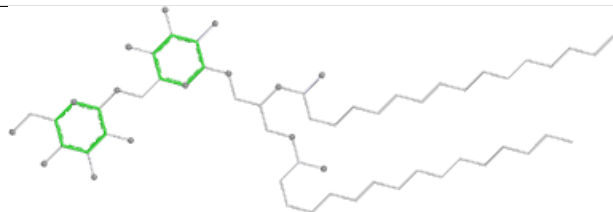


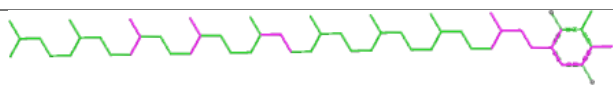
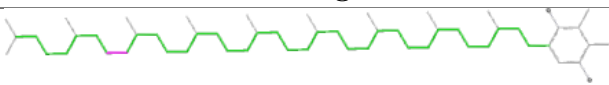
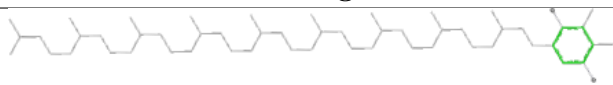
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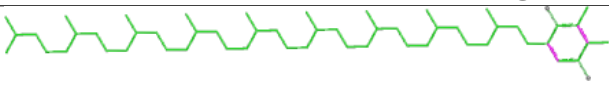
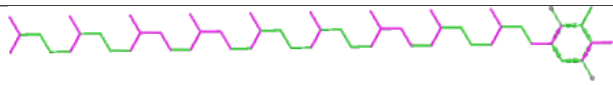
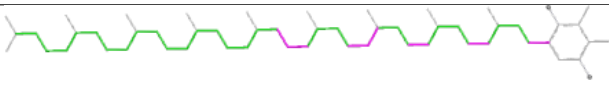
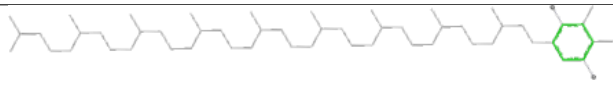


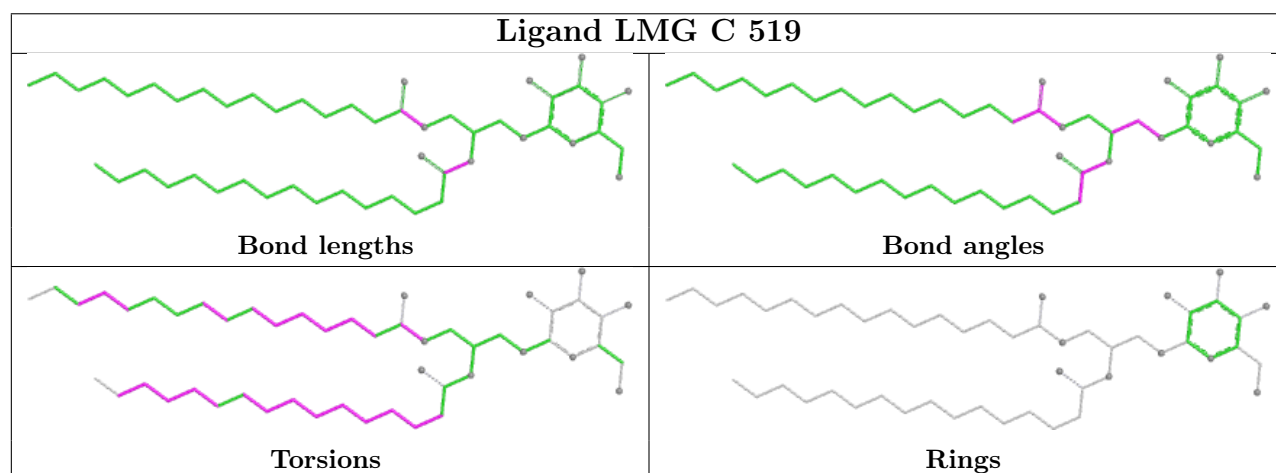
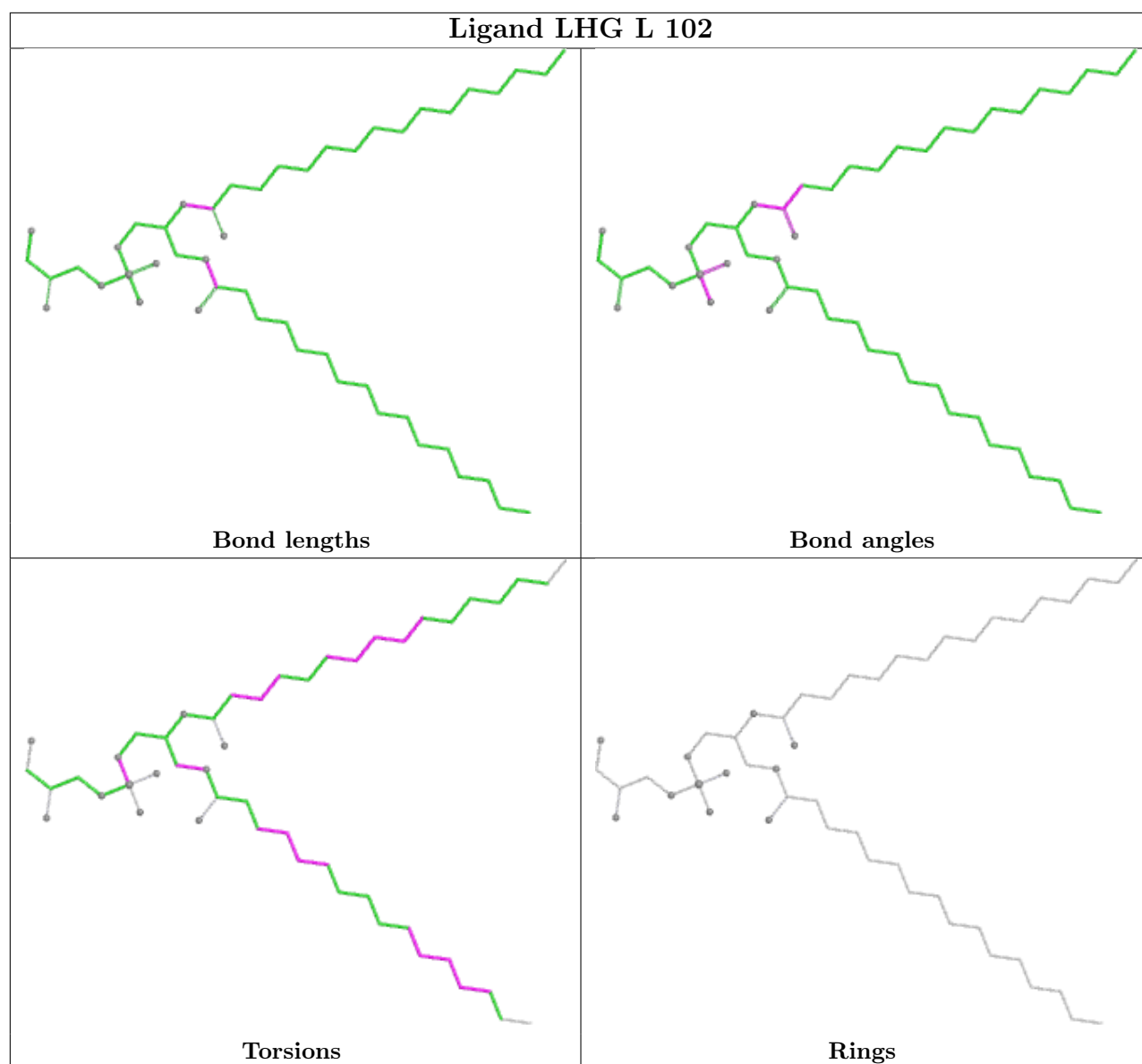
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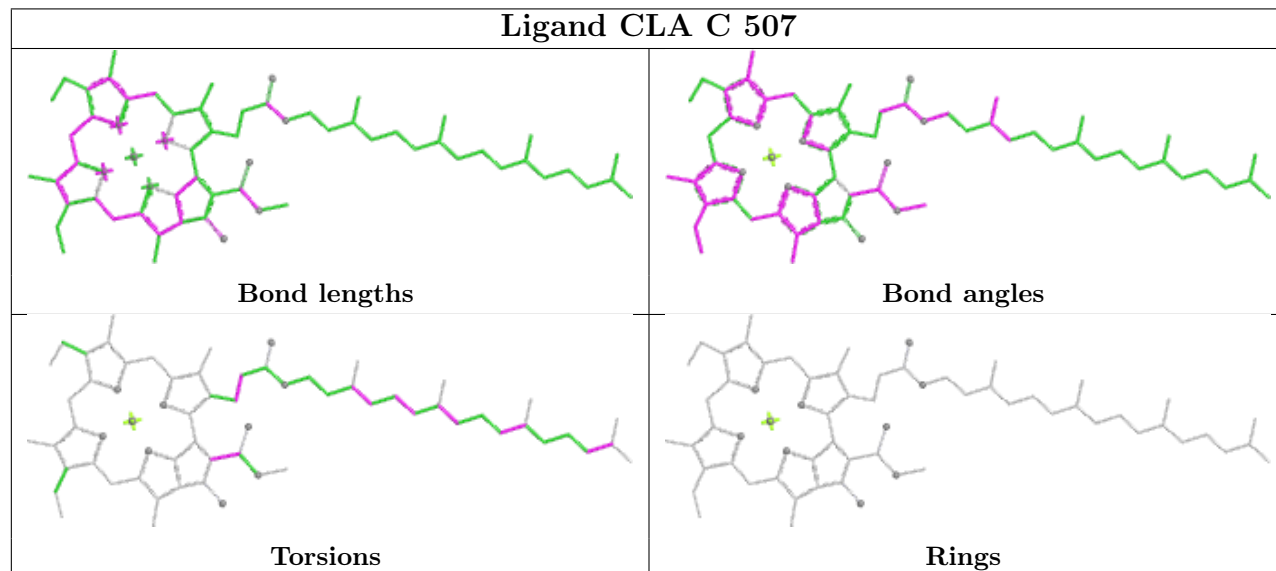
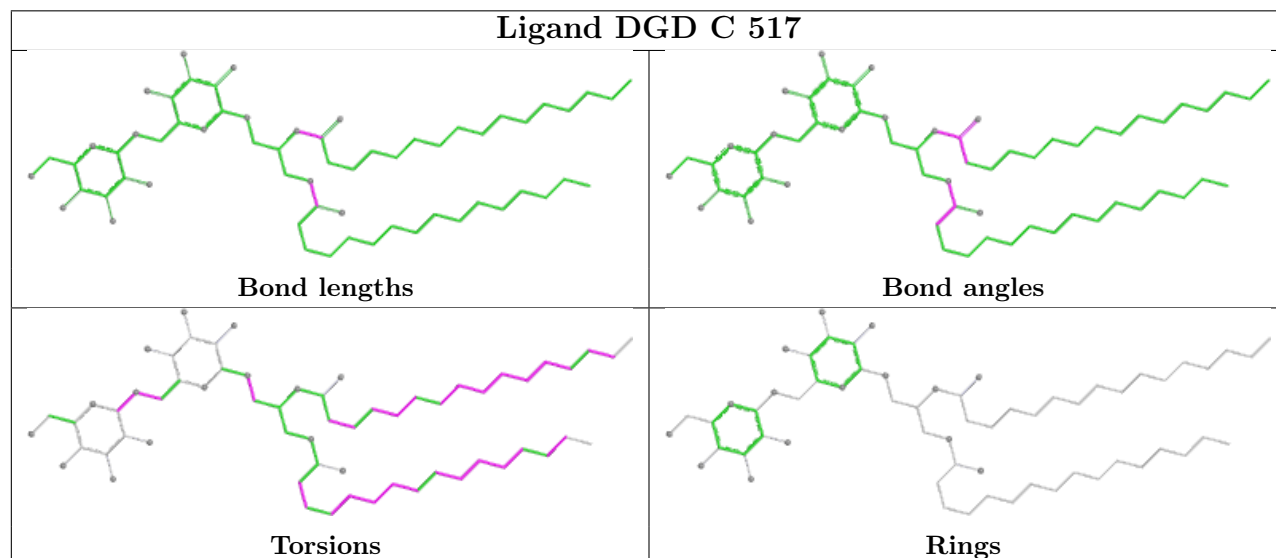
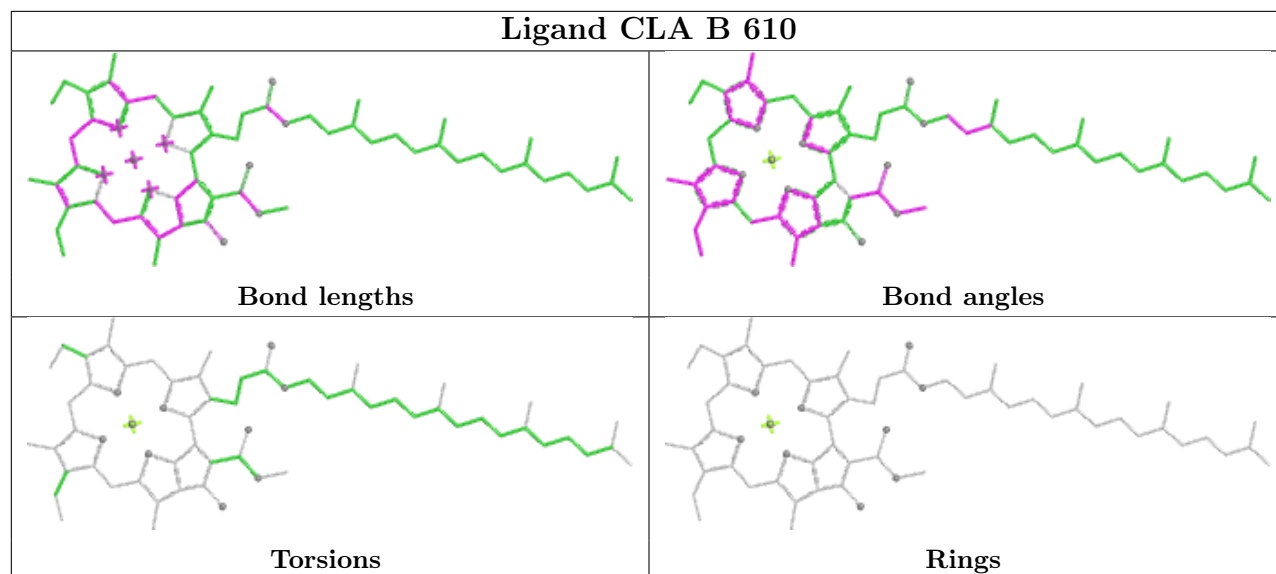


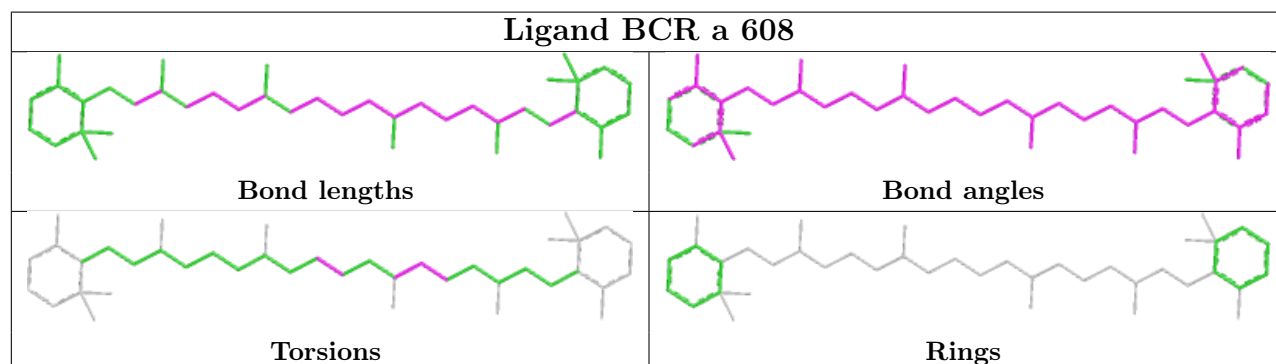
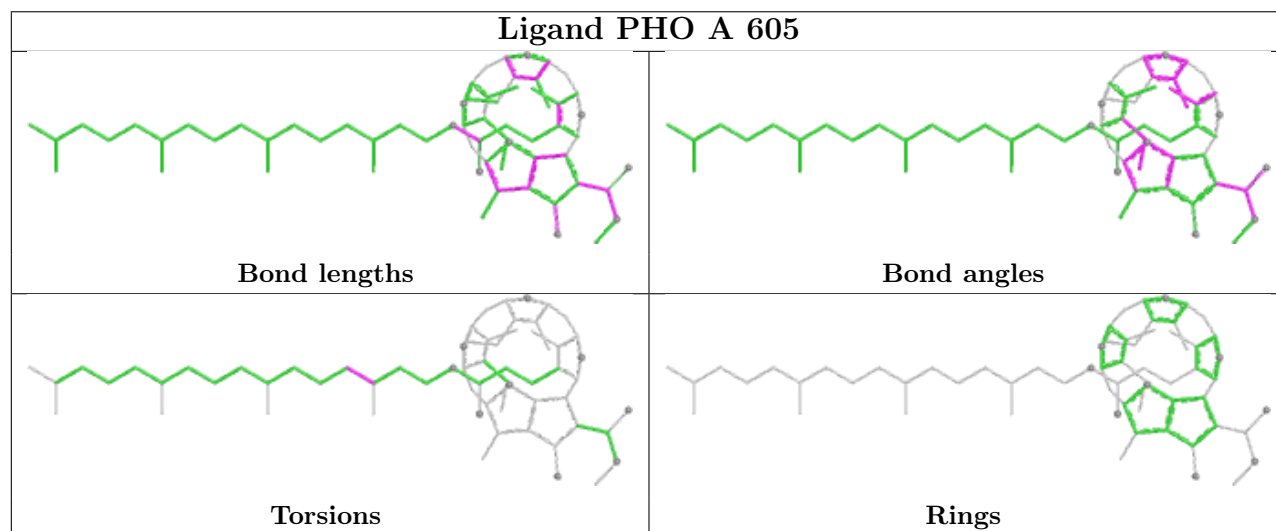
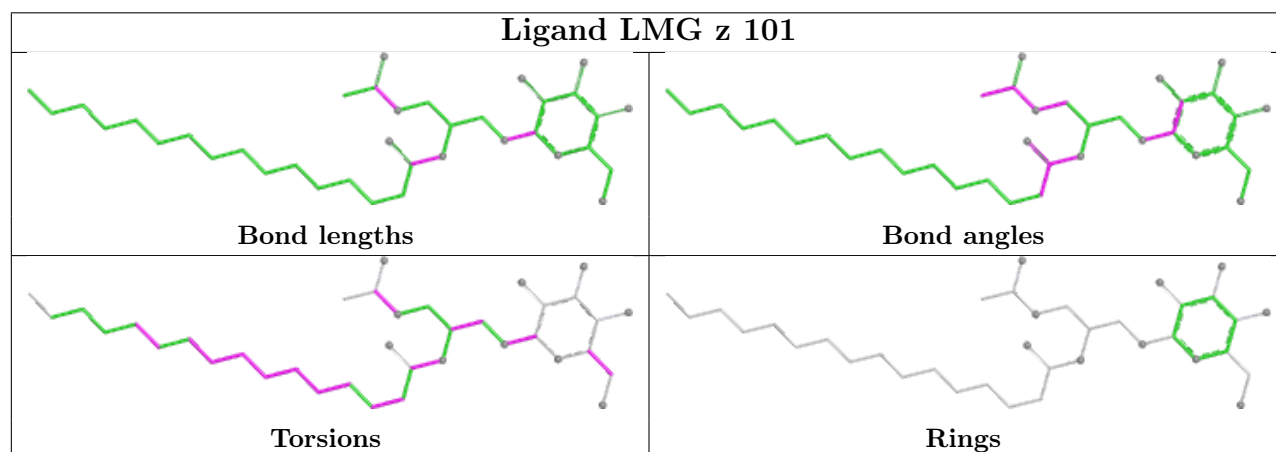
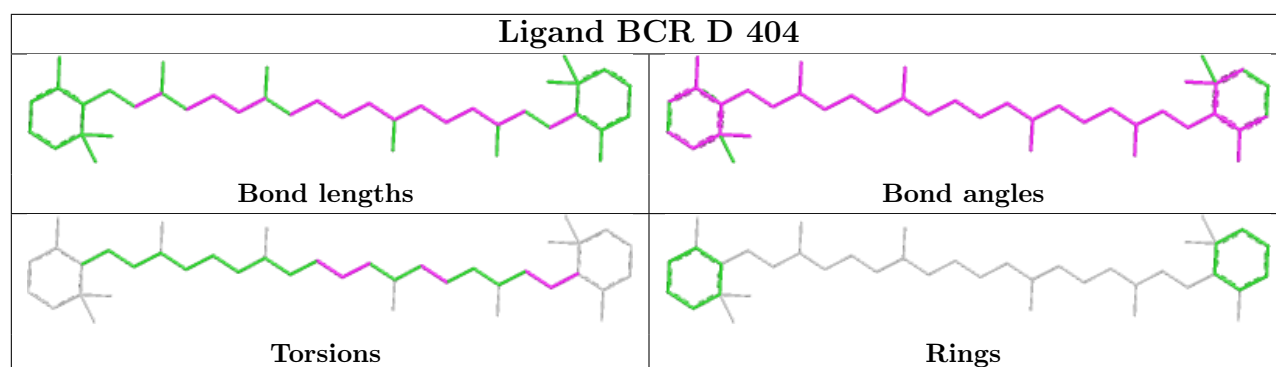
Ligand DGD d 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

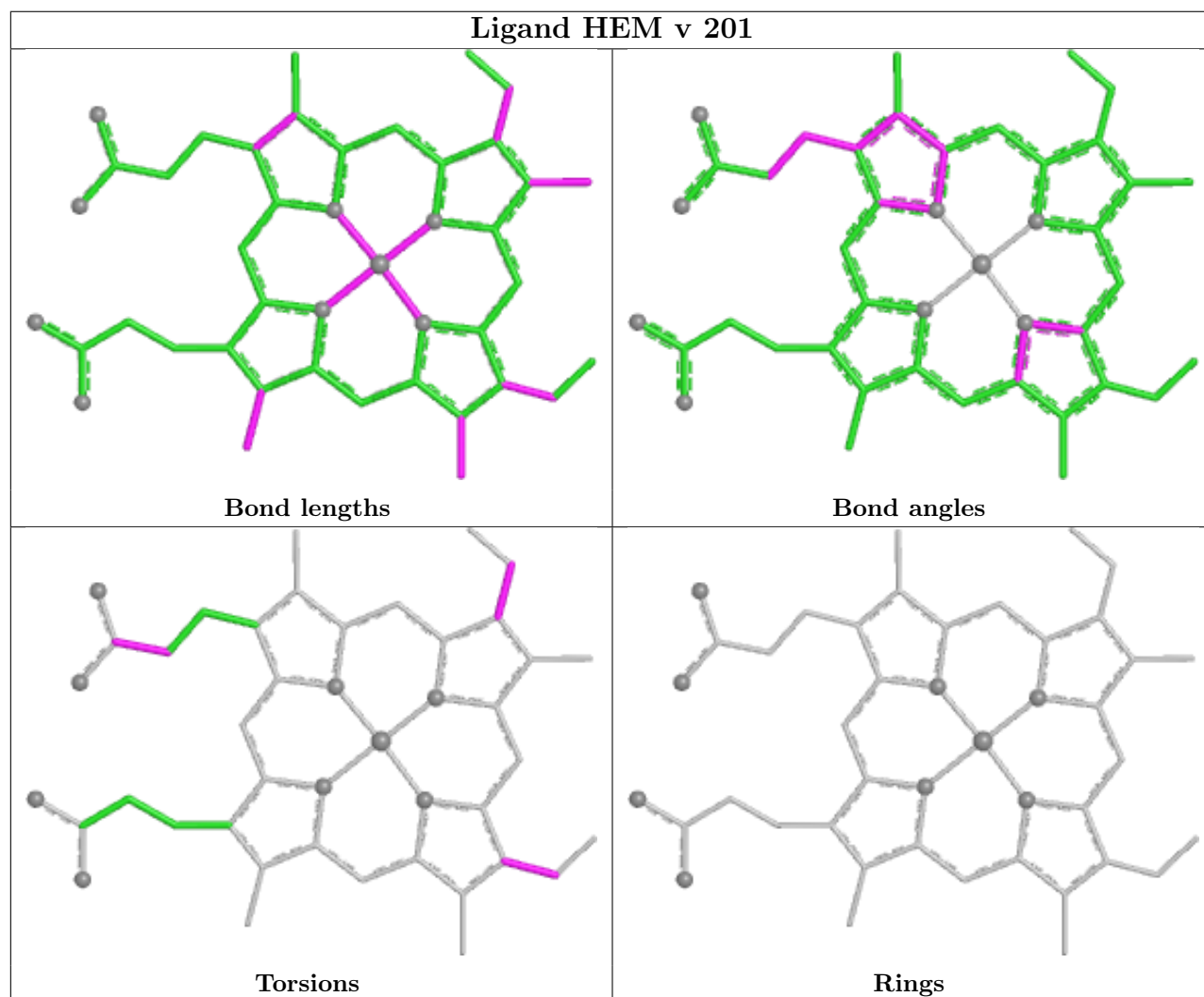
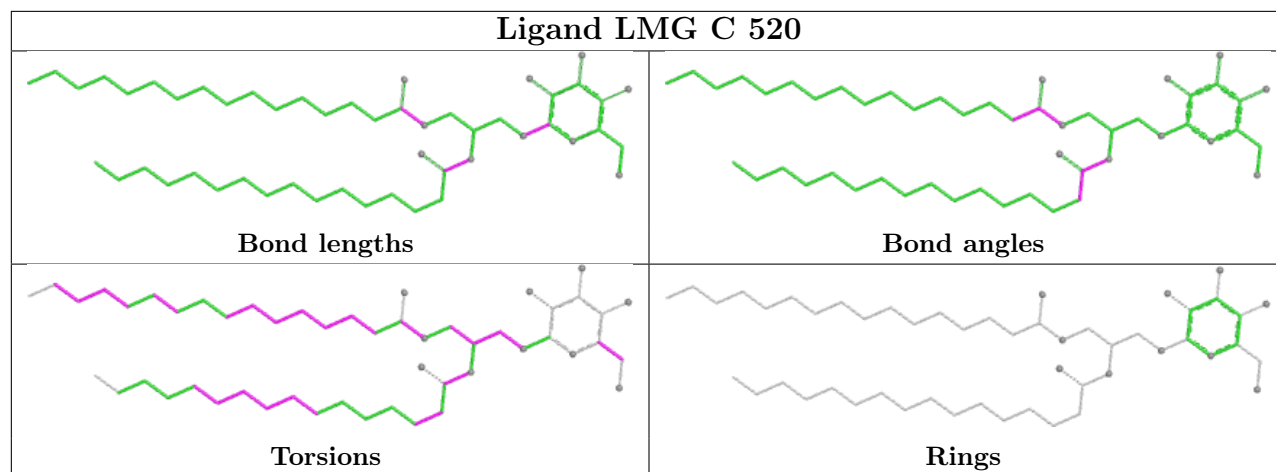
Ligand PL9 d 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

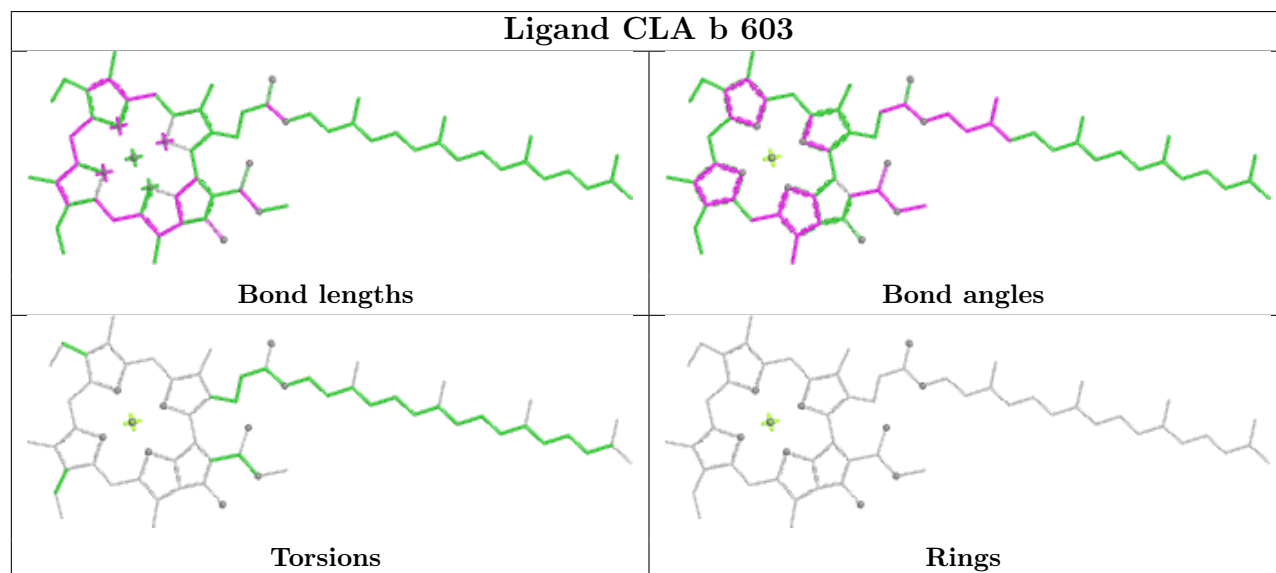
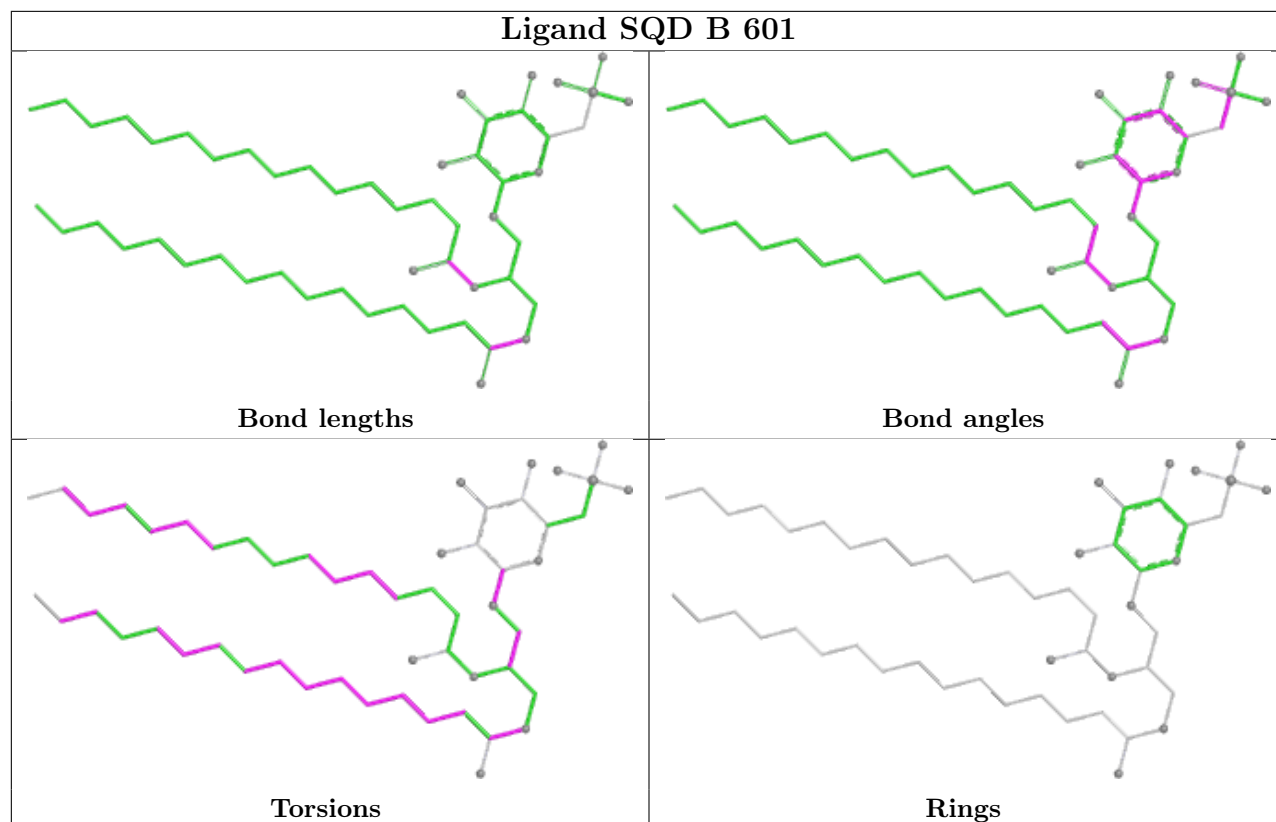
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Bond lengths	Bond angles
	
Torsions	Rings



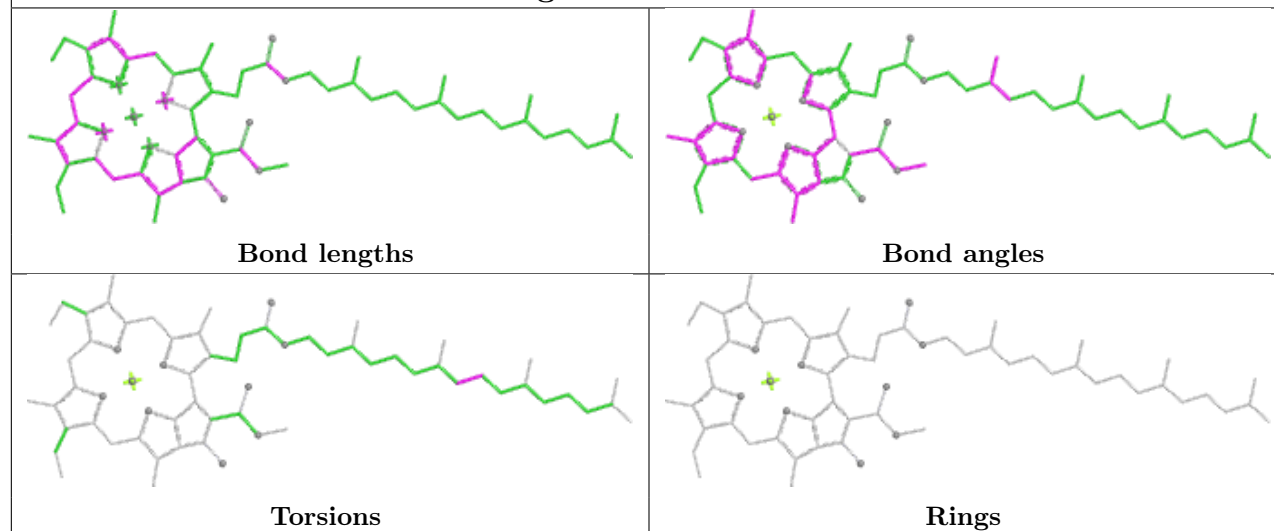




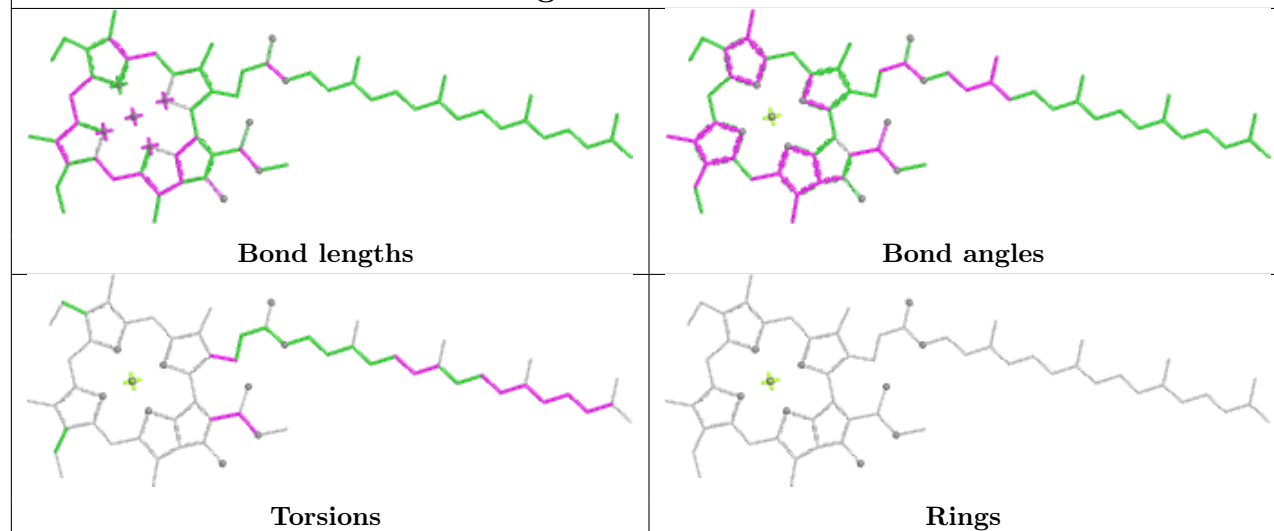




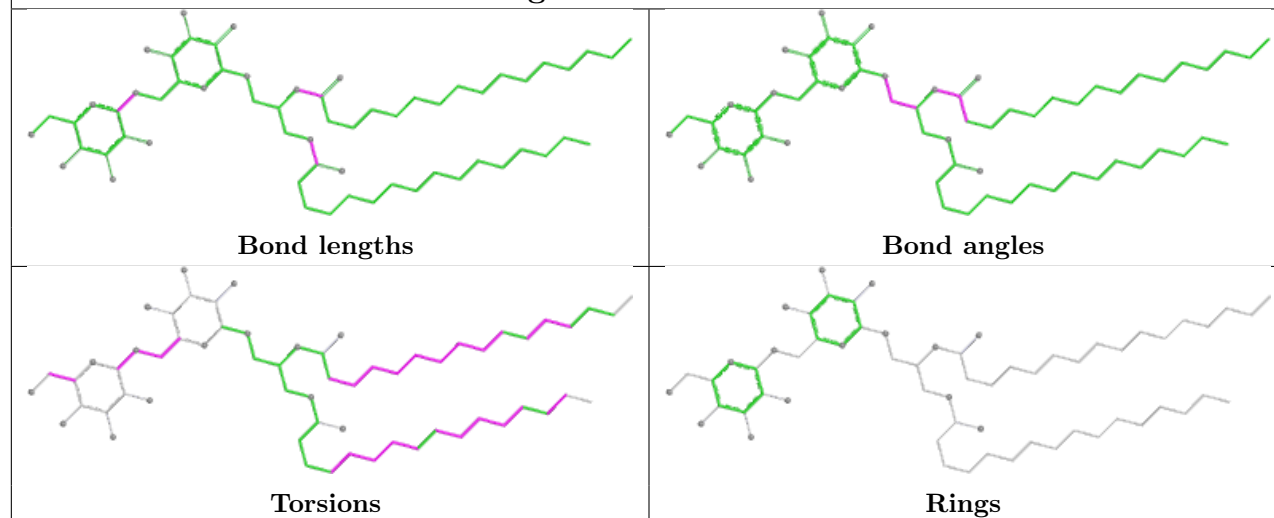
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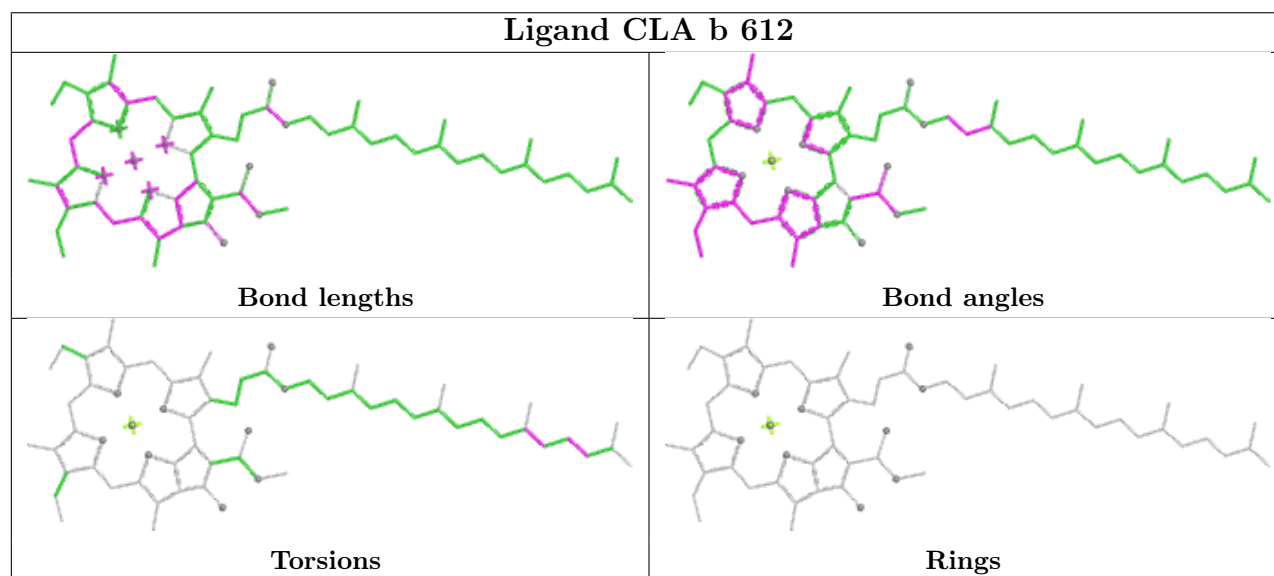
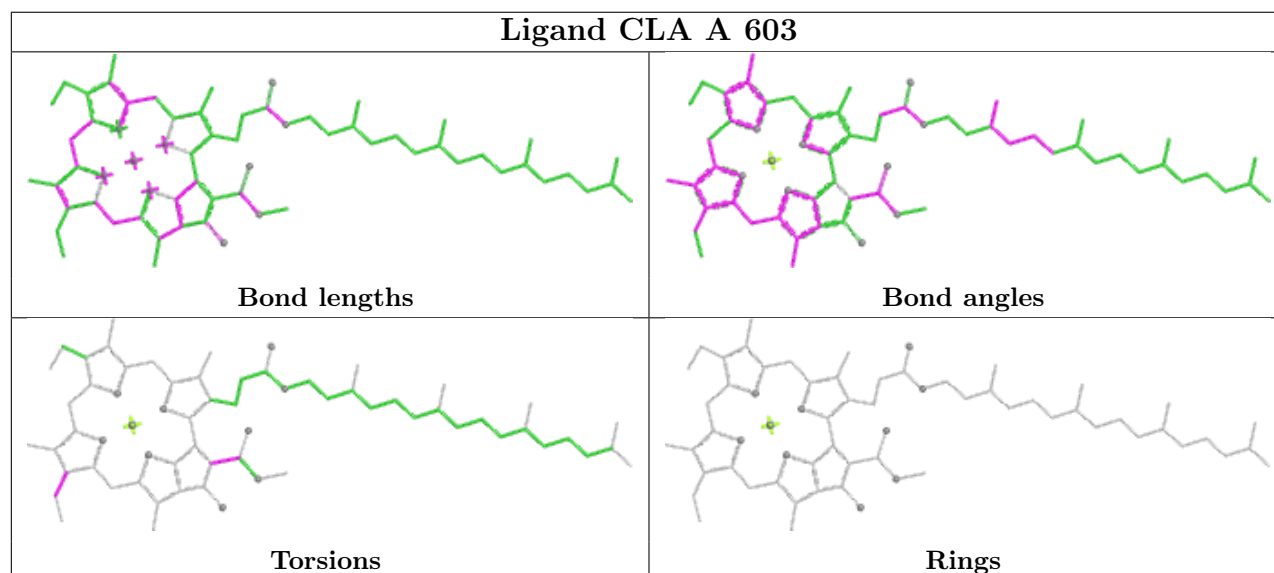
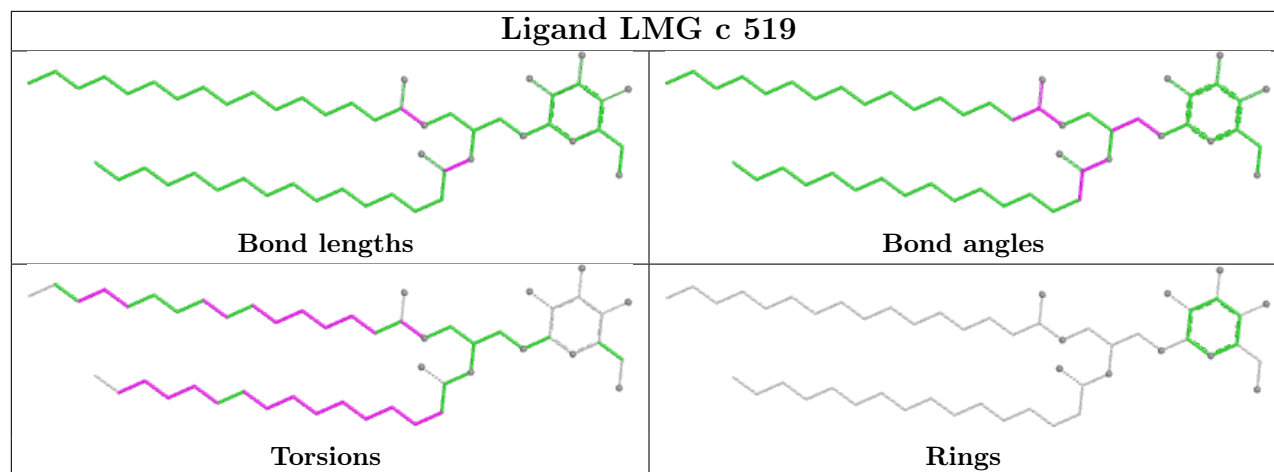


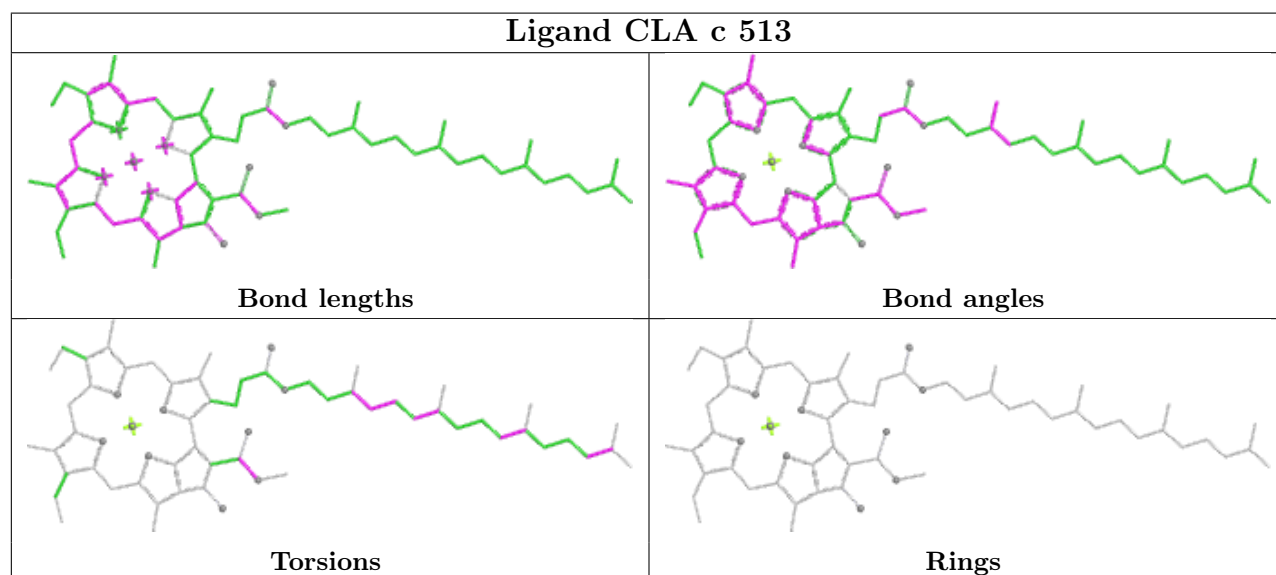
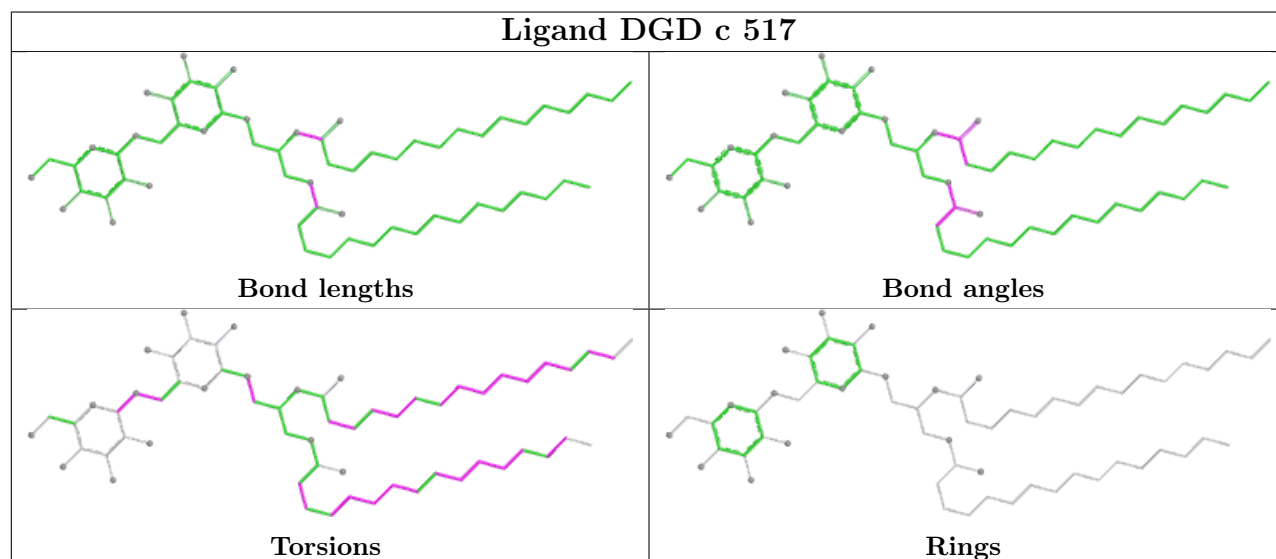
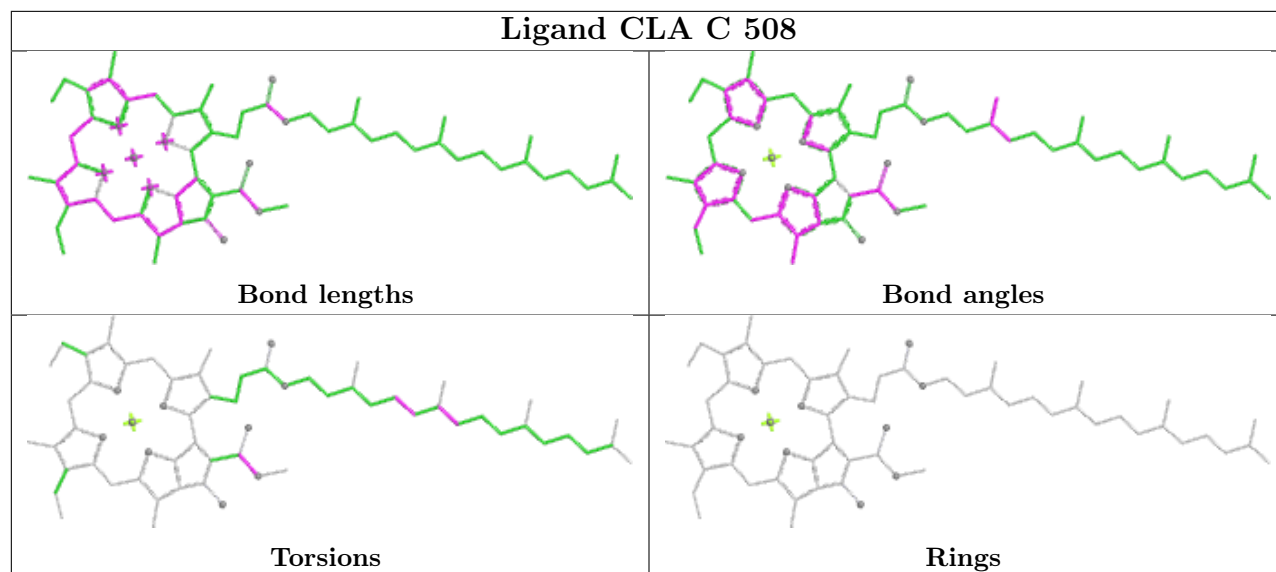
Ligand CLA c 506

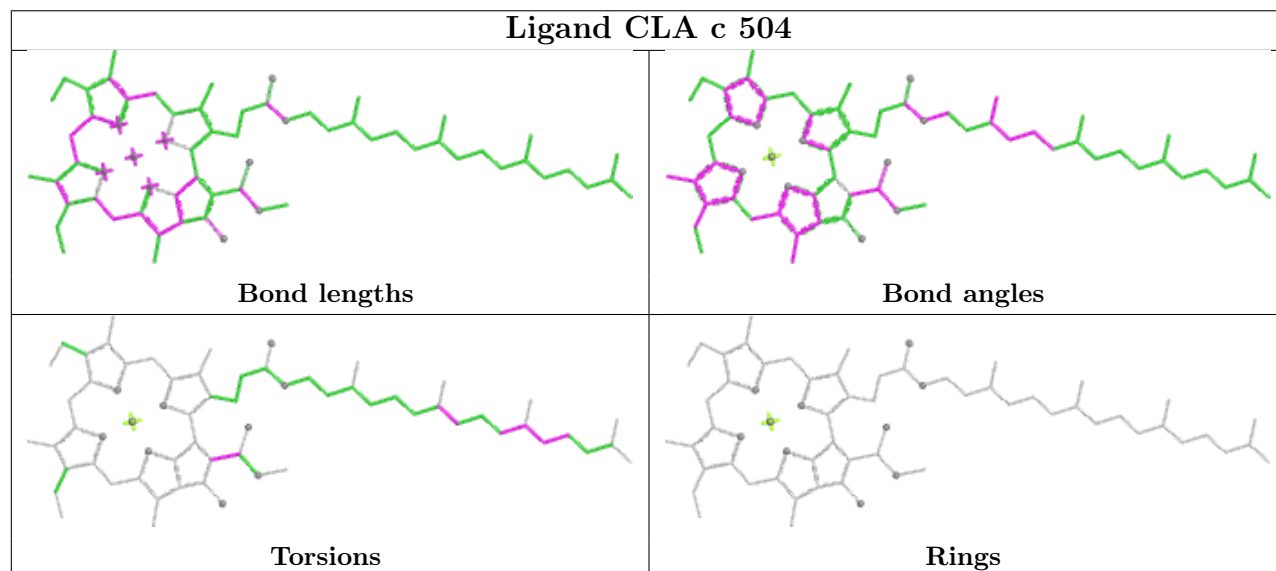
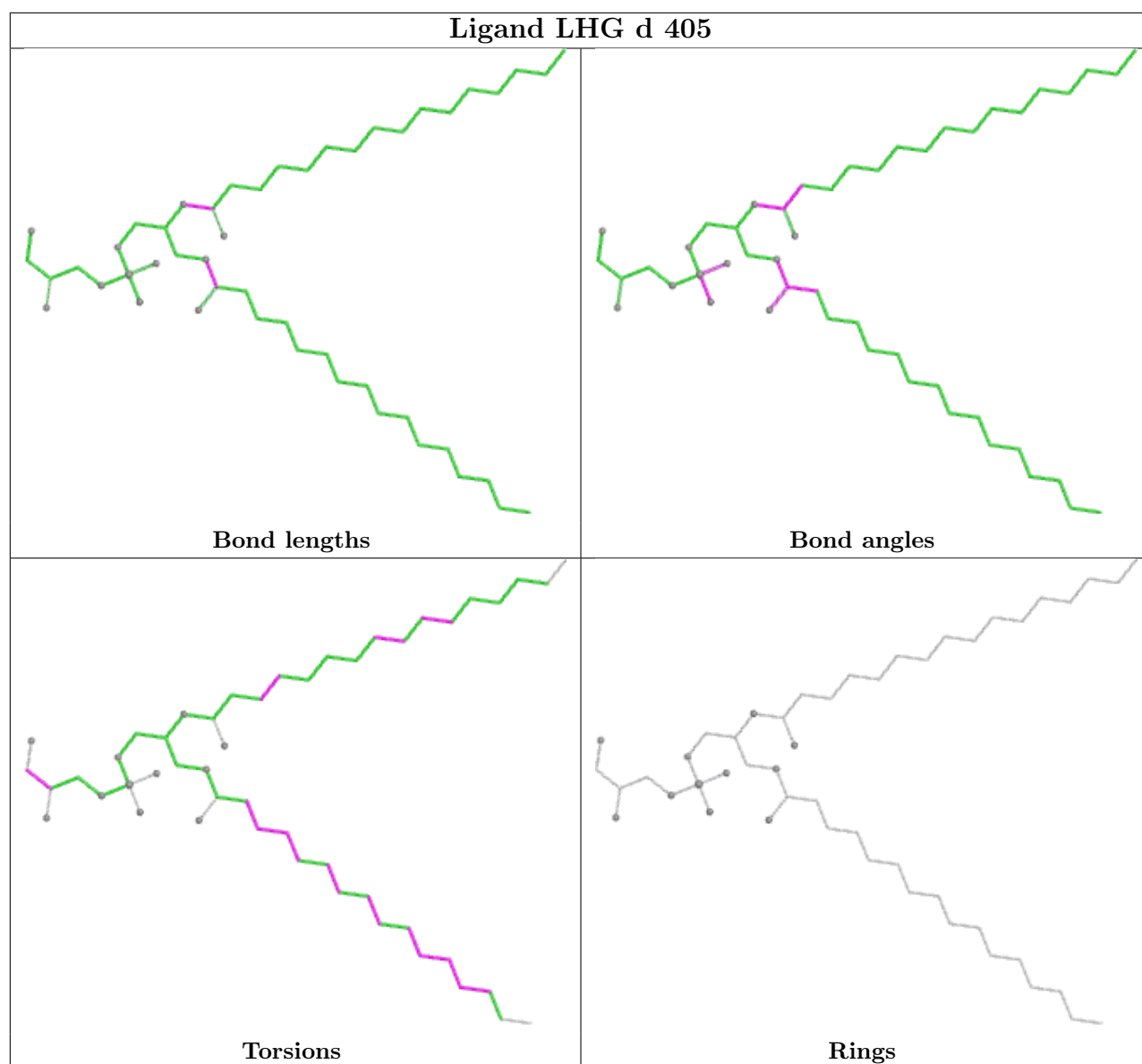


Ligand DGD C 516

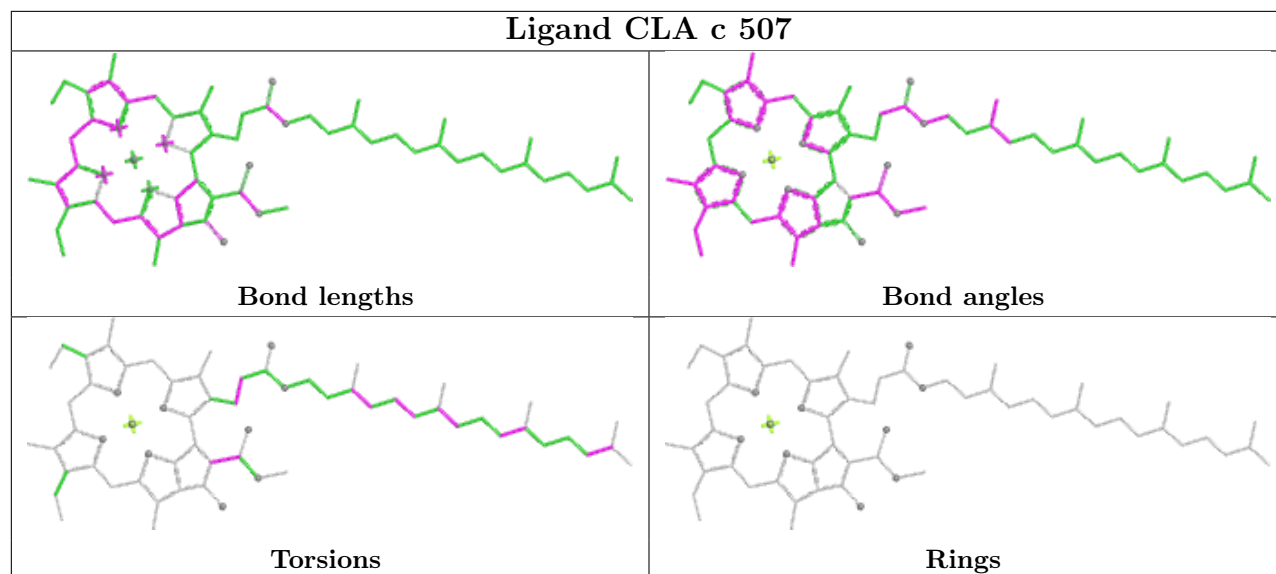




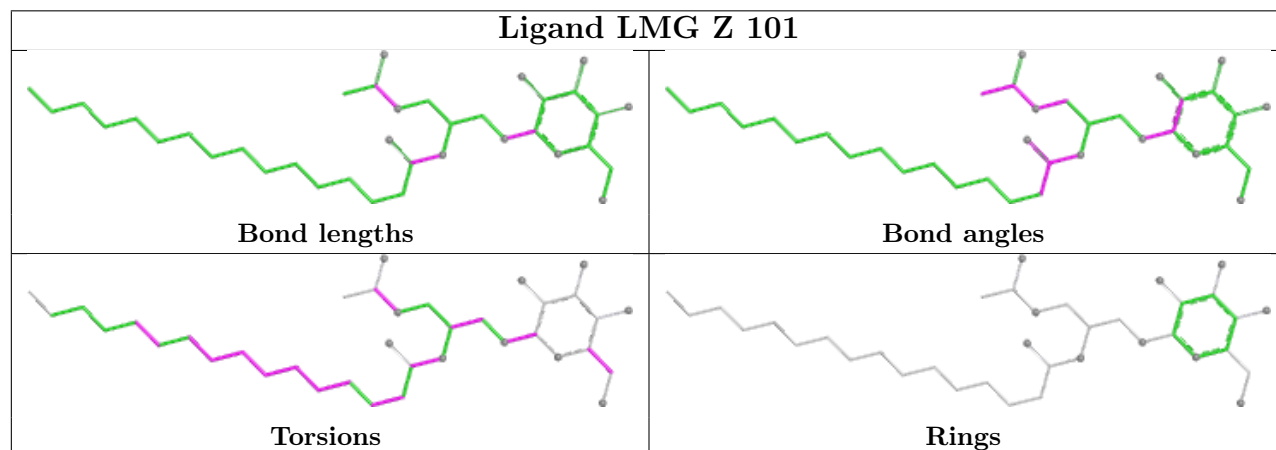


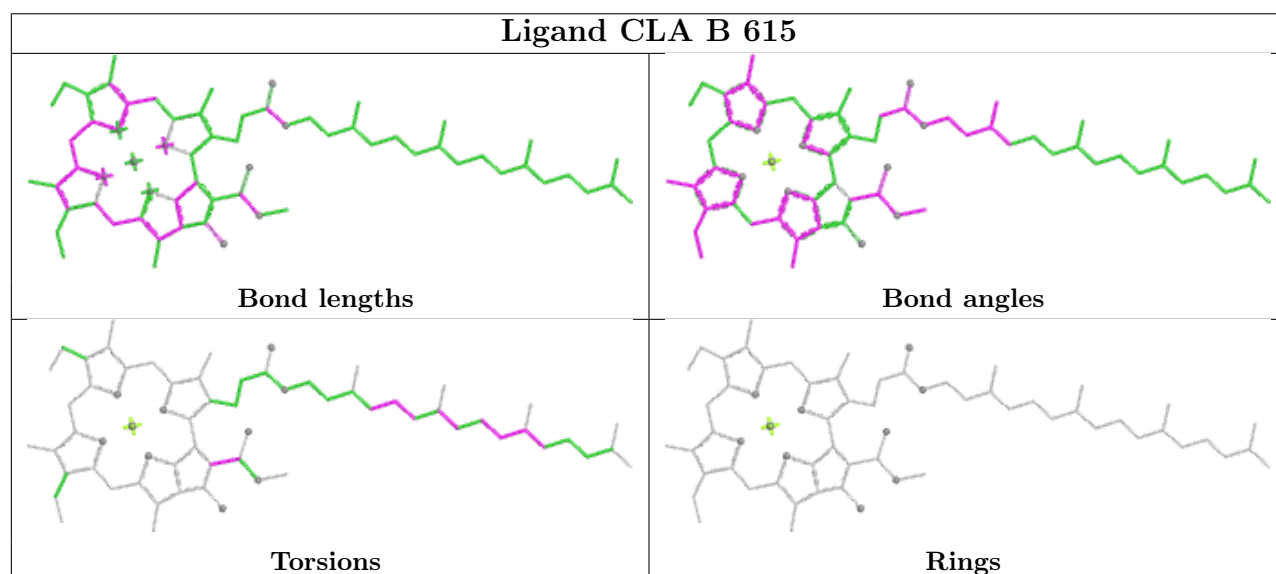
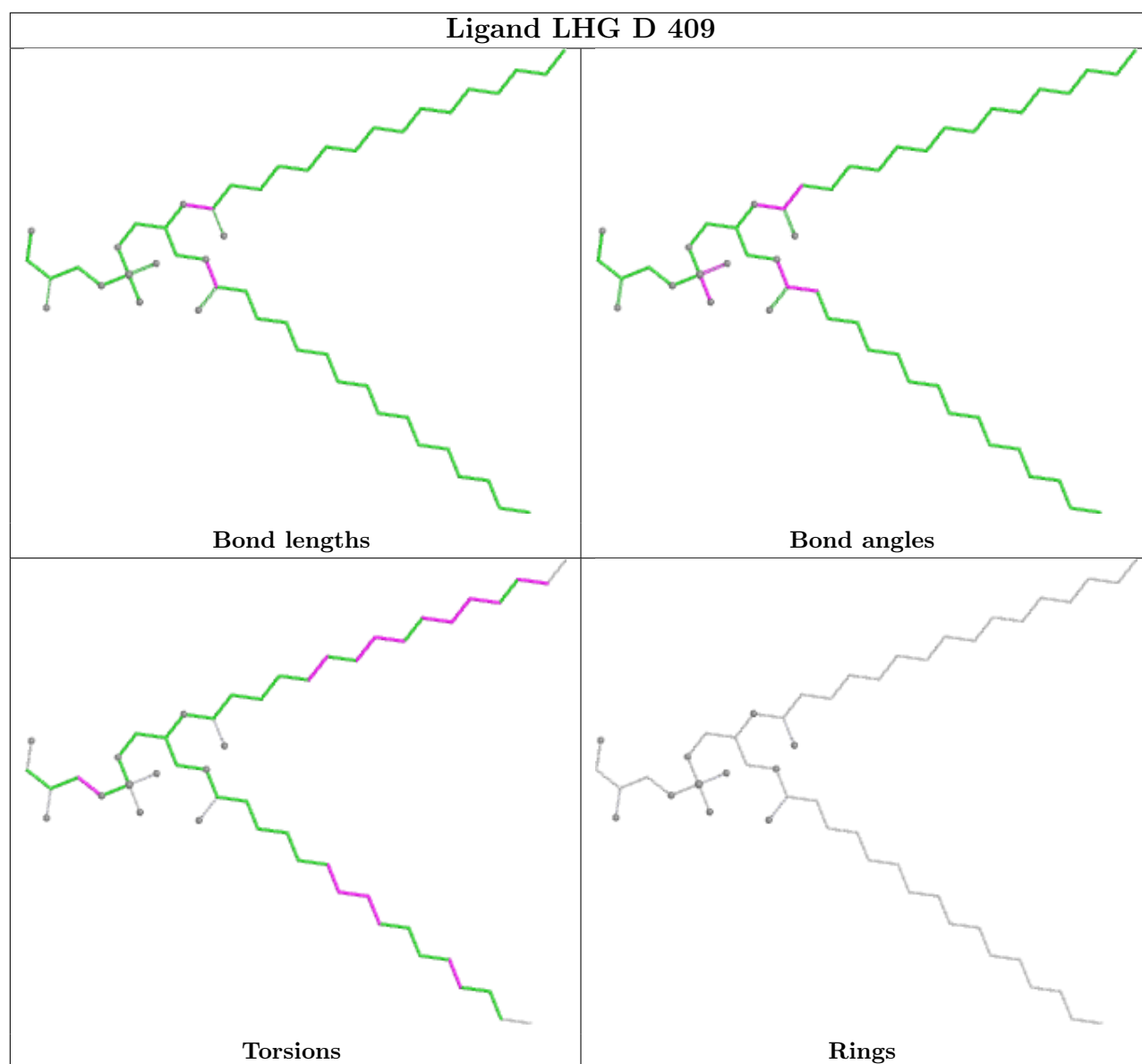


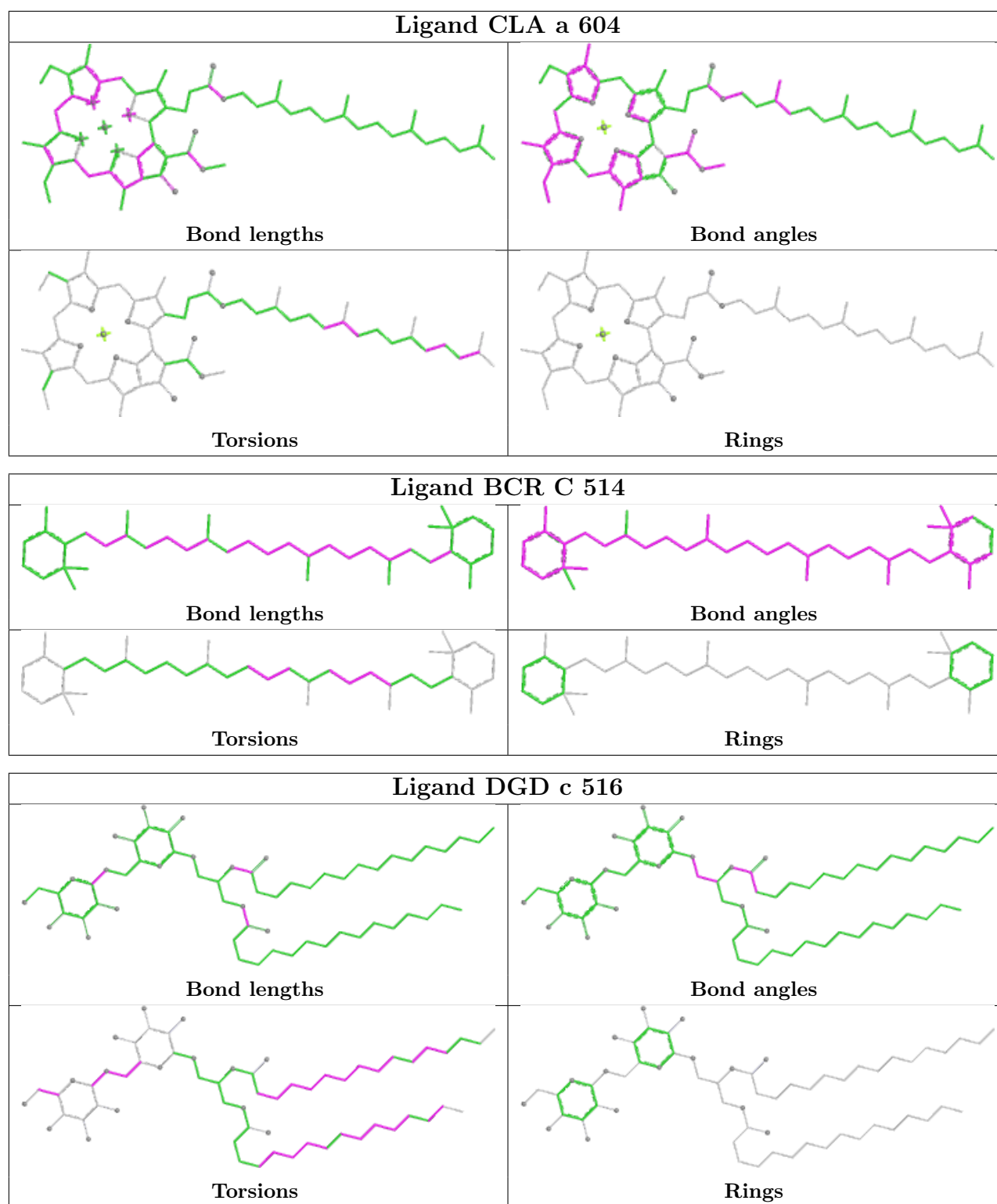
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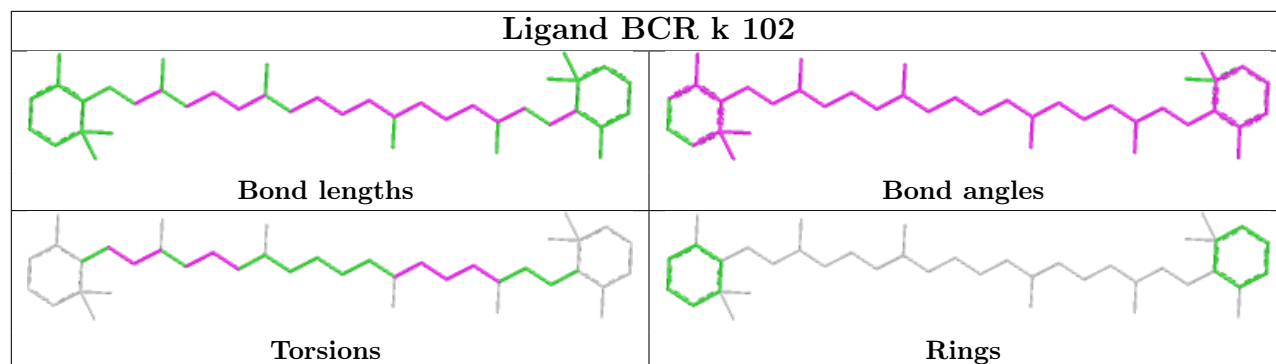
Ligand LMG Z 101



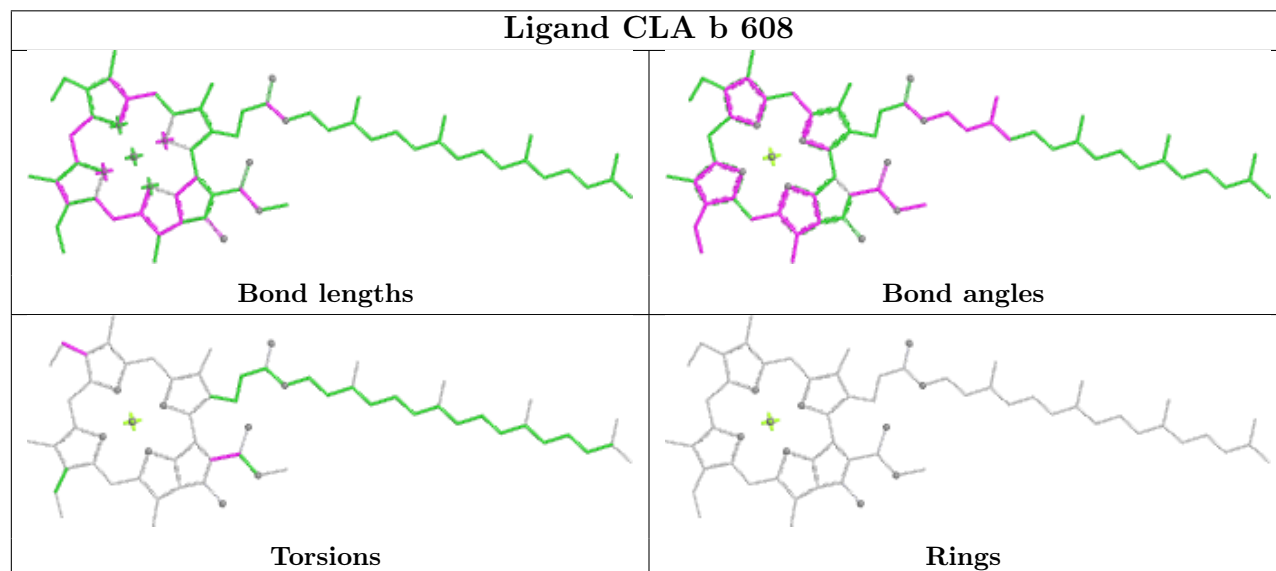




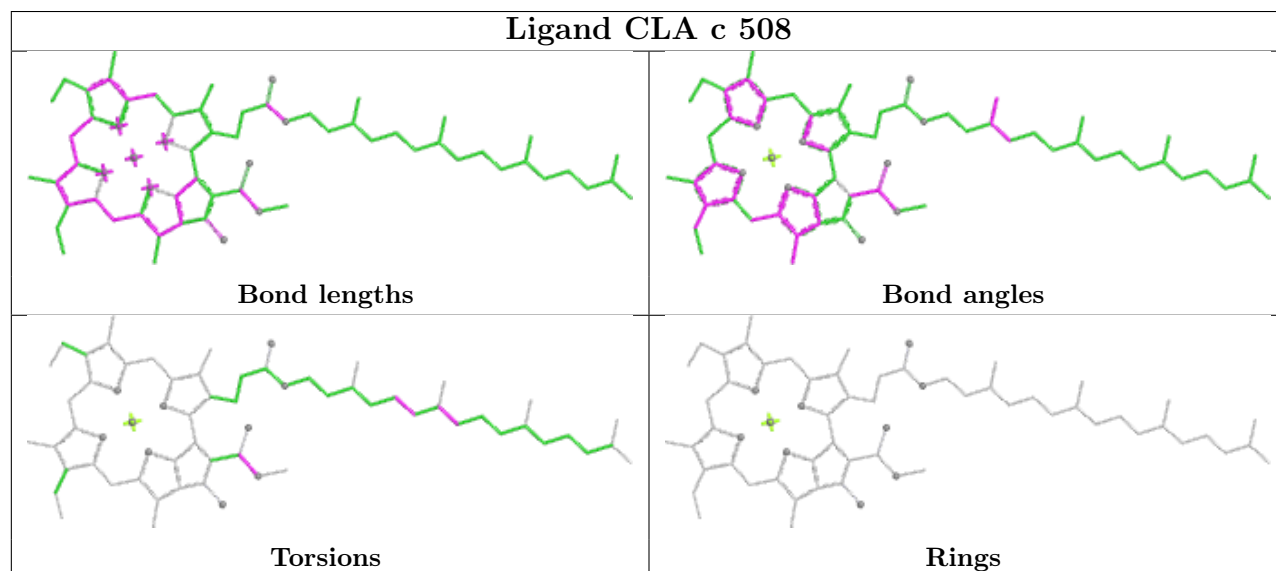
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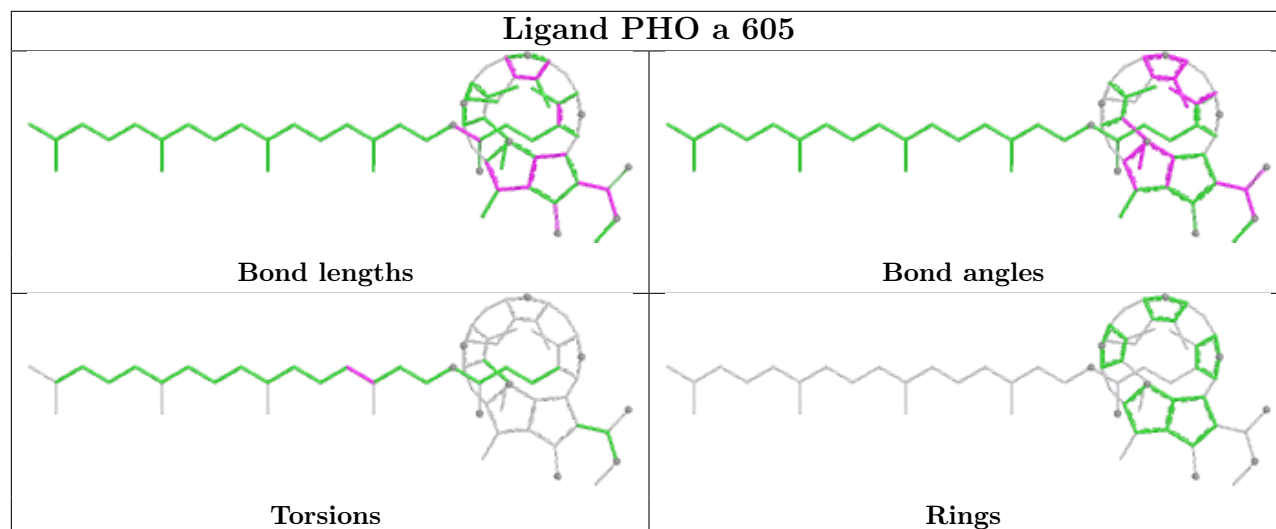
Ligand CLA b 608



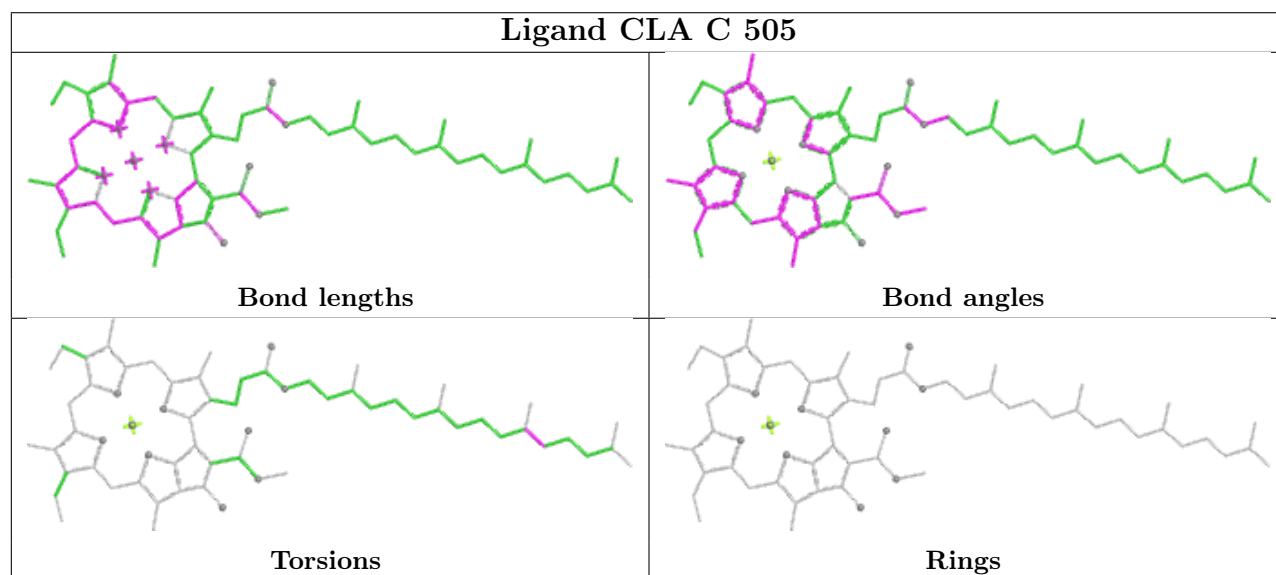
Ligand CLA c 508



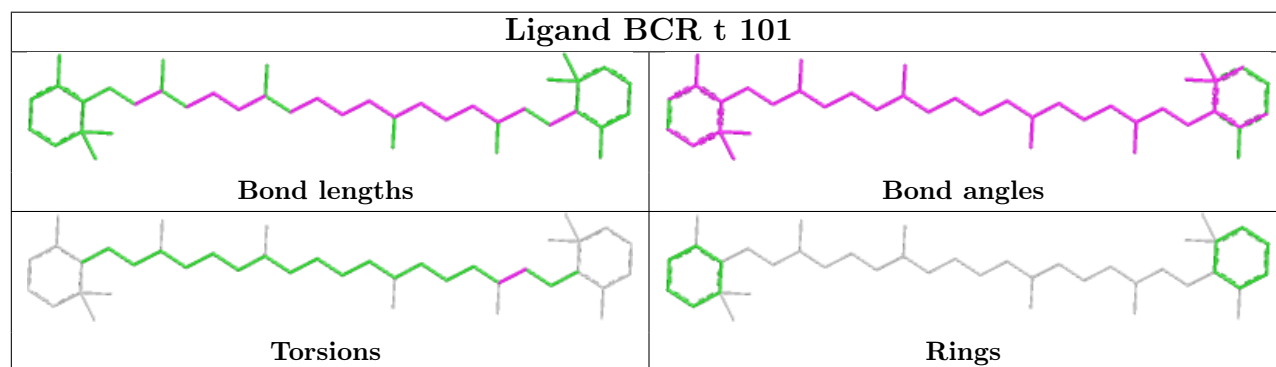
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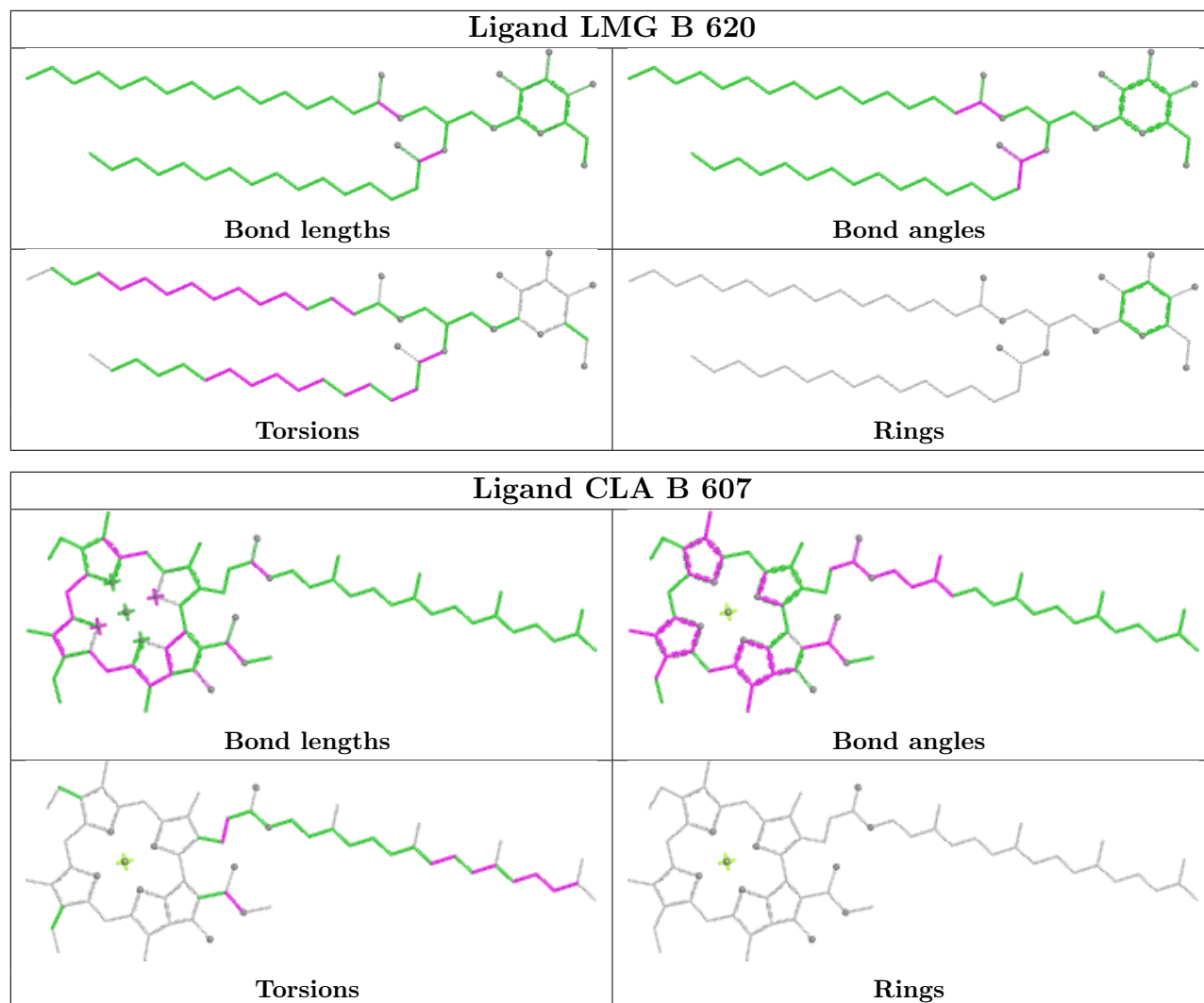


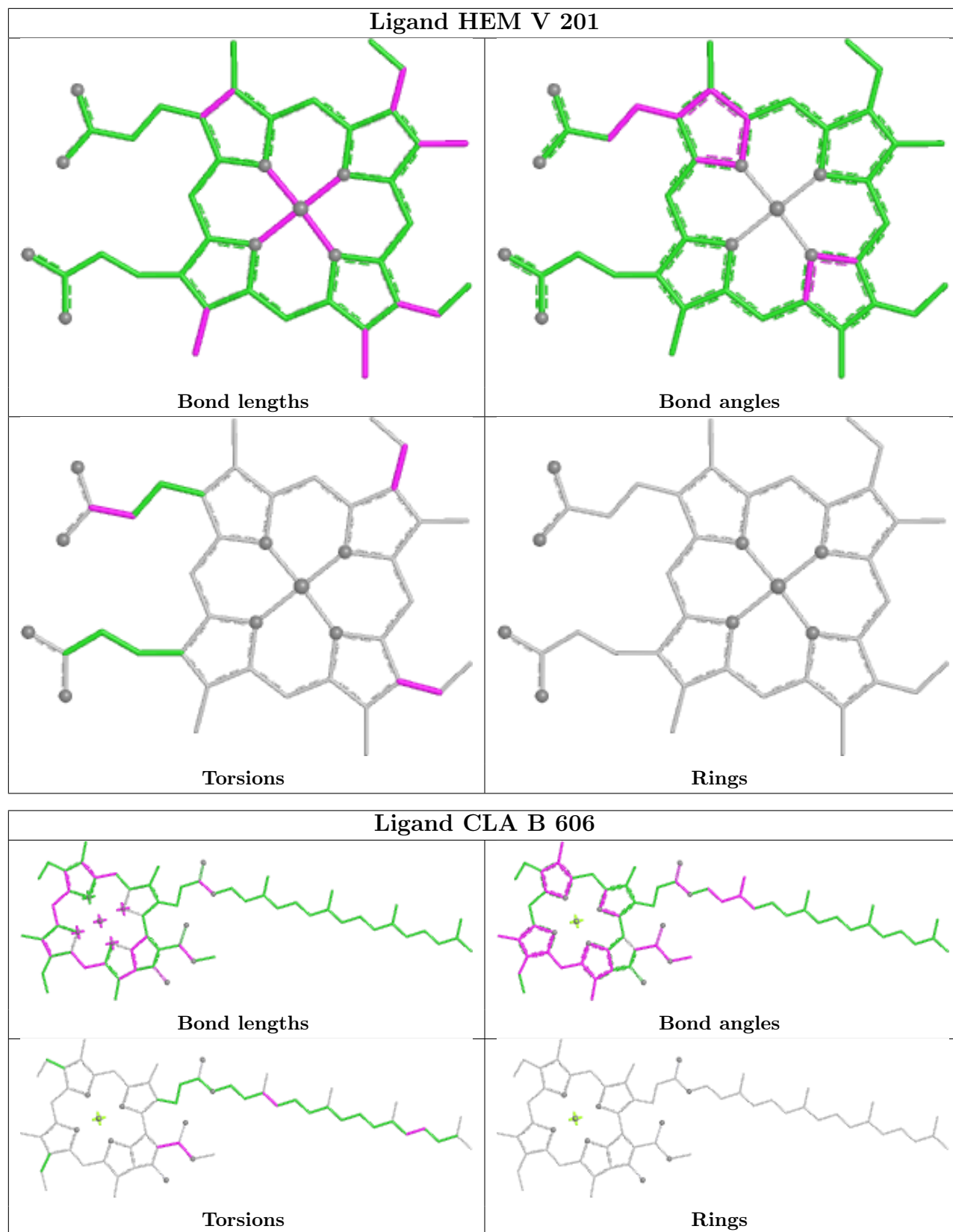
Ligand CLA C 505

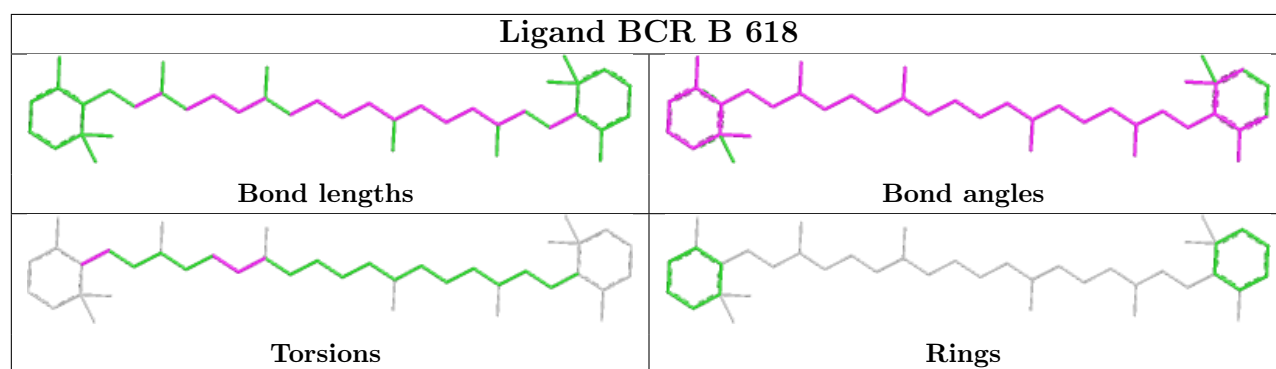
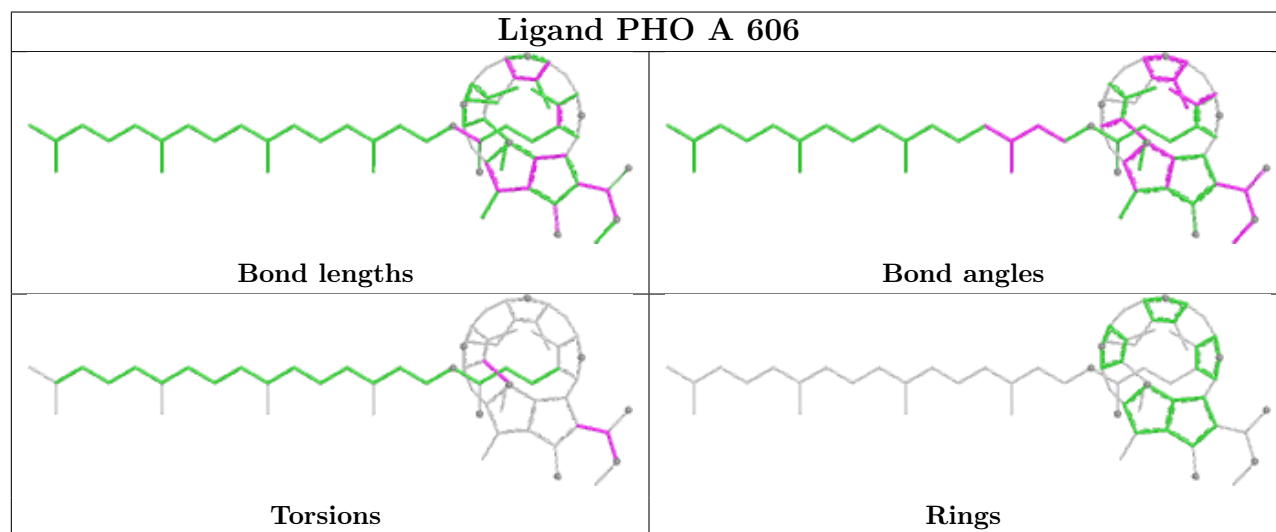
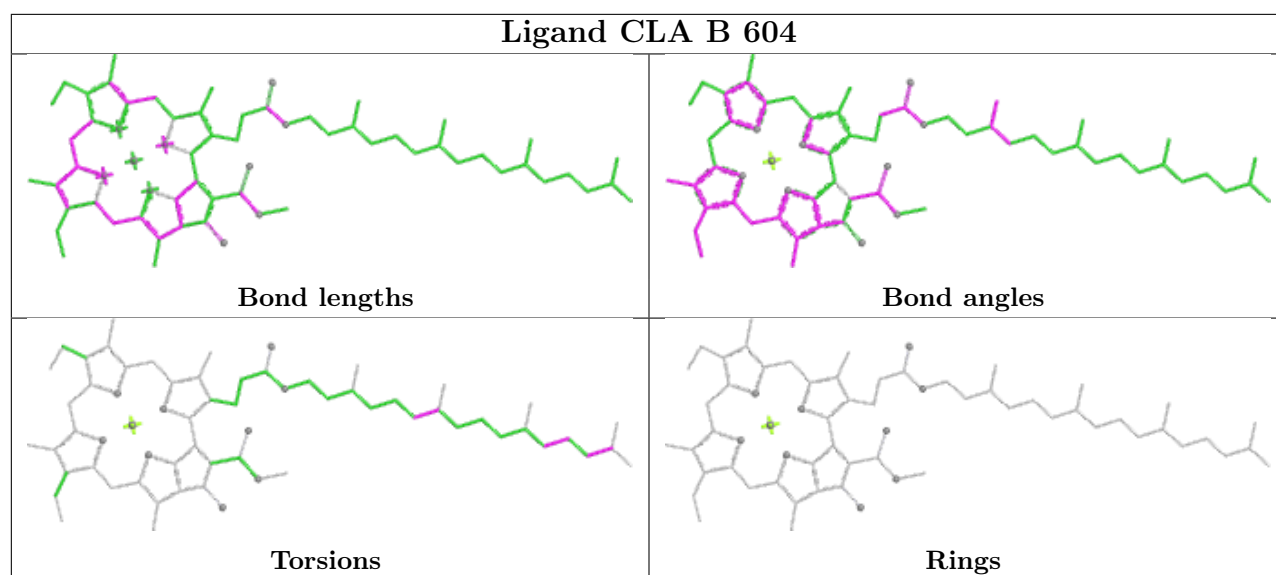


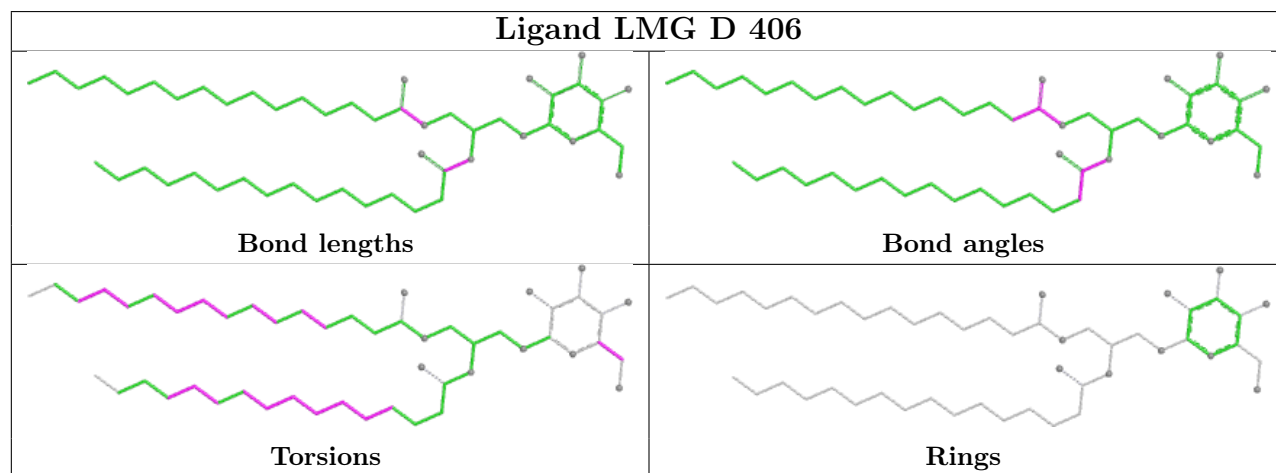
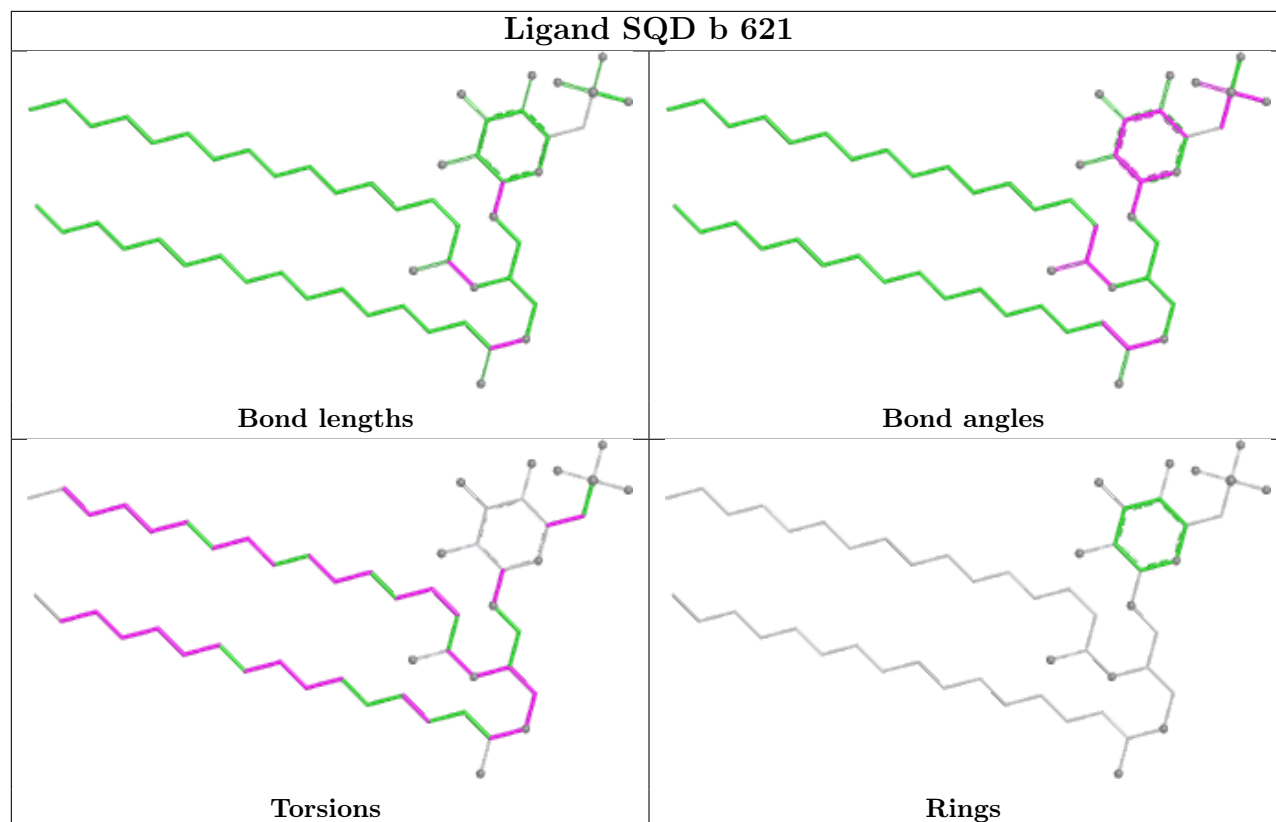
Ligand BCR t 101

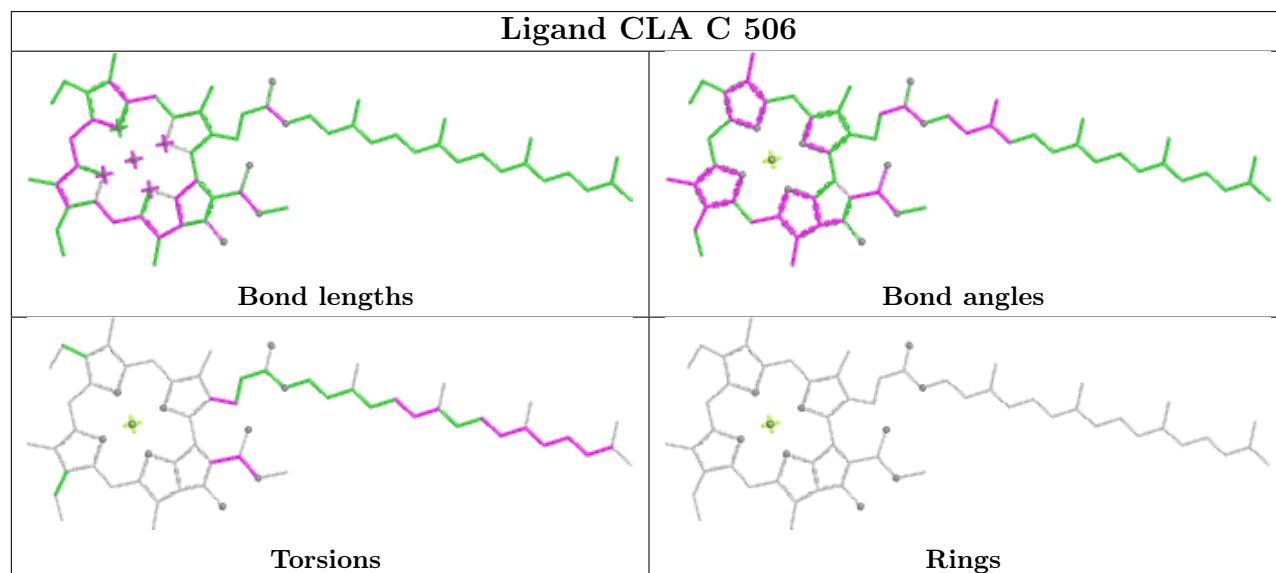
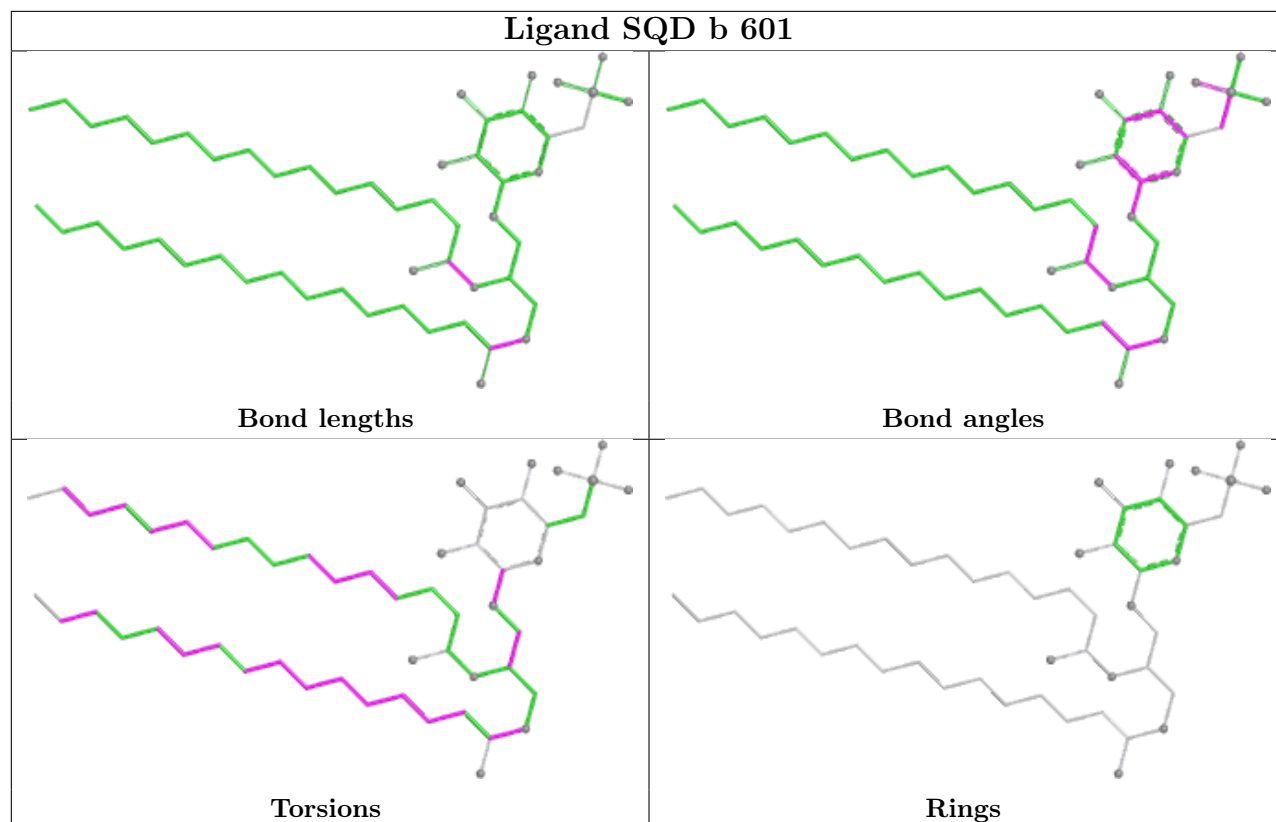


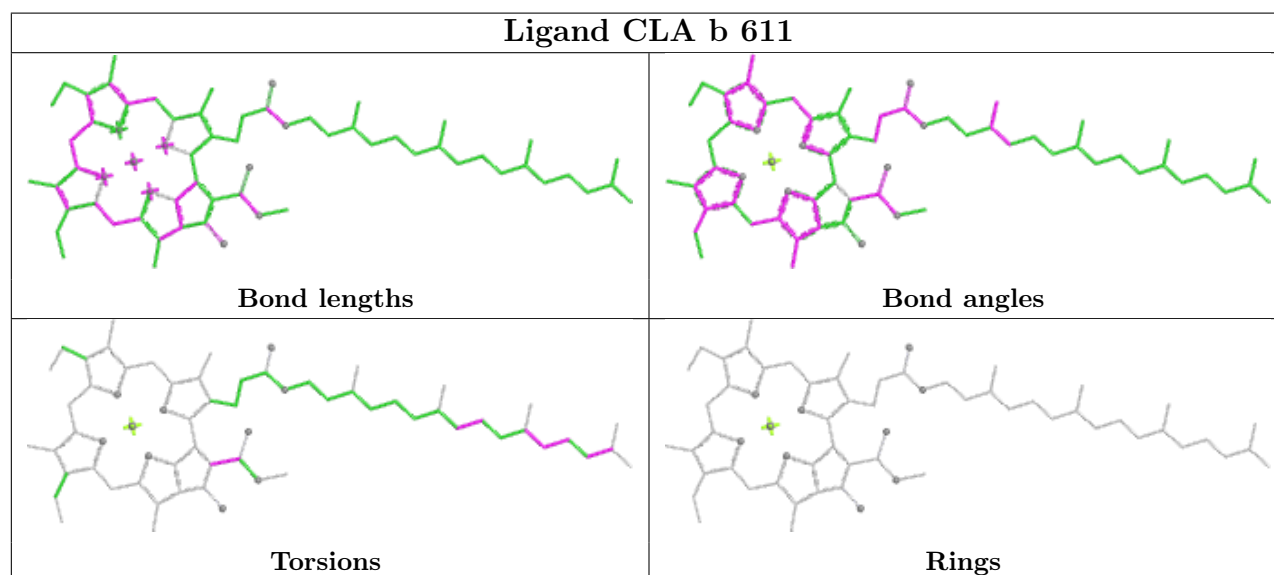
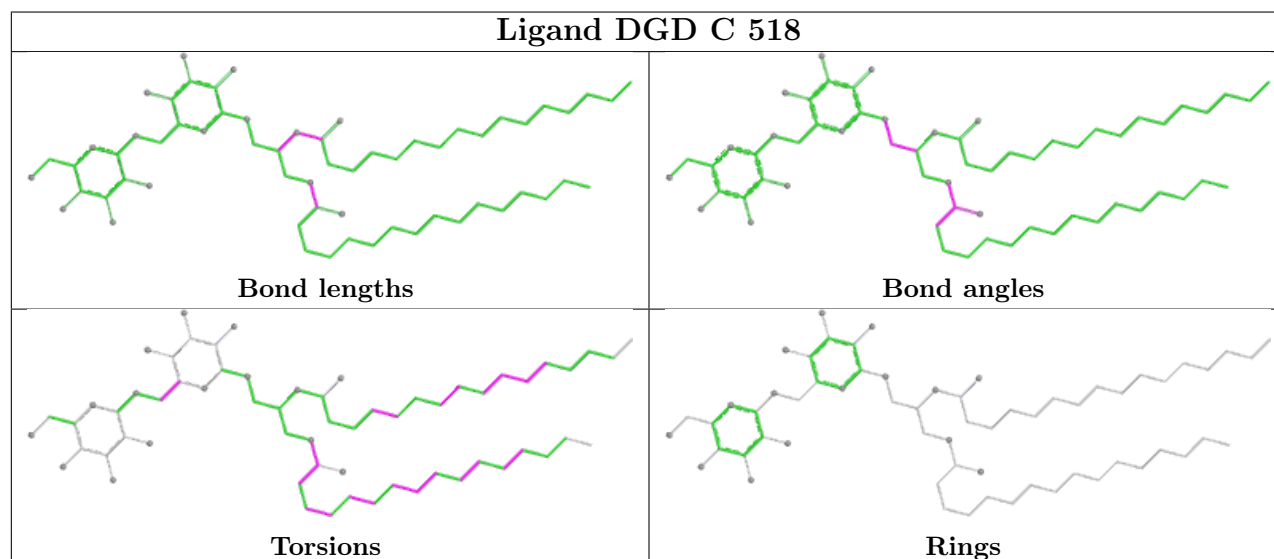
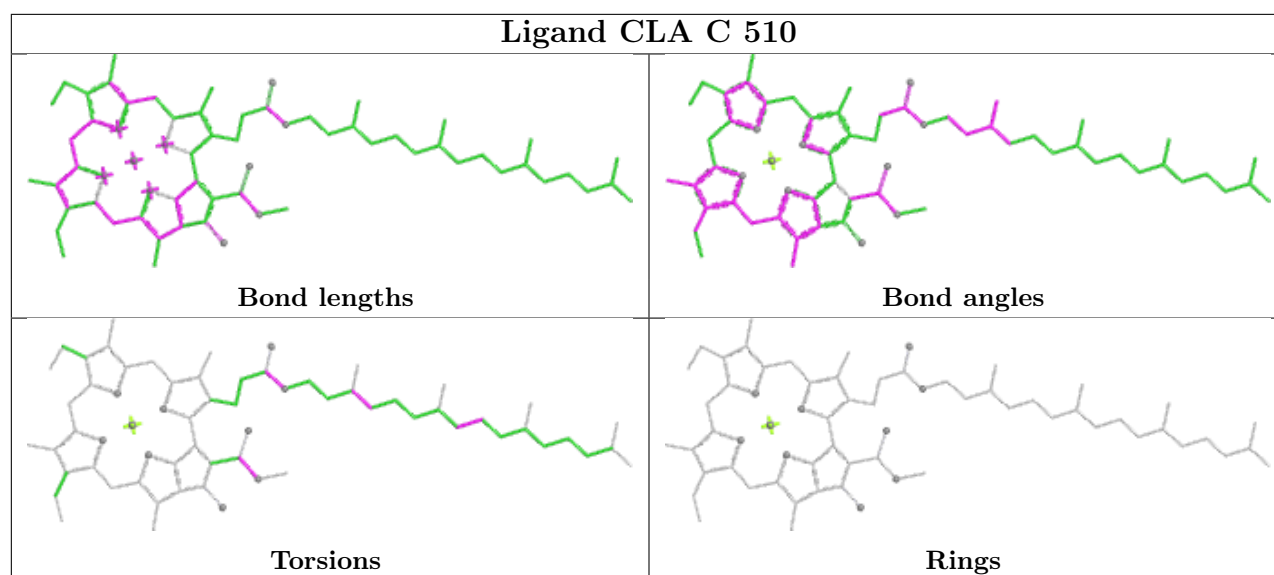


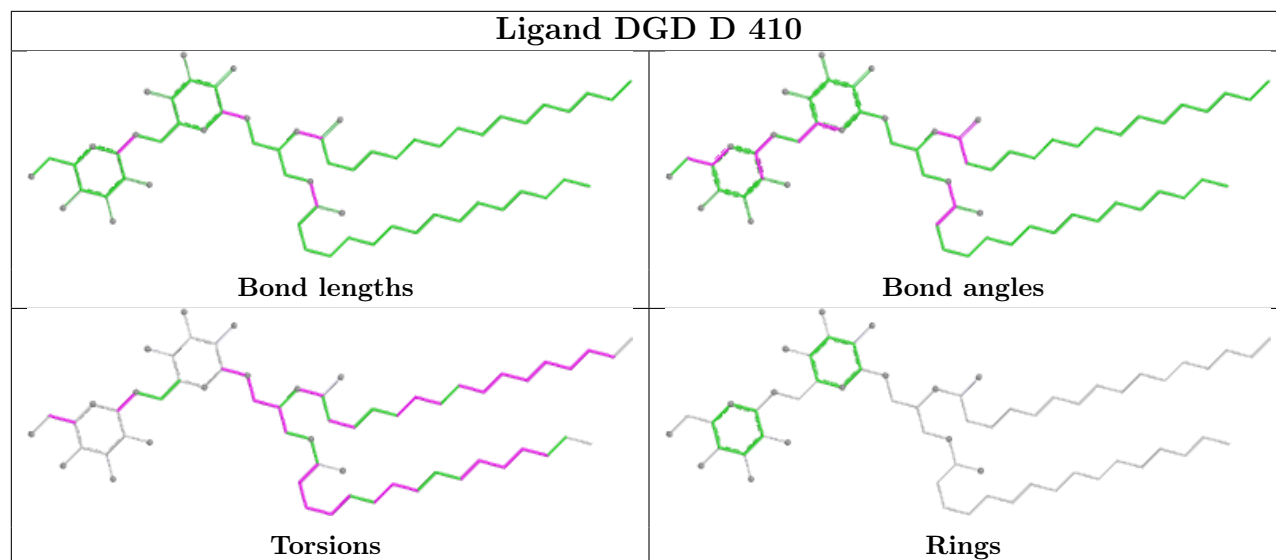
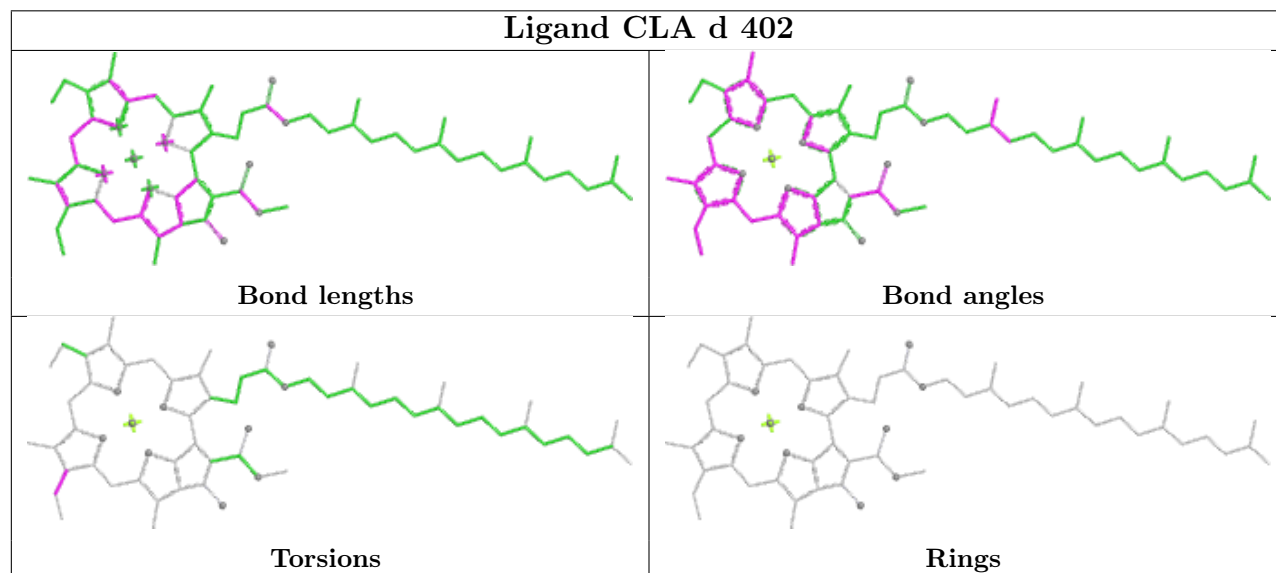
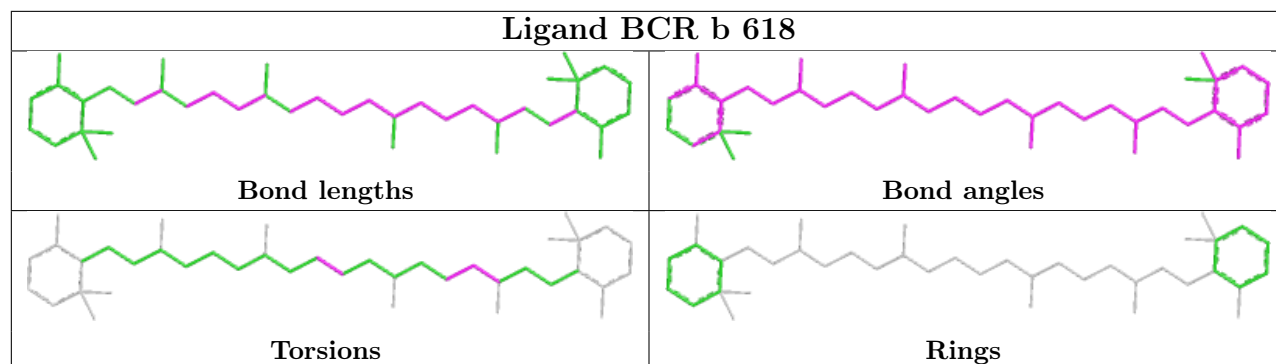


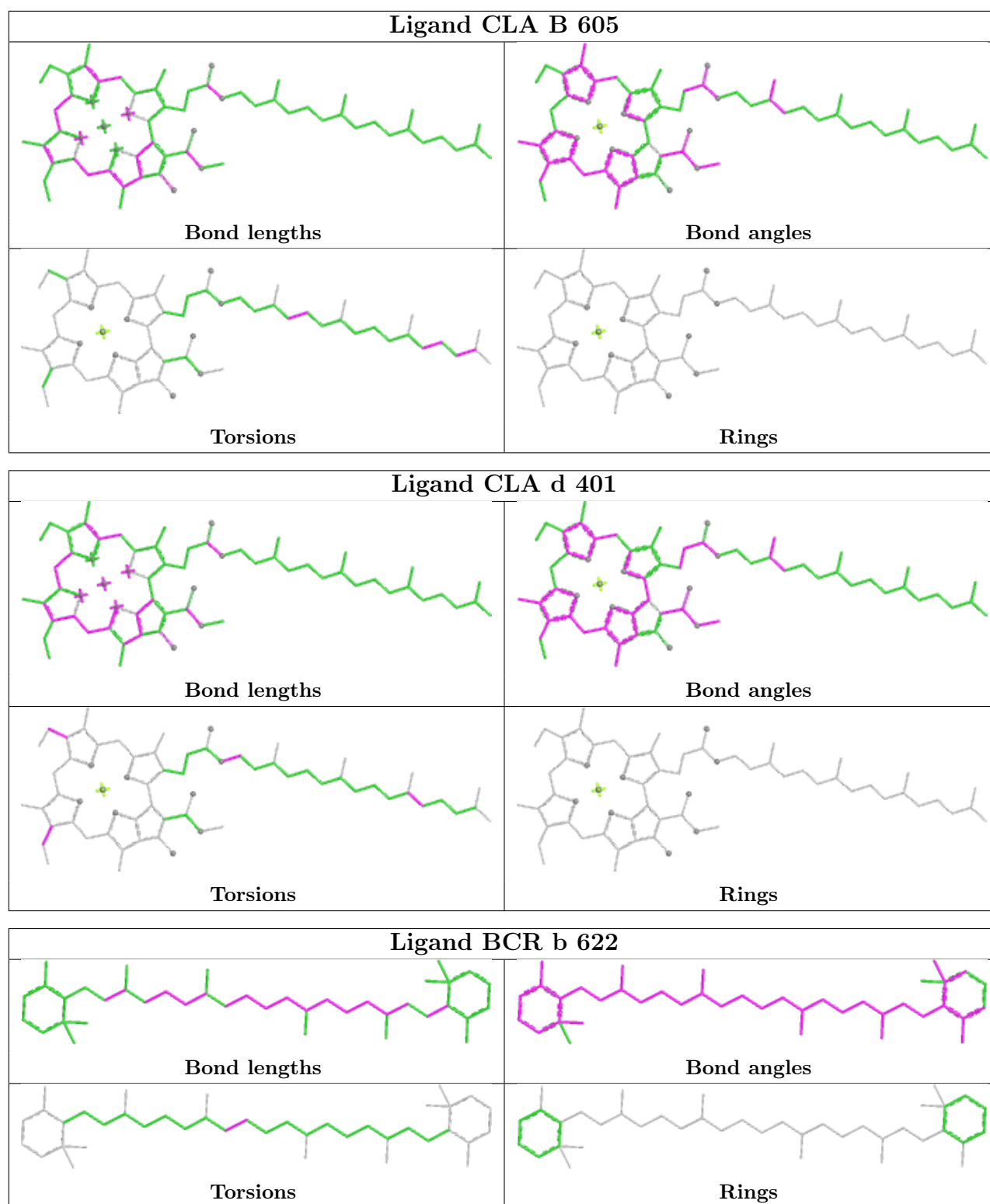




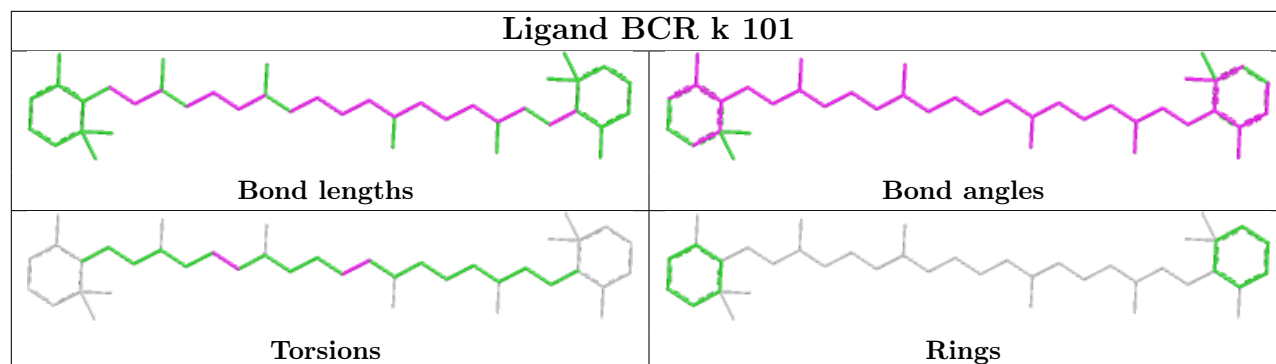




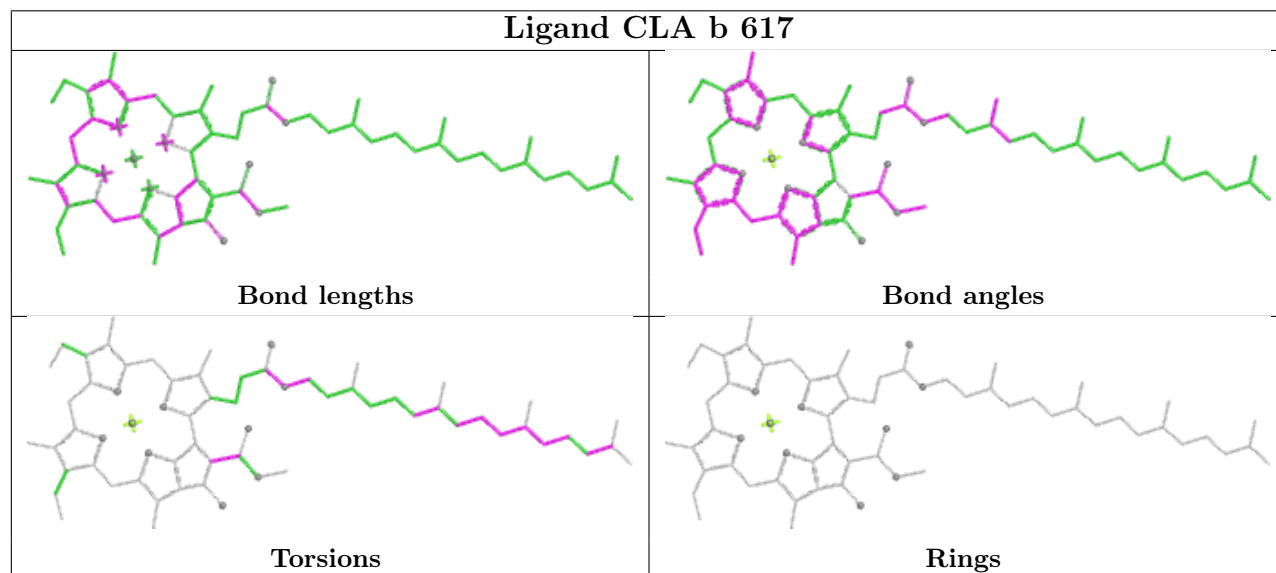




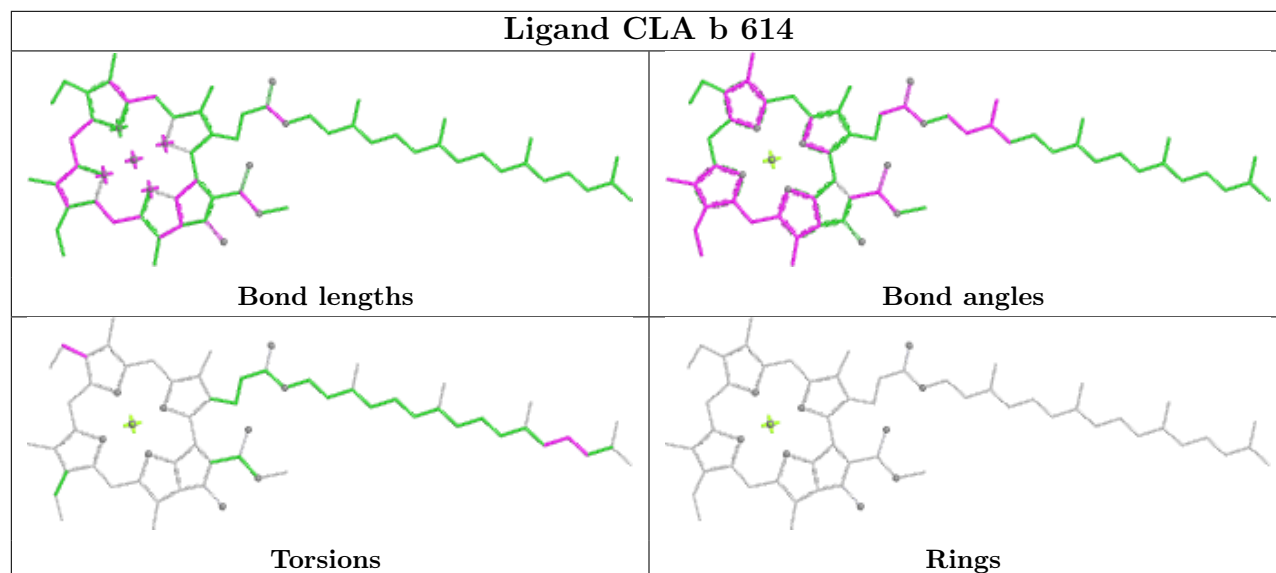
Ligand BCR k 101

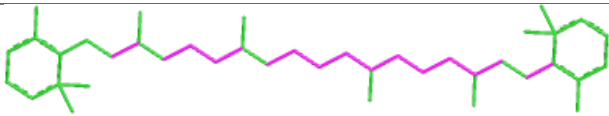
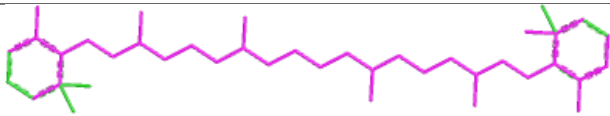
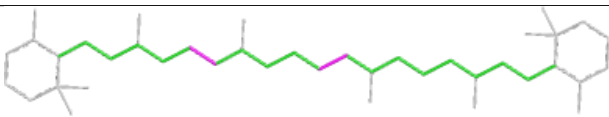
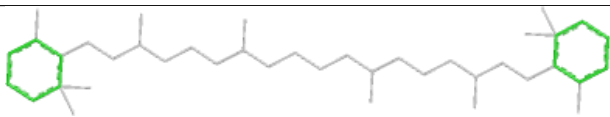


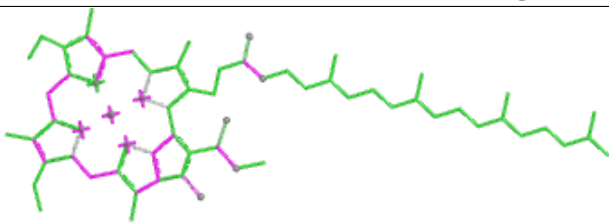
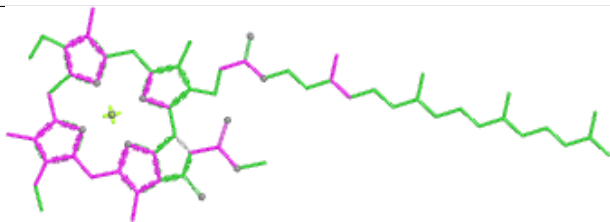
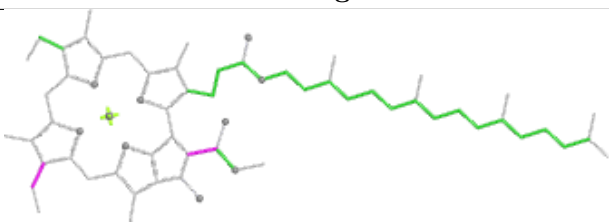
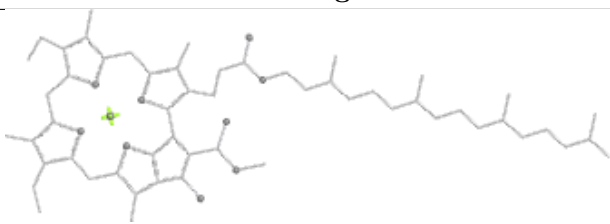
Ligand CLA b 617

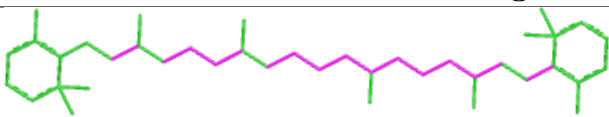
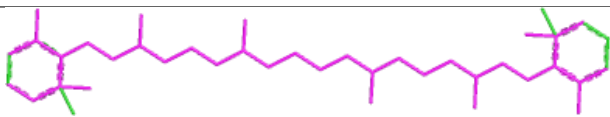
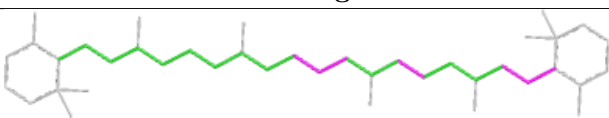
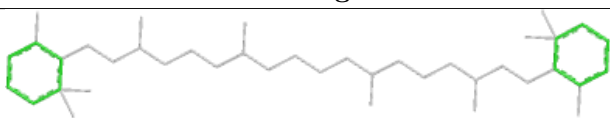


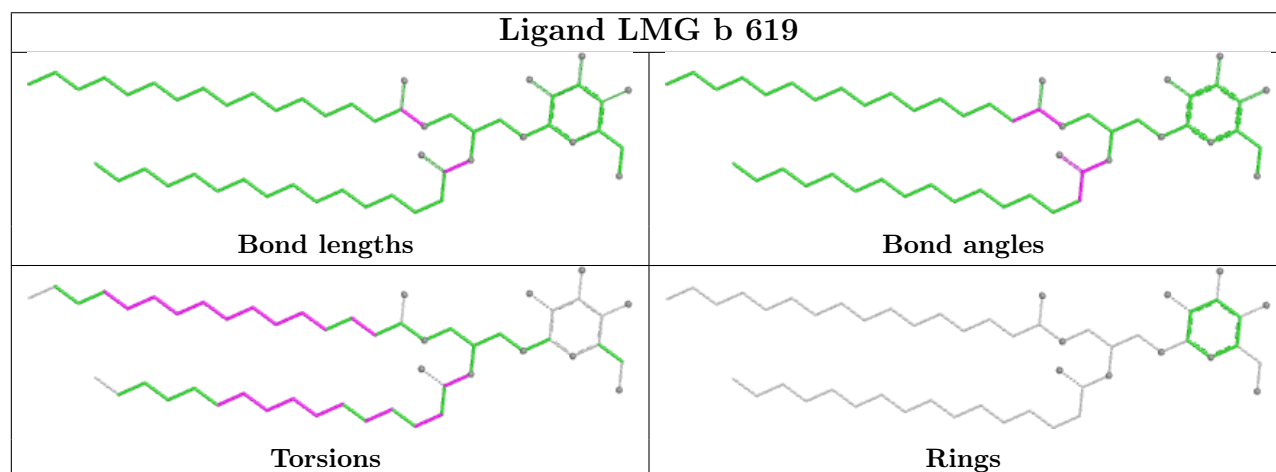
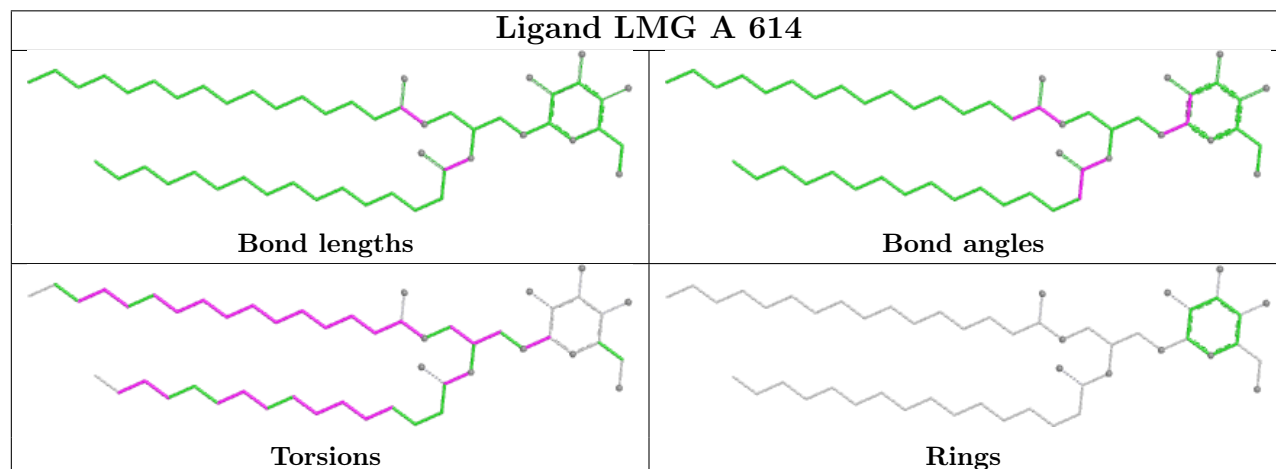
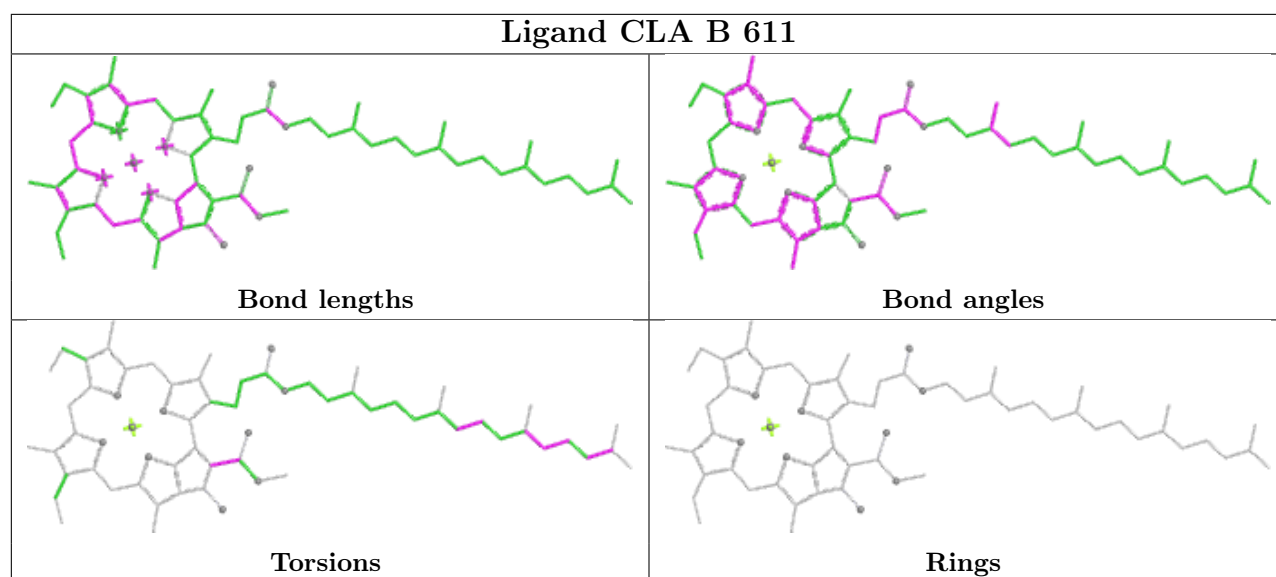
Ligand CLA b 614

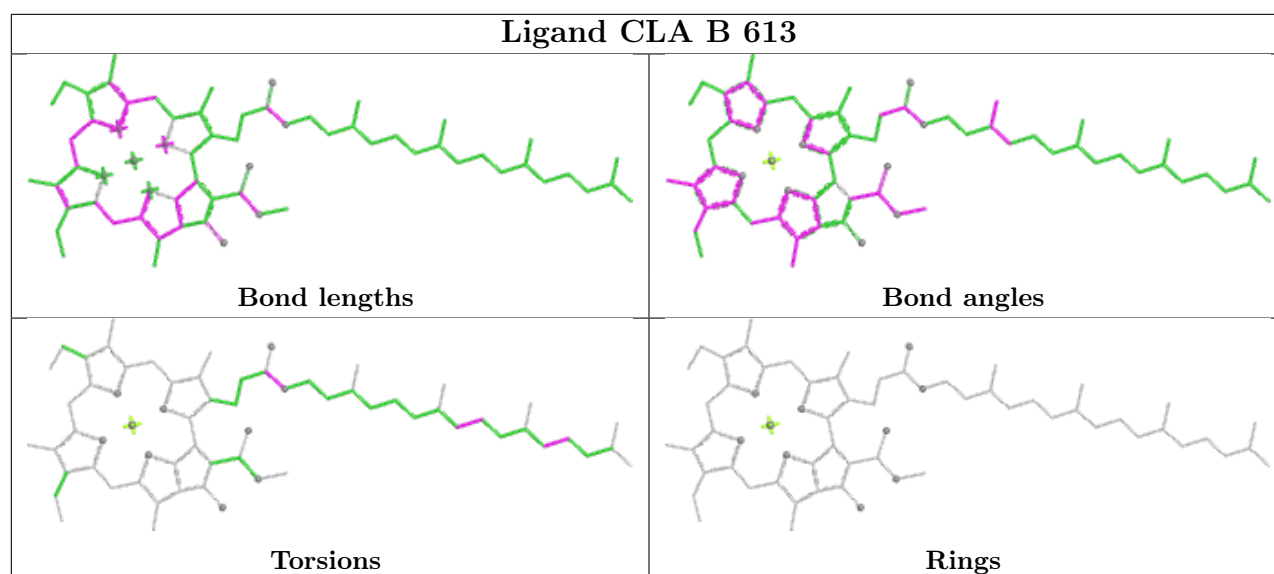
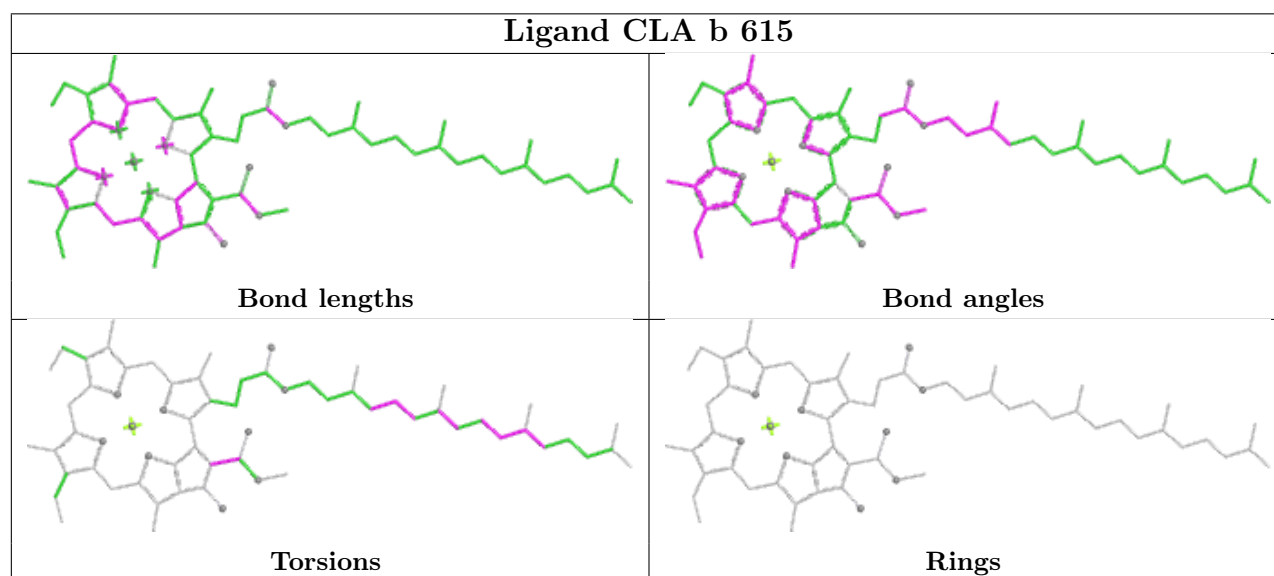
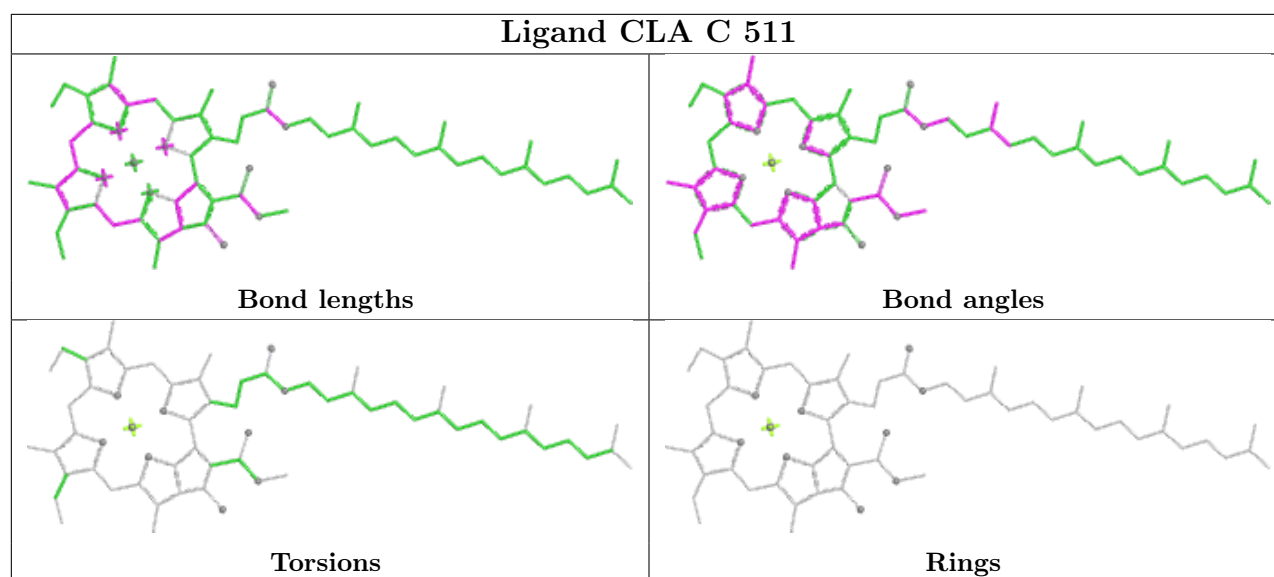


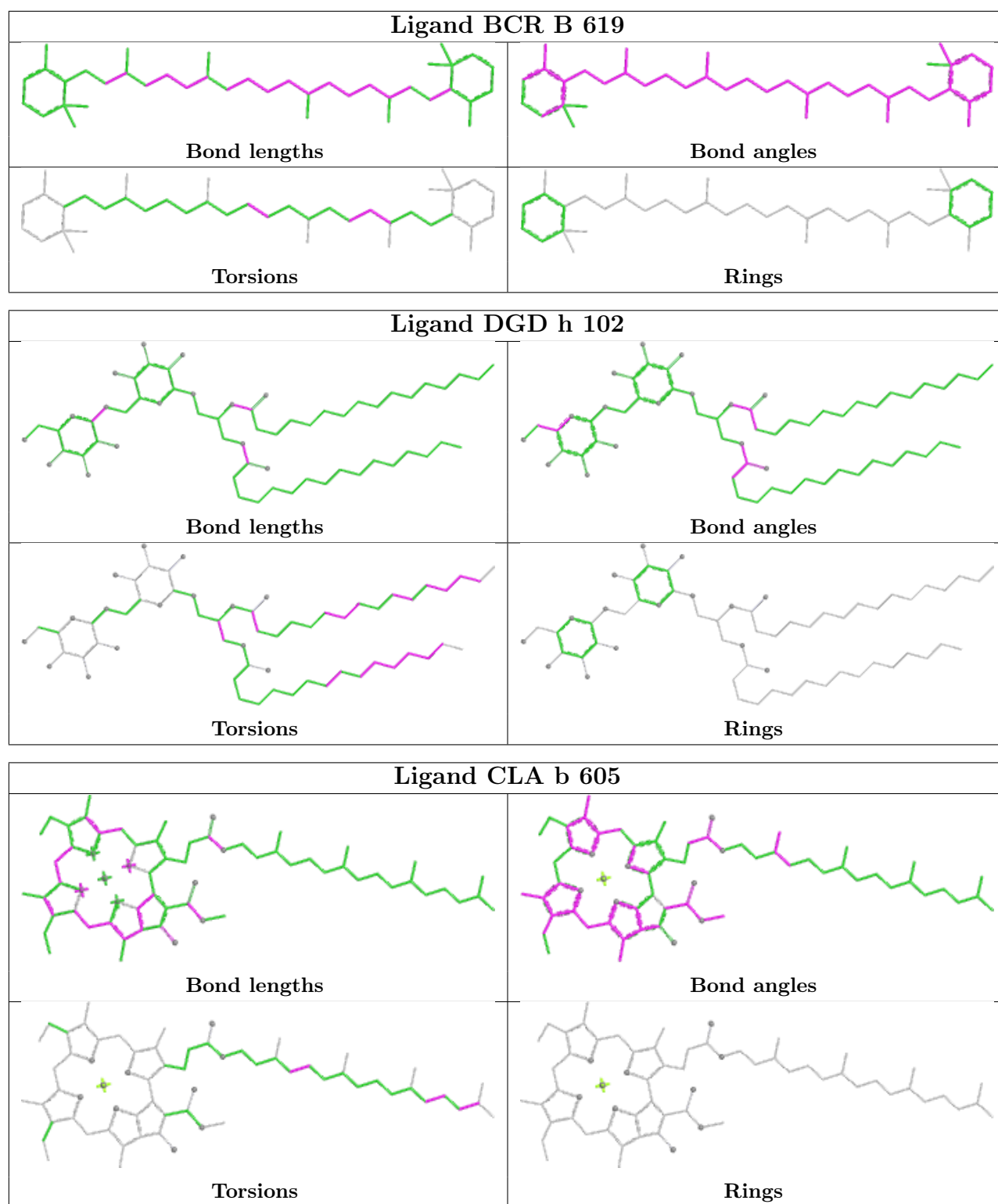
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

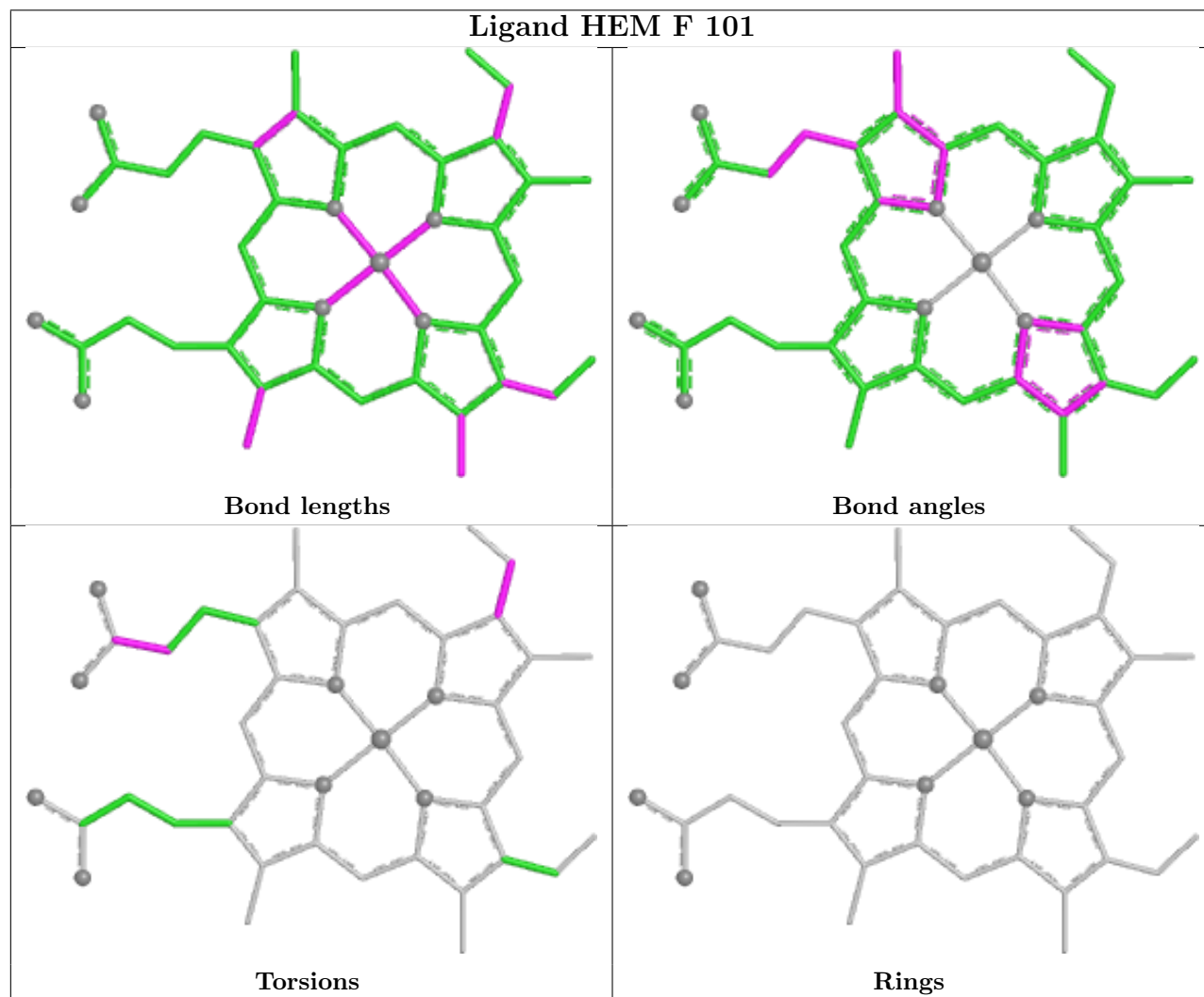
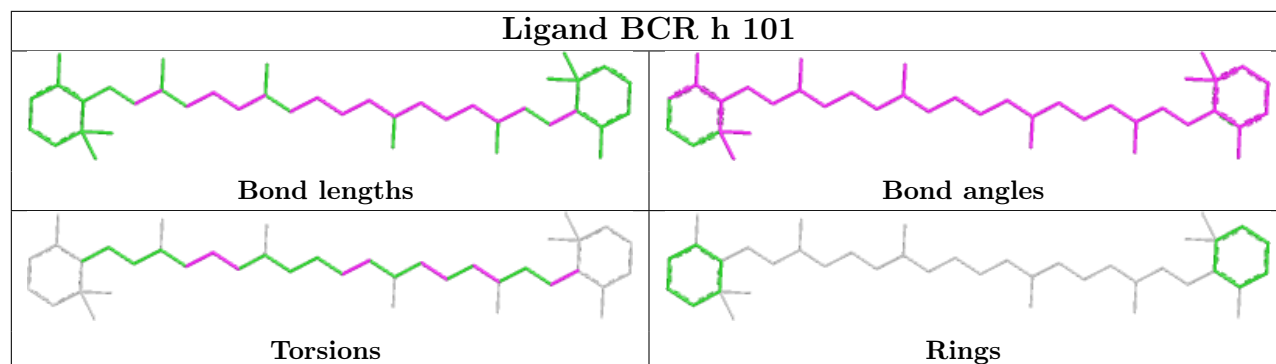
Ligand CLA a 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

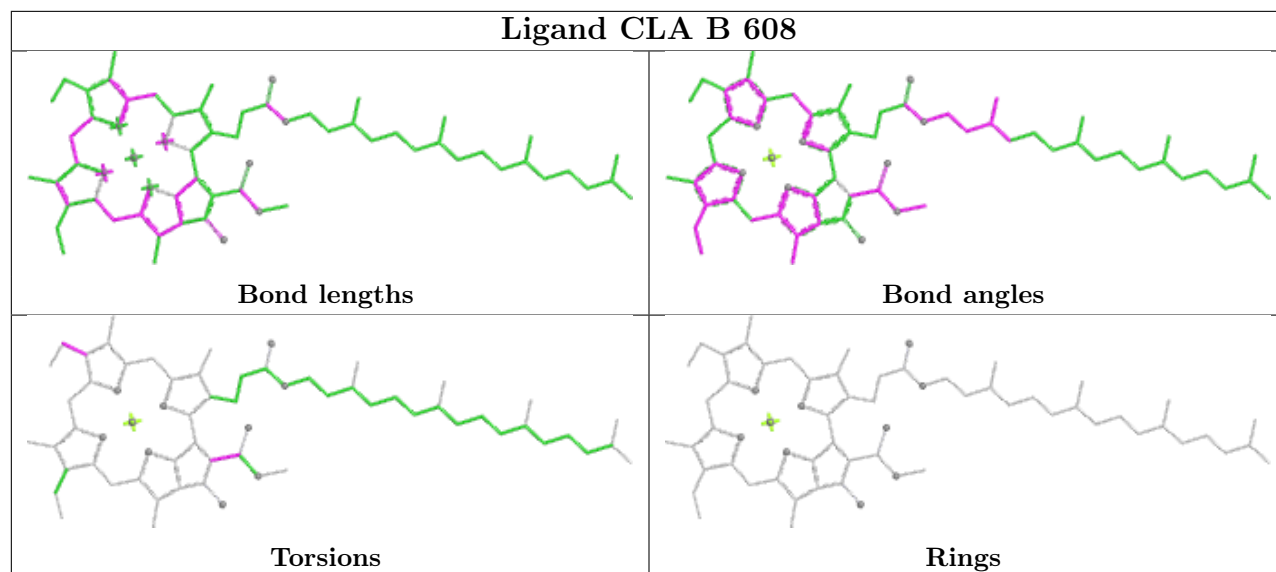




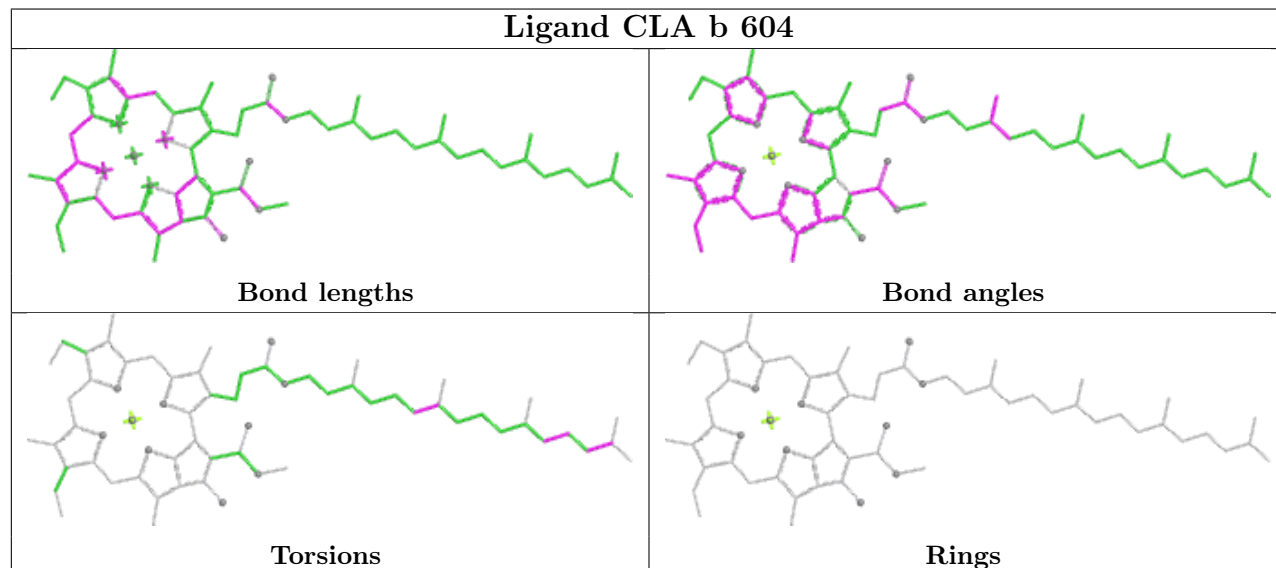




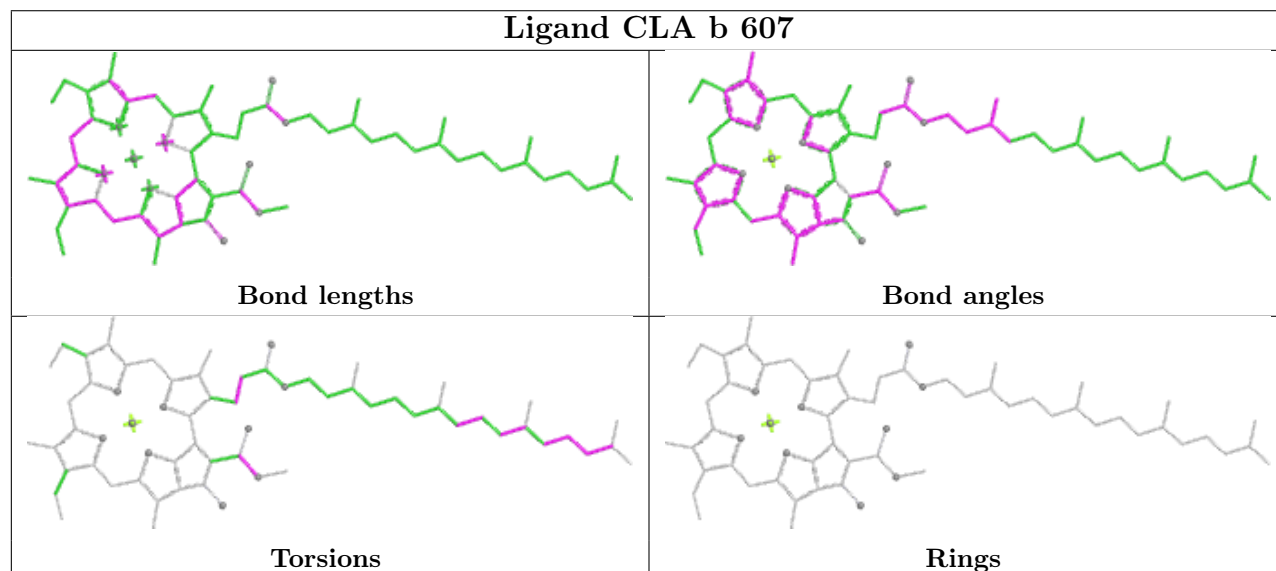
Ligand CLA B 608

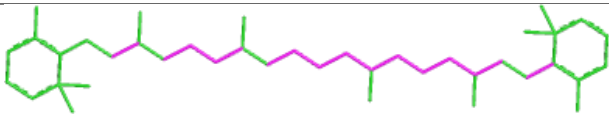
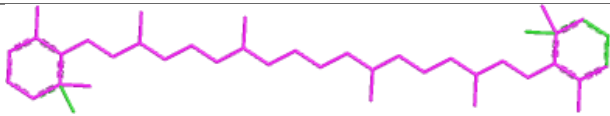
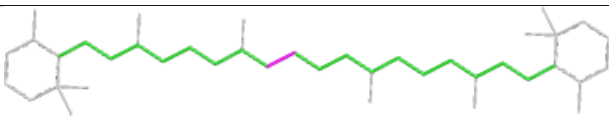
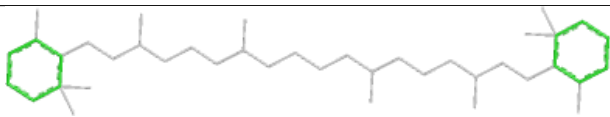


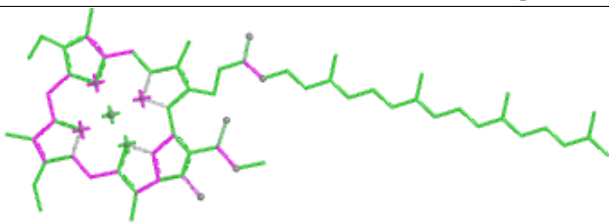
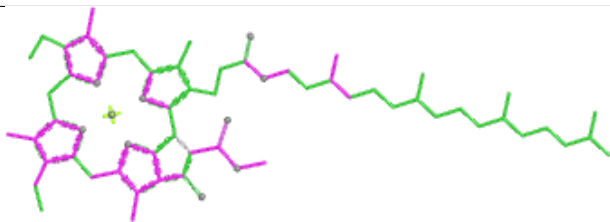
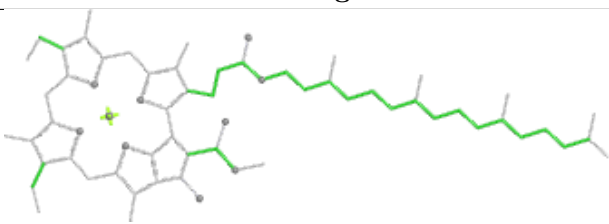
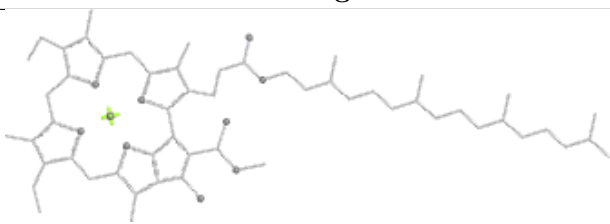
Ligand CLA b 604

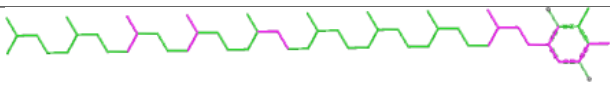
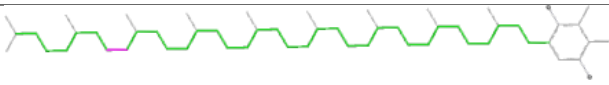
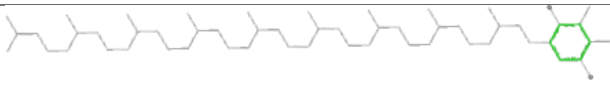


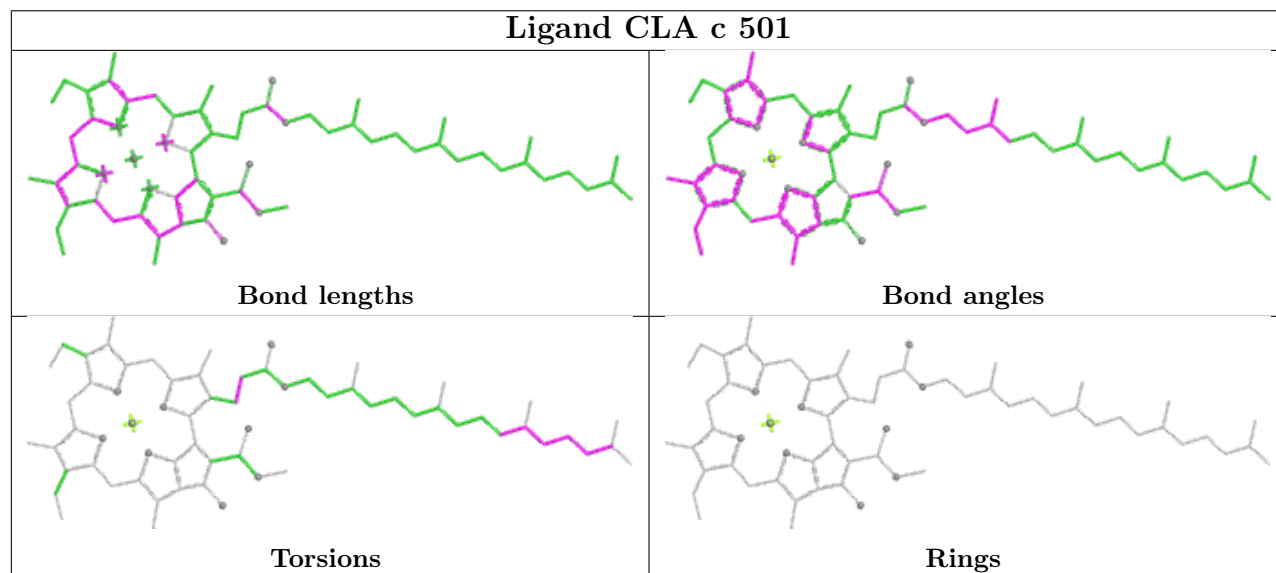
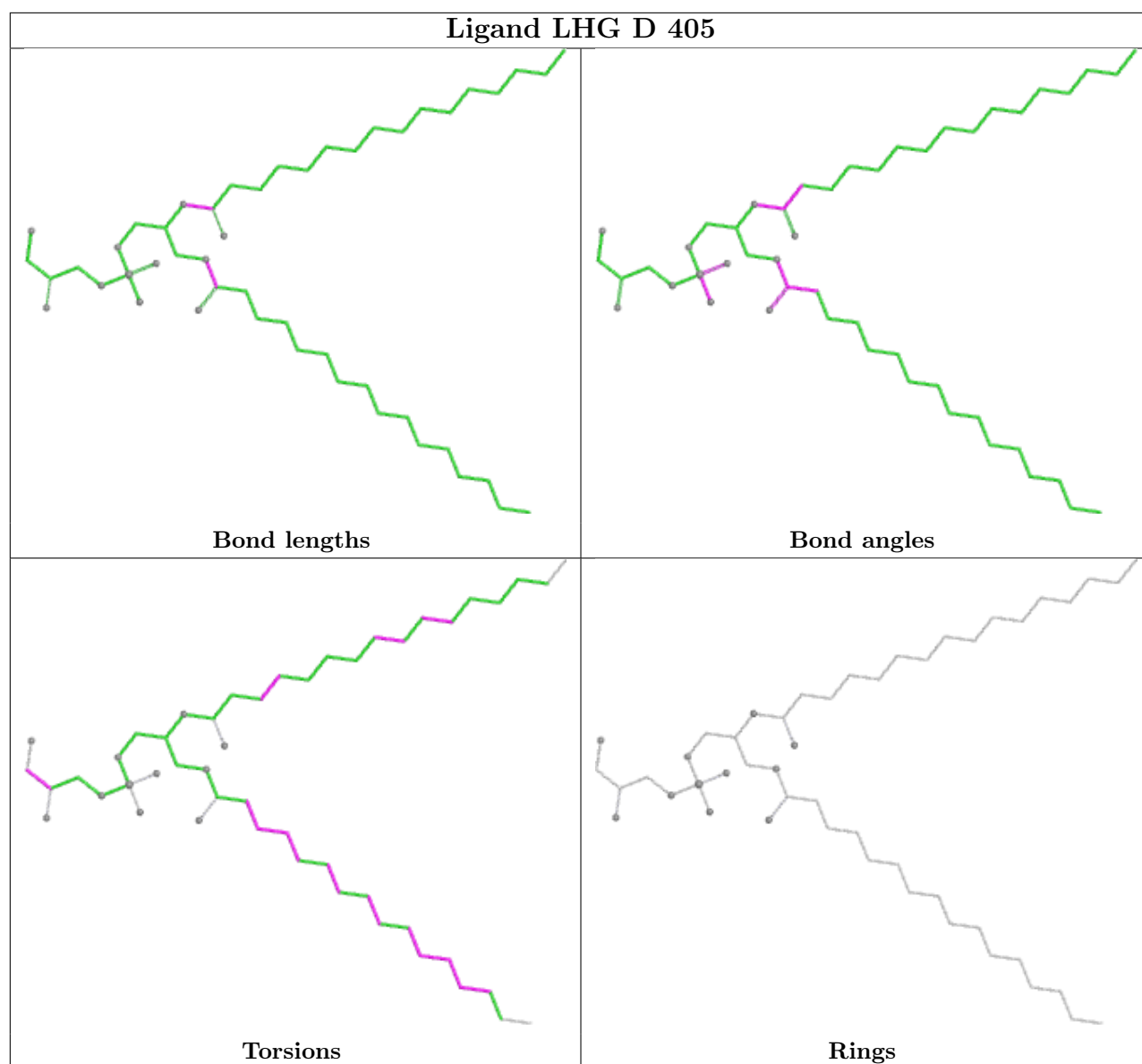
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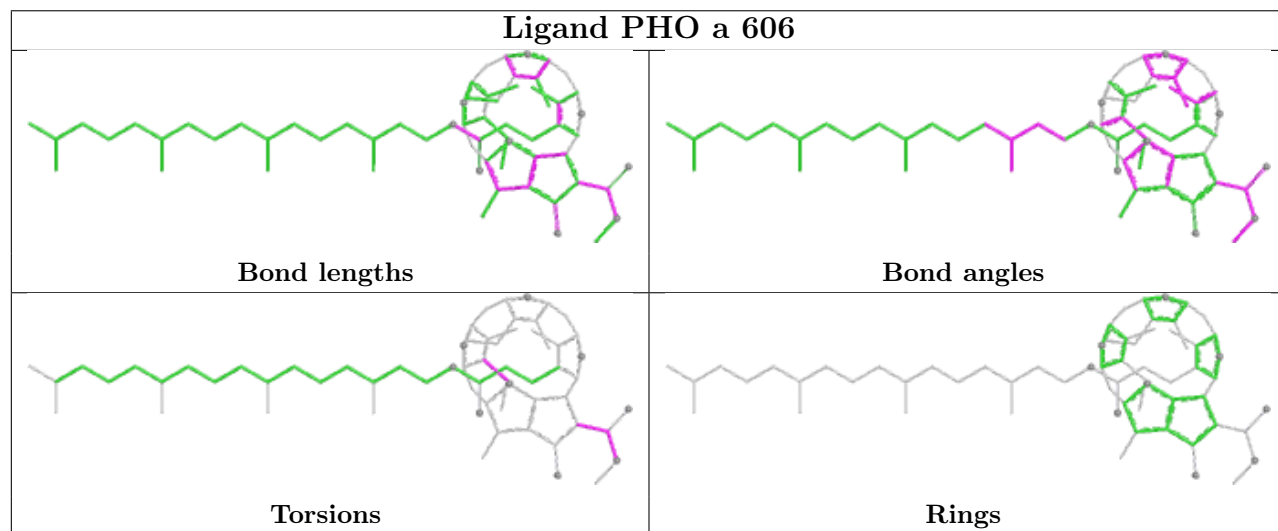
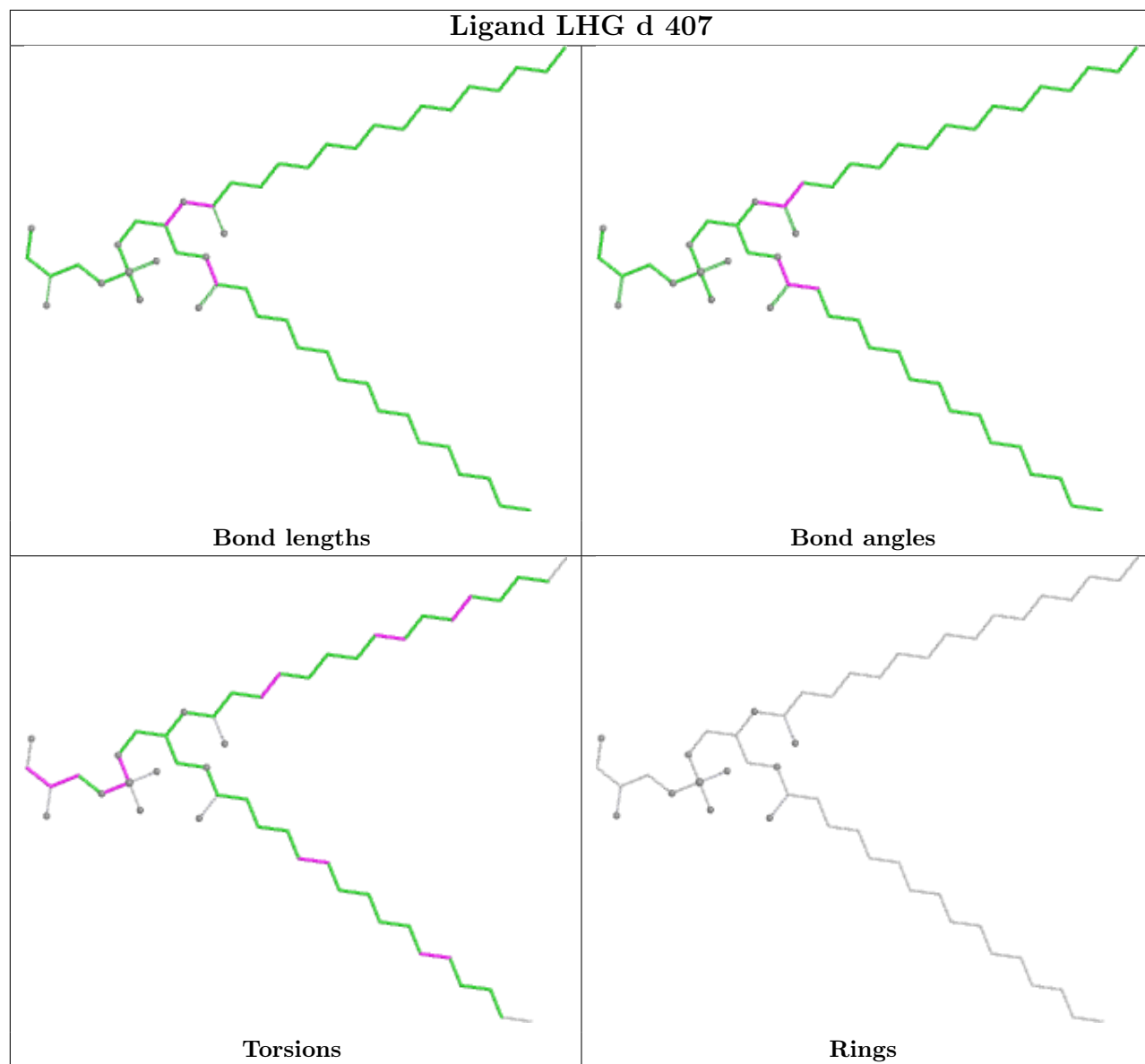


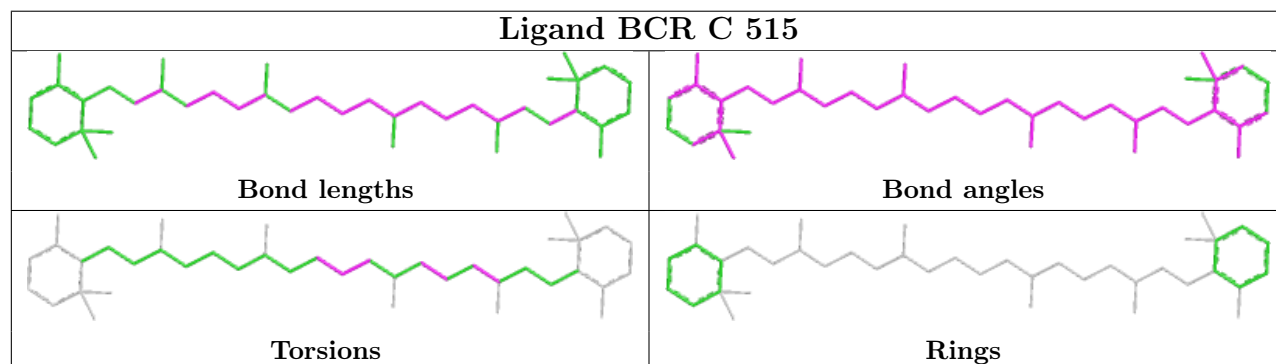
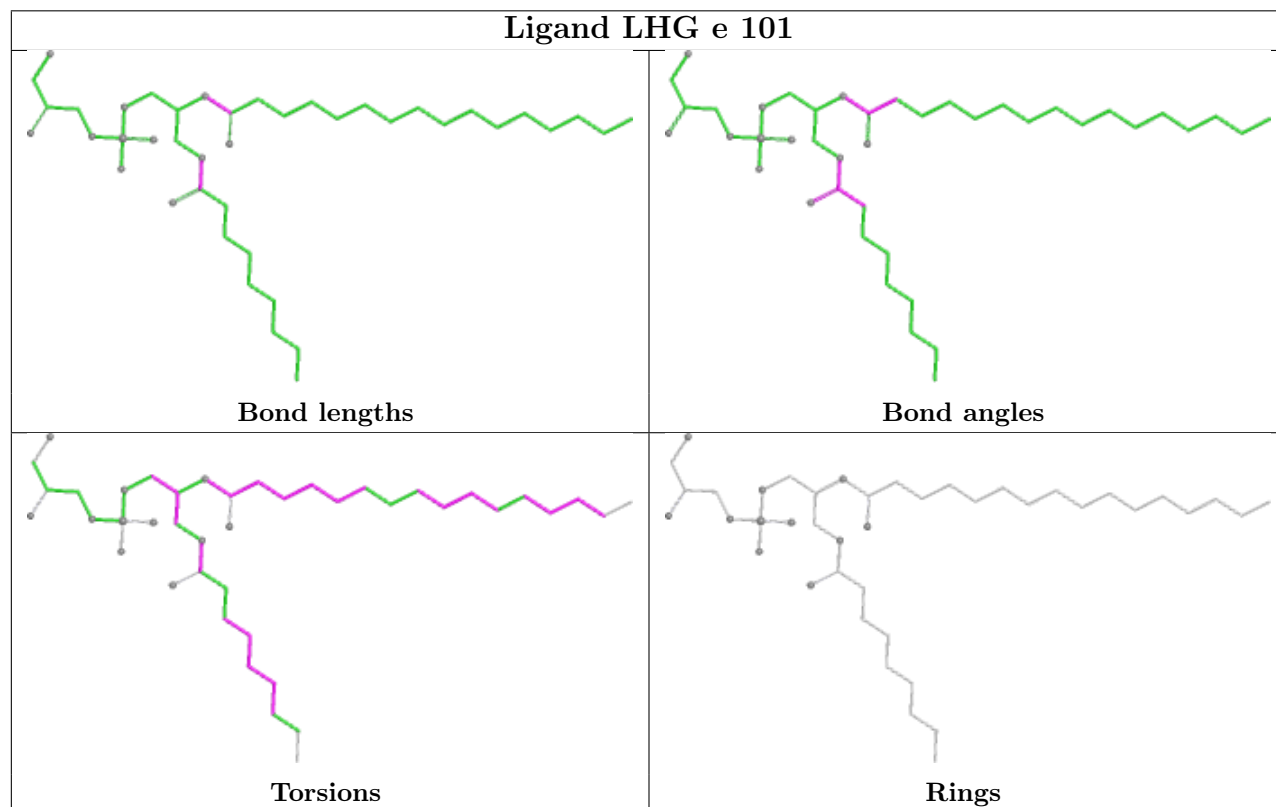
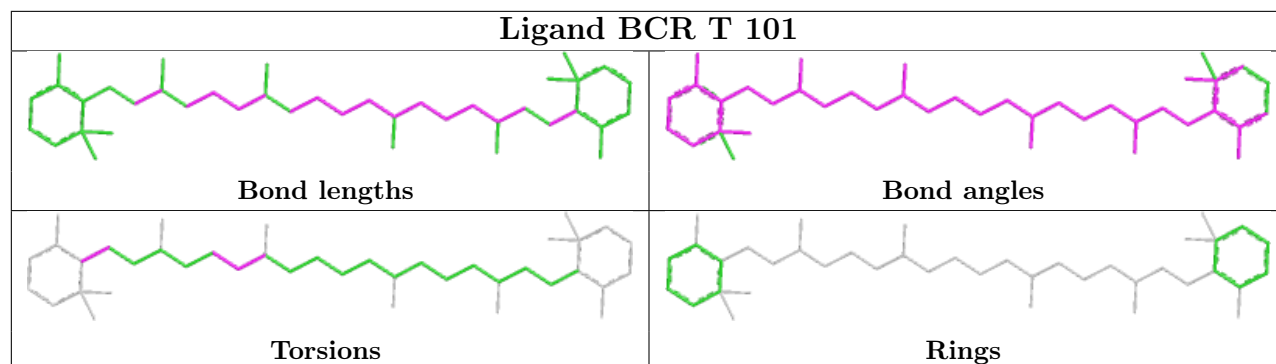
Ligand BCR B 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

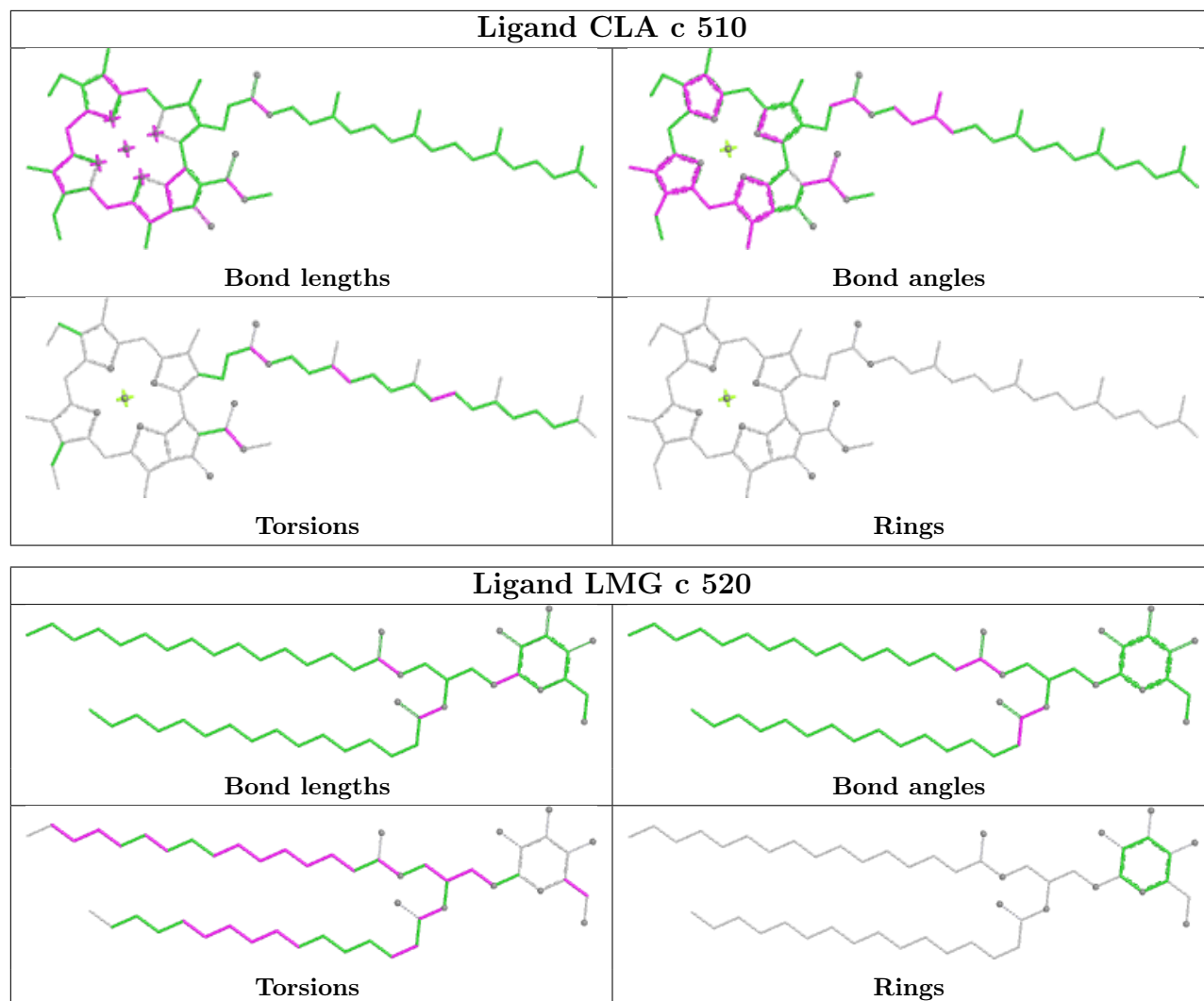
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Bond lengths	Bond angles
	
Torsions	Rings

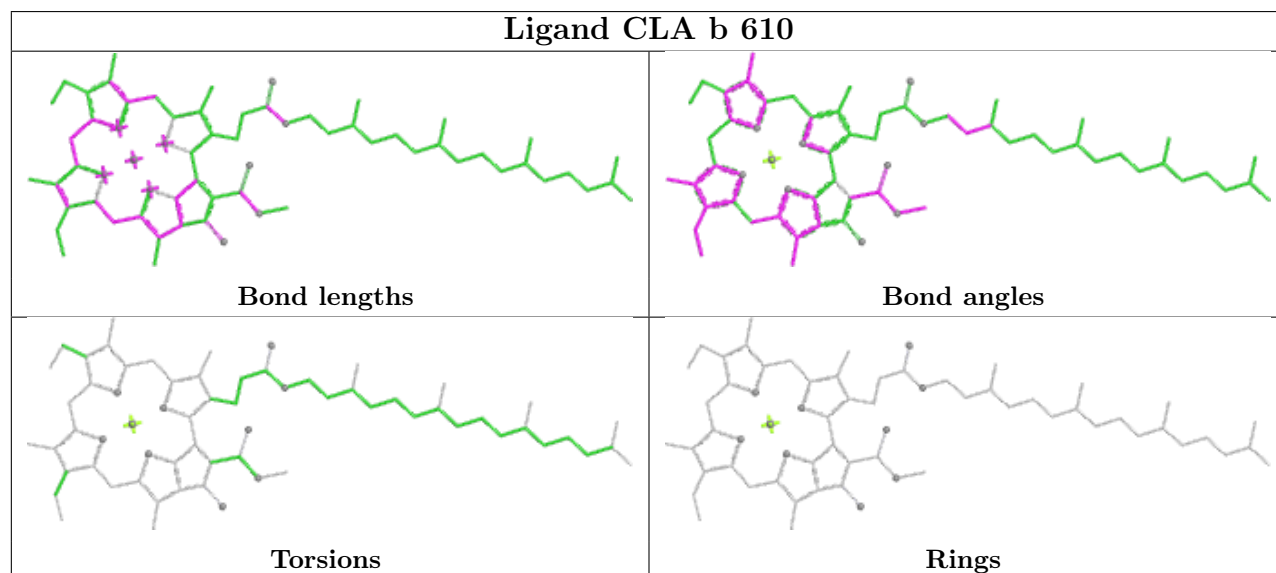
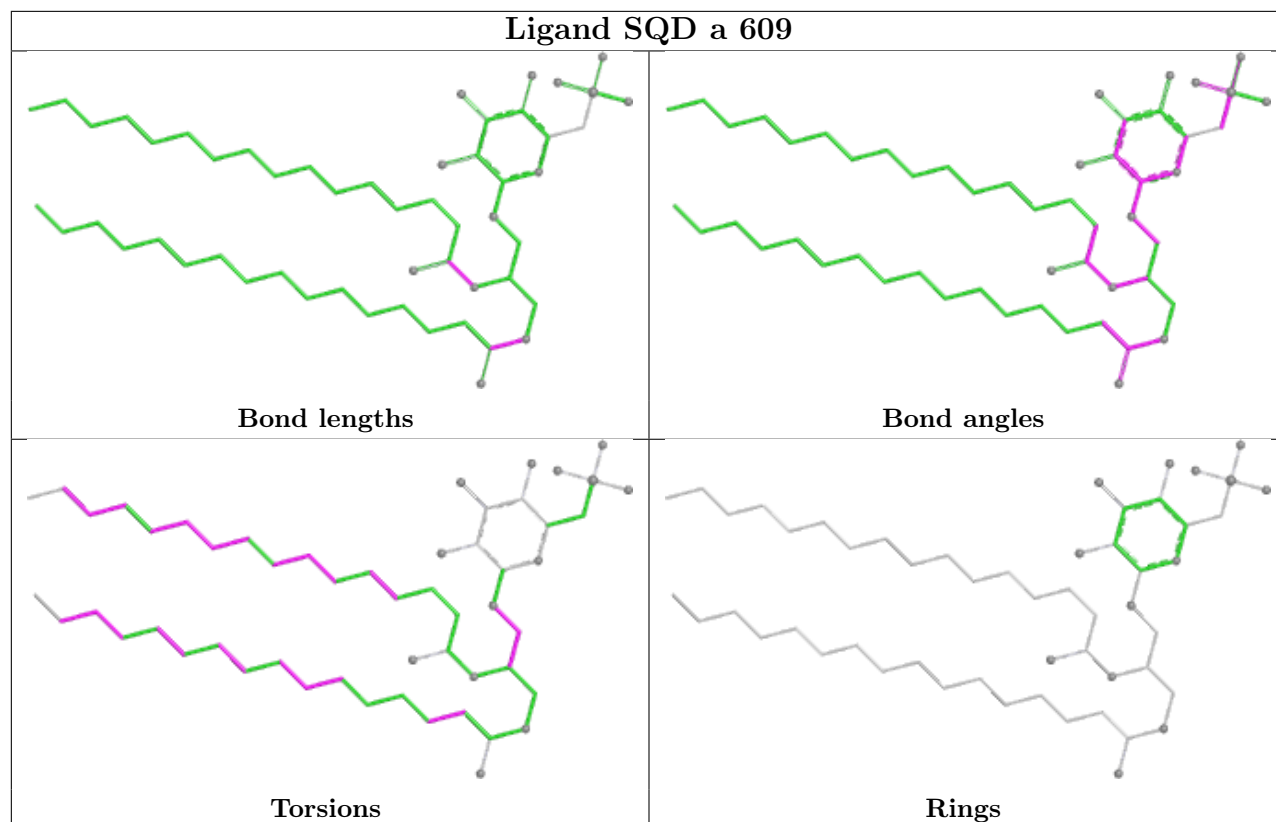
Ligand PL9 D 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

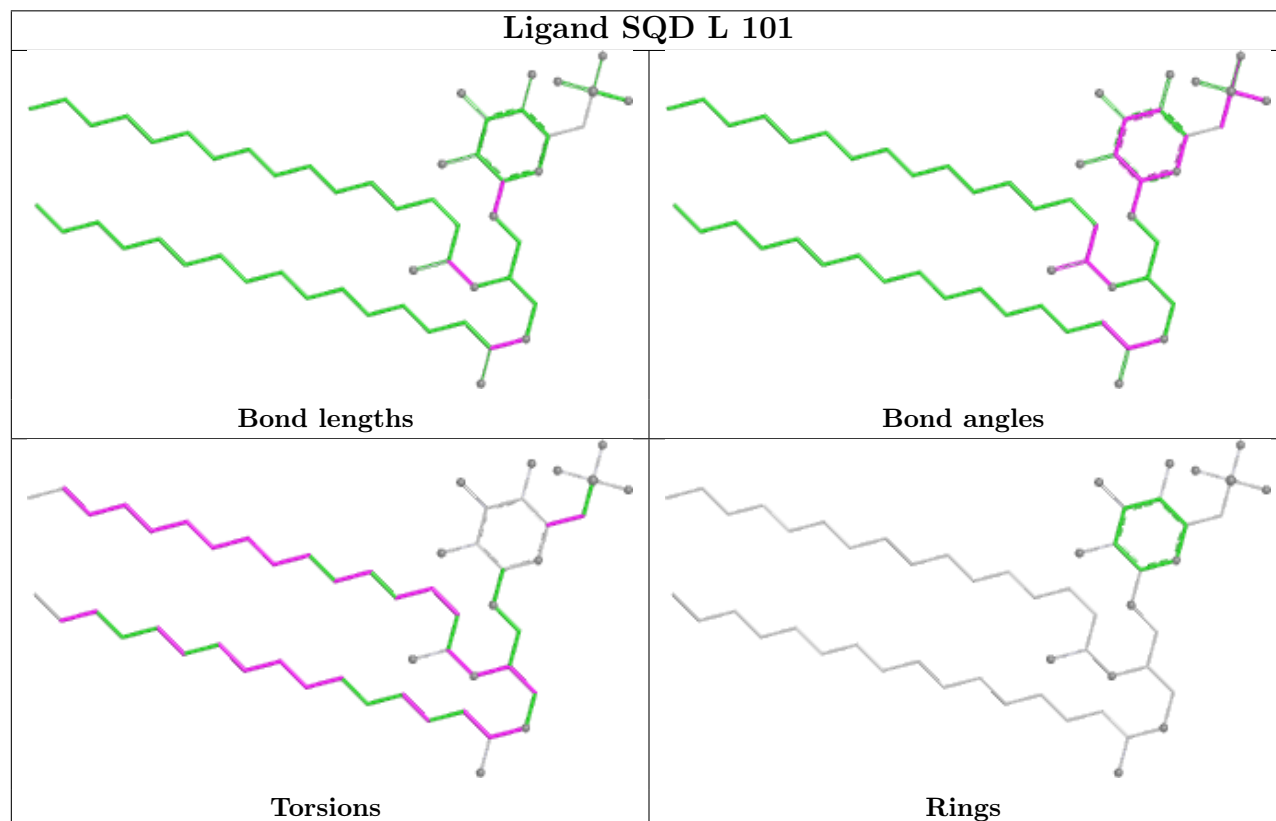
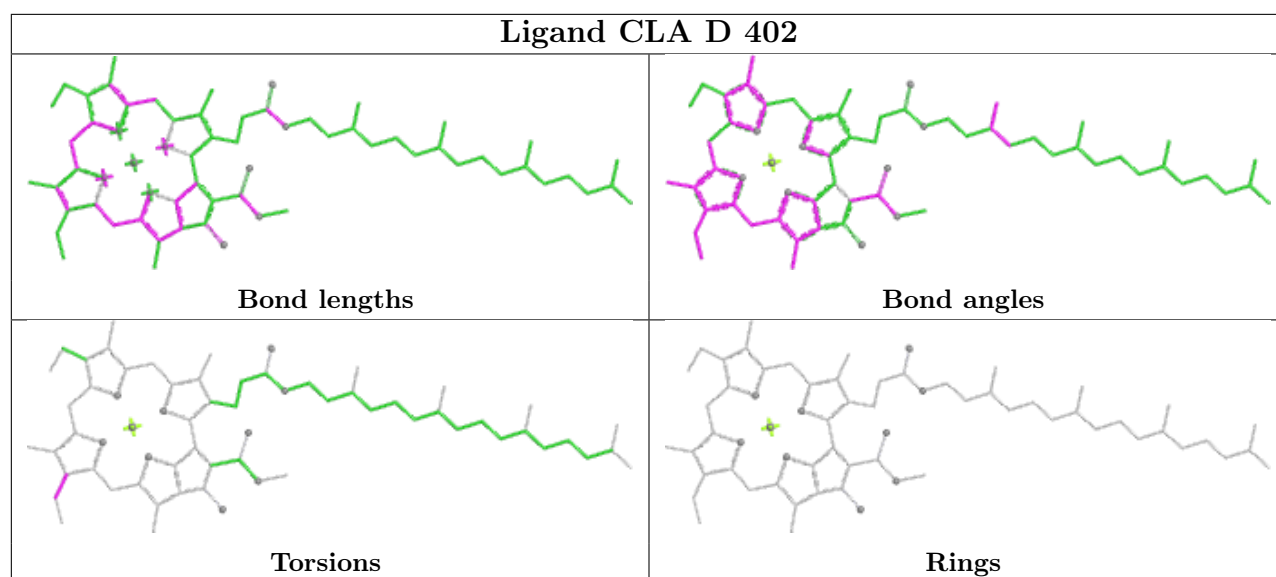


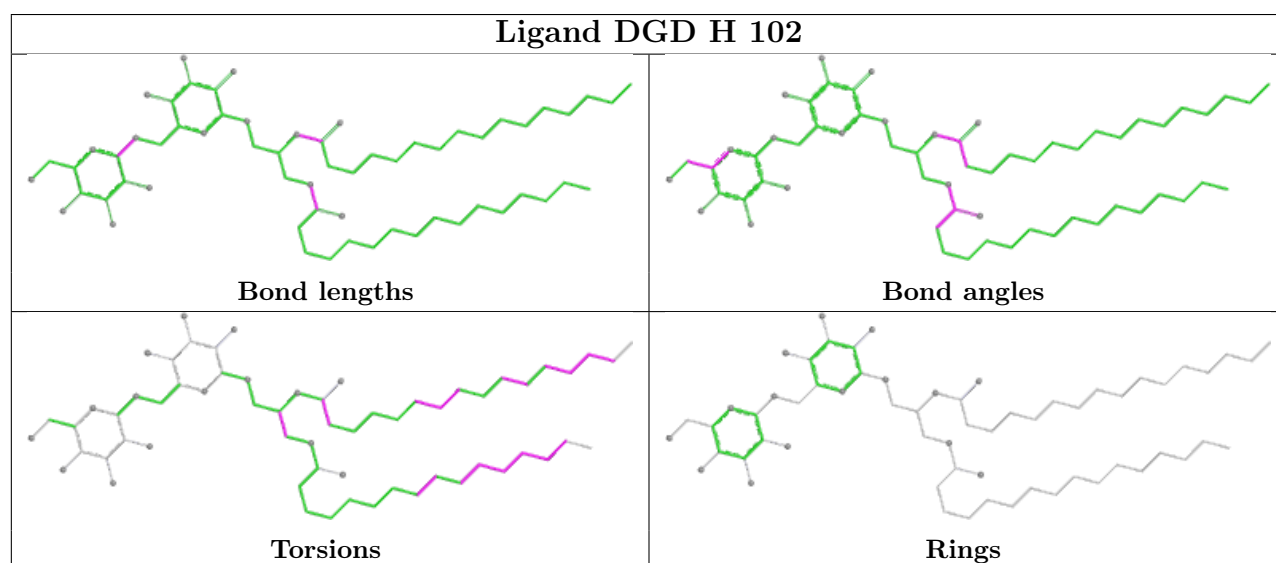
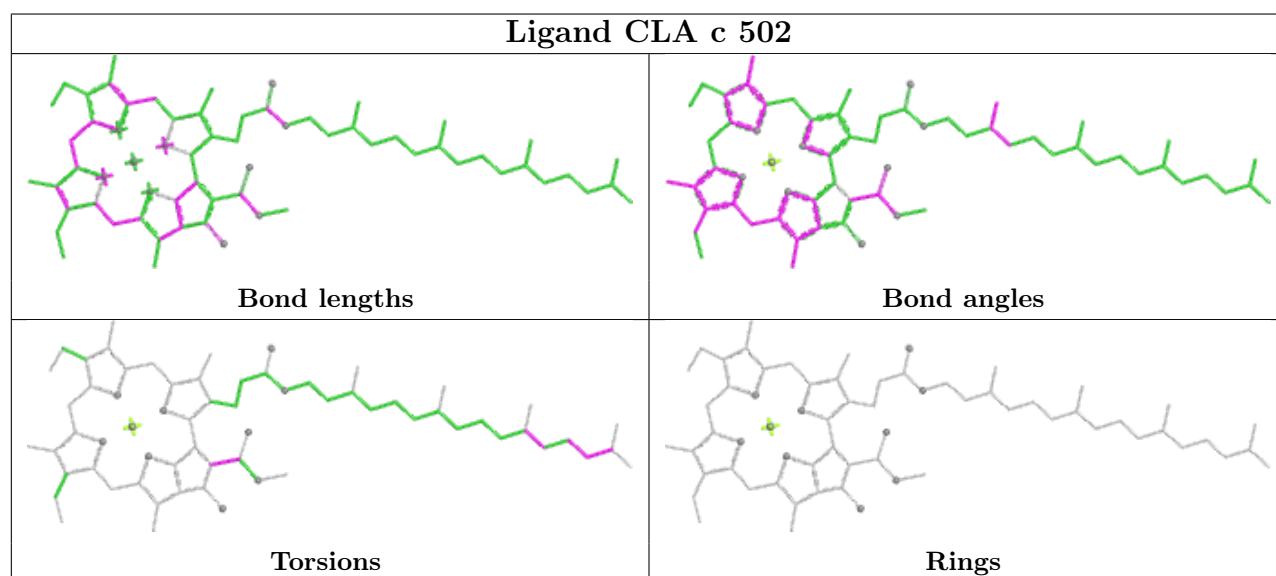
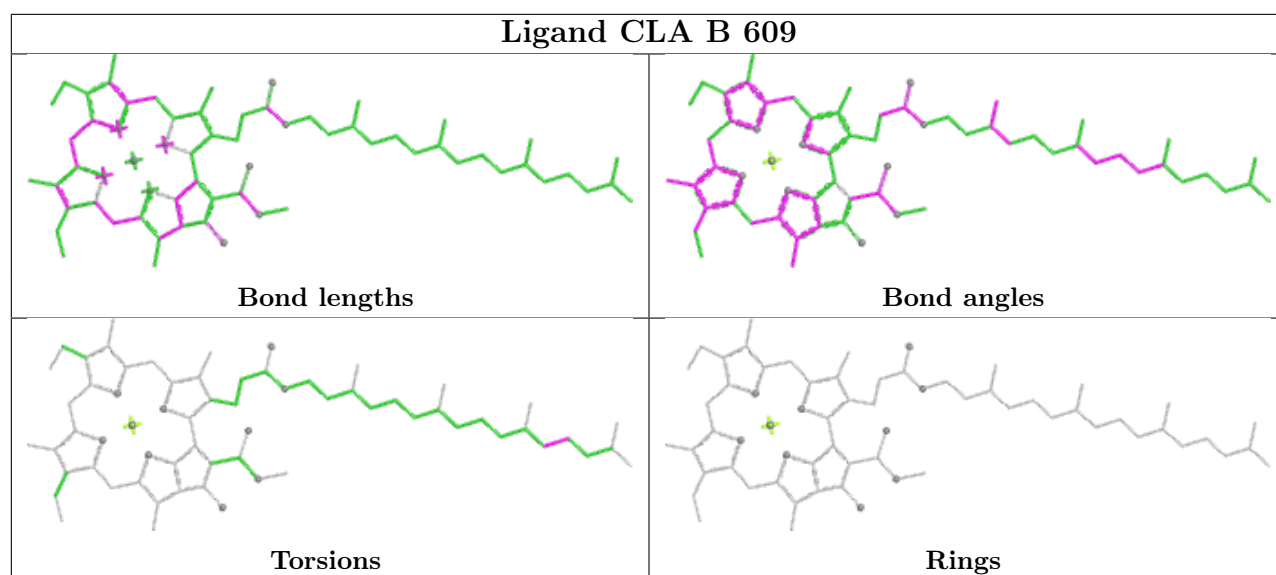


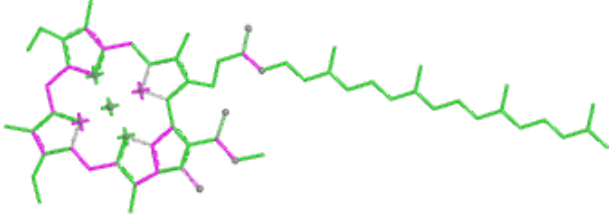
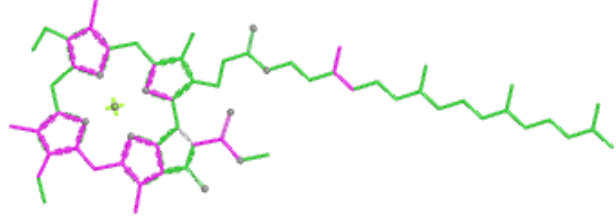
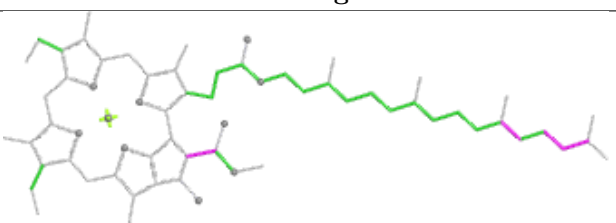
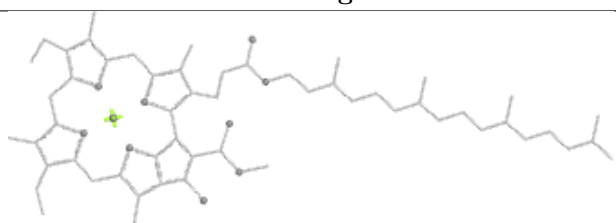
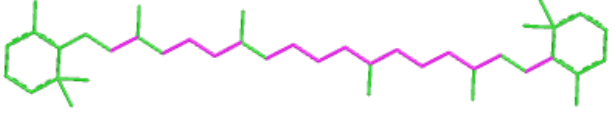
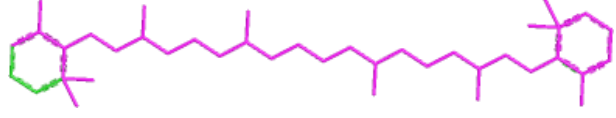
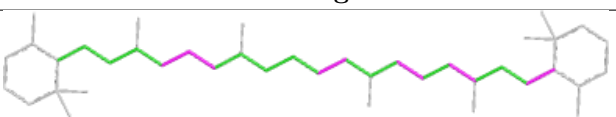
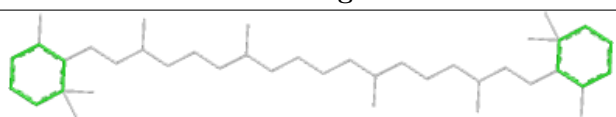
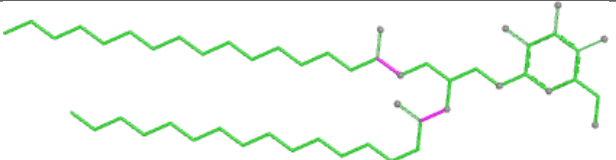
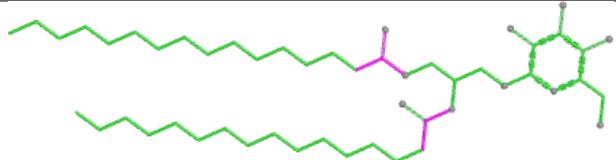
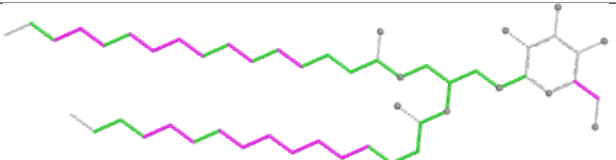
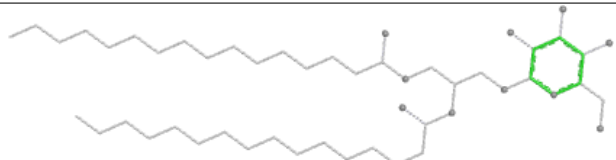




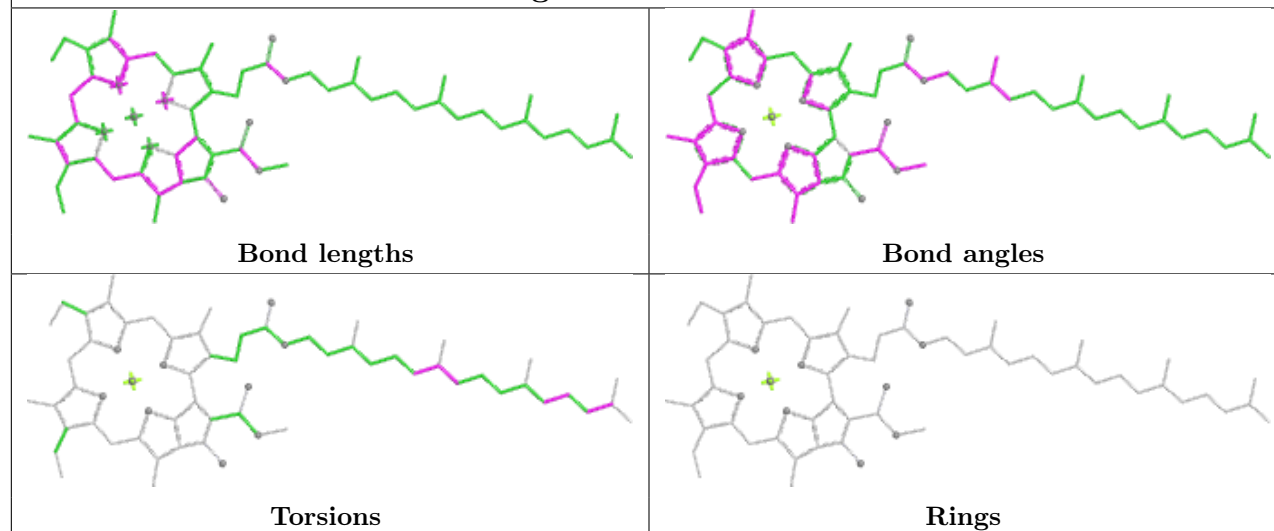




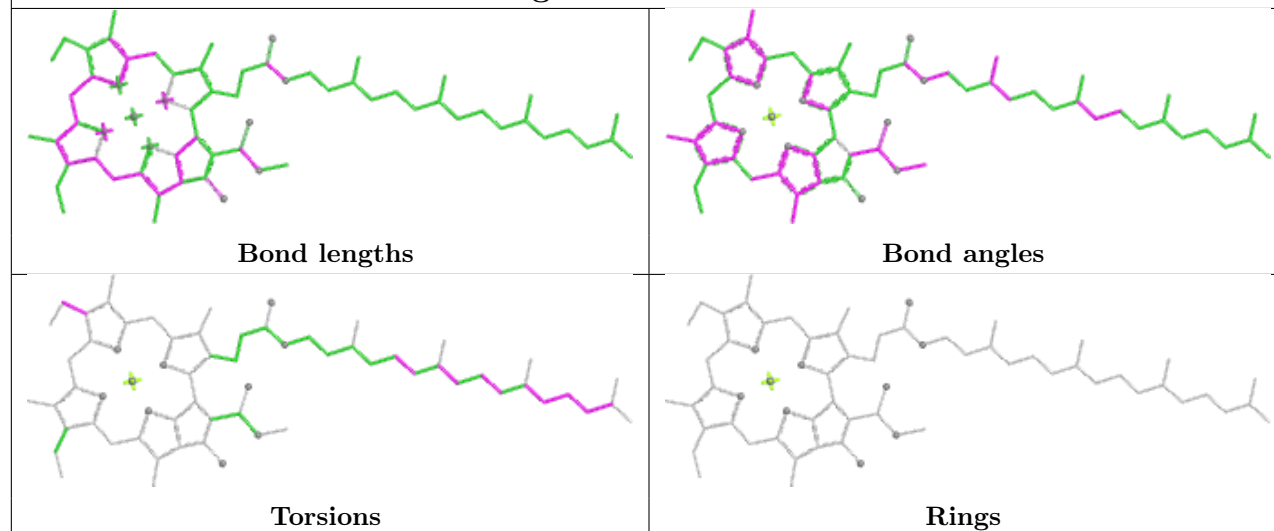


Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

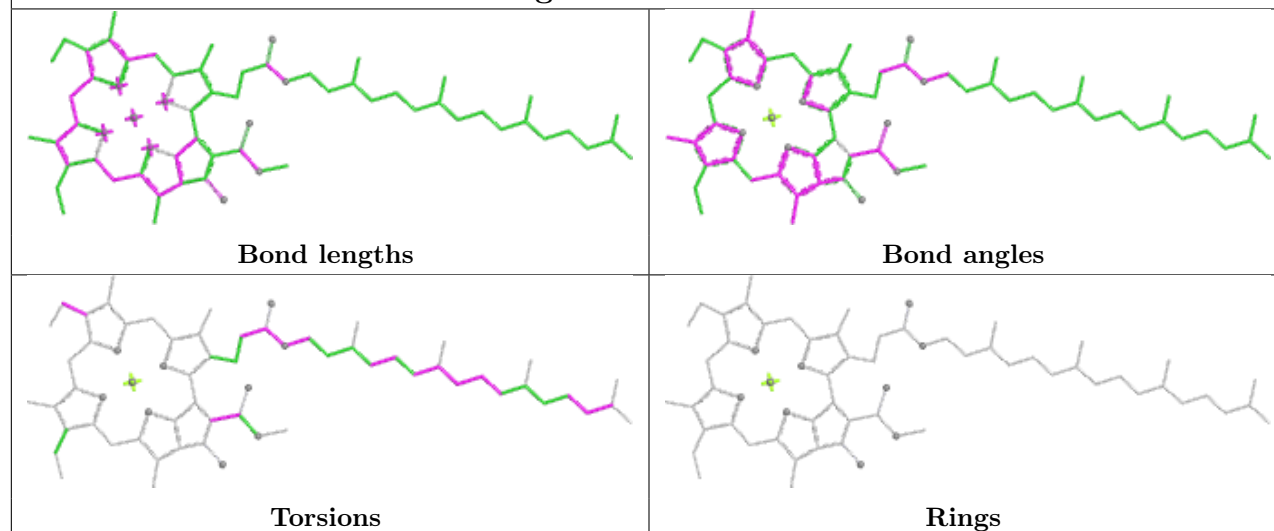
Ligand CLA A 604

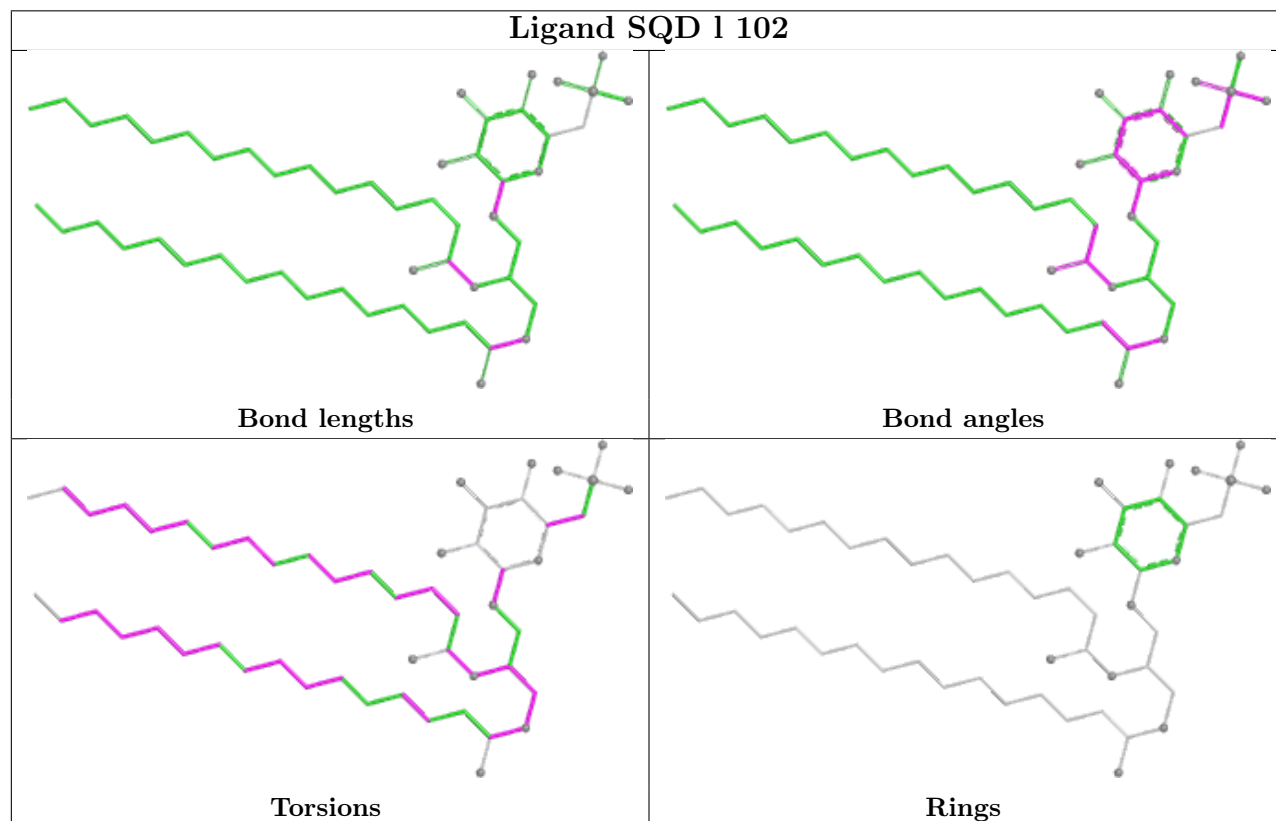
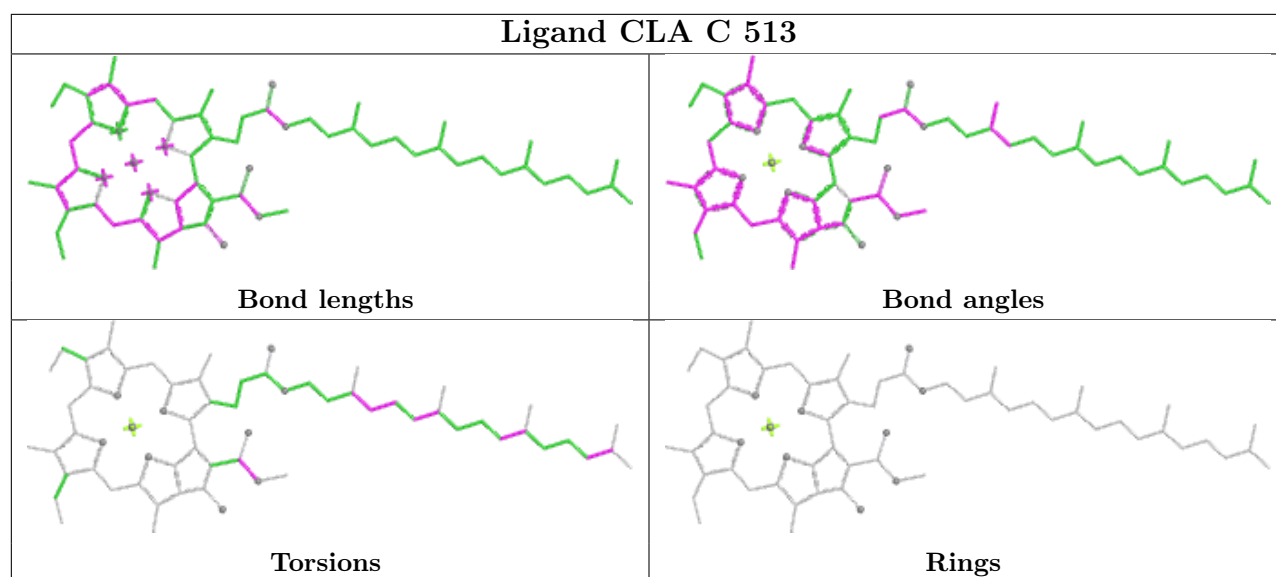


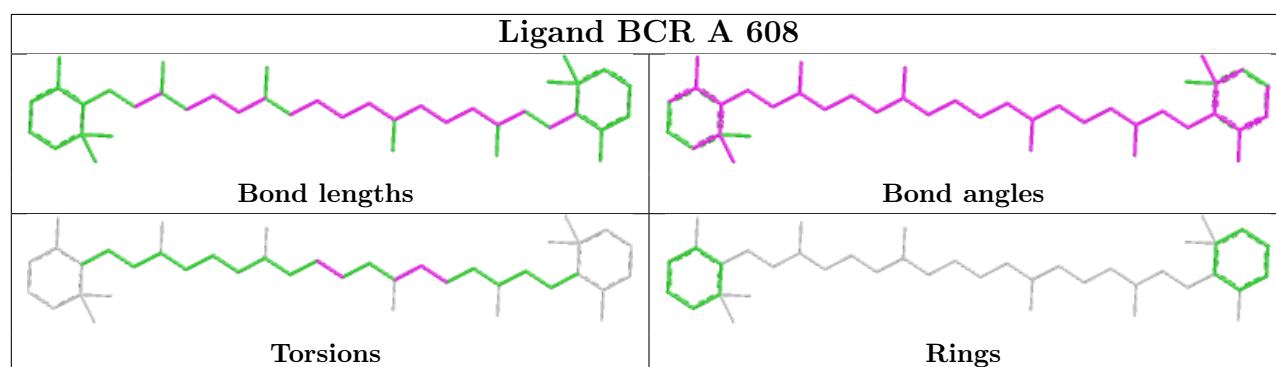
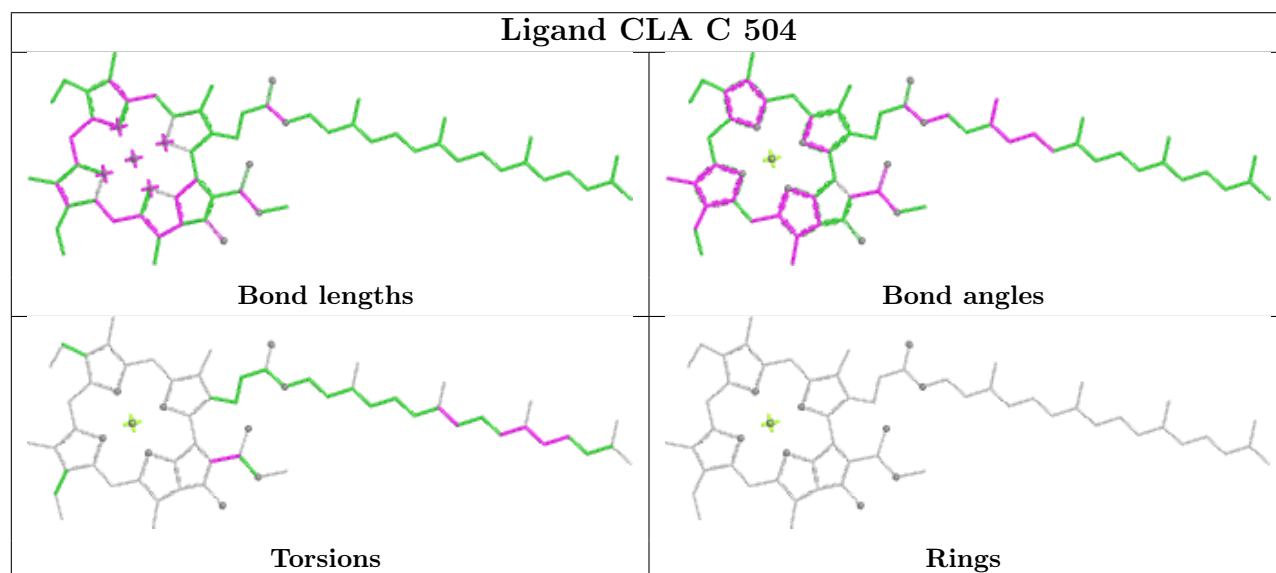
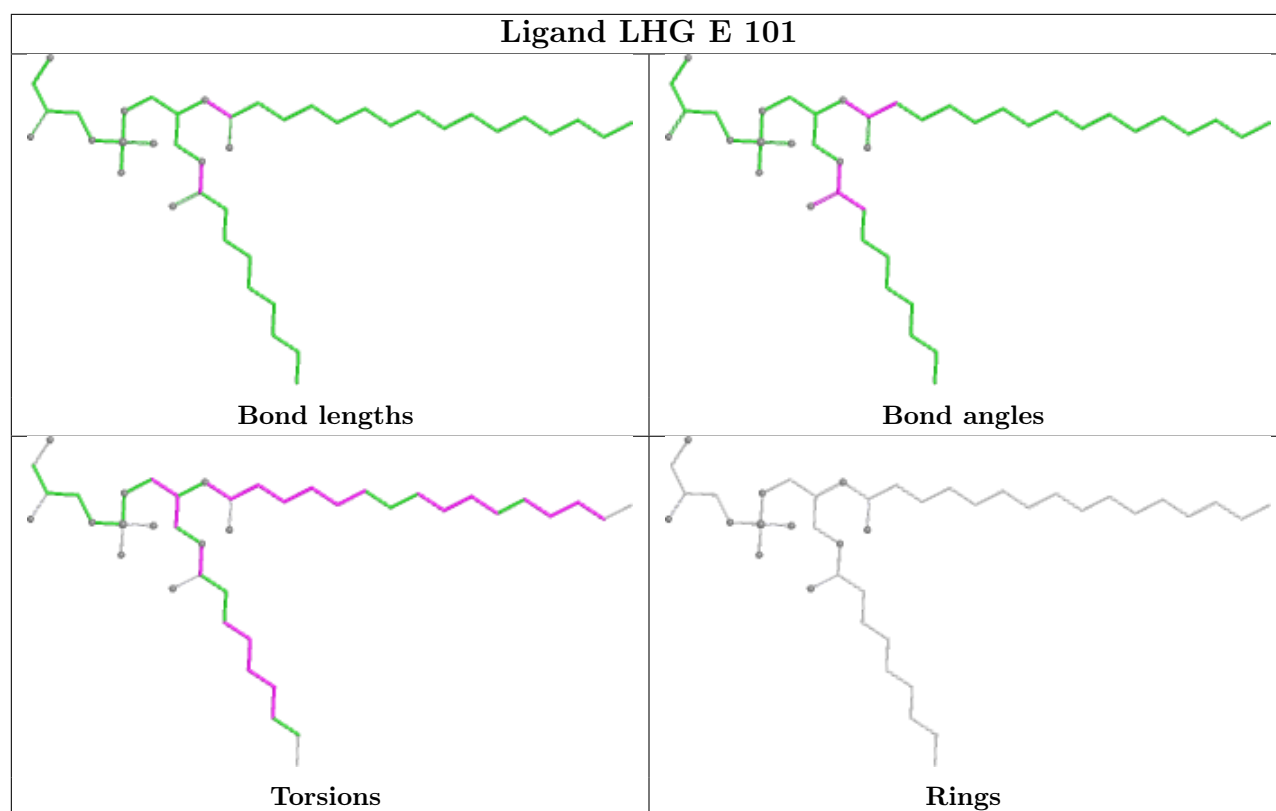
Ligand CLA B 616

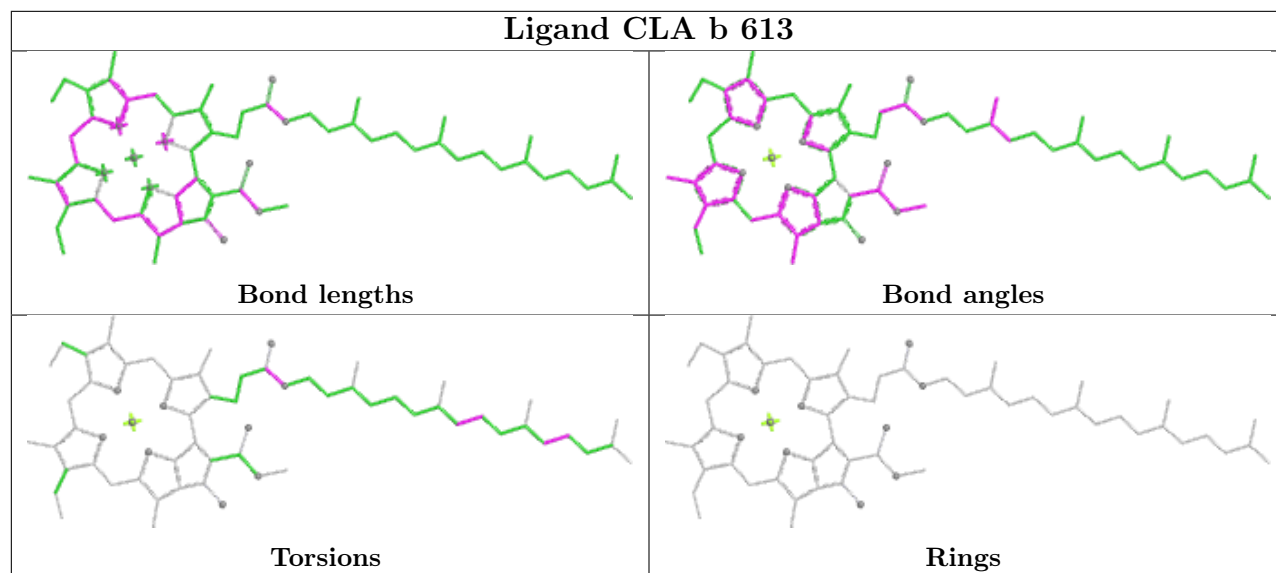
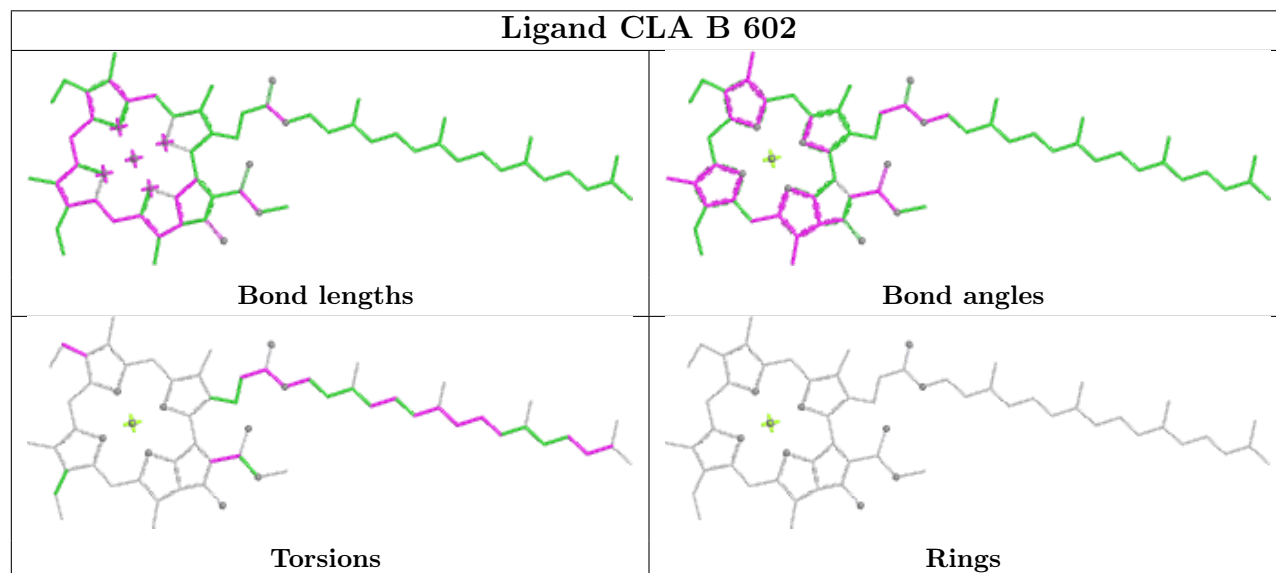
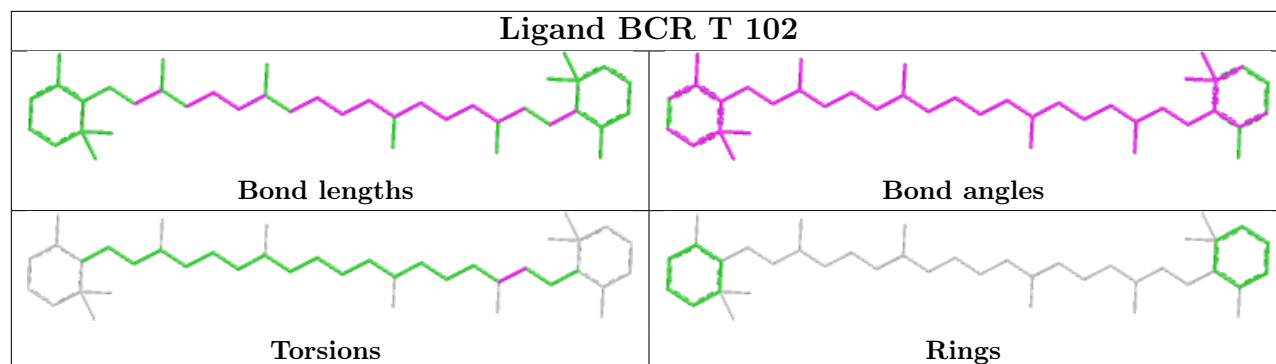


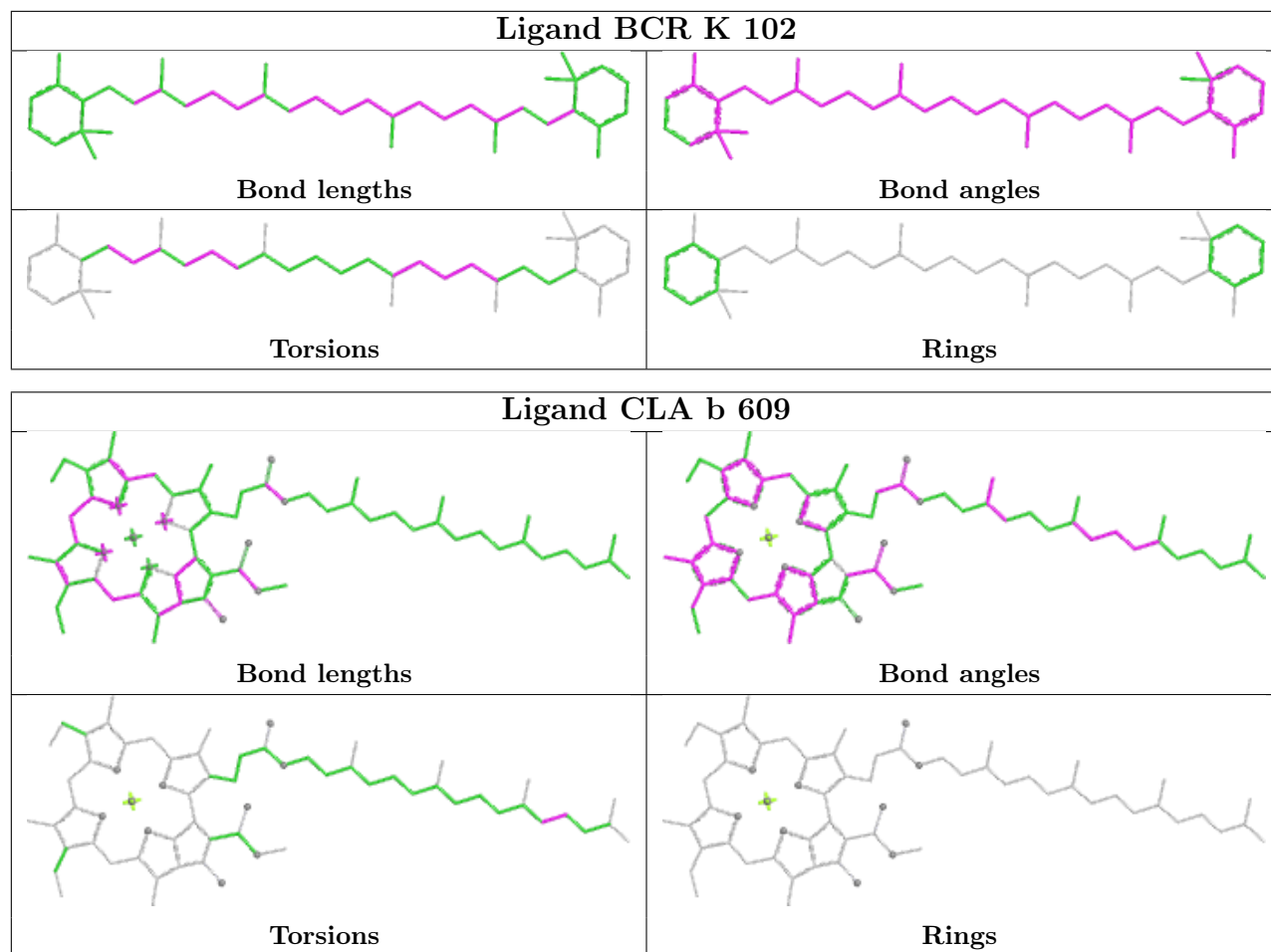
Ligand CLA b 602











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%)	-0.59	0 100 100	16, 22, 43, 53	0
1	a	334/334 (100%)	-0.63	0 100 100	16, 22, 43, 53	0
2	B	504/504 (100%)	-0.62	0 100 100	18, 27, 49, 70	0
2	b	504/504 (100%)	-0.63	1 (0%) 91 84	18, 27, 49, 70	0
3	C	451/461 (97%)	-0.64	0 100 100	21, 31, 44, 56	0
3	c	451/461 (97%)	-0.75	0 100 100	21, 31, 44, 56	0
4	D	342/342 (100%)	-0.63	1 (0%) 90 81	17, 23, 39, 61	0
4	d	342/342 (100%)	-0.62	0 100 100	17, 23, 39, 61	0
5	E	81/81 (100%)	-0.65	0 100 100	27, 40, 57, 63	0
5	e	81/81 (100%)	-0.70	0 100 100	27, 40, 57, 63	0
6	F	34/34 (100%)	-0.65	0 100 100	28, 33, 58, 61	0
6	f	34/34 (100%)	-0.67	0 100 100	28, 33, 58, 61	0
7	H	65/65 (100%)	-0.59	0 100 100	23, 34, 40, 58	0
7	h	65/65 (100%)	-0.54	0 100 100	23, 34, 40, 58	0
8	I	38/38 (100%)	-0.54	0 100 100	30, 34, 65, 68	0
8	i	38/38 (100%)	-0.93	0 100 100	30, 34, 65, 68	0
9	J	38/40 (95%)	-0.95	0 100 100	26, 37, 68, 72	0
9	j	38/40 (95%)	-0.81	0 100 100	26, 37, 68, 72	0
10	K	37/37 (100%)	-0.77	0 100 100	33, 38, 45, 47	0
10	k	37/37 (100%)	-0.48	0 100 100	33, 38, 45, 47	0
11	L	37/37 (100%)	-0.54	0 100 100	17, 22, 50, 59	0
11	l	37/37 (100%)	-0.67	0 100 100	17, 22, 50, 59	0
12	M	34/34 (100%)	-0.26	1 (2%) 53 46	21, 23, 36, 52	0
12	m	34/34 (100%)	-0.32	0 100 100	21, 23, 36, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	-0.63	0 100 100	18, 32, 55, 71	0
13	o	243/243 (100%)	-0.64	1 (0%) 88 78	18, 32, 55, 71	0
14	T	30/30 (100%)	-0.17	0 100 100	19, 23, 44, 52	0
14	t	30/30 (100%)	-0.53	0 100 100	19, 23, 44, 52	0
15	U	97/97 (100%)	-0.58	0 100 100	23, 30, 48, 50	0
15	u	97/97 (100%)	-0.59	0 100 100	23, 30, 48, 50	0
16	V	137/137 (100%)	-0.69	0 100 100	23, 28, 39, 48	0
16	v	137/137 (100%)	-0.70	0 100 100	23, 28, 39, 48	0
17	X	39/39 (100%)	-0.73	0 100 100	33, 40, 66, 68	0
17	x	39/39 (100%)	-0.83	0 100 100	33, 40, 66, 68	0
18	Y	29/29 (100%)	-0.72	0 100 100	42, 48, 75, 77	0
18	y	29/29 (100%)	-0.51	0 100 100	42, 48, 75, 77	0
19	Z	62/62 (100%)	-0.72	0 100 100	39, 48, 68, 72	0
19	z	62/62 (100%)	-0.48	0 100 100	39, 48, 68, 72	0
All	All	5264/5288 (99%)	-0.64	4 (0%) 92 87	16, 28, 51, 77	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	183	LEU	2.5
12	M	23	ILE	2.4
2	b	268	PHE	2.4
13	o	101	ILE	2.0

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
30	CA	F	102	1/1	0.11	0.12	56,56,56,56	0
30	CA	B	621	1/1	0.28	0.13	76,76,76,76	0
30	CA	f	102	1/1	0.41	0.16	56,56,56,56	0
27	BCT	a	612	4/4	0.43	0.31	39,39,40,42	0
26	CL	u	201	1/1	0.59	0.52	50,50,50,50	0
25	SQD	b	621	54/54	0.63	0.13	58,66,80,80	0
25	SQD	l	102	54/54	0.66	0.13	58,66,80,80	0
25	SQD	l	101	54/54	0.66	0.13	57,69,84,85	0
25	SQD	L	101	54/54	0.71	0.12	57,69,84,85	0
24	BCR	T	102	40/40	0.71	0.13	27,33,39,39	0
22	CLA	b	602	65/65	0.75	0.12	32,41,66,66	0
24	BCR	t	101	40/40	0.77	0.12	27,33,39,39	0
29	LMG	c	520	51/55	0.78	0.15	43,76,81,82	0
26	CL	a	610	1/1	0.78	0.17	24,24,24,24	0
22	CLA	b	607	65/65	0.79	0.12	24,28,40,41	0
29	LMG	b	619	51/55	0.79	0.18	29,39,51,54	0
22	CLA	a	604	65/65	0.80	0.15	19,21,63,65	0
29	LMG	C	520	51/55	0.80	0.13	43,76,81,82	0
24	BCR	A	608	40/40	0.82	0.13	22,27,32,32	0
22	CLA	b	608	65/65	0.82	0.14	17,20,32,34	0
32	LHG	E	101	42/49	0.82	0.15	69,83,86,86	0
24	BCR	T	101	40/40	0.83	0.13	23,27,28,29	0
22	CLA	C	513	65/65	0.83	0.12	39,45,64,64	0
24	BCR	C	514	40/40	0.83	0.11	37,43,47,47	0
25	SQD	a	609	54/54	0.83	0.14	49,57,66,67	0
26	CL	A	611	1/1	0.83	0.08	21,21,21,21	0
28	PL9	A	613	55/55	0.84	0.17	52,69,78,78	0
23	PHO	A	606	64/64	0.84	0.08	19,22,28,32	0
28	PL9	d	408	55/55	0.85	0.13	19,23,29,32	0
29	LMG	A	614	51/55	0.85	0.14	53,59,64,65	0
26	CL	A	610	1/1	0.85	0.10	24,24,24,24	0
24	BCR	d	404	40/40	0.85	0.12	25,30,48,49	0
24	BCR	k	101	40/40	0.85	0.12	34,38,39,39	0
26	CL	U	201	1/1	0.85	0.13	50,50,50,50	0
22	CLA	a	603	65/65	0.85	0.11	15,19,25,34	0
24	BCR	C	515	40/40	0.85	0.11	30,37,40,41	0
24	BCR	c	514	40/40	0.85	0.12	37,43,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	a	608	40/40	0.86	0.14	22,27,32,32	0
27	BCT	A	612	4/4	0.86	0.10	39,39,40,42	0
22	CLA	C	507	65/65	0.86	0.11	29,33,52,53	0
29	LMG	Z	101	37/55	0.86	0.08	55,84,88,88	0
22	CLA	C	508	65/65	0.87	0.12	25,29,54,58	0
22	CLA	C	511	65/65	0.87	0.09	29,34,37,38	0
25	SQD	A	609	54/54	0.87	0.12	49,57,66,67	0
22	CLA	A	604	65/65	0.87	0.15	19,21,63,65	0
28	PL9	D	408	55/55	0.87	0.15	19,23,29,32	0
24	BCR	B	618	40/40	0.87	0.10	23,27,28,29	0
22	CLA	c	501	65/65	0.87	0.11	29,32,44,46	0
31	DGD	C	516	62/66	0.87	0.14	23,33,61,62	0
32	LHG	d	409	49/49	0.87	0.13	26,33,62,64	0
29	LMG	B	620	51/55	0.87	0.14	29,39,51,54	0
22	CLA	D	403	65/65	0.88	0.14	24,27,65,67	0
29	LMG	z	101	37/55	0.88	0.09	55,84,88,88	0
22	CLA	A	603	65/65	0.88	0.12	15,19,25,34	0
22	CLA	B	602	65/65	0.88	0.08	32,41,66,66	0
22	CLA	B	607	65/65	0.88	0.10	24,28,40,41	0
22	CLA	b	613	65/65	0.88	0.12	20,24,30,31	0
31	DGD	d	410	62/66	0.88	0.12	77,89,103,103	0
32	LHG	D	407	49/49	0.88	0.16	24,28,37,40	0
24	BCR	b	622	40/40	0.88	0.12	25,37,44,45	0
22	CLA	b	617	65/65	0.88	0.10	22,29,77,78	0
24	BCR	K	102	40/40	0.89	0.11	29,33,37,37	0
29	LMG	C	519	51/55	0.89	0.16	31,57,72,73	0
22	CLA	B	613	65/65	0.89	0.12	20,24,30,31	0
22	CLA	C	504	65/65	0.89	0.11	25,28,54,54	0
29	LMG	d	406	51/55	0.89	0.14	26,35,65,67	0
22	CLA	b	614	65/65	0.89	0.10	19,22,45,47	0
24	BCR	b	618	40/40	0.89	0.13	21,28,40,40	0
22	CLA	c	512	65/65	0.89	0.10	37,41,62,63	0
30	CA	b	620	1/1	0.89	0.13	76,76,76,76	0
22	CLA	b	615	65/65	0.89	0.12	20,24,60,61	0
22	CLA	d	403	65/65	0.89	0.12	24,27,65,67	0
25	SQD	d	411	43/54	0.89	0.10	67,74,78,79	0
31	DGD	D	410	62/66	0.89	0.11	77,89,103,103	0
22	CLA	C	509	65/65	0.89	0.09	29,32,46,47	0
23	PHO	a	606	64/64	0.89	0.08	19,22,28,32	0
32	LHG	D	409	49/49	0.89	0.13	26,33,62,64	0
29	LMG	a	614	51/55	0.89	0.11	53,59,64,65	0
24	BCR	K	101	40/40	0.89	0.10	34,38,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	c	515	40/40	0.90	0.12	30,37,40,41	0
31	DGD	C	517	62/66	0.90	0.11	23,35,62,63	0
31	DGD	C	518	62/66	0.90	0.11	22,31,52,56	0
31	DGD	c	516	62/66	0.90	0.12	23,33,61,62	0
24	BCR	D	404	40/40	0.90	0.12	25,30,48,49	0
24	BCR	B	622	40/40	0.90	0.12	25,37,44,45	0
22	CLA	b	612	65/65	0.90	0.10	19,21,32,34	0
28	PL9	a	613	55/55	0.90	0.14	52,69,78,78	0
32	LHG	d	407	49/49	0.90	0.13	24,28,37,40	0
26	CL	a	611	1/1	0.90	0.05	21,21,21,21	0
22	CLA	c	503	65/65	0.90	0.09	27,31,35,36	0
22	CLA	c	502	65/65	0.91	0.10	24,26,39,42	0
24	BCR	H	101	40/40	0.91	0.13	26,33,42,42	0
31	DGD	c	518	62/66	0.91	0.11	22,31,52,56	0
22	CLA	C	512	65/65	0.91	0.10	37,41,62,63	0
25	SQD	D	411	43/54	0.91	0.10	67,74,78,79	0
22	CLA	C	501	65/65	0.91	0.11	29,32,44,46	0
22	CLA	c	513	65/65	0.91	0.09	39,45,64,64	0
22	CLA	D	401	65/65	0.91	0.10	13,18,34,35	0
22	CLA	D	402	65/65	0.91	0.11	14,18,29,35	0
22	CLA	b	603	65/65	0.91	0.09	23,26,32,32	0
32	LHG	l	103	49/49	0.91	0.12	23,31,43,44	0
24	BCR	B	619	40/40	0.92	0.11	21,28,40,40	0
22	CLA	d	402	65/65	0.92	0.11	14,18,29,35	0
22	CLA	c	511	65/65	0.92	0.09	29,34,37,38	0
22	CLA	B	611	65/65	0.92	0.09	21,25,32,37	0
22	CLA	B	615	65/65	0.92	0.10	20,24,60,61	0
22	CLA	B	616	65/65	0.92	0.10	25,27,45,46	0
22	CLA	B	617	65/65	0.92	0.10	22,29,77,78	0
32	LHG	e	101	42/49	0.92	0.10	69,83,86,86	0
22	CLA	c	510	65/65	0.92	0.07	24,28,35,37	0
22	CLA	B	609	65/65	0.93	0.09	20,24,31,31	0
22	CLA	B	606	65/65	0.93	0.08	19,23,34,35	0
29	LMG	D	406	51/55	0.93	0.11	26,35,65,67	0
24	BCR	k	102	40/40	0.93	0.08	29,33,37,37	0
22	CLA	C	506	65/65	0.93	0.09	31,38,74,75	0
32	LHG	D	405	49/49	0.93	0.13	29,34,41,41	0
22	CLA	B	608	65/65	0.93	0.09	17,20,32,34	0
23	PHO	a	605	64/64	0.93	0.10	16,21,25,26	0
22	CLA	c	507	65/65	0.93	0.07	29,33,52,53	0
24	BCR	h	101	40/40	0.93	0.09	26,33,42,42	0
25	SQD	B	601	54/54	0.93	0.12	50,63,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	SQD	b	601	54/54	0.93	0.12	50,63,68,68	0
22	CLA	c	508	65/65	0.93	0.09	25,29,54,58	0
22	CLA	b	616	65/65	0.94	0.07	25,27,45,46	0
22	CLA	b	604	65/65	0.94	0.08	18,22,31,35	0
22	CLA	b	610	65/65	0.94	0.09	23,28,31,32	0
32	LHG	d	405	49/49	0.94	0.10	29,34,41,41	0
22	CLA	B	612	65/65	0.94	0.08	19,21,32,34	0
29	LMG	c	519	51/55	0.94	0.13	31,57,72,73	0
23	PHO	A	605	64/64	0.94	0.07	16,21,25,26	0
22	CLA	c	509	65/65	0.94	0.07	29,32,46,47	0
32	LHG	L	102	49/49	0.94	0.11	23,31,43,44	0
31	DGD	h	102	62/66	0.94	0.14	26,32,38,40	0
33	HEM	F	101	43/43	0.94	0.09	39,42,45,47	0
33	HEM	f	101	43/43	0.94	0.09	39,42,45,47	0
31	DGD	c	517	62/66	0.95	0.07	23,35,62,63	0
22	CLA	b	609	65/65	0.95	0.09	20,24,31,31	0
22	CLA	C	510	65/65	0.95	0.05	24,28,35,37	0
30	CA	O	301	1/1	0.95	0.03	49,49,49,49	0
31	DGD	H	102	62/66	0.95	0.09	26,32,38,40	0
22	CLA	A	607	65/65	0.95	0.08	21,24,71,72	0
22	CLA	c	506	65/65	0.95	0.08	31,38,74,75	0
22	CLA	b	605	65/65	0.95	0.08	19,22,50,51	0
22	CLA	C	502	65/65	0.95	0.09	24,26,39,42	0
22	CLA	c	504	65/65	0.96	0.07	25,28,54,54	0
22	CLA	c	505	65/65	0.96	0.07	28,30,44,45	0
22	CLA	b	606	65/65	0.96	0.06	19,23,34,35	0
22	CLA	C	503	65/65	0.96	0.08	27,31,35,36	0
22	CLA	a	607	65/65	0.96	0.07	21,24,71,72	0
22	CLA	C	505	65/65	0.96	0.07	28,30,44,45	0
22	CLA	d	401	65/65	0.96	0.06	13,18,34,35	0
22	CLA	B	603	65/65	0.96	0.08	23,26,32,32	0
34	MG	j	101	1/1	0.96	0.06	27,27,27,27	0
22	CLA	B	614	65/65	0.97	0.08	19,22,45,47	0
30	CA	o	301	1/1	0.97	0.03	49,49,49,49	0
22	CLA	b	611	65/65	0.97	0.06	21,25,32,37	0
22	CLA	B	610	65/65	0.97	0.07	23,28,31,32	0
33	HEM	V	201	43/43	0.97	0.08	23,24,27,29	0
33	HEM	v	201	43/43	0.97	0.09	23,24,27,29	0
22	CLA	B	605	65/65	0.97	0.07	19,22,50,51	0
22	CLA	B	604	65/65	0.98	0.07	18,22,31,35	0
21	FE2	a	602	1/1	0.99	0.19	26,26,26,26	0
20	OEX	A	601	10/10	0.99	0.06	22,23,26,26	0

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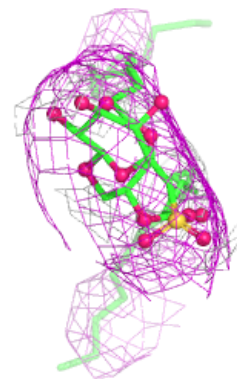
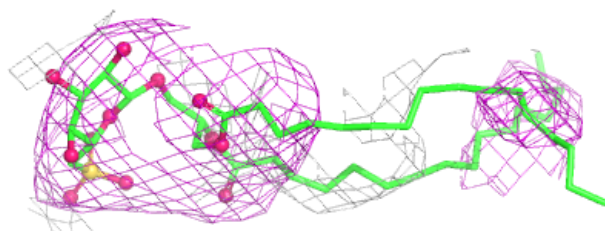
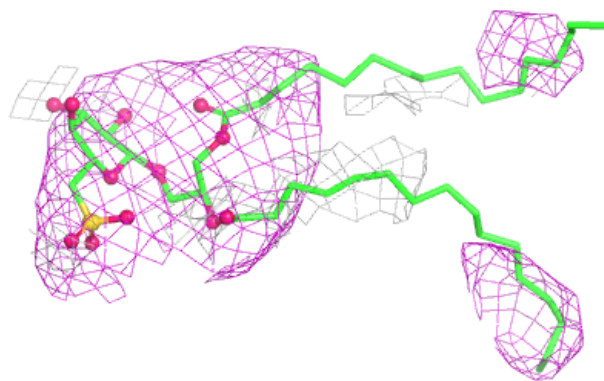
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	OEX	a	601	10/10	0.99	0.06	22,23,26,26	0
34	MG	J	101	1/1	1.00	0.04	27,27,27,27	0
21	FE2	A	602	1/1	1.00	0.04	26,26,26,26	0

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.

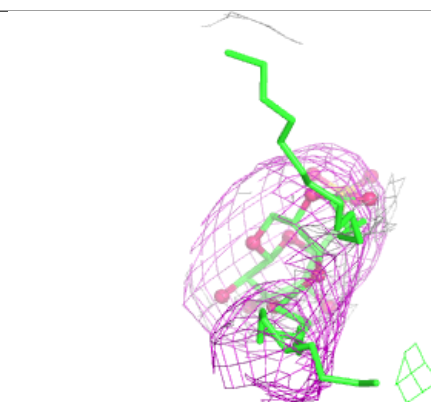
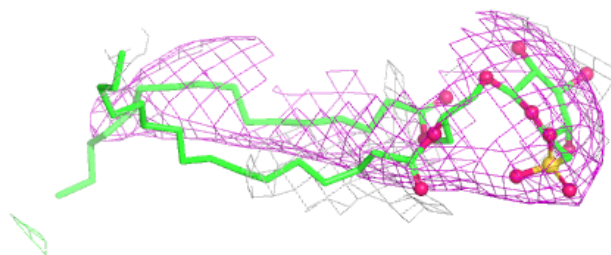
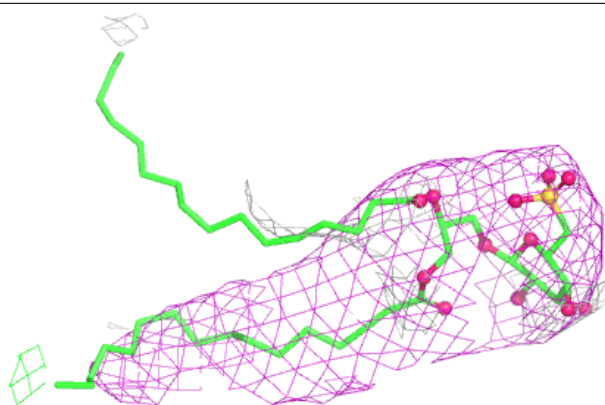
Electron density around SQD b 621:

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

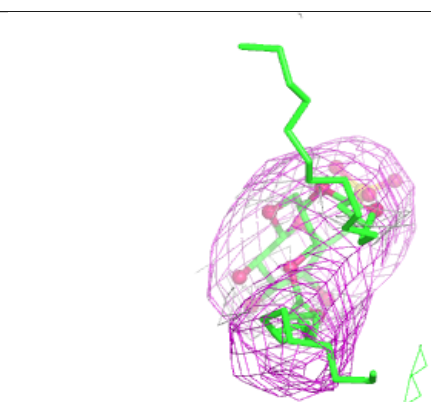
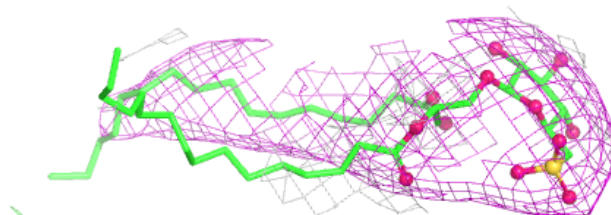
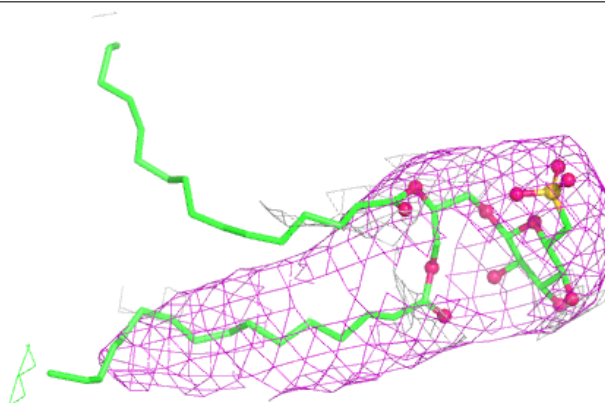


Electron density around SQD 1 102:

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

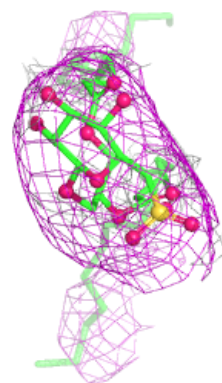
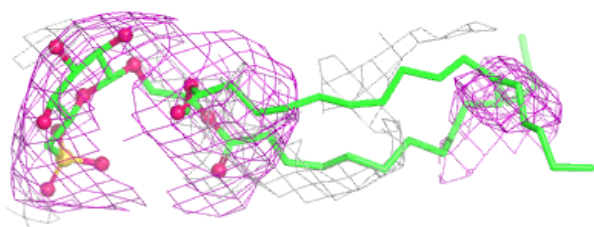
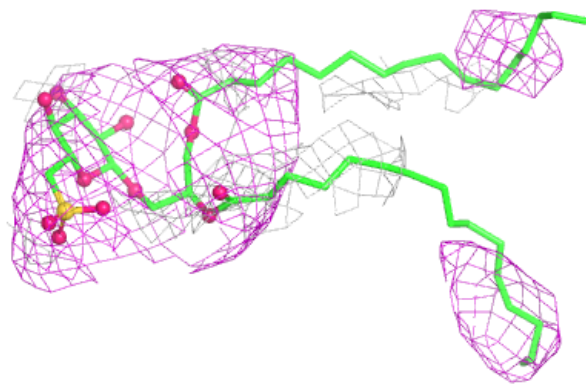
**Electron density around SQD 1 101:**

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

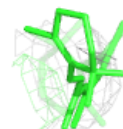
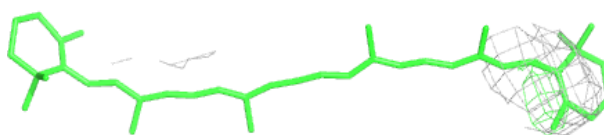


Electron density around SQD L 101:

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

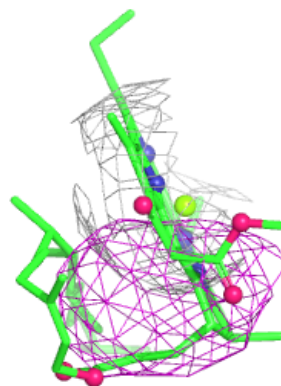
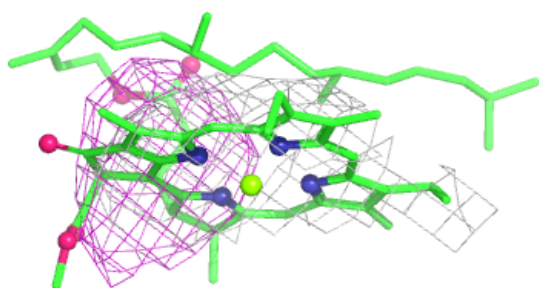
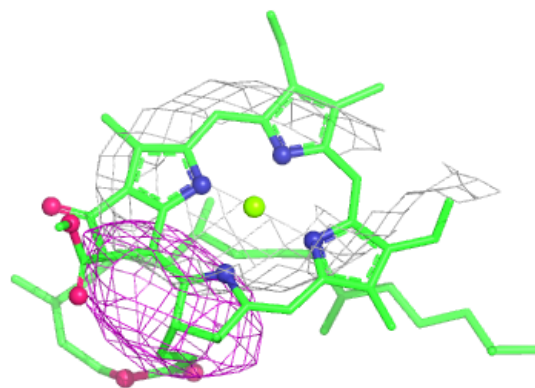
**Electron density around BCR T 102:**

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

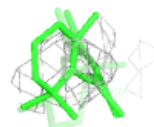
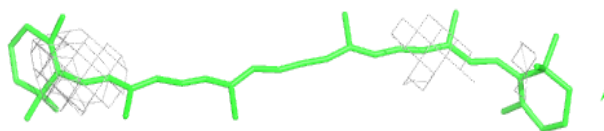


Electron density around CLA b 602:

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

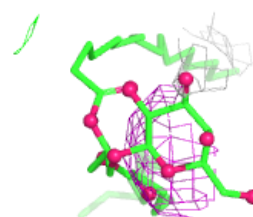
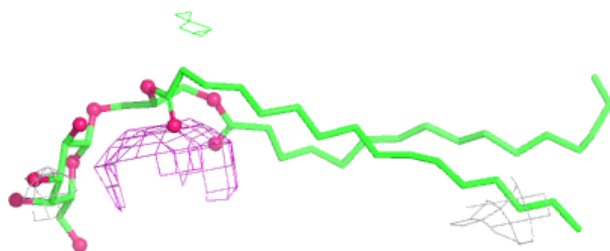
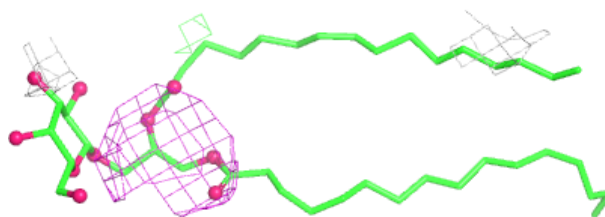
**Electron density around BCR t 101:**

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

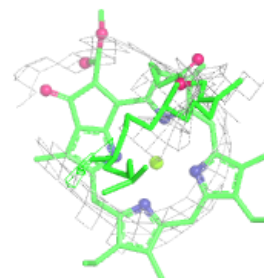
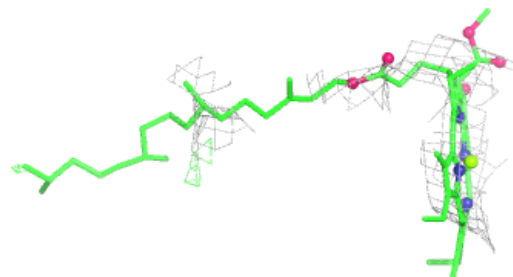


Electron density around LMG c 520:

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

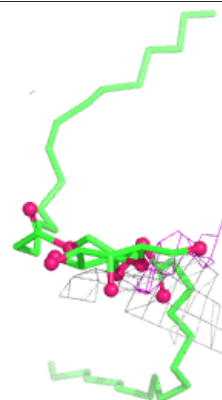
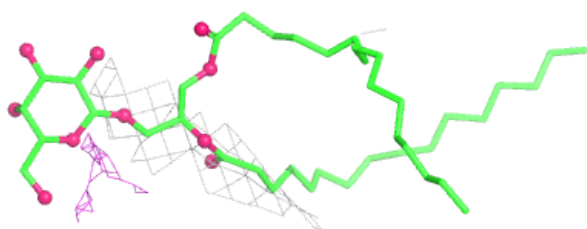
**Electron density around CLA b 607:**

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

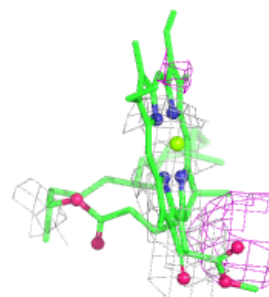
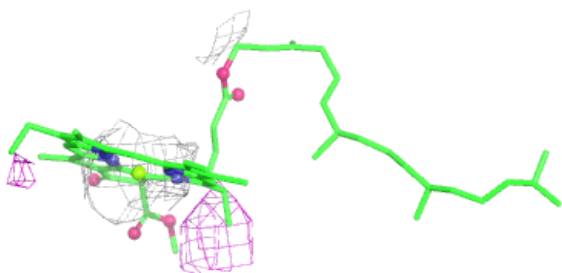
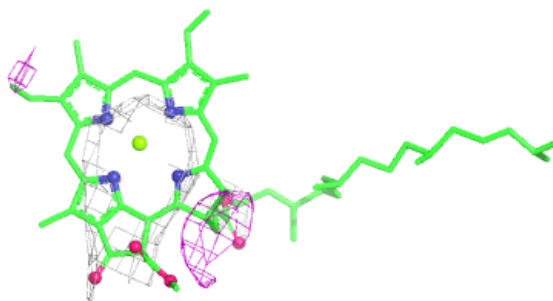


Electron density around LMG b 619:

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

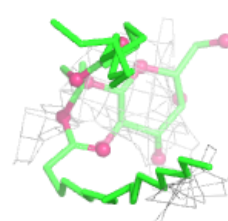
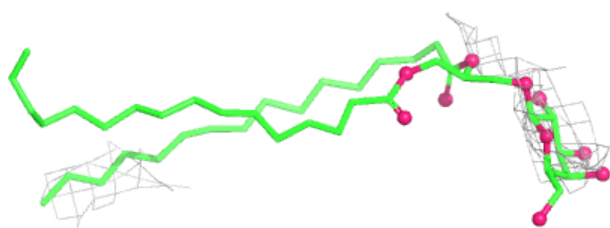
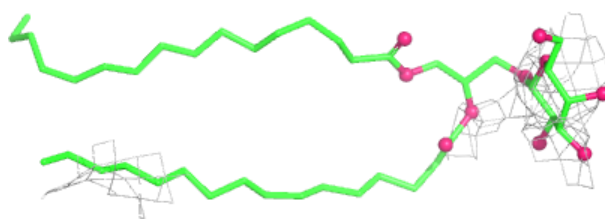
**Electron density around CLA a 604:**

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

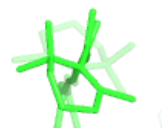
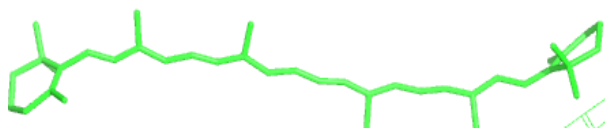


Electron density around LMG C 520:

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

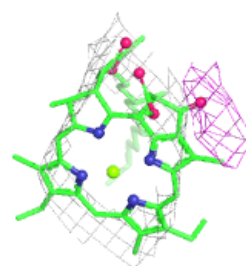
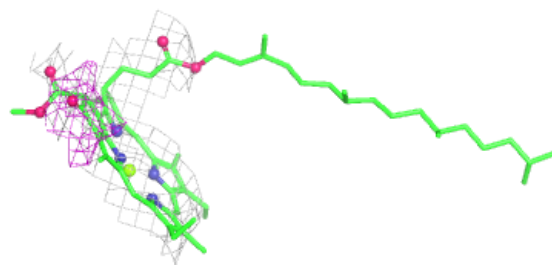
**Electron density around BCR A 608:**

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

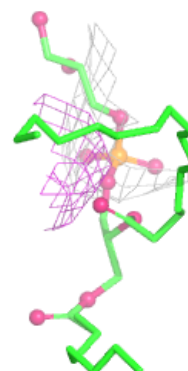
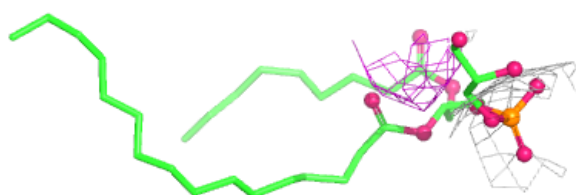


Electron density around CLA b 608:

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

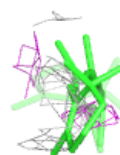
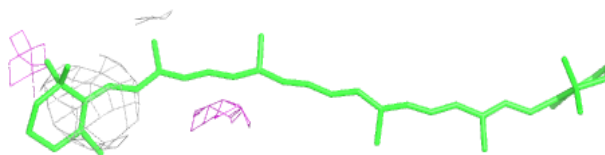
**Electron density around LHG E 101:**

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

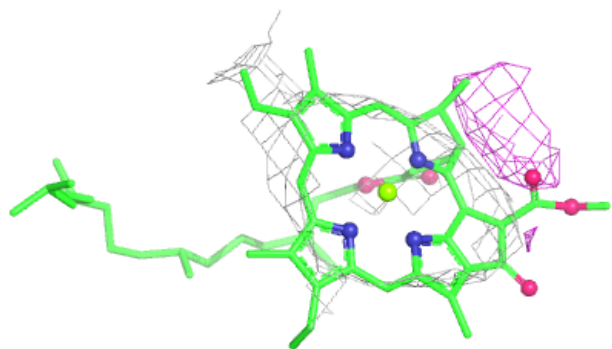
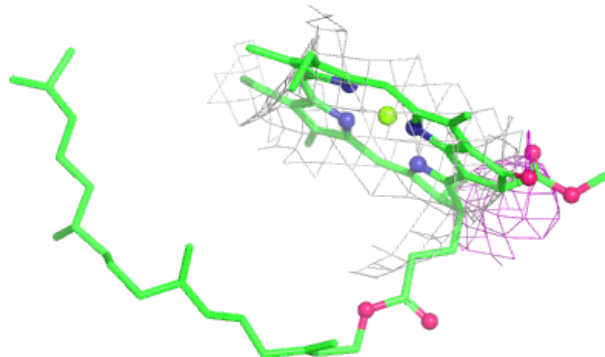


Electron density around BCR T 101:

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

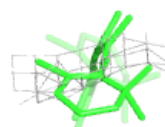
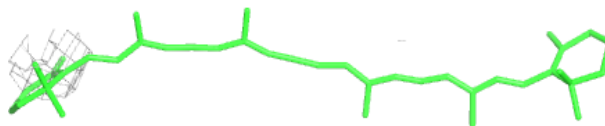
**Electron density around CLA C 513:**

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

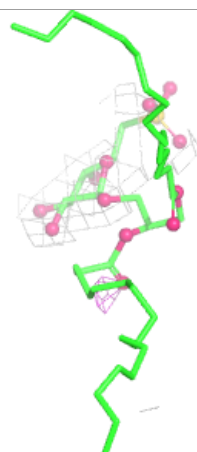
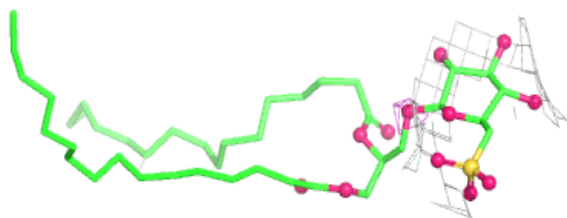
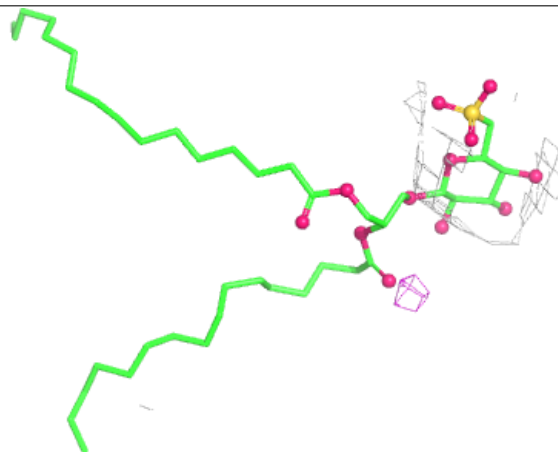


Electron density around BCR C 514:

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

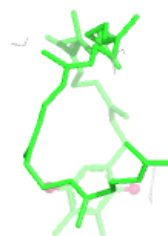
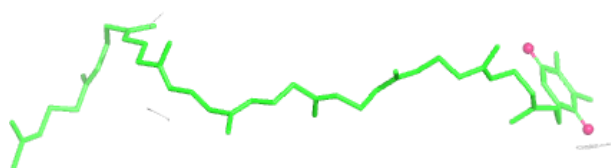
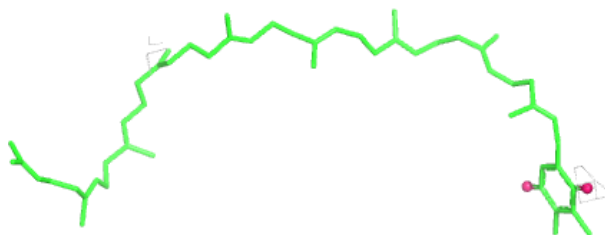
**Electron density around SQD a 609:**

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

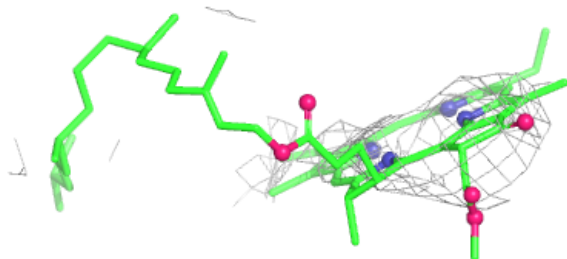
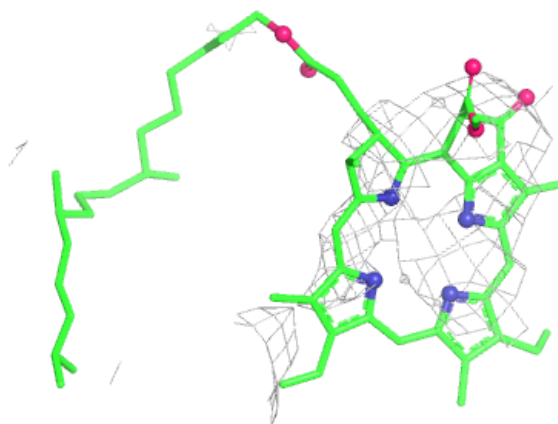


Electron density around PL9 A 613:

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

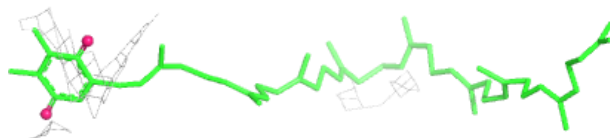
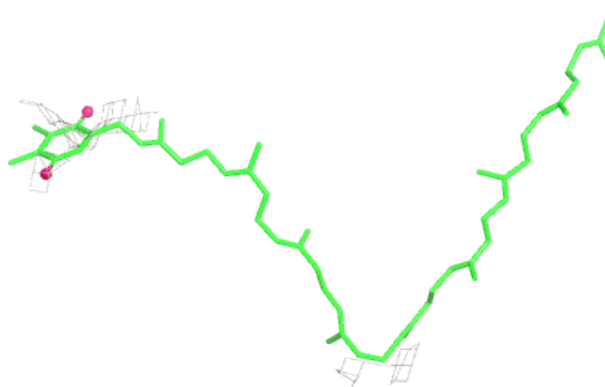
**Electron density around PHO A 606:**

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

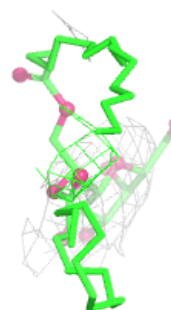
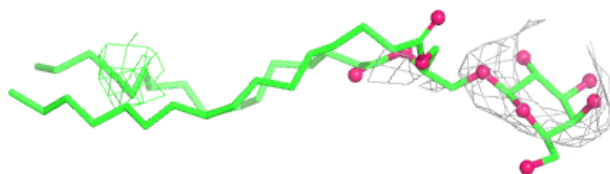
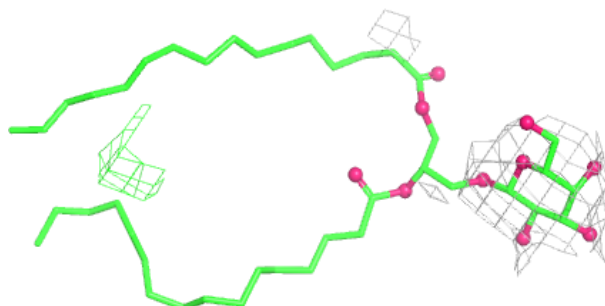


Electron density around PL9 d 408:

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

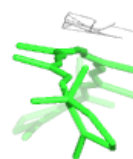
**Electron density around LMG A 614:**

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

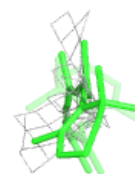


Electron density around BCR d 404:

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

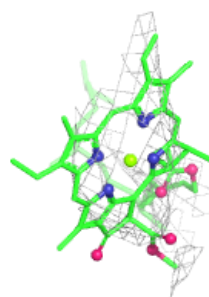
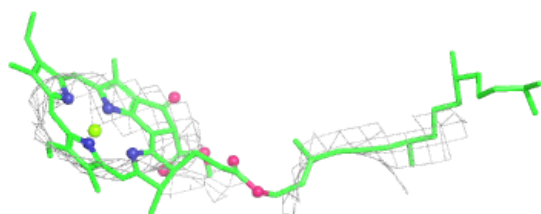
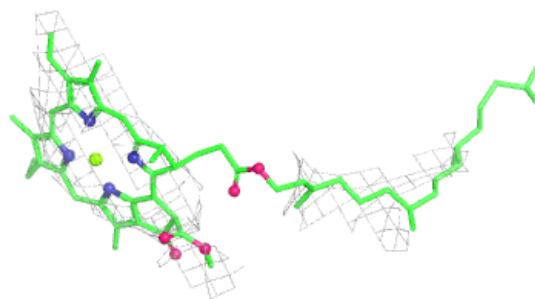
**Electron density around BCR k 101:**

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

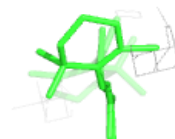
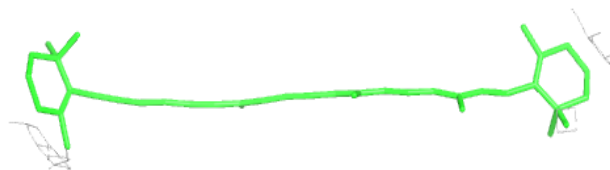
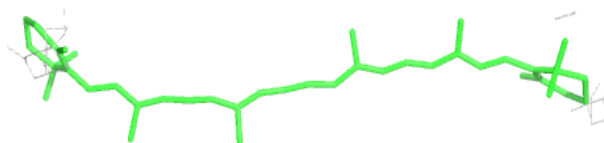


Electron density around CLA a 603:

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

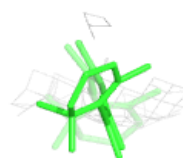
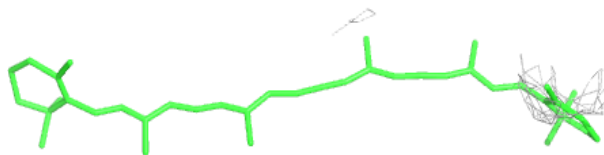
**Electron density around BCR C 515:**

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

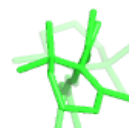
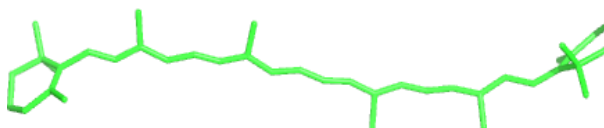


Electron density around BCR c 514:

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

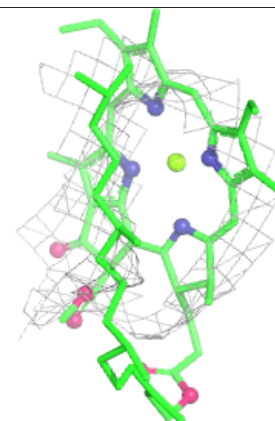
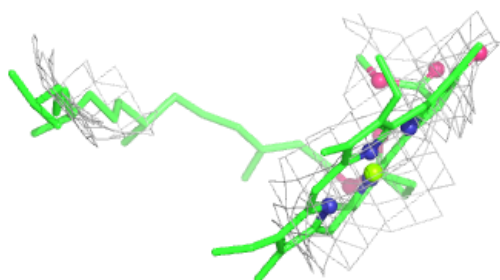
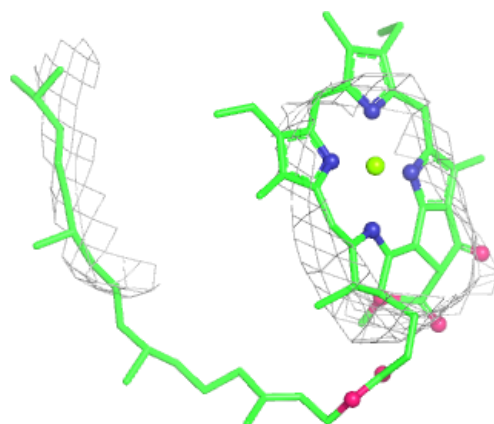
**Electron density around BCR a 608:**

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

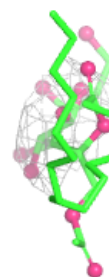
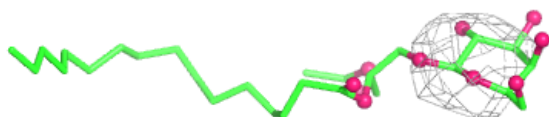
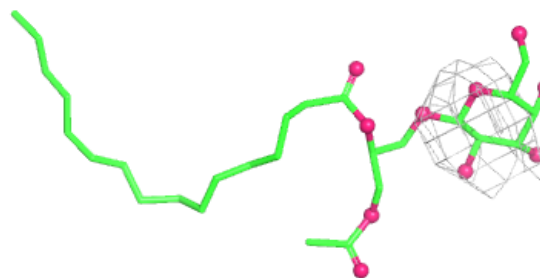


Electron density around CLA C 507:

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

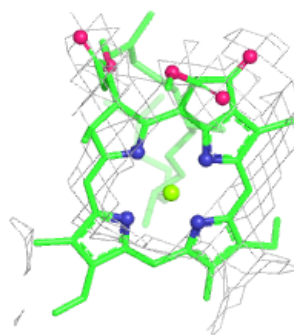
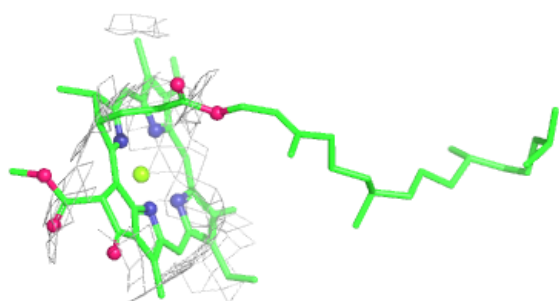
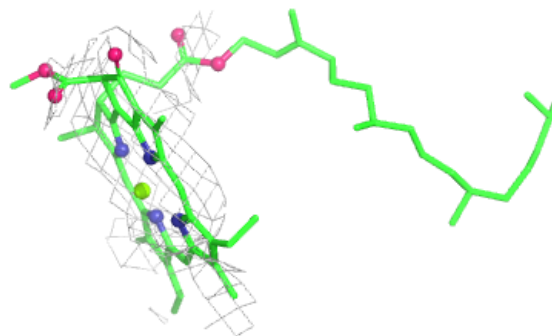
**Electron density around LMG Z 101:**

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

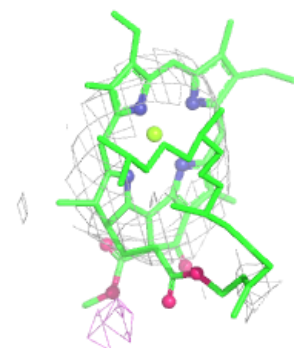
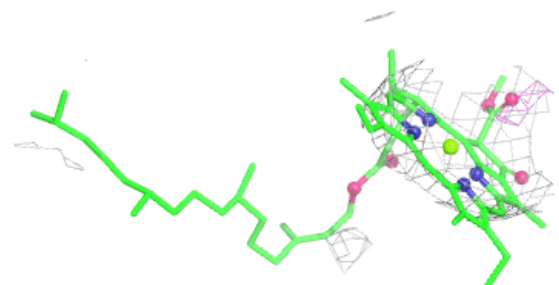
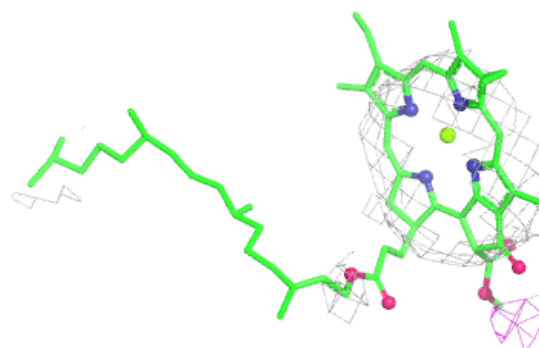


Electron density around CLA C 508:

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

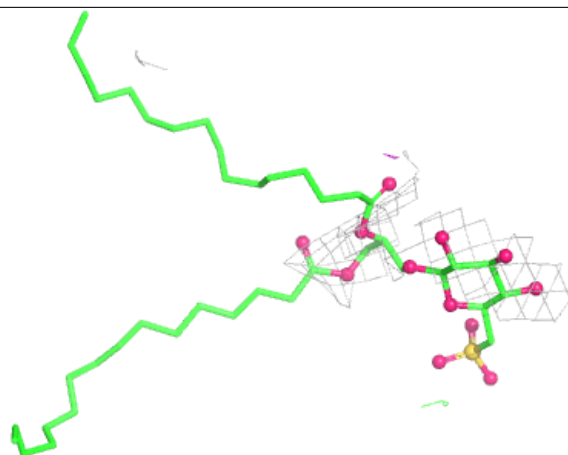
**Electron density around CLA C 511:**

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



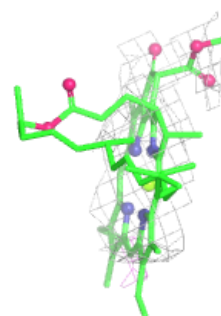
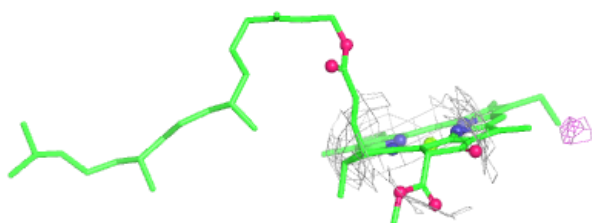
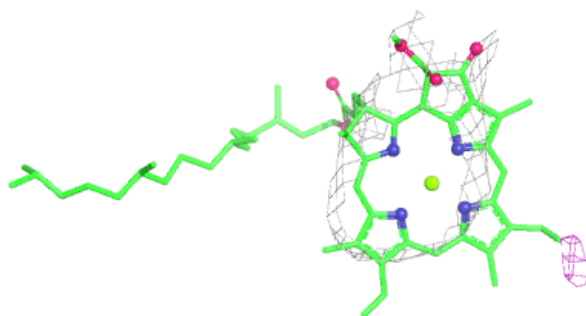
Electron density around SQD A 609:

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

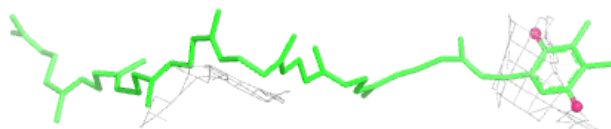
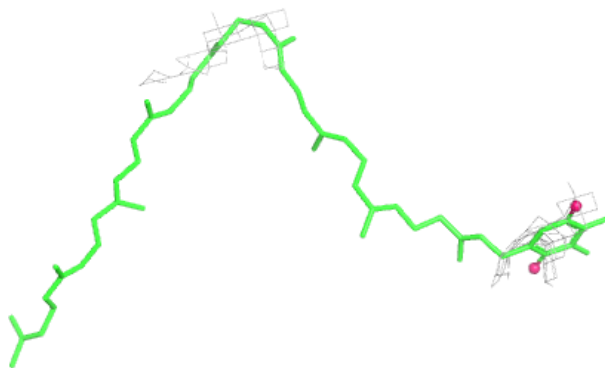


Electron density around CLA A 604:

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

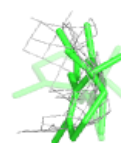
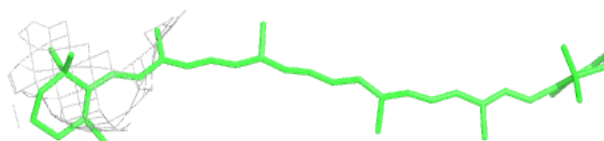
**Electron density around PL9 D 408:**

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

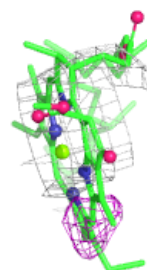
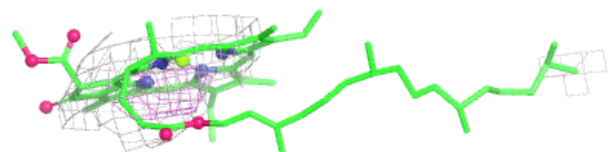
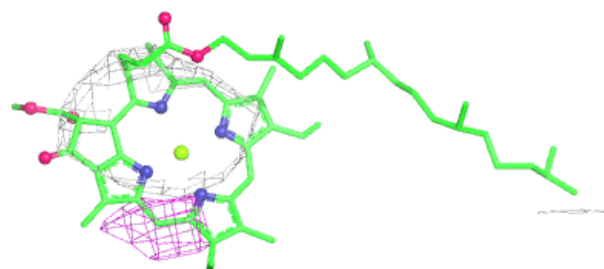


Electron density around BCR B 618:

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

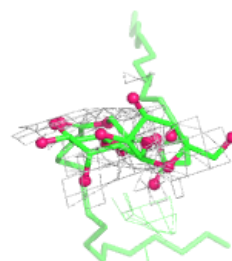
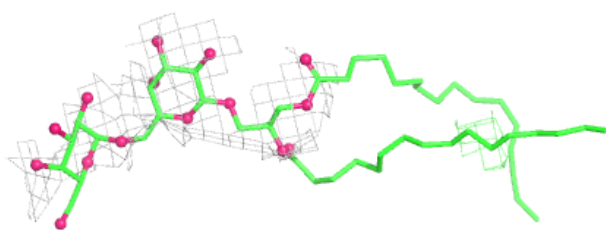
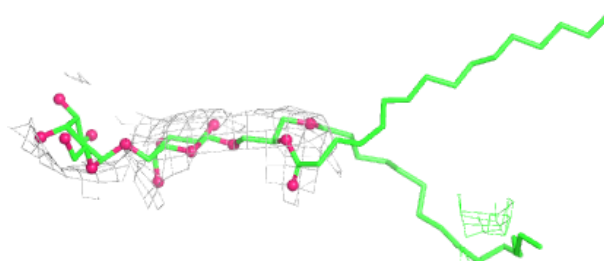
**Electron density around CLA c 501:**

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

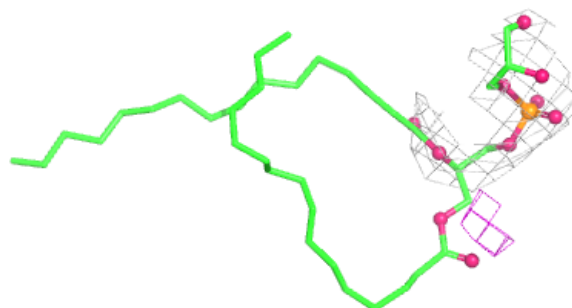


Electron density around DGD C 516:

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

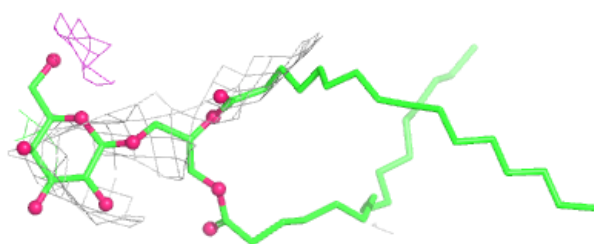
**Electron density around LHG d 409:**

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

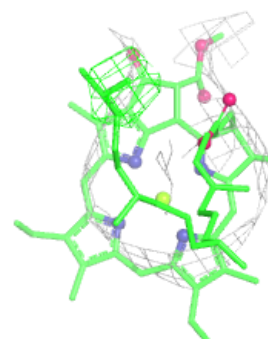
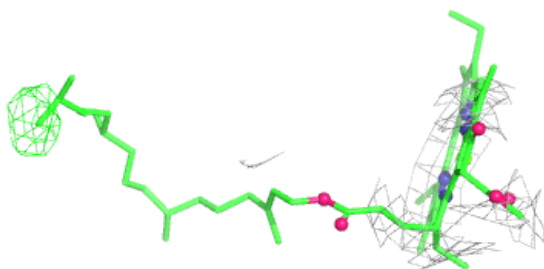
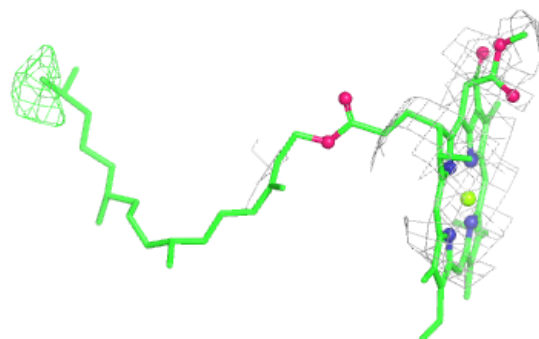


Electron density around LMG B 620:

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

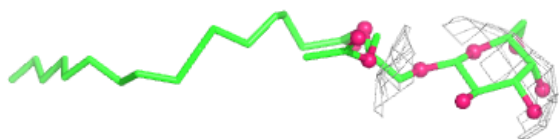
**Electron density around CLA D 403:**

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

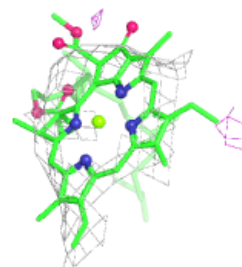
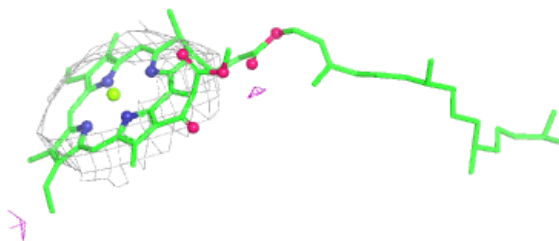
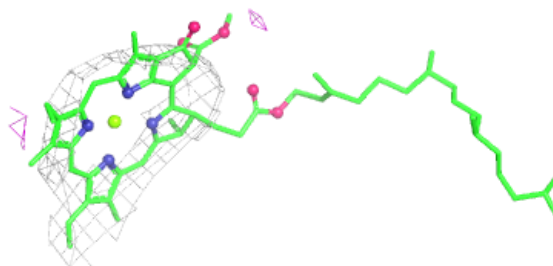


Electron density around LMG z 101:

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

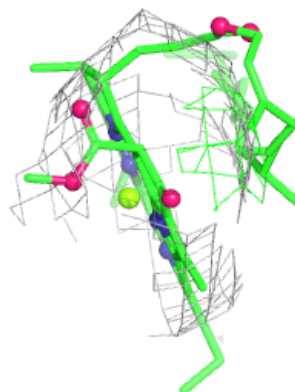
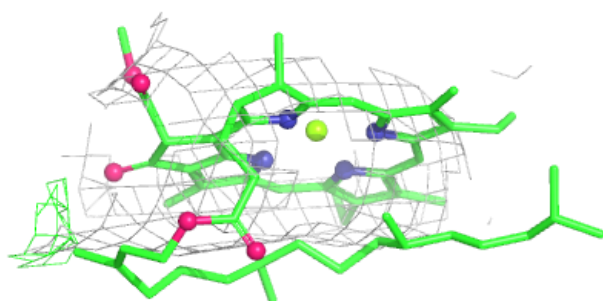
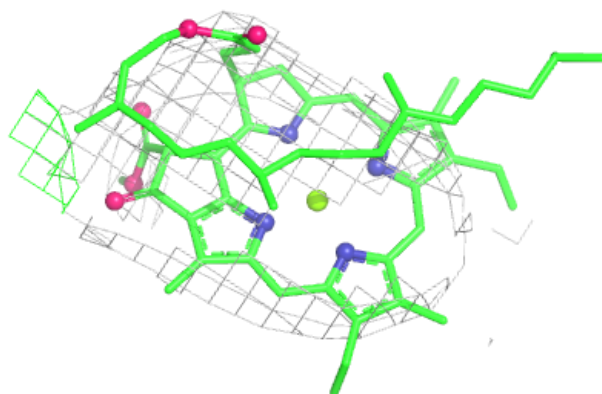
**Electron density around CLA A 603:**

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

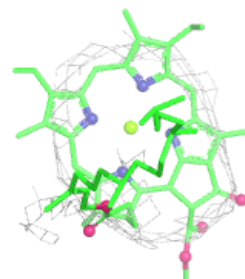
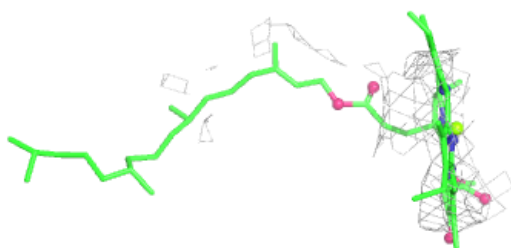
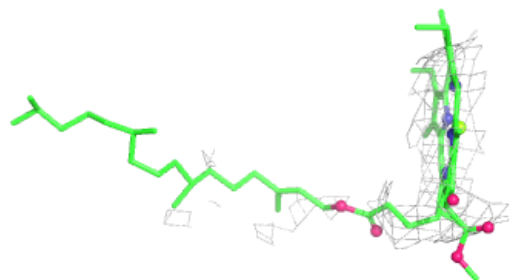


Electron density around CLA B 602:

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

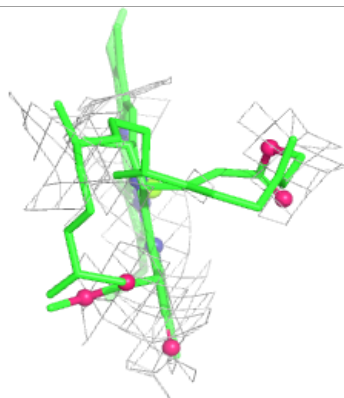
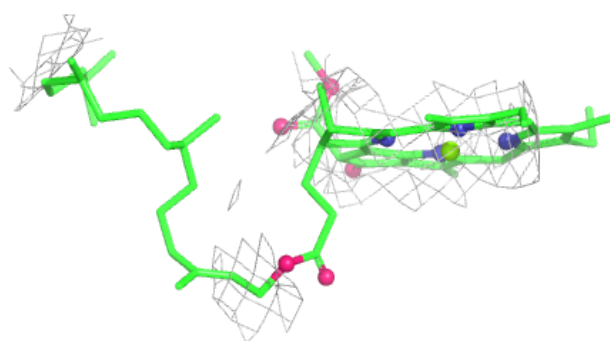
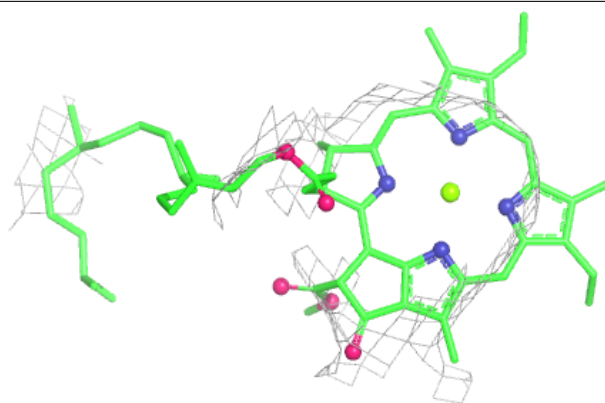
**Electron density around CLA B 607:**

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

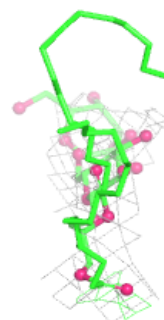
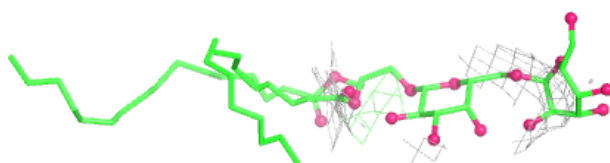
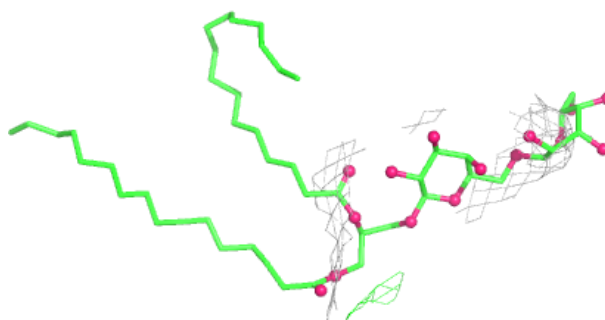


Electron density around CLA b 613:

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

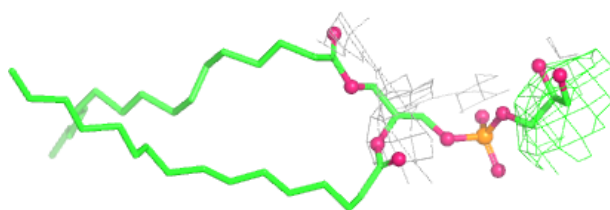
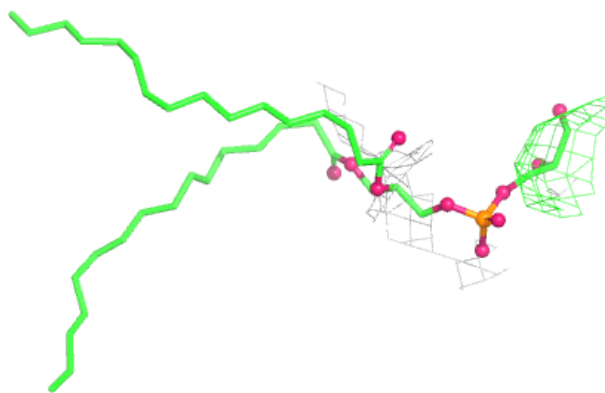
**Electron density around DGD d 410:**

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

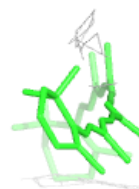
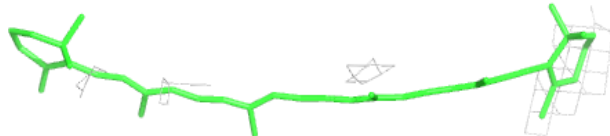
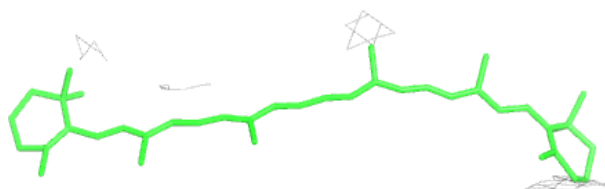


Electron density around LHG D 407:

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

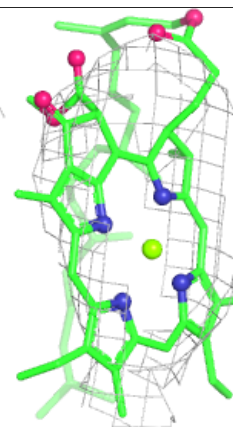
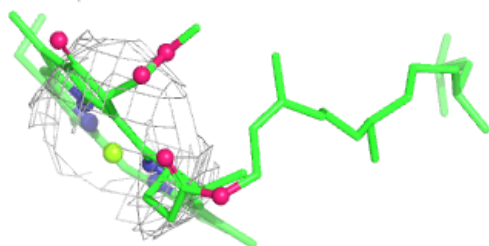
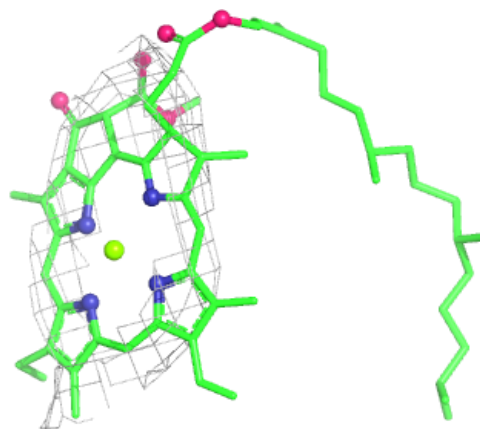
**Electron density around BCR b 622:**

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

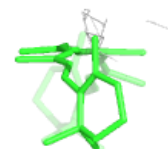
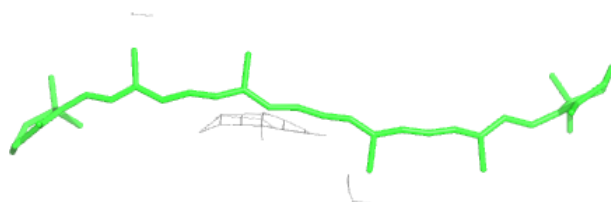


Electron density around CLA b 617:

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

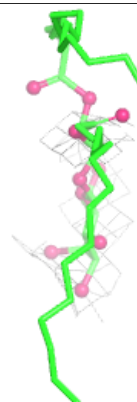
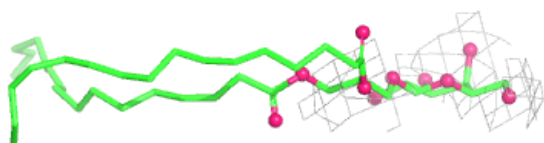
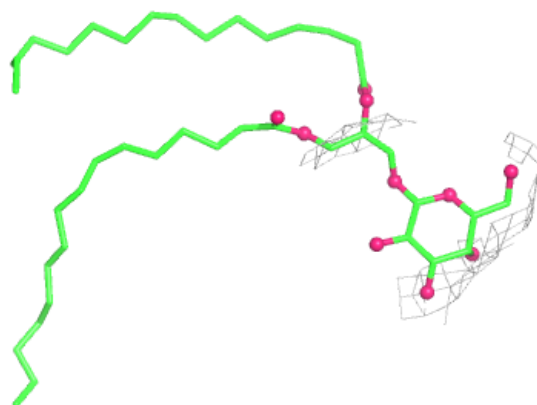
**Electron density around BCR K 102:**

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

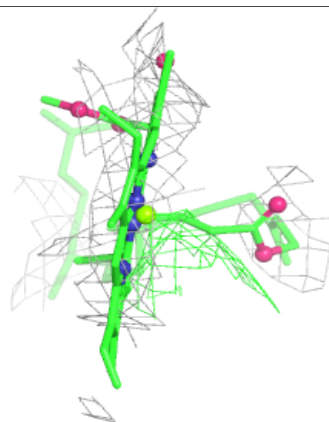
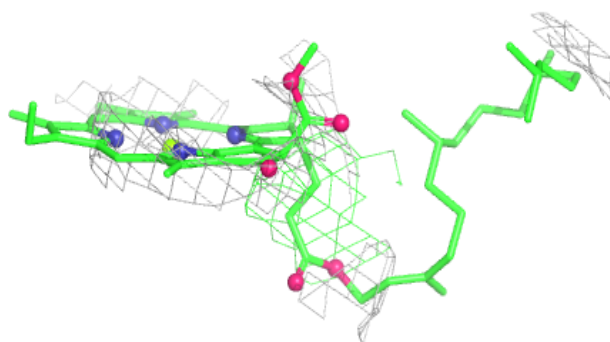
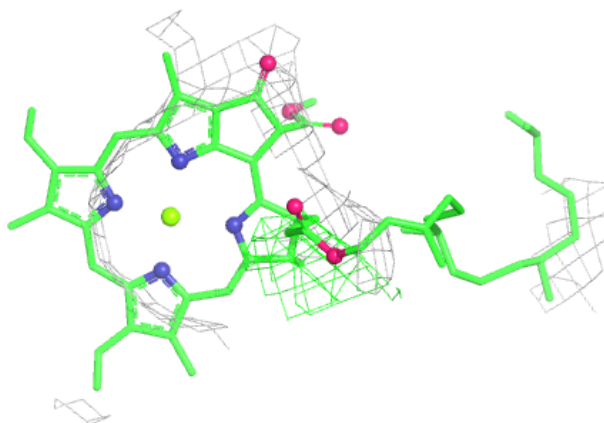


Electron density around LMG C 519:

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

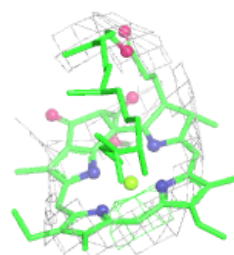
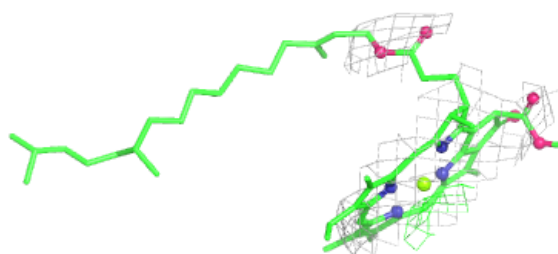
**Electron density around CLA B 613:**

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

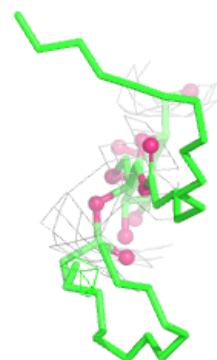
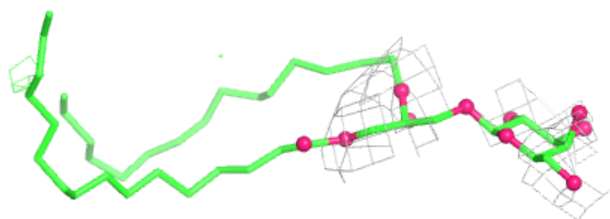
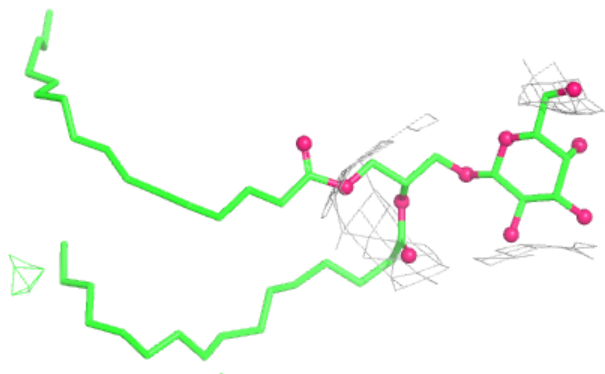


Electron density around CLA C 504:

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

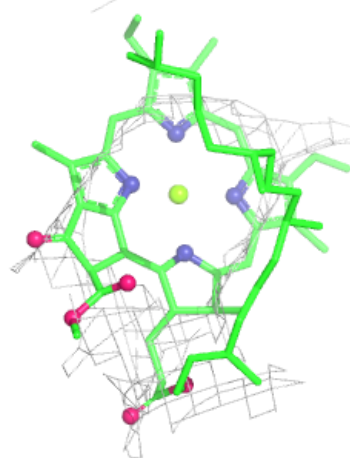
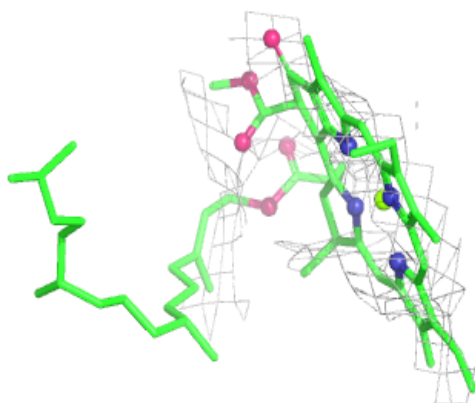
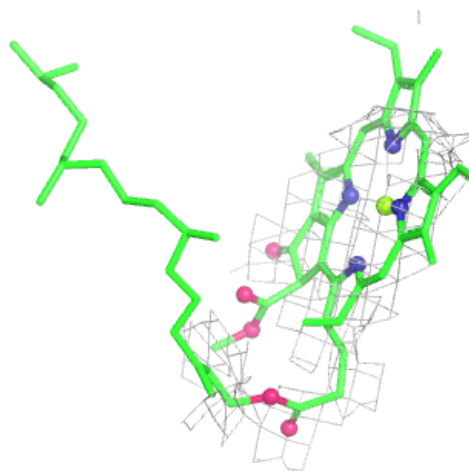
**Electron density around LMG d 406:**

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



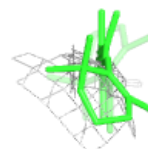
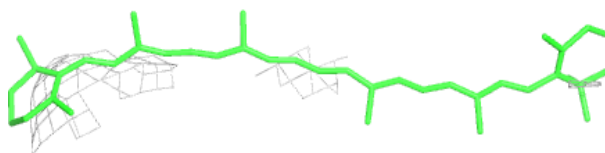
Electron density around CLA b 614:

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



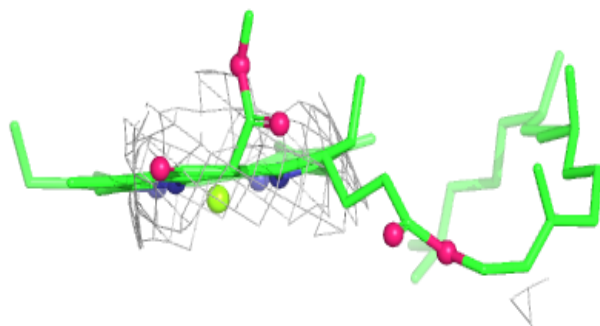
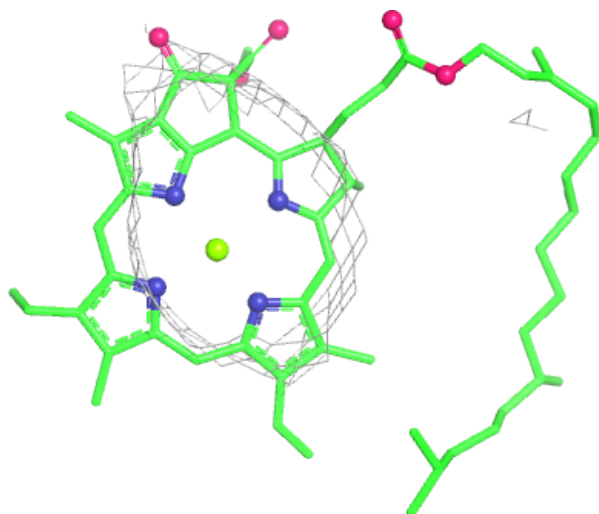
Electron density around BCR b 618:

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



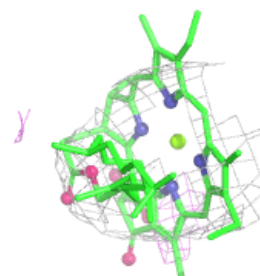
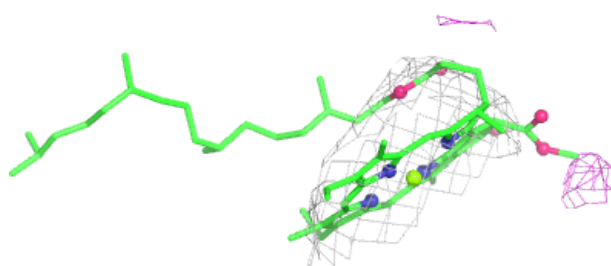
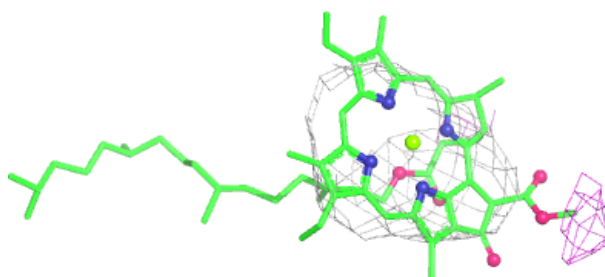
Electron density around CLA c 512:

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

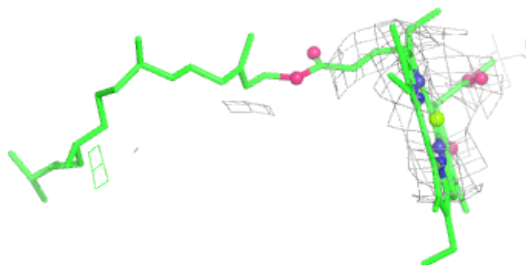
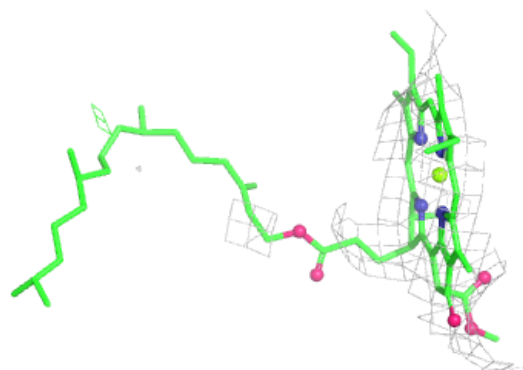


Electron density around CLA b 615:

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

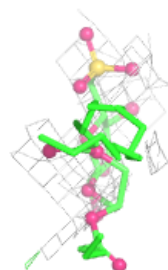
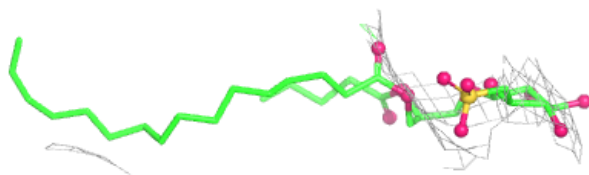
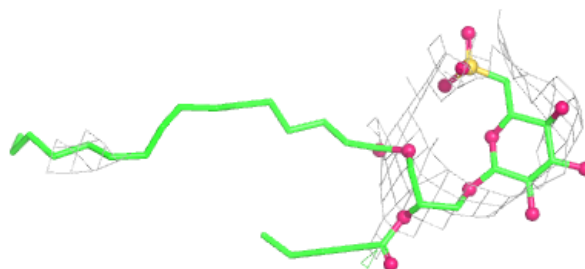
**Electron density around CLA d 403:**

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

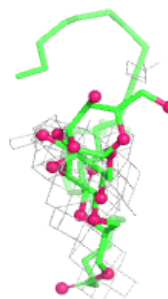
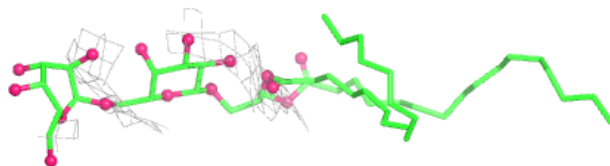


Electron density around SQD d 411:

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

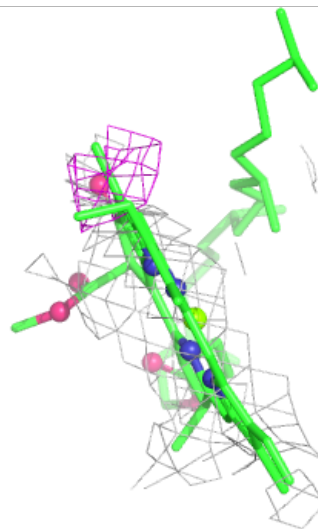
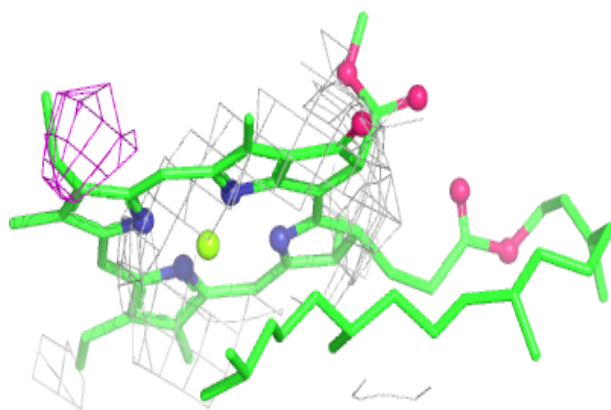
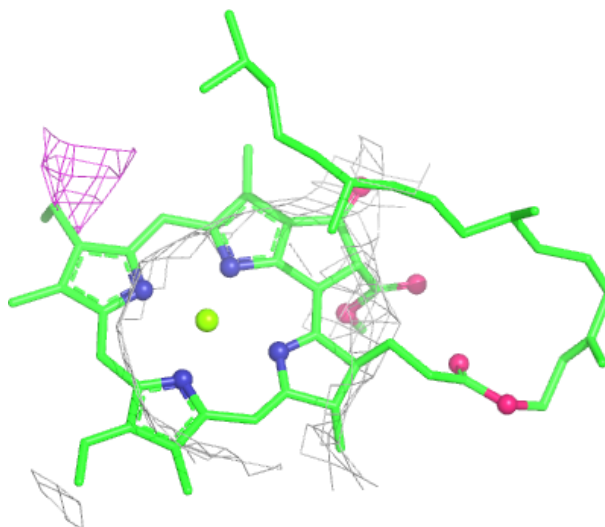
**Electron density around DGD D 410:**

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



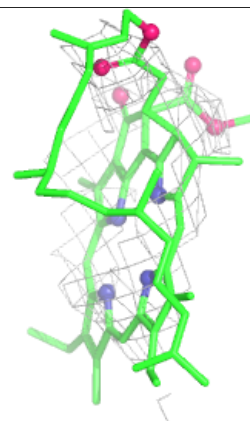
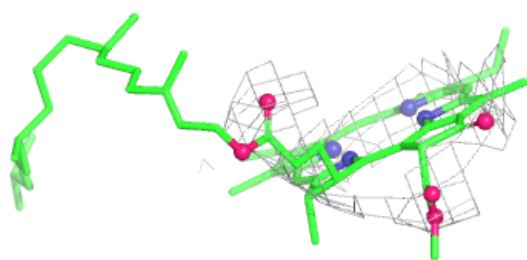
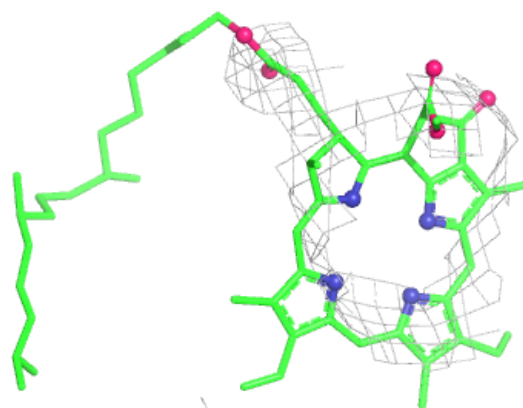
Electron density around CLA C 509:

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

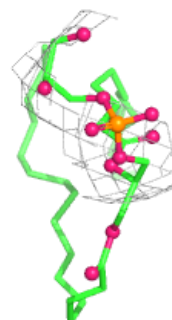


Electron density around PHO a 606:

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

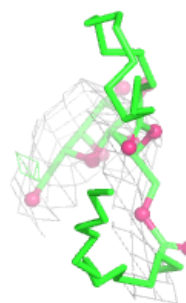
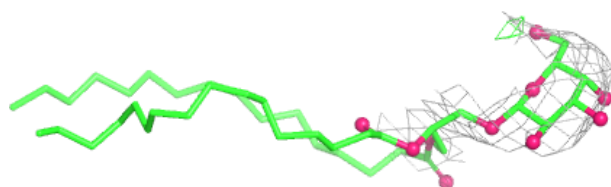
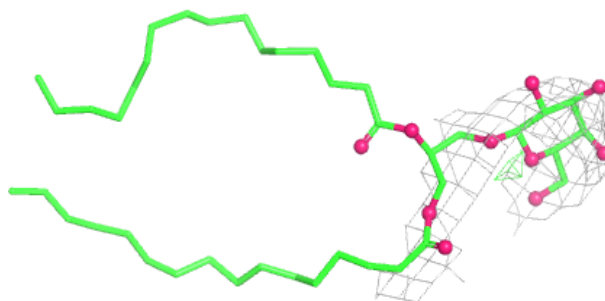
**Electron density around LHG D 409:**

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

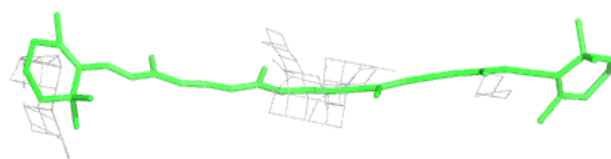
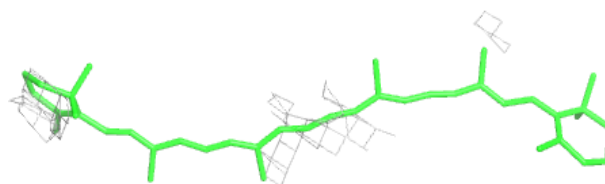


Electron density around LMG a 614:

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

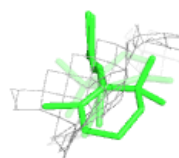
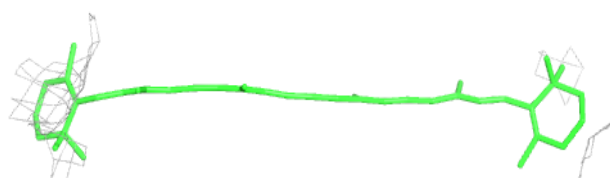
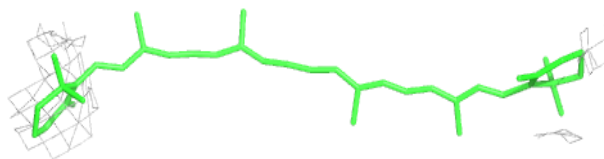
**Electron density around BCR K 101:**

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

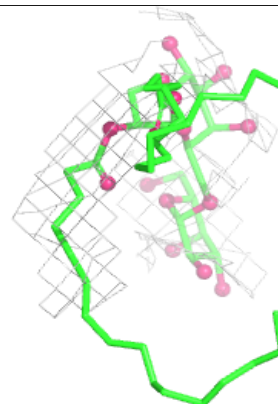
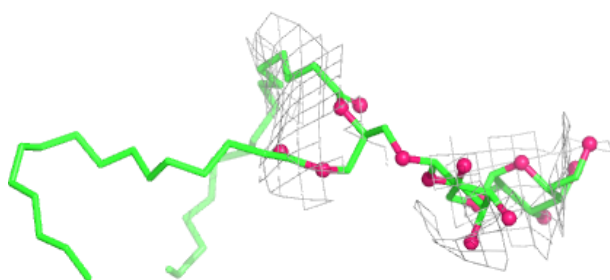
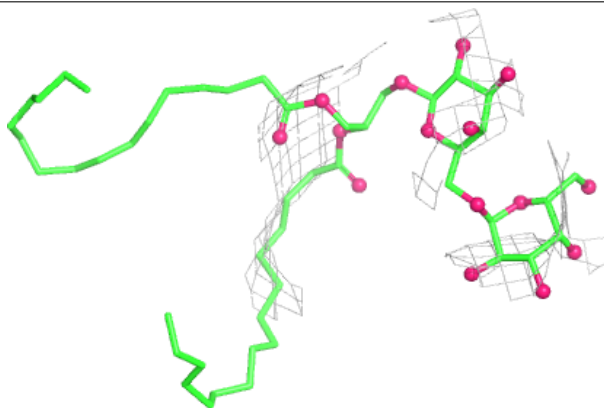


Electron density around BCR c 515:

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

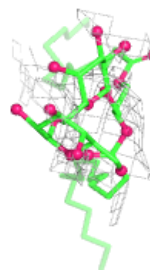
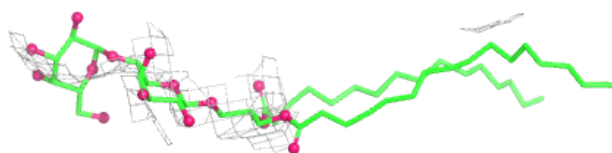
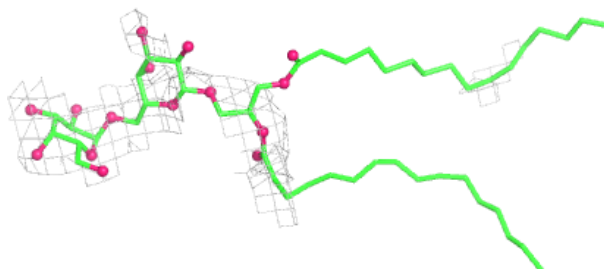
**Electron density around DGD C 517:**

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

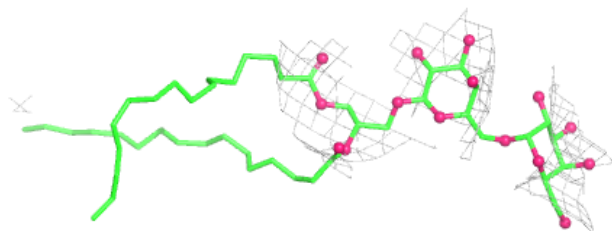
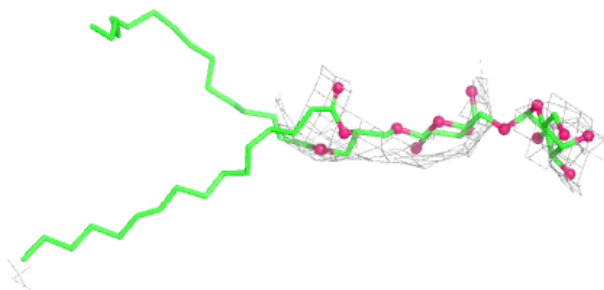


Electron density around DGD C 518:

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

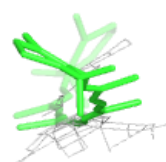
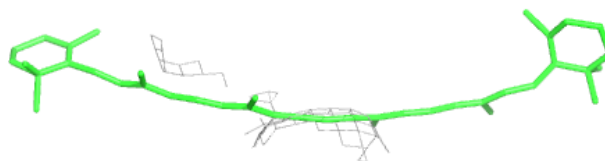
**Electron density around DGD c 516:**

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

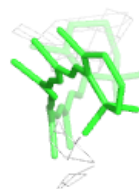
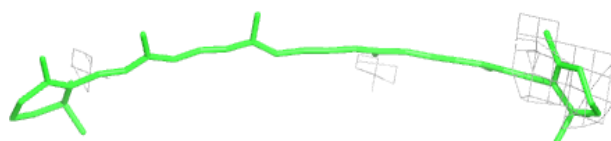
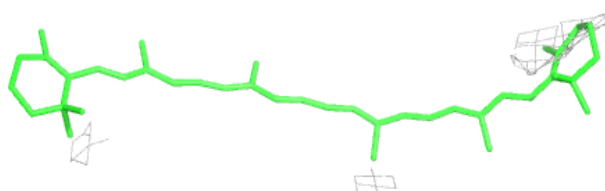


Electron density around BCR D 404:

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

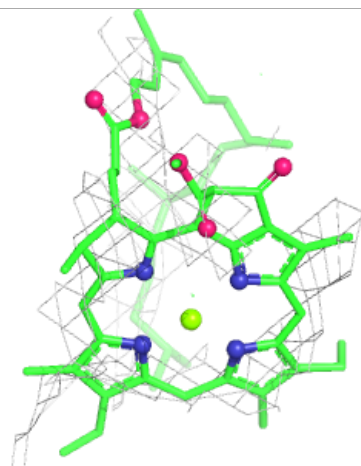
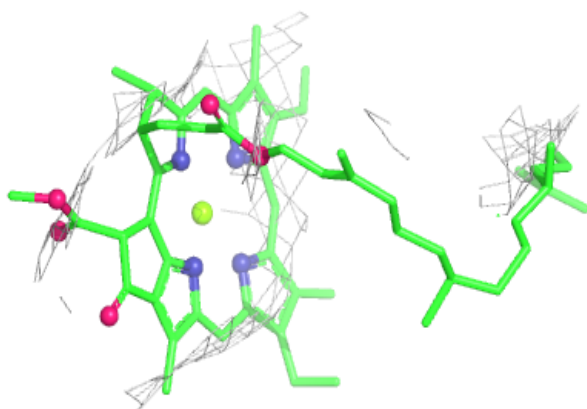
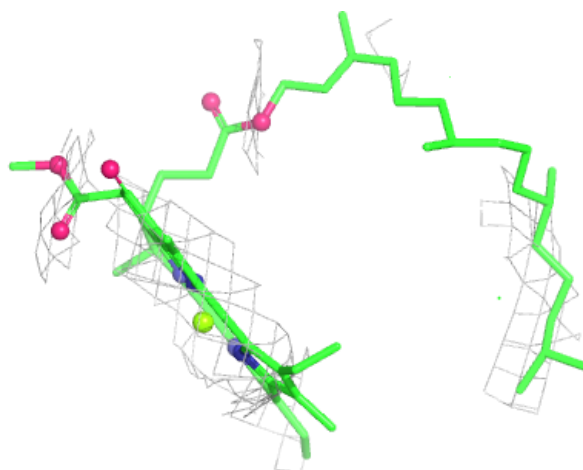
**Electron density around BCR B 622:**

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



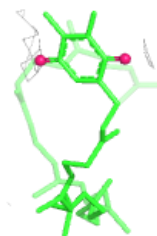
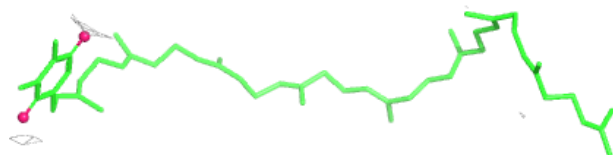
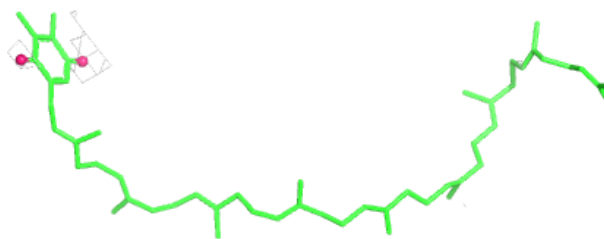
Electron density around CLA b 612:

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

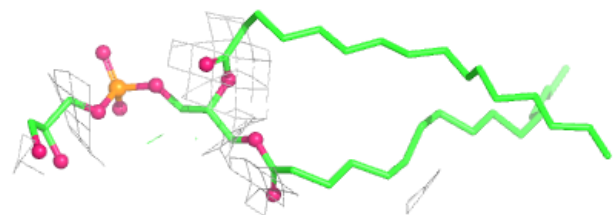
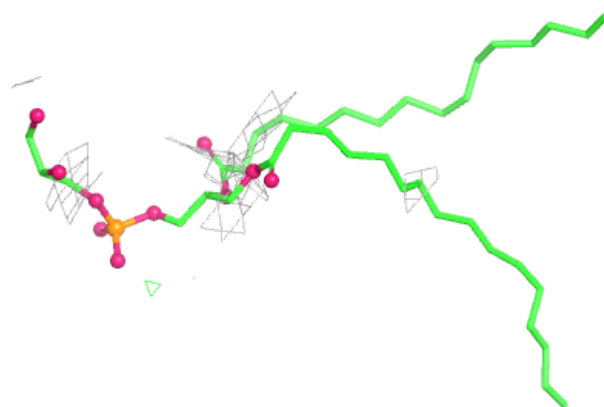


Electron density around PL9 a 613:

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

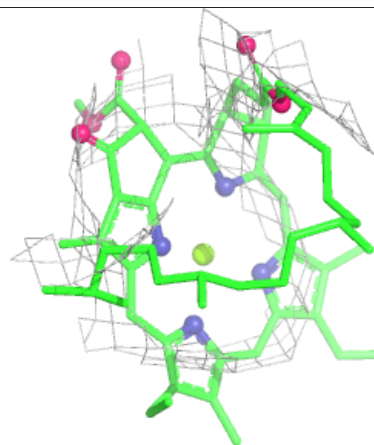
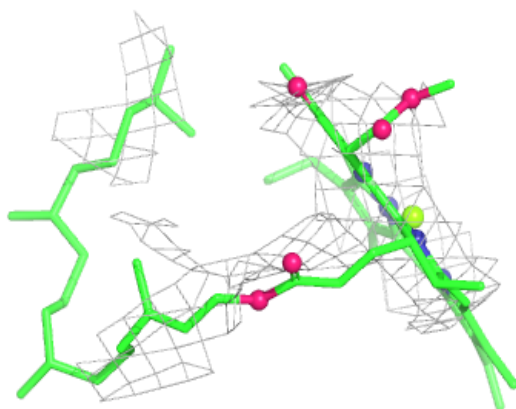
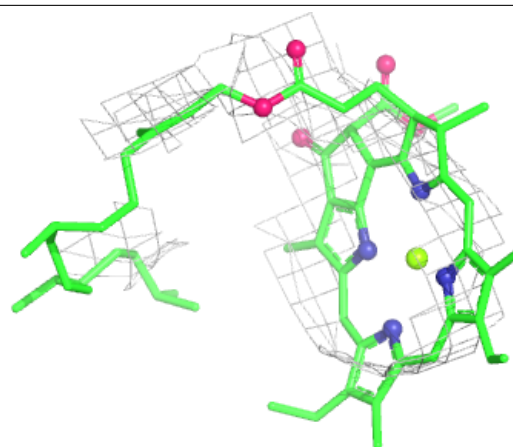
**Electron density around LHG d 407:**

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



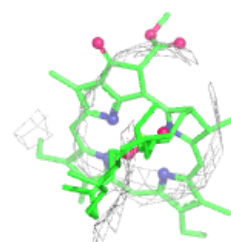
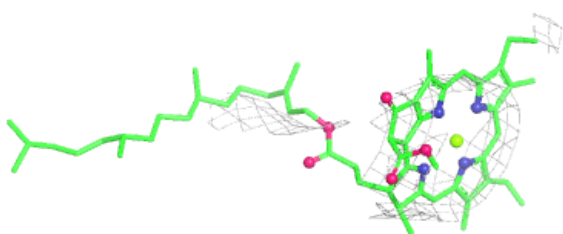
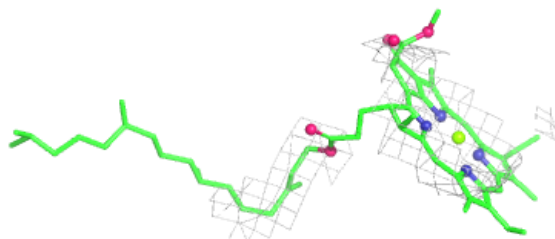
Electron density around CLA c 503:

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

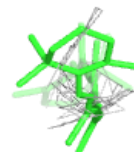
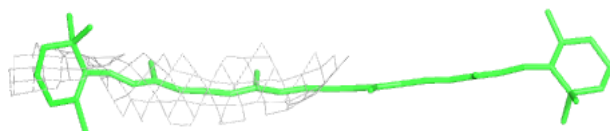
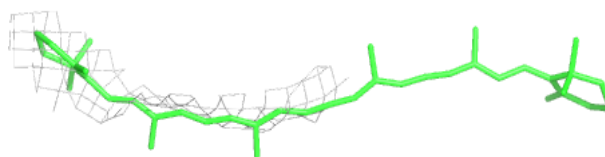


Electron density around CLA c 502:

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

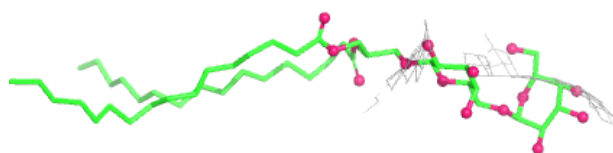
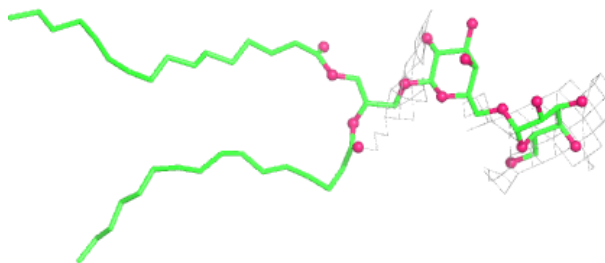
**Electron density around BCR H 101:**

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



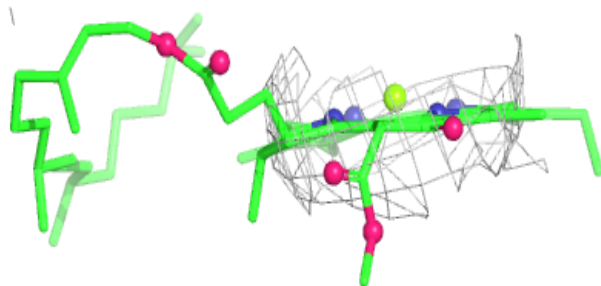
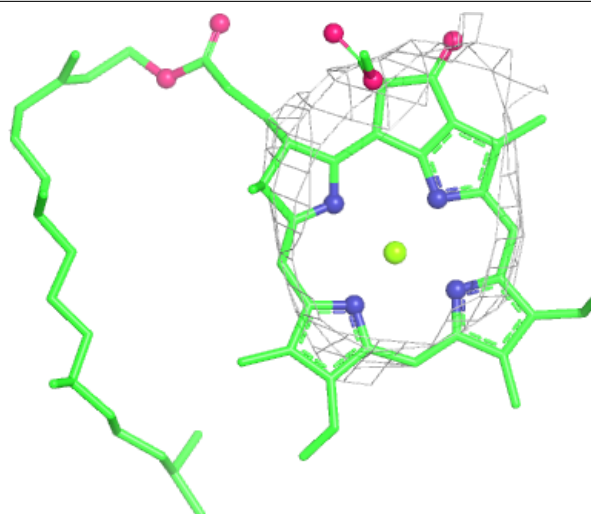
Electron density around DGD c 518:

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



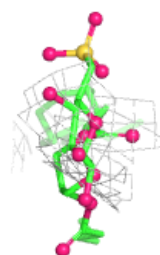
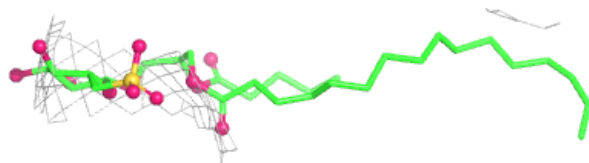
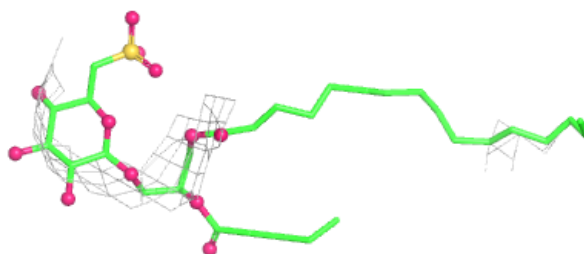
Electron density around CLA C 512:

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

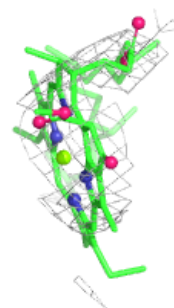
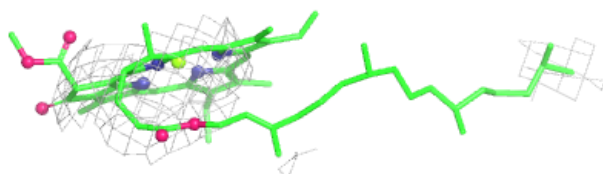
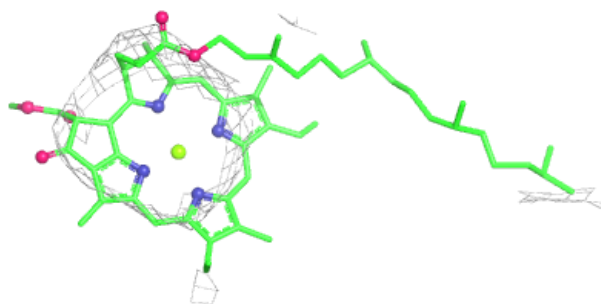


Electron density around SQD D 411:

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

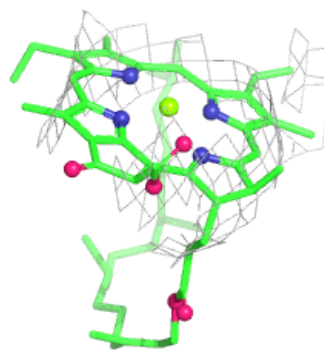
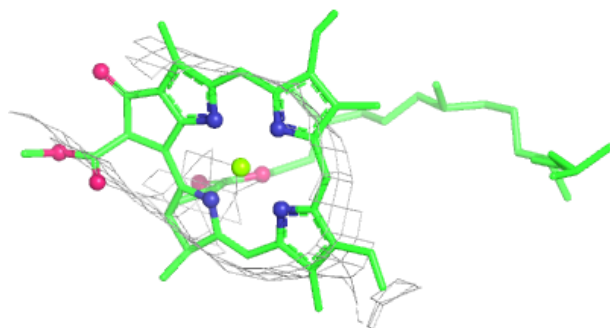
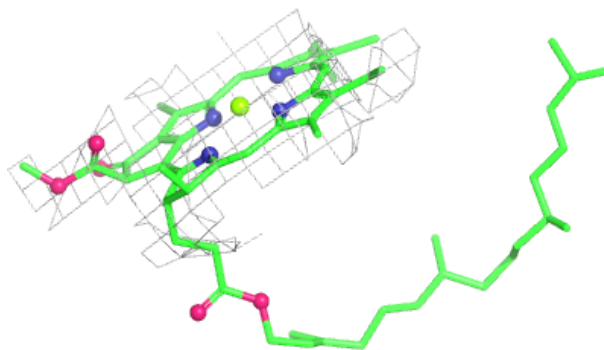
**Electron density around CLA C 501:**

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

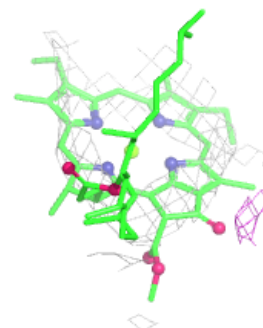
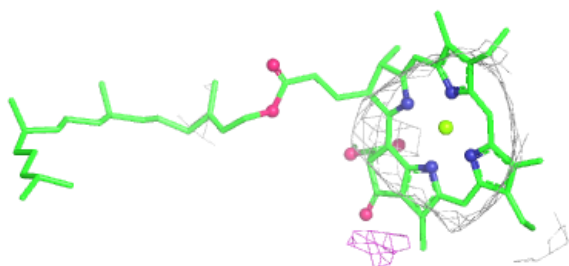
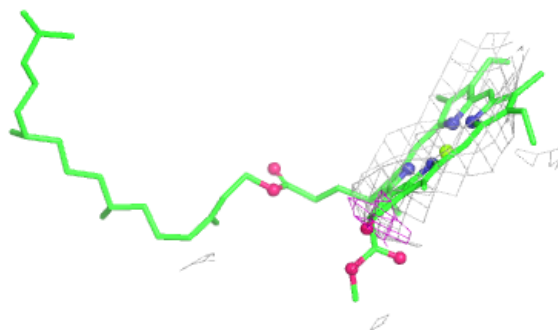


Electron density around CLA c 513:

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

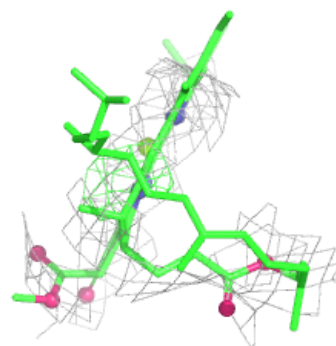
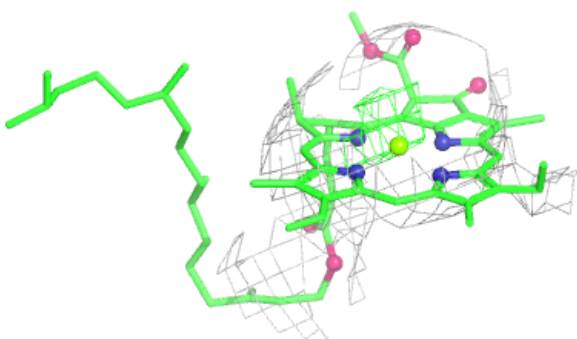
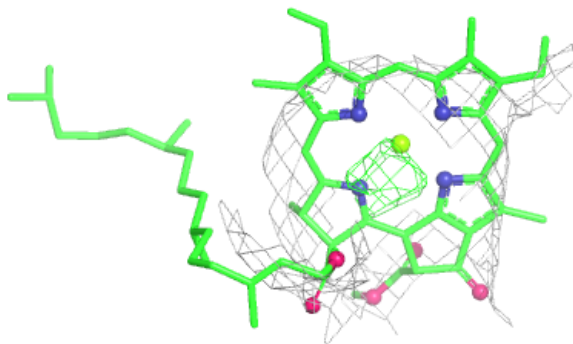
**Electron density around CLA D 401:**

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

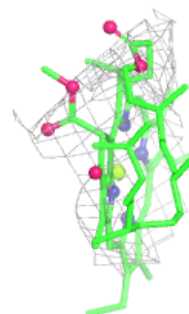
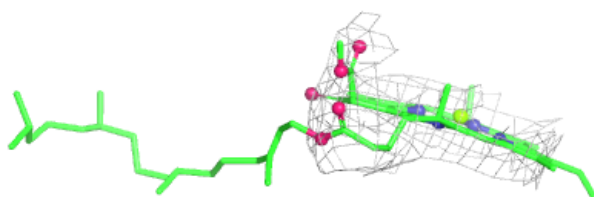
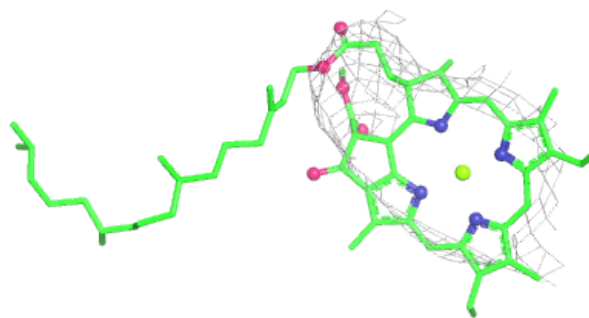


Electron density around CLA D 402:

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

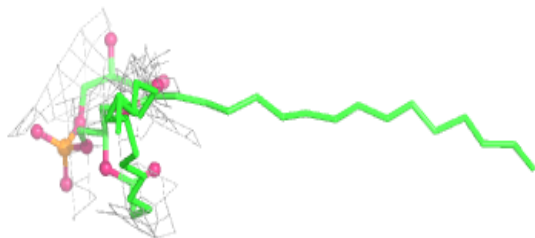
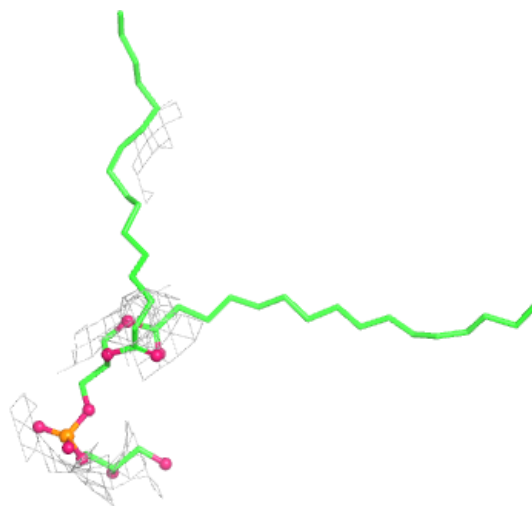
**Electron density around CLA b 603:**

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



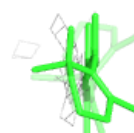
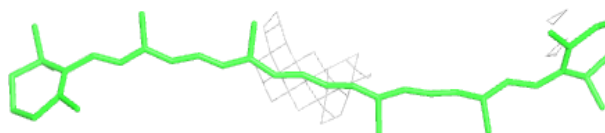
Electron density around LHG 1 103:

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

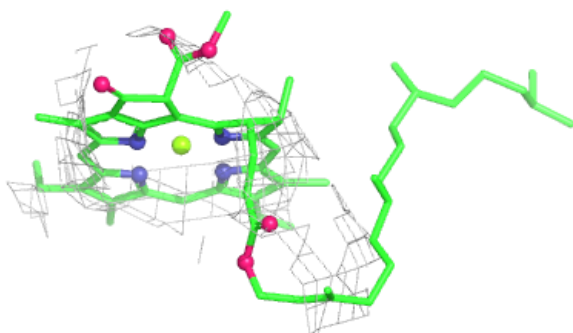
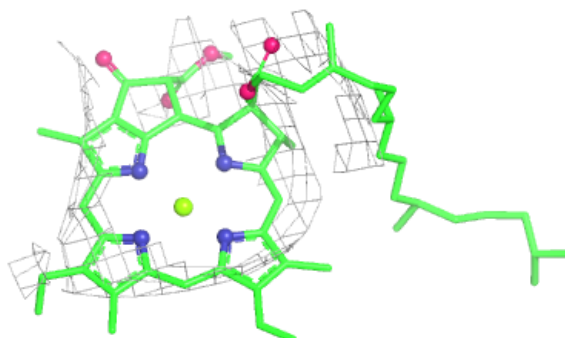


Electron density around BCR B 619:

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

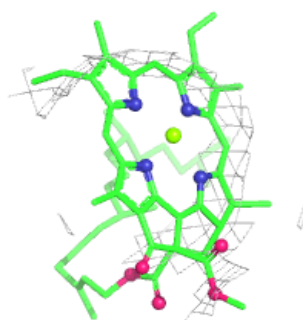
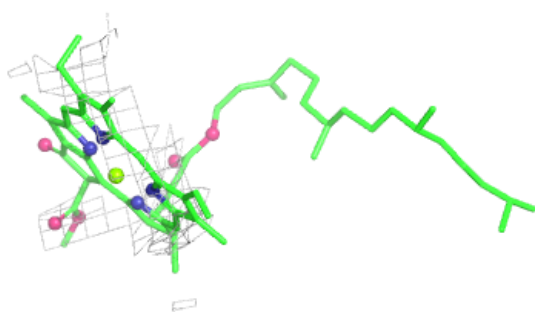
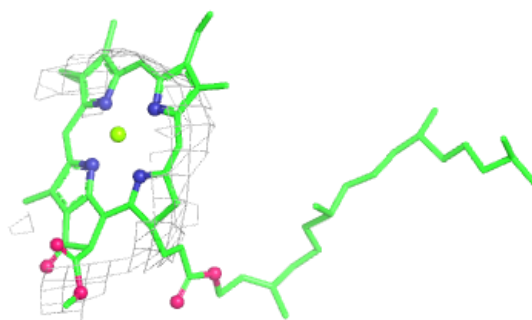
**Electron density around CLA d 402:**

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



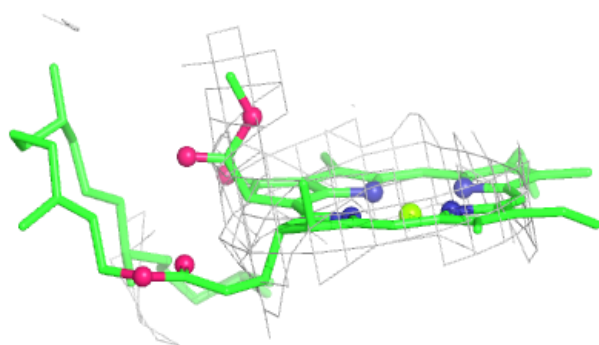
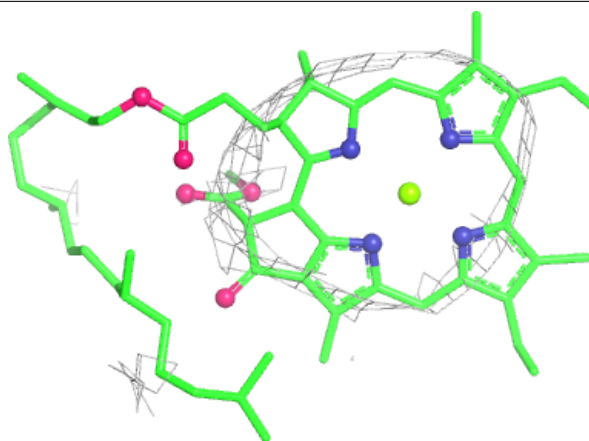
Electron density around CLA c 511:

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



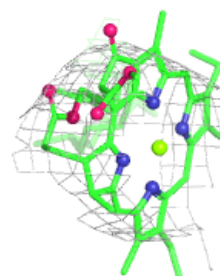
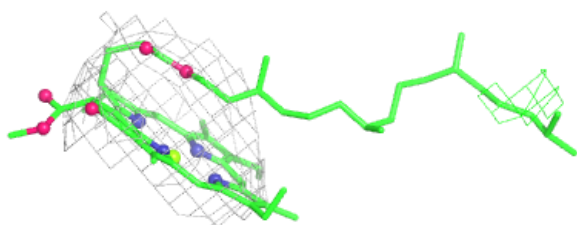
Electron density around CLA B 611:

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



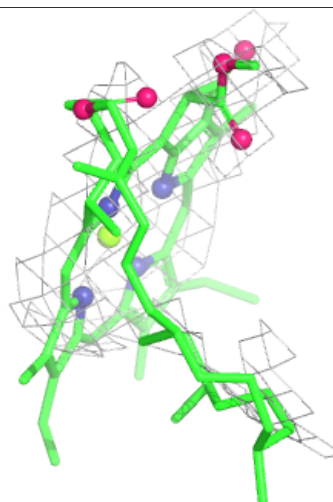
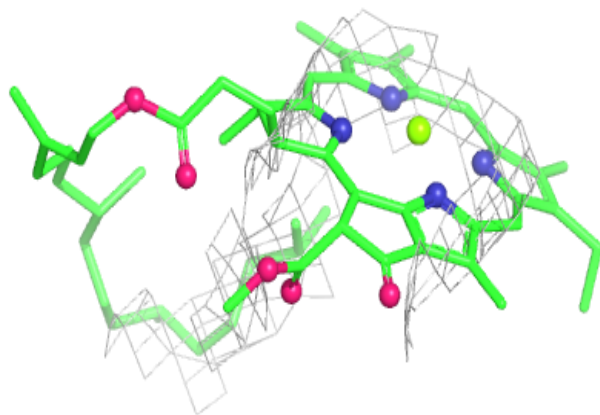
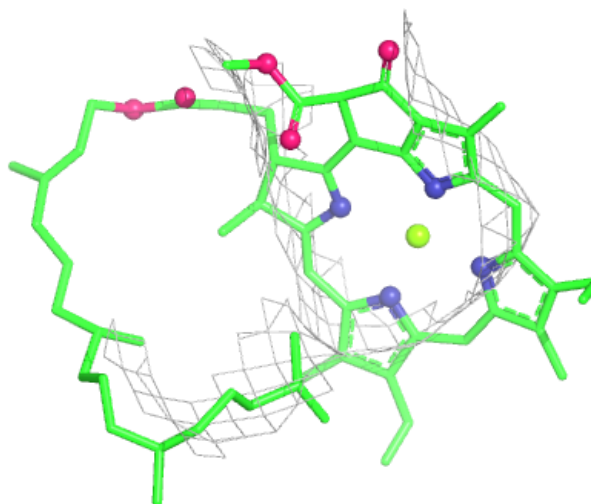
Electron density around CLA B 615:

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



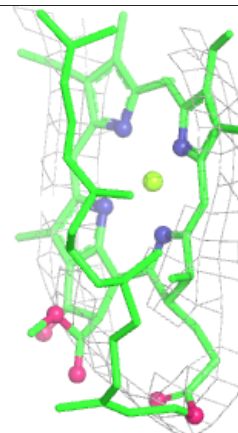
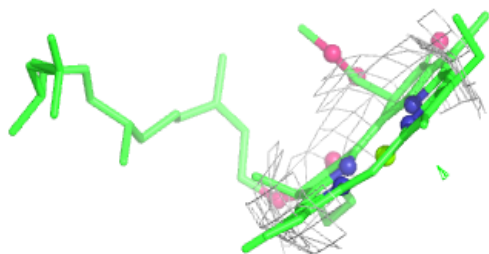
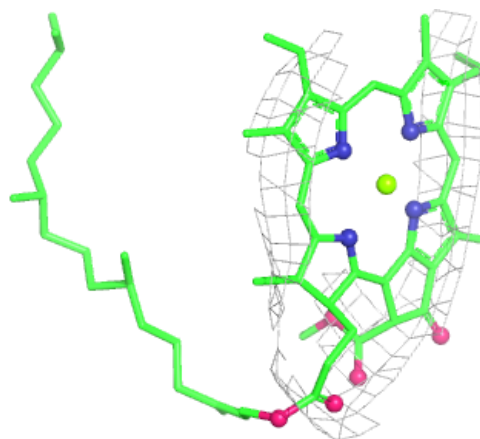
Electron density around CLA B 616:

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



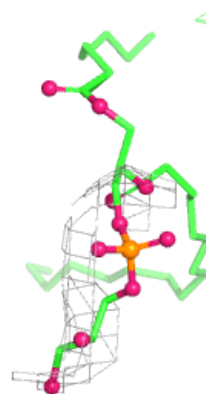
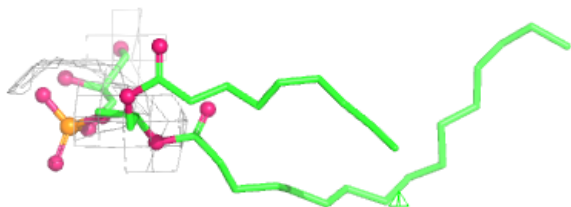
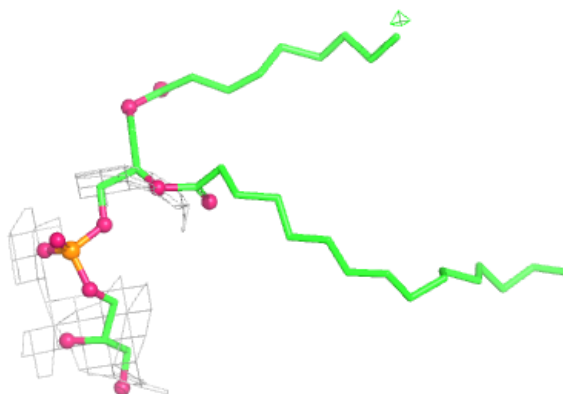
Electron density around CLA B 617:

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



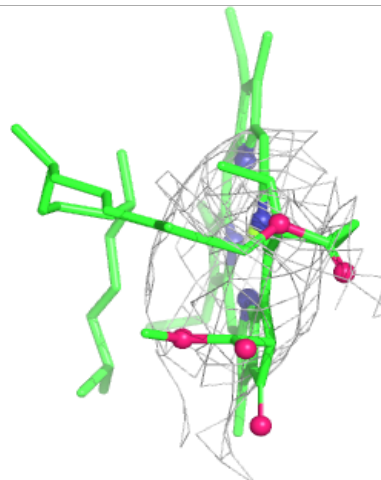
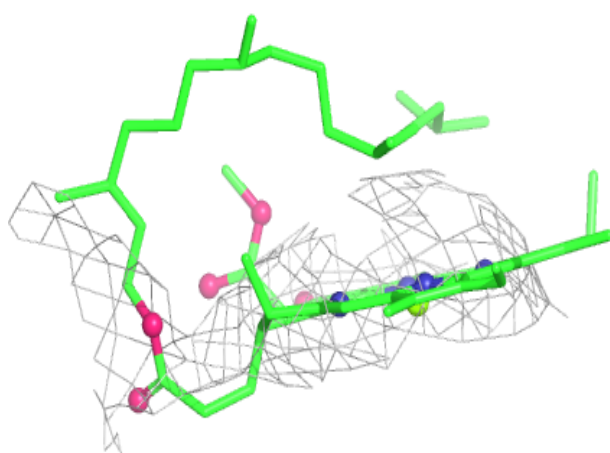
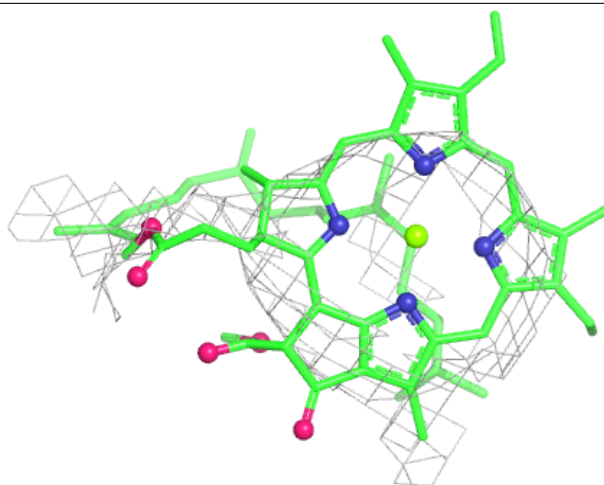
Electron density around LHG e 101:

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



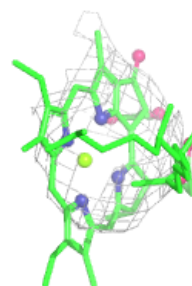
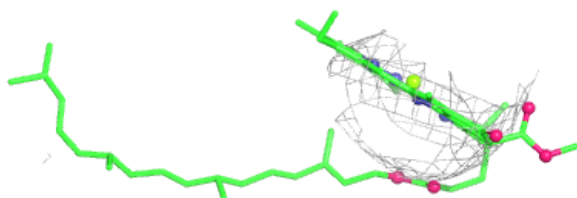
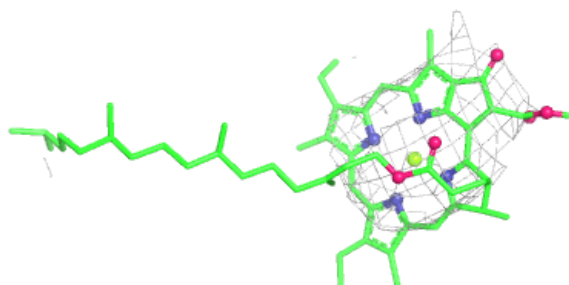
Electron density around CLA c 510:

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

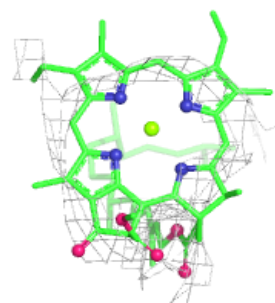
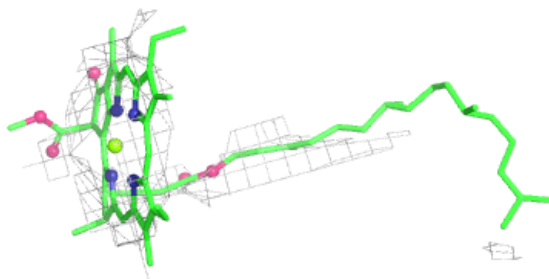


Electron density around CLA B 609:

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

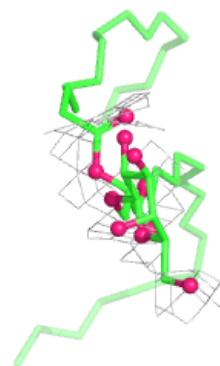
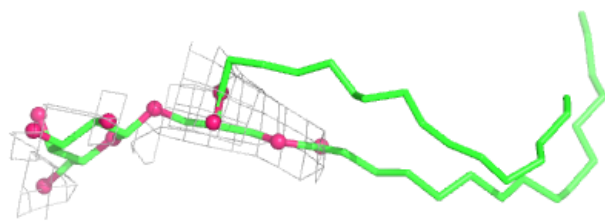
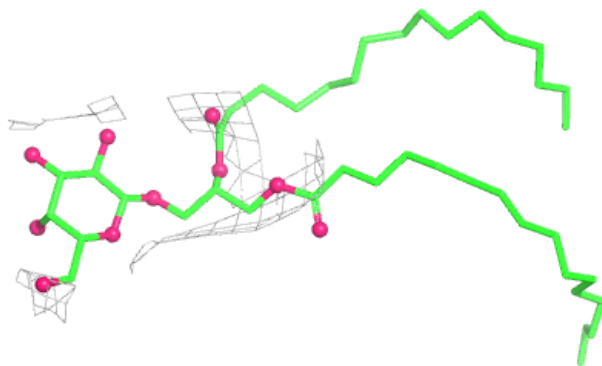
**Electron density around CLA B 606:**

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

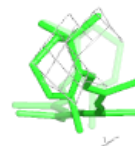


Electron density around LMG D 406:

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

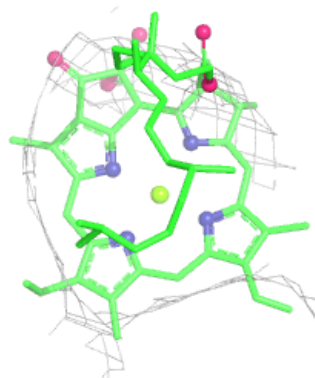
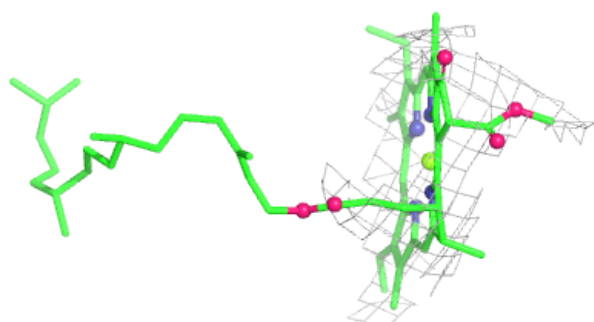
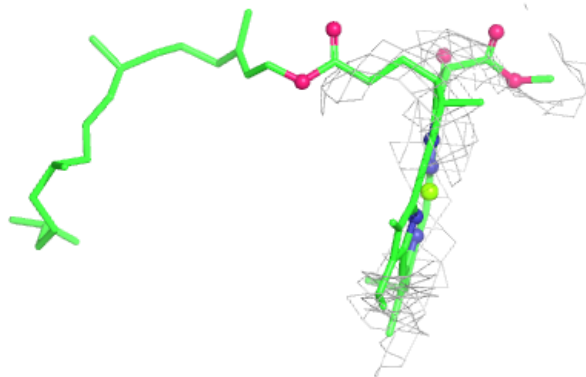
**Electron density around BCR k 102:**

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

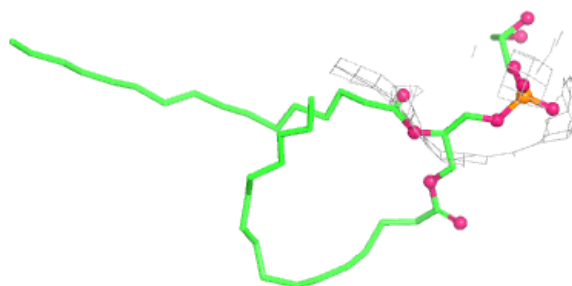


Electron density around CLA C 506:

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

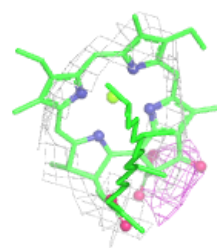
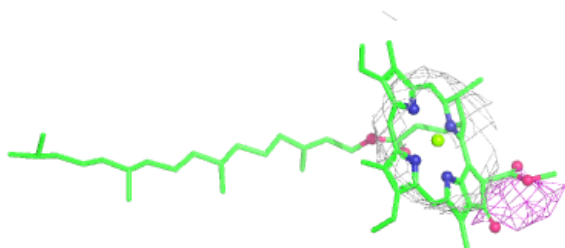
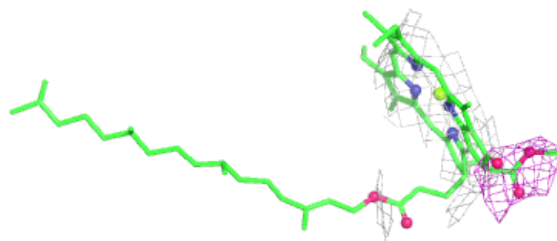
**Electron density around LHG D 405:**

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



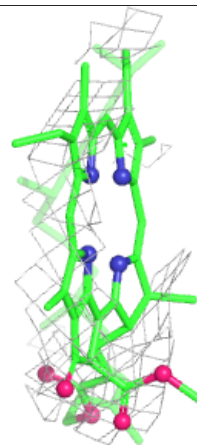
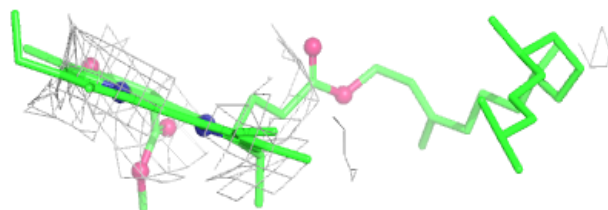
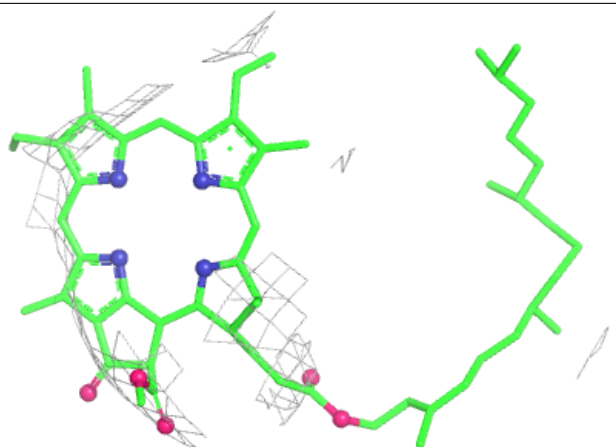
Electron density around CLA B 608:

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



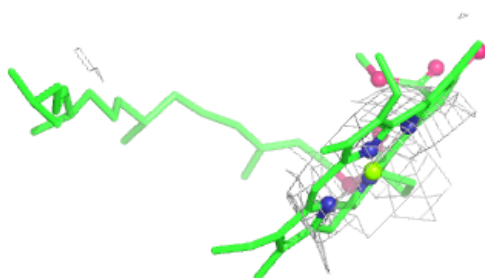
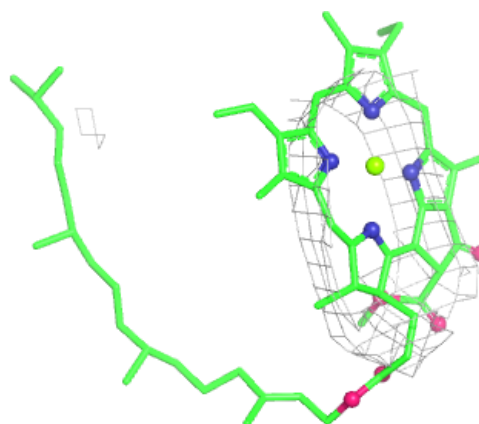
Electron density around PHO a 605:

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

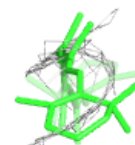
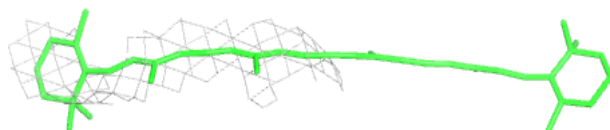


Electron density around CLA c 507:

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

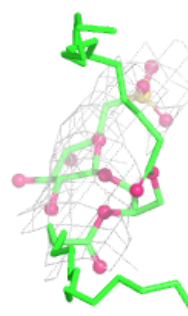
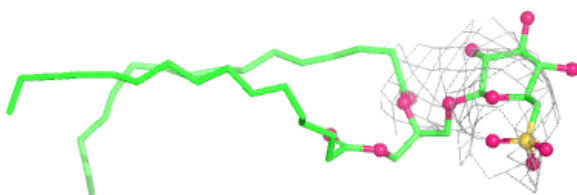
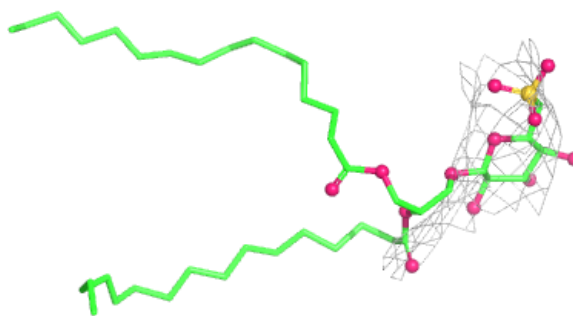
**Electron density around BCR h 101:**

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

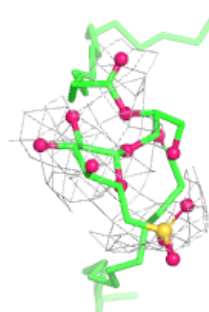
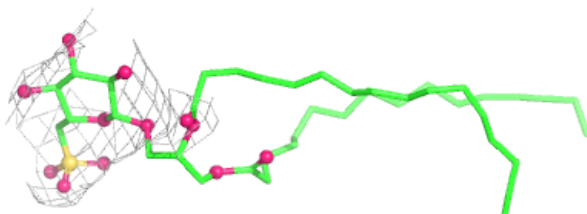
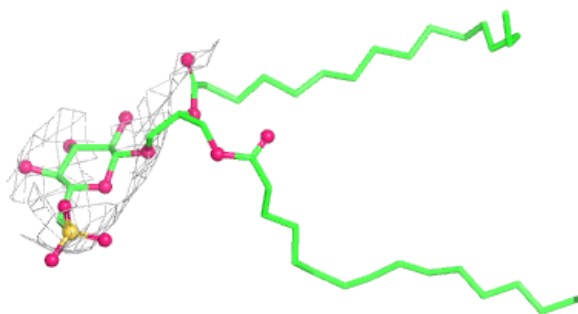


Electron density around SQD B 601:

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

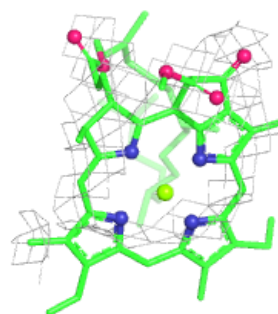
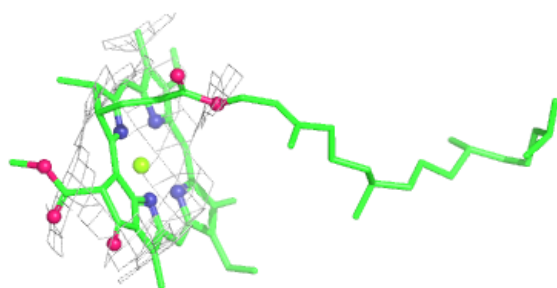
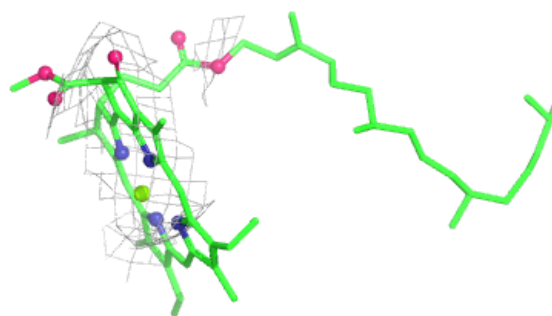
**Electron density around SQD b 601:**

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



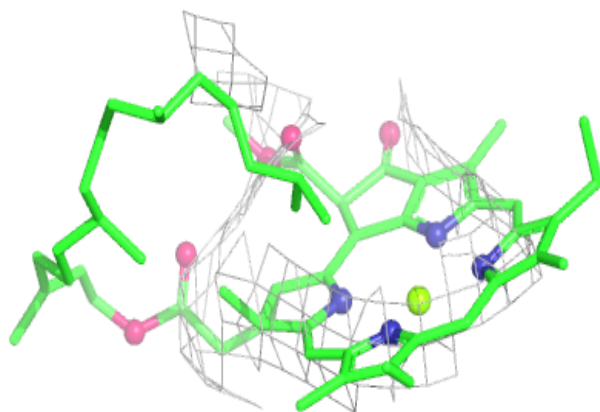
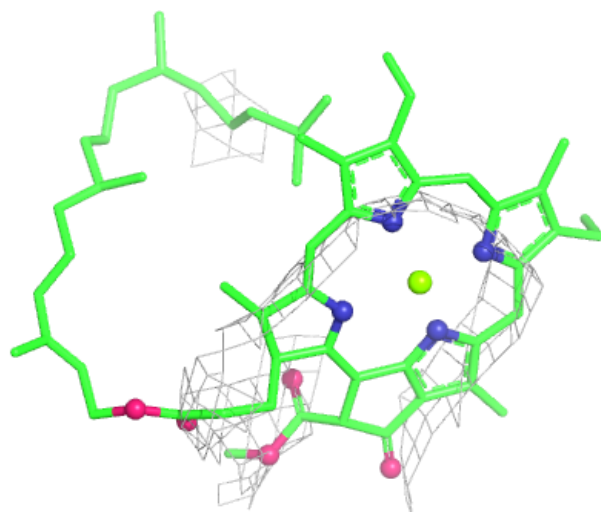
Electron density around CLA c 508:

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



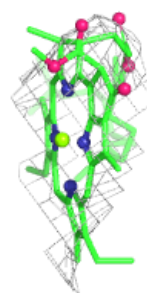
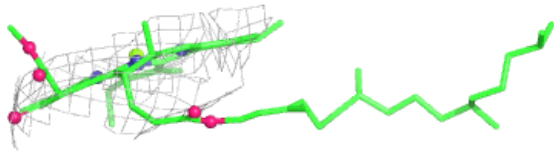
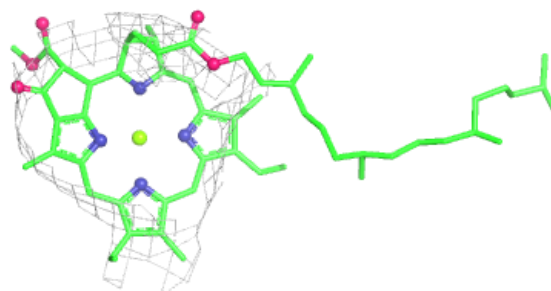
Electron density around CLA b 616:

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

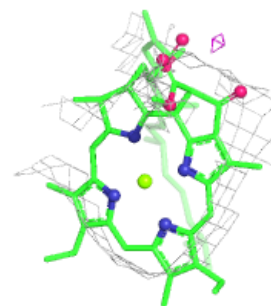
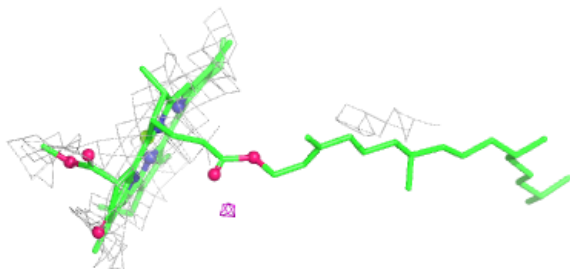
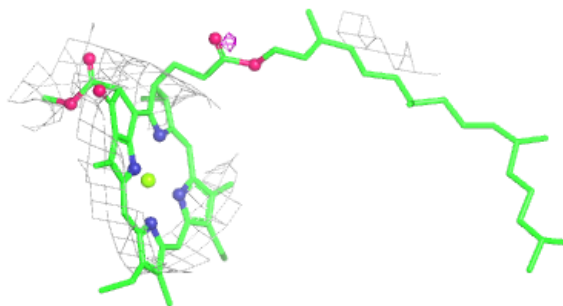


Electron density around CLA b 604:

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

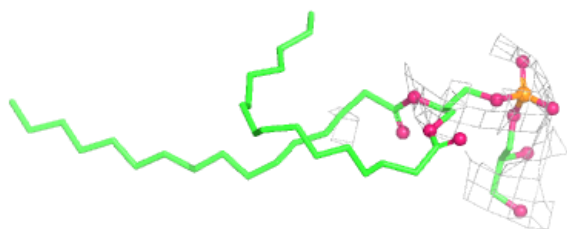
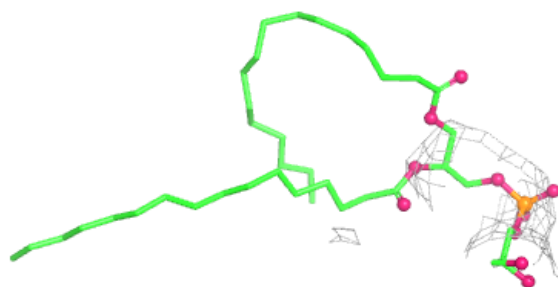
**Electron density around CLA b 610:**

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



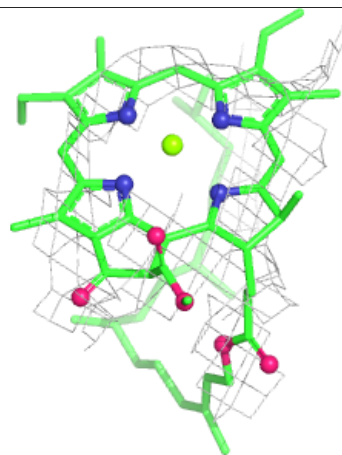
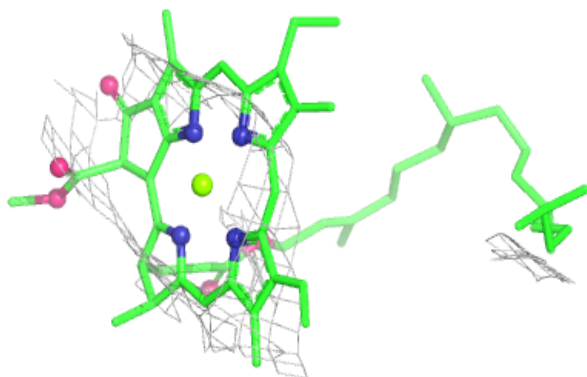
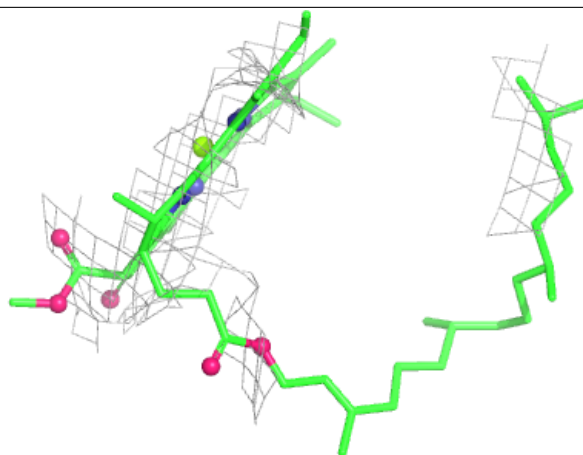
Electron density around LHG d 405:

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



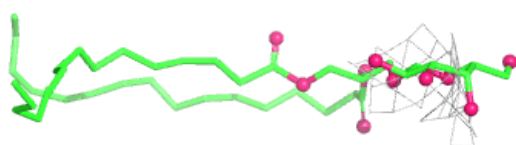
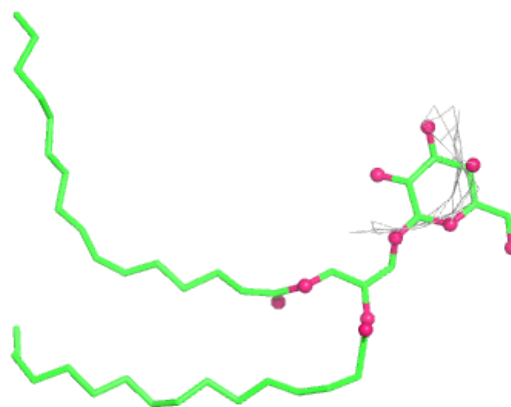
Electron density around CLA B 612:

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



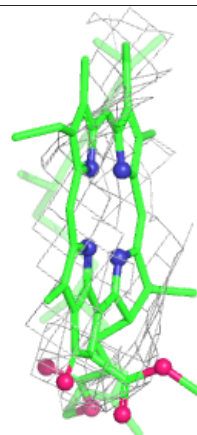
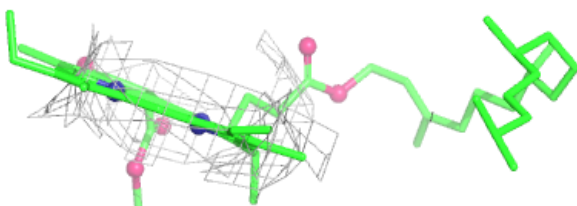
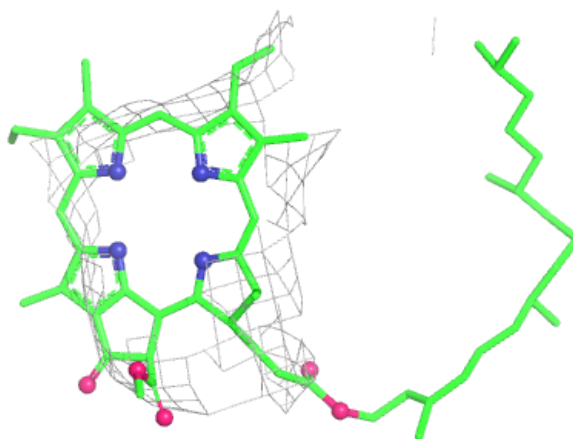
Electron density around LMG c 519:

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



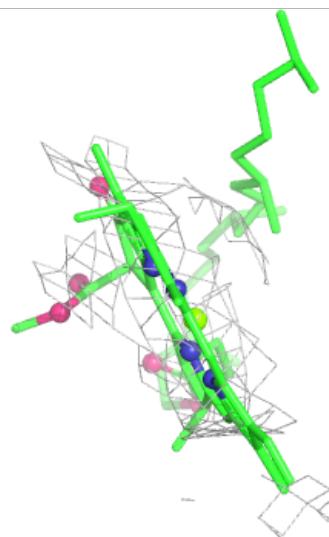
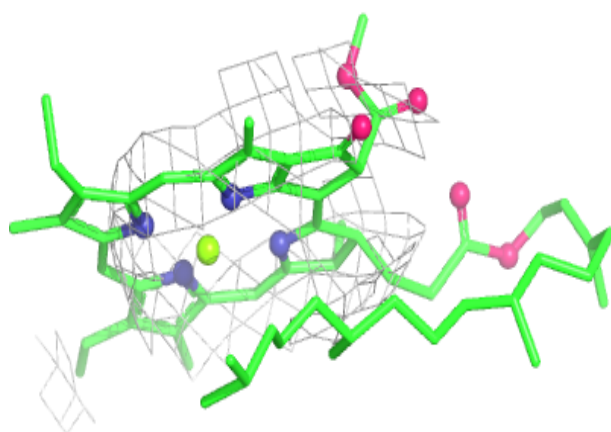
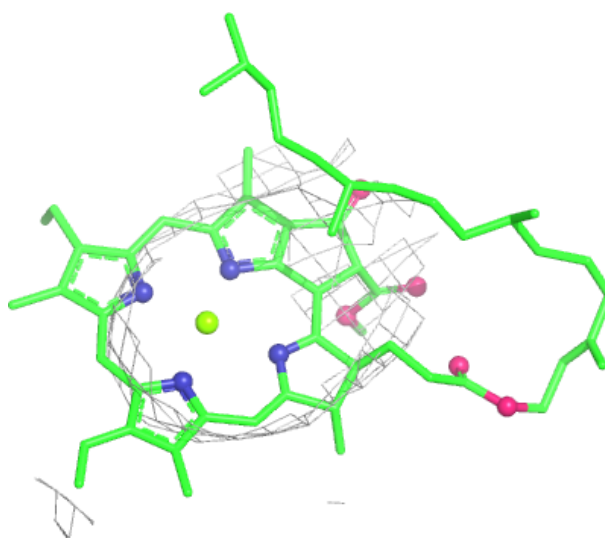
Electron density around PHO A 605:

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



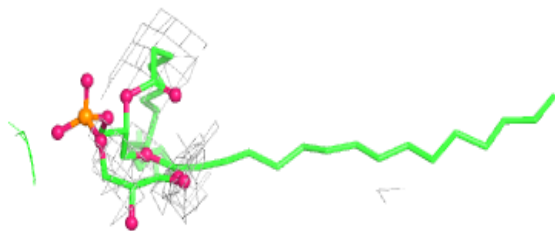
Electron density around CLA c 509:

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



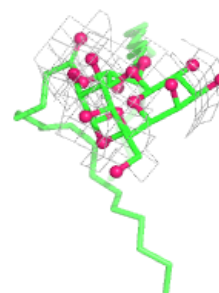
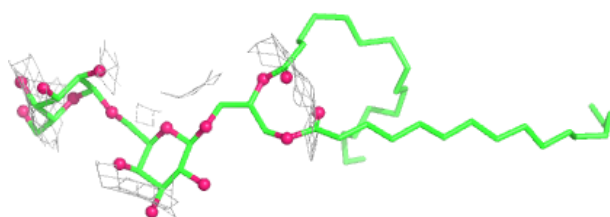
Electron density around LHG L 102:

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

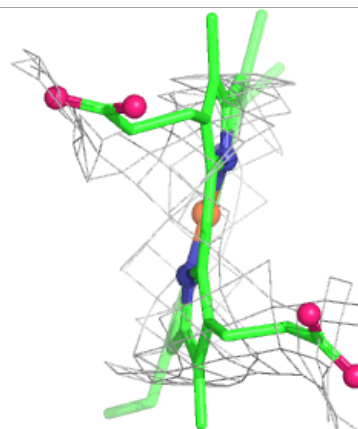
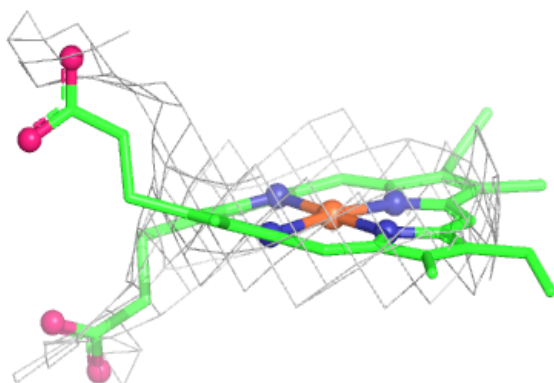
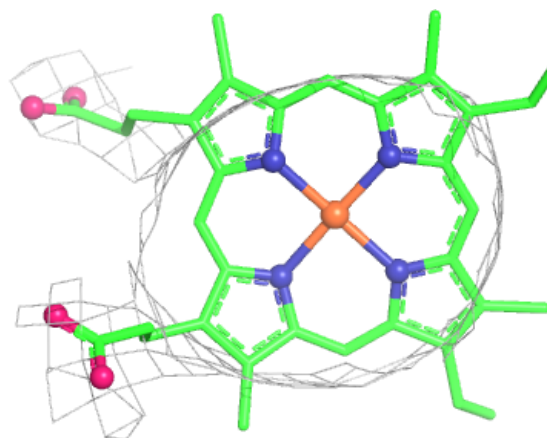


Electron density around DGD h 102:

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

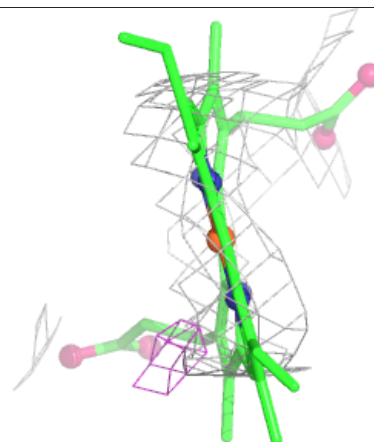
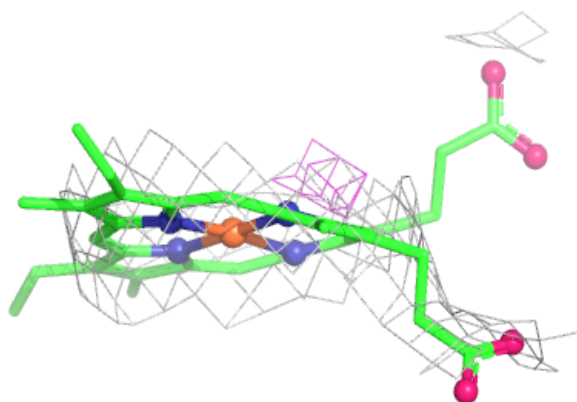
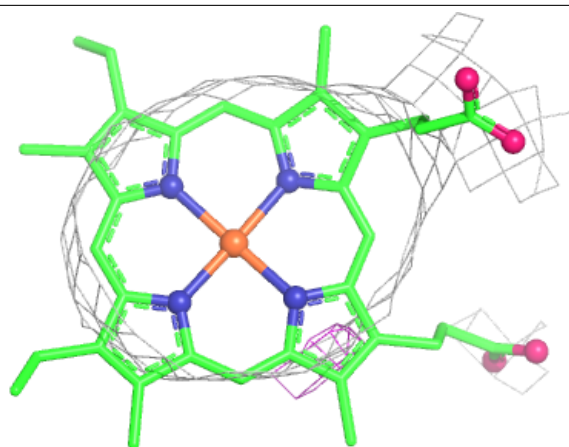
**Electron density around HEM F 101:**

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

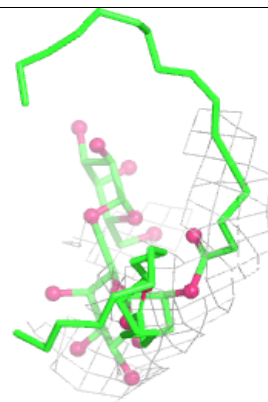
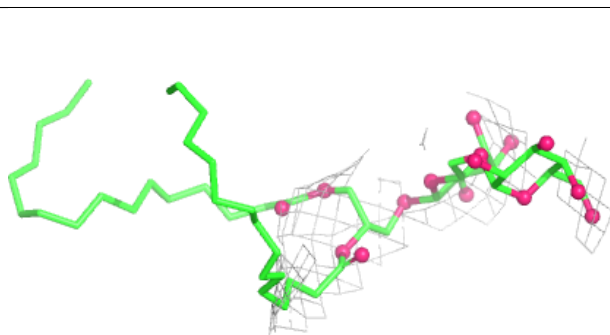
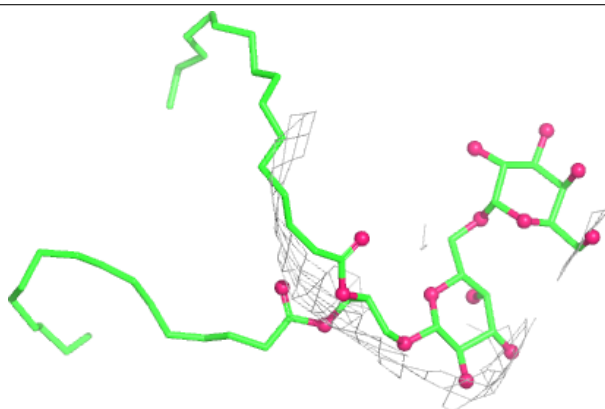


Electron density around HEM f 101:

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

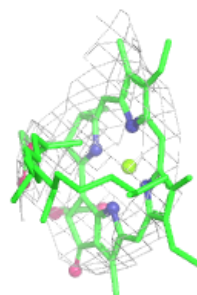
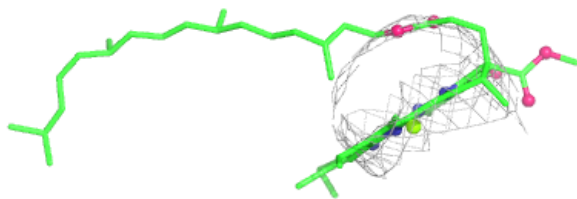
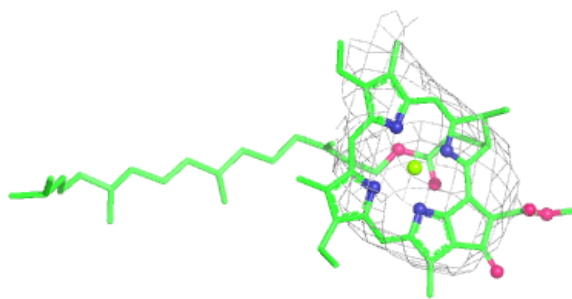
**Electron density around DGD c 517:**

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



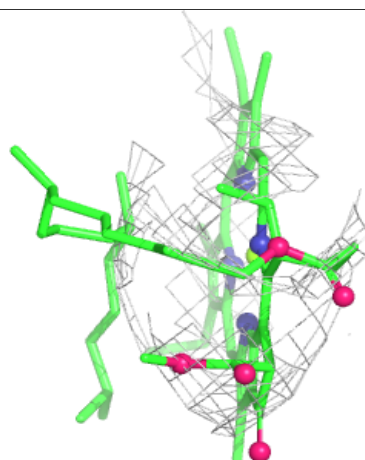
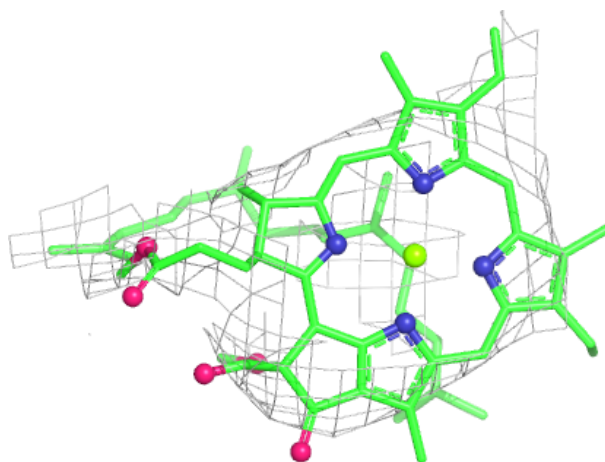
Electron density around CLA b 609:

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



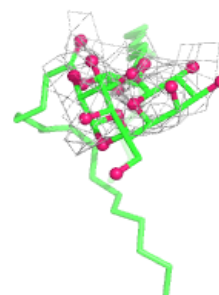
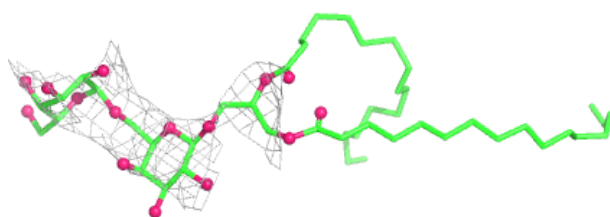
Electron density around CLA C 510:

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

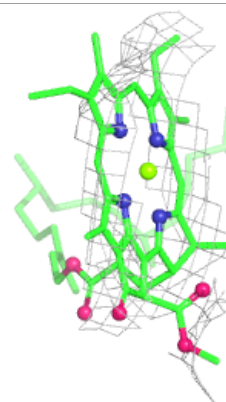
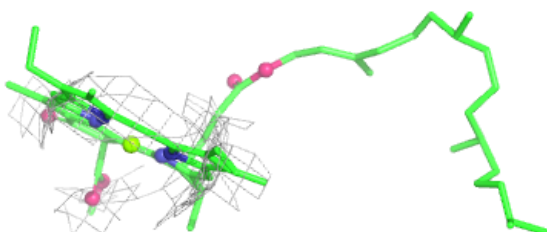
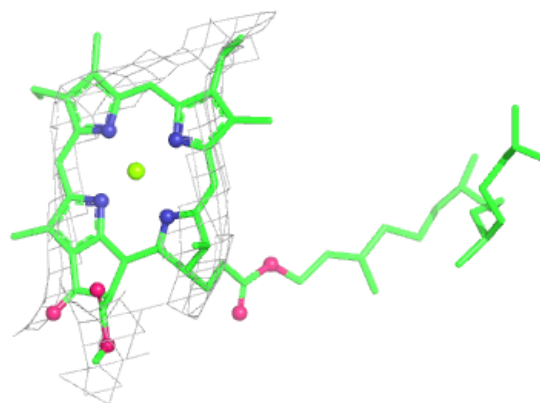


Electron density around DGD H 102:

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

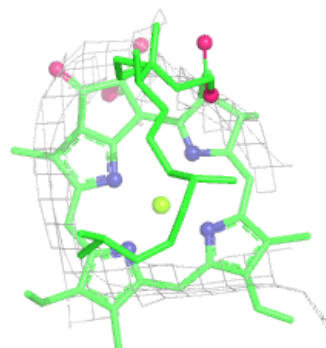
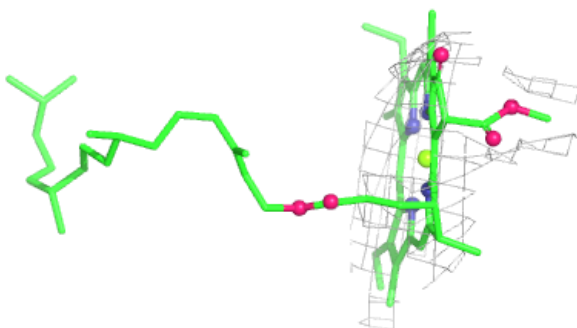
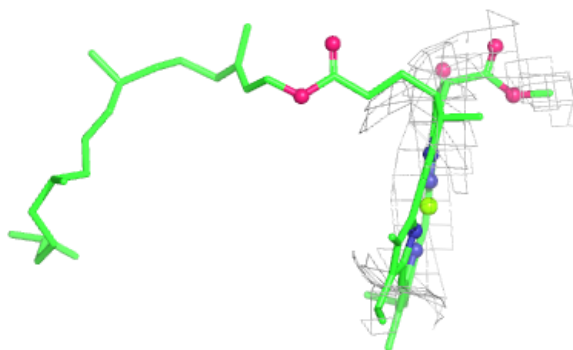
**Electron density around CLA A 607:**

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

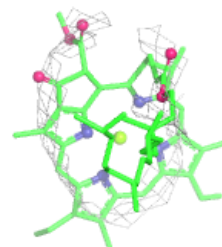
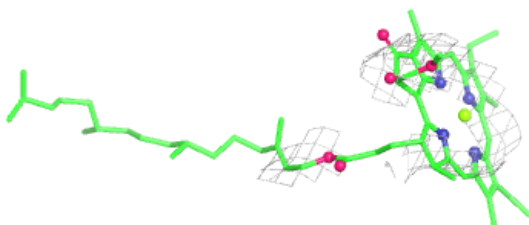
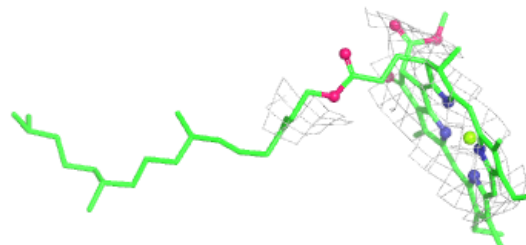


Electron density around CLA c 506:

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

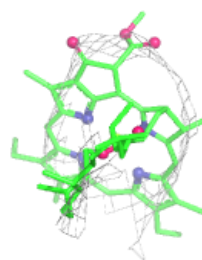
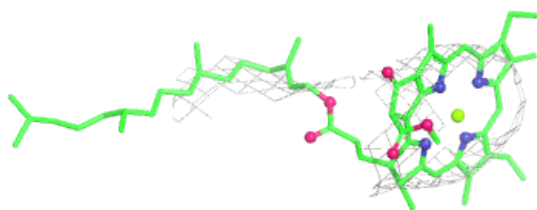
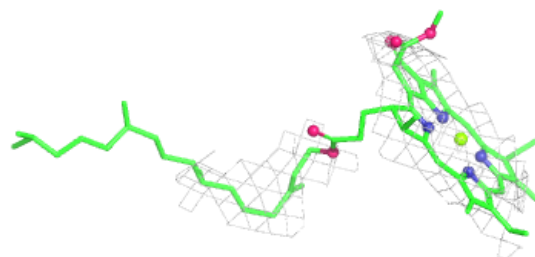
**Electron density around CLA b 605:**

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

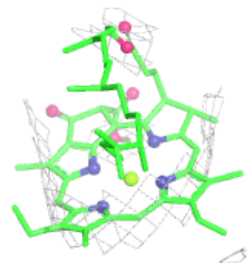
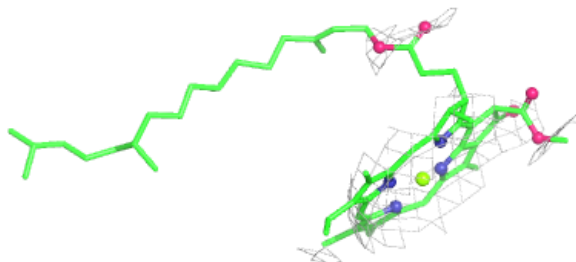


Electron density around CLA C 502:

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

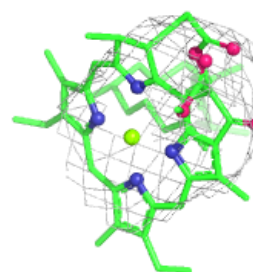
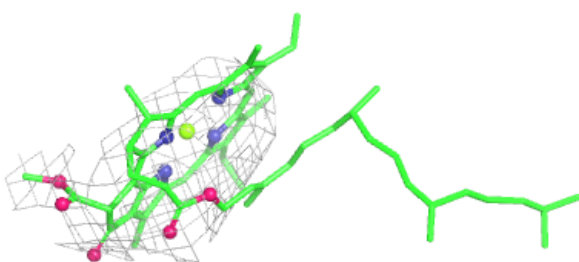
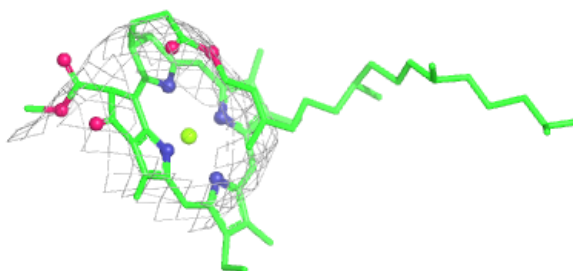
**Electron density around CLA c 504:**

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

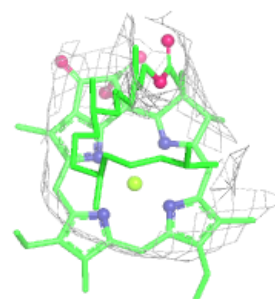
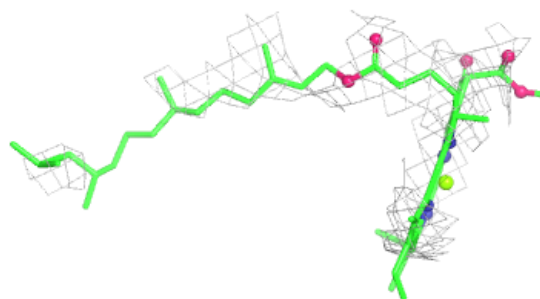


Electron density around CLA c 505:

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

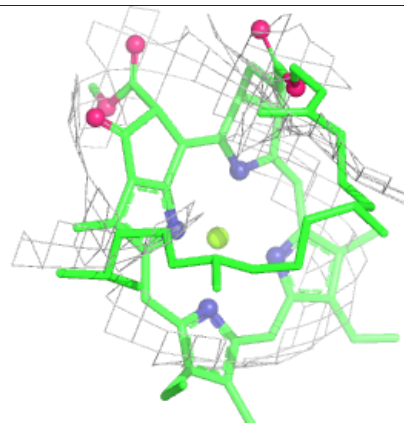
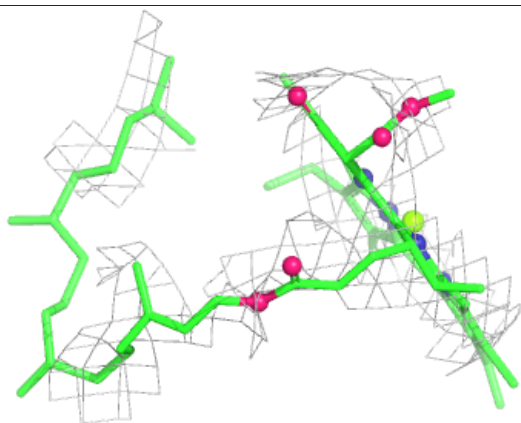
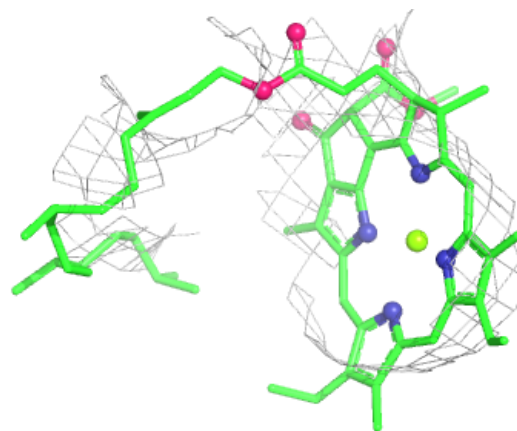
**Electron density around CLA b 606:**

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

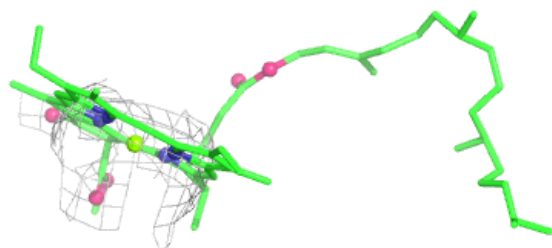
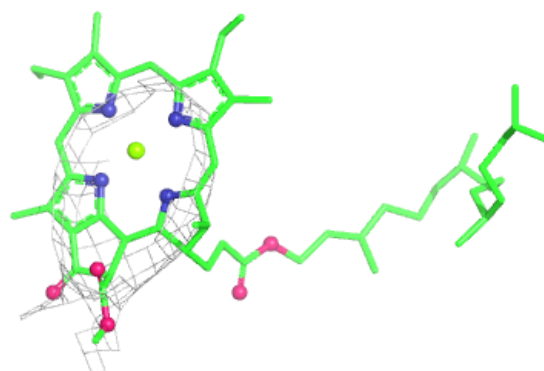


Electron density around CLA C 503:

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

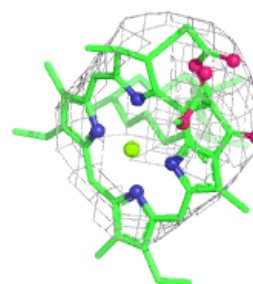
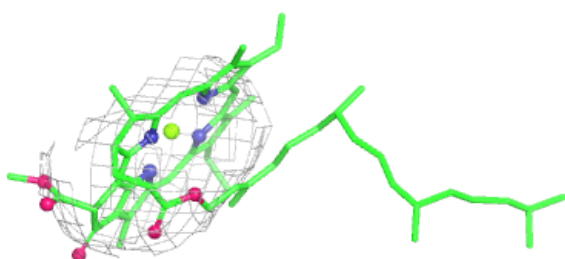
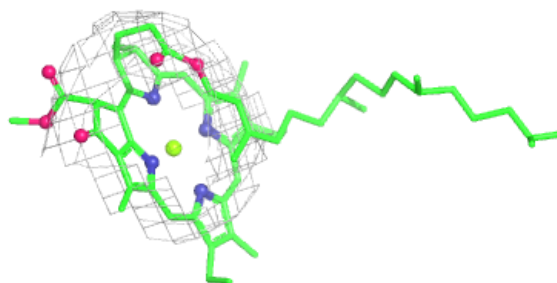
**Electron density around CLA a 607:**

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

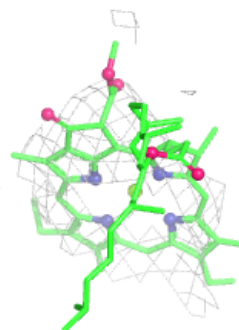
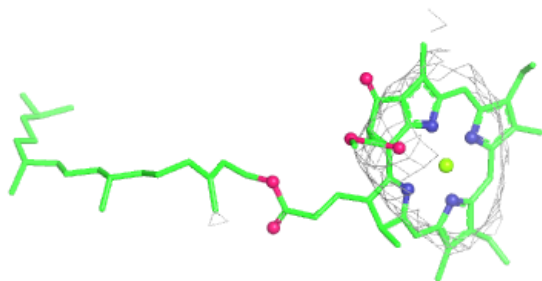
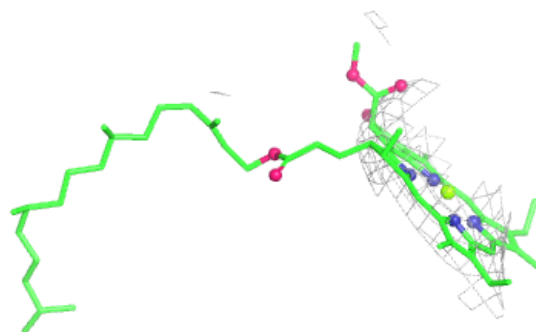


Electron density around CLA C 505:

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

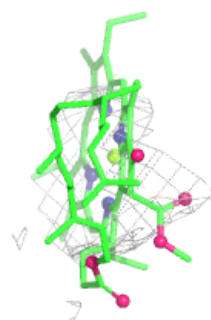
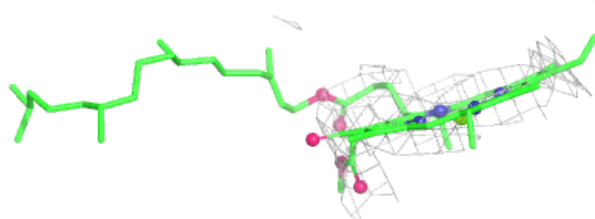
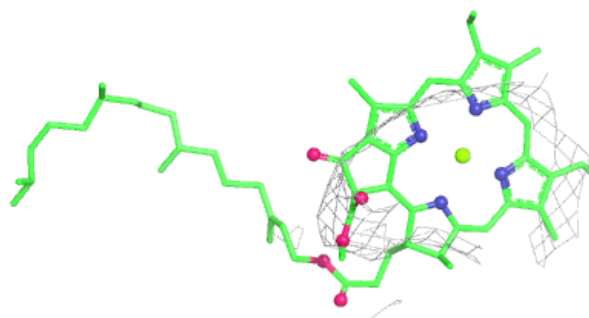
**Electron density around CLA d 401:**

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



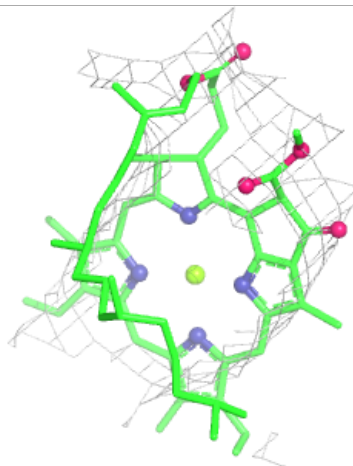
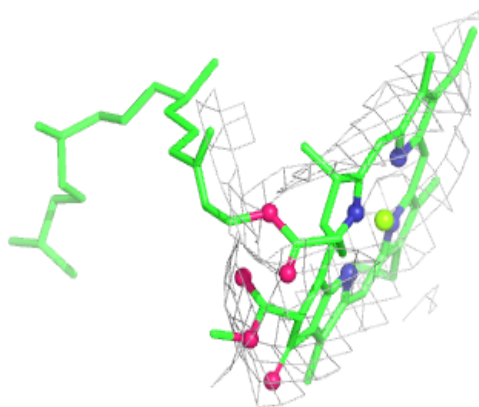
Electron density around CLA B 603:

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



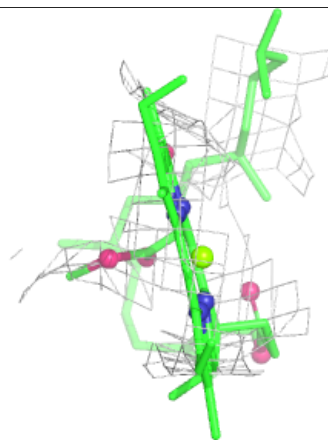
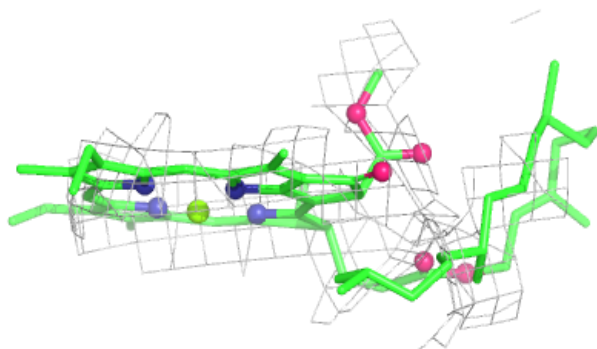
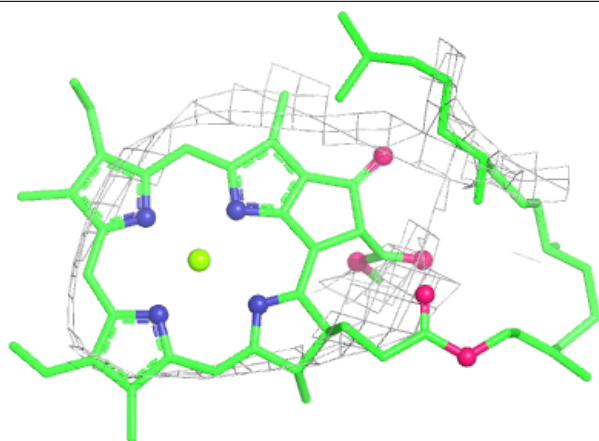
Electron density around CLA B 614:

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



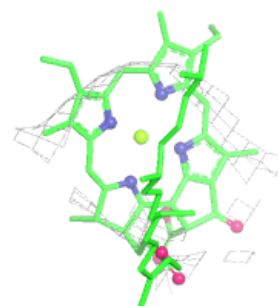
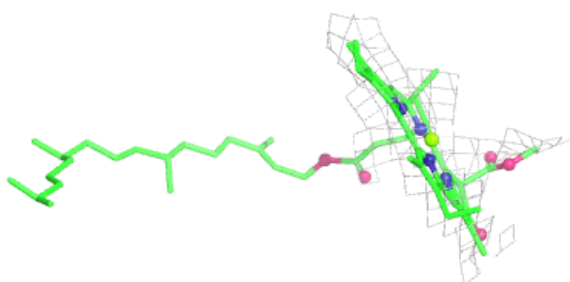
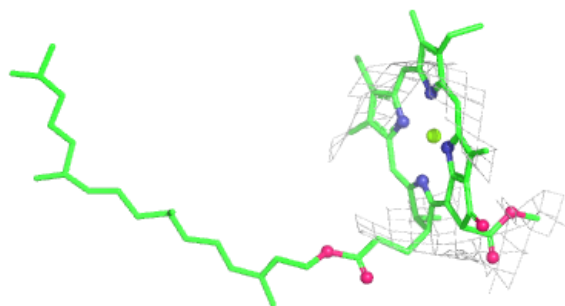
Electron density around CLA b 611:

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

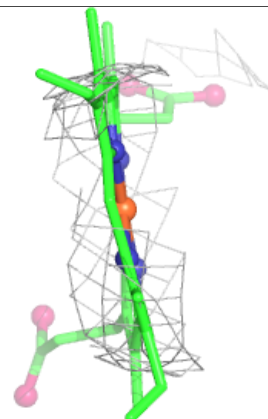
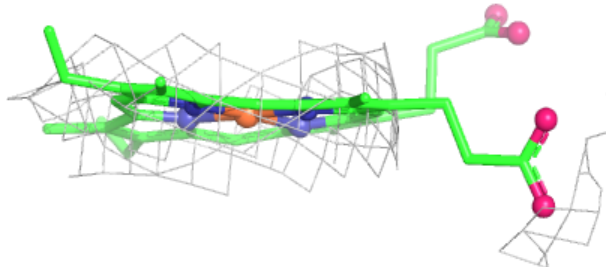
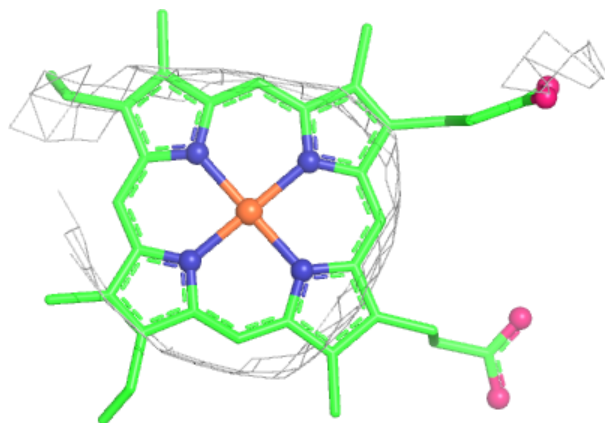


Electron density around CLA B 610:

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

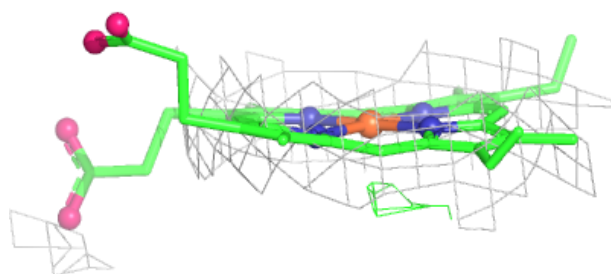
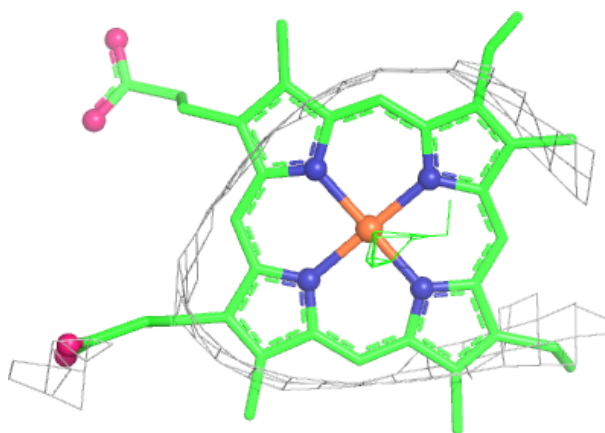
**Electron density around HEM V 201:**

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

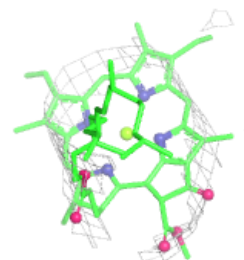
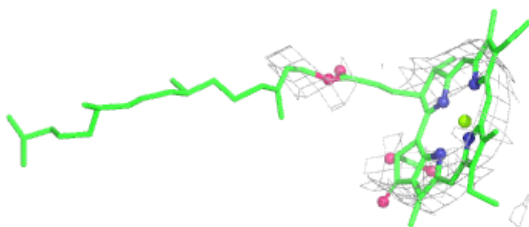
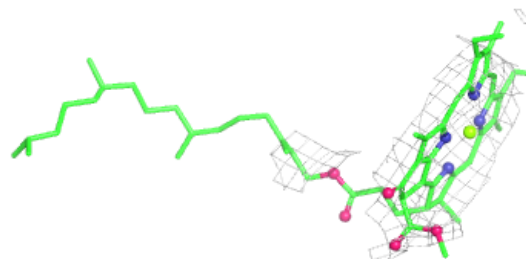


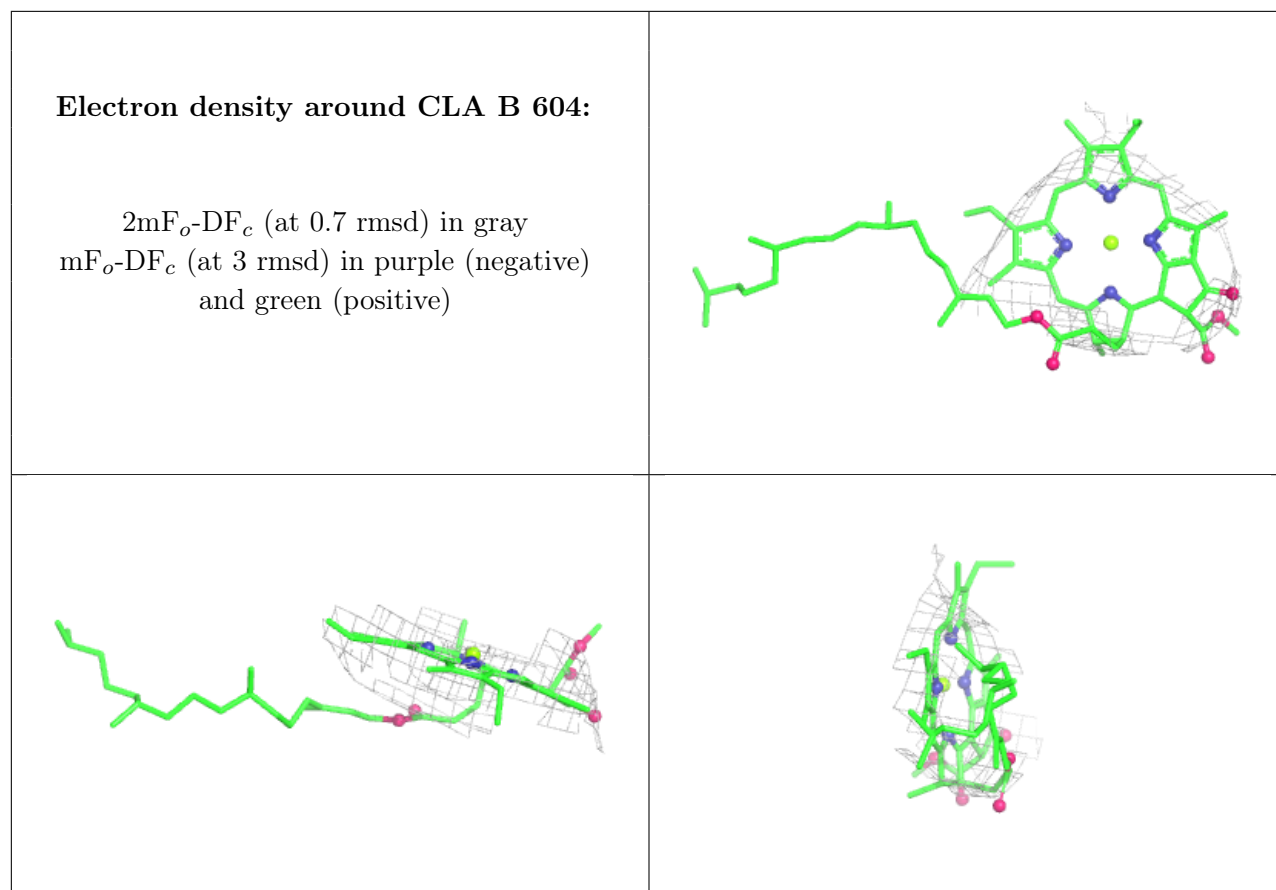
Electron density around HEM v 201:

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

**Electron density around CLA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.