



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:21 pm BST

PDB ID : 4RVY
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11

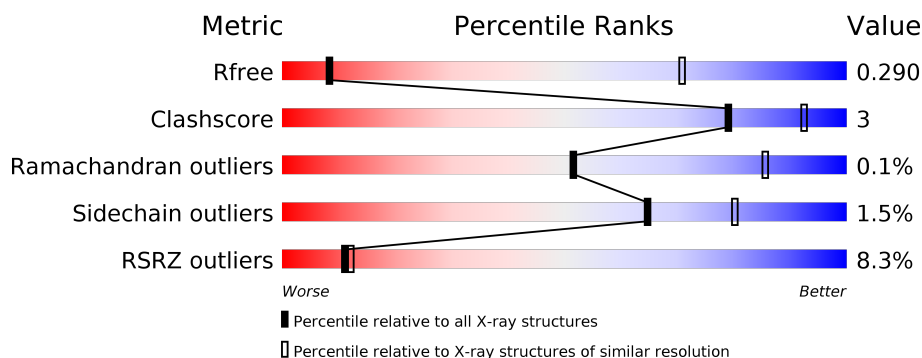
1 Overall quality at a glance

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}	130704	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)
RSRZ outliers	127900	1023 (7.08-3.76)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>6%</div> <div>94%</div> <div>6%</div> </div>

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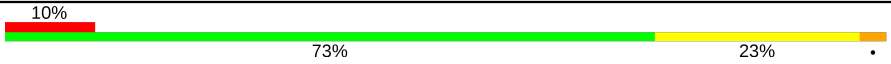
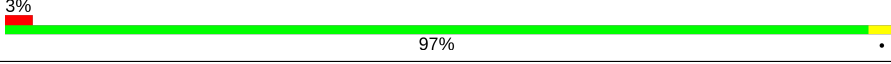
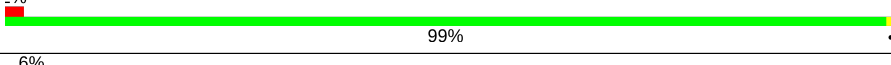
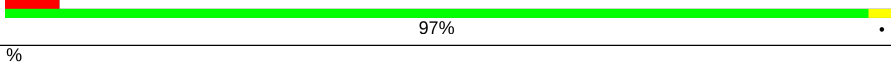
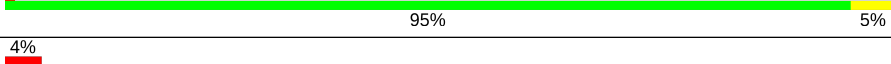
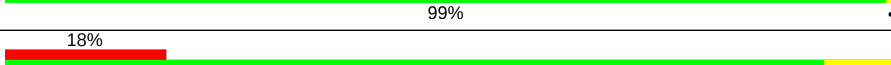
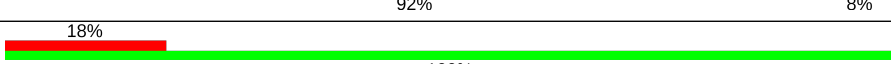
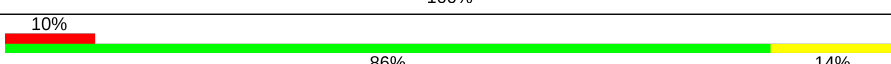
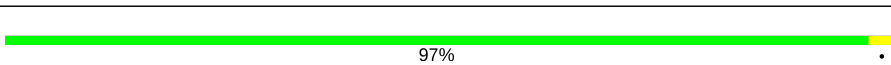
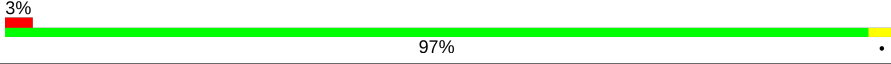
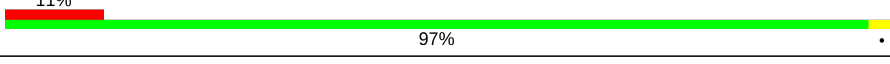

buster-report : 1.1.7 (2018)
 Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
 Refmac : 5.8.0158
 CCP4 : 7.0.044 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.11

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Mol	Chain	Length	Quality of chain
1	a	334	
2	B	504	
2	b	504	
3	C	461	
3	c	461	
4	D	342	
4	d	342	
5	E	81	
5	e	81	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	243	
13	o	243	

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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	-	-	X
22	CLA	A	604	X	-	-	X
22	CLA	A	607	X	-	-	-
22	CLA	B	602	X	-	-	X
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	X
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	616	X	-	-	X
22	CLA	B	617	X	-	-	X
22	CLA	C	501	X	-	-	X
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	X
22	CLA	C	508	X	-	-	X
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	X
22	CLA	C	513	X	-	-	X
22	CLA	D	401	X	-	-	-
22	CLA	D	402	X	-	-	X
22	CLA	D	403	X	-	-	X
22	CLA	a	603	X	-	-	X
22	CLA	a	604	X	-	-	X
22	CLA	a	607	X	-	-	X
22	CLA	b	602	X	-	-	X
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	X
22	CLA	b	607	X	-	-	X
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	X
22	CLA	b	615	X	-	-	X
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	X
22	CLA	c	501	X	-	-	X
22	CLA	c	502	X	-	-	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	-	-	X
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	X
22	CLA	c	513	X	-	-	X
22	CLA	d	401	X	-	-	-
22	CLA	d	402	X	-	-	X
22	CLA	d	403	X	-	-	X
23	PHO	A	605	-	-	-	X
24	BCR	A	608	-	-	-	X
24	BCR	B	622	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	C	515	-	-	-	X
24	BCR	D	404	-	-	-	X
24	BCR	H	101	-	-	-	X
24	BCR	K	101	-	-	-	X
24	BCR	K	102	-	X	-	-
24	BCR	T	101	-	-	-	X
24	BCR	T	102	-	-	-	X
24	BCR	a	608	-	-	-	X
24	BCR	b	618	-	-	-	X
24	BCR	b	622	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	c	515	-	-	-	X
24	BCR	d	404	-	-	-	X
24	BCR	k	101	-	-	-	X
24	BCR	k	102	-	X	-	X
24	BCR	t	101	-	-	-	X
25	SQD	A	609	-	-	-	X
25	SQD	D	411	-	-	-	X
25	SQD	L	101	-	-	-	X
25	SQD	a	609	-	-	-	X
25	SQD	b	601	-	-	-	X
25	SQD	b	621	-	-	-	X
25	SQD	d	411	-	-	-	X
26	CL	a	610	-	-	-	X
28	PL9	A	613	-	-	-	X
28	PL9	D	408	-	-	-	X
28	PL9	a	613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	PL9	d	408	-	-	-	X
29	LMG	A	614	-	-	-	X
29	LMG	C	519	-	-	-	X
29	LMG	C	520	-	-	-	X
29	LMG	D	406	-	-	-	X
29	LMG	Z	101	-	-	-	X
29	LMG	a	614	-	-	-	X
29	LMG	c	520	-	-	-	X
29	LMG	d	406	-	-	-	X
29	LMG	z	101	-	-	-	X
30	CA	B	621	-	-	-	X
30	CA	F	102	-	-	-	X
30	CA	b	620	-	-	-	X
30	CA	f	102	-	-	-	X
31	DGD	C	518	-	-	-	X
31	DGD	D	410	-	-	-	X
31	DGD	d	410	-	-	-	X
32	LHG	D	409	-	-	-	X
32	LHG	E	101	-	-	-	X
32	LHG	d	409	-	-	-	X
32	LHG	e	101	-	-	-	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			

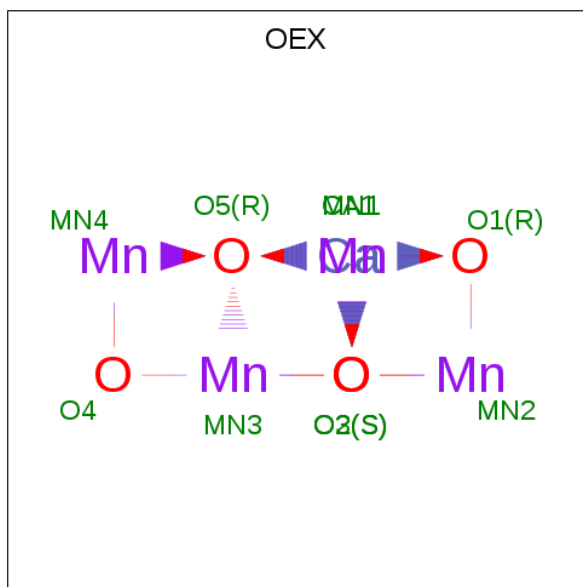
- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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 (three-letter code: OEX) (formula: CaMn_4O_5).

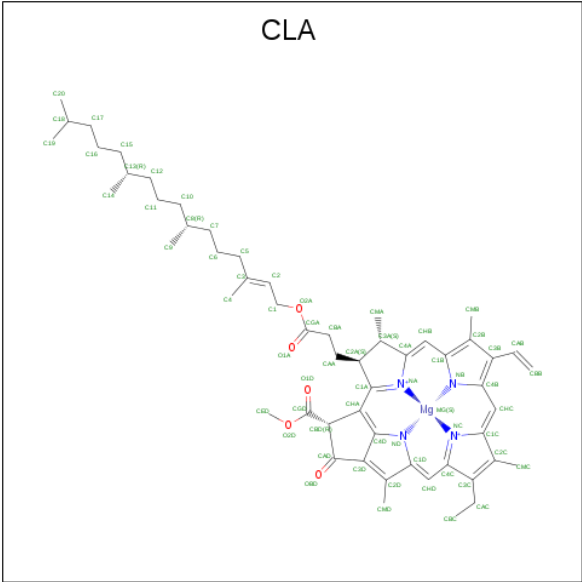


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 21 is FE (II) ION (three-letter code: 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 (three-letter code: 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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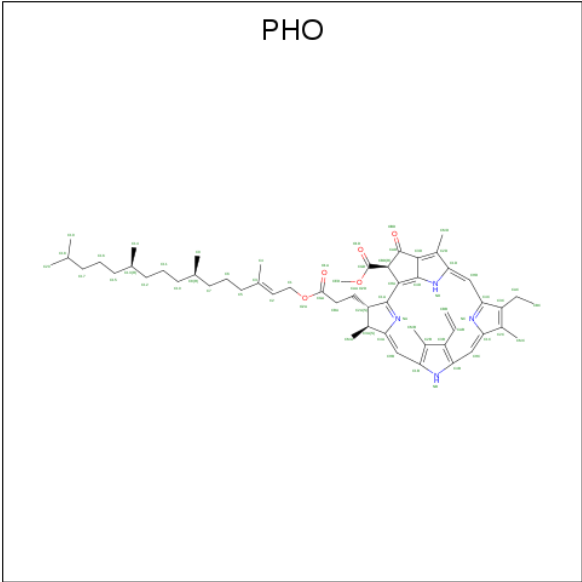
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 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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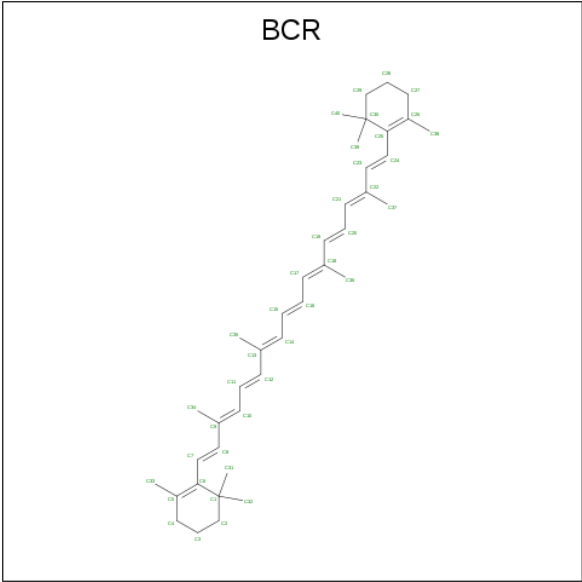
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 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 (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



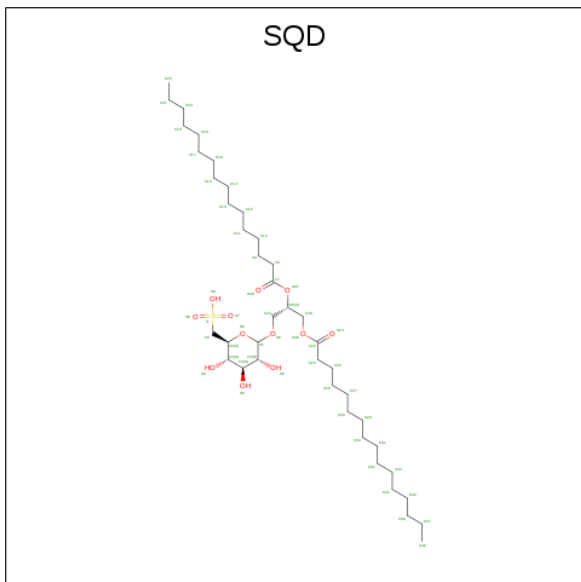
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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 (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

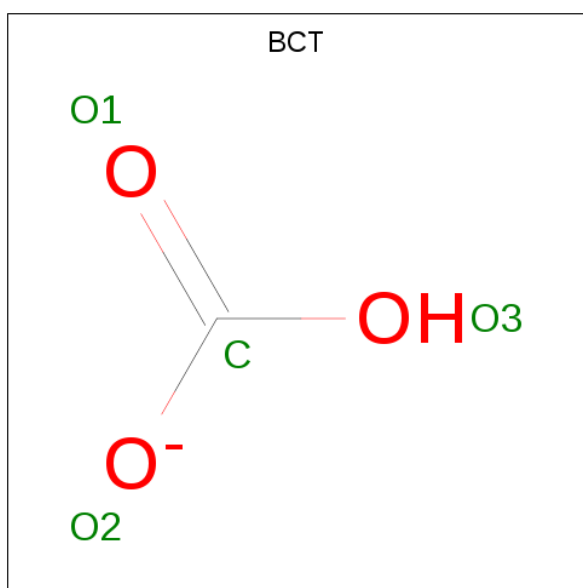


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	S	0	0
			54	41	12	1		
25	a	1	Total	C	O	S	0	0
			54	41	12	1		
25	B	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	D	1	Total	C	O	S	0	0
			43	30	12	1		
25	d	1	Total	C	O	S	0	0
			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 (three-letter code: CL) (formula: Cl).

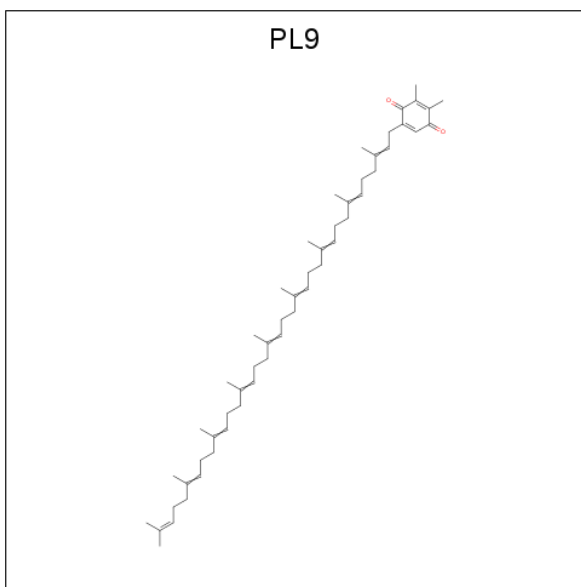
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	2	Total	Cl	0	0
			2	2		
26	u	1	Total	Cl	0	0
			1	1		
26	a	2	Total	Cl	0	0
			2	2		
26	U	1	Total	Cl	0	0
			1	1		

- Molecule 27 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



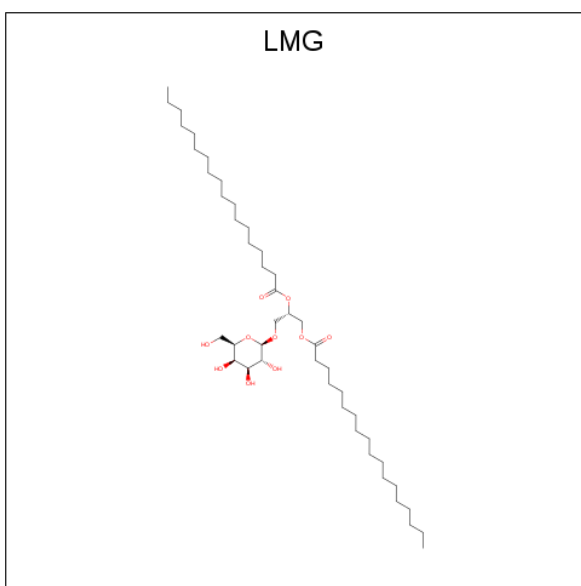
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			4	1	3		
27	a	1	Total	C	O	0	0
			4	1	3		

- 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 (three-letter code: 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 (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

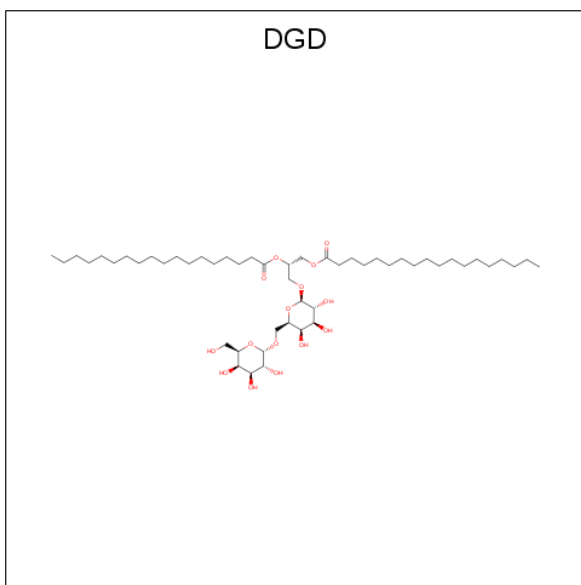


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 51 41 10	0	0
29	a	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	b	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	D	1	Total C O 51 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 (three-letter code: CA) (formula: Ca).

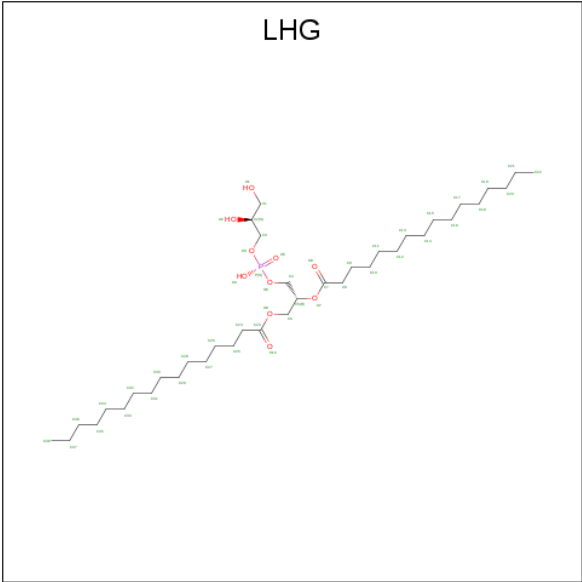
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total Ca 1 1	0	0
30	F	1	Total Ca 1 1	0	0
30	o	1	Total Ca 1 1	0	0
30	O	1	Total Ca 1 1	0	0
30	b	1	Total Ca 1 1	0	0
30	f	1	Total Ca 1 1	0	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



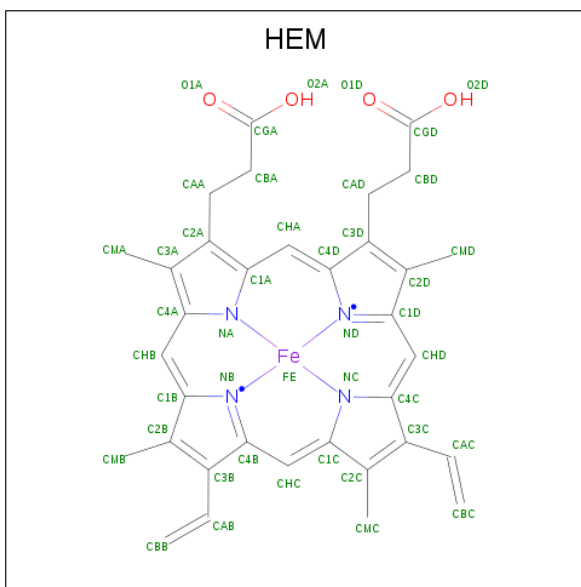
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	D	1	Total	C	O	0	0
			62	47	15		
31	d	1	Total	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 1,3-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: 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 (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

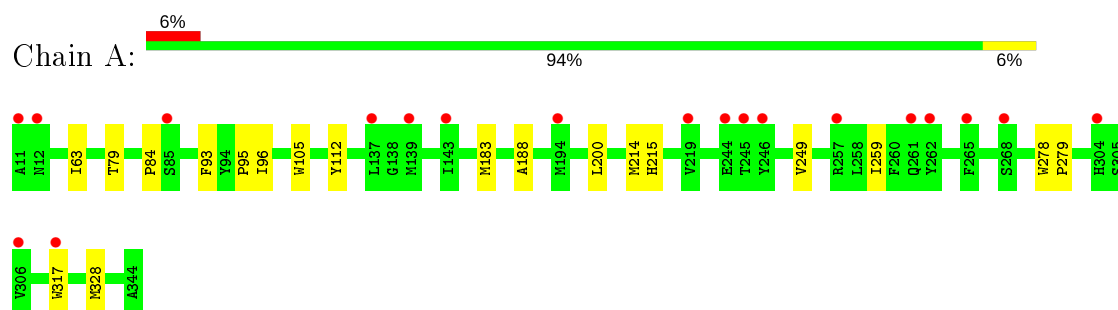
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

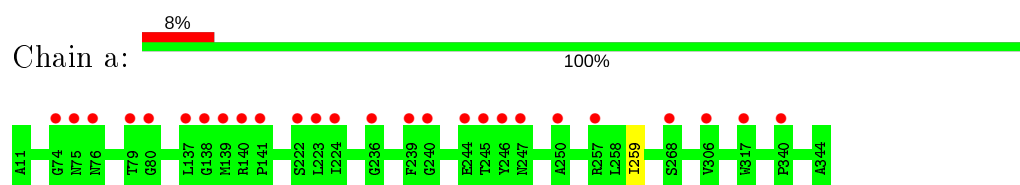
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

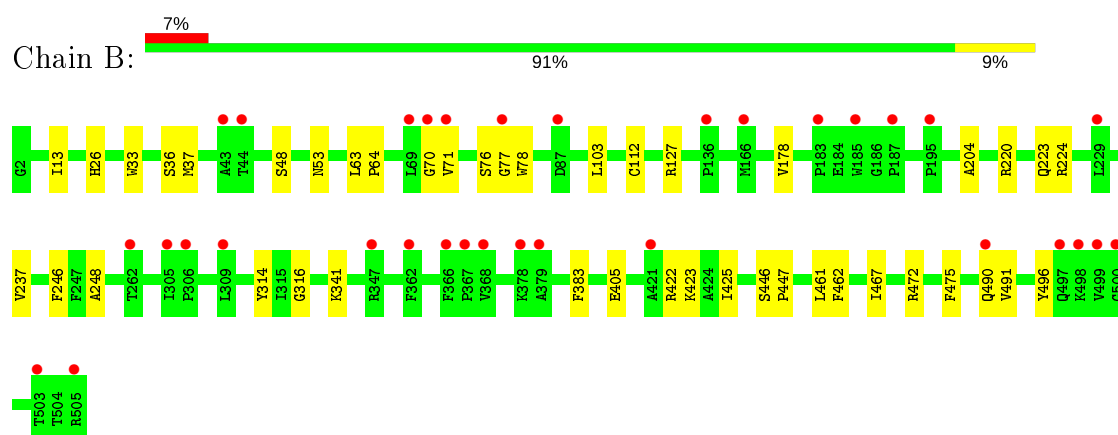
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

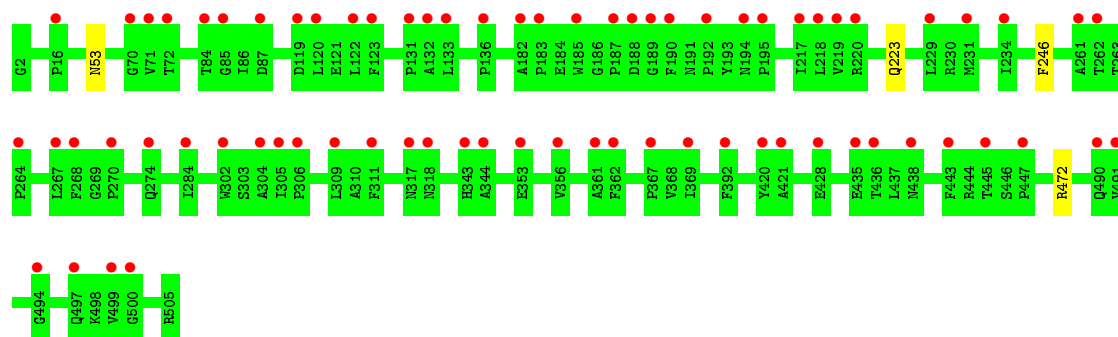


- Molecule 2: Photosystem II CP47 reaction center protein

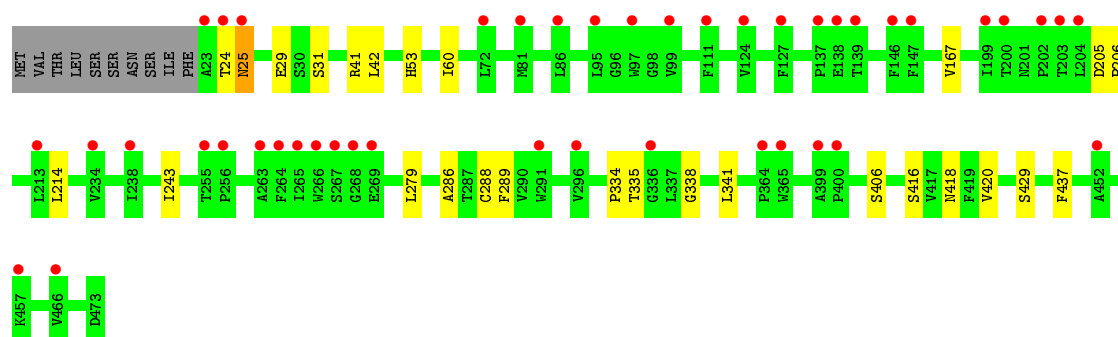


- Molecule 2: Photosystem II CP47 reaction center protein

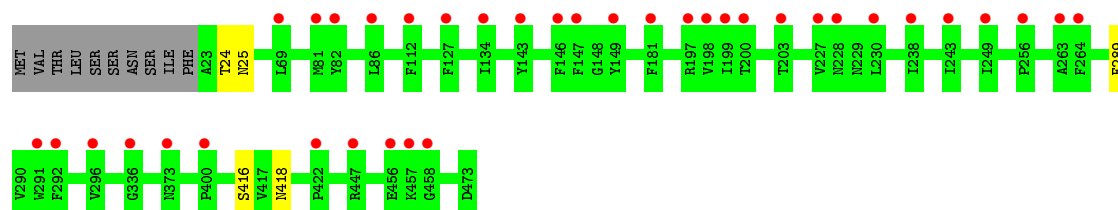




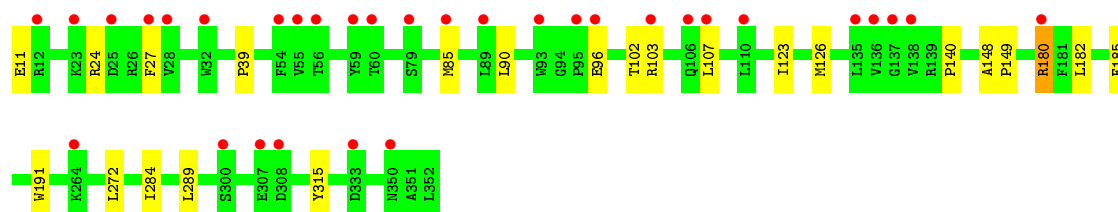
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

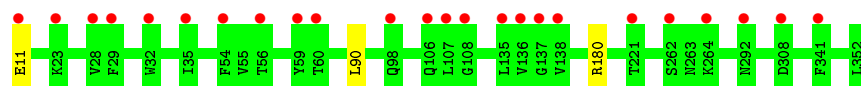


• Molecule 4: Photosystem II D2 protein

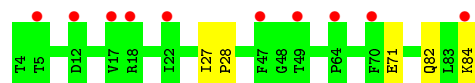


• Molecule 4: Photosystem II D2 protein

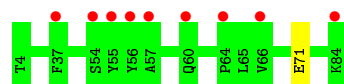




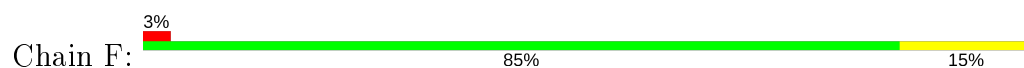
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



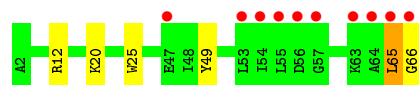
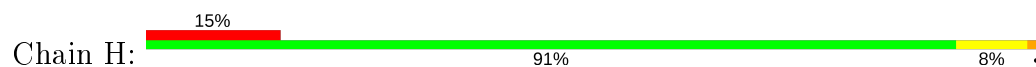
- Molecule 6: Cytochrome b559 subunit beta



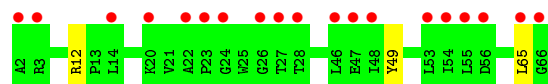
- Molecule 6: Cytochrome b559 subunit beta



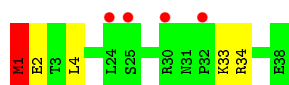
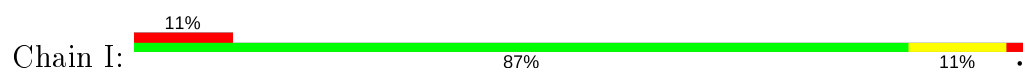
- Molecule 7: Photosystem II reaction center protein H



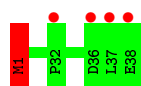
- Molecule 7: Photosystem II reaction center protein H



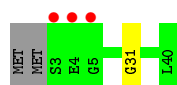
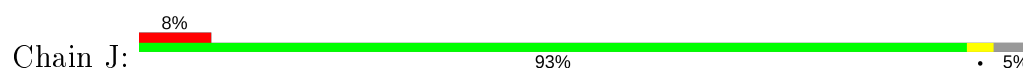
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



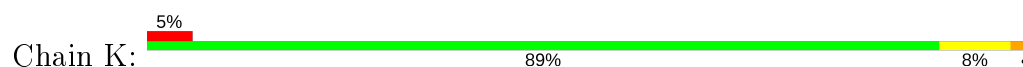
- Molecule 9: Photosystem II reaction center protein J



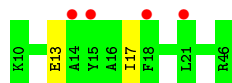
- Molecule 9: Photosystem II reaction center protein J



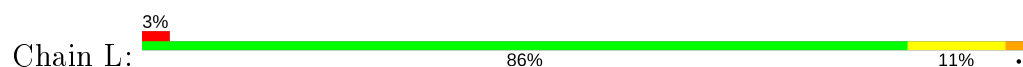
- Molecule 10: Photosystem II reaction center protein K



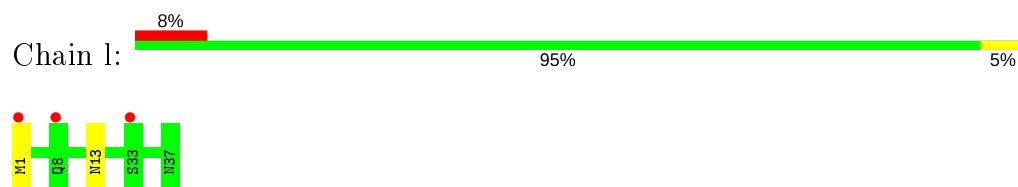
- Molecule 10: Photosystem II reaction center protein K



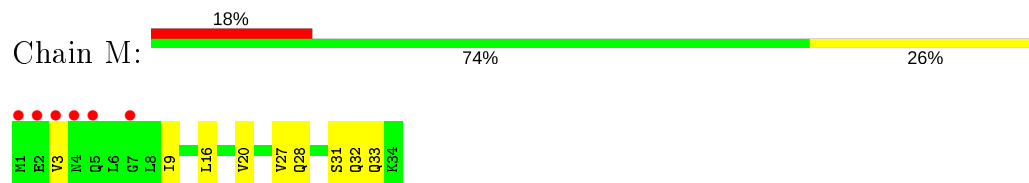
- Molecule 11: Photosystem II reaction center protein L



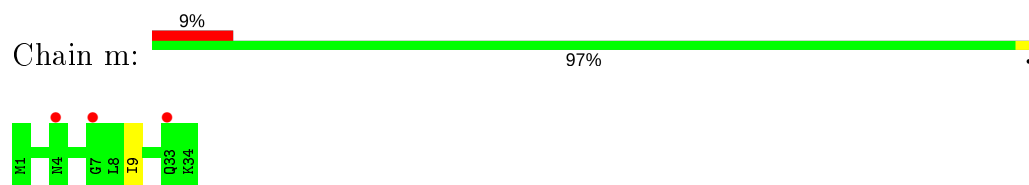
- Molecule 11: Photosystem II reaction center protein L



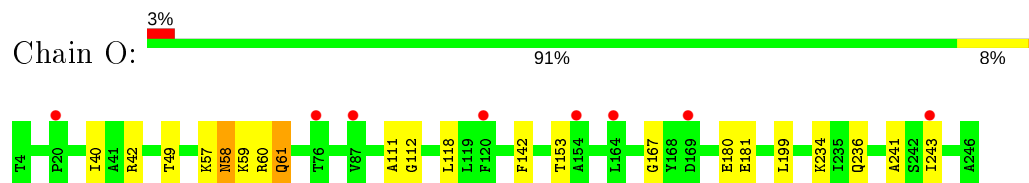
- Molecule 12: Photosystem II reaction center protein M



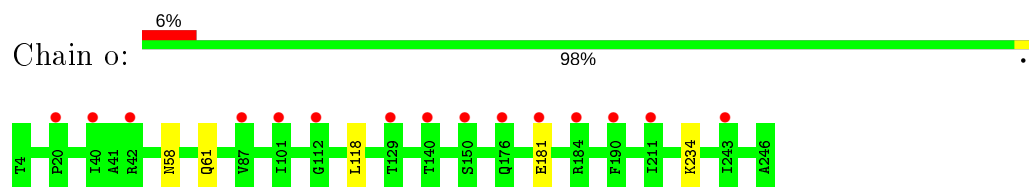
- Molecule 12: Photosystem II reaction center protein M



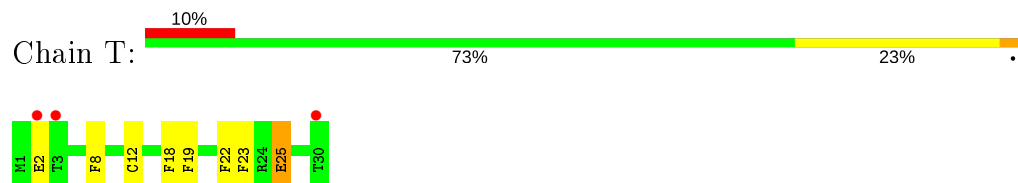
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

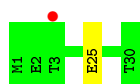


- Molecule 14: Photosystem II reaction center protein T

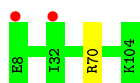


- Molecule 14: Photosystem II reaction center protein T

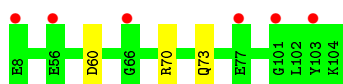




- Molecule 15: Photosystem II 12 kDa extrinsic protein



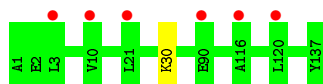
- Molecule 15: Photosystem II 12 kDa extrinsic protein



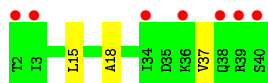
- Molecule 16: Cytochrome c-550



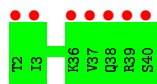
- Molecule 16: Cytochrome c-550



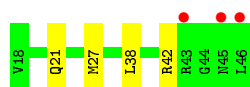
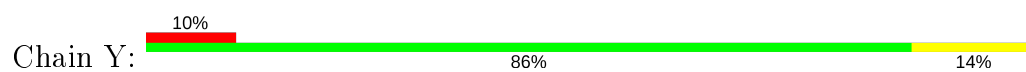
- Molecule 17: Photosystem II reaction center X protein



- Molecule 17: Photosystem II reaction center X protein



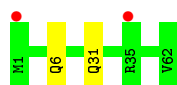
- Molecule 18: Photosystem II reaction center protein Ycf12



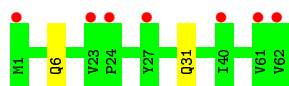
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.61Å 228.09Å 308.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.30 – 5.50 102.29 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (102.30-5.50) 100.0 (102.29-5.50)	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 0.281 , 0.290	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 , 61.9	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	0.87	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: LHG, MG, OEX, PHO, DGD, CL, CA, CLA, PL9, FE2, BCT, HEM, SQD, BCR, LMG

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	0.53	0/2705	0.55	0/3689
1	a	0.53	0/2705	0.55	0/3689
2	B	0.50	0/4109	0.54	0/5600
2	b	0.50	0/4109	0.54	0/5600
3	C	0.46	0/3599	0.51	0/4900
3	c	0.46	0/3599	0.51	0/4900
4	D	0.53	0/2821	0.55	0/3844
4	d	0.53	0/2821	0.55	0/3844
5	E	0.43	0/681	0.51	0/928
5	e	0.43	0/681	0.51	0/928
6	F	0.49	0/284	0.45	0/387
6	f	0.49	0/284	0.45	0/387
7	H	0.47	0/524	0.50	0/713
7	h	0.47	0/524	0.50	0/713
8	I	2.22	2/319 (0.6%)	1.25	4/429 (0.9%)
8	i	2.22	2/319 (0.6%)	1.25	4/429 (0.9%)
9	J	0.46	0/278	0.43	0/376
9	j	0.46	0/278	0.43	0/376
10	K	0.42	0/303	0.50	0/416
10	k	0.43	0/303	0.50	0/416
11	L	0.55	0/311	0.51	0/422
11	l	0.55	0/311	0.51	0/422
12	M	0.47	0/270	0.59	0/367
12	m	0.47	0/270	0.59	0/367
13	O	0.45	0/1896	0.58	0/2571
13	o	0.45	0/1896	0.58	0/2571
14	T	0.53	0/265	0.54	0/359
14	t	0.53	0/265	0.54	0/359
15	U	0.46	0/785	0.55	0/1064
15	u	0.46	0/785	0.55	0/1064
16	V	0.47	0/1085	0.53	0/1473
16	v	0.47	0/1085	0.53	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.43	0/290	0.47	0/392
17	x	0.43	0/290	0.47	0/392
18	Y	0.41	0/216	0.45	0/289
18	y	0.41	0/216	0.45	0/289
19	Z	0.41	0/490	0.45	0/669
19	z	0.41	0/490	0.45	0/669
All	All	0.55	4/42462 (0.0%)	0.55	8/57776 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	MET	N-CA	36.97	2.20	1.46
8	I	1	MET	N-CA	36.95	2.20	1.46
8	I	1	MET	CA-C	12.27	1.84	1.52
8	i	1	MET	CA-C	12.26	1.84	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	MET	N-CA-CB	-17.88	78.41	110.60
8	I	1	MET	N-CA-CB	-17.86	78.45	110.60
8	I	1	MET	N-CA-C	-12.99	75.92	111.00
8	i	1	MET	N-CA-C	-12.98	75.94	111.00
8	I	1	MET	CA-C-N	-6.32	103.29	117.20
8	i	1	MET	CA-C-N	-6.30	103.33	117.20
8	I	1	MET	CB-CA-C	-6.21	97.97	110.40
8	i	1	MET	CB-CA-C	-6.21	97.97	110.40

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	16	0
1	a	2620	0	2517	0	0
2	B	3969	0	3828	47	0
2	b	3969	0	3828	0	0
3	C	3486	0	3407	20	0
3	c	3486	0	3407	0	0
4	D	2726	0	2627	21	0
4	d	2726	0	2627	0	0
5	E	662	0	648	3	0
5	e	662	0	648	0	0
6	F	275	0	282	3	0
6	f	275	0	282	0	0
7	H	511	0	532	4	0
7	h	511	0	532	0	0
8	I	312	0	329	16	0
8	i	312	0	329	0	0
9	J	272	0	279	1	0
9	j	272	0	279	0	0
10	K	293	0	305	5	0
10	k	293	0	305	0	0
11	L	304	0	316	6	0
11	l	304	0	316	0	0
12	M	267	0	288	21	0
12	m	267	0	287	0	0
13	O	1865	0	1838	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	o	1865	0	1838	0	0
14	T	256	0	262	12	0
14	t	256	0	262	0	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	0	0
17	X	287	0	317	3	0
17	x	287	0	317	0	0
18	Y	215	0	246	2	0
18	y	215	0	246	0	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	10	0
22	B	1040	0	1152	32	0
22	C	845	0	936	29	0
22	D	195	0	216	8	0
22	a	195	0	216	0	0
22	b	1040	0	1152	0	0
22	c	845	0	936	0	0
22	d	195	0	216	0	0
23	A	128	0	148	6	0
23	a	128	0	148	0	0
24	A	40	0	48	1	0
24	B	120	0	140	8	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	9	0
24	a	40	0	48	0	0
24	b	80	0	92	0	0
24	c	80	0	93	0	0
24	d	40	0	48	0	0
24	h	40	0	46	0	0
24	k	80	0	93	0	0
24	t	40	0	47	0	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	5	0
25	a	54	0	78	0	0
25	b	108	0	112	0	0
25	d	43	0	53	0	0
25	l	108	0	59	0	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	0	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	0	0
29	b	51	0	72	0	0
29	c	102	0	144	0	0
29	d	51	0	72	0	0
29	z	37	0	44	0	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	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	0	0
31	d	62	0	82	0	0
31	h	62	0	82	0	0
32	D	147	0	222	13	0
32	E	42	0	57	2	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	0	0
32	e	42	0	57	0	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	0	0
33	v	43	0	30	0	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	49594	0	50450	263	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 3.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:37:CYS:SG	33:V:201:HEM:HAB	1.52	1.48
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:40:CYS:SG	33:V:201:HEM:HAC	1.57	1.44
8:I:1:MET:CA	8:I:1:MET:C	1.84	1.44
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
1:A:214:MET:HG2	28:A:613:PL9:H102	1.20	1.17
12:M:16:LEU:HD22	12:M:16:LEU:HD11	2.95	1.11
12:M:16:LEU:HD13	12:M:16:LEU:HD13	0.00	1.07
8:I:1:MET:CA	8:I:1:MET:N	2.20	1.04
12:M:16:LEU:CD1	12:M:16:LEU:HD22	2.70	0.98
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:CG2	12:M:20:VAL:HG11	2.72	0.95
32:D:409:LHG:H372	32:D:409:LHG:H132	1.48	0.93
2:B:76:SER:OG	13:O:112:GLY:CA	56.52	0.92
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.35	0.91
1:A:214:MET:HG2	28:A:613:PL9:C10	2.02	0.88
25:L:101:SQD:H342	14:T:12:CYS:HB3	1.90	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	3.05	0.86
32:D:409:LHG:H352	32:D:409:LHG:H151	1.59	0.83
8:I:1:MET:CB	8:I:1:MET:N	2.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:509:CLA:HBB1	22:C:509:CLA:HMB1	1.63	0.81
8:I:1:MET:CG	8:I:1:MET:H2	1.73	0.80
8:I:1:MET:SD	8:I:1:MET:N	2.43	0.78
2:B:76:SER:OG	13:O:112:GLY:HA2	56.41	0.77
12:M:33:GLN:HB2	12:M:33:GLN:HB2	0.00	0.77
8:I:1:MET:CA	8:I:2:GLU:N	2.50	0.75
8:I:1:MET:CB	8:I:1:MET:C	2.56	0.74
12:M:20:VAL:HG11	12:M:20:VAL:HG21	2.52	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	0.97	0.73
32:D:409:LHG:H112	32:D:409:LHG:H382	1.72	0.72
22:D:402:CLA:HBB1	22:D:402:CLA:HMB1	1.71	0.72
12:M:16:LEU:CD1	12:M:16:LEU:CD2	2.49	0.71
22:A:603:CLA:HBB1	22:A:603:CLA:HMB1	1.73	0.70
22:B:614:CLA:HBB1	22:B:614:CLA:HMB1	1.73	0.70
25:B:601:SQD:H252	24:T:101:BCR:H373	44.10	0.70
16:V:37:CYS:SG	33:V:201:HEM:C3B	2.85	0.70
22:C:508:CLA:HBB1	22:C:508:CLA:HMB1	1.75	0.69
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
22:B:615:CLA:H18	29:B:620:LMG:H421	1.76	0.67
12:M:28:GLN:O	12:M:31:SER:OG	3.31	0.67
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.77	0.67
23:A:606:PHO:HBB1	23:A:606:PHO:HMB1	1.76	0.67
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.76	0.67
10:K:17:ILE:HD13	10:K:17:ILE:N	2.08	0.67
22:C:506:CLA:HMC2	22:C:507:CLA:H102	1.77	0.66
16:V:40:CYS:SG	33:V:201:HEM:CBC	2.81	0.65
2:B:77:GLY:C	13:O:111:ALA:HB1	64.18	0.65
8:I:1:MET:C	8:I:1:MET:N	2.50	0.65
22:B:617:CLA:HMB1	22:B:617:CLA:HBB1	1.79	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
1:A:183:MET:HA	22:A:603:CLA:HMD2	1.81	0.63
29:Z:101:LMG:O2	29:Z:101:LMG:HC71	1.99	0.63
32:D:409:LHG:H112	32:D:409:LHG:C38	2.30	0.61
25:L:101:SQD:H45	14:T:23:PHE:CD1	2.35	0.61
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:SER:OG	13:O:112:GLY:C	55.95	0.60
22:C:510:CLA:H43	32:D:409:LHG:H383	1.84	0.60
23:A:605:PHO:HMB1	23:A:605:PHO:HBB1	1.84	0.60
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	0.00	0.59
22:B:611:CLA:HBB1	22:B:611:CLA:HHC	1.85	0.59
28:A:613:PL9:H502	4:D:39:PRO:HG3	1.85	0.58
2:B:76:SER:O	13:O:111:ALA:HA	62.72	0.58
2:B:462:PHE:CE1	22:B:614:CLA:HMB3	2.38	0.58
2:B:103:LEU:HD21	22:B:606:CLA:HMC3	1.86	0.57
22:B:616:CLA:H2	22:B:617:CLA:HBB2	1.87	0.57
12:M:28:GLN:CB	12:M:28:GLN:HA	2.06	0.57
12:M:31:SER:O	12:M:32:GLN:HG2	4.82	0.56
2:B:76:SER:OG	13:O:112:GLY:N	57.94	0.56
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.40	0.56
2:B:127:ARG:NH1	2:B:127:ARG:HG3	2.12	0.56
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
8:I:1:MET:CE	8:I:4:LEU:HB2	2.37	0.55
10:K:17:ILE:H	10:K:17:ILE:CD1	2.00	0.55
2:B:26:HIS:HB2	22:B:613:CLA:HMB2	1.89	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
3:C:41:ARG:NH1	22:C:511:CLA:HMD1	2.22	0.54
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.54
22:B:614:CLA:H122	29:B:620:LMG:H232	1.88	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
12:M:20:VAL:CG1	12:M:20:VAL:HG22	2.78	0.53
22:C:506:CLA:HBB1	22:C:506:CLA:HMB1	1.90	0.53
25:B:601:SQD:C25	24:T:101:BCR:H373	44.11	0.53
2:B:446:SER:HB2	2:B:447:PRO:CD	2.38	0.53
22:C:513:CLA:HMB1	22:C:513:CLA:HBB1	1.91	0.52
4:D:123:ILE:HD11	31:H:102:DGD:HAE1	1.92	0.52
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.92	0.52
2:B:76:SER:O	13:O:112:GLY:N	60.38	0.52
22:A:603:CLA:CBF	22:D:402:CLA:HAC2	2.40	0.52
22:C:510:CLA:C4	32:D:409:LHG:H383	2.40	0.52
22:C:503:CLA:HBB1	22:C:503:CLA:HMB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:L:101:SQD:O6	14:T:23:PHE:CD1	2.92	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	2.55	0.52
2:B:248:ALA:HA	22:B:604:CLA:H42	1.92	0.51
2:B:37:MET:CE	24:B:622:BCR:H282	2.71	0.51
22:C:508:CLA:H92	32:D:409:LHG:H371	1.93	0.51
25:B:601:SQD:H252	24:T:101:BCR:C37	44.21	0.51
22:D:403:CLA:H192	17:X:15:LEU:HD11	1.93	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
11:L:13:ASN:C	11:L:13:ASN:HD22	2.15	0.50
8:I:1:MET:C	8:I:1:MET:SD	2.90	0.50
2:B:112:CYS:HG	14:T:18:PHE:HZ	45.04	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
3:C:437:PHE:CZ	22:C:510:CLA:HMB3	2.47	0.50
2:B:36:SER:OG	24:B:618:BCR:H362	13.46	0.49
2:B:341:LYS:HA	2:B:405:GLU:HG2	1.94	0.49
29:B:620:LMG:H242	4:D:284:ILE:HD13	1.94	0.49
22:C:501:CLA:H42	22:C:502:CLA:HMD1	1.94	0.49
2:B:422:ARG:O	2:B:425:ILE:HG12	2.13	0.49
2:B:48:SER:O	13:O:57:LYS:HE3	52.61	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
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
22:A:604:CLA:HMD3	4:D:182:LEU:HD11	1.95	0.49
31:C:517:DGD:HB22	29:C:519:LMG:H302	1.95	0.49
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
22:B:615:CLA:H171	14:T:8:PHE:CE1	20.74	0.48
2:B:462:PHE:CZ	22:B:614:CLA:HMB3	2.49	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
29:A:614:LMG:H291	3:C:214:LEU:O	2.14	0.47
22:B:615:CLA:H151	14:T:8:PHE:HE1	22.71	0.47
3:C:25:ASN:HD21	3:C:31:SER:HA	1.79	0.47
3:C:437:PHE:CE1	22:C:510:CLA:HMB3	2.50	0.47
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.70	0.47
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:L:18:TYR:OH	25:L:101:SQD:C24	2.78	0.47
22:B:609:CLA:HMB1	22:B:609:CLA:HBB1	1.97	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	7.62	0.47
1:A:200:LEU:HG	31:C:518:DGD:HAT2	1.97	0.47
2:B:127:ARG:CG	2:B:127:ARG:HH11	2.18	0.46
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.46
24:B:618:BCR:H371	24:B:618:BCR:H24C	1.83	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: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
2:B:237:VAL:HG12	22:B:613:CLA:HMD1	1.98	0.46
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.16	0.46
8:I:1:MET:HE1	8:I:4:LEU:HB2	1.98	0.46
22:B:617:CLA:HED2	22:B:617:CLA:H43	1.98	0.45
2:B:467:ILE:HG13	4:D:126:MET:HE2	2.04	0.45
22:A:607:CLA:H162	22:A:607:CLA:H122	1.76	0.45
22:B:611:CLA:OBD	22:B:611:CLA:H152	2.16	0.45
24:T:101:BCR:H371	24:T:101:BCR:H24C	1.83	0.45
24:T:102:BCR:H371	24:T:102:BCR:H24C	1.78	0.45
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.51	0.45
8:I:1:MET:HE3	8:I:4:LEU:HB2	1.98	0.45
22:C:510:CLA:H192	22:C:510:CLA:HBC3	1.99	0.45
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.81	0.45
1:A:215:HIS:HA	28:A:613:PL9:O1	2.17	0.44
22:B:606:CLA:H41	22:B:606:CLA:H62	1.77	0.44
22:A:607:CLA:H192	22:C:505:CLA:H142	2.00	0.44
29:A:614:LMG:H231	29:A:614:LMG:H201	1.86	0.44
2:B:78:TRP:N	13:O:111:ALA:HB1	63.04	0.44
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.99	0.44
12:M:27:VAL:HG12	12:M:28:GLN:HG2	6.64	0.44
3:C:334:PRO:HA	13:O:153:THR:OG1	2.17	0.44
22:D:403:CLA:H121	17:X:18:ALA:HB2	1.99	0.44
22:D:403:CLA:HBB1	22:D:403:CLA:HMB1	2.00	0.44
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.53	0.44
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.44
5:E:82:GLN:C	5:E:84:LYS:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:608:BCR:H24C	24:A:608:BCR:H371	1.84	0.44
24:B:618:BCR:C38	14:T:19:PHE:HZ	34.43	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
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
22:A:604:CLA:HBB1	22:A:604:CLA:HMB1	2.00	0.43
2:B:13:ILE:HG12	22:B:613:CLA:HAC2	2.00	0.43
2:B:467:ILE:HG13	4:D:126:MET:CE	2.48	0.43
24:B:622:BCR:H371	24:B:622:BCR:H24C	1.89	0.43
4:D:85:MET:CE	4:D:96:GLU:HG2	2.49	0.43
14:T:22:PHE:HB3	24:T:102:BCR:H271	2.00	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
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.52	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
2:B:71:VAL:HG23	22:B:607:CLA:HMA2	2.01	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
3:C:53:HIS:CB	22:C:512:CLA:HMD1	2.49	0.43
4:D:102:THR:OG1	31:D:410:DGD:HG31	2.19	0.43
10:K:10:LYS:N	10:K:10:LYS:HD2	2.34	0.43
22:C:510:CLA:HBB1	22:C:510:CLA:HMB1	2.01	0.42
22:A:603:CLA:CAD	22:D:402:CLA:HAC2	2.50	0.42
22:B:605:CLA:H43	22:B:606:CLA:H2	2.01	0.42
12:M:20:VAL:CG1	12:M:20:VAL:HG13	0.97	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:C:504:CLA:H201	32:D:409:LHG:H342	2.01	0.42
23:A:605:PHO:ND	23:A:605:PHO:NC	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
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	2.01	0.42
4:D:272:LEU:C	4:D:272:LEU:HD23	2.40	0.42
32:D:409:LHG:H302	32:D:409:LHG:H332	1.88	0.42
4:D:27:PHE:HD1	32:E:101:LHG:HC12	1.85	0.42
2:B:220:ARG:HG3	7:H:20:LYS:HD3	2.01	0.42
3:C:29:GLU:CD	3:C:29:GLU:H	2.22	0.42
24:H:101:BCR:H24C	24:H:101:BCR:H371	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:612:CLA:H142	32:L:102:LHG:H361	2.02	0.42
13:O:59:LYS:HD2	13:O:61:GLN:CG	2.50	0.42
2:B:204:ALA:CB	22:B:603:CLA:HAB	2.50	0.42
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.55	0.42
4:D:185:PHE:CG	22:D:401:CLA:HMD3	2.55	0.42
25:B:601:SQD:H252	24:T:101:BCR:C22	45.35	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
22:A:603:CLA:HBD	22:D:402:CLA:HAC2	2.02	0.41
2:B:423:LYS:HD3	2:B:423:LYS:HA	1.94	0.41
22:B:605:CLA:H161	22:B:605:CLA:H141	1.93	0.41
22:C:502:CLA:H61	22:C:512:CLA:H42	2.03	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
12:M:16:LEU:CD1	12:M:16:LEU:CD1	0.00	0.41
23:A:606:PHO:HMA2	28:A:613:PL9:C22	2.51	0.41
22:B:611:CLA:CBB	22:B:611:CLA:HHC	2.50	0.41
22:B:607:CLA:HBB1	22:B:607:CLA:HMB1	2.03	0.41
12:M:28:GLN:HA	12:M:28:GLN:CA	0.97	0.41
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.56	0.41
3:C:243:ILE:HG22	22:C:506:CLA:HMC1	2.03	0.41
3:C:406:SER:HA	3:C:420:VAL:HG23	2.03	0.41
22:B:609:CLA:HMB1	4:D:126:MET:HB3	2.04	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	6.90	0.40
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.04	0.40
2:B:78:TRP:HD1	13:O:112:GLY:HA2	55.87	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
13:O:180:GLU:CD	13:O:180:GLU:H	2.24	0.40
23:A:606:PHO:ND	23:A:606:PHO:NC	2.70	0.40
3:C:286:ALA:HB2	22:C:502:CLA:CMD	2.51	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

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:73:GLN:OE1	16:V:70:GLU:CD[3_544]	0.80	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	41	76
1	a	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	41	76
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%)	47	81
3	c	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	47	81
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
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	34	72
13	o	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	34	72
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%)	51	85

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%)	76	86
2	b	402/402 (100%)	398 (99%)	4 (1%)	76	86
3	C	352/362 (97%)	348 (99%)	4 (1%)	73	84
3	c	352/362 (97%)	348 (99%)	4 (1%)	73	84
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	84
4	d	277/277 (100%)	274 (99%)	3 (1%)	73	84
5	E	72/72 (100%)	71 (99%)	1 (1%)	67	80
5	e	72/72 (100%)	71 (99%)	1 (1%)	67	80
6	F	28/28 (100%)	27 (96%)	1 (4%)	35	59
6	f	28/28 (100%)	27 (96%)	1 (4%)	35	59
7	H	54/54 (100%)	51 (94%)	3 (6%)	21	47
7	h	54/54 (100%)	51 (94%)	3 (6%)	21	47
8	I	35/35 (100%)	34 (97%)	1 (3%)	42	64
8	i	35/35 (100%)	34 (97%)	1 (3%)	42	64
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%)	16	42
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	42
11	L	35/35 (100%)	33 (94%)	2 (6%)	20	47
11	l	35/35 (100%)	33 (94%)	2 (6%)	20	47
12	M	31/31 (100%)	30 (97%)	1 (3%)	39	61
12	m	31/31 (100%)	30 (97%)	1 (3%)	39	61
13	O	206/206 (100%)	202 (98%)	4 (2%)	57	75
13	o	206/206 (100%)	202 (98%)	4 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	27/27 (100%)	26 (96%)	1 (4%)	34	58
14	t	27/27 (100%)	26 (96%)	1 (4%)	34	58
15	U	84/84 (100%)	83 (99%)	1 (1%)	71	84
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	84
16	V	117/117 (100%)	116 (99%)	1 (1%)	78	88
16	v	117/117 (100%)	116 (99%)	1 (1%)	78	88
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%)	27	53
18	y	22/22 (100%)	21 (96%)	1 (4%)	27	53
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	57
19	z	52/52 (100%)	50 (96%)	2 (4%)	33	57
All	All	4302/4326 (99%)	4238 (98%)	64 (2%)	65	80

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	223	GLN
2	B	246	PHE
2	B	472	ARG
2	b	53	ASN
2	b	223	GLN
2	b	246	PHE
2	b	472	ARG
3	C	24	THR
3	C	25	ASN
3	C	289	PHE
3	C	418	ASN
3	c	24	THR
3	c	25	ASN
3	c	289	PHE
3	c	418	ASN
4	D	11	GLU
4	D	90	LEU
4	D	180	ARG
4	d	11	GLU
4	d	90	LEU

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Mol	Chain	Res	Type
4	d	180	ARG
5	E	71	GLU
5	e	71	GLU
6	F	44	GLN
6	f	44	GLN
7	H	12	ARG
7	H	49	TYR
7	H	65	LEU
7	h	12	ARG
7	h	49	TYR
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	118	LEU
13	O	181	GLU
13	O	234	LYS
13	o	61	GLN
13	o	118	LEU
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	6	GLN
19	Z	31	GLN
19	z	6	GLN

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Mol	Chain	Res	Type
19	z	31	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	315	ASN
1	a	261	GLN
1	a	315	ASN
2	B	53	ASN
2	B	223	GLN
2	B	281	GLN
2	B	331	ASN
2	b	53	ASN
2	b	223	GLN
2	b	281	GLN
2	b	331	ASN
3	C	25	ASN
3	C	373	ASN
3	c	25	ASN
3	c	373	ASN
4	D	83	ASN
4	D	332	GLN
4	d	83	ASN
4	d	332	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	82	GLN
13	O	124	ASN
13	O	147	ASN
13	o	82	GLN
13	o	124	ASN
13	o	147	ASN
16	V	34	GLN
16	v	34	GLN
19	Z	58	ASN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
32	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.07	3 (6%)
22	CLA	B	617	-	59,73,73	2.20	13 (22%)	67,113,113	2.05	19 (28%)
22	CLA	c	513	-	59,73,73	2.66	14 (23%)	67,113,113	2.09	16 (23%)
25	SQD	a	609	-	53,54,54	0.99	3 (5%)	62,65,65	1.53	11 (17%)
32	LHG	d	409	-	48,48,48	0.94	2 (4%)	51,54,54	0.89	3 (5%)
24	BCR	b	622	-	41,41,41	3.80	14 (34%)	56,56,56	7.07	39 (69%)
22	CLA	A	607	-	59,73,73	2.17	13 (22%)	67,113,113	2.04	17 (25%)
29	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.30	4 (8%)
31	DGD	c	516	-	63,63,67	0.88	3 (4%)	77,77,81	0.97	2 (2%)
24	BCR	K	101	-	41,41,41	3.83	14 (34%)	56,56,56	8.02	36 (64%)
22	CLA	d	402	-	59,73,73	1.98	13 (22%)	67,113,113	2.00	15 (22%)
28	PL9	d	408	-	55,55,55	0.80	1 (1%)	68,69,69	1.33	9 (13%)
22	CLA	c	511	3	59,73,73	2.50	14 (23%)	67,113,113	2.26	14 (20%)
22	CLA	B	610	-	59,73,73	2.19	14 (23%)	67,113,113	2.09	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	502	-	59,73,73	2.21	14 (23%)	67,113,113	1.97	14 (20%)
22	CLA	B	614	-	59,73,73	2.29	15 (25%)	67,113,113	2.01	17 (25%)
24	BCR	T	102	-	41,41,41	3.72	14 (34%)	56,56,56	8.43	41 (73%)
27	BCT	A	612	21	0,3,3	0.00	-	0,3,3	0.00	-
24	BCR	K	102	-	41,41,41	3.76	14 (34%)	56,56,56	7.77	41 (73%)
32	LHG	d	407	-	48,48,48	0.90	2 (4%)	51,54,54	0.84	2 (3%)
28	PL9	a	613	-	55,55,55	0.71	2 (3%)	68,69,69	1.57	13 (19%)
29	LMG	B	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.00	3 (5%)
22	CLA	b	602	-	59,73,73	2.55	14 (23%)	67,113,113	2.19	14 (20%)
31	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.94	4 (5%)
22	CLA	D	403	-	59,73,73	2.39	16 (27%)	67,113,113	2.05	15 (22%)
22	CLA	c	508	-	59,73,73	2.45	15 (25%)	67,113,113	2.03	12 (17%)
22	CLA	b	612	-	59,73,73	2.10	13 (22%)	67,113,113	2.10	15 (22%)
22	CLA	B	609	-	59,73,73	2.07	13 (22%)	67,113,113	2.00	18 (26%)
22	CLA	b	605	-	59,73,73	2.36	14 (23%)	67,113,113	2.28	16 (23%)
24	BCR	C	515	-	41,41,41	3.82	14 (34%)	56,56,56	8.21	38 (67%)
31	DGD	C	518	-	63,63,67	0.79	3 (4%)	77,77,81	0.90	3 (3%)
22	CLA	b	611	-	59,73,73	2.24	14 (23%)	67,113,113	2.01	15 (22%)
22	CLA	B	606	-	59,73,73	2.32	13 (22%)	67,113,113	2.01	16 (23%)
20	OEX	A	601	1,3	0,15,15	0.00	-	-	-	-
32	LHG	D	407	-	48,48,48	0.90	2 (4%)	51,54,54	0.84	2 (3%)
22	CLA	B	612	-	59,73,73	2.10	13 (22%)	67,113,113	2.11	15 (22%)
22	CLA	b	617	-	59,73,73	2.20	13 (22%)	67,113,113	2.06	19 (28%)
22	CLA	B	605	-	59,73,73	2.36	14 (23%)	67,113,113	2.29	16 (23%)
23	PHO	A	605	-	67,69,69	1.91	13 (19%)	85,99,99	1.90	16 (18%)
22	CLA	C	505	-	59,73,73	2.29	15 (25%)	67,113,113	2.06	14 (20%)
31	DGD	c	517	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	2 (2%)
27	BCT	a	612	21	0,3,3	0.00	-	0,3,3	0.00	-
33	HEM	F	101	5,6	27,50,50	2.12	6 (22%)	17,82,82	2.05	4 (23%)
23	PHO	a	605	-	67,69,69	1.92	13 (19%)	85,99,99	1.91	16 (18%)
22	CLA	A	603	-	59,73,73	2.11	13 (22%)	67,113,113	1.93	16 (23%)
22	CLA	C	501	-	59,73,73	2.31	14 (23%)	67,113,113	2.13	16 (23%)
24	BCR	h	101	-	41,41,41	3.79	14 (34%)	56,56,56	8.24	41 (73%)
31	DGD	D	410	-	63,63,67	0.99	4 (6%)	77,77,81	1.03	6 (7%)
22	CLA	c	503	-	59,73,73	2.51	14 (23%)	67,113,113	1.97	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	613	-	59,73,73	2.35	13 (22%)	67,113,113	2.12	15 (22%)
24	BCR	B	619	-	41,41,41	3.65	14 (34%)	56,56,56	7.73	41 (73%)
32	LHG	D	405	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	4 (7%)
22	CLA	b	608	-	59,73,73	2.27	13 (22%)	67,113,113	2.01	15 (22%)
24	BCR	B	622	-	41,41,41	3.80	14 (34%)	56,56,56	7.07	39 (69%)
31	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	0.98	2 (2%)
25	SQD	D	411	-	42,43,54	1.21	4 (9%)	51,54,65	1.45	7 (13%)
22	CLA	b	606	-	59,73,73	2.32	13 (22%)	67,113,113	2.00	16 (23%)
25	SQD	d	411	-	42,43,54	1.21	3 (7%)	51,54,65	1.46	7 (13%)
25	SQD	l	101	-	53,54,54	1.04	4 (7%)	62,65,65	1.36	8 (12%)
25	SQD	l	102	-	53,54,54	1.08	4 (7%)	62,65,65	1.44	9 (14%)
22	CLA	B	603	-	59,73,73	2.34	14 (23%)	67,113,113	1.91	14 (20%)
22	CLA	c	504	-	59,73,73	2.33	13 (22%)	67,113,113	2.15	15 (22%)
24	BCR	A	608	-	41,41,41	3.71	14 (34%)	56,56,56	7.75	37 (66%)
22	CLA	C	508	-	59,73,73	2.45	15 (25%)	67,113,113	2.03	12 (17%)
22	CLA	B	602	-	59,73,73	2.55	15 (25%)	67,113,113	2.18	14 (20%)
24	BCR	t	101	-	41,41,41	3.72	14 (34%)	56,56,56	8.43	41 (73%)
29	LMG	D	406	34	51,51,55	0.87	2 (3%)	59,59,63	0.78	2 (3%)
29	LMG	z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.30	4 (8%)
25	SQD	B	601	-	53,54,54	1.04	3 (5%)	62,65,65	1.22	6 (9%)
24	BCR	c	514	-	41,41,41	3.85	15 (36%)	56,56,56	8.41	36 (64%)
22	CLA	b	610	-	59,73,73	2.19	14 (23%)	67,113,113	2.07	14 (20%)
25	SQD	L	101	-	53,54,54	1.04	4 (7%)	62,65,65	1.36	8 (12%)
28	PL9	A	613	-	55,55,55	0.71	2 (3%)	68,69,69	1.56	13 (19%)
22	CLA	B	616	-	59,73,73	2.47	15 (25%)	67,113,113	2.10	15 (22%)
22	CLA	D	401	-	59,73,73	2.12	15 (25%)	67,113,113	1.97	17 (25%)
22	CLA	c	509	-	59,73,73	2.39	14 (23%)	67,113,113	2.22	17 (25%)
24	BCR	k	101	-	41,41,41	3.83	14 (34%)	56,56,56	8.02	36 (64%)
24	BCR	C	514	-	41,41,41	3.86	15 (36%)	56,56,56	8.41	36 (64%)
24	BCR	D	404	-	41,41,41	3.81	14 (34%)	56,56,56	7.78	40 (71%)
29	LMG	A	614	-	51,51,55	0.94	2 (3%)	59,59,63	0.96	4 (6%)
22	CLA	c	510	-	59,73,73	2.24	14 (23%)	67,113,113	2.09	16 (23%)
31	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	2 (2%)
22	CLA	B	607	-	59,73,73	2.47	14 (23%)	67,113,113	2.13	17 (25%)
23	PHO	A	606	-	67,69,69	2.02	15 (22%)	85,99,99	1.92	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	507	-	59,73,73	2.50	14 (23%)	67,113,113	2.26	18 (26%)
22	CLA	C	504	-	59,73,73	2.33	13 (22%)	67,113,113	2.15	15 (22%)
24	BCR	a	608	-	41,41,41	3.71	14 (34%)	56,56,56	7.74	37 (66%)
22	CLA	d	401	-	59,73,73	2.11	15 (25%)	67,113,113	1.97	17 (25%)
29	LMG	C	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	4 (6%)
24	BCR	d	404	-	41,41,41	3.81	14 (34%)	56,56,56	7.77	40 (71%)
22	CLA	c	501	-	59,73,73	2.31	14 (23%)	67,113,113	2.13	16 (23%)
24	BCR	b	618	-	41,41,41	3.65	14 (34%)	56,56,56	7.73	41 (73%)
29	LMG	d	406	34	51,51,55	0.87	2 (3%)	59,59,63	0.79	2 (3%)
23	PHO	a	606	-	67,69,69	2.02	15 (22%)	85,99,99	1.92	18 (21%)
22	CLA	B	608	-	59,73,73	2.27	13 (22%)	67,113,113	2.02	15 (22%)
22	CLA	b	604	-	59,73,73	2.21	15 (25%)	67,113,113	2.13	17 (25%)
24	BCR	H	101	-	41,41,41	3.79	14 (34%)	56,56,56	8.24	41 (73%)
29	LMG	a	614	-	51,51,55	0.94	2 (3%)	59,59,63	0.96	4 (6%)
22	CLA	C	513	-	59,73,73	2.66	14 (23%)	67,113,113	2.10	16 (23%)
22	CLA	b	616	-	59,73,73	2.47	15 (25%)	67,113,113	2.10	15 (22%)
29	LMG	c	520	-	51,51,55	1.01	3 (5%)	59,59,63	0.98	2 (3%)
22	CLA	a	603	-	59,73,73	2.11	13 (22%)	67,113,113	1.93	15 (22%)
22	CLA	D	402	-	59,73,73	1.98	13 (22%)	67,113,113	2.00	15 (22%)
20	OEX	a	601	1,3	0,15,15	0.00	-	-	-	-
24	BCR	T	101	-	41,41,41	3.65	14 (34%)	56,56,56	7.51	38 (67%)
22	CLA	C	502	-	59,73,73	2.21	15 (25%)	67,113,113	1.97	14 (20%)
25	SQD	b	621	-	53,54,54	1.08	4 (7%)	62,65,65	1.44	9 (14%)
22	CLA	b	607	-	59,73,73	2.47	14 (23%)	67,113,113	2.13	17 (25%)
24	BCR	c	515	-	41,41,41	3.82	14 (34%)	56,56,56	8.20	38 (67%)
32	LHG	L	102	-	48,48,48	0.89	2 (4%)	51,54,54	0.98	2 (3%)
22	CLA	a	604	-	59,73,73	2.28	12 (20%)	67,113,113	2.16	17 (25%)
29	LMG	c	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	4 (6%)
22	CLA	c	505	-	59,73,73	2.29	15 (25%)	67,113,113	2.05	15 (22%)
29	LMG	C	520	-	51,51,55	1.01	3 (5%)	59,59,63	0.98	2 (3%)
33	HEM	f	101	5,6	27,50,50	2.12	6 (22%)	17,82,82	2.04	4 (23%)
29	LMG	b	619	-	51,51,55	0.94	2 (3%)	59,59,63	1.00	3 (5%)
31	DGD	H	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.94	4 (5%)
22	CLA	b	603	-	59,73,73	2.35	14 (23%)	67,113,113	1.92	15 (22%)
22	CLA	b	609	-	59,73,73	2.08	13 (22%)	67,113,113	2.00	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	604	-	59,73,73	2.28	12 (20%)	67,113,113	2.17	17 (25%)
22	CLA	B	611	-	59,73,73	2.25	14 (23%)	67,113,113	2.01	15 (22%)
22	CLA	C	512	-	59,73,73	2.71	15 (25%)	67,113,113	2.09	18 (26%)
22	CLA	b	615	-	59,73,73	2.21	15 (25%)	67,113,113	2.10	17 (25%)
33	HEM	v	201	16	27,50,50	2.15	7 (25%)	17,82,82	1.89	4 (23%)
31	DGD	c	518	-	63,63,67	0.79	3 (4%)	77,77,81	0.90	3 (3%)
22	CLA	C	506	-	59,73,73	2.34	14 (23%)	67,113,113	2.13	15 (22%)
22	CLA	C	507	-	59,73,73	2.50	14 (23%)	67,113,113	2.27	17 (25%)
22	CLA	B	613	-	59,73,73	2.35	13 (22%)	67,113,113	2.11	15 (22%)
32	LHG	d	405	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	4 (7%)
24	BCR	k	102	-	41,41,41	3.76	14 (34%)	56,56,56	7.77	41 (73%)
32	LHG	l	103	-	48,48,48	0.89	2 (4%)	51,54,54	0.97	2 (3%)
22	CLA	c	512	-	59,73,73	2.71	15 (25%)	67,113,113	2.09	18 (26%)
22	CLA	B	615	-	59,73,73	2.21	15 (25%)	67,113,113	2.10	17 (25%)
24	BCR	B	618	-	41,41,41	3.65	14 (34%)	56,56,56	7.51	38 (67%)
22	CLA	c	506	-	59,73,73	2.34	14 (23%)	67,113,113	2.13	14 (20%)
22	CLA	d	403	-	59,73,73	2.40	16 (27%)	67,113,113	2.06	15 (22%)
32	LHG	e	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.06	3 (6%)
22	CLA	B	604	-	59,73,73	2.21	15 (25%)	67,113,113	2.13	17 (25%)
25	SQD	A	609	-	53,54,54	0.99	3 (5%)	62,65,65	1.53	11 (17%)
22	CLA	C	509	-	59,73,73	2.38	14 (23%)	67,113,113	2.21	17 (25%)
32	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	0.90	3 (5%)
22	CLA	a	607	-	59,73,73	2.16	13 (22%)	67,113,113	2.04	17 (25%)
25	SQD	b	601	-	53,54,54	1.05	3 (5%)	62,65,65	1.22	6 (9%)
33	HEM	V	201	16	27,50,50	2.15	6 (22%)	17,82,82	1.89	4 (23%)
28	PL9	D	408	-	55,55,55	0.80	1 (1%)	68,69,69	1.33	9 (13%)
22	CLA	C	511	3	59,73,73	2.50	14 (23%)	67,113,113	2.26	14 (20%)
22	CLA	C	510	-	59,73,73	2.23	14 (23%)	67,113,113	2.09	16 (23%)
22	CLA	b	614	-	59,73,73	2.29	15 (25%)	67,113,113	2.02	17 (25%)
31	DGD	d	410	-	63,63,67	0.99	4 (6%)	77,77,81	1.02	6 (7%)
22	CLA	C	503	-	59,73,73	2.51	14 (23%)	67,113,113	1.98	12 (17%)

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
32	LHG	E	101	-	-	25/46/46/53	-
22	CLA	B	617	-	3/3/20/25	16/37/135/135	-
22	CLA	c	513	-	2/2/20/25	10/37/135/135	-
25	SQD	a	609	-	-	16/49/69/69	0/1/1/1
32	LHG	d	409	-	-	12/53/53/53	-
24	BCR	b	622	-	-	2/29/63/63	0/2/2/2
22	CLA	A	607	-	1/1/20/25	16/37/135/135	-
31	DGD	c	516	-	-	24/51/91/95	0/2/2/2
24	BCR	K	101	-	-	2/29/63/63	0/2/2/2
22	CLA	d	402	-	1/1/20/25	5/37/135/135	-
28	PL9	d	408	-	-	1/53/73/73	0/1/1/1
22	CLA	c	511	3	2/2/20/25	2/37/135/135	-
22	CLA	B	610	-	2/2/20/25	4/37/135/135	-
22	CLA	c	502	-	1/1/20/25	8/37/135/135	-
22	CLA	B	614	-	3/3/20/25	2/37/135/135	-
24	BCR	T	102	-	-	2/29/63/63	0/2/2/2
24	BCR	K	102	-	-	10/29/63/63	0/2/2/2
32	LHG	d	407	-	-	14/53/53/53	-
28	PL9	a	613	-	-	9/53/73/73	0/1/1/1
29	LMG	B	620	-	-	19/46/66/70	0/1/1/1
22	CLA	b	602	-	2/2/20/25	17/37/135/135	-
31	DGD	h	102	-	-	15/51/91/95	0/2/2/2
22	CLA	D	403	-	2/2/20/25	15/37/135/135	-
22	CLA	c	508	-	2/2/20/25	7/37/135/135	-
22	CLA	b	612	-	2/2/20/25	3/37/135/135	-
22	CLA	B	609	-	1/1/20/25	1/37/135/135	-
22	CLA	b	605	-	3/3/20/25	7/37/135/135	-
22	CLA	B	612	-	2/2/20/25	3/37/135/135	-
31	DGD	C	518	-	-	16/51/91/95	0/2/2/2
24	BCR	k	101	-	-	2/29/63/63	0/2/2/2
22	CLA	B	606	-	3/3/20/25	6/37/135/135	-
29	LMG	Z	101	-	-	18/31/51/70	0/1/1/1
32	LHG	D	407	-	-	14/53/53/53	-
24	BCR	C	515	-	-	4/29/63/63	0/2/2/2
22	CLA	b	617	-	3/3/20/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	605	-	3/3/20/25	7/37/135/135	-
24	BCR	h	101	-	-	8/29/63/63	0/2/2/2
22	CLA	C	505	-	1/1/20/25	4/37/135/135	-
31	DGD	c	517	-	-	25/51/91/95	0/2/2/2
33	HEM	F	101	5,6	-	0/6/54/54	-
23	PHO	a	605	-	-	4/53/103/103	0/5/6/6
22	CLA	A	603	-	3/3/20/25	3/37/135/135	-
22	CLA	C	501	-	2/2/20/25	11/37/135/135	-
23	PHO	A	605	-	-	4/53/103/103	0/5/6/6
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
31	DGD	D	410	-	-	32/51/91/95	0/2/2/2
22	CLA	c	503	-	3/3/20/25	1/37/135/135	-
22	CLA	b	613	-	3/3/20/25	4/37/135/135	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
32	LHG	D	405	-	-	13/53/53/53	-
22	CLA	b	608	-	3/3/20/25	2/37/135/135	-
24	BCR	B	622	-	-	2/29/63/63	0/2/2/2
31	DGD	C	516	-	-	24/51/91/95	0/2/2/2
25	SQD	D	411	-	-	16/38/58/69	0/1/1/1
22	CLA	b	606	-	3/3/20/25	6/37/135/135	-
25	SQD	d	411	-	-	16/38/58/69	0/1/1/1
24	BCR	A	608	-	-	4/29/63/63	0/2/2/2
25	SQD	l	102	-	-	29/49/69/69	0/1/1/1
22	CLA	B	603	-	3/3/20/25	4/37/135/135	-
22	CLA	c	504	-	3/3/20/25	9/37/135/135	-
25	SQD	l	101	-	-	28/49/69/69	0/1/1/1
23	PHO	A	606	-	-	5/53/103/103	0/5/6/6
22	CLA	B	602	-	2/2/20/25	17/37/135/135	-
22	CLA	c	507	-	3/3/20/25	10/37/135/135	-
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
29	LMG	z	101	-	-	18/31/51/70	0/1/1/1
22	CLA	b	610	-	2/2/20/25	4/37/135/135	-
25	SQD	L	101	-	-	28/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	A	613	-	-	9/53/73/73	0/1/1/1
22	CLA	B	616	-	3/3/20/25	10/37/135/135	-
22	CLA	D	401	-	1/1/20/25	4/37/135/135	-
22	CLA	c	509	-	3/3/20/25	9/37/135/135	-
22	CLA	b	611	-	3/3/20/25	8/37/135/135	-
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
24	BCR	D	404	-	-	6/29/63/63	0/2/2/2
29	LMG	A	614	-	-	31/46/66/70	0/1/1/1
22	CLA	c	510	-	3/3/20/25	9/37/135/135	-
31	DGD	C	517	-	-	25/51/91/95	0/2/2/2
22	CLA	B	607	-	2/2/20/25	9/37/135/135	-
22	CLA	C	508	-	2/2/20/25	7/37/135/135	-
24	BCR	t	101	-	-	2/29/63/63	0/2/2/2
22	CLA	C	504	-	3/3/20/25	9/37/135/135	-
24	BCR	a	608	-	-	4/29/63/63	0/2/2/2
22	CLA	d	401	-	1/1/20/25	4/37/135/135	-
29	LMG	C	519	-	-	22/46/66/70	0/1/1/1
24	BCR	d	404	-	-	6/29/63/63	0/2/2/2
22	CLA	c	501	-	2/2/20/25	11/37/135/135	-
24	BCR	b	618	-	-	4/29/63/63	0/2/2/2
29	LMG	d	406	34	-	16/46/66/70	0/1/1/1
23	PHO	a	606	-	-	5/53/103/103	0/5/6/6
22	CLA	B	608	-	3/3/20/25	2/37/135/135	-
22	CLA	b	604	-	3/3/20/25	5/37/135/135	-
24	BCR	H	101	-	-	8/29/63/63	0/2/2/2
29	LMG	a	614	-	-	31/46/66/70	0/1/1/1
22	CLA	C	513	-	2/2/20/25	10/37/135/135	-
22	CLA	b	616	-	3/3/20/25	10/37/135/135	-
29	LMG	c	520	-	-	26/46/66/70	0/1/1/1
22	CLA	a	603	-	3/3/20/25	3/37/135/135	-
22	CLA	D	402	-	1/1/20/25	5/37/135/135	-
24	BCR	T	101	-	-	5/29/63/63	0/2/2/2
22	CLA	C	502	-	1/1/20/25	8/37/135/135	-
25	SQD	b	621	-	-	29/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	607	-	2/2/20/25	9/37/135/135	-
24	BCR	c	515	-	-	4/29/63/63	0/2/2/2
32	LHG	L	102	-	-	17/53/53/53	-
22	CLA	a	604	-	2/2/20/25	8/37/135/135	-
29	LMG	c	519	-	-	22/46/66/70	0/1/1/1
22	CLA	c	505	-	1/1/20/25	3/37/135/135	-
29	LMG	C	520	-	-	26/46/66/70	0/1/1/1
33	HEM	f	101	5,6	-	0/6/54/54	-
29	LMG	b	619	-	-	19/46/66/70	0/1/1/1
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
22	CLA	b	603	-	3/3/20/25	4/37/135/135	-
22	CLA	b	609	-	1/1/20/25	1/37/135/135	-
22	CLA	A	604	-	2/2/20/25	8/37/135/135	-
22	CLA	B	611	-	3/3/20/25	8/37/135/135	-
22	CLA	C	512	-	3/3/20/25	10/37/135/135	-
22	CLA	b	615	-	3/3/20/25	12/37/135/135	-
33	HEM	v	201	16	-	0/6/54/54	-
31	DGD	c	518	-	-	17/51/91/95	0/2/2/2
22	CLA	C	506	-	3/3/20/25	14/37/135/135	-
22	CLA	C	507	-	3/3/20/25	10/37/135/135	-
22	CLA	B	613	-	3/3/20/25	4/37/135/135	-
32	LHG	d	405	-	-	13/53/53/53	-
24	BCR	k	102	-	-	10/29/63/63	0/2/2/2
32	LHG	l	103	-	-	17/53/53/53	-
22	CLA	c	512	-	3/3/20/25	10/37/135/135	-
22	CLA	B	615	-	3/3/20/25	12/37/135/135	-
24	BCR	B	618	-	-	5/29/63/63	0/2/2/2
22	CLA	c	506	-	3/3/20/25	14/37/135/135	-
22	CLA	d	403	-	2/2/20/25	15/37/135/135	-
32	LHG	e	101	-	-	25/46/46/53	-
22	CLA	B	604	-	3/3/20/25	5/37/135/135	-
25	SQD	A	609	-	-	16/49/69/69	0/1/1/1
22	CLA	C	509	-	3/3/20/25	9/37/135/135	-
32	LHG	D	409	-	-	12/53/53/53	-
22	CLA	a	607	-	1/1/20/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SQD	b	601	-	-	23/49/69/69	0/1/1/1
33	HEM	V	201	16	-	0/6/54/54	-
28	PL9	D	408	-	-	1/53/73/73	0/1/1/1
22	CLA	C	511	3	2/2/20/25	2/37/135/135	-
22	CLA	C	510	-	3/3/20/25	9/37/135/135	-
22	CLA	b	614	-	3/3/20/25	2/37/135/135	-
31	DGD	d	410	-	-	32/51/91/95	0/2/2/2
22	CLA	C	503	-	3/3/20/25	1/37/135/135	-

All (1487) 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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
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
22	c	510	CLA	MG-NA	9.03	2.27	2.06
22	C	510	CLA	MG-NA	9.00	2.27	2.06
24	C	514	BCR	C8-C9	-8.81	1.27	1.45
24	c	514	BCR	C8-C9	-8.78	1.27	1.45
22	B	612	CLA	MG-NA	8.75	2.27	2.06
24	d	404	BCR	C8-C9	-8.75	1.27	1.45
24	C	514	BCR	C12-C13	-8.73	1.27	1.45
24	K	102	BCR	C8-C9	-8.73	1.27	1.45
24	k	102	BCR	C8-C9	-8.72	1.27	1.45
24	D	404	BCR	C8-C9	-8.71	1.27	1.45
24	c	514	BCR	C12-C13	-8.71	1.27	1.45
22	b	612	CLA	MG-NA	8.70	2.26	2.06
24	h	101	BCR	C19-C18	-8.68	1.27	1.45
24	H	101	BCR	C19-C18	-8.67	1.27	1.45
24	k	101	BCR	C19-C18	-8.65	1.27	1.45
24	B	622	BCR	C8-C9	-8.65	1.27	1.45
24	b	622	BCR	C8-C9	-8.64	1.27	1.45
24	c	515	BCR	C8-C9	-8.63	1.27	1.45
24	C	515	BCR	C8-C9	-8.61	1.27	1.45
24	K	101	BCR	C19-C18	-8.60	1.27	1.45
24	K	101	BCR	C8-C9	-8.59	1.27	1.45
24	T	102	BCR	C8-C9	-8.57	1.27	1.45
24	k	101	BCR	C8-C9	-8.56	1.27	1.45
24	t	101	BCR	C8-C9	-8.55	1.27	1.45
24	b	622	BCR	C12-C13	-8.53	1.27	1.45
24	c	515	BCR	C19-C18	-8.50	1.27	1.45
24	B	622	BCR	C12-C13	-8.50	1.27	1.45
24	D	404	BCR	C19-C18	-8.50	1.27	1.45
24	C	514	BCR	C19-C18	-8.49	1.27	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	BCR	C19-C18	-8.48	1.27	1.45
24	K	101	BCR	C12-C13	-8.48	1.27	1.45
24	t	101	BCR	C12-C13	-8.48	1.27	1.45
22	B	604	CLA	MG-NA	8.48	2.26	2.06
24	c	514	BCR	C19-C18	-8.47	1.27	1.45
24	B	618	BCR	C8-C9	-8.47	1.27	1.45
24	k	101	BCR	C12-C13	-8.46	1.27	1.45
24	T	101	BCR	C8-C9	-8.46	1.27	1.45
24	C	515	BCR	C12-C13	-8.46	1.27	1.45
24	C	515	BCR	C19-C18	-8.45	1.27	1.45
22	b	604	CLA	MG-NA	8.45	2.26	2.06
24	H	101	BCR	C12-C13	-8.44	1.27	1.45
24	T	102	BCR	C12-C13	-8.44	1.27	1.45
24	H	101	BCR	C8-C9	-8.43	1.27	1.45
24	h	101	BCR	C8-C9	-8.42	1.27	1.45
24	c	515	BCR	C12-C13	-8.41	1.27	1.45
24	h	101	BCR	C12-C13	-8.41	1.27	1.45
24	B	619	BCR	C8-C9	-8.40	1.27	1.45
24	b	618	BCR	C8-C9	-8.39	1.27	1.45
24	k	102	BCR	C19-C18	-8.38	1.27	1.45
24	K	102	BCR	C19-C18	-8.38	1.27	1.45
24	a	608	BCR	C8-C9	-8.38	1.28	1.45
24	A	608	BCR	C8-C9	-8.36	1.28	1.45
24	b	622	BCR	C19-C18	-8.35	1.28	1.45
24	B	622	BCR	C19-C18	-8.33	1.28	1.45
24	d	404	BCR	C12-C13	-8.32	1.28	1.45
24	B	619	BCR	C19-C18	-8.31	1.28	1.45
24	D	404	BCR	C12-C13	-8.30	1.28	1.45
24	b	618	BCR	C19-C18	-8.30	1.28	1.45
24	k	102	BCR	C12-C13	-8.28	1.28	1.45
24	B	618	BCR	C12-C13	-8.28	1.28	1.45
24	T	101	BCR	C12-C13	-8.27	1.28	1.45
24	K	102	BCR	C12-C13	-8.26	1.28	1.45
24	A	608	BCR	C12-C13	-8.23	1.28	1.45
24	a	608	BCR	C12-C13	-8.21	1.28	1.45
24	A	608	BCR	C19-C18	-8.20	1.28	1.45
24	t	101	BCR	C19-C18	-8.16	1.28	1.45
24	b	618	BCR	C12-C13	-8.16	1.28	1.45
24	a	608	BCR	C19-C18	-8.15	1.28	1.45
24	B	619	BCR	C12-C13	-8.15	1.28	1.45
22	c	502	CLA	MG-NA	8.15	2.25	2.06
24	T	102	BCR	C19-C18	-8.13	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	MG-NA	8.13	2.25	2.06
24	B	618	BCR	C19-C18	-8.06	1.28	1.45
24	T	101	BCR	C19-C18	-8.02	1.28	1.45
22	c	504	CLA	MG-NC	7.98	2.25	2.06
22	C	504	CLA	MG-NC	7.97	2.25	2.06
24	d	404	BCR	C20-C21	-7.59	1.19	1.43
24	k	101	BCR	C20-C21	-7.57	1.20	1.43
24	D	404	BCR	C20-C21	-7.56	1.20	1.43
24	K	101	BCR	C20-C21	-7.55	1.20	1.43
24	C	514	BCR	C20-C21	-7.55	1.20	1.43
24	h	101	BCR	C20-C21	-7.55	1.20	1.43
24	c	514	BCR	C20-C21	-7.54	1.20	1.43
24	H	101	BCR	C20-C21	-7.53	1.20	1.43
24	c	514	BCR	C16-C17	-7.51	1.20	1.43
24	c	515	BCR	C16-C17	-7.51	1.20	1.43
24	C	514	BCR	C16-C17	-7.50	1.20	1.43
24	K	101	BCR	C16-C17	-7.49	1.20	1.43
24	C	515	BCR	C16-C17	-7.49	1.20	1.43
24	C	515	BCR	C20-C21	-7.47	1.20	1.43
24	c	515	BCR	C20-C21	-7.46	1.20	1.43
24	k	101	BCR	C16-C17	-7.45	1.20	1.43
24	k	102	BCR	C20-C21	-7.43	1.20	1.43
24	K	102	BCR	C20-C21	-7.42	1.20	1.43
22	B	611	CLA	MG-NA	7.40	2.23	2.06
22	b	611	CLA	MG-NA	7.39	2.23	2.06
24	d	404	BCR	C16-C17	-7.39	1.20	1.43
24	D	404	BCR	C16-C17	-7.38	1.20	1.43
24	H	101	BCR	C16-C17	-7.38	1.20	1.43
24	B	622	BCR	C16-C17	-7.38	1.20	1.43
24	b	622	BCR	C16-C17	-7.38	1.20	1.43
24	h	101	BCR	C16-C17	-7.37	1.20	1.43
24	b	622	BCR	C20-C21	-7.37	1.20	1.43
24	A	608	BCR	C20-C21	-7.37	1.20	1.43
24	a	608	BCR	C20-C21	-7.35	1.20	1.43
24	B	622	BCR	C20-C21	-7.34	1.20	1.43
24	t	101	BCR	C16-C17	-7.33	1.20	1.43
24	b	618	BCR	C20-C21	-7.33	1.20	1.43
24	T	102	BCR	C16-C17	-7.33	1.20	1.43
24	B	619	BCR	C20-C21	-7.30	1.20	1.43
24	A	608	BCR	C16-C17	-7.30	1.20	1.43
24	K	102	BCR	C16-C17	-7.29	1.20	1.43
24	k	102	BCR	C16-C17	-7.29	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	608	BCR	C16-C17	-7.29	1.20	1.43
24	t	101	BCR	C20-C21	-7.28	1.20	1.43
24	T	102	BCR	C20-C21	-7.26	1.21	1.43
24	B	618	BCR	C20-C21	-7.24	1.21	1.43
24	T	101	BCR	C20-C21	-7.21	1.21	1.43
22	a	603	CLA	MG-NA	7.20	2.23	2.06
22	A	603	CLA	MG-NA	7.17	2.23	2.06
24	T	101	BCR	C16-C17	-7.15	1.21	1.43
24	B	618	BCR	C16-C17	-7.14	1.21	1.43
24	B	619	BCR	C16-C17	-7.14	1.21	1.43
24	b	618	BCR	C16-C17	-7.13	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
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
22	B	610	CLA	MG-NA	6.55	2.21	2.06
22	b	610	CLA	MG-NA	6.54	2.21	2.06
22	b	615	CLA	MG-NA	6.39	2.21	2.06
22	B	615	CLA	MG-NA	6.39	2.21	2.06
24	c	515	BCR	C21-C22	-6.38	1.27	1.35
22	b	610	CLA	MG-NC	6.37	2.21	2.06
24	k	101	BCR	C21-C22	-6.36	1.27	1.35
24	K	101	BCR	C21-C22	-6.33	1.27	1.35
24	C	515	BCR	C21-C22	-6.31	1.27	1.35
22	B	610	CLA	MG-NC	6.31	2.21	2.06
24	D	404	BCR	C21-C22	-6.27	1.27	1.35
22	b	609	CLA	MG-NA	6.27	2.21	2.06
24	h	101	BCR	C21-C22	-6.26	1.27	1.35
24	d	404	BCR	C21-C22	-6.26	1.27	1.35
22	B	609	CLA	MG-NA	6.26	2.21	2.06
24	H	101	BCR	C21-C22	-6.25	1.27	1.35
24	B	622	BCR	C21-C22	-6.25	1.27	1.35
24	k	102	BCR	C21-C22	-6.23	1.27	1.35
24	K	102	BCR	C21-C22	-6.23	1.27	1.35
24	C	514	BCR	C17-C18	-6.23	1.27	1.35
24	c	514	BCR	C17-C18	-6.21	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	622	BCR	C16-C15	-6.21	1.19	1.36
24	b	622	BCR	C16-C15	-6.20	1.19	1.36
24	b	622	BCR	C21-C22	-6.20	1.27	1.35
24	c	514	BCR	C16-C15	-6.19	1.19	1.36
24	K	101	BCR	C17-C18	-6.18	1.27	1.35
24	k	101	BCR	C17-C18	-6.18	1.27	1.35
24	C	514	BCR	C16-C15	-6.16	1.20	1.36
24	c	514	BCR	C21-C22	-6.14	1.27	1.35
24	C	514	BCR	C21-C22	-6.13	1.27	1.35
24	B	619	BCR	C21-C22	-6.12	1.27	1.35
24	b	618	BCR	C21-C22	-6.09	1.27	1.35
24	A	608	BCR	C17-C18	-6.09	1.27	1.35
24	C	515	BCR	C16-C15	-6.08	1.20	1.36
22	b	611	CLA	MG-NC	6.08	2.20	2.06
22	B	611	CLA	MG-NC	6.08	2.20	2.06
24	k	101	BCR	C16-C15	-6.07	1.20	1.36
24	c	515	BCR	C16-C15	-6.07	1.20	1.36
24	a	608	BCR	C17-C18	-6.07	1.27	1.35
24	K	101	BCR	C16-C15	-6.06	1.20	1.36
22	C	507	CLA	C3B-C2B	6.05	1.48	1.40
22	c	507	CLA	C3B-C2B	6.04	1.48	1.40
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
24	C	515	BCR	C17-C18	-6.00	1.27	1.35
24	T	102	BCR	C21-C22	-5.99	1.27	1.35
24	d	404	BCR	C17-C18	-5.99	1.27	1.35
24	t	101	BCR	C21-C22	-5.99	1.27	1.35
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	a	608	BCR	C16-C15	-5.98	1.20	1.36
24	D	404	BCR	C17-C18	-5.98	1.27	1.35
24	b	622	BCR	C17-C18	-5.97	1.27	1.35
24	h	101	BCR	C16-C15	-5.97	1.20	1.36
24	B	622	BCR	C17-C18	-5.96	1.27	1.35
24	B	618	BCR	C16-C15	-5.96	1.20	1.36
22	d	401	CLA	MG-NA	5.96	2.20	2.06
24	H	101	BCR	C16-C15	-5.95	1.20	1.36
24	A	608	BCR	C16-C15	-5.95	1.20	1.36
24	T	101	BCR	C16-C15	-5.94	1.20	1.36
24	D	404	BCR	C16-C15	-5.94	1.20	1.36
24	c	515	BCR	C17-C18	-5.93	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	BCR	C16-C15	-5.93	1.20	1.36
24	k	102	BCR	C16-C15	-5.93	1.20	1.36
24	K	102	BCR	C16-C15	-5.92	1.20	1.36
24	T	102	BCR	C16-C15	-5.92	1.20	1.36
24	T	101	BCR	C21-C22	-5.90	1.28	1.35
24	H	101	BCR	C17-C18	-5.90	1.28	1.35
24	t	101	BCR	C16-C15	-5.90	1.20	1.36
24	K	102	BCR	C17-C18	-5.89	1.28	1.35
24	k	102	BCR	C17-C18	-5.89	1.28	1.35
24	h	101	BCR	C17-C18	-5.88	1.28	1.35
24	A	608	BCR	C21-C22	-5.87	1.28	1.35
24	a	608	BCR	C21-C22	-5.83	1.28	1.35
24	B	618	BCR	C21-C22	-5.82	1.28	1.35
22	c	513	CLA	C3B-C2B	5.81	1.48	1.40
22	C	513	CLA	C3B-C2B	5.79	1.48	1.40
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	c	514	BCR	C11-C12	-5.73	1.19	1.34
24	k	101	BCR	C11-C12	-5.72	1.19	1.34
24	C	514	BCR	C11-C12	-5.71	1.19	1.34
24	K	101	BCR	C11-C12	-5.69	1.19	1.34
24	a	608	BCR	C20-C19	-5.69	1.19	1.34
24	T	102	BCR	C17-C18	-5.69	1.28	1.35
22	A	607	CLA	MG-NA	5.69	2.19	2.06
24	C	515	BCR	C20-C19	-5.68	1.19	1.34
24	t	101	BCR	C17-C18	-5.68	1.28	1.35
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
22	b	603	CLA	C3B-C2B	5.65	1.48	1.40
24	D	404	BCR	C20-C19	-5.65	1.20	1.34
24	c	515	BCR	C20-C19	-5.65	1.20	1.34
24	A	608	BCR	C20-C19	-5.65	1.20	1.34
24	K	101	BCR	C20-C19	-5.65	1.20	1.34
22	B	603	CLA	C3B-C2B	5.64	1.48	1.40
24	T	102	BCR	C11-C12	-5.63	1.20	1.34
24	h	101	BCR	C20-C19	-5.61	1.20	1.34
24	H	101	BCR	C20-C19	-5.61	1.20	1.34
24	b	622	BCR	C11-C12	-5.60	1.20	1.34
24	t	101	BCR	C11-C12	-5.60	1.20	1.34
24	k	101	BCR	C20-C19	-5.60	1.20	1.34
24	d	404	BCR	C20-C19	-5.60	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	622	BCR	C11-C12	-5.60	1.20	1.34
24	c	514	BCR	C20-C19	-5.59	1.20	1.34
22	b	617	CLA	C3B-C2B	5.59	1.48	1.40
24	C	514	BCR	C20-C19	-5.58	1.20	1.34
24	D	404	BCR	C11-C12	-5.57	1.20	1.34
24	d	404	BCR	C11-C12	-5.57	1.20	1.34
24	T	101	BCR	C17-C18	-5.55	1.28	1.35
22	c	508	CLA	C3B-C2B	5.55	1.48	1.40
24	B	619	BCR	C16-C15	-5.54	1.21	1.36
24	B	618	BCR	C17-C18	-5.53	1.28	1.35
22	B	617	CLA	C3B-C2B	5.52	1.48	1.40
24	B	622	BCR	C20-C19	-5.52	1.20	1.34
22	c	508	CLA	C3C-C2C	5.52	1.48	1.36
24	b	618	BCR	C16-C15	-5.52	1.21	1.36
24	c	515	BCR	C11-C12	-5.52	1.20	1.34
22	c	503	CLA	C3B-C2B	5.51	1.48	1.40
22	b	603	CLA	CHC-C1C	5.51	1.49	1.35
22	C	503	CLA	C3B-C2B	5.51	1.48	1.40
24	b	622	BCR	C20-C19	-5.50	1.20	1.34
23	A	606	PHO	C3B-C2B	5.49	1.48	1.37
22	C	508	CLA	C3B-C2B	5.49	1.48	1.40
24	h	101	BCR	C11-C12	-5.49	1.20	1.34
23	a	606	PHO	C3B-C2B	5.49	1.48	1.37
24	K	102	BCR	C20-C19	-5.48	1.20	1.34
22	C	508	CLA	C3C-C2C	5.47	1.48	1.36
24	K	102	BCR	C11-C12	-5.47	1.20	1.34
22	B	603	CLA	CHC-C1C	5.47	1.49	1.35
22	b	603	CLA	C3C-C2C	5.47	1.48	1.36
24	C	515	BCR	C11-C12	-5.47	1.20	1.34
24	H	101	BCR	C11-C12	-5.47	1.20	1.34
24	k	102	BCR	C20-C19	-5.47	1.20	1.34
24	k	102	BCR	C11-C12	-5.45	1.20	1.34
24	T	102	BCR	C20-C19	-5.44	1.20	1.34
22	c	512	CLA	C3C-C2C	5.44	1.48	1.36
22	C	513	CLA	C3C-C2C	5.43	1.48	1.36
22	B	603	CLA	C3C-C2C	5.43	1.48	1.36
22	C	512	CLA	C3C-C2C	5.41	1.48	1.36
24	t	101	BCR	C20-C19	-5.41	1.20	1.34
22	B	613	CLA	CHC-C1C	5.41	1.48	1.35
22	b	613	CLA	CHC-C1C	5.41	1.48	1.35
22	C	502	CLA	CHC-C1C	5.40	1.48	1.35
22	c	513	CLA	C3C-C2C	5.40	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	502	CLA	CHC-C1C	5.40	1.48	1.35
22	B	606	CLA	MG-NC	5.39	2.19	2.06
22	b	606	CLA	MG-NC	5.38	2.19	2.06
22	c	512	CLA	CHC-C1C	5.36	1.48	1.35
23	A	605	PHO	CHB-C1B	5.36	1.49	1.38
22	C	503	CLA	C3C-C2C	5.36	1.48	1.36
22	c	501	CLA	C3B-C2B	5.36	1.47	1.40
23	a	605	PHO	CHB-C1B	5.35	1.49	1.38
22	C	501	CLA	C3B-C2B	5.35	1.47	1.40
24	b	618	BCR	C20-C19	-5.35	1.20	1.34
22	C	512	CLA	CHC-C1C	5.34	1.48	1.35
22	c	513	CLA	CHC-C1C	5.34	1.48	1.35
22	C	513	CLA	CHC-C1C	5.34	1.48	1.35
24	B	619	BCR	C20-C19	-5.34	1.20	1.34
22	c	512	CLA	C3B-C2B	5.33	1.47	1.40
22	c	503	CLA	CHC-C1C	5.33	1.48	1.35
22	C	503	CLA	CHC-C1C	5.33	1.48	1.35
24	b	618	BCR	C11-C12	-5.33	1.20	1.34
24	b	618	BCR	C17-C18	-5.33	1.28	1.35
24	B	619	BCR	C11-C12	-5.32	1.20	1.34
22	b	602	CLA	CHC-C1C	5.32	1.48	1.35
24	C	514	BCR	C11-C10	-5.32	1.27	1.43
24	B	619	BCR	C17-C18	-5.32	1.28	1.35
22	c	503	CLA	C3C-C2C	5.31	1.48	1.36
24	B	618	BCR	C11-C12	-5.30	1.20	1.34
22	C	512	CLA	C3B-C2B	5.29	1.47	1.40
24	c	514	BCR	C11-C10	-5.29	1.27	1.43
22	B	602	CLA	CHC-C1C	5.28	1.48	1.35
24	a	608	BCR	C11-C12	-5.28	1.21	1.34
22	b	616	CLA	C3C-C2C	5.28	1.48	1.36
22	B	602	CLA	O2D-CGD	5.28	1.46	1.33
22	c	507	CLA	C3C-C2C	5.28	1.48	1.36
22	B	616	CLA	C3C-C2C	5.28	1.47	1.36
33	F	101	HEM	C3D-C2D	5.28	1.53	1.37
22	b	602	CLA	O2D-CGD	5.27	1.46	1.33
22	C	507	CLA	CHC-C1C	5.27	1.48	1.35
22	C	501	CLA	CHC-C1C	5.27	1.48	1.35
33	f	101	HEM	C3D-C2D	5.27	1.53	1.37
22	c	504	CLA	C3B-C2B	5.27	1.47	1.40
22	c	501	CLA	CHC-C1C	5.27	1.48	1.35
22	c	507	CLA	CHC-C1C	5.27	1.48	1.35
22	b	602	CLA	C3C-C2C	5.26	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	101	BCR	C11-C12	-5.26	1.21	1.34
22	B	606	CLA	CHC-C1C	5.26	1.48	1.35
24	A	608	BCR	C11-C12	-5.26	1.21	1.34
22	A	603	CLA	C3C-C2C	5.26	1.47	1.36
22	B	617	CLA	MG-NC	5.26	2.18	2.06
22	C	507	CLA	C3C-C2C	5.25	1.47	1.36
22	b	606	CLA	CHC-C1C	5.25	1.48	1.35
22	B	602	CLA	C3C-C2C	5.25	1.47	1.36
24	H	101	BCR	C11-C10	-5.24	1.27	1.43
22	c	506	CLA	CHC-C1C	5.24	1.48	1.35
22	b	617	CLA	MG-NC	5.23	2.18	2.06
22	C	504	CLA	C3B-C2B	5.23	1.47	1.40
24	h	101	BCR	C11-C10	-5.23	1.27	1.43
22	C	506	CLA	CHC-C1C	5.23	1.48	1.35
22	b	607	CLA	CHC-C1C	5.22	1.48	1.35
22	B	607	CLA	C3C-C2C	5.22	1.47	1.36
22	B	606	CLA	C3C-C2C	5.22	1.47	1.36
24	d	404	BCR	C11-C10	-5.22	1.27	1.43
24	D	404	BCR	C11-C10	-5.22	1.27	1.43
22	D	403	CLA	C3B-C2B	5.22	1.47	1.40
22	c	505	CLA	C3B-C2B	5.21	1.47	1.40
22	C	505	CLA	CHC-C1C	5.21	1.48	1.35
24	C	515	BCR	C11-C10	-5.21	1.27	1.43
23	A	605	PHO	C3B-C2B	5.20	1.47	1.37
22	B	613	CLA	C3B-C2B	5.20	1.47	1.40
22	B	607	CLA	CHC-C1C	5.20	1.48	1.35
22	B	611	CLA	C3C-C2C	5.20	1.47	1.36
22	a	603	CLA	C3C-C2C	5.19	1.47	1.36
22	A	607	CLA	CHC-C1C	5.19	1.48	1.35
22	b	607	CLA	C3C-C2C	5.19	1.47	1.36
22	b	606	CLA	C3C-C2C	5.18	1.47	1.36
22	B	614	CLA	CHC-C1C	5.18	1.48	1.35
22	B	611	CLA	CHC-C1C	5.18	1.48	1.35
24	c	515	BCR	C11-C10	-5.18	1.27	1.43
23	a	605	PHO	C3B-C2B	5.18	1.47	1.37
22	d	403	CLA	CHC-C1C	5.18	1.48	1.35
22	c	505	CLA	CHC-C1C	5.18	1.48	1.35
22	C	505	CLA	C3B-C2B	5.17	1.47	1.40
22	D	401	CLA	C3B-C2B	5.17	1.47	1.40
22	d	403	CLA	C3B-C2B	5.17	1.47	1.40
22	b	611	CLA	CHC-C1C	5.17	1.48	1.35
22	b	611	CLA	C3C-C2C	5.17	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	513	CLA	O2D-CGD	5.16	1.45	1.33
22	b	613	CLA	C3B-C2B	5.16	1.47	1.40
22	a	607	CLA	CHC-C1C	5.15	1.48	1.35
24	b	622	BCR	C11-C10	-5.15	1.27	1.43
22	c	508	CLA	CHC-C1C	5.15	1.48	1.35
22	C	508	CLA	CHC-C1C	5.15	1.48	1.35
22	b	614	CLA	CHC-C1C	5.15	1.48	1.35
24	B	622	BCR	C11-C10	-5.15	1.27	1.43
24	K	101	BCR	C11-C10	-5.14	1.27	1.43
22	d	403	CLA	C3C-C2C	5.14	1.47	1.36
22	c	509	CLA	O2D-CGD	5.14	1.45	1.33
24	C	514	BCR	C15-C14	-5.14	1.27	1.43
22	C	505	CLA	C3C-C2C	5.14	1.47	1.36
22	c	505	CLA	C3C-C2C	5.14	1.47	1.36
22	c	513	CLA	O2D-CGD	5.14	1.45	1.33
22	D	403	CLA	C3C-C2C	5.14	1.47	1.36
22	D	403	CLA	CHC-C1C	5.14	1.48	1.35
22	d	401	CLA	C3B-C2B	5.13	1.47	1.40
24	k	101	BCR	C11-C10	-5.13	1.27	1.43
22	c	506	CLA	O2D-CGD	5.13	1.45	1.33
23	A	606	PHO	CHB-C1B	5.13	1.48	1.38
22	C	509	CLA	O2D-CGD	5.13	1.45	1.33
23	a	606	PHO	CHB-C1B	5.12	1.48	1.38
22	C	511	CLA	O2D-CGD	5.12	1.45	1.33
22	A	607	CLA	C3B-C2B	5.12	1.47	1.40
22	B	607	CLA	C3B-C2B	5.12	1.47	1.40
24	c	514	BCR	C15-C14	-5.12	1.27	1.43
22	b	615	CLA	CHC-C1C	5.12	1.48	1.35
22	A	607	CLA	C3C-C2C	5.11	1.47	1.36
22	c	507	CLA	O2D-CGD	5.11	1.45	1.33
22	B	615	CLA	CHC-C1C	5.11	1.48	1.35
22	c	511	CLA	O2D-CGD	5.11	1.45	1.33
22	C	506	CLA	O2D-CGD	5.11	1.45	1.33
22	c	508	CLA	O2D-CGD	5.11	1.45	1.33
22	b	609	CLA	C3C-C2C	5.10	1.47	1.36
22	b	617	CLA	CHC-C1C	5.10	1.48	1.35
22	a	607	CLA	C3B-C2B	5.10	1.47	1.40
22	B	609	CLA	C3C-C2C	5.09	1.47	1.36
22	c	510	CLA	C3C-C2C	5.09	1.47	1.36
24	B	622	BCR	C15-C14	-5.09	1.27	1.43
22	C	506	CLA	C3C-C2C	5.09	1.47	1.36
22	C	510	CLA	C3C-C2C	5.09	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	608	BCR	C11-C10	-5.09	1.27	1.43
24	C	515	BCR	C15-C14	-5.09	1.27	1.43
24	T	101	BCR	C20-C19	-5.09	1.21	1.34
22	b	607	CLA	C3B-C2B	5.08	1.47	1.40
24	b	622	BCR	C15-C14	-5.08	1.27	1.43
22	a	607	CLA	C3C-C2C	5.08	1.47	1.36
22	b	610	CLA	CHC-C1C	5.08	1.48	1.35
24	a	608	BCR	C11-C10	-5.08	1.27	1.43
22	B	617	CLA	CHC-C1C	5.08	1.48	1.35
22	B	616	CLA	CHC-C1C	5.08	1.48	1.35
24	H	101	BCR	C15-C14	-5.08	1.27	1.43
22	C	508	CLA	O2D-CGD	5.08	1.45	1.33
22	C	511	CLA	C3C-C2C	5.07	1.47	1.36
24	c	515	BCR	C15-C14	-5.07	1.27	1.43
22	A	603	CLA	C3B-C2B	5.07	1.47	1.40
22	C	509	CLA	OBD-CAD	5.06	1.29	1.22
24	h	101	BCR	C15-C14	-5.06	1.27	1.43
22	a	603	CLA	C3B-C2B	5.06	1.47	1.40
22	b	616	CLA	CHC-C1C	5.06	1.47	1.35
22	c	511	CLA	CHC-C1C	5.06	1.47	1.35
22	c	506	CLA	C3C-C2C	5.06	1.47	1.36
22	c	509	CLA	OBD-CAD	5.06	1.29	1.22
24	k	102	BCR	C11-C10	-5.06	1.27	1.43
22	B	610	CLA	CHC-C1C	5.06	1.47	1.35
24	K	102	BCR	C11-C10	-5.06	1.27	1.43
22	C	507	CLA	O2D-CGD	5.05	1.45	1.33
22	c	506	CLA	C3B-C2B	5.05	1.47	1.40
22	A	603	CLA	CHC-C1C	5.05	1.47	1.35
22	B	608	CLA	C3C-C2C	5.05	1.47	1.36
22	C	506	CLA	C3B-C2B	5.05	1.47	1.40
24	B	618	BCR	C20-C19	-5.05	1.21	1.34
22	a	603	CLA	CHC-C1C	5.05	1.47	1.35
22	b	609	CLA	C3B-C2B	5.04	1.47	1.40
22	B	609	CLA	O2D-CGD	5.04	1.45	1.33
22	C	512	CLA	O2D-CGD	5.04	1.45	1.33
23	a	605	PHO	C3C-C2C	5.04	1.47	1.36
22	c	511	CLA	C3C-C2C	5.04	1.47	1.36
24	T	102	BCR	C11-C10	-5.03	1.27	1.43
24	T	101	BCR	C11-C10	-5.03	1.27	1.43
22	C	511	CLA	CHC-C1C	5.03	1.47	1.35
22	C	509	CLA	CHC-C1C	5.03	1.47	1.35
23	A	605	PHO	C3C-C2C	5.03	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	101	BCR	C15-C14	-5.03	1.27	1.43
22	c	512	CLA	O2D-CGD	5.03	1.45	1.33
22	B	609	CLA	C3B-C2B	5.03	1.47	1.40
22	b	609	CLA	O2D-CGD	5.03	1.45	1.33
22	b	608	CLA	C3C-C2C	5.02	1.47	1.36
22	B	604	CLA	C3B-C2B	5.02	1.47	1.40
22	c	509	CLA	CHC-C1C	5.02	1.47	1.35
22	b	614	CLA	C3C-C2C	5.02	1.47	1.36
22	c	509	CLA	C3C-C2C	5.02	1.47	1.36
24	K	101	BCR	C15-C14	-5.02	1.27	1.43
22	c	510	CLA	C3B-C2B	5.02	1.47	1.40
24	d	404	BCR	C15-C14	-5.02	1.27	1.43
24	t	101	BCR	C11-C10	-5.02	1.27	1.43
24	B	618	BCR	C11-C10	-5.02	1.27	1.43
24	D	404	BCR	C15-C14	-5.01	1.27	1.43
22	A	607	CLA	OBD-CAD	5.01	1.29	1.22
22	B	608	CLA	CHC-C1C	5.01	1.47	1.35
24	t	101	BCR	C15-C14	-5.01	1.27	1.43
24	T	102	BCR	C15-C14	-5.01	1.27	1.43
22	C	508	CLA	MG-NC	5.01	2.18	2.06
22	b	604	CLA	C3B-C2B	5.01	1.47	1.40
22	c	508	CLA	MG-NC	5.01	2.18	2.06
22	B	602	CLA	C3B-C2B	5.01	1.47	1.40
22	b	617	CLA	C3C-C2C	5.00	1.47	1.36
22	C	502	CLA	O2D-CGD	5.00	1.45	1.33
22	C	510	CLA	C3B-C2B	5.00	1.47	1.40
22	C	509	CLA	C3C-C2C	4.99	1.47	1.36
22	B	614	CLA	C3C-C2C	4.99	1.47	1.36
22	B	607	CLA	O2D-CGD	4.98	1.45	1.33
22	b	608	CLA	C3B-C2B	4.98	1.47	1.40
22	c	505	CLA	O2D-CGD	4.98	1.45	1.33
22	a	607	CLA	OBD-CAD	4.98	1.29	1.22
24	k	102	BCR	C15-C14	-4.98	1.28	1.43
33	V	201	HEM	C3D-C2D	4.98	1.52	1.37
22	C	501	CLA	C3C-C2C	4.98	1.47	1.36
22	B	610	CLA	C3C-C2C	4.97	1.47	1.36
22	b	610	CLA	C3C-C2C	4.97	1.47	1.36
22	B	608	CLA	C3B-C2B	4.97	1.47	1.40
22	C	504	CLA	C3C-C2C	4.97	1.47	1.36
22	b	602	CLA	C3B-C2B	4.97	1.47	1.40
22	B	617	CLA	C3C-C2C	4.97	1.47	1.36
22	b	608	CLA	CHC-C1C	4.97	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	510	CLA	OBD-CAD	4.97	1.29	1.22
22	c	509	CLA	C3B-C2B	4.96	1.47	1.40
24	K	102	BCR	C15-C14	-4.96	1.28	1.43
22	c	502	CLA	O2D-CGD	4.96	1.45	1.33
22	d	402	CLA	C3C-C2C	4.96	1.47	1.36
23	A	606	PHO	O2D-CGD	4.96	1.45	1.33
22	b	604	CLA	CHC-C1C	4.95	1.47	1.35
33	v	201	HEM	C3D-C2D	4.95	1.52	1.37
23	a	606	PHO	O2D-CGD	4.95	1.45	1.33
22	b	608	CLA	MG-NC	4.95	2.18	2.06
22	C	505	CLA	O2D-CGD	4.94	1.45	1.33
22	D	402	CLA	C3C-C2C	4.94	1.47	1.36
22	b	607	CLA	O2D-CGD	4.94	1.45	1.33
22	C	504	CLA	CHC-C1C	4.94	1.47	1.35
22	c	501	CLA	C3C-C2C	4.94	1.47	1.36
22	B	605	CLA	C3C-C2C	4.94	1.47	1.36
24	A	608	BCR	C15-C14	-4.93	1.28	1.43
22	c	504	CLA	C3C-C2C	4.93	1.47	1.36
22	c	504	CLA	CHC-C1C	4.93	1.47	1.35
24	B	622	BCR	C23-C22	-4.93	1.35	1.45
24	C	515	BCR	C23-C22	-4.93	1.35	1.45
23	a	606	PHO	C3C-C2C	4.93	1.47	1.36
22	C	511	CLA	C3B-C2B	4.92	1.47	1.40
24	B	619	BCR	C11-C10	-4.92	1.28	1.43
22	d	401	CLA	C3C-C2C	4.92	1.47	1.36
22	C	510	CLA	OBD-CAD	4.92	1.29	1.22
24	b	622	BCR	C23-C22	-4.92	1.35	1.45
22	D	401	CLA	C3C-C2C	4.92	1.47	1.36
22	b	615	CLA	C3C-C2C	4.92	1.47	1.36
24	b	618	BCR	C11-C10	-4.91	1.28	1.43
22	c	502	CLA	C3C-C2C	4.91	1.47	1.36
24	a	608	BCR	C15-C14	-4.91	1.28	1.43
23	A	606	PHO	C3C-C2C	4.90	1.47	1.36
22	B	615	CLA	C3C-C2C	4.90	1.47	1.36
22	c	510	CLA	O2D-CGD	4.90	1.45	1.33
22	c	511	CLA	C3B-C2B	4.90	1.47	1.40
22	B	604	CLA	CHC-C1C	4.90	1.47	1.35
22	b	614	CLA	C3B-C2B	4.90	1.47	1.40
22	b	605	CLA	C3C-C2C	4.90	1.47	1.36
22	C	502	CLA	C3C-C2C	4.89	1.47	1.36
22	C	510	CLA	O2D-CGD	4.89	1.45	1.33
22	B	608	CLA	MG-NC	4.89	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	BCR	C23-C22	-4.88	1.35	1.45
22	B	614	CLA	C3B-C2B	4.88	1.47	1.40
22	B	606	CLA	O2D-CGD	4.87	1.45	1.33
22	b	606	CLA	O2D-CGD	4.87	1.45	1.33
22	B	616	CLA	O2D-CGD	4.87	1.45	1.33
22	d	402	CLA	OBD-CAD	4.87	1.29	1.22
22	B	604	CLA	O2D-CGD	4.86	1.45	1.33
22	B	617	CLA	O2D-CGD	4.86	1.45	1.33
22	A	603	CLA	O2D-CGD	4.86	1.45	1.33
22	b	613	CLA	C3C-C2C	4.86	1.47	1.36
22	a	603	CLA	O2D-CGD	4.85	1.45	1.33
22	b	617	CLA	O2D-CGD	4.85	1.45	1.33
22	C	509	CLA	C3B-C2B	4.85	1.47	1.40
22	a	603	CLA	OBD-CAD	4.85	1.29	1.22
22	b	616	CLA	O2D-CGD	4.85	1.45	1.33
22	b	604	CLA	O2D-CGD	4.84	1.45	1.33
22	B	613	CLA	C3C-C2C	4.84	1.47	1.36
22	A	604	CLA	C3B-C2B	4.84	1.47	1.40
22	D	402	CLA	OBD-CAD	4.83	1.29	1.22
24	D	404	BCR	C23-C22	-4.82	1.35	1.45
22	B	617	CLA	OBD-CAD	4.82	1.29	1.22
22	A	604	CLA	C3C-C2C	4.82	1.47	1.36
24	d	404	BCR	C23-C22	-4.81	1.35	1.45
22	d	402	CLA	C3B-C2B	4.81	1.47	1.40
22	b	616	CLA	C3B-C2B	4.81	1.47	1.40
22	D	402	CLA	C3B-C2B	4.81	1.47	1.40
22	B	613	CLA	O2D-CGD	4.80	1.44	1.33
22	b	617	CLA	OBD-CAD	4.80	1.29	1.22
22	b	611	CLA	C3B-C2B	4.80	1.47	1.40
22	b	613	CLA	O2D-CGD	4.79	1.44	1.33
22	B	616	CLA	C3B-C2B	4.79	1.47	1.40
22	D	401	CLA	OBD-CAD	4.79	1.29	1.22
22	b	604	CLA	OBD-CAD	4.79	1.29	1.22
22	A	603	CLA	OBD-CAD	4.78	1.29	1.22
22	b	602	CLA	O2A-CGA	4.78	1.47	1.33
22	C	503	CLA	O2D-CGD	4.78	1.44	1.33
22	a	604	CLA	C3C-C2C	4.78	1.46	1.36
24	K	101	BCR	C23-C22	-4.78	1.35	1.45
22	B	602	CLA	O2A-CGA	4.78	1.47	1.33
22	c	503	CLA	O2D-CGD	4.78	1.44	1.33
22	a	604	CLA	C3B-C2B	4.78	1.47	1.40
22	d	401	CLA	OBD-CAD	4.77	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	O2D-CGD	4.77	1.44	1.33
24	T	101	BCR	C23-C22	-4.77	1.35	1.45
22	b	608	CLA	O2D-CGD	4.77	1.44	1.33
22	B	610	CLA	C3B-C2B	4.77	1.47	1.40
22	b	604	CLA	C3C-C2C	4.77	1.46	1.36
22	B	615	CLA	O2D-CGD	4.77	1.44	1.33
22	B	604	CLA	C3C-C2C	4.77	1.46	1.36
24	B	618	BCR	C23-C22	-4.77	1.35	1.45
22	B	611	CLA	C3B-C2B	4.77	1.47	1.40
24	B	619	BCR	C15-C14	-4.77	1.28	1.43
22	C	510	CLA	CHC-C1C	4.76	1.47	1.35
24	b	618	BCR	C15-C14	-4.76	1.28	1.43
24	K	102	BCR	C23-C22	-4.76	1.35	1.45
22	b	615	CLA	O2D-CGD	4.75	1.44	1.33
22	c	510	CLA	CHC-C1C	4.75	1.47	1.35
24	k	101	BCR	C23-C22	-4.75	1.35	1.45
24	C	514	BCR	C23-C22	-4.74	1.35	1.45
24	H	101	BCR	C23-C22	-4.74	1.35	1.45
22	A	604	CLA	CHC-C1C	4.74	1.47	1.35
24	B	618	BCR	C15-C14	-4.74	1.28	1.43
24	k	102	BCR	C23-C22	-4.74	1.35	1.45
22	B	604	CLA	OBD-CAD	4.74	1.28	1.22
22	D	402	CLA	MG-NA	4.74	2.17	2.06
24	T	101	BCR	C15-C14	-4.73	1.28	1.43
22	b	605	CLA	CHC-C1C	4.73	1.47	1.35
22	a	604	CLA	CHC-C1C	4.73	1.47	1.35
23	a	606	PHO	C1A-NA	-4.73	1.28	1.37
22	B	603	CLA	OBD-CAD	4.73	1.28	1.22
24	c	514	BCR	C23-C22	-4.73	1.35	1.45
22	B	612	CLA	CHC-C1C	4.73	1.47	1.35
22	b	603	CLA	OBD-CAD	4.73	1.28	1.22
22	B	612	CLA	C3C-C2C	4.72	1.46	1.36
22	b	612	CLA	CHC-C1C	4.72	1.47	1.35
22	c	511	CLA	MG-NC	4.72	2.17	2.06
22	c	504	CLA	O2D-CGD	4.72	1.44	1.33
22	c	511	CLA	OBD-CAD	4.72	1.28	1.22
22	C	511	CLA	OBD-CAD	4.72	1.28	1.22
22	B	605	CLA	CHC-C1C	4.72	1.47	1.35
22	d	402	CLA	MG-NA	4.72	2.17	2.06
22	A	604	CLA	O2D-CGD	4.71	1.44	1.33
22	b	612	CLA	C3C-C2C	4.71	1.46	1.36
22	C	504	CLA	O2D-CGD	4.71	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	401	CLA	O2D-CGD	4.71	1.44	1.33
22	c	513	CLA	OBD-CAD	4.71	1.28	1.22
22	C	502	CLA	C3B-C2B	4.71	1.46	1.40
22	b	610	CLA	C3B-C2B	4.71	1.46	1.40
23	A	606	PHO	C1A-NA	-4.71	1.28	1.37
22	D	403	CLA	O2D-CGD	4.70	1.44	1.33
22	C	511	CLA	MG-NC	4.70	2.17	2.06
24	h	101	BCR	C23-C22	-4.69	1.35	1.45
22	c	502	CLA	C3B-C2B	4.69	1.46	1.40
22	b	607	CLA	OBD-CAD	4.69	1.28	1.22
22	d	403	CLA	O2D-CGD	4.69	1.44	1.33
22	b	609	CLA	MG-NC	4.68	2.17	2.06
22	C	513	CLA	OBD-CAD	4.68	1.28	1.22
22	a	604	CLA	O2D-CGD	4.67	1.44	1.33
22	b	605	CLA	C3B-C2B	4.67	1.46	1.40
23	A	606	PHO	CHC-C1C	4.67	1.47	1.38
22	B	609	CLA	MG-NC	4.67	2.17	2.06
23	a	606	PHO	CHC-C1C	4.66	1.47	1.38
22	d	401	CLA	O2D-CGD	4.66	1.44	1.33
22	B	607	CLA	OBD-CAD	4.65	1.28	1.22
22	a	604	CLA	OBD-CAD	4.64	1.28	1.22
22	b	609	CLA	CHC-C1C	4.64	1.46	1.35
22	D	401	CLA	CHC-C1C	4.63	1.46	1.35
22	c	501	CLA	O2D-CGD	4.63	1.44	1.33
22	C	501	CLA	O2D-CGD	4.63	1.44	1.33
22	d	401	CLA	CHC-C1C	4.62	1.46	1.35
22	B	605	CLA	C3B-C2B	4.62	1.46	1.40
23	a	605	PHO	O2D-CGD	4.61	1.44	1.33
22	B	609	CLA	CHC-C1C	4.61	1.46	1.35
22	D	402	CLA	CHC-C1C	4.61	1.46	1.35
22	B	611	CLA	O2D-CGD	4.60	1.44	1.33
22	d	402	CLA	CHC-C1C	4.60	1.46	1.35
22	c	508	CLA	C3D-C2D	4.60	1.47	1.39
23	A	605	PHO	O2D-CGD	4.59	1.44	1.33
22	b	611	CLA	O2D-CGD	4.59	1.44	1.33
22	C	504	CLA	OBD-CAD	4.59	1.28	1.22
22	c	502	CLA	OBD-CAD	4.57	1.28	1.22
29	b	619	LMG	O8-C28	4.57	1.46	1.33
22	A	604	CLA	OBD-CAD	4.57	1.28	1.22
24	b	618	BCR	C23-C22	-4.57	1.36	1.45
22	b	614	CLA	O2D-CGD	4.57	1.44	1.33
22	B	602	CLA	OBD-CAD	4.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	411	SQD	O48-C23	4.55	1.46	1.33
22	B	614	CLA	O2D-CGD	4.55	1.44	1.33
29	B	620	LMG	O8-C28	4.55	1.46	1.33
24	B	619	BCR	C23-C22	-4.55	1.36	1.45
22	b	602	CLA	OBD-CAD	4.55	1.28	1.22
22	b	610	CLA	OBD-CAD	4.54	1.28	1.22
22	B	615	CLA	C3B-C2B	4.54	1.46	1.40
22	c	504	CLA	OBD-CAD	4.53	1.28	1.22
22	c	501	CLA	OBD-CAD	4.53	1.28	1.22
22	C	508	CLA	C3D-C2D	4.53	1.47	1.39
22	b	610	CLA	O2D-CGD	4.53	1.44	1.33
22	B	612	CLA	O2D-CGD	4.52	1.44	1.33
22	b	612	CLA	O2D-CGD	4.52	1.44	1.33
29	c	520	LMG	O7-C10	4.52	1.47	1.34
29	C	520	LMG	O7-C10	4.52	1.47	1.34
31	D	410	DGD	O1G-C1A	4.52	1.46	1.33
22	B	610	CLA	O2D-CGD	4.51	1.44	1.33
23	a	605	PHO	C1A-NA	-4.51	1.28	1.37
25	d	411	SQD	O48-C23	4.51	1.46	1.33
22	c	505	CLA	OBD-CAD	4.51	1.28	1.22
22	C	501	CLA	OBD-CAD	4.51	1.28	1.22
22	B	603	CLA	C3D-C2D	4.51	1.47	1.39
23	A	605	PHO	C1A-NA	-4.51	1.28	1.37
22	C	502	CLA	OBD-CAD	4.50	1.28	1.22
22	c	507	CLA	OBD-CAD	4.50	1.28	1.22
22	B	607	CLA	MG-NC	4.50	2.17	2.06
24	T	102	BCR	C23-C22	-4.50	1.36	1.45
31	d	410	DGD	O1G-C1A	4.50	1.46	1.33
25	b	601	SQD	O48-C23	4.50	1.46	1.33
24	t	101	BCR	C23-C22	-4.49	1.36	1.45
32	e	101	LHG	O8-C23	4.49	1.46	1.33
22	b	615	CLA	C3B-C2B	4.49	1.46	1.40
22	b	607	CLA	MG-NC	4.49	2.16	2.06
25	D	411	SQD	O47-C7	4.49	1.47	1.34
31	D	410	DGD	O2G-C1B	4.48	1.46	1.34
22	C	506	CLA	OBD-CAD	4.48	1.28	1.22
22	B	610	CLA	OBD-CAD	4.48	1.28	1.22
22	B	606	CLA	C3B-C2B	4.48	1.46	1.40
25	d	411	SQD	O47-C7	4.48	1.46	1.34
25	B	601	SQD	O48-C23	4.48	1.46	1.33
22	b	616	CLA	OBD-CAD	4.48	1.28	1.22
22	C	507	CLA	OBD-CAD	4.48	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	OBD-CAD	4.47	1.28	1.22
22	b	603	CLA	C3D-C2D	4.47	1.47	1.39
32	E	101	LHG	O8-C23	4.47	1.46	1.33
31	d	410	DGD	O2G-C1B	4.47	1.46	1.34
22	B	603	CLA	O2D-CGD	4.46	1.44	1.33
22	b	605	CLA	O2D-CGD	4.46	1.44	1.33
22	B	605	CLA	O2D-CGD	4.46	1.44	1.33
22	C	505	CLA	OBD-CAD	4.45	1.28	1.22
22	b	606	CLA	C3B-C2B	4.44	1.46	1.40
22	b	611	CLA	OBD-CAD	4.44	1.28	1.22
24	a	608	BCR	C23-C22	-4.44	1.36	1.45
22	c	506	CLA	OBD-CAD	4.44	1.28	1.22
25	l	102	SQD	O48-C23	4.44	1.46	1.33
22	c	508	CLA	OBD-CAD	4.44	1.28	1.22
22	b	603	CLA	O2D-CGD	4.44	1.44	1.33
22	d	403	CLA	OBD-CAD	4.43	1.28	1.22
22	b	613	CLA	OBD-CAD	4.43	1.28	1.22
22	b	612	CLA	C3B-C2B	4.43	1.46	1.40
22	C	502	CLA	MG-NC	4.43	2.16	2.06
22	B	616	CLA	OBD-CAD	4.43	1.28	1.22
22	B	611	CLA	OBD-CAD	4.43	1.28	1.22
23	a	606	PHO	CHD-C1D	4.43	1.47	1.38
22	B	617	CLA	C3D-C2D	4.42	1.47	1.39
23	A	606	PHO	CHD-C1D	4.42	1.47	1.38
22	c	513	CLA	C3D-C2D	4.42	1.47	1.39
25	l	102	SQD	O47-C7	4.42	1.46	1.34
25	b	621	SQD	O48-C23	4.42	1.46	1.33
22	b	617	CLA	C3D-C2D	4.41	1.47	1.39
22	c	502	CLA	MG-NC	4.41	2.16	2.06
22	C	513	CLA	C3D-C2D	4.41	1.47	1.39
22	D	403	CLA	OBD-CAD	4.40	1.28	1.22
24	A	608	BCR	C23-C22	-4.40	1.36	1.45
25	b	621	SQD	O47-C7	4.40	1.46	1.34
22	B	604	CLA	C3D-C2D	4.40	1.47	1.39
23	a	605	PHO	CHC-C1C	4.39	1.47	1.38
22	C	511	CLA	C3D-C2D	4.39	1.47	1.39
22	B	613	CLA	OBD-CAD	4.39	1.28	1.22
22	B	612	CLA	C3B-C2B	4.39	1.46	1.40
22	b	604	CLA	C3D-C2D	4.38	1.47	1.39
25	l	101	SQD	O47-C7	4.38	1.46	1.34
22	c	504	CLA	C3D-C2D	4.38	1.47	1.39
29	C	520	LMG	O8-C28	4.37	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	511	CLA	C3D-C2D	4.37	1.47	1.39
25	L	101	SQD	O47-C7	4.36	1.46	1.34
22	c	506	CLA	O2A-CGA	4.35	1.46	1.33
22	a	607	CLA	O2D-CGD	4.35	1.43	1.33
22	b	606	CLA	OBD-CAD	4.35	1.28	1.22
22	A	607	CLA	O2D-CGD	4.34	1.43	1.33
22	C	504	CLA	C3D-C2D	4.34	1.47	1.39
22	C	512	CLA	C3D-C2D	4.34	1.47	1.39
23	A	605	PHO	CHC-C1C	4.34	1.47	1.38
29	c	520	LMG	O8-C28	4.34	1.46	1.33
22	C	506	CLA	O2A-CGA	4.32	1.46	1.33
22	B	611	CLA	C3D-C2D	4.31	1.47	1.39
22	B	606	CLA	OBD-CAD	4.31	1.28	1.22
22	b	611	CLA	C3D-C2D	4.31	1.47	1.39
22	c	512	CLA	C3D-C2D	4.31	1.47	1.39
22	b	615	CLA	OBD-CAD	4.30	1.28	1.22
29	z	101	LMG	O7-C10	4.29	1.46	1.34
22	b	609	CLA	OBD-CAD	4.29	1.28	1.22
22	C	501	CLA	C3D-C2D	4.29	1.47	1.39
33	v	201	HEM	C3C-C2C	-4.28	1.34	1.40
22	a	604	CLA	C3D-C2D	4.28	1.47	1.39
22	c	501	CLA	C3D-C2D	4.28	1.47	1.39
25	b	601	SQD	O47-C7	4.28	1.46	1.34
33	V	201	HEM	C3C-C2C	-4.28	1.34	1.40
25	B	601	SQD	O47-C7	4.28	1.46	1.34
22	B	608	CLA	OBD-CAD	4.28	1.28	1.22
22	D	401	CLA	O2A-CGA	4.27	1.45	1.33
29	c	519	LMG	O8-C28	4.27	1.45	1.33
29	Z	101	LMG	O7-C10	4.27	1.46	1.34
22	D	402	CLA	C3D-C2D	4.27	1.47	1.39
22	b	608	CLA	OBD-CAD	4.27	1.28	1.22
22	B	614	CLA	C3D-C2D	4.27	1.47	1.39
22	C	509	CLA	O2A-CGA	4.26	1.45	1.33
22	b	614	CLA	C3D-C2D	4.26	1.47	1.39
22	B	609	CLA	OBD-CAD	4.26	1.28	1.22
22	C	512	CLA	OBD-CAD	4.26	1.28	1.22
22	b	617	CLA	O2A-CGA	4.26	1.45	1.33
22	d	402	CLA	C3D-C2D	4.26	1.47	1.39
29	C	519	LMG	O8-C28	4.25	1.45	1.33
22	B	615	CLA	OBD-CAD	4.25	1.28	1.22
29	c	519	LMG	O7-C10	4.25	1.46	1.34
22	c	512	CLA	O2A-CGA	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	E	101	LHG	O7-C7	4.25	1.46	1.34
22	c	509	CLA	O2A-CGA	4.25	1.45	1.33
29	A	614	LMG	O7-C10	4.25	1.46	1.34
22	B	617	CLA	O2A-CGA	4.25	1.45	1.33
22	D	402	CLA	O2D-CGD	4.24	1.43	1.33
22	A	604	CLA	C3D-C2D	4.24	1.47	1.39
29	a	614	LMG	O7-C10	4.24	1.46	1.34
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	507	CLA	O2A-CGA	4.23	1.45	1.33
22	c	512	CLA	OBD-CAD	4.23	1.28	1.22
22	c	507	CLA	O2A-CGA	4.23	1.45	1.33
29	a	614	LMG	O8-C28	4.23	1.45	1.33
29	C	519	LMG	O7-C10	4.22	1.46	1.34
22	d	401	CLA	O2A-CGA	4.22	1.45	1.33
22	C	512	CLA	O2A-CGA	4.21	1.45	1.33
22	d	402	CLA	O2D-CGD	4.21	1.43	1.33
22	B	610	CLA	C3D-C2D	4.19	1.46	1.39
22	B	609	CLA	C3D-C2D	4.19	1.46	1.39
22	a	607	CLA	O2A-CGA	4.19	1.45	1.33
22	b	609	CLA	C3D-C2D	4.19	1.46	1.39
22	C	503	CLA	O2A-CGA	4.19	1.45	1.33
22	c	513	CLA	O2A-CGA	4.17	1.45	1.33
22	c	503	CLA	O2A-CGA	4.17	1.45	1.33
22	D	403	CLA	C3D-C2D	4.17	1.46	1.39
22	A	607	CLA	O2A-CGA	4.16	1.45	1.33
22	C	513	CLA	O2A-CGA	4.16	1.45	1.33
22	d	403	CLA	O2A-CGA	4.16	1.45	1.33
22	b	610	CLA	C3D-C2D	4.16	1.46	1.39
22	B	616	CLA	C3D-C2D	4.16	1.46	1.39
22	b	606	CLA	C3D-C2D	4.15	1.46	1.39
22	B	614	CLA	OBD-CAD	4.15	1.28	1.22
22	b	616	CLA	C3D-C2D	4.15	1.46	1.39
22	d	403	CLA	C3D-C2D	4.15	1.46	1.39
22	b	616	CLA	O2A-CGA	4.14	1.45	1.33
22	c	511	CLA	O2A-CGA	4.14	1.45	1.33
22	b	614	CLA	OBD-CAD	4.14	1.28	1.22
25	A	609	SQD	O47-C7	4.13	1.46	1.34
22	D	403	CLA	O2A-CGA	4.13	1.45	1.33
25	a	609	SQD	O47-C7	4.13	1.45	1.34
22	B	616	CLA	O2A-CGA	4.13	1.45	1.33
22	C	511	CLA	O2A-CGA	4.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	MG-NC	4.13	2.16	2.06
32	d	409	LHG	O8-C23	4.13	1.45	1.33
32	D	409	LHG	O8-C23	4.12	1.45	1.33
22	c	509	CLA	MG-NC	4.12	2.16	2.06
25	L	101	SQD	O48-C23	4.12	1.45	1.33
22	B	606	CLA	C3D-C2D	4.12	1.46	1.39
22	b	610	CLA	O2A-CGA	4.11	1.45	1.33
25	l	101	SQD	O48-C23	4.10	1.45	1.33
22	b	612	CLA	OBD-CAD	4.09	1.28	1.22
31	C	517	DGD	O1G-C1A	4.09	1.45	1.33
31	c	517	DGD	O1G-C1A	4.09	1.45	1.33
22	C	502	CLA	O2A-CGA	4.09	1.45	1.33
33	f	101	HEM	C3C-C2C	-4.08	1.34	1.40
22	B	612	CLA	OBD-CAD	4.08	1.28	1.22
22	B	610	CLA	O2A-CGA	4.08	1.45	1.33
22	c	510	CLA	C3D-C2D	4.08	1.46	1.39
22	C	510	CLA	C3D-C2D	4.07	1.46	1.39
33	F	101	HEM	C3C-C2C	-4.07	1.34	1.40
22	C	501	CLA	O2A-CGA	4.07	1.45	1.33
22	d	402	CLA	MG-NC	4.07	2.15	2.06
22	b	607	CLA	O2A-CGA	4.07	1.45	1.33
22	D	402	CLA	MG-NC	4.06	2.15	2.06
22	b	615	CLA	O2A-CGA	4.06	1.45	1.33
22	c	502	CLA	O2A-CGA	4.06	1.45	1.33
22	B	607	CLA	O2A-CGA	4.06	1.45	1.33
22	c	505	CLA	C3D-C2D	4.06	1.46	1.39
22	B	608	CLA	C3D-C2D	4.05	1.46	1.39
22	a	603	CLA	C3D-C2D	4.05	1.46	1.39
22	c	501	CLA	O2A-CGA	4.05	1.45	1.33
22	C	507	CLA	C3D-C2D	4.05	1.46	1.39
22	B	615	CLA	C3D-C2D	4.05	1.46	1.39
22	c	502	CLA	C3D-C2D	4.04	1.46	1.39
22	C	505	CLA	C3D-C2D	4.04	1.46	1.39
22	c	507	CLA	C3D-C2D	4.04	1.46	1.39
33	v	201	HEM	C3B-CAB	4.04	1.56	1.47
22	B	615	CLA	O2A-CGA	4.04	1.45	1.33
22	b	615	CLA	C3D-C2D	4.04	1.46	1.39
22	b	608	CLA	C3D-C2D	4.03	1.46	1.39
32	L	102	LHG	O8-C23	4.03	1.45	1.33
22	C	501	CLA	MG-NC	4.03	2.15	2.06
22	C	502	CLA	C3D-C2D	4.02	1.46	1.39
32	l	103	LHG	O8-C23	4.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	O2A-CGA	4.02	1.45	1.33
22	C	508	CLA	O2A-CGA	4.02	1.45	1.33
25	A	609	SQD	O48-C23	4.02	1.45	1.33
22	C	504	CLA	O2A-CGA	4.01	1.45	1.33
33	V	201	HEM	C3B-CAB	4.01	1.56	1.47
22	A	603	CLA	C3D-C2D	4.01	1.46	1.39
22	A	607	CLA	C3D-C2D	4.01	1.46	1.39
22	c	501	CLA	MG-NC	4.00	2.15	2.06
22	c	508	CLA	O2A-CGA	4.00	1.45	1.33
22	b	613	CLA	C3D-C2D	4.00	1.46	1.39
22	c	509	CLA	C3D-C2D	4.00	1.46	1.39
22	c	506	CLA	C3D-C2D	4.00	1.46	1.39
25	a	609	SQD	O48-C23	4.00	1.45	1.33
22	C	506	CLA	C3D-C2D	3.99	1.46	1.39
31	h	102	DGD	O1G-C1A	3.99	1.45	1.33
22	c	504	CLA	O2A-CGA	3.99	1.45	1.33
22	C	509	CLA	C3D-C2D	3.99	1.46	1.39
32	d	405	LHG	O8-C23	3.98	1.45	1.33
31	c	516	DGD	O2G-C1B	3.98	1.45	1.34
22	B	604	CLA	O2A-CGA	3.98	1.45	1.33
22	c	510	CLA	O2A-CGA	3.97	1.45	1.33
32	D	405	LHG	O8-C23	3.97	1.45	1.33
31	H	102	DGD	O1G-C1A	3.97	1.45	1.33
29	b	619	LMG	O7-C10	3.97	1.45	1.34
22	a	607	CLA	C3D-C2D	3.97	1.46	1.39
22	B	603	CLA	MG-NC	3.97	2.15	2.06
33	f	101	HEM	C3B-C2B	-3.97	1.34	1.40
22	b	603	CLA	MG-NC	3.96	2.15	2.06
22	B	613	CLA	C3D-C2D	3.96	1.46	1.39
32	d	407	LHG	O8-C23	3.96	1.44	1.33
31	C	516	DGD	O2G-C1B	3.96	1.45	1.34
22	C	510	CLA	O2A-CGA	3.95	1.44	1.33
22	D	402	CLA	O2A-CGA	3.95	1.44	1.33
22	d	402	CLA	O2A-CGA	3.95	1.44	1.33
32	D	407	LHG	O8-C23	3.94	1.44	1.33
23	a	605	PHO	O2A-CGA	3.94	1.44	1.33
29	D	406	LMG	O7-C10	3.94	1.45	1.34
29	B	620	LMG	O7-C10	3.94	1.45	1.34
31	C	518	DGD	O1G-C1A	3.94	1.44	1.33
22	B	607	CLA	C3D-C2D	3.93	1.46	1.39
33	F	101	HEM	C3B-C2B	-3.93	1.34	1.40
29	d	406	LMG	O7-C10	3.93	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	518	DGD	O1G-C1A	3.93	1.44	1.33
23	A	605	PHO	O2A-CGA	3.92	1.44	1.33
22	b	609	CLA	O2A-CGA	3.92	1.44	1.33
32	D	409	LHG	O7-C7	3.92	1.45	1.34
32	d	409	LHG	O7-C7	3.92	1.45	1.34
22	B	609	CLA	O2A-CGA	3.91	1.44	1.33
31	c	516	DGD	O1G-C1A	3.91	1.44	1.33
33	v	201	HEM	C3B-C2B	-3.91	1.34	1.40
33	V	201	HEM	C3C-CAC	3.90	1.55	1.47
22	C	503	CLA	C3D-C2D	3.89	1.46	1.39
33	v	201	HEM	C3C-CAC	3.89	1.55	1.47
22	b	607	CLA	C3D-C2D	3.89	1.46	1.39
22	b	612	CLA	C3D-C2D	3.88	1.46	1.39
31	C	516	DGD	O1G-C1A	3.88	1.44	1.33
22	c	505	CLA	O2A-CGA	3.88	1.44	1.33
22	B	611	CLA	O2A-CGA	3.87	1.44	1.33
31	H	102	DGD	O2G-C1B	3.87	1.45	1.34
22	B	612	CLA	C3D-C2D	3.87	1.46	1.39
31	h	102	DGD	O2G-C1B	3.87	1.45	1.34
33	V	201	HEM	C3B-C2B	-3.86	1.35	1.40
22	C	505	CLA	O2A-CGA	3.85	1.44	1.33
22	c	503	CLA	C3D-C2D	3.85	1.46	1.39
22	b	611	CLA	O2A-CGA	3.85	1.44	1.33
22	a	604	CLA	O2A-CGA	3.83	1.44	1.33
22	c	503	CLA	OBD-CAD	3.83	1.27	1.22
32	l	103	LHG	O7-C7	3.82	1.45	1.34
22	C	503	CLA	OBD-CAD	3.82	1.27	1.22
32	L	102	LHG	O7-C7	3.82	1.45	1.34
22	B	605	CLA	O2A-CGA	3.80	1.44	1.33
33	f	101	HEM	C3B-CAB	3.79	1.55	1.47
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	B	602	CLA	C3D-C2D	3.78	1.46	1.39
22	A	604	CLA	O2A-CGA	3.78	1.44	1.33
32	D	407	LHG	O7-C7	3.78	1.45	1.34
22	b	605	CLA	OBD-CAD	3.77	1.27	1.22
22	b	602	CLA	C3D-C2D	3.77	1.46	1.39
33	F	101	HEM	C3B-CAB	3.77	1.55	1.47
31	c	517	DGD	O2G-C1B	3.75	1.44	1.34
22	b	606	CLA	O2A-CGA	3.74	1.44	1.33
23	A	606	PHO	O2A-CGA	3.74	1.44	1.33
31	C	517	DGD	O2G-C1B	3.73	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	606	PHO	O2A-CGA	3.73	1.44	1.33
22	B	606	CLA	O2A-CGA	3.72	1.44	1.33
22	B	614	CLA	O2A-CGA	3.72	1.44	1.33
22	B	605	CLA	OBD-CAD	3.72	1.27	1.22
22	B	613	CLA	O2A-CGA	3.71	1.44	1.33
23	A	605	PHO	CHD-C1D	3.71	1.45	1.38
23	a	605	PHO	CHD-C1D	3.71	1.45	1.38
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	613	CLA	O2A-CGA	3.70	1.44	1.33
22	d	401	CLA	C3D-C2D	3.69	1.46	1.39
22	D	401	CLA	C3D-C2D	3.69	1.46	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
23	A	606	PHO	OBD-CAD	3.66	1.28	1.22
22	b	605	CLA	C3D-C2D	3.66	1.46	1.39
22	B	605	CLA	C3D-C2D	3.66	1.46	1.39
23	a	606	PHO	OBD-CAD	3.63	1.28	1.22
33	F	101	HEM	C3C-CAC	3.62	1.55	1.47
33	f	101	HEM	C3C-CAC	3.59	1.55	1.47
22	C	512	CLA	MG-NC	3.59	2.14	2.06
22	c	512	CLA	MG-NC	3.58	2.14	2.06
22	A	603	CLA	O2A-CGA	3.54	1.43	1.33
22	a	603	CLA	O2A-CGA	3.52	1.43	1.33
22	b	602	CLA	C1D-C2D	3.51	1.50	1.42
22	B	602	CLA	C1D-C2D	3.51	1.50	1.42
22	b	612	CLA	MG-NC	3.50	2.14	2.06
22	B	612	CLA	MG-NC	3.49	2.14	2.06
22	B	612	CLA	O2A-CGA	3.47	1.43	1.33
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	603	CLA	O2A-CGA	3.45	1.43	1.33
22	b	607	CLA	C1D-C2D	3.43	1.50	1.42
22	C	505	CLA	MG-NC	3.42	2.14	2.06
22	B	607	CLA	C1D-C2D	3.42	1.50	1.42
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	603	CLA	C1D-C2D	3.39	1.50	1.42
31	C	518	DGD	O2G-C1B	3.37	1.43	1.34
22	C	501	CLA	C1D-C2D	3.36	1.50	1.42
22	c	501	CLA	C1D-C2D	3.35	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	C1D-C2D	3.34	1.50	1.42
23	a	606	PHO	CHC-C4B	3.34	1.48	1.40
22	C	513	CLA	C1D-C2D	3.32	1.50	1.42
22	c	513	CLA	C1D-C2D	3.32	1.50	1.42
22	B	614	CLA	MG-NC	3.32	2.14	2.06
22	b	608	CLA	O2A-CGA	3.31	1.43	1.33
23	A	606	PHO	CHC-C4B	3.30	1.48	1.40
22	B	608	CLA	O2A-CGA	3.30	1.43	1.33
22	C	506	CLA	MG-NC	3.29	2.14	2.06
22	c	506	CLA	MG-NC	3.28	2.14	2.06
22	b	614	CLA	MG-NC	3.28	2.14	2.06
22	C	503	CLA	C1D-C2D	3.28	1.50	1.42
22	c	506	CLA	C1D-C2D	3.27	1.50	1.42
22	C	506	CLA	C1D-C2D	3.26	1.50	1.42
22	c	503	CLA	C1D-C2D	3.24	1.49	1.42
22	A	604	CLA	C1D-C2D	3.23	1.49	1.42
22	D	402	CLA	C1D-C2D	3.22	1.49	1.42
22	c	510	CLA	C1D-C2D	3.22	1.49	1.42
22	a	604	CLA	C1D-C2D	3.21	1.49	1.42
22	C	504	CLA	C1D-C2D	3.21	1.49	1.42
22	b	610	CLA	C1D-C2D	3.20	1.49	1.42
22	c	504	CLA	C1D-C2D	3.19	1.49	1.42
22	d	402	CLA	C1D-C2D	3.18	1.49	1.42
22	B	608	CLA	C1D-C2D	3.18	1.49	1.42
22	b	608	CLA	C1D-C2D	3.17	1.49	1.42
32	D	405	LHG	O7-C7	3.17	1.43	1.34
22	C	510	CLA	C1D-C2D	3.17	1.49	1.42
22	C	509	CLA	C1D-C2D	3.17	1.49	1.42
22	D	403	CLA	C1B-CHB	3.16	1.49	1.41
22	B	610	CLA	C1D-C2D	3.15	1.49	1.42
32	d	405	LHG	O7-C7	3.15	1.43	1.34
22	A	603	CLA	MG-NC	3.14	2.13	2.06
22	d	403	CLA	C1B-CHB	3.14	1.49	1.41
22	B	608	CLA	C1B-CHB	3.13	1.49	1.41
22	c	509	CLA	C1D-C2D	3.13	1.49	1.42
22	C	507	CLA	C1D-C2D	3.12	1.49	1.42
22	c	507	CLA	C1D-C2D	3.12	1.49	1.42
22	b	608	CLA	C1B-CHB	3.12	1.49	1.41
22	c	506	CLA	C1B-CHB	3.11	1.49	1.41
22	a	603	CLA	MG-NC	3.10	2.13	2.06
22	b	615	CLA	C1D-C2D	3.10	1.49	1.42
22	B	606	CLA	C1B-CHB	3.10	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	C1B-CHB	3.10	1.49	1.41
22	B	605	CLA	C1D-C2D	3.09	1.49	1.42
22	c	510	CLA	C1B-CHB	3.09	1.49	1.41
22	b	605	CLA	C1D-C2D	3.09	1.49	1.42
22	C	510	CLA	C1B-CHB	3.08	1.49	1.41
22	C	506	CLA	C1B-CHB	3.08	1.49	1.41
22	b	606	CLA	C1B-CHB	3.08	1.49	1.41
22	B	604	CLA	MG-NC	3.08	2.13	2.06
22	B	603	CLA	C1B-CHB	3.08	1.49	1.41
22	c	508	CLA	C1D-C2D	3.07	1.49	1.42
22	B	614	CLA	C1B-CHB	3.07	1.49	1.41
22	C	511	CLA	C1B-CHB	3.07	1.49	1.41
22	b	603	CLA	C1B-CHB	3.07	1.49	1.41
22	b	604	CLA	MG-NC	3.06	2.13	2.06
22	b	616	CLA	C1D-C2D	3.06	1.49	1.42
22	c	511	CLA	C1B-CHB	3.06	1.49	1.41
22	B	615	CLA	C1D-C2D	3.06	1.49	1.42
22	c	513	CLA	C1B-CHB	3.05	1.49	1.41
22	C	508	CLA	C1D-C2D	3.04	1.49	1.42
22	C	512	CLA	C1D-C2D	3.04	1.49	1.42
22	C	513	CLA	C1B-CHB	3.04	1.49	1.41
22	c	512	CLA	C1B-CHB	3.04	1.49	1.41
22	B	616	CLA	C1D-C2D	3.04	1.49	1.42
22	c	512	CLA	C1D-C2D	3.04	1.49	1.42
22	B	615	CLA	C1B-CHB	3.04	1.49	1.41
22	c	504	CLA	C1B-CHB	3.02	1.49	1.41
22	C	505	CLA	C1B-CHB	3.02	1.49	1.41
22	C	512	CLA	C1B-CHB	3.02	1.49	1.41
23	a	605	PHO	CHD-C4C	3.02	1.47	1.40
22	B	602	CLA	C4B-CHC	3.02	1.49	1.41
22	A	607	CLA	C1B-CHB	3.02	1.49	1.41
22	b	615	CLA	C1B-CHB	3.02	1.49	1.41
22	b	613	CLA	C1D-C2D	3.02	1.49	1.42
22	b	607	CLA	C1B-CHB	3.02	1.49	1.41
22	B	613	CLA	C1D-C2D	3.01	1.49	1.42
22	c	508	CLA	C1B-CHB	3.01	1.49	1.41
22	C	504	CLA	C1B-CHB	3.01	1.49	1.41
22	B	604	CLA	C1D-C2D	3.01	1.49	1.42
22	C	508	CLA	C1B-CHB	3.01	1.49	1.41
22	c	507	CLA	C1B-CHB	3.01	1.49	1.41
22	a	607	CLA	C1B-CHB	3.00	1.49	1.41
22	B	612	CLA	C1D-C2D	3.00	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	C1B-CHB	3.00	1.49	1.41
22	b	602	CLA	C4B-CHC	3.00	1.49	1.41
22	b	604	CLA	C1D-C2D	2.99	1.49	1.42
22	B	607	CLA	C1B-CHB	2.99	1.49	1.41
23	A	605	PHO	CHD-C4C	2.99	1.47	1.40
22	b	612	CLA	C1D-C2D	2.98	1.49	1.42
22	c	505	CLA	C1B-CHB	2.98	1.49	1.41
22	C	505	CLA	C1D-C2D	2.97	1.49	1.42
22	D	403	CLA	C1D-C2D	2.96	1.49	1.42
22	b	617	CLA	C1D-C2D	2.95	1.49	1.42
22	c	505	CLA	C1D-C2D	2.95	1.49	1.42
22	d	403	CLA	C1D-C2D	2.94	1.49	1.42
23	a	605	PHO	OBD-CAD	2.94	1.27	1.22
22	B	605	CLA	C1B-CHB	2.94	1.49	1.41
22	b	611	CLA	C1D-C2D	2.94	1.49	1.42
23	A	605	PHO	OBD-CAD	2.93	1.27	1.22
22	b	604	CLA	C1B-CHB	2.93	1.49	1.41
22	C	511	CLA	C1D-C2D	2.92	1.49	1.42
22	c	502	CLA	C1D-C2D	2.92	1.49	1.42
22	B	611	CLA	C1D-C2D	2.92	1.49	1.42
22	C	502	CLA	C1D-C2D	2.91	1.49	1.42
22	B	617	CLA	C1D-C2D	2.91	1.49	1.42
22	b	605	CLA	C1B-CHB	2.91	1.49	1.41
22	A	603	CLA	C1D-C2D	2.91	1.49	1.42
22	B	604	CLA	C1B-CHB	2.91	1.49	1.41
22	c	511	CLA	C1D-C2D	2.89	1.49	1.42
22	B	610	CLA	C1B-CHB	2.88	1.49	1.41
22	b	613	CLA	C1B-CHB	2.87	1.49	1.41
22	C	513	CLA	C4B-CHC	2.87	1.49	1.41
22	b	610	CLA	C1B-CHB	2.87	1.49	1.41
22	c	513	CLA	C4B-CHC	2.87	1.49	1.41
22	B	614	CLA	C1D-C2D	2.86	1.49	1.42
22	b	614	CLA	C1D-C2D	2.86	1.49	1.42
22	B	613	CLA	C1B-CHB	2.86	1.48	1.41
23	A	606	PHO	C3D-C4D	-2.85	1.34	1.43
22	a	603	CLA	C1D-C2D	2.85	1.49	1.42
23	a	606	PHO	CHD-C4C	2.84	1.47	1.40
23	A	606	PHO	C3D-C2D	2.84	1.46	1.39
23	a	605	PHO	CHC-C4B	2.84	1.47	1.40
23	A	606	PHO	CHD-C4C	2.83	1.47	1.40
22	c	501	CLA	C1B-CHB	2.82	1.48	1.41
22	C	503	CLA	C4B-CHC	2.82	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	605	PHO	CHC-C4B	2.82	1.47	1.40
23	a	606	PHO	C3D-C2D	2.82	1.46	1.39
23	a	606	PHO	C3D-C4D	-2.82	1.34	1.43
22	c	503	CLA	C4B-CHC	2.81	1.48	1.41
22	C	507	CLA	MG-NC	2.81	2.12	2.06
22	c	507	CLA	MG-NC	2.80	2.12	2.06
22	C	503	CLA	C1C-C2C	2.80	1.50	1.44
22	C	501	CLA	C1B-CHB	2.80	1.48	1.41
22	b	616	CLA	C1B-CHB	2.79	1.48	1.41
22	b	606	CLA	C1D-C2D	2.79	1.48	1.42
22	B	616	CLA	C1B-CHB	2.79	1.48	1.41
22	B	606	CLA	C1D-C2D	2.78	1.48	1.42
22	c	505	CLA	C4B-CHC	2.78	1.48	1.41
25	A	609	SQD	C6-S	-2.77	1.67	1.77
22	c	504	CLA	CHD-C4C	2.77	1.49	1.41
22	c	503	CLA	C1C-C2C	2.77	1.49	1.44
25	a	609	SQD	C6-S	-2.77	1.67	1.77
22	a	603	CLA	C1B-CHB	2.77	1.48	1.41
22	C	505	CLA	C4B-CHC	2.77	1.48	1.41
22	C	502	CLA	C1B-CHB	2.76	1.48	1.41
22	A	603	CLA	C1B-CHB	2.76	1.48	1.41
22	B	617	CLA	C1B-CHB	2.76	1.48	1.41
22	C	503	CLA	C1B-CHB	2.76	1.48	1.41
22	C	501	CLA	C4B-CHC	2.76	1.48	1.41
22	c	502	CLA	C1B-CHB	2.76	1.48	1.41
22	b	617	CLA	C1B-CHB	2.76	1.48	1.41
22	b	603	CLA	C4B-CHC	2.76	1.48	1.41
22	B	603	CLA	C4B-CHC	2.76	1.48	1.41
22	B	611	CLA	C1B-CHB	2.76	1.48	1.41
22	b	611	CLA	C1B-CHB	2.75	1.48	1.41
23	a	605	PHO	C3D-C4D	-2.75	1.34	1.43
22	c	503	CLA	C1B-CHB	2.74	1.48	1.41
28	A	613	PL9	C6-C5	2.74	1.49	1.35
23	A	605	PHO	C3D-C4D	-2.73	1.35	1.43
28	a	613	PL9	C6-C5	2.73	1.49	1.35
22	C	504	CLA	CHD-C4C	2.73	1.48	1.41
22	B	615	CLA	C1C-NC	-2.72	1.33	1.37
22	c	501	CLA	C4B-CHC	2.72	1.48	1.41
22	c	509	CLA	C1B-CHB	2.72	1.48	1.41
22	C	509	CLA	C1B-CHB	2.72	1.48	1.41
22	c	507	CLA	C4B-CHC	2.71	1.48	1.41
22	C	507	CLA	C4B-CHC	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	C1B-CHB	2.70	1.48	1.41
25	b	601	SQD	C6-S	-2.70	1.67	1.77
22	b	602	CLA	C1C-C2C	2.70	1.49	1.44
22	B	602	CLA	C1C-C2C	2.69	1.49	1.44
22	a	607	CLA	C4B-CHC	2.69	1.48	1.41
22	b	615	CLA	C1C-NC	-2.68	1.33	1.37
22	b	602	CLA	C1B-CHB	2.68	1.48	1.41
28	d	408	PL9	C6-C5	2.68	1.49	1.35
28	D	408	PL9	C6-C5	2.68	1.49	1.35
29	z	101	LMG	O8-C28	2.68	1.46	1.33
25	B	601	SQD	C6-S	-2.68	1.67	1.77
22	A	607	CLA	C4B-CHC	2.67	1.48	1.41
29	Z	101	LMG	O8-C28	2.67	1.46	1.33
22	c	507	CLA	C1C-C2C	2.66	1.49	1.44
31	H	102	DGD	O5D-C1E	2.66	1.44	1.40
25	d	411	SQD	C6-S	-2.65	1.67	1.77
22	b	611	CLA	C4B-CHC	2.65	1.48	1.41
25	D	411	SQD	C6-S	-2.64	1.67	1.77
31	h	102	DGD	O5D-C1E	2.63	1.44	1.40
22	B	612	CLA	C1B-CHB	2.63	1.48	1.41
22	c	506	CLA	C4B-CHC	2.63	1.48	1.41
22	C	512	CLA	C4B-CHC	2.62	1.48	1.41
22	b	612	CLA	C1B-CHB	2.62	1.48	1.41
22	b	607	CLA	C4B-CHC	2.62	1.48	1.41
22	C	506	CLA	C4B-CHC	2.62	1.48	1.41
22	C	507	CLA	C1C-C2C	2.62	1.49	1.44
22	a	607	CLA	C1D-C2D	2.62	1.48	1.42
22	c	501	CLA	CHD-C4C	2.62	1.48	1.41
22	B	611	CLA	C4B-CHC	2.62	1.48	1.41
22	C	512	CLA	CHD-C4C	2.61	1.48	1.41
22	a	603	CLA	C4B-CHC	2.61	1.48	1.41
22	A	607	CLA	C1D-C2D	2.61	1.48	1.42
22	d	403	CLA	C4B-CHC	2.61	1.48	1.41
22	c	512	CLA	CHD-C4C	2.61	1.48	1.41
22	B	607	CLA	C4B-CHC	2.61	1.48	1.41
24	k	102	BCR	C24-C25	-2.61	1.35	1.45
22	b	613	CLA	C4B-CHC	2.60	1.48	1.41
24	c	515	BCR	C24-C25	-2.60	1.35	1.45
22	c	512	CLA	C4B-CHC	2.60	1.48	1.41
24	K	102	BCR	C24-C25	-2.60	1.35	1.45
22	D	403	CLA	C4B-CHC	2.60	1.48	1.41
22	A	603	CLA	C4B-CHC	2.60	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	CLA	CHD-C4C	2.59	1.48	1.41
22	B	613	CLA	C4B-CHC	2.59	1.48	1.41
22	C	508	CLA	C4B-CHC	2.59	1.48	1.41
22	c	508	CLA	C4B-CHC	2.59	1.48	1.41
24	C	515	BCR	C24-C25	-2.57	1.36	1.45
24	c	514	BCR	C24-C25	-2.57	1.36	1.45
24	h	101	BCR	C24-C25	-2.57	1.36	1.45
24	H	101	BCR	C24-C25	-2.56	1.36	1.45
24	C	514	BCR	C24-C25	-2.56	1.36	1.45
22	b	609	CLA	C1B-CHB	2.56	1.48	1.41
23	a	605	PHO	C3D-C2D	2.55	1.46	1.39
22	c	513	CLA	C1C-C2C	2.55	1.49	1.44
22	C	512	CLA	C1C-C2C	2.55	1.49	1.44
22	B	609	CLA	C1B-CHB	2.55	1.48	1.41
22	B	609	CLA	C1D-C2D	2.54	1.48	1.42
24	k	101	BCR	C24-C25	-2.54	1.36	1.45
25	l	102	SQD	C6-S	-2.54	1.68	1.77
24	K	101	BCR	C24-C25	-2.54	1.36	1.45
22	b	609	CLA	C1D-C2D	2.53	1.48	1.42
22	D	401	CLA	C4B-CHC	2.53	1.48	1.41
22	d	401	CLA	C4B-CHC	2.53	1.48	1.41
22	B	613	CLA	CHD-C4C	2.53	1.48	1.41
22	B	610	CLA	C4B-CHC	2.53	1.48	1.41
25	b	621	SQD	C6-S	-2.52	1.68	1.77
22	B	617	CLA	C4B-CHC	2.52	1.48	1.41
22	b	608	CLA	CHD-C4C	2.52	1.48	1.41
22	C	511	CLA	C4B-CHC	2.52	1.48	1.41
22	c	512	CLA	C1C-C2C	2.52	1.49	1.44
24	t	101	BCR	C24-C25	-2.52	1.36	1.45
23	A	605	PHO	C3D-C2D	2.52	1.46	1.39
22	C	513	CLA	C1C-C2C	2.52	1.49	1.44
22	b	614	CLA	C4B-CHC	2.52	1.48	1.41
22	B	614	CLA	C4B-CHC	2.51	1.48	1.41
22	b	613	CLA	CHD-C4C	2.51	1.48	1.41
22	b	610	CLA	C4B-CHC	2.51	1.48	1.41
22	C	502	CLA	C4B-CHC	2.51	1.48	1.41
24	B	618	BCR	C24-C25	-2.50	1.36	1.45
24	T	101	BCR	C24-C25	-2.50	1.36	1.45
22	B	608	CLA	CHD-C4C	2.50	1.48	1.41
22	C	506	CLA	CHD-C4C	2.50	1.48	1.41
22	d	401	CLA	C1B-CHB	2.50	1.47	1.41
22	c	511	CLA	C4B-CHC	2.49	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	102	BCR	C24-C25	-2.49	1.36	1.45
22	c	502	CLA	C4B-CHC	2.48	1.47	1.41
22	D	401	CLA	C1B-CHB	2.48	1.47	1.41
24	D	404	BCR	C24-C25	-2.47	1.36	1.45
22	b	617	CLA	C4B-CHC	2.47	1.47	1.41
22	C	505	CLA	CHD-C4C	2.47	1.48	1.41
22	B	603	CLA	CHD-C4C	2.47	1.48	1.41
22	c	503	CLA	CHD-C4C	2.47	1.48	1.41
22	B	602	CLA	CHD-C4C	2.47	1.48	1.41
22	c	507	CLA	CHD-C4C	2.47	1.48	1.41
24	d	404	BCR	C24-C25	-2.47	1.36	1.45
22	B	606	CLA	C4B-CHC	2.47	1.47	1.41
22	c	506	CLA	CHD-C4C	2.46	1.48	1.41
22	d	402	CLA	C4B-CHC	2.46	1.47	1.41
22	c	505	CLA	CHD-C4C	2.46	1.48	1.41
22	d	403	CLA	CHD-C4C	2.46	1.48	1.41
22	b	607	CLA	CHD-C4C	2.46	1.48	1.41
22	b	606	CLA	C4B-CHC	2.46	1.47	1.41
22	b	603	CLA	CHD-C4C	2.46	1.48	1.41
22	b	602	CLA	CHD-C4C	2.46	1.48	1.41
22	B	616	CLA	CHD-C4C	2.46	1.48	1.41
22	C	503	CLA	CHD-C4C	2.46	1.48	1.41
22	b	612	CLA	C4B-CHC	2.45	1.47	1.41
22	D	402	CLA	C4B-CHC	2.45	1.47	1.41
25	L	101	SQD	C6-S	-2.45	1.68	1.77
22	C	507	CLA	CHD-C4C	2.44	1.48	1.41
25	l	101	SQD	C6-S	-2.44	1.68	1.77
24	a	608	BCR	C24-C25	-2.44	1.36	1.45
24	A	608	BCR	C24-C25	-2.44	1.36	1.45
22	B	607	CLA	CHD-C4C	2.44	1.48	1.41
22	c	511	CLA	CHD-C4C	2.44	1.48	1.41
22	a	604	CLA	C1B-CHB	2.44	1.47	1.41
22	D	403	CLA	CHD-C4C	2.43	1.48	1.41
22	b	616	CLA	CHD-C4C	2.43	1.48	1.41
22	D	401	CLA	C1D-C2D	2.43	1.48	1.42
22	C	511	CLA	CHD-C4C	2.42	1.48	1.41
22	B	612	CLA	C4B-CHC	2.42	1.47	1.41
24	b	622	BCR	C24-C25	-2.42	1.36	1.45
22	B	616	CLA	C4B-CHC	2.42	1.47	1.41
22	d	402	CLA	C1B-CHB	2.42	1.47	1.41
22	b	616	CLA	C4B-CHC	2.42	1.47	1.41
22	c	513	CLA	CHD-C4C	2.41	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	CHD-C4C	2.41	1.48	1.41
22	C	513	CLA	CHD-C4C	2.41	1.48	1.41
22	D	402	CLA	C1B-CHB	2.41	1.47	1.41
22	A	604	CLA	C1B-CHB	2.41	1.47	1.41
22	c	509	CLA	C4B-CHC	2.39	1.47	1.41
22	A	603	CLA	CHD-C4C	2.39	1.48	1.41
22	c	510	CLA	CHD-C4C	2.39	1.48	1.41
22	c	501	CLA	C1C-C2C	2.38	1.49	1.44
24	B	622	BCR	C24-C25	-2.38	1.36	1.45
22	d	401	CLA	C1D-C2D	2.38	1.48	1.42
23	A	606	PHO	C3B-C4B	2.38	1.48	1.43
22	C	509	CLA	C4B-CHC	2.38	1.47	1.41
22	c	509	CLA	CHD-C4C	2.37	1.47	1.41
22	a	603	CLA	CHD-C4C	2.36	1.47	1.41
22	C	501	CLA	C1C-C2C	2.36	1.49	1.44
23	a	606	PHO	C3B-C4B	2.36	1.48	1.43
22	b	604	CLA	C4B-CHC	2.36	1.47	1.41
22	b	614	CLA	CHD-C4C	2.36	1.47	1.41
22	B	604	CLA	C4B-CHC	2.35	1.47	1.41
22	c	510	CLA	C4B-CHC	2.35	1.47	1.41
22	C	508	CLA	CHD-C4C	2.35	1.47	1.41
22	c	508	CLA	CHD-C4C	2.34	1.47	1.41
22	B	614	CLA	CHD-C4C	2.33	1.47	1.41
22	C	510	CLA	C4B-CHC	2.33	1.47	1.41
22	C	505	CLA	C1C-C2C	2.33	1.49	1.44
22	C	506	CLA	C1C-C2C	2.33	1.49	1.44
22	d	403	CLA	C1C-C2C	2.32	1.49	1.44
22	C	509	CLA	CHD-C4C	2.32	1.47	1.41
22	c	506	CLA	C1C-C2C	2.32	1.49	1.44
22	D	403	CLA	C1C-C2C	2.32	1.49	1.44
22	B	609	CLA	CHD-C4C	2.31	1.47	1.41
24	b	618	BCR	C24-C25	-2.31	1.36	1.45
22	c	505	CLA	C1C-C2C	2.31	1.49	1.44
22	C	508	CLA	C4C-C3C	2.31	1.49	1.45
22	B	605	CLA	CHD-C4C	2.31	1.47	1.41
22	A	604	CLA	CHD-C4C	2.31	1.47	1.41
24	B	619	BCR	C24-C25	-2.30	1.37	1.45
22	B	603	CLA	C1C-C2C	2.30	1.49	1.44
22	B	607	CLA	C1C-C2C	2.30	1.49	1.44
22	B	608	CLA	C4B-CHC	2.29	1.47	1.41
22	c	508	CLA	C4C-C3C	2.29	1.49	1.45
22	b	607	CLA	C1C-C2C	2.29	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	604	CLA	CHD-C4C	2.29	1.47	1.41
22	b	608	CLA	C4B-CHC	2.29	1.47	1.41
22	b	609	CLA	CHD-C4C	2.29	1.47	1.41
22	C	510	CLA	MG-NC	2.29	2.11	2.06
22	B	614	CLA	C1C-C2C	2.29	1.49	1.44
22	b	614	CLA	C1C-C2C	2.29	1.49	1.44
22	b	605	CLA	CHD-C4C	2.28	1.47	1.41
22	c	504	CLA	C4B-CHC	2.27	1.47	1.41
22	b	611	CLA	CHD-C4C	2.27	1.47	1.41
22	B	611	CLA	CHD-C4C	2.26	1.47	1.41
28	a	613	PL9	C2-C3	2.26	1.40	1.34
22	C	510	CLA	C1C-C2C	2.26	1.48	1.44
22	B	615	CLA	C4B-CHC	2.26	1.47	1.41
22	b	603	CLA	C1C-C2C	2.25	1.48	1.44
22	c	510	CLA	C1C-C2C	2.25	1.48	1.44
22	a	607	CLA	CHD-C4C	2.24	1.47	1.41
29	Z	101	LMG	O1-C1	2.24	1.44	1.40
22	C	504	CLA	C4B-CHC	2.24	1.47	1.41
22	b	615	CLA	C4B-CHC	2.24	1.47	1.41
22	b	615	CLA	CHD-C4C	2.24	1.47	1.41
22	A	607	CLA	CHD-C4C	2.23	1.47	1.41
22	B	611	CLA	C1C-NC	-2.23	1.34	1.37
22	c	510	CLA	MG-NC	2.23	2.11	2.06
22	B	615	CLA	CHD-C4C	2.23	1.47	1.41
22	b	604	CLA	C1C-NC	-2.23	1.34	1.37
28	A	613	PL9	C2-C3	2.23	1.40	1.34
29	z	101	LMG	O1-C1	2.22	1.44	1.40
31	d	410	DGD	O5D-C1E	2.22	1.44	1.40
22	C	511	CLA	C1C-C2C	2.21	1.48	1.44
22	B	616	CLA	C1C-C2C	2.21	1.48	1.44
22	b	616	CLA	C1C-C2C	2.20	1.48	1.44
22	b	611	CLA	C1C-NC	-2.20	1.34	1.37
22	b	605	CLA	C4B-CHC	2.19	1.47	1.41
22	C	512	CLA	C4C-C3C	2.19	1.48	1.45
22	c	512	CLA	C4C-C3C	2.19	1.48	1.45
22	B	605	CLA	C4B-CHC	2.19	1.47	1.41
22	c	511	CLA	C1C-C2C	2.19	1.48	1.44
22	b	604	CLA	CHD-C4C	2.19	1.47	1.41
22	B	604	CLA	C1C-NC	-2.18	1.34	1.37
22	c	505	CLA	C4C-C3C	2.17	1.48	1.45
22	c	509	CLA	C4C-C3C	2.17	1.48	1.45
29	c	520	LMG	O1-C1	2.17	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	C4C-C3C	2.17	1.48	1.45
22	C	509	CLA	C4C-C3C	2.16	1.48	1.45
31	D	410	DGD	O5D-C1E	2.16	1.43	1.40
22	B	604	CLA	C1C-C2C	2.16	1.48	1.44
22	B	604	CLA	CHD-C4C	2.15	1.47	1.41
22	D	403	CLA	C4C-C3C	2.15	1.48	1.45
22	B	617	CLA	CHD-C4C	2.15	1.47	1.41
25	l	101	SQD	O6-C1	2.15	1.43	1.40
22	b	617	CLA	CHD-C4C	2.14	1.47	1.41
22	b	605	CLA	MG-NC	2.14	2.11	2.06
31	d	410	DGD	O3G-C1D	2.14	1.43	1.40
29	C	520	LMG	O1-C1	2.13	1.43	1.40
22	B	605	CLA	MG-NC	2.13	2.11	2.06
22	c	508	CLA	C1C-C2C	2.13	1.48	1.44
22	D	401	CLA	C4C-C3C	2.12	1.48	1.45
25	l	102	SQD	O6-C1	2.12	1.43	1.40
22	d	401	CLA	CHD-C4C	2.12	1.47	1.41
22	C	508	CLA	C1C-C2C	2.12	1.48	1.44
22	B	610	CLA	CHD-C4C	2.12	1.47	1.41
22	b	604	CLA	C1C-C2C	2.12	1.48	1.44
22	d	403	CLA	C1C-NC	-2.12	1.34	1.37
22	c	502	CLA	CHD-C4C	2.11	1.47	1.41
22	C	502	CLA	CHD-C4C	2.11	1.47	1.41
22	B	612	CLA	CHD-C4C	2.11	1.47	1.41
22	C	505	CLA	C4C-C3C	2.11	1.48	1.45
22	b	609	CLA	C4B-CHC	2.11	1.46	1.41
25	b	621	SQD	O6-C1	2.10	1.43	1.40
22	D	401	CLA	CHD-C4C	2.10	1.47	1.41
22	B	609	CLA	C4B-CHC	2.09	1.46	1.41
31	C	518	DGD	O2G-C2G	-2.09	1.41	1.46
22	A	604	CLA	C4B-CHC	2.09	1.46	1.41
25	L	101	SQD	O6-C1	2.09	1.43	1.40
31	c	518	DGD	O2G-C2G	-2.09	1.41	1.46
22	d	401	CLA	C4C-C3C	2.08	1.48	1.45
23	a	606	PHO	CHB-C4A	-2.08	1.34	1.40
23	A	606	PHO	CHB-C4A	-2.08	1.34	1.40
22	a	604	CLA	C4B-CHC	2.08	1.46	1.41
22	B	615	CLA	C1C-C2C	2.08	1.48	1.44
22	b	612	CLA	CHD-C4C	2.08	1.47	1.41
22	b	610	CLA	CHD-C4C	2.08	1.47	1.41
22	B	613	CLA	C1C-C2C	2.07	1.48	1.44
22	D	403	CLA	C1C-NC	-2.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	410	DGD	O3G-C1D	2.07	1.43	1.40
24	c	514	BCR	C8-C7	-2.06	1.26	1.33
22	b	613	CLA	C1C-C2C	2.05	1.48	1.44
22	d	402	CLA	CHD-C4C	2.05	1.47	1.41
22	d	401	CLA	C1C-C2C	2.05	1.48	1.44
22	D	402	CLA	CHD-C4C	2.05	1.47	1.41
24	C	514	BCR	C8-C7	-2.04	1.26	1.33
22	B	616	CLA	C4C-C3C	2.04	1.48	1.45
22	b	615	CLA	C1C-C2C	2.04	1.48	1.44
22	b	606	CLA	C1C-C2C	2.04	1.48	1.44
22	b	614	CLA	C1C-NC	-2.04	1.34	1.37
22	B	614	CLA	C1C-NC	-2.04	1.34	1.37
22	b	616	CLA	C4C-C3C	2.03	1.48	1.45
22	B	605	CLA	C1C-C2C	2.03	1.48	1.44
22	D	401	CLA	C1C-C2C	2.03	1.48	1.44
33	v	201	HEM	CMA-C3A	2.03	1.55	1.51
22	B	602	CLA	C4C-C3C	2.03	1.48	1.45
22	C	502	CLA	C1C-C2C	2.03	1.48	1.44
22	c	502	CLA	C1C-C2C	2.03	1.48	1.44
31	c	516	DGD	O5D-C1E	2.02	1.43	1.40
22	B	606	CLA	CHD-C4C	2.02	1.46	1.41
33	f	101	HEM	CAA-C2A	2.02	1.55	1.52
22	C	502	CLA	C1C-NC	-2.01	1.34	1.37
33	V	201	HEM	CAA-C2A	2.01	1.55	1.52
22	b	605	CLA	C1C-C2C	2.01	1.48	1.44
33	F	101	HEM	CAA-C2A	2.01	1.55	1.52
22	b	610	CLA	C1C-NC	-2.01	1.34	1.37
22	B	610	CLA	C1C-NC	-2.01	1.34	1.37
25	D	411	SQD	O6-C1	2.01	1.43	1.40
33	v	201	HEM	CAA-C2A	2.00	1.55	1.52

All (2262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	BCR	C20-C21-C22	26.91	165.72	127.31
24	h	101	BCR	C20-C21-C22	26.91	165.71	127.31
24	c	514	BCR	C15-C16-C17	26.83	178.43	123.47
24	C	514	BCR	C15-C16-C17	26.78	178.33	123.47
24	T	102	BCR	C20-C21-C22	26.60	165.27	127.31
24	t	101	BCR	C20-C21-C22	26.58	165.24	127.31
24	C	515	BCR	C20-C21-C22	25.73	164.04	127.31
24	c	515	BCR	C20-C21-C22	25.67	163.95	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	101	BCR	C20-C21-C22	25.57	163.81	127.31
24	k	101	BCR	C20-C21-C22	25.55	163.77	127.31
24	t	101	BCR	C16-C17-C18	25.44	163.61	127.31
24	T	102	BCR	C16-C17-C18	25.43	163.60	127.31
24	t	101	BCR	C15-C16-C17	25.37	175.44	123.47
24	T	102	BCR	C15-C16-C17	25.35	175.40	123.47
24	h	101	BCR	C15-C16-C17	25.31	175.33	123.47
24	H	101	BCR	C15-C16-C17	25.31	175.32	123.47
24	a	608	BCR	C20-C21-C22	25.16	163.21	127.31
24	A	608	BCR	C20-C21-C22	25.15	163.21	127.31
24	c	514	BCR	C16-C17-C18	25.08	163.11	127.31
24	C	514	BCR	C16-C17-C18	25.06	163.08	127.31
24	T	101	BCR	C16-C17-C18	24.20	161.85	127.31
24	B	618	BCR	C16-C17-C18	24.19	161.83	127.31
24	C	515	BCR	C15-C16-C17	23.71	172.04	123.47
24	c	515	BCR	C15-C16-C17	23.67	171.97	123.47
24	k	101	BCR	C16-C17-C18	23.33	160.61	127.31
24	K	101	BCR	C16-C17-C18	23.32	160.59	127.31
24	D	404	BCR	C15-C16-C17	23.23	171.05	123.47
24	d	404	BCR	C15-C16-C17	23.21	171.02	123.47
24	C	514	BCR	C20-C21-C22	23.07	160.23	127.31
24	c	514	BCR	C20-C21-C22	23.05	160.21	127.31
24	d	404	BCR	C20-C21-C22	22.49	159.41	127.31
24	D	404	BCR	C20-C21-C22	22.47	159.38	127.31
24	k	102	BCR	C15-C16-C17	22.39	169.34	123.47
24	K	102	BCR	C15-C16-C17	22.36	169.28	123.47
24	d	404	BCR	C16-C17-C18	22.32	159.16	127.31
24	D	404	BCR	C16-C17-C18	22.31	159.15	127.31
24	b	618	BCR	C20-C21-C22	21.92	158.60	127.31
24	B	619	BCR	C20-C21-C22	21.92	158.59	127.31
24	C	515	BCR	C16-C15-C14	21.81	168.15	123.47
24	c	515	BCR	C16-C15-C14	21.79	168.10	123.47
24	A	608	BCR	C16-C17-C18	21.54	158.06	127.31
24	a	608	BCR	C16-C17-C18	21.52	158.03	127.31
24	B	622	BCR	C15-C16-C17	21.18	166.85	123.47
24	b	622	BCR	C15-C16-C17	21.14	166.79	123.47
24	K	102	BCR	C20-C21-C22	20.98	157.25	127.31
24	k	102	BCR	C20-C21-C22	20.93	157.18	127.31
24	c	514	BCR	C16-C15-C14	20.73	165.94	123.47
24	C	514	BCR	C16-C15-C14	20.71	165.91	123.47
24	K	101	BCR	C15-C16-C17	20.71	165.89	123.47
24	k	101	BCR	C15-C16-C17	20.70	165.89	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C16-C17-C18	20.63	156.75	127.31
24	b	618	BCR	C16-C17-C18	20.62	156.74	127.31
24	C	515	BCR	C16-C17-C18	20.61	156.73	127.31
24	c	515	BCR	C16-C17-C18	20.61	156.72	127.31
24	h	101	BCR	C16-C17-C18	20.53	156.61	127.31
24	H	101	BCR	C16-C17-C18	20.52	156.59	127.31
24	B	622	BCR	C16-C15-C14	20.36	165.18	123.47
24	b	622	BCR	C16-C15-C14	20.34	165.14	123.47
24	D	404	BCR	C16-C15-C14	20.18	164.82	123.47
24	d	404	BCR	C16-C15-C14	20.18	164.81	123.47
24	T	101	BCR	C15-C16-C17	19.72	163.86	123.47
24	B	618	BCR	C15-C16-C17	19.67	163.77	123.47
24	k	102	BCR	C16-C15-C14	19.23	162.86	123.47
24	K	102	BCR	C16-C15-C14	19.20	162.80	123.47
24	K	102	BCR	C16-C17-C18	18.73	154.04	127.31
24	k	102	BCR	C16-C17-C18	18.72	154.02	127.31
24	T	102	BCR	C16-C15-C14	18.41	161.18	123.47
24	t	101	BCR	C16-C15-C14	18.39	161.15	123.47
24	A	608	BCR	C15-C16-C17	18.14	160.63	123.47
24	a	608	BCR	C15-C16-C17	18.12	160.60	123.47
24	B	618	BCR	C20-C21-C22	18.05	153.07	127.31
24	T	101	BCR	C20-C21-C22	18.05	153.07	127.31
24	B	622	BCR	C16-C17-C18	17.24	151.91	127.31
24	b	622	BCR	C16-C17-C18	17.22	151.88	127.31
24	C	514	BCR	C21-C20-C19	16.94	176.07	123.22
24	c	514	BCR	C21-C20-C19	16.92	176.01	123.22
24	k	101	BCR	C16-C15-C14	16.56	157.39	123.47
24	K	101	BCR	C16-C15-C14	16.55	157.37	123.47
24	C	515	BCR	C21-C20-C19	16.29	174.06	123.22
24	c	515	BCR	C21-C20-C19	16.29	174.04	123.22
24	H	101	BCR	C16-C15-C14	16.11	156.47	123.47
24	h	101	BCR	C16-C15-C14	16.08	156.42	123.47
24	b	618	BCR	C15-C16-C17	16.04	156.33	123.47
24	B	619	BCR	C15-C16-C17	16.03	156.31	123.47
24	b	618	BCR	C16-C15-C14	15.86	155.97	123.47
24	B	619	BCR	C16-C15-C14	15.86	155.96	123.47
24	B	618	BCR	C19-C18-C17	15.48	142.69	118.94
24	T	101	BCR	C19-C18-C17	15.46	142.66	118.94
24	h	101	BCR	C21-C20-C19	14.97	169.92	123.22
24	H	101	BCR	C21-C20-C19	14.97	169.92	123.22
24	a	608	BCR	C16-C15-C14	14.62	153.43	123.47
24	K	101	BCR	C21-C20-C19	14.62	168.84	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	101	BCR	C21-C20-C19	14.62	168.83	123.22
24	A	608	BCR	C16-C15-C14	14.62	153.41	123.47
24	b	618	BCR	C21-C20-C19	14.61	168.82	123.22
24	B	619	BCR	C21-C20-C19	14.60	168.76	123.22
24	c	515	BCR	C11-C10-C9	14.47	147.97	127.31
24	C	515	BCR	C11-C10-C9	14.47	147.96	127.31
24	b	618	BCR	C19-C18-C17	14.37	141.00	118.94
24	B	619	BCR	C19-C18-C17	14.37	140.99	118.94
24	K	102	BCR	C15-C14-C13	14.16	147.51	127.31
24	k	102	BCR	C15-C14-C13	14.15	147.51	127.31
24	T	101	BCR	C16-C15-C14	14.12	152.40	123.47
24	B	618	BCR	C16-C15-C14	14.10	152.35	123.47
24	b	622	BCR	C20-C21-C22	13.99	147.27	127.31
24	B	622	BCR	C20-C21-C22	13.98	147.26	127.31
24	H	101	BCR	C11-C10-C9	13.83	147.04	127.31
24	h	101	BCR	C11-C10-C9	13.82	147.04	127.31
24	K	102	BCR	C21-C20-C19	13.72	166.04	123.22
24	k	102	BCR	C21-C20-C19	13.72	166.03	123.22
24	B	619	BCR	C15-C14-C13	13.56	146.66	127.31
24	b	618	BCR	C15-C14-C13	13.55	146.65	127.31
24	T	102	BCR	C21-C20-C19	13.33	164.81	123.22
24	B	619	BCR	C11-C10-C9	13.32	146.32	127.31
24	t	101	BCR	C21-C20-C19	13.31	164.76	123.22
24	b	618	BCR	C11-C10-C9	13.30	146.29	127.31
24	T	102	BCR	C19-C18-C17	13.25	139.28	118.94
24	t	101	BCR	C19-C18-C17	13.20	139.20	118.94
24	k	101	BCR	C11-C10-C9	13.02	145.89	127.31
24	K	101	BCR	C11-C10-C9	13.01	145.88	127.31
24	A	608	BCR	C21-C20-C19	12.72	162.90	123.22
24	a	608	BCR	C21-C20-C19	12.70	162.84	123.22
24	K	101	BCR	C19-C18-C17	12.69	138.41	118.94
24	C	514	BCR	C20-C19-C18	12.68	162.05	126.42
24	c	514	BCR	C20-C19-C18	12.68	162.03	126.42
24	d	404	BCR	C21-C20-C19	12.67	162.76	123.22
24	D	404	BCR	C21-C20-C19	12.67	162.75	123.22
24	k	101	BCR	C19-C18-C17	12.64	138.34	118.94
24	T	102	BCR	C11-C10-C9	12.62	145.32	127.31
24	t	101	BCR	C11-C10-C9	12.54	145.20	127.31
24	A	608	BCR	C19-C18-C17	12.47	138.07	118.94
24	a	608	BCR	C19-C18-C17	12.44	138.03	118.94
24	C	515	BCR	C20-C19-C18	12.36	161.13	126.42
24	c	515	BCR	C20-C19-C18	12.34	161.08	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	622	BCR	C11-C10-C9	12.28	144.84	127.31
24	B	622	BCR	C11-C10-C9	12.27	144.82	127.31
24	k	102	BCR	C20-C19-C18	12.25	160.84	126.42
24	k	102	BCR	C19-C18-C17	12.24	137.73	118.94
24	K	102	BCR	C19-C18-C17	12.24	137.73	118.94
24	K	102	BCR	C20-C19-C18	12.23	160.78	126.42
24	c	514	BCR	C10-C11-C12	11.93	160.46	123.22
24	C	514	BCR	C10-C11-C12	11.93	160.44	123.22
22	C	507	CLA	C4A-NA-C1A	11.82	112.02	106.71
22	c	511	CLA	C4A-NA-C1A	11.79	112.01	106.71
24	b	622	BCR	C10-C11-C12	11.77	159.94	123.22
24	B	622	BCR	C10-C11-C12	11.75	159.90	123.22
22	C	511	CLA	C4A-NA-C1A	11.73	111.98	106.71
24	T	101	BCR	C12-C13-C14	11.72	136.92	118.94
24	B	618	BCR	C12-C13-C14	11.69	136.88	118.94
22	c	507	CLA	C4A-NA-C1A	11.69	111.96	106.71
24	b	622	BCR	C11-C12-C13	11.58	158.93	126.42
24	B	622	BCR	C11-C12-C13	11.55	158.86	126.42
24	H	101	BCR	C15-C14-C13	11.52	143.76	127.31
24	h	101	BCR	C15-C14-C13	11.51	143.73	127.31
24	C	515	BCR	C15-C14-C13	11.50	143.73	127.31
24	c	515	BCR	C15-C14-C13	11.50	143.72	127.31
24	A	608	BCR	C11-C10-C9	11.40	143.59	127.31
24	k	101	BCR	C15-C14-C13	11.37	143.54	127.31
24	a	608	BCR	C11-C10-C9	11.37	143.54	127.31
24	K	101	BCR	C15-C14-C13	11.35	143.51	127.31
24	k	102	BCR	C11-C12-C13	11.32	158.21	126.42
24	K	102	BCR	C11-C12-C13	11.31	158.18	126.42
24	B	618	BCR	C21-C20-C19	11.22	158.22	123.22
24	T	101	BCR	C21-C20-C19	11.21	158.19	123.22
24	K	101	BCR	C20-C19-C18	11.17	157.79	126.42
24	k	101	BCR	C20-C19-C18	11.14	157.72	126.42
24	a	608	BCR	C23-C22-C21	11.11	135.99	118.94
24	A	608	BCR	C23-C22-C21	11.09	135.96	118.94
24	B	618	BCR	C11-C10-C9	11.03	143.05	127.31
24	T	101	BCR	C11-C10-C9	11.01	143.03	127.31
22	B	605	CLA	C4A-NA-C1A	10.95	111.63	106.71
24	H	101	BCR	C20-C19-C18	10.90	157.04	126.42
24	h	101	BCR	C20-C19-C18	10.89	157.02	126.42
24	a	608	BCR	C12-C13-C14	10.86	135.60	118.94
22	b	605	CLA	C4A-NA-C1A	10.85	111.58	106.71
24	A	608	BCR	C12-C13-C14	10.85	135.59	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	102	BCR	C10-C11-C12	10.80	156.93	123.22
24	K	102	BCR	C10-C11-C12	10.79	156.90	123.22
24	a	608	BCR	C15-C14-C13	10.79	142.71	127.31
24	A	608	BCR	C15-C14-C13	10.77	142.68	127.31
24	b	622	BCR	C20-C19-C18	10.76	156.64	126.42
24	B	622	BCR	C20-C19-C18	10.75	156.61	126.42
24	B	618	BCR	C20-C19-C18	10.74	156.58	126.42
24	T	101	BCR	C20-C19-C18	10.73	156.55	126.42
24	h	101	BCR	C19-C18-C17	10.72	135.40	118.94
24	H	101	BCR	C19-C18-C17	10.72	135.40	118.94
24	b	618	BCR	C20-C19-C18	10.71	156.50	126.42
24	B	619	BCR	C20-C19-C18	10.69	156.44	126.42
24	c	514	BCR	C11-C12-C13	10.60	156.18	126.42
24	T	102	BCR	C36-C18-C17	-10.60	108.08	122.92
24	C	514	BCR	C11-C12-C13	10.59	156.18	126.42
24	t	101	BCR	C36-C18-C17	-10.59	108.09	122.92
24	d	404	BCR	C15-C14-C13	10.58	142.41	127.31
24	c	514	BCR	C19-C18-C17	10.56	135.15	118.94
24	D	404	BCR	C15-C14-C13	10.55	142.36	127.31
24	C	514	BCR	C19-C18-C17	10.54	135.11	118.94
22	B	616	CLA	C4A-NA-C1A	10.41	111.39	106.71
22	b	616	CLA	C4A-NA-C1A	10.41	111.38	106.71
24	D	404	BCR	C11-C10-C9	10.39	142.15	127.31
24	d	404	BCR	C11-C10-C9	10.36	142.10	127.31
24	T	102	BCR	C15-C14-C13	10.34	142.07	127.31
24	t	101	BCR	C15-C14-C13	10.28	141.99	127.31
24	b	622	BCR	C21-C20-C19	10.18	155.00	123.22
22	b	602	CLA	C4A-NA-C1A	10.18	111.28	106.71
22	B	602	CLA	C4A-NA-C1A	10.17	111.28	106.71
24	B	622	BCR	C21-C20-C19	10.17	154.94	123.22
24	T	102	BCR	C10-C11-C12	10.16	154.93	123.22
22	C	513	CLA	C4A-NA-C1A	10.15	111.27	106.71
24	t	101	BCR	C10-C11-C12	10.14	154.86	123.22
24	c	515	BCR	C10-C11-C12	10.14	154.85	123.22
24	C	515	BCR	C10-C11-C12	10.12	154.81	123.22
24	T	102	BCR	C11-C12-C13	10.11	154.83	126.42
24	t	101	BCR	C11-C12-C13	10.11	154.81	126.42
22	c	513	CLA	C4A-NA-C1A	10.04	111.22	106.71
22	c	504	CLA	C4A-NA-C1A	10.01	111.20	106.71
22	C	509	CLA	C4A-NA-C1A	9.93	111.17	106.71
22	C	504	CLA	C4A-NA-C1A	9.92	111.17	106.71
22	c	509	CLA	C4A-NA-C1A	9.89	111.15	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	622	BCR	C15-C14-C13	9.83	141.34	127.31
24	b	622	BCR	C15-C14-C13	9.83	141.34	127.31
24	B	622	BCR	C19-C18-C17	9.77	133.93	118.94
24	b	622	BCR	C19-C18-C17	9.77	133.93	118.94
24	C	514	BCR	C7-C8-C9	9.76	140.99	126.23
24	a	608	BCR	C37-C22-C21	-9.76	109.26	122.92
24	a	608	BCR	C11-C12-C13	9.75	153.80	126.42
24	A	608	BCR	C11-C12-C13	9.74	153.78	126.42
24	A	608	BCR	C37-C22-C21	-9.72	109.31	122.92
24	c	514	BCR	C7-C8-C9	9.70	140.90	126.23
24	C	514	BCR	C15-C14-C13	9.70	141.16	127.31
24	c	514	BCR	C15-C14-C13	9.70	141.15	127.31
22	b	613	CLA	C4A-NA-C1A	9.69	111.06	106.71
22	c	506	CLA	C4A-NA-C1A	9.69	111.06	106.71
24	K	102	BCR	C12-C13-C14	9.62	133.71	118.94
24	A	608	BCR	C10-C11-C12	9.62	153.24	123.22
22	C	506	CLA	C4A-NA-C1A	9.62	111.03	106.71
24	a	608	BCR	C10-C11-C12	9.61	153.22	123.22
24	k	102	BCR	C12-C13-C14	9.61	133.69	118.94
24	c	515	BCR	C19-C18-C17	9.61	133.68	118.94
24	C	515	BCR	C19-C18-C17	9.60	133.68	118.94
22	B	613	CLA	C4A-NA-C1A	9.60	111.02	106.71
24	C	515	BCR	C12-C13-C14	9.57	133.63	118.94
22	C	505	CLA	C4A-NA-C1A	9.56	111.01	106.71
24	c	515	BCR	C12-C13-C14	9.55	133.59	118.94
24	D	404	BCR	C20-C19-C18	9.52	153.17	126.42
24	d	404	BCR	C20-C19-C18	9.52	153.17	126.42
24	b	618	BCR	C12-C13-C14	9.51	133.54	118.94
24	D	404	BCR	C19-C18-C17	9.51	133.53	118.94
24	d	404	BCR	C19-C18-C17	9.51	133.53	118.94
24	B	619	BCR	C12-C13-C14	9.50	133.52	118.94
24	h	101	BCR	C10-C11-C12	9.49	152.83	123.22
24	H	101	BCR	C10-C11-C12	9.47	152.78	123.22
24	H	101	BCR	C12-C13-C14	9.46	133.46	118.94
24	h	101	BCR	C12-C13-C14	9.45	133.44	118.94
22	d	403	CLA	C4A-NA-C1A	9.44	110.95	106.71
22	C	510	CLA	C4A-NA-C1A	9.44	110.95	106.71
22	c	505	CLA	C4A-NA-C1A	9.41	110.94	106.71
24	d	404	BCR	C11-C12-C13	9.41	152.85	126.42
22	c	510	CLA	C4A-NA-C1A	9.41	110.94	106.71
24	D	404	BCR	C11-C12-C13	9.39	152.80	126.42
24	T	101	BCR	C11-C12-C13	9.39	152.78	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	618	BCR	C11-C12-C13	9.38	152.77	126.42
24	T	102	BCR	C20-C19-C18	9.37	152.73	126.42
22	D	403	CLA	C4A-NA-C1A	9.36	110.92	106.71
24	t	101	BCR	C20-C19-C18	9.34	152.66	126.42
22	B	610	CLA	C4A-NA-C1A	9.31	110.89	106.71
24	K	102	BCR	C7-C8-C9	9.31	140.31	126.23
24	k	102	BCR	C7-C8-C9	9.30	140.29	126.23
24	T	102	BCR	C7-C8-C9	9.29	140.28	126.23
24	t	101	BCR	C7-C8-C9	9.29	140.28	126.23
24	h	101	BCR	C11-C12-C13	9.26	152.44	126.42
24	H	101	BCR	C11-C12-C13	9.26	152.42	126.42
22	c	512	CLA	C4A-NA-C1A	9.24	110.86	106.71
22	b	610	CLA	C4A-NA-C1A	9.22	110.85	106.71
22	B	612	CLA	C4A-NA-C1A	9.21	110.85	106.71
22	C	512	CLA	C4A-NA-C1A	9.19	110.84	106.71
22	b	612	CLA	C4A-NA-C1A	9.14	110.82	106.71
24	D	404	BCR	C30-C25-C26	-9.10	109.80	122.61
24	d	404	BCR	C30-C25-C26	-9.08	109.82	122.61
22	B	614	CLA	C4A-NA-C1A	9.05	110.78	106.71
22	b	614	CLA	C4A-NA-C1A	9.00	110.75	106.71
22	C	508	CLA	C4A-NA-C1A	8.98	110.74	106.71
24	b	618	BCR	C23-C22-C21	8.96	132.69	118.94
22	B	607	CLA	C4A-NA-C1A	8.95	110.73	106.71
22	C	503	CLA	C4A-NA-C1A	8.95	110.73	106.71
24	B	619	BCR	C23-C22-C21	8.95	132.67	118.94
24	K	102	BCR	C11-C10-C9	8.92	140.04	127.31
24	k	102	BCR	C11-C10-C9	8.91	140.02	127.31
22	c	501	CLA	C4A-NA-C1A	8.90	110.71	106.71
22	c	503	CLA	C4A-NA-C1A	8.90	110.71	106.71
24	B	622	BCR	C7-C8-C9	8.89	139.67	126.23
22	c	508	CLA	C4A-NA-C1A	8.88	110.70	106.71
24	b	622	BCR	C7-C8-C9	8.87	139.64	126.23
22	C	501	CLA	C4A-NA-C1A	8.87	110.69	106.71
22	b	607	CLA	C4A-NA-C1A	8.85	110.69	106.71
24	t	101	BCR	C23-C22-C21	8.81	132.46	118.94
24	B	619	BCR	C36-C18-C19	-8.78	104.24	118.08
24	T	102	BCR	C23-C22-C21	8.78	132.41	118.94
24	b	618	BCR	C36-C18-C19	-8.78	104.25	118.08
24	h	101	BCR	C23-C22-C21	8.74	132.36	118.94
24	H	101	BCR	C23-C22-C21	8.74	132.36	118.94
22	B	611	CLA	C4A-NA-C1A	8.69	110.61	106.71
24	B	618	BCR	C36-C18-C17	-8.69	110.75	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	101	BCR	C36-C18-C17	-8.68	110.77	122.92
24	b	618	BCR	C24-C23-C22	8.67	139.34	126.23
22	b	611	CLA	C4A-NA-C1A	8.67	110.60	106.71
24	B	619	BCR	C24-C23-C22	8.63	139.28	126.23
24	T	101	BCR	C10-C11-C12	8.63	150.14	123.22
24	B	618	BCR	C10-C11-C12	8.62	150.12	123.22
24	A	608	BCR	C20-C19-C18	8.55	150.43	126.42
24	C	515	BCR	C11-C12-C13	8.54	150.40	126.42
24	a	608	BCR	C20-C19-C18	8.53	150.38	126.42
24	k	101	BCR	C33-C5-C4	-8.52	97.25	113.62
24	c	515	BCR	C11-C12-C13	8.52	150.34	126.42
24	K	101	BCR	C33-C5-C4	-8.51	97.27	113.62
22	B	617	CLA	C4A-NA-C1A	8.49	110.52	106.71
22	b	617	CLA	C4A-NA-C1A	8.44	110.50	106.71
24	K	102	BCR	C23-C22-C21	8.37	131.79	118.94
24	k	102	BCR	C23-C22-C21	8.37	131.78	118.94
24	k	101	BCR	C11-C12-C13	8.35	149.87	126.42
24	K	101	BCR	C11-C12-C13	8.34	149.85	126.42
24	D	404	BCR	C29-C30-C25	8.32	123.29	110.48
24	T	101	BCR	C15-C14-C13	8.30	139.15	127.31
24	B	618	BCR	C15-C14-C13	8.29	139.15	127.31
24	d	404	BCR	C29-C30-C25	8.29	123.25	110.48
24	A	608	BCR	C36-C18-C17	-8.24	111.38	122.92
24	C	514	BCR	C11-C10-C9	8.21	139.02	127.31
24	a	608	BCR	C36-C18-C17	-8.21	111.43	122.92
24	c	514	BCR	C11-C10-C9	8.20	139.01	127.31
24	d	404	BCR	C32-C1-C6	8.19	123.58	110.30
24	D	404	BCR	C32-C1-C6	8.19	123.58	110.30
22	B	606	CLA	C4A-NA-C1A	8.15	110.37	106.71
22	A	607	CLA	C4A-NA-C1A	8.08	110.34	106.71
22	a	607	CLA	C4A-NA-C1A	8.08	110.34	106.71
22	b	606	CLA	C4A-NA-C1A	8.08	110.34	106.71
22	b	615	CLA	C4A-NA-C1A	8.07	110.33	106.71
22	B	615	CLA	C4A-NA-C1A	8.03	110.32	106.71
24	d	404	BCR	C12-C13-C14	8.01	131.23	118.94
22	B	608	CLA	C4A-NA-C1A	8.01	110.31	106.71
24	D	404	BCR	C12-C13-C14	7.99	131.20	118.94
22	c	502	CLA	C4A-NA-C1A	7.98	110.29	106.71
24	A	608	BCR	C7-C8-C9	7.98	138.29	126.23
22	C	502	CLA	C4A-NA-C1A	7.93	110.27	106.71
22	b	608	CLA	C4A-NA-C1A	7.92	110.27	106.71
24	a	608	BCR	C7-C8-C9	7.89	138.16	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	618	BCR	C8-C9-C10	7.89	131.05	118.94
24	T	101	BCR	C8-C9-C10	7.86	131.00	118.94
24	k	101	BCR	C10-C11-C12	7.85	147.73	123.22
22	B	604	CLA	C4A-NA-C1A	7.85	110.24	106.71
24	B	619	BCR	C7-C8-C9	7.85	138.10	126.23
24	K	101	BCR	C10-C11-C12	7.84	147.69	123.22
24	b	618	BCR	C7-C8-C9	7.84	138.08	126.23
24	a	608	BCR	C35-C13-C14	-7.83	111.95	122.92
24	A	608	BCR	C35-C13-C14	-7.83	111.95	122.92
24	h	101	BCR	C7-C8-C9	7.83	138.06	126.23
24	H	101	BCR	C7-C8-C9	7.82	138.04	126.23
24	B	619	BCR	C10-C11-C12	7.80	147.56	123.22
24	b	618	BCR	C10-C11-C12	7.79	147.54	123.22
22	b	604	CLA	C4A-NA-C1A	7.79	110.21	106.71
22	A	604	CLA	C4A-NA-C1A	7.74	110.19	106.71
22	a	604	CLA	C4A-NA-C1A	7.71	110.17	106.71
24	a	608	BCR	C27-C26-C25	7.69	133.90	122.73
24	T	101	BCR	C35-C13-C12	-7.69	105.96	118.08
24	B	618	BCR	C35-C13-C12	-7.67	105.99	118.08
24	A	608	BCR	C27-C26-C25	7.65	133.84	122.73
22	b	603	CLA	C4A-NA-C1A	7.63	110.14	106.71
24	k	101	BCR	C7-C8-C9	7.62	137.74	126.23
23	A	606	PHO	CMD-C2D-C1D	7.61	136.78	125.06
24	K	101	BCR	C7-C8-C9	7.58	137.68	126.23
23	a	606	PHO	CMD-C2D-C1D	7.57	136.73	125.06
24	k	101	BCR	C33-C5-C6	7.54	132.99	124.53
24	H	101	BCR	C37-C22-C21	-7.51	112.40	122.92
22	B	603	CLA	C4A-NA-C1A	7.50	110.08	106.71
24	K	101	BCR	C33-C5-C6	7.50	132.95	124.53
24	h	101	BCR	C37-C22-C21	-7.46	112.47	122.92
24	C	514	BCR	C38-C26-C27	-7.44	99.32	113.62
24	k	101	BCR	C12-C13-C14	7.44	130.35	118.94
23	a	605	PHO	CMD-C2D-C1D	7.43	136.51	125.06
24	c	514	BCR	C38-C26-C27	-7.41	99.37	113.62
24	K	101	BCR	C12-C13-C14	7.41	130.31	118.94
24	b	622	BCR	C33-C5-C6	7.40	132.84	124.53
23	A	605	PHO	CMD-C2D-C1D	7.40	136.46	125.06
24	B	622	BCR	C33-C5-C6	7.38	132.82	124.53
24	B	618	BCR	C36-C18-C19	-7.31	106.56	118.08
24	T	101	BCR	C36-C18-C19	-7.30	106.57	118.08
24	T	102	BCR	C12-C13-C14	7.30	130.14	118.94
24	t	101	BCR	C12-C13-C14	7.27	130.10	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	402	CLA	C2C-C1C-NC	7.27	116.78	109.97
22	D	402	CLA	C2C-C1C-NC	7.26	116.77	109.97
24	K	101	BCR	C37-C22-C21	-7.24	112.78	122.92
24	b	618	BCR	C30-C25-C26	-7.23	112.43	122.61
24	B	619	BCR	C30-C25-C26	-7.23	112.43	122.61
24	d	404	BCR	C10-C11-C12	7.19	145.65	123.22
24	k	101	BCR	C37-C22-C21	-7.19	112.85	122.92
24	D	404	BCR	C10-C11-C12	7.18	145.61	123.22
24	b	622	BCR	C12-C13-C14	7.14	129.91	118.94
24	B	622	BCR	C12-C13-C14	7.14	129.89	118.94
24	B	622	BCR	C36-C18-C17	-7.12	112.95	122.92
24	b	622	BCR	C36-C18-C17	-7.12	112.95	122.92
24	T	101	BCR	C24-C23-C22	6.97	136.77	126.23
24	B	618	BCR	C24-C23-C22	6.93	136.70	126.23
24	a	608	BCR	C38-C26-C27	-6.85	100.45	113.62
24	H	101	BCR	C36-C18-C19	-6.85	107.29	118.08
24	h	101	BCR	C36-C18-C19	-6.85	107.29	118.08
24	K	101	BCR	C36-C18-C19	-6.85	107.29	118.08
22	a	604	CLA	C2C-C1C-NC	6.84	116.38	109.97
24	A	608	BCR	C38-C26-C27	-6.84	100.48	113.62
22	A	604	CLA	C2C-C1C-NC	6.83	116.37	109.97
24	c	514	BCR	C36-C18-C17	-6.83	113.36	122.92
24	C	514	BCR	C36-C18-C17	-6.81	113.38	122.92
22	B	605	CLA	C2C-C1C-NC	6.79	116.33	109.97
22	b	605	CLA	C2C-C1C-NC	6.77	116.31	109.97
24	k	101	BCR	C36-C18-C19	-6.77	107.41	118.08
22	b	609	CLA	C2C-C1C-NC	6.73	116.28	109.97
22	B	609	CLA	C2C-C1C-NC	6.73	116.28	109.97
24	B	622	BCR	C8-C7-C6	6.72	146.06	127.20
24	b	622	BCR	C8-C7-C6	6.71	146.04	127.20
24	T	101	BCR	C23-C22-C21	6.71	129.23	118.94
24	H	101	BCR	C8-C9-C10	6.69	129.20	118.94
24	h	101	BCR	C8-C9-C10	6.67	129.18	118.94
24	C	515	BCR	C23-C22-C21	6.67	129.18	118.94
24	B	618	BCR	C23-C22-C21	6.66	129.16	118.94
24	k	102	BCR	C36-C18-C19	-6.63	107.62	118.08
24	c	515	BCR	C23-C22-C21	6.61	129.09	118.94
24	C	515	BCR	C24-C23-C22	6.61	136.22	126.23
24	K	102	BCR	C36-C18-C19	-6.60	107.68	118.08
24	B	618	BCR	C34-C9-C10	-6.59	113.69	122.92
24	T	101	BCR	C34-C9-C10	-6.57	113.71	122.92
24	c	515	BCR	C24-C23-C22	6.56	136.15	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	101	BCR	C29-C30-C25	6.52	120.51	110.48
24	K	101	BCR	C29-C30-C25	6.52	120.51	110.48
24	K	102	BCR	C37-C22-C21	-6.49	113.83	122.92
24	k	102	BCR	C37-C22-C21	-6.48	113.85	122.92
24	c	514	BCR	C33-C5-C6	6.47	131.80	124.53
33	F	101	HEM	CBD-CAD-C3D	-6.47	100.56	112.48
22	D	401	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	a	603	CLA	C4A-NA-C1A	6.46	109.61	106.71
33	f	101	HEM	CBD-CAD-C3D	-6.45	100.60	112.48
24	C	514	BCR	C33-C5-C6	6.40	131.72	124.53
22	A	603	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	h	101	BCR	C32-C1-C6	6.35	120.60	110.30
24	H	101	BCR	C32-C1-C6	6.34	120.59	110.30
22	d	401	CLA	C4A-NA-C1A	6.31	109.54	106.71
24	A	608	BCR	C8-C9-C10	6.27	128.57	118.94
22	b	604	CLA	C2C-C1C-NC	6.27	115.85	109.97
24	B	619	BCR	C11-C12-C13	6.26	144.01	126.42
24	b	618	BCR	C11-C12-C13	6.26	144.01	126.42
24	B	619	BCR	C8-C9-C10	6.25	128.53	118.94
24	T	102	BCR	C8-C9-C10	6.24	128.51	118.94
24	a	608	BCR	C8-C9-C10	6.22	128.49	118.94
24	b	618	BCR	C8-C9-C10	6.22	128.48	118.94
24	k	101	BCR	C36-C18-C17	-6.20	114.24	122.92
24	t	101	BCR	C8-C9-C10	6.19	128.44	118.94
24	B	619	BCR	C23-C24-C25	6.18	144.56	127.20
24	b	618	BCR	C23-C24-C25	6.18	144.55	127.20
22	B	604	CLA	C2C-C1C-NC	6.17	115.75	109.97
24	K	101	BCR	C36-C18-C17	-6.16	114.29	122.92
24	K	102	BCR	C8-C7-C6	6.14	144.44	127.20
24	k	102	BCR	C8-C7-C6	6.12	144.40	127.20
24	C	514	BCR	C24-C23-C22	6.12	135.48	126.23
24	c	514	BCR	C24-C23-C22	6.09	135.44	126.23
24	B	622	BCR	C24-C23-C22	6.09	135.44	126.23
22	a	607	CLA	C2C-C1C-NC	6.07	115.66	109.97
24	b	622	BCR	C24-C23-C22	6.06	135.39	126.23
22	A	607	CLA	C2C-C1C-NC	6.05	115.64	109.97
22	c	509	CLA	C2C-C1C-NC	6.04	115.64	109.97
22	B	610	CLA	C2C-C1C-NC	6.04	115.63	109.97
22	C	509	CLA	C2C-C1C-NC	6.03	115.62	109.97
24	B	618	BCR	C7-C8-C9	6.03	135.35	126.23
22	b	610	CLA	C2C-C1C-NC	6.02	115.61	109.97
22	B	612	CLA	C2C-C1C-NC	6.01	115.60	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	515	BCR	C31-C1-C6	6.00	120.03	110.30
24	T	101	BCR	C7-C8-C9	6.00	135.30	126.23
22	C	504	CLA	C2C-C1C-NC	6.00	115.59	109.97
22	c	501	CLA	O2D-CGD-CBD	5.98	121.90	111.27
22	b	612	CLA	C2C-C1C-NC	5.98	115.57	109.97
22	c	504	CLA	C2C-C1C-NC	5.98	115.57	109.97
22	C	501	CLA	O2D-CGD-CBD	5.98	121.89	111.27
24	c	515	BCR	C31-C1-C6	5.97	119.98	110.30
24	H	101	BCR	C34-C9-C10	-5.96	114.58	122.92
22	D	401	CLA	C2C-C1C-NC	5.95	115.55	109.97
22	d	401	CLA	C2C-C1C-NC	5.95	115.55	109.97
22	B	608	CLA	C2C-C1C-NC	5.95	115.54	109.97
24	K	102	BCR	C36-C18-C17	-5.95	114.59	122.92
24	h	101	BCR	C34-C9-C10	-5.93	114.62	122.92
24	k	102	BCR	C36-C18-C17	-5.91	114.65	122.92
24	C	514	BCR	C38-C26-C25	5.89	131.15	124.53
22	b	608	CLA	C2C-C1C-NC	5.88	115.48	109.97
24	b	618	BCR	C38-C26-C27	-5.87	102.34	113.62
24	B	619	BCR	C38-C26-C27	-5.86	102.35	113.62
24	H	101	BCR	C30-C25-C26	-5.85	114.37	122.61
24	c	514	BCR	C38-C26-C25	5.85	131.10	124.53
24	B	619	BCR	C37-C22-C21	-5.85	114.73	122.92
24	C	514	BCR	C12-C13-C14	5.85	127.91	118.94
24	b	618	BCR	C37-C22-C21	-5.84	114.74	122.92
24	b	618	BCR	C36-C18-C17	-5.83	114.75	122.92
24	h	101	BCR	C33-C5-C4	-5.83	102.42	113.62
24	c	514	BCR	C12-C13-C14	5.83	127.88	118.94
24	B	619	BCR	C36-C18-C17	-5.82	114.77	122.92
22	b	614	CLA	C2C-C1C-NC	5.82	115.42	109.97
24	H	101	BCR	C33-C5-C4	-5.82	102.44	113.62
22	b	615	CLA	C2C-C1C-NC	5.82	115.42	109.97
22	B	615	CLA	C2C-C1C-NC	5.81	115.42	109.97
24	h	101	BCR	C30-C25-C26	-5.81	114.43	122.61
24	B	619	BCR	C35-C13-C14	-5.80	114.80	122.92
24	D	404	BCR	C23-C22-C21	5.80	127.84	118.94
22	c	510	CLA	C2C-C1C-NC	5.80	115.40	109.97
24	d	404	BCR	C23-C22-C21	5.79	127.83	118.94
24	c	515	BCR	C7-C8-C9	5.79	134.99	126.23
22	B	614	CLA	C2C-C1C-NC	5.79	115.40	109.97
24	b	618	BCR	C35-C13-C14	-5.79	114.82	122.92
24	C	515	BCR	C7-C8-C9	5.78	134.97	126.23
22	C	510	CLA	C2C-C1C-NC	5.75	115.36	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	C2C-C1C-NC	5.73	115.34	109.97
22	c	506	CLA	C2C-C1C-NC	5.71	115.32	109.97
24	k	101	BCR	C30-C25-C26	-5.71	114.57	122.61
24	K	101	BCR	C30-C25-C26	-5.70	114.59	122.61
24	B	619	BCR	C29-C30-C25	5.69	119.23	110.48
24	b	618	BCR	C29-C30-C25	5.68	119.23	110.48
24	C	514	BCR	C8-C7-C6	5.66	143.11	127.20
24	c	514	BCR	C8-C7-C6	5.64	143.05	127.20
22	B	602	CLA	O2D-CGD-CBD	5.64	121.28	111.27
24	B	618	BCR	C38-C26-C27	-5.63	102.81	113.62
22	b	602	CLA	O2D-CGD-CBD	5.63	121.27	111.27
24	T	101	BCR	C38-C26-C27	-5.60	102.86	113.62
22	C	501	CLA	C2C-C1C-NC	5.55	115.17	109.97
22	A	603	CLA	C2C-C1C-NC	5.55	115.17	109.97
24	K	101	BCR	C24-C23-C22	5.55	134.61	126.23
22	a	603	CLA	C2C-C1C-NC	5.54	115.16	109.97
22	c	501	CLA	C2C-C1C-NC	5.52	115.14	109.97
24	k	101	BCR	C24-C23-C22	5.52	134.58	126.23
22	B	606	CLA	C2C-C1C-NC	5.52	115.14	109.97
22	b	606	CLA	C2C-C1C-NC	5.51	115.13	109.97
24	b	622	BCR	C2-C1-C6	5.51	118.96	110.48
24	B	622	BCR	C2-C1-C6	5.50	118.95	110.48
22	b	607	CLA	C2C-C1C-NC	5.45	115.08	109.97
22	c	505	CLA	C2C-C1C-NC	5.44	115.07	109.97
22	B	607	CLA	C2C-C1C-NC	5.44	115.07	109.97
24	K	102	BCR	C8-C9-C10	5.44	127.29	118.94
24	k	102	BCR	C8-C9-C10	5.44	127.28	118.94
22	C	505	CLA	C2C-C1C-NC	5.44	115.06	109.97
24	t	101	BCR	C33-C5-C4	-5.43	103.19	113.62
22	c	508	CLA	C2C-C1C-NC	5.42	115.05	109.97
24	k	101	BCR	C8-C9-C10	5.42	127.26	118.94
24	D	404	BCR	C36-C18-C17	-5.42	115.33	122.92
24	T	102	BCR	C33-C5-C4	-5.41	103.22	113.62
22	C	511	CLA	C2C-C1C-NC	5.41	115.04	109.97
24	K	101	BCR	C8-C9-C10	5.41	127.24	118.94
22	c	502	CLA	C2C-C1C-NC	5.40	115.03	109.97
22	C	502	CLA	C2C-C1C-NC	5.40	115.03	109.97
22	c	511	CLA	C2C-C1C-NC	5.40	115.03	109.97
22	b	613	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	d	404	BCR	C36-C18-C17	-5.40	115.36	122.92
24	h	101	BCR	C33-C5-C6	5.39	130.58	124.53
22	B	616	CLA	C2C-C1C-NC	5.39	115.02	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	BCR	C29-C30-C25	5.38	118.76	110.48
22	C	508	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	C	514	BCR	C29-C30-C25	5.37	118.75	110.48
22	B	613	CLA	C2C-C1C-NC	5.36	115.00	109.97
22	B	611	CLA	C2C-C1C-NC	5.35	114.98	109.97
22	b	611	CLA	C2C-C1C-NC	5.34	114.98	109.97
22	b	616	CLA	C2C-C1C-NC	5.33	114.97	109.97
24	H	101	BCR	C33-C5-C6	5.33	130.52	124.53
24	a	608	BCR	C30-C25-C26	-5.31	115.13	122.61
24	A	608	BCR	C30-C25-C26	-5.31	115.13	122.61
22	d	403	CLA	C2C-C1C-NC	5.30	114.94	109.97
22	b	612	CLA	C3C-C4C-NC	5.29	116.50	110.57
22	B	612	CLA	C3C-C4C-NC	5.29	116.50	110.57
22	b	617	CLA	C2C-C1C-NC	5.29	114.92	109.97
24	C	515	BCR	C37-C22-C21	-5.27	115.54	122.92
22	D	403	CLA	C2C-C1C-NC	5.26	114.90	109.97
24	H	101	BCR	C35-C13-C12	-5.25	109.81	118.08
24	h	101	BCR	C35-C13-C12	-5.24	109.82	118.08
24	k	101	BCR	C8-C7-C6	5.24	141.91	127.20
22	C	507	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	K	102	BCR	C35-C13-C14	-5.24	115.59	122.92
24	t	101	BCR	C37-C22-C23	-5.24	109.83	118.08
24	a	608	BCR	C24-C23-C22	5.23	134.14	126.23
24	K	101	BCR	C23-C22-C21	5.23	126.96	118.94
24	K	101	BCR	C8-C7-C6	5.22	141.87	127.20
24	k	102	BCR	C35-C13-C14	-5.22	115.61	122.92
33	V	201	HEM	CBD-CAD-C3D	-5.22	102.86	112.48
33	v	201	HEM	CBD-CAD-C3D	-5.21	102.87	112.48
24	A	608	BCR	C24-C23-C22	5.21	134.11	126.23
24	C	515	BCR	C35-C13-C12	-5.21	109.88	118.08
24	k	101	BCR	C23-C22-C21	5.20	126.93	118.94
22	d	401	CLA	C3C-C4C-NC	5.20	116.40	110.57
22	d	402	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
22	D	402	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
24	c	515	BCR	C35-C13-C12	-5.19	109.90	118.08
24	c	515	BCR	C8-C7-C6	5.19	141.77	127.20
24	T	102	BCR	C37-C22-C23	-5.19	109.90	118.08
22	B	617	CLA	C2C-C1C-NC	5.19	114.83	109.97
24	c	515	BCR	C37-C22-C21	-5.18	115.67	122.92
24	C	515	BCR	C8-C7-C6	5.17	141.72	127.20
24	D	404	BCR	C8-C9-C10	5.17	126.87	118.94
22	B	605	CLA	C3C-C4C-NC	5.16	116.36	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	C2C-C1C-NC	5.16	114.81	109.97
24	D	404	BCR	C34-C9-C10	-5.16	115.70	122.92
22	D	401	CLA	C3C-C4C-NC	5.15	116.35	110.57
23	a	605	PHO	C3D-C2D-C1D	-5.15	98.37	105.87
24	K	102	BCR	C23-C24-C25	5.15	141.66	127.20
22	B	606	CLA	C3C-C4C-NC	5.14	116.34	110.57
24	k	102	BCR	C23-C24-C25	5.14	141.65	127.20
24	d	404	BCR	C34-C9-C10	-5.14	115.72	122.92
24	D	404	BCR	C24-C23-C22	5.14	134.00	126.23
22	C	512	CLA	O2D-CGD-CBD	5.13	120.39	111.27
24	k	101	BCR	C34-C9-C10	-5.13	115.74	122.92
24	d	404	BCR	C8-C9-C10	5.12	126.80	118.94
22	C	503	CLA	C2C-C1C-NC	5.12	114.77	109.97
24	K	101	BCR	C34-C9-C10	-5.12	115.75	122.92
22	c	512	CLA	O2D-CGD-CBD	5.12	120.37	111.27
22	c	503	CLA	C2C-C1C-NC	5.11	114.76	109.97
22	c	506	CLA	O2D-CGD-CBD	5.11	120.35	111.27
22	C	506	CLA	O2D-CGD-CBD	5.11	120.35	111.27
22	b	606	CLA	C3C-C4C-NC	5.11	116.30	110.57
23	A	605	PHO	C3D-C2D-C1D	-5.10	98.43	105.87
24	H	101	BCR	C29-C30-C25	5.10	118.33	110.48
24	d	404	BCR	C24-C23-C22	5.10	133.93	126.23
24	B	619	BCR	C40-C30-C25	5.09	118.55	110.30
22	b	605	CLA	C3C-C4C-NC	5.08	116.27	110.57
24	b	618	BCR	C40-C30-C25	5.07	118.53	110.30
24	d	404	BCR	C39-C30-C29	-5.05	88.70	108.91
24	D	404	BCR	C39-C30-C29	-5.05	88.71	108.91
24	h	101	BCR	C29-C30-C25	5.05	118.25	110.48
22	b	617	CLA	C3C-C4C-NC	5.03	116.22	110.57
24	c	514	BCR	C33-C5-C4	-5.02	103.97	113.62
22	B	617	CLA	C3C-C4C-NC	5.02	116.20	110.57
22	b	609	CLA	C4A-NA-C1A	5.02	108.96	106.71
24	C	514	BCR	C33-C5-C4	-5.01	103.99	113.62
24	T	101	BCR	C2-C1-C6	5.00	118.18	110.48
24	C	515	BCR	C36-C18-C19	-5.00	110.20	118.08
24	c	515	BCR	C29-C30-C25	4.99	118.17	110.48
24	B	618	BCR	C2-C1-C6	4.99	118.16	110.48
24	c	515	BCR	C38-C26-C27	-4.99	104.03	113.62
24	C	515	BCR	C38-C26-C27	-4.99	104.04	113.62
24	C	515	BCR	C29-C30-C25	4.98	118.15	110.48
22	b	602	CLA	C2C-C1C-NC	4.98	114.63	109.97
24	c	515	BCR	C36-C18-C19	-4.97	110.25	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	101	BCR	C24-C23-C22	4.96	133.73	126.23
22	D	402	CLA	C4A-NA-C1A	4.95	108.93	106.71
22	B	602	CLA	C2C-C1C-NC	4.95	114.61	109.97
22	B	609	CLA	C4A-NA-C1A	4.95	108.93	106.71
24	k	101	BCR	C35-C13-C14	-4.94	116.00	122.92
24	K	101	BCR	C35-C13-C14	-4.94	116.01	122.92
22	A	604	CLA	C1C-C2C-C3C	-4.93	101.78	106.96
23	A	606	PHO	C3D-C2D-C1D	-4.91	98.71	105.87
24	B	622	BCR	C33-C5-C4	-4.91	104.18	113.62
24	T	102	BCR	C24-C23-C22	4.91	133.65	126.23
24	b	622	BCR	C33-C5-C4	-4.91	104.19	113.62
22	B	604	CLA	O2D-CGD-CBD	4.90	119.98	111.27
24	B	622	BCR	C38-C26-C27	-4.90	104.20	113.62
22	a	604	CLA	C1C-C2C-C3C	-4.90	101.81	106.96
24	c	514	BCR	C2-C1-C6	4.90	118.02	110.48
24	c	515	BCR	C36-C18-C17	-4.90	116.06	122.92
22	C	504	CLA	O2D-CGD-CBD	4.88	119.95	111.27
24	b	622	BCR	C38-C26-C27	-4.88	104.24	113.62
22	b	604	CLA	O2D-CGD-CBD	4.88	119.94	111.27
22	c	504	CLA	O2D-CGD-CBD	4.88	119.94	111.27
22	d	402	CLA	C4A-NA-C1A	4.88	108.90	106.71
23	a	606	PHO	C3D-C2D-C1D	-4.88	98.76	105.87
24	C	514	BCR	C2-C1-C6	4.87	117.97	110.48
24	D	404	BCR	C8-C7-C6	4.86	140.87	127.20
24	d	404	BCR	C8-C7-C6	4.86	140.85	127.20
22	c	512	CLA	C2C-C1C-NC	4.86	114.52	109.97
24	C	515	BCR	C36-C18-C17	-4.86	116.12	122.92
24	K	101	BCR	C4-C5-C6	4.86	129.78	122.73
22	B	616	CLA	C3C-C4C-NC	4.85	116.01	110.57
24	D	404	BCR	C7-C8-C9	4.85	133.57	126.23
22	A	604	CLA	O2D-CGD-CBD	4.85	119.88	111.27
24	d	404	BCR	C7-C8-C9	4.85	133.56	126.23
22	b	616	CLA	C3C-C4C-NC	4.84	116.00	110.57
24	k	101	BCR	C4-C5-C6	4.84	129.76	122.73
22	a	604	CLA	O2D-CGD-CBD	4.84	119.86	111.27
22	D	402	CLA	C3C-C4C-NC	4.82	115.98	110.57
22	b	609	CLA	O2D-CGD-CBD	4.82	119.84	111.27
22	b	603	CLA	C2C-C1C-NC	4.82	114.49	109.97
24	D	404	BCR	C4-C5-C6	4.81	129.72	122.73
22	B	609	CLA	O2D-CGD-CBD	4.81	119.82	111.27
24	B	622	BCR	C23-C22-C21	4.81	126.32	118.94
22	C	512	CLA	C2C-C1C-NC	4.81	114.48	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	402	CLA	C3C-C4C-NC	4.80	115.95	110.57
24	d	404	BCR	C4-C5-C6	4.79	129.69	122.73
24	a	608	BCR	C36-C18-C19	-4.78	110.54	118.08
24	C	515	BCR	C38-C26-C25	4.78	129.90	124.53
24	A	608	BCR	C36-C18-C19	-4.78	110.55	118.08
22	B	603	CLA	C2C-C1C-NC	4.78	114.45	109.97
24	c	515	BCR	C38-C26-C25	4.77	129.89	124.53
24	b	622	BCR	C23-C22-C21	4.77	126.27	118.94
22	b	613	CLA	O2D-CGD-CBD	4.75	119.71	111.27
22	B	613	CLA	O2D-CGD-CBD	4.73	119.68	111.27
22	C	509	CLA	O2D-CGD-CBD	4.72	119.66	111.27
24	b	618	BCR	C27-C26-C25	4.72	129.58	122.73
22	C	513	CLA	C2C-C1C-NC	4.72	114.39	109.97
22	b	602	CLA	C4D-C3D-CAD	4.72	111.10	108.47
24	B	619	BCR	C33-C5-C4	-4.70	104.58	113.62
24	B	619	BCR	C27-C26-C25	4.70	129.56	122.73
22	c	509	CLA	O2D-CGD-CBD	4.70	119.62	111.27
22	b	604	CLA	C1C-C2C-C3C	-4.70	102.01	106.96
29	z	101	LMG	O7-C10-C11	4.69	121.60	111.50
29	Z	101	LMG	O7-C10-C11	4.69	121.60	111.50
22	B	604	CLA	C1C-C2C-C3C	-4.68	102.03	106.96
24	C	514	BCR	C27-C26-C25	4.68	129.53	122.73
24	b	618	BCR	C33-C5-C4	-4.68	104.62	113.62
22	c	513	CLA	C2C-C1C-NC	4.68	114.36	109.97
24	k	102	BCR	C35-C13-C12	-4.68	110.70	118.08
24	c	514	BCR	C27-C26-C25	4.68	129.53	122.73
22	C	506	CLA	C3C-C4C-NC	4.68	115.82	110.57
25	A	609	SQD	O6-C1-C2	4.68	115.61	108.30
24	K	102	BCR	C35-C13-C12	-4.68	110.71	118.08
25	a	609	SQD	O6-C1-C2	4.67	115.59	108.30
22	b	604	CLA	C3C-C4C-NC	4.66	115.80	110.57
24	K	101	BCR	C23-C24-C25	4.66	140.29	127.20
24	k	101	BCR	C23-C24-C25	4.66	140.28	127.20
22	b	615	CLA	O2D-CGD-CBD	4.65	119.53	111.27
24	D	404	BCR	C33-C5-C4	-4.65	104.68	113.62
22	B	602	CLA	C4D-C3D-CAD	4.65	111.06	108.47
22	B	615	CLA	O2D-CGD-CBD	4.64	119.52	111.27
22	c	506	CLA	C3C-C4C-NC	4.64	115.78	110.57
22	B	604	CLA	C3C-C4C-NC	4.64	115.78	110.57
22	B	609	CLA	C3C-C4C-NC	4.64	115.77	110.57
22	B	613	CLA	C3C-C4C-NC	4.63	115.76	110.57
22	B	605	CLA	C1C-C2C-C3C	-4.61	102.11	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
22	A	603	CLA	C3C-C4C-NC	4.60	115.73	110.57
25	L	101	SQD	O6-C1-C2	4.60	115.49	108.30
22	b	613	CLA	C3C-C4C-NC	4.60	115.73	110.57
24	d	404	BCR	C33-C5-C4	-4.60	104.78	113.62
24	c	514	BCR	C35-C13-C12	-4.60	110.83	118.08
24	C	514	BCR	C35-C13-C12	-4.60	110.84	118.08
24	C	515	BCR	C35-C13-C14	-4.59	116.50	122.92
24	c	515	BCR	C35-C13-C14	-4.58	116.51	122.92
22	b	609	CLA	C3C-C4C-NC	4.58	115.71	110.57
22	C	508	CLA	O2D-CGD-CBD	4.58	119.40	111.27
22	B	610	CLA	C3C-C4C-NC	4.58	115.70	110.57
24	B	619	BCR	C2-C1-C6	4.57	117.52	110.48
22	a	603	CLA	C3C-C4C-NC	4.56	115.69	110.57
24	b	618	BCR	C2-C1-C6	4.56	117.50	110.48
22	c	508	CLA	O2D-CGD-CBD	4.56	119.36	111.27
25	l	101	SQD	O6-C1-C2	4.56	115.42	108.30
22	B	611	CLA	C3C-C4C-NC	4.55	115.67	110.57
22	C	504	CLA	C1C-C2C-C3C	-4.54	102.18	106.96
22	c	502	CLA	C3C-C4C-NC	4.54	115.66	110.57
31	d	410	DGD	O2G-C1B-C2B	4.53	121.27	111.50
22	B	610	CLA	O2D-CGD-CBD	4.53	119.31	111.27
22	b	610	CLA	O2D-CGD-CBD	4.53	119.31	111.27
22	b	611	CLA	C3C-C4C-NC	4.53	115.65	110.57
31	D	410	DGD	O2G-C1B-C2B	4.52	121.25	111.50
24	T	102	BCR	C34-C9-C8	-4.52	110.96	118.08
22	c	511	CLA	C3C-C4C-NC	4.52	115.64	110.57
22	C	511	CLA	C3C-C4C-NC	4.52	115.64	110.57
24	t	101	BCR	C34-C9-C8	-4.51	110.98	118.08
22	C	502	CLA	C3C-C4C-NC	4.50	115.62	110.57
22	c	505	CLA	O2D-CGD-CBD	4.49	119.25	111.27
22	C	505	CLA	O2D-CGD-CBD	4.49	119.24	111.27
22	c	504	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
22	b	610	CLA	C3C-C4C-NC	4.48	115.60	110.57
24	d	404	BCR	C35-C13-C12	-4.48	111.02	118.08
22	A	604	CLA	C3B-C4B-NB	4.47	114.99	109.21
24	D	404	BCR	C35-C13-C12	-4.47	111.03	118.08
22	A	604	CLA	C3C-C4C-NC	4.46	115.58	110.57
24	T	101	BCR	C37-C22-C23	-4.45	111.06	118.08
24	b	622	BCR	C35-C13-C14	-4.44	116.70	122.92
22	a	604	CLA	C3C-C4C-NC	4.44	115.55	110.57
22	b	614	CLA	C3C-C4C-NC	4.44	115.55	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	402	CLA	O2D-CGD-CBD	4.44	119.15	111.27
23	A	606	PHO	C4C-C3C-C2C	-4.43	101.87	106.78
22	a	604	CLA	C3B-C4B-NB	4.43	114.94	109.21
22	B	609	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
22	c	509	CLA	C3C-C4C-NC	4.43	115.54	110.57
24	d	404	BCR	C36-C18-C19	-4.43	111.10	118.08
23	a	606	PHO	C4C-C3C-C2C	-4.43	101.88	106.78
24	B	622	BCR	C35-C13-C14	-4.42	116.73	122.92
24	B	618	BCR	C37-C22-C23	-4.42	111.11	118.08
24	H	101	BCR	C35-C13-C14	-4.42	116.73	122.92
24	h	101	BCR	C35-C13-C14	-4.42	116.73	122.92
22	d	402	CLA	O2D-CGD-CBD	4.42	119.11	111.27
22	b	609	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
22	c	501	CLA	O2D-CGD-O1D	-4.41	115.22	123.84
24	D	404	BCR	C36-C18-C19	-4.41	111.13	118.08
22	c	505	CLA	C3C-C4C-NC	4.40	115.51	110.57
22	C	501	CLA	O2D-CGD-O1D	-4.40	115.23	123.84
24	t	101	BCR	C8-C7-C6	4.40	139.56	127.20
22	C	505	CLA	C3C-C4C-NC	4.40	115.50	110.57
24	T	102	BCR	C8-C7-C6	4.40	139.55	127.20
22	C	503	CLA	C3C-C4C-NC	4.40	115.50	110.57
22	C	509	CLA	C3C-C4C-NC	4.39	115.50	110.57
22	c	509	CLA	C4D-C3D-CAD	4.39	110.92	108.47
22	B	614	CLA	C3C-C4C-NC	4.39	115.49	110.57
24	t	101	BCR	C29-C30-C25	4.39	117.23	110.48
22	c	503	CLA	C3C-C4C-NC	4.38	115.49	110.57
22	C	507	CLA	O2D-CGD-CBD	4.38	119.06	111.27
24	T	102	BCR	C29-C30-C25	4.37	117.21	110.48
24	c	514	BCR	C30-C25-C26	-4.37	116.45	122.61
22	c	507	CLA	O2D-CGD-CBD	4.37	119.03	111.27
24	c	514	BCR	C32-C1-C6	4.37	117.38	110.30
24	K	101	BCR	C1-C6-C5	-4.37	116.46	122.61
24	k	101	BCR	C1-C6-C5	-4.36	116.47	122.61
24	C	514	BCR	C32-C1-C6	4.36	117.36	110.30
22	c	513	CLA	O2D-CGD-CBD	4.35	119.00	111.27
24	C	514	BCR	C30-C25-C26	-4.35	116.49	122.61
22	C	513	CLA	O2D-CGD-CBD	4.35	118.99	111.27
25	a	609	SQD	O47-C7-C8	4.34	120.86	111.50
25	A	609	SQD	O47-C7-C8	4.34	120.86	111.50
24	D	404	BCR	C23-C24-C25	4.33	139.37	127.20
22	c	508	CLA	C3C-C4C-NC	4.33	115.43	110.57
24	T	101	BCR	C30-C25-C26	-4.33	116.51	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	BCR	C23-C24-C25	4.33	139.35	127.20
22	C	509	CLA	C4D-C3D-CAD	4.32	110.88	108.47
24	d	404	BCR	C38-C26-C27	-4.31	105.33	113.62
22	c	509	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
24	D	404	BCR	C38-C26-C27	-4.31	105.34	113.62
25	A	609	SQD	O9-S-C6	4.31	112.06	106.94
22	A	607	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
22	b	609	CLA	C3B-C4B-NB	4.30	114.77	109.21
24	B	618	BCR	C30-C25-C26	-4.30	116.55	122.61
22	C	508	CLA	C3C-C4C-NC	4.30	115.39	110.57
25	a	609	SQD	O9-S-C6	4.30	112.05	106.94
22	a	607	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
22	B	608	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
22	b	607	CLA	C3C-C4C-NC	4.28	115.38	110.57
22	B	609	CLA	C3B-C4B-NB	4.28	114.74	109.21
25	b	621	SQD	O6-C1-C2	4.28	114.98	108.30
22	B	607	CLA	C3C-C4C-NC	4.27	115.36	110.57
31	C	516	DGD	O2G-C1B-C2B	4.27	120.71	111.50
24	h	101	BCR	C28-C27-C26	4.27	121.70	114.08
22	C	509	CLA	C1C-C2C-C3C	-4.26	102.47	106.96
22	b	614	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
24	H	101	BCR	C28-C27-C26	4.26	121.68	114.08
22	B	614	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
22	B	612	CLA	O2D-CGD-CBD	4.25	118.83	111.27
23	a	605	PHO	C2D-C1D-ND	4.25	116.21	109.79
31	c	516	DGD	O2G-C1B-C2B	4.25	120.66	111.50
24	b	618	BCR	C8-C7-C6	4.25	139.13	127.20
22	B	603	CLA	C3C-C4C-NC	4.25	115.33	110.57
24	B	619	BCR	C8-C7-C6	4.25	139.13	127.20
22	b	612	CLA	O2D-CGD-CBD	4.24	118.81	111.27
25	l	102	SQD	O6-C1-C2	4.24	114.92	108.30
22	b	607	CLA	O2D-CGD-O1D	-4.23	115.56	123.84
23	a	605	PHO	O2D-CGD-CBD	4.23	118.79	111.27
22	C	510	CLA	C3C-C4C-NC	4.23	115.31	110.57
22	b	608	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
22	B	607	CLA	O2D-CGD-O1D	-4.23	115.58	123.84
23	A	605	PHO	O2D-CGD-CBD	4.22	118.77	111.27
23	A	605	PHO	C2D-C1D-ND	4.22	116.16	109.79
22	c	510	CLA	C3C-C4C-NC	4.21	115.30	110.57
22	c	512	CLA	C3C-C4C-NC	4.21	115.29	110.57
24	C	514	BCR	C23-C22-C21	4.21	125.40	118.94
24	t	101	BCR	C2-C1-C6	4.21	116.96	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	C3B-C4B-NB	4.20	114.64	109.21
22	b	604	CLA	C3B-C4B-NB	4.20	114.64	109.21
24	c	514	BCR	C23-C22-C21	4.20	125.39	118.94
22	b	602	CLA	C3C-C4C-NC	4.20	115.28	110.57
22	b	603	CLA	C3C-C4C-NC	4.20	115.28	110.57
24	B	619	BCR	C33-C5-C6	4.20	129.24	124.53
22	B	604	CLA	C3B-C4B-NB	4.19	114.63	109.21
24	K	101	BCR	C38-C26-C27	-4.19	105.56	113.62
24	T	102	BCR	C30-C25-C26	-4.19	116.71	122.61
24	k	101	BCR	C38-C26-C27	-4.19	105.57	113.62
24	T	102	BCR	C2-C1-C6	4.19	116.93	110.48
24	t	101	BCR	C30-C25-C26	-4.19	116.72	122.61
24	c	514	BCR	C36-C18-C19	-4.18	111.49	118.08
24	b	618	BCR	C33-C5-C6	4.18	129.22	124.53
22	C	513	CLA	C3C-C4C-NC	4.17	115.25	110.57
22	C	512	CLA	C3C-C4C-NC	4.17	115.25	110.57
22	c	501	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
24	C	514	BCR	C36-C18-C19	-4.17	111.51	118.08
22	b	608	CLA	C3B-C4B-NB	4.17	114.60	109.21
22	A	607	CLA	O2D-CGD-CBD	4.17	118.67	111.27
22	C	501	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
23	a	605	PHO	C4C-C3C-C2C	-4.16	102.17	106.78
22	A	607	CLA	C3C-C4C-NC	4.16	115.24	110.57
24	B	618	BCR	C29-C30-C25	4.16	116.88	110.48
22	c	511	CLA	O2D-CGD-CBD	4.15	118.65	111.27
24	T	102	BCR	C35-C13-C14	-4.15	117.11	122.92
24	T	101	BCR	C35-C13-C14	-4.15	117.11	122.92
24	T	101	BCR	C29-C30-C25	4.15	116.87	110.48
25	d	411	SQD	O6-C1-C2	4.15	114.78	108.30
22	B	602	CLA	C3C-C4C-NC	4.14	115.22	110.57
25	D	411	SQD	O6-C1-C2	4.14	114.77	108.30
24	t	101	BCR	C23-C24-C25	4.14	138.83	127.20
23	A	605	PHO	C4C-C3C-C2C	-4.14	102.20	106.78
24	B	618	BCR	C35-C13-C14	-4.14	117.13	122.92
24	C	515	BCR	C33-C5-C4	-4.14	105.67	113.62
22	C	511	CLA	O2D-CGD-CBD	4.13	118.61	111.27
24	c	515	BCR	C33-C5-C4	-4.13	105.67	113.62
22	a	607	CLA	C3C-C4C-NC	4.13	115.20	110.57
22	B	615	CLA	C3C-C4C-NC	4.13	115.20	110.57
24	T	102	BCR	C23-C24-C25	4.13	138.80	127.20
22	a	607	CLA	O2D-CGD-CBD	4.13	118.60	111.27
22	b	615	CLA	C3C-C4C-NC	4.13	115.20	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	101	BCR	C35-C13-C14	-4.12	117.14	122.92
24	C	514	BCR	C23-C24-C25	4.12	138.78	127.20
22	c	507	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
22	c	513	CLA	C3C-C4C-NC	4.12	115.19	110.57
24	B	618	BCR	C38-C26-C25	4.12	129.15	124.53
24	c	514	BCR	C23-C24-C25	4.11	138.73	127.20
22	C	507	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
24	C	515	BCR	C8-C9-C10	4.09	125.22	118.94
24	b	618	BCR	C35-C13-C12	-4.09	111.64	118.08
23	A	606	PHO	CAC-C3C-C4C	4.08	129.68	125.22
23	a	606	PHO	CAC-C3C-C4C	4.08	129.68	125.22
24	T	101	BCR	C38-C26-C25	4.08	129.11	124.53
23	a	605	PHO	C2C-C1C-NC	4.08	115.95	109.79
24	B	622	BCR	C8-C9-C10	4.08	125.19	118.94
24	b	622	BCR	C8-C9-C10	4.07	125.19	118.94
24	B	619	BCR	C35-C13-C12	-4.07	111.67	118.08
22	d	403	CLA	C3C-C4C-NC	4.07	115.13	110.57
22	c	502	CLA	O2D-CGD-CBD	4.06	118.49	111.27
24	b	622	BCR	C30-C25-C26	-4.06	116.89	122.61
23	A	606	PHO	O2D-CGD-CBD	4.06	118.48	111.27
22	C	502	CLA	O2D-CGD-CBD	4.06	118.48	111.27
24	c	515	BCR	C8-C9-C10	4.06	125.17	118.94
23	A	605	PHO	C2C-C1C-NC	4.05	115.91	109.79
24	t	101	BCR	C33-C5-C6	4.05	129.08	124.53
23	a	606	PHO	O2D-CGD-CBD	4.05	118.47	111.27
24	h	101	BCR	C8-C7-C6	4.05	138.58	127.20
24	H	101	BCR	C8-C7-C6	4.04	138.54	127.20
24	h	101	BCR	C38-C26-C27	-4.03	105.87	113.62
22	D	403	CLA	C3C-C4C-NC	4.03	115.09	110.57
24	H	101	BCR	C38-C26-C27	-4.03	105.88	113.62
23	a	605	PHO	C3C-C4C-NC	4.02	116.52	110.28
22	c	507	CLA	C3C-C4C-NC	4.02	115.08	110.57
24	B	622	BCR	C30-C25-C26	-4.01	116.96	122.61
22	d	403	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
24	h	101	BCR	C36-C18-C17	-4.01	117.31	122.92
24	H	101	BCR	C36-C18-C17	-4.00	117.31	122.92
24	T	102	BCR	C33-C5-C6	4.00	129.02	124.53
22	C	503	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
22	b	602	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	A	605	PHO	C3C-C4C-NC	3.99	116.46	110.28
22	C	513	CLA	C4D-C3D-CAD	3.99	110.69	108.47
24	T	102	BCR	C37-C22-C21	-3.99	117.34	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	403	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
24	a	608	BCR	C23-C24-C25	3.98	138.38	127.20
24	b	622	BCR	C27-C26-C25	3.98	128.51	122.73
22	B	607	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
32	E	101	LHG	O7-C7-C8	3.98	120.07	111.50
22	B	617	CLA	O2D-CGD-CBD	3.97	118.33	111.27
32	e	101	LHG	O7-C7-C8	3.97	120.06	111.50
24	t	101	BCR	C37-C22-C21	-3.97	117.36	122.92
22	B	602	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
24	B	622	BCR	C27-C26-C25	3.97	128.49	122.73
24	A	608	BCR	C23-C24-C25	3.97	138.34	127.20
22	b	603	CLA	O2D-CGD-CBD	3.96	118.31	111.27
25	b	621	SQD	O47-C7-C8	3.96	120.03	111.50
22	C	506	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
22	C	507	CLA	C3C-C4C-NC	3.95	115.00	110.57
22	c	503	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
22	c	510	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
25	l	102	SQD	O47-C7-C8	3.95	120.01	111.50
22	B	603	CLA	O2D-CGD-CBD	3.94	118.28	111.27
24	k	102	BCR	C30-C25-C26	-3.94	117.06	122.61
22	b	607	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
22	b	617	CLA	O2D-CGD-CBD	3.94	118.27	111.27
22	B	606	CLA	C4-C3-C5	3.92	121.87	115.27
24	K	102	BCR	C30-C25-C26	-3.92	117.09	122.61
22	b	606	CLA	C4-C3-C5	3.92	121.86	115.27
22	c	513	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
24	k	102	BCR	C38-C26-C27	-3.91	106.10	113.62
29	B	620	LMG	O7-C10-C11	3.91	119.93	111.50
22	C	513	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
22	C	511	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
24	K	102	BCR	C38-C26-C27	-3.90	106.12	113.62
29	b	619	LMG	O7-C10-C11	3.90	119.91	111.50
22	c	510	CLA	C3B-C4B-NB	3.90	114.25	109.21
22	a	603	CLA	C3B-C4B-NB	3.90	114.25	109.21
24	C	515	BCR	C31-C1-C2	-3.90	93.32	108.91
24	c	515	BCR	C31-C1-C2	-3.90	93.32	108.91
22	C	510	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
22	c	506	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
22	b	610	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
22	C	510	CLA	C3B-C4B-NB	3.89	114.23	109.21
25	b	621	SQD	O7-S-C6	3.88	111.56	106.94
22	c	513	CLA	C4D-C3D-CAD	3.88	110.63	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	C3C-C4C-NC	3.88	114.92	110.57
22	B	610	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
22	A	603	CLA	C3B-C4B-NB	3.88	114.22	109.21
22	c	511	CLA	C1C-C2C-C3C	-3.87	102.88	106.96
24	T	101	BCR	C23-C24-C25	3.87	138.08	127.20
24	c	514	BCR	C32-C1-C2	-3.87	93.42	108.91
24	B	618	BCR	C23-C24-C25	3.87	138.07	127.20
24	B	619	BCR	C40-C30-C29	-3.87	93.43	108.91
24	b	618	BCR	C40-C30-C29	-3.87	93.44	108.91
24	C	514	BCR	C32-C1-C2	-3.86	93.45	108.91
22	c	501	CLA	C3C-C4C-NC	3.86	114.90	110.57
29	C	520	LMG	O7-C10-C11	3.86	119.81	111.50
25	l	102	SQD	O7-S-C6	3.85	111.51	106.94
22	A	603	CLA	CMB-C2B-C3B	3.85	131.87	124.68
22	c	508	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
22	b	615	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
22	C	501	CLA	C3C-C4C-NC	3.84	114.88	110.57
22	B	615	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	C	515	BCR	C2-C1-C6	3.83	116.38	110.48
22	b	606	CLA	O2D-CGD-CBD	3.83	118.08	111.27
22	b	608	CLA	C3C-C4C-NC	3.83	114.86	110.57
24	d	404	BCR	C37-C22-C21	-3.83	117.56	122.92
29	c	520	LMG	O7-C10-C11	3.82	119.74	111.50
22	B	606	CLA	O2D-CGD-CBD	3.82	118.06	111.27
23	a	605	PHO	C4A-NA-C1A	3.82	111.22	108.14
22	c	503	CLA	O2D-CGD-CBD	3.82	118.05	111.27
22	a	603	CLA	CMB-C2B-C3B	3.82	131.82	124.68
22	A	603	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
24	c	515	BCR	C2-C1-C6	3.81	116.35	110.48
29	C	519	LMG	O7-C10-C11	3.81	119.71	111.50
25	l	102	SQD	C3-C4-C5	3.80	117.01	110.24
22	C	510	CLA	O2D-CGD-CBD	3.79	118.01	111.27
25	b	621	SQD	C3-C4-C5	3.79	117.01	110.24
24	D	404	BCR	C37-C22-C21	-3.79	117.61	122.92
29	z	101	LMG	O1-C1-C2	3.79	114.22	108.30
22	C	503	CLA	O2D-CGD-CBD	3.79	118.00	111.27
28	D	408	PL9	C40-C39-C41	3.79	121.64	115.27
22	C	508	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
22	a	603	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
22	c	510	CLA	O2D-CGD-CBD	3.78	117.99	111.27
23	A	606	PHO	C2D-C1D-ND	3.78	115.50	109.79
29	c	519	LMG	O7-C10-C11	3.78	119.64	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	618	BCR	C8-C7-C6	3.76	137.77	127.20
23	A	605	PHO	C4A-NA-C1A	3.76	111.18	108.14
29	Z	101	LMG	O1-C1-C2	3.76	114.17	108.30
23	a	606	PHO	C2D-C1D-ND	3.76	115.46	109.79
28	d	408	PL9	C40-C39-C41	3.75	121.58	115.27
22	B	616	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
22	B	607	CLA	C4D-C3D-CAD	3.75	110.56	108.47
22	d	402	CLA	C3B-C4B-NB	3.75	114.06	109.21
25	l	101	SQD	O47-C7-C8	3.74	119.57	111.50
24	T	101	BCR	C8-C7-C6	3.74	137.71	127.20
25	D	411	SQD	O47-C7-C8	3.74	119.56	111.50
22	A	607	CLA	C3B-C4B-NB	3.74	114.04	109.21
25	d	411	SQD	O47-C7-C8	3.74	119.55	111.50
25	L	101	SQD	O47-C7-C8	3.73	119.54	111.50
22	D	402	CLA	C3B-C4B-NB	3.73	114.03	109.21
22	a	607	CLA	C3B-C4B-NB	3.73	114.03	109.21
22	b	616	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
24	K	102	BCR	C33-C5-C4	-3.72	106.47	113.62
31	C	517	DGD	O2G-C1B-C2B	3.72	119.52	111.50
22	B	607	CLA	O2D-CGD-CBD	3.71	117.86	111.27
24	k	102	BCR	C33-C5-C4	-3.71	106.49	113.62
24	c	514	BCR	C37-C22-C21	-3.71	117.73	122.92
22	b	607	CLA	O2D-CGD-CBD	3.71	117.85	111.27
23	a	606	PHO	C2B-C1B-NB	3.70	115.37	109.79
31	c	517	DGD	O2G-C1B-C2B	3.70	119.47	111.50
24	C	514	BCR	C37-C22-C21	-3.70	117.75	122.92
23	A	606	PHO	C2B-C1B-NB	3.70	115.37	109.79
25	L	101	SQD	O7-S-C6	3.69	111.33	106.94
23	a	606	PHO	C3C-C4C-NC	3.69	116.00	110.28
24	d	404	BCR	C35-C13-C14	-3.69	117.75	122.92
23	A	606	PHO	C3C-C4C-NC	3.69	116.00	110.28
22	b	607	CLA	C4D-C3D-CAD	3.69	110.53	108.47
24	D	404	BCR	C35-C13-C14	-3.68	117.76	122.92
24	c	515	BCR	C33-C5-C6	3.68	128.66	124.53
24	C	515	BCR	C33-C5-C6	3.68	128.66	124.53
28	a	613	PL9	C20-C19-C21	3.67	121.45	115.27
22	C	512	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
22	c	512	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
22	c	504	CLA	C3B-C4B-NB	3.67	113.96	109.21
24	K	102	BCR	C32-C1-C6	3.67	116.25	110.30
22	b	605	CLA	C3B-C4B-NB	3.67	113.95	109.21
24	h	101	BCR	C24-C23-C22	3.67	131.77	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	l	101	SQD	O7-S-C6	3.66	111.29	106.94
24	B	618	BCR	C27-C26-C25	3.65	128.04	122.73
24	K	102	BCR	C2-C1-C6	3.65	116.11	110.48
22	B	605	CLA	C3B-C4B-NB	3.65	113.93	109.21
22	B	612	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
28	A	613	PL9	C20-C19-C21	3.65	121.41	115.27
22	C	511	CLA	C3B-C4B-NB	3.65	113.93	109.21
24	T	101	BCR	C27-C26-C25	3.65	128.03	122.73
24	k	102	BCR	C32-C1-C6	3.64	116.21	110.30
24	H	101	BCR	C24-C23-C22	3.64	131.74	126.23
22	b	611	CLA	O2D-CGD-CBD	3.64	117.74	111.27
22	c	509	CLA	C3B-C4B-NB	3.64	113.92	109.21
24	k	102	BCR	C2-C1-C6	3.63	116.07	110.48
22	B	611	CLA	O2D-CGD-CBD	3.63	117.72	111.27
22	C	509	CLA	C3B-C4B-NB	3.63	113.90	109.21
22	C	503	CLA	CMB-C2B-C3B	3.63	131.47	124.68
22	b	605	CLA	O2D-CGD-CBD	3.62	117.71	111.27
22	b	612	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
22	C	505	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
22	b	603	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
22	c	505	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
22	B	605	CLA	O2D-CGD-CBD	3.61	117.68	111.27
22	C	504	CLA	C3B-C4B-NB	3.61	113.87	109.21
22	c	511	CLA	C3B-C4B-NB	3.61	113.87	109.21
22	C	502	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
24	k	101	BCR	C27-C26-C25	3.60	127.95	122.73
22	c	508	CLA	C3B-C4B-NB	3.59	113.85	109.21
22	c	503	CLA	CMB-C2B-C3B	3.59	131.39	124.68
22	c	502	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
24	K	101	BCR	C27-C26-C25	3.58	127.93	122.73
22	d	401	CLA	C3B-C4B-NB	3.58	113.84	109.21
22	a	607	CLA	C4-C3-C5	3.58	121.29	115.27
22	D	401	CLA	C3B-C4B-NB	3.58	113.83	109.21
22	C	508	CLA	C3B-C4B-NB	3.58	113.83	109.21
22	a	604	CLA	CMB-C2B-C3B	3.58	131.37	124.68
22	B	603	CLA	C1C-C2C-C3C	-3.58	103.20	106.96
22	A	604	CLA	CMB-C2B-C3B	3.57	131.36	124.68
24	a	608	BCR	C35-C13-C12	-3.57	112.45	118.08
24	A	608	BCR	C35-C13-C12	-3.57	112.46	118.08
22	A	607	CLA	C4-C3-C5	3.56	121.26	115.27
22	B	611	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
22	b	611	CLA	C1C-C2C-C3C	-3.55	103.22	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C3B-C4B-NB	3.55	113.79	109.21
22	d	403	CLA	C3B-C4B-NB	3.54	113.79	109.21
22	b	610	CLA	C3B-C4B-NB	3.54	113.78	109.21
22	B	615	CLA	C3B-C4B-NB	3.53	113.77	109.21
22	B	613	CLA	CAC-C3C-C4C	3.53	129.39	124.81
22	B	604	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
22	b	606	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
22	D	403	CLA	C3B-C4B-NB	3.53	113.77	109.21
24	b	618	BCR	C37-C22-C23	-3.52	112.53	118.08
22	b	615	CLA	C3B-C4B-NB	3.52	113.76	109.21
24	H	101	BCR	C23-C24-C25	3.51	137.07	127.20
22	b	613	CLA	CAC-C3C-C4C	3.51	129.37	124.81
22	b	617	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
24	h	101	BCR	C23-C24-C25	3.51	137.06	127.20
22	b	614	CLA	C3B-C4B-NB	3.50	113.74	109.21
24	B	619	BCR	C37-C22-C23	-3.50	112.56	118.08
22	B	614	CLA	C3B-C4B-NB	3.50	113.74	109.21
24	a	608	BCR	C33-C5-C4	-3.50	106.89	113.62
22	B	617	CLA	C4C-C3C-C2C	-3.50	101.80	106.90
24	D	404	BCR	C1-C6-C5	-3.49	117.69	122.61
24	A	608	BCR	C33-C5-C4	-3.49	106.91	113.62
22	B	606	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
23	a	606	PHO	C4A-NA-C1A	3.49	110.96	108.14
24	k	102	BCR	C24-C23-C22	3.49	131.50	126.23
24	K	102	BCR	C24-C23-C22	3.49	131.50	126.23
24	d	404	BCR	C1-C6-C5	-3.48	117.72	122.61
22	b	616	CLA	C3B-C4B-NB	3.47	113.70	109.21
22	b	605	CLA	CED-O2D-CGD	3.47	123.78	115.94
22	b	611	CLA	C3B-C4B-NB	3.47	113.69	109.21
24	T	102	BCR	C4-C5-C6	3.46	127.76	122.73
22	b	604	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
22	B	605	CLA	CED-O2D-CGD	3.46	123.77	115.94
22	B	611	CLA	C3B-C4B-NB	3.46	113.69	109.21
22	B	606	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
24	T	102	BCR	C27-C26-C25	3.46	127.75	122.73
22	d	401	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
22	b	612	CLA	C3B-C4B-NB	3.45	113.68	109.21
24	t	101	BCR	C27-C26-C25	3.45	127.75	122.73
24	A	608	BCR	C34-C9-C8	-3.45	112.64	118.08
22	d	401	CLA	CMB-C2B-C3B	3.45	131.14	124.68
22	D	401	CLA	CMB-C2B-C3B	3.45	131.14	124.68
24	D	404	BCR	C27-C26-C25	3.45	127.74	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	404	BCR	C32-C1-C2	-3.45	95.11	108.91
24	T	102	BCR	C36-C18-C19	-3.45	112.64	118.08
24	d	404	BCR	C27-C26-C25	3.45	127.74	122.73
23	A	606	PHO	C4A-NA-C1A	3.45	110.92	108.14
24	t	101	BCR	C4-C5-C6	3.45	127.73	122.73
22	D	401	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
24	d	404	BCR	C32-C1-C2	-3.44	95.15	108.91
22	b	615	CLA	C4-C3-C5	3.44	121.06	115.27
22	c	504	CLA	C3C-C4C-NC	3.44	114.42	110.57
22	B	615	CLA	C4-C3-C5	3.43	121.05	115.27
22	C	504	CLA	C3C-C4C-NC	3.43	114.42	110.57
22	b	606	CLA	C4C-C3C-C2C	-3.41	101.92	106.90
25	b	601	SQD	O9-S-C6	3.41	111.00	106.94
22	B	616	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	a	608	BCR	C34-C9-C8	-3.41	112.70	118.08
22	B	604	CLA	C4D-C3D-CAD	3.41	110.37	108.47
24	t	101	BCR	C36-C18-C19	-3.41	112.71	118.08
22	d	401	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
25	B	601	SQD	O9-S-C6	3.40	110.98	106.94
25	B	601	SQD	O47-C7-C8	3.39	118.80	111.50
23	a	605	PHO	C2B-C1B-NB	3.39	114.90	109.79
22	D	401	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
24	K	101	BCR	C2-C1-C6	3.39	115.69	110.48
25	b	601	SQD	O47-C7-C8	3.38	118.79	111.50
24	T	102	BCR	C35-C13-C12	-3.38	112.75	118.08
23	A	605	PHO	C2B-C1B-NB	3.38	114.89	109.79
24	k	101	BCR	C2-C1-C6	3.38	115.68	110.48
24	t	101	BCR	C35-C13-C12	-3.38	112.76	118.08
25	a	609	SQD	O8-S-C6	3.37	111.12	105.74
24	C	515	BCR	C40-C30-C25	3.36	115.76	110.30
24	H	101	BCR	C27-C26-C25	3.36	127.61	122.73
22	B	612	CLA	C3B-C4B-NB	3.36	113.56	109.21
22	c	502	CLA	CAC-C3C-C4C	3.36	129.17	124.81
22	b	615	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
24	c	515	BCR	C40-C30-C25	3.35	115.74	110.30
22	b	617	CLA	CAC-C3C-C4C	3.35	129.16	124.81
22	b	604	CLA	C4D-C3D-CAD	3.35	110.34	108.47
22	C	511	CLA	C4D-C3D-CAD	3.35	110.34	108.47
22	C	512	CLA	C4D-C3D-CAD	3.35	110.34	108.47
22	C	502	CLA	CAC-C3C-C4C	3.35	129.16	124.81
25	A	609	SQD	O8-S-C6	3.35	111.07	105.74
22	B	611	CLA	C4C-C3C-C2C	-3.35	102.02	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	101	BCR	C27-C26-C25	3.34	127.58	122.73
22	B	617	CLA	CAC-C3C-C4C	3.34	129.15	124.81
22	c	511	CLA	C4D-C3D-CAD	3.34	110.33	108.47
22	C	506	CLA	C4D-C3D-CAD	3.34	110.33	108.47
32	d	405	LHG	O8-C23-C24	3.33	122.36	111.91
32	D	405	LHG	O8-C23-C24	3.33	122.36	111.91
22	B	615	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
22	b	611	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
22	B	613	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
22	b	605	CLA	C4D-C3D-CAD	3.33	110.33	108.47
22	b	604	CLA	CMC-C2C-C1C	3.32	130.10	125.04
22	C	512	CLA	C4-C3-C5	3.32	120.86	115.27
22	D	402	CLA	CBC-CAC-C3C	-3.32	103.29	112.43
22	b	613	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
22	D	401	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
22	A	604	CLA	CAC-C3C-C4C	3.31	129.10	124.81
22	B	617	CLA	C3B-C4B-NB	3.31	113.49	109.21
22	c	512	CLA	C4D-C3D-CAD	3.31	110.31	108.47
25	A	609	SQD	C1-C2-C3	-3.30	103.11	110.00
25	a	609	SQD	C1-C2-C3	-3.30	103.12	110.00
22	c	512	CLA	C4-C3-C5	3.30	120.82	115.27
23	a	605	PHO	C4D-ND-C1D	-3.30	100.83	106.76
22	d	402	CLA	CBC-CAC-C3C	-3.30	103.34	112.43
22	d	401	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
29	a	614	LMG	O7-C10-C11	3.29	118.59	111.50
22	B	610	CLA	CAC-C3C-C4C	3.29	129.07	124.81
29	A	614	LMG	O7-C10-C11	3.28	118.58	111.50
23	A	605	PHO	C4D-ND-C1D	-3.28	100.86	106.76
22	c	506	CLA	C4D-C3D-CAD	3.28	110.30	108.47
22	C	511	CLA	C1-O2A-CGA	3.27	125.03	116.44
22	B	613	CLA	C4-C3-C5	3.27	120.77	115.27
22	b	610	CLA	CAC-C3C-C4C	3.27	129.05	124.81
22	a	604	CLA	CAC-C3C-C4C	3.27	129.05	124.81
22	b	616	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
22	B	604	CLA	CMC-C2C-C1C	3.26	130.01	125.04
22	B	616	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
22	b	617	CLA	C3B-C4B-NB	3.26	113.42	109.21
22	B	609	CLA	CMB-C2B-C3B	3.25	130.76	124.68
24	K	102	BCR	C31-C1-C6	3.25	115.57	110.30
22	b	609	CLA	CMB-C2B-C3B	3.25	130.76	124.68
24	k	102	BCR	C31-C1-C6	3.25	115.56	110.30
22	d	403	CLA	O2D-CGD-CBD	3.25	117.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	511	CLA	C1-O2A-CGA	3.24	124.95	116.44
22	C	505	CLA	C4D-C3D-CAD	3.24	110.28	108.47
22	b	613	CLA	C4-C3-C5	3.24	120.72	115.27
22	C	508	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
22	C	502	CLA	C3B-C4B-NB	3.24	113.39	109.21
22	b	613	CLA	CMB-C2B-C3B	3.24	130.73	124.68
22	c	505	CLA	C4D-C3D-CAD	3.24	110.27	108.47
22	c	508	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
22	c	502	CLA	C3B-C4B-NB	3.23	113.38	109.21
22	B	613	CLA	CMB-C2B-C3B	3.23	130.71	124.68
24	T	101	BCR	C32-C1-C6	3.22	115.53	110.30
22	B	612	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
22	D	403	CLA	O2D-CGD-CBD	3.22	116.99	111.27
22	B	605	CLA	C4D-C3D-CAD	3.22	110.27	108.47
22	b	612	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
22	D	401	CLA	O2D-CGD-CBD	3.21	116.98	111.27
22	d	401	CLA	O2D-CGD-CBD	3.21	116.98	111.27
23	a	606	PHO	C2C-C1C-NC	3.21	114.63	109.79
24	B	618	BCR	C32-C1-C6	3.21	115.50	110.30
23	a	606	PHO	C4-C3-C5	3.21	120.66	115.27
24	B	619	BCR	C34-C9-C10	-3.20	118.44	122.92
24	A	608	BCR	C30-C25-C24	3.20	124.83	115.78
24	B	619	BCR	C34-C9-C8	-3.20	113.04	118.08
23	A	606	PHO	C2C-C1C-NC	3.20	114.61	109.79
24	b	618	BCR	C34-C9-C8	-3.19	113.04	118.08
32	D	409	LHG	O7-C7-C8	3.19	118.38	111.50
22	c	513	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
33	v	201	HEM	C1D-C2D-C3D	-3.19	104.78	107.00
22	b	608	CLA	CED-O2D-CGD	3.19	123.14	115.94
22	B	608	CLA	CED-O2D-CGD	3.18	123.14	115.94
24	a	608	BCR	C30-C25-C24	3.18	124.78	115.78
22	b	607	CLA	C3B-C4B-NB	3.18	113.32	109.21
25	D	411	SQD	O7-S-C6	3.18	110.72	106.94
24	b	618	BCR	C34-C9-C10	-3.18	118.47	122.92
24	A	608	BCR	C40-C30-C25	3.17	115.44	110.30
31	C	518	DGD	O3G-C3G-C2G	-3.17	103.25	110.90
23	A	606	PHO	C4-C3-C5	3.17	120.60	115.27
25	d	411	SQD	O7-S-C6	3.17	110.70	106.94
32	d	409	LHG	O7-C7-C8	3.17	118.32	111.50
22	b	603	CLA	C4-C3-C5	3.16	120.59	115.27
22	C	507	CLA	CBC-CAC-C3C	-3.16	103.71	112.43
22	B	607	CLA	C3B-C4B-NB	3.16	113.30	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	CBC-CAC-C3C	-3.16	103.72	112.43
24	B	619	BCR	C38-C26-C25	3.16	128.08	124.53
24	a	608	BCR	C40-C30-C25	3.16	115.42	110.30
22	b	613	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
24	B	622	BCR	C34-C9-C8	-3.16	113.10	118.08
24	b	618	BCR	C38-C26-C25	3.15	128.07	124.53
22	C	513	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
22	c	507	CLA	C4D-C3D-CAD	3.15	110.23	108.47
31	c	518	DGD	O3G-C3G-C2G	-3.15	103.30	110.90
24	B	622	BCR	C36-C18-C19	-3.15	113.11	118.08
24	b	622	BCR	C36-C18-C19	-3.15	113.12	118.08
33	V	201	HEM	C1D-C2D-C3D	-3.15	104.81	107.00
22	B	616	CLA	O2D-CGD-CBD	3.14	116.86	111.27
24	b	622	BCR	C34-C9-C8	-3.14	113.13	118.08
22	B	603	CLA	C4-C3-C5	3.14	120.56	115.27
22	c	502	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
22	B	613	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
22	C	507	CLA	C4D-C3D-CAD	3.12	110.21	108.47
22	A	604	CLA	C4-C3-C5	3.12	120.52	115.27
22	b	616	CLA	C4D-C3D-CAD	3.12	110.21	108.47
22	b	616	CLA	O2D-CGD-CBD	3.11	116.80	111.27
32	L	102	LHG	O7-C7-C8	3.11	118.21	111.50
22	a	604	CLA	C4-C3-C5	3.11	120.51	115.27
22	b	608	CLA	CBC-CAC-C3C	-3.11	103.85	112.43
22	c	510	CLA	C4D-C3D-CAD	3.11	110.20	108.47
22	B	608	CLA	CBC-CAC-C3C	-3.11	103.86	112.43
32	l	103	LHG	O7-C7-C8	3.11	118.20	111.50
25	D	411	SQD	O9-S-C6	3.11	110.64	106.94
22	C	510	CLA	C4D-C3D-CAD	3.11	110.20	108.47
25	d	411	SQD	O9-S-C6	3.11	110.63	106.94
22	c	506	CLA	C4-C3-C5	3.10	120.49	115.27
22	C	502	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
23	a	605	PHO	C1C-C2C-C3C	-3.10	102.95	106.51
22	c	504	CLA	CMB-C2B-C3B	3.10	130.48	124.68
22	C	506	CLA	C4-C3-C5	3.10	120.48	115.27
22	a	603	CLA	C4D-C3D-CAD	3.10	110.20	108.47
22	A	603	CLA	C4D-C3D-CAD	3.10	110.20	108.47
25	b	601	SQD	O6-C1-C2	3.10	113.14	108.30
22	C	504	CLA	CMB-C2B-C3B	3.09	130.47	124.68
25	B	601	SQD	O6-C1-C2	3.09	113.13	108.30
22	C	507	CLA	C4-C3-C5	3.09	120.47	115.27
22	B	603	CLA	CMB-C2B-C3B	3.09	130.45	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	CMB-C2B-C3B	3.09	130.45	124.68
22	c	511	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
22	c	506	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
22	A	604	CLA	CMC-C2C-C1C	3.08	129.73	125.04
22	A	603	CLA	O2D-CGD-CBD	3.08	116.74	111.27
22	c	507	CLA	C4-C3-C5	3.08	120.45	115.27
22	C	511	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	A	605	PHO	C1C-C2C-C3C	-3.08	102.98	106.51
22	C	506	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
22	a	603	CLA	O2D-CGD-CBD	3.07	116.72	111.27
22	B	610	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
22	B	616	CLA	C4D-C3D-CAD	3.06	110.18	108.47
24	d	404	BCR	C3-C2-C1	3.06	125.54	114.60
22	a	604	CLA	CMC-C2C-C1C	3.06	129.69	125.04
22	c	513	CLA	CMB-C2B-C3B	3.05	130.39	124.68
22	b	603	CLA	C3B-C4B-NB	3.05	113.15	109.21
24	K	102	BCR	C27-C26-C25	3.05	127.16	122.73
22	b	615	CLA	CAC-C3C-C4C	3.05	128.77	124.81
22	B	615	CLA	CAC-C3C-C4C	3.05	128.77	124.81
24	k	102	BCR	C27-C26-C25	3.05	127.15	122.73
23	A	606	PHO	C4D-ND-C1D	-3.05	101.29	106.76
24	K	102	BCR	C34-C9-C10	-3.04	118.66	122.92
24	D	404	BCR	C3-C2-C1	3.04	125.48	114.60
22	B	612	CLA	CMC-C2C-C1C	3.04	129.67	125.04
22	C	501	CLA	C3B-C4B-NB	3.04	113.14	109.21
22	B	617	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	b	610	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
22	b	604	CLA	C4-C3-C5	3.03	120.37	115.27
22	C	504	CLA	C4-C3-C5	3.03	120.37	115.27
22	b	617	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	c	501	CLA	C3B-C4B-NB	3.02	113.12	109.21
22	c	504	CLA	C4-C3-C5	3.02	120.35	115.27
22	C	513	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	b	612	CLA	CMC-C2C-C1C	3.02	129.64	125.04
23	a	606	PHO	C4D-ND-C1D	-3.02	101.34	106.76
24	c	515	BCR	C30-C25-C26	-3.02	118.36	122.61
24	k	102	BCR	C34-C9-C10	-3.02	118.70	122.92
24	C	515	BCR	C30-C25-C26	-3.01	118.37	122.61
22	B	604	CLA	C4-C3-C5	3.01	120.34	115.27
24	a	608	BCR	C33-C5-C6	3.01	127.91	124.53
22	B	603	CLA	C3B-C4B-NB	3.01	113.10	109.21
32	D	405	LHG	O8-C23-O10	-3.01	116.00	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
32	d	405	LHG	O8-C23-O10	-3.00	116.02	123.59
22	b	603	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
28	a	613	PL9	C7-C3-C4	3.00	119.31	116.88
32	E	101	LHG	O8-C23-C24	2.99	121.28	111.91
22	B	615	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
22	C	513	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	B	622	BCR	C37-C22-C21	-2.98	118.74	122.92
22	B	602	CLA	O2A-CGA-CBA	2.98	121.27	111.91
24	T	102	BCR	C30-C25-C24	2.98	124.22	115.78
22	c	512	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	t	101	BCR	C30-C25-C24	2.98	124.22	115.78
22	C	504	CLA	CAC-C3C-C4C	2.98	128.68	124.81
22	c	505	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
22	C	505	CLA	CMC-C2C-C1C	2.98	129.58	125.04
24	B	622	BCR	C35-C13-C12	-2.98	113.38	118.08
24	C	515	BCR	C34-C9-C8	-2.98	113.38	118.08
22	b	615	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
22	c	505	CLA	CMC-C2C-C1C	2.98	129.57	125.04
24	c	515	BCR	C34-C9-C8	-2.97	113.39	118.08
22	b	617	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
22	b	602	CLA	O2A-CGA-CBA	2.97	121.23	111.91
24	b	622	BCR	C35-C13-C12	-2.97	113.40	118.08
32	e	101	LHG	O8-C23-C24	2.97	121.23	111.91
24	A	608	BCR	C33-C5-C6	2.97	127.86	124.53
22	c	504	CLA	CAC-C3C-C4C	2.97	128.66	124.81
24	H	101	BCR	C4-C5-C6	2.97	127.04	122.73
22	B	604	CLA	CMB-C2B-C3B	2.97	130.23	124.68
22	C	505	CLA	CAC-C3C-C4C	2.97	128.66	124.81
22	C	505	CLA	C4C-C3C-C2C	-2.97	102.58	106.90
22	c	505	CLA	CAC-C3C-C4C	2.96	128.66	124.81
28	A	613	PL9	C30-C29-C31	2.96	120.25	115.27
22	C	512	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
24	b	622	BCR	C37-C22-C21	-2.96	118.78	122.92
25	d	411	SQD	O48-C23-C24	2.96	121.18	111.91
22	B	617	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
28	d	408	PL9	C53-C6-C1	2.95	121.02	114.99
22	b	604	CLA	CMB-C2B-C3B	2.95	130.19	124.68
24	A	608	BCR	C34-C9-C10	-2.95	118.80	122.92
25	B	601	SQD	O48-C23-C24	2.94	121.15	111.91
23	a	606	PHO	C1-C2-C3	-2.94	120.95	126.04
23	A	606	PHO	C1-C2-C3	-2.94	120.95	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	411	SQD	O48-C23-C24	2.94	121.14	111.91
24	a	608	BCR	C34-C9-C10	-2.94	118.80	122.92
22	b	613	CLA	C3B-C4B-NB	2.94	113.01	109.21
24	h	101	BCR	C4-C5-C6	2.94	127.00	122.73
31	H	102	DGD	O2G-C1B-C2B	2.94	117.84	111.50
22	b	603	CLA	C4D-C3D-CAD	2.94	110.11	108.47
22	B	609	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	c	513	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	b	618	BCR	C1-C6-C5	-2.94	118.48	122.61
25	b	601	SQD	O48-C23-C24	2.94	121.12	111.91
24	K	102	BCR	C40-C30-C25	2.94	115.06	110.30
24	A	608	BCR	C31-C1-C6	2.94	115.06	110.30
31	h	102	DGD	O2G-C1B-C2B	2.93	117.82	111.50
28	D	408	PL9	C53-C6-C1	2.93	120.98	114.99
28	a	613	PL9	C30-C29-C31	2.93	120.20	115.27
22	d	403	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
22	B	613	CLA	C3B-C4B-NB	2.93	113.00	109.21
24	k	102	BCR	C40-C30-C25	2.93	115.05	110.30
29	c	519	LMG	O8-C28-C29	2.93	121.09	111.91
24	B	619	BCR	C1-C6-C5	-2.92	118.49	122.61
28	A	613	PL9	C7-C3-C4	2.92	119.25	116.88
22	b	615	CLA	CBC-CAC-C3C	-2.92	104.37	112.43
22	B	615	CLA	CBC-CAC-C3C	-2.92	104.37	112.43
24	a	608	BCR	C31-C1-C6	2.92	115.04	110.30
22	b	609	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	C	501	CLA	C4D-C3D-CAD	2.92	110.10	108.47
29	C	519	LMG	O8-C28-C29	2.92	121.07	111.91
22	B	607	CLA	C4-C3-C5	2.91	120.17	115.27
22	B	608	CLA	C1-C2-C3	-2.91	121.02	126.04
22	D	403	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
22	c	504	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
22	D	401	CLA	C4D-C3D-CAD	2.90	110.09	108.47
22	c	503	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
28	a	613	PL9	C25-C24-C26	2.90	120.15	115.27
22	d	401	CLA	C4D-C3D-CAD	2.90	110.09	108.47
22	A	603	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	A	608	BCR	C8-C7-C6	2.90	135.34	127.20
22	A	607	CLA	C4D-C3D-CAD	2.90	110.09	108.47
22	b	607	CLA	C4-C3-C5	2.90	120.14	115.27
22	b	608	CLA	C1-C2-C3	-2.90	121.03	126.04
22	C	503	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
22	C	505	CLA	C3B-C4B-NB	2.89	112.95	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	C	512	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	B	611	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
31	h	102	DGD	O1G-C1A-C2A	2.89	120.97	111.91
22	c	509	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
24	T	101	BCR	C37-C22-C21	-2.89	118.88	122.92
22	C	509	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
28	A	613	PL9	C32-C33-C34	-2.89	120.71	127.66
24	B	618	BCR	C37-C22-C21	-2.88	118.89	122.92
31	H	102	DGD	O1G-C1A-C2A	2.88	120.95	111.91
22	B	617	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	c	507	CLA	C3B-C4B-NB	2.88	112.93	109.21
28	a	613	PL9	C32-C33-C34	-2.88	120.73	127.66
31	h	102	DGD	O1G-C1A-O1A	-2.88	116.33	123.59
22	b	617	CLA	CMB-C2B-C3B	2.88	130.06	124.68
22	c	512	CLA	CMB-C2B-C3B	2.88	130.06	124.68
22	D	402	CLA	C4-C3-C5	2.88	120.11	115.27
22	b	611	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
28	A	613	PL9	C15-C14-C16	2.87	120.11	115.27
22	c	506	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	c	505	CLA	C3B-C4B-NB	2.87	112.92	109.21
24	a	608	BCR	C8-C7-C6	2.87	135.27	127.20
22	b	607	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
22	a	603	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
22	c	501	CLA	C4D-C3D-CAD	2.87	110.07	108.47
28	A	613	PL9	C25-C24-C26	2.87	120.10	115.27
28	a	613	PL9	C15-C14-C16	2.87	120.09	115.27
28	a	613	PL9	C53-C6-C1	2.86	120.85	114.99
31	H	102	DGD	O1G-C1A-O1A	-2.86	116.38	123.59
22	B	603	CLA	C4D-C3D-CAD	2.86	110.06	108.47
22	C	507	CLA	C3B-C4B-NB	2.86	112.91	109.21
22	b	608	CLA	C4-C3-C5	2.86	120.08	115.27
22	d	402	CLA	C4-C3-C5	2.86	120.08	115.27
24	t	101	BCR	C39-C30-C25	2.86	114.93	110.30
28	A	613	PL9	C53-C6-C1	2.86	120.83	114.99
22	B	612	CLA	C1-C2-C3	-2.86	121.11	126.04
22	b	612	CLA	C1-C2-C3	-2.85	121.11	126.04
22	b	609	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
22	a	607	CLA	C4D-C3D-CAD	2.85	110.06	108.47
22	B	608	CLA	C4-C3-C5	2.85	120.06	115.27
24	B	618	BCR	C39-C30-C25	2.84	114.91	110.30
22	C	507	CLA	CMB-C2B-C3B	2.84	130.00	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	609	SQD	C45-O47-C7	-2.84	110.80	117.79
22	C	506	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	B	609	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
22	B	602	CLA	CMC-C2C-C1C	2.84	129.37	125.04
22	B	607	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
22	b	611	CLA	C4D-C3D-CAD	2.84	110.05	108.47
22	B	605	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
22	b	608	CLA	O2D-CGD-CBD	2.83	116.30	111.27
25	a	609	SQD	C45-O47-C7	-2.83	110.82	117.79
22	c	507	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	b	602	CLA	CMC-C2C-C1C	2.83	129.34	125.04
23	a	605	PHO	CAC-C3C-C4C	2.82	128.30	125.22
24	T	102	BCR	C39-C30-C25	2.82	114.87	110.30
22	B	608	CLA	O2D-CGD-CBD	2.82	116.28	111.27
22	C	510	CLA	CMB-C2B-C3B	2.82	129.94	124.68
22	B	603	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
24	k	101	BCR	C35-C13-C12	-2.81	113.65	118.08
25	a	609	SQD	C44-O6-C1	-2.81	108.25	113.74
22	C	512	CLA	C3B-C4B-NB	2.81	112.84	109.21
22	C	510	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
25	A	609	SQD	C44-O6-C1	-2.81	108.25	113.74
22	c	510	CLA	CMB-C2B-C3B	2.81	129.93	124.68
24	h	101	BCR	C39-C30-C29	-2.81	97.68	108.91
22	B	611	CLA	C4D-C3D-CAD	2.81	110.03	108.47
24	H	101	BCR	C39-C30-C29	-2.80	97.69	108.91
25	l	101	SQD	C1-O5-C5	-2.80	108.18	113.69
23	A	605	PHO	CAC-C3C-C4C	2.80	128.28	125.22
22	D	402	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	A	603	CLA	CAC-C3C-C4C	2.80	128.44	124.81
22	b	605	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
22	b	614	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
22	b	605	CLA	C4-C3-C5	2.79	119.97	115.27
22	d	401	CLA	CAC-C3C-C4C	2.79	128.43	124.81
22	C	503	CLA	C3B-C4B-NB	2.79	112.82	109.21
22	d	402	CLA	CAC-C3C-C4C	2.79	128.43	124.81
22	D	402	CLA	CAC-C3C-C4C	2.79	128.43	124.81
24	K	101	BCR	C35-C13-C12	-2.79	113.68	118.08
22	C	502	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	c	512	CLA	C3B-C4B-NB	2.79	112.81	109.21
28	a	613	PL9	C35-C34-C36	2.78	119.95	115.27
22	b	603	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	c	508	CLA	CMB-C2B-C3B	2.78	129.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	101	BCR	C39-C30-C25	2.78	114.81	110.30
22	B	602	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
22	B	606	CLA	C3B-C4B-NB	2.78	112.80	109.21
22	c	502	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	B	607	CLA	O1D-CGD-CBD	-2.78	118.80	124.48
22	b	613	CLA	CED-O2D-CGD	2.77	122.21	115.94
22	d	402	CLA	CMB-C2B-C3B	2.77	129.86	124.68
22	b	607	CLA	O1D-CGD-CBD	-2.77	118.81	124.48
22	c	510	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	C	514	BCR	C39-C30-C29	-2.77	97.83	108.91
22	C	508	CLA	CMB-C2B-C3B	2.77	129.86	124.68
25	L	101	SQD	C1-O5-C5	-2.77	108.26	113.69
24	K	102	BCR	C31-C1-C2	-2.77	97.84	108.91
28	A	613	PL9	C35-C34-C36	2.77	119.92	115.27
24	c	514	BCR	C39-C30-C29	-2.76	97.85	108.91
22	b	602	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
22	c	503	CLA	C3B-C4B-NB	2.76	112.78	109.21
24	k	102	BCR	C31-C1-C2	-2.76	97.85	108.91
22	C	508	CLA	C4-C3-C5	2.76	119.92	115.27
24	H	101	BCR	C32-C1-C31	-2.76	100.06	108.53
22	B	614	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
22	B	615	CLA	C4D-C3D-CAD	2.76	110.01	108.47
22	B	613	CLA	CED-O2D-CGD	2.76	122.17	115.94
24	h	101	BCR	C32-C1-C31	-2.76	100.07	108.53
22	B	605	CLA	C4-C3-C5	2.75	119.91	115.27
22	a	603	CLA	CAC-C3C-C4C	2.75	128.38	124.81
24	B	622	BCR	C1-C6-C5	-2.75	118.74	122.61
22	b	615	CLA	C4D-C3D-CAD	2.74	110.00	108.47
22	c	508	CLA	C4-C3-C5	2.74	119.89	115.27
24	b	622	BCR	C29-C30-C25	2.74	114.70	110.48
22	D	401	CLA	CAC-C3C-C4C	2.74	128.36	124.81
28	a	613	PL9	C40-C39-C41	2.74	119.88	115.27
22	C	510	CLA	CHD-C4C-C3C	-2.74	120.82	124.84
22	c	505	CLA	CMB-C2B-C3B	2.74	129.80	124.68
22	c	513	CLA	C3B-C4B-NB	2.73	112.74	109.21
22	C	505	CLA	CMB-C2B-C3B	2.73	129.79	124.68
25	l	101	SQD	O48-C23-C24	2.73	120.47	111.91
29	B	620	LMG	O8-C28-C29	2.73	120.47	111.91
22	b	606	CLA	C3B-C4B-NB	2.73	112.74	109.21
22	B	612	CLA	CAC-C3C-C4C	2.73	128.35	124.81
24	b	622	BCR	C1-C6-C5	-2.73	118.77	122.61
25	l	102	SQD	O48-C23-C24	2.73	120.46	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	622	BCR	C29-C30-C25	2.73	114.68	110.48
24	k	102	BCR	C37-C22-C23	-2.73	113.78	118.08
25	L	101	SQD	O48-C23-C24	2.72	120.46	111.91
24	K	102	BCR	C37-C22-C23	-2.72	113.79	118.08
22	C	503	CLA	C4D-C3D-CAD	2.72	109.99	108.47
28	A	613	PL9	C40-C39-C41	2.72	119.84	115.27
22	C	513	CLA	C3B-C4B-NB	2.71	112.72	109.21
25	b	621	SQD	O48-C23-C24	2.71	120.42	111.91
22	C	506	CLA	C3B-C4B-NB	2.71	112.72	109.21
22	c	501	CLA	CAC-C3C-C4C	2.71	128.33	124.81
22	c	503	CLA	C4D-C3D-CAD	2.71	109.98	108.47
22	c	510	CLA	CHD-C4C-C3C	-2.71	120.86	124.84
29	b	619	LMG	O8-C28-C29	2.71	120.40	111.91
22	a	604	CLA	CBC-CAC-C3C	-2.70	104.97	112.43
22	b	602	CLA	C3B-C4B-NB	2.70	112.70	109.21
22	d	401	CLA	C4-C3-C5	2.70	119.82	115.27
22	b	612	CLA	CAC-C3C-C4C	2.70	128.31	124.81
22	c	506	CLA	C3B-C4B-NB	2.70	112.70	109.21
24	D	404	BCR	C2-C1-C6	2.70	114.64	110.48
22	C	501	CLA	CAC-C3C-C4C	2.70	128.31	124.81
22	A	607	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
22	A	604	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
25	l	102	SQD	O9-S-C6	2.69	110.13	106.94
22	c	510	CLA	CMC-C2C-C1C	2.68	129.13	125.04
25	l	102	SQD	C4-C3-C2	2.68	115.51	110.82
22	B	609	CLA	O2A-CGA-CBA	2.68	120.33	111.91
22	C	511	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
25	L	101	SQD	O8-S-C6	2.68	110.01	105.74
22	B	609	CLA	CAC-C3C-C4C	2.68	128.29	124.81
22	c	511	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
25	b	621	SQD	O9-S-C6	2.68	110.12	106.94
22	b	609	CLA	O2A-CGA-CBA	2.67	120.30	111.91
22	d	403	CLA	CAC-C3C-C4C	2.67	128.28	124.81
25	l	101	SQD	O8-S-C6	2.67	110.00	105.74
22	a	607	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
22	B	602	CLA	C3B-C4B-NB	2.67	112.66	109.21
22	D	401	CLA	C4-C3-C5	2.67	119.76	115.27
25	b	621	SQD	C4-C3-C2	2.67	115.48	110.82
22	C	503	CLA	C4-C3-C5	2.67	119.76	115.27
22	B	611	CLA	O2A-CGA-CBA	2.66	120.25	111.91
24	d	404	BCR	C2-C1-C6	2.66	114.58	110.48
24	k	102	BCR	C29-C30-C25	2.66	114.57	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	503	CLA	C4-C3-C5	2.66	119.74	115.27
22	b	611	CLA	O2A-CGA-CBA	2.66	120.24	111.91
22	c	513	CLA	CMC-C2C-C1C	2.65	129.08	125.04
22	B	617	CLA	O2A-CGA-CBA	2.65	120.24	111.91
24	b	618	BCR	C1-C6-C7	2.65	123.28	115.78
22	C	513	CLA	CMC-C2C-C1C	2.65	129.07	125.04
22	C	510	CLA	CMC-C2C-C1C	2.65	129.07	125.04
22	b	609	CLA	CAC-C3C-C4C	2.65	128.24	124.81
22	b	604	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
24	k	101	BCR	C39-C30-C29	-2.64	98.34	108.91
24	K	101	BCR	C39-C30-C29	-2.64	98.35	108.91
22	b	608	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
22	D	403	CLA	CAC-C3C-C4C	2.64	128.23	124.81
22	B	612	CLA	CHD-C4C-C3C	-2.64	120.96	124.84
24	B	619	BCR	C1-C6-C7	2.64	123.24	115.78
22	B	614	CLA	O2D-CGD-CBD	2.64	115.95	111.27
22	B	610	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
22	c	511	CLA	C4-C3-C5	2.63	119.70	115.27
22	c	509	CLA	CAC-C3C-C4C	2.63	128.22	124.81
22	b	612	CLA	CHD-C4C-C3C	-2.63	120.97	124.84
22	b	610	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	B	612	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	b	614	CLA	O2D-CGD-CBD	2.63	115.94	111.27
22	B	608	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
22	b	617	CLA	O2A-CGA-CBA	2.63	120.15	111.91
24	B	618	BCR	C39-C30-C29	-2.63	98.40	108.91
24	h	101	BCR	C29-C28-C27	-2.63	105.51	111.38
22	c	502	CLA	C4-C3-C5	2.62	119.68	115.27
22	b	612	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	d	403	CLA	CED-O2D-CGD	2.62	121.87	115.94
24	T	101	BCR	C39-C30-C29	-2.62	98.42	108.91
22	B	604	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
22	C	511	CLA	C4-C3-C5	2.62	119.68	115.27
31	C	516	DGD	O3G-C3G-C2G	-2.62	104.59	110.90
24	K	102	BCR	C29-C30-C25	2.62	114.51	110.48
22	C	502	CLA	C4-C3-C5	2.62	119.67	115.27
24	B	622	BCR	C23-C24-C25	2.61	134.54	127.20
31	D	410	DGD	O5D-C1E-C2E	2.61	112.38	108.30
22	b	616	CLA	C4-C3-C5	2.61	119.67	115.27
22	C	507	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
22	B	616	CLA	C4-C3-C5	2.61	119.66	115.27
24	b	622	BCR	C23-C24-C25	2.61	134.53	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	403	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	D	403	CLA	CED-O2D-CGD	2.61	121.84	115.94
22	c	507	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
31	c	516	DGD	O3G-C3G-C2G	-2.61	104.61	110.90
22	B	614	CLA	CMB-C2B-C3B	2.61	129.55	124.68
22	c	502	CLA	C4D-C3D-CAD	2.61	109.92	108.47
24	H	101	BCR	C29-C28-C27	-2.60	105.56	111.38
22	C	501	CLA	CMC-C2C-C1C	2.60	129.00	125.04
24	C	515	BCR	C23-C24-C25	2.60	134.51	127.20
22	C	504	CLA	C1-O2A-CGA	2.60	123.26	116.44
24	A	608	BCR	C29-C30-C25	2.60	114.48	110.48
22	D	403	CLA	C4D-C3D-CAD	2.59	109.92	108.47
22	c	504	CLA	C1-O2A-CGA	2.59	123.25	116.44
22	D	403	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	C	509	CLA	CAC-C3C-C4C	2.59	128.17	124.81
22	C	512	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	b	614	CLA	CMB-C2B-C3B	2.59	129.52	124.68
24	C	514	BCR	C39-C30-C25	2.59	114.50	110.30
22	A	607	CLA	CED-O2D-CGD	2.59	121.79	115.94
22	d	403	CLA	CMB-C2B-C3B	2.59	129.52	124.68
31	d	410	DGD	O5D-C1E-C2E	2.59	112.34	108.30
22	D	403	CLA	CMB-C2B-C3B	2.59	129.52	124.68
22	A	607	CLA	CAC-C3C-C4C	2.59	128.17	124.81
22	C	506	CLA	CAC-C3C-C4C	2.59	128.17	124.81
22	c	509	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
22	a	603	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
31	d	410	DGD	O1G-C1A-C2A	2.58	120.01	111.91
31	D	410	DGD	O1G-C1A-C2A	2.58	120.01	111.91
22	A	603	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
24	c	515	BCR	C23-C24-C25	2.58	134.45	127.20
22	a	607	CLA	CED-O2D-CGD	2.58	121.77	115.94
24	a	608	BCR	C29-C30-C25	2.58	114.45	110.48
22	C	512	CLA	C1-C2-C3	-2.58	121.58	126.04
24	B	618	BCR	C4-C5-C6	2.58	126.47	122.73
22	b	614	CLA	C4-C3-C5	2.58	119.61	115.27
22	b	613	CLA	CMC-C2C-C1C	2.58	128.96	125.04
24	k	102	BCR	C34-C9-C8	-2.58	114.02	118.08
31	c	518	DGD	O1G-C1A-C2A	2.58	119.99	111.91
31	C	518	DGD	O1G-C1A-C2A	2.57	119.98	111.91
24	c	514	BCR	C39-C30-C25	2.57	114.47	110.30
24	T	101	BCR	C4-C5-C6	2.57	126.46	122.73
22	b	614	CLA	CHD-C4C-C3C	-2.57	121.06	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
28	d	408	PL9	C7-C3-C4	2.57	118.96	116.88
28	A	613	PL9	C37-C38-C39	-2.56	121.49	127.66
22	c	501	CLA	CMC-C2C-C1C	2.56	128.94	125.04
22	c	512	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	C	502	CLA	C4D-C3D-CAD	2.56	109.90	108.47
28	D	408	PL9	C7-C3-C4	2.56	118.95	116.88
22	b	609	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
22	B	614	CLA	C4-C3-C5	2.56	119.57	115.27
22	d	401	CLA	CHD-C4C-C3C	-2.55	121.08	124.84
24	K	102	BCR	C34-C9-C8	-2.55	114.05	118.08
25	b	601	SQD	O8-S-C6	2.55	109.81	105.74
22	B	612	CLA	C4D-C3D-CAD	2.55	109.89	108.47
22	c	506	CLA	CAC-C3C-C4C	2.55	128.12	124.81
28	a	613	PL9	C37-C38-C39	-2.55	121.52	127.66
24	K	102	BCR	C33-C5-C6	2.55	127.39	124.53
22	c	512	CLA	C1-C2-C3	-2.54	121.64	126.04
22	a	607	CLA	CAC-C3C-C4C	2.54	128.11	124.81
22	B	614	CLA	CHD-C4C-C3C	-2.54	121.10	124.84
28	a	613	PL9	C10-C9-C11	2.54	119.55	115.27
22	C	501	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
22	D	401	CLA	CMC-C2C-C1C	2.54	128.91	125.04
22	c	501	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
22	a	607	CLA	CMB-C2B-C3B	2.54	129.43	124.68
25	B	601	SQD	O8-S-C6	2.54	109.78	105.74
22	D	403	CLA	C4-C3-C5	2.54	119.54	115.27
22	b	611	CLA	C4-C3-C5	2.54	119.54	115.27
22	D	401	CLA	CHD-C4C-C3C	-2.54	121.11	124.84
24	B	622	BCR	C37-C22-C23	-2.53	114.08	118.08
22	d	403	CLA	C4D-C3D-CAD	2.53	109.88	108.47
22	d	401	CLA	CMC-C2C-C1C	2.53	128.89	125.04
33	F	101	HEM	C1D-C2D-C3D	-2.53	105.24	107.00
22	c	501	CLA	C1-O2A-CGA	2.53	123.08	116.44
22	B	611	CLA	C4-C3-C5	2.53	119.52	115.27
22	a	607	CLA	CMC-C2C-C1C	2.53	128.89	125.04
22	C	506	CLA	CMB-C2B-C3B	2.53	129.40	124.68
22	c	506	CLA	CMB-C2B-C3B	2.53	129.40	124.68
28	A	613	PL9	C10-C9-C11	2.53	119.52	115.27
22	A	607	CLA	CMB-C2B-C3B	2.52	129.40	124.68
22	B	613	CLA	CMC-C2C-C1C	2.52	128.88	125.04
22	A	607	CLA	CMC-C2C-C1C	2.52	128.88	125.04
24	k	102	BCR	C33-C5-C6	2.52	127.36	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	CMC-C2C-C1C	2.52	128.88	125.04
22	B	609	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
31	c	517	DGD	O2G-C1B-O1B	-2.52	117.62	123.70
25	a	609	SQD	C1-O5-C5	-2.52	108.75	113.69
22	C	501	CLA	C1-O2A-CGA	2.52	123.05	116.44
31	C	517	DGD	O2G-C1B-O1B	-2.52	117.62	123.70
24	b	622	BCR	C37-C22-C23	-2.51	114.11	118.08
32	D	405	LHG	O7-C7-C8	2.51	116.92	111.50
24	B	618	BCR	C2-C3-C4	2.51	116.99	111.38
22	d	403	CLA	C4-C3-C5	2.51	119.49	115.27
24	C	515	BCR	C1-C6-C5	-2.50	119.09	122.61
22	C	507	CLA	O1D-CGD-CBD	-2.50	119.36	124.48
22	B	602	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	B	614	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	b	614	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
22	b	612	CLA	C4D-C3D-CAD	2.49	109.86	108.47
24	c	515	BCR	C1-C6-C5	-2.49	119.10	122.61
22	C	501	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
22	c	503	CLA	CMC-C2C-C1C	2.49	128.84	125.04
24	T	101	BCR	C2-C3-C4	2.49	116.95	111.38
24	h	101	BCR	C39-C30-C25	2.49	114.34	110.30
32	d	405	LHG	O7-C7-C8	2.49	116.87	111.50
25	A	609	SQD	C1-O5-C5	-2.49	108.80	113.69
24	H	101	BCR	C39-C30-C25	2.49	114.33	110.30
33	f	101	HEM	C1D-C2D-C3D	-2.48	105.27	107.00
24	D	404	BCR	C30-C25-C24	2.48	122.80	115.78
24	d	404	BCR	C30-C25-C24	2.48	122.80	115.78
22	c	507	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
22	b	602	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
29	c	520	LMG	O8-C28-C29	2.47	119.67	111.91
22	c	501	CLA	C4C-C3C-C2C	-2.47	103.29	106.90
24	B	622	BCR	C38-C26-C25	2.47	127.31	124.53
29	C	520	LMG	O8-C28-C29	2.47	119.66	111.91
29	a	614	LMG	O1-C1-C2	2.47	112.16	108.30
33	F	101	HEM	CBA-CAA-C2A	-2.47	107.93	112.49
22	C	512	CLA	CED-O2D-CGD	2.47	121.52	115.94
33	f	101	HEM	CBA-CAA-C2A	-2.47	107.94	112.49
22	c	502	CLA	CMC-C2C-C1C	2.47	128.79	125.04
23	A	606	PHO	CED-O2D-CGD	2.46	121.51	115.94
24	B	618	BCR	C1-C6-C5	-2.46	119.14	122.61
22	c	512	CLA	CED-O2D-CGD	2.46	121.50	115.94
24	T	101	BCR	C1-C6-C5	-2.46	119.15	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	101	BCR	C1-C6-C5	-2.45	119.16	122.61
23	a	606	PHO	CED-O2D-CGD	2.45	121.48	115.94
22	b	617	CLA	C4D-C3D-CAD	2.45	109.84	108.47
22	c	509	CLA	O2A-CGA-CBA	2.45	119.59	111.91
22	C	502	CLA	CMC-C2C-C1C	2.45	128.77	125.04
22	B	610	CLA	C1-C2-C3	-2.45	121.81	126.04
22	C	510	CLA	CAC-C3C-C4C	2.45	127.99	124.81
22	C	507	CLA	CMC-C2C-C1C	2.45	128.77	125.04
22	b	607	CLA	C1-C2-C3	-2.45	121.81	126.04
22	A	604	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
29	A	614	LMG	O1-C1-C2	2.44	112.12	108.30
24	T	102	BCR	C1-C6-C5	-2.44	119.17	122.61
22	C	509	CLA	O2A-CGA-CBA	2.44	119.58	111.91
22	C	513	CLA	CAC-C3C-C4C	2.44	127.98	124.81
22	b	612	CLA	CMB-C2B-C3B	2.44	129.25	124.68
22	C	513	CLA	C4-C3-C5	2.44	119.38	115.27
29	D	406	LMG	O8-C28-O10	-2.44	117.44	123.59
22	a	604	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
24	B	618	BCR	C33-C5-C4	-2.44	108.94	113.62
29	d	406	LMG	O8-C28-O10	-2.44	117.44	123.59
22	B	607	CLA	C1-C2-C3	-2.44	121.83	126.04
24	T	102	BCR	C31-C1-C6	2.44	114.25	110.30
24	t	101	BCR	C40-C30-C39	-2.43	101.07	108.53
22	c	510	CLA	CAC-C3C-C4C	2.43	127.96	124.81
22	C	512	CLA	O2A-CGA-CBA	2.43	119.53	111.91
24	T	101	BCR	C33-C5-C4	-2.43	108.95	113.62
22	c	507	CLA	CMC-C2C-C1C	2.43	128.74	125.04
24	b	622	BCR	C38-C26-C25	2.43	127.25	124.53
22	c	513	CLA	C4-C3-C5	2.43	119.35	115.27
24	T	102	BCR	C40-C30-C39	-2.42	101.09	108.53
22	B	610	CLA	CMB-C2B-C3B	2.42	129.21	124.68
22	C	505	CLA	CED-O2D-CGD	2.42	121.42	115.94
22	c	505	CLA	CED-O2D-CGD	2.42	121.41	115.94
22	C	511	CLA	CAC-C3C-C4C	2.42	127.94	124.81
22	b	608	CLA	CMB-C2B-C3B	2.41	129.20	124.68
22	c	511	CLA	CAC-C3C-C4C	2.41	127.94	124.81
22	b	610	CLA	C1-C2-C3	-2.41	121.87	126.04
24	b	622	BCR	C3-C4-C5	2.41	118.38	114.08
24	B	622	BCR	C3-C4-C5	2.41	118.38	114.08
22	b	602	CLA	CMB-C2B-C3B	2.41	129.19	124.68
22	d	402	CLA	CHC-C1C-C2C	-2.41	120.06	126.72
22	B	612	CLA	CMB-C2B-C3B	2.41	129.18	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	CAC-C3C-C4C	2.41	127.93	124.81
23	A	606	PHO	O2D-CGD-O1D	-2.41	119.14	123.84
22	C	508	CLA	C1D-CHD-C4C	2.41	125.73	122.56
22	B	602	CLA	CMB-C2B-C3B	2.40	129.17	124.68
22	B	617	CLA	C4D-C3D-CAD	2.40	109.81	108.47
22	d	402	CLA	CHD-C4C-C3C	-2.40	121.31	124.84
22	c	512	CLA	O2A-CGA-CBA	2.40	119.45	111.91
22	D	402	CLA	CHD-C4C-C3C	-2.40	121.31	124.84
24	h	101	BCR	C30-C25-C24	2.40	122.57	115.78
24	H	101	BCR	C30-C25-C24	2.40	122.57	115.78
22	C	504	CLA	CMC-C2C-C1C	2.40	128.69	125.04
22	b	606	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
22	b	610	CLA	CMB-C2B-C3B	2.40	129.17	124.68
22	D	402	CLA	CHC-C1C-C2C	-2.40	120.09	126.72
22	c	513	CLA	CAC-C3C-C4C	2.40	127.92	124.81
22	b	615	CLA	CMB-C2B-C3B	2.40	129.16	124.68
31	D	410	DGD	O6D-C5D-C6D	2.40	111.50	106.67
22	A	604	CLA	C4D-C3D-CAD	2.39	109.81	108.47
24	t	101	BCR	C31-C1-C6	2.39	114.18	110.30
22	A	604	CLA	C4C-C3C-C2C	-2.39	103.41	106.90
22	B	617	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
22	B	608	CLA	CMB-C2B-C3B	2.39	129.15	124.68
24	B	622	BCR	C40-C30-C25	2.39	114.17	110.30
22	B	606	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
24	b	622	BCR	C40-C30-C25	2.39	114.17	110.30
22	B	616	CLA	CMB-C2B-C3B	2.38	129.14	124.68
22	b	615	CLA	CMC-C2C-C1C	2.38	128.67	125.04
22	C	506	CLA	CMC-C2C-C1C	2.38	128.67	125.04
22	b	617	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
22	C	512	CLA	CAC-C3C-C4C	2.38	127.90	124.81
28	a	613	PL9	C45-C44-C46	2.38	119.28	115.27
22	c	508	CLA	C1D-CHD-C4C	2.38	125.70	122.56
22	B	615	CLA	CMB-C2B-C3B	2.38	129.13	124.68
22	a	604	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
23	a	606	PHO	O2D-CGD-O1D	-2.38	119.18	123.84
22	b	615	CLA	C1-O2A-CGA	2.38	122.68	116.44
22	b	616	CLA	CMB-C2B-C3B	2.37	129.12	124.68
22	B	615	CLA	C1-O2A-CGA	2.37	122.67	116.44
28	A	613	PL9	C45-C44-C46	2.37	119.26	115.27
22	B	614	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
22	b	614	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
22	B	607	CLA	O2A-CGA-CBA	2.37	119.34	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	607	CLA	O2A-CGA-CBA	2.37	119.34	111.91
22	C	513	CLA	O2A-CGA-CBA	2.37	119.34	111.91
22	c	513	CLA	O2A-CGA-CBA	2.37	119.33	111.91
29	B	620	LMG	O7-C10-O9	-2.37	117.99	123.70
22	B	610	CLA	CED-O2D-CGD	2.36	121.28	115.94
22	B	611	CLA	CMB-C2B-C3B	2.36	129.10	124.68
22	b	610	CLA	CED-O2D-CGD	2.36	121.28	115.94
22	d	402	CLA	CMC-C2C-C1C	2.36	128.64	125.04
22	c	506	CLA	CMC-C2C-C1C	2.36	128.63	125.04
24	k	102	BCR	C4-C5-C6	2.36	126.16	122.73
22	C	501	CLA	CMB-C2B-C3B	2.36	129.09	124.68
31	d	410	DGD	O6D-C5D-C6D	2.36	111.43	106.67
24	B	619	BCR	C4-C5-C6	2.36	126.15	122.73
22	c	504	CLA	CMC-C2C-C1C	2.36	128.63	125.04
22	c	504	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
24	K	102	BCR	C1-C6-C5	-2.35	119.30	122.61
22	B	603	CLA	C1-C2-C3	-2.35	121.97	126.04
22	B	615	CLA	CMC-C2C-C1C	2.35	128.62	125.04
22	c	501	CLA	CMB-C2B-C3B	2.35	129.08	124.68
31	d	410	DGD	O6E-C5E-C6E	2.35	112.29	106.44
22	D	402	CLA	CMC-C2C-C1C	2.35	128.62	125.04
28	D	408	PL9	C35-C34-C36	2.35	119.23	115.27
24	K	102	BCR	C4-C5-C6	2.35	126.15	122.73
22	C	504	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
31	D	410	DGD	O6E-C5E-C6E	2.35	112.28	106.44
22	b	611	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	B	611	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	b	603	CLA	C1-C2-C3	-2.35	121.98	126.04
24	c	514	BCR	C3-C4-C5	2.35	118.27	114.08
24	B	622	BCR	C1-C6-C7	2.35	122.42	115.78
24	k	102	BCR	C1-C6-C5	-2.35	119.31	122.61
24	b	622	BCR	C1-C6-C7	2.35	122.42	115.78
22	B	612	CLA	CBC-CAC-C3C	-2.35	105.97	112.43
22	D	402	CLA	C4C-C3C-C2C	-2.35	103.48	106.90
24	h	101	BCR	C28-C29-C30	2.34	122.99	114.60
22	b	604	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
24	b	618	BCR	C4-C5-C6	2.34	126.13	122.73
22	d	402	CLA	C4C-C3C-C2C	-2.34	103.48	106.90
24	b	618	BCR	C29-C28-C27	-2.34	106.14	111.38
24	C	514	BCR	C3-C4-C5	2.34	118.26	114.08
24	H	101	BCR	C28-C29-C30	2.34	122.97	114.60
28	d	408	PL9	C7-C8-C9	-2.34	122.90	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	408	PL9	C35-C34-C36	2.34	119.21	115.27
24	B	622	BCR	C32-C1-C6	2.34	114.09	110.30
29	b	619	LMG	O7-C10-O9	-2.34	118.05	123.70
22	B	604	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
22	b	611	CLA	CMB-C2B-C3B	2.34	129.05	124.68
24	T	102	BCR	C32-C1-C2	-2.33	99.57	108.91
22	C	510	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
28	D	408	PL9	C7-C8-C9	-2.33	122.91	126.79
24	t	101	BCR	C32-C1-C2	-2.33	99.60	108.91
22	b	612	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
22	C	509	CLA	CMB-C2B-C3B	2.32	129.03	124.68
22	c	509	CLA	CMB-C2B-C3B	2.32	129.02	124.68
22	B	605	CLA	CAC-C3C-C4C	2.32	127.82	124.81
22	b	617	CLA	C1-O2A-CGA	2.32	122.53	116.44
24	B	619	BCR	C29-C28-C27	-2.32	106.19	111.38
22	B	617	CLA	C1-O2A-CGA	2.32	122.52	116.44
22	b	602	CLA	O1D-CGD-CBD	-2.32	119.75	124.48
23	a	606	PHO	C1C-C2C-C3C	-2.32	103.85	106.51
22	b	614	CLA	O2A-CGA-CBA	2.32	119.17	111.91
22	A	603	CLA	C4-C3-C5	2.31	119.16	115.27
22	a	604	CLA	C4D-C3D-CAD	2.31	109.76	108.47
22	B	614	CLA	O2A-CGA-CBA	2.31	119.16	111.91
22	C	512	CLA	C1-O2A-CGA	2.31	122.50	116.44
22	C	502	CLA	CMB-C2B-C3B	2.31	129.00	124.68
24	b	622	BCR	C32-C1-C6	2.31	114.04	110.30
29	a	614	LMG	O8-C28-C29	2.31	119.15	111.91
22	B	602	CLA	O1D-CGD-CBD	-2.31	119.77	124.48
22	c	508	CLA	CAC-C3C-C4C	2.30	127.80	124.81
24	c	515	BCR	C27-C26-C25	2.30	126.07	122.73
22	b	603	CLA	CED-O2D-CGD	2.30	121.14	115.94
22	B	603	CLA	CED-O2D-CGD	2.30	121.14	115.94
22	c	510	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
24	C	515	BCR	C27-C26-C25	2.30	126.06	122.73
23	A	606	PHO	CHD-C1D-ND	-2.30	119.80	124.58
29	A	614	LMG	O8-C28-C29	2.29	119.11	111.91
22	b	606	CLA	CED-O2D-CGD	2.29	121.12	115.94
24	k	101	BCR	C28-C27-C26	2.29	118.17	114.08
22	c	513	CLA	CHD-C4C-NC	-2.29	120.59	124.20
22	B	606	CLA	CED-O2D-CGD	2.29	121.12	115.94
24	K	101	BCR	C28-C27-C26	2.29	118.17	114.08
28	d	408	PL9	C10-C9-C11	2.29	119.12	115.27
23	a	606	PHO	CHD-C1D-ND	-2.29	119.82	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	601	SQD	C3-C4-C5	2.29	114.32	110.24
22	b	605	CLA	CAC-C3C-C4C	2.28	127.77	124.81
22	C	513	CLA	CHD-C4C-NC	-2.28	120.61	124.20
23	A	606	PHO	C1C-C2C-C3C	-2.28	103.89	106.51
28	D	408	PL9	C10-C9-C11	2.28	119.11	115.27
24	k	101	BCR	C30-C25-C24	2.28	122.22	115.78
24	A	608	BCR	C37-C22-C23	-2.27	114.49	118.08
24	D	404	BCR	C37-C22-C23	-2.27	114.49	118.08
22	c	502	CLA	CMB-C2B-C3B	2.27	128.93	124.68
32	d	407	LHG	O8-C23-C24	2.27	119.03	111.91
25	b	601	SQD	C3-C4-C5	2.27	114.29	110.24
22	b	606	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
32	D	407	LHG	O8-C23-C24	2.27	119.03	111.91
23	a	605	PHO	CMB-C2B-C1B	2.27	128.56	125.06
22	A	603	CLA	CMC-C2C-C1C	2.27	128.49	125.04
22	B	606	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
22	b	611	CLA	CAC-C3C-C4C	2.27	127.75	124.81
22	B	611	CLA	CAC-C3C-C4C	2.27	127.75	124.81
22	b	609	CLA	C11-C12-C13	-2.26	108.60	115.92
24	K	101	BCR	C30-C25-C24	2.26	122.18	115.78
22	b	613	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
22	a	603	CLA	C4-C3-C5	2.26	119.08	115.27
22	c	512	CLA	C1-O2A-CGA	2.26	122.38	116.44
22	B	613	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
22	b	609	CLA	C4-C3-C5	2.26	119.07	115.27
22	B	609	CLA	C11-C12-C13	-2.26	108.62	115.92
28	d	408	PL9	C27-C28-C29	-2.26	122.22	127.66
22	B	616	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
24	a	608	BCR	C37-C22-C23	-2.26	114.52	118.08
22	a	607	CLA	O2A-CGA-CBA	2.25	118.97	111.91
22	B	609	CLA	C4-C3-C5	2.25	119.06	115.27
28	D	408	PL9	C27-C28-C29	-2.25	122.24	127.66
22	b	616	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	a	605	PHO	CHD-C1D-ND	-2.25	119.90	124.58
31	D	410	DGD	O2G-C1B-O1B	-2.25	118.27	123.70
22	C	508	CLA	CAC-C3C-C4C	2.25	127.73	124.81
23	A	605	PHO	CMB-C2B-C1B	2.25	128.52	125.06
23	A	606	PHO	CMB-C2B-C1B	2.25	128.52	125.06
29	c	519	LMG	O8-C28-O10	-2.24	117.93	123.59
31	d	410	DGD	O2G-C1B-O1B	-2.24	118.28	123.70
22	C	509	CLA	CHD-C4C-NC	-2.24	120.67	124.20
24	d	404	BCR	C37-C22-C23	-2.24	114.55	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	605	PHO	CHD-C1D-ND	-2.24	119.91	124.58
22	b	616	CLA	CED-O2D-CGD	2.24	121.00	115.94
22	A	607	CLA	C1-O2A-CGA	2.24	122.32	116.44
22	A	607	CLA	O2A-CGA-CBA	2.24	118.93	111.91
29	Z	101	LMG	O7-C10-O9	-2.24	118.30	123.70
22	a	607	CLA	C1-O2A-CGA	2.24	122.31	116.44
29	z	101	LMG	O7-C10-O9	-2.24	118.30	123.70
22	c	502	CLA	CHD-C4C-C3C	-2.23	121.56	124.84
22	B	616	CLA	CED-O2D-CGD	2.23	120.99	115.94
22	a	603	CLA	CMC-C2C-C1C	2.23	128.44	125.04
29	C	519	LMG	O8-C28-O10	-2.23	117.96	123.59
22	c	504	CLA	C4D-C3D-CAD	2.23	109.72	108.47
25	a	609	SQD	O48-C23-C24	2.23	118.89	111.91
29	c	519	LMG	O1-C7-C8	-2.23	105.53	110.90
22	c	509	CLA	CHD-C4C-NC	-2.22	120.70	124.20
22	D	401	CLA	CED-O2D-CGD	2.22	120.97	115.94
29	C	519	LMG	O1-C7-C8	-2.22	105.53	110.90
22	d	401	CLA	CED-O2D-CGD	2.22	120.96	115.94
22	c	510	CLA	O2A-CGA-CBA	2.22	118.88	111.91
25	A	609	SQD	O48-C23-C24	2.22	118.88	111.91
22	b	605	CLA	O2A-CGA-CBA	2.22	118.88	111.91
22	C	502	CLA	CHD-C4C-C3C	-2.22	121.57	124.84
25	d	411	SQD	O48-C23-O10	-2.22	117.99	123.59
22	b	617	CLA	CED-O2D-CGD	2.22	120.96	115.94
22	b	614	CLA	CMC-C2C-C1C	2.22	128.42	125.04
22	A	604	CLA	CED-O2D-CGD	2.22	120.95	115.94
22	C	507	CLA	CED-O2D-CGD	2.22	120.95	115.94
22	b	608	CLA	C4D-C3D-CAD	2.22	109.71	108.47
32	E	101	LHG	O8-C23-O10	-2.22	118.00	123.59
22	C	510	CLA	O2A-CGA-CBA	2.22	118.86	111.91
22	b	603	CLA	C1-O2A-CGA	2.21	122.25	116.44
22	B	605	CLA	O2A-CGA-CBA	2.21	118.86	111.91
23	a	606	PHO	CMB-C2B-C1B	2.21	128.47	125.06
29	d	406	LMG	O7-C10-C11	2.21	116.27	111.50
22	B	603	CLA	C1-O2A-CGA	2.21	122.25	116.44
25	D	411	SQD	O48-C23-O10	-2.21	118.01	123.59
22	B	617	CLA	CED-O2D-CGD	2.21	120.94	115.94
24	a	608	BCR	C28-C27-C26	-2.21	110.13	114.08
24	c	515	BCR	C37-C22-C23	-2.21	114.60	118.08
22	a	604	CLA	CED-O2D-CGD	2.21	120.93	115.94
29	D	406	LMG	O7-C10-C11	2.21	116.26	111.50
22	b	614	CLA	C1D-CHD-C4C	2.20	125.47	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	609	SQD	O48-C23-O10	-2.20	118.03	123.59
24	t	101	BCR	C38-C26-C27	-2.20	109.39	113.62
22	b	605	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
22	B	617	CLA	CHD-C4C-C3C	-2.20	121.60	124.84
24	C	515	BCR	C37-C22-C23	-2.20	114.61	118.08
22	b	606	CLA	C4D-C3D-CAD	2.20	109.70	108.47
23	a	605	PHO	C1C-NC-C4C	-2.20	102.37	106.51
24	A	608	BCR	C28-C27-C26	-2.20	110.16	114.08
22	c	507	CLA	CED-O2D-CGD	2.20	120.91	115.94
22	B	605	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
32	e	101	LHG	O8-C23-O10	-2.19	118.06	123.59
22	B	614	CLA	C1-C2-C3	-2.19	122.25	126.04
22	B	615	CLA	CED-O2D-CGD	2.19	120.89	115.94
22	B	614	CLA	CMC-C2C-C1C	2.19	128.38	125.04
22	B	614	CLA	C1D-CHD-C4C	2.19	125.45	122.56
25	a	609	SQD	O48-C23-O10	-2.19	118.06	123.59
22	c	507	CLA	O2A-CGA-CBA	2.19	118.77	111.91
22	C	507	CLA	O2A-CGA-CBA	2.19	118.77	111.91
22	b	615	CLA	CED-O2D-CGD	2.19	120.88	115.94
22	b	617	CLA	CHD-C4C-C3C	-2.19	121.62	124.84
22	C	501	CLA	C4-C3-C5	2.18	118.94	115.27
33	v	201	HEM	C4C-C3C-C2C	2.18	108.42	106.90
22	b	614	CLA	C1-C2-C3	-2.18	122.27	126.04
22	c	501	CLA	C4-C3-C5	2.18	118.94	115.27
31	H	102	DGD	O6E-C5E-C6E	2.18	111.85	106.44
22	C	504	CLA	C4D-C3D-CAD	2.18	109.68	108.47
22	B	605	CLA	CMC-C2C-C1C	2.18	128.35	125.04
32	D	409	LHG	O4-P-O5	2.18	123.00	112.24
23	A	605	PHO	C1C-NC-C4C	-2.18	102.41	106.51
22	B	616	CLA	C1-O2A-CGA	2.17	122.15	116.44
22	c	511	CLA	CED-O2D-CGD	2.17	120.85	115.94
22	C	511	CLA	CED-O2D-CGD	2.17	120.85	115.94
24	c	514	BCR	C40-C30-C29	-2.17	100.22	108.91
31	h	102	DGD	O6E-C5E-C6E	2.17	111.83	106.44
32	d	409	LHG	O4-P-O5	2.17	122.95	112.24
22	b	606	CLA	CHD-C4C-C3C	-2.17	121.66	124.84
24	C	514	BCR	C40-C30-C29	-2.16	100.25	108.91
22	b	608	CLA	C1-O2A-CGA	2.16	122.11	116.44
24	T	102	BCR	C38-C26-C27	-2.16	109.47	113.62
22	b	616	CLA	C1-O2A-CGA	2.16	122.10	116.44
33	V	201	HEM	C4C-C3C-C2C	2.16	108.40	106.90
33	V	201	HEM	CMA-C3A-C4A	-2.16	125.15	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	604	CLA	C1-O2A-CGA	2.15	122.09	116.44
22	B	606	CLA	CHD-C4C-C3C	-2.15	121.68	124.84
22	d	401	CLA	O2A-CGA-CBA	2.15	118.65	111.91
22	b	617	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
22	B	608	CLA	C1-O2A-CGA	2.15	122.07	116.44
22	D	401	CLA	O2A-CGA-CBA	2.14	118.63	111.91
22	A	607	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
22	b	605	CLA	CMC-C2C-C1C	2.14	128.30	125.04
22	D	402	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
24	d	404	BCR	C38-C26-C25	2.14	126.93	124.53
22	b	609	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
33	v	201	HEM	CMA-C3A-C4A	-2.14	125.18	128.46
22	B	607	CLA	CMB-C2B-C3B	2.14	128.68	124.68
32	d	407	LHG	O7-C7-C8	2.14	116.11	111.50
22	B	607	CLA	C1-O2A-CGA	2.14	122.05	116.44
22	c	509	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
22	B	605	CLA	CHD-C4C-NC	-2.13	120.84	124.20
22	b	607	CLA	CMB-C2B-C3B	2.13	128.67	124.68
22	b	610	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
32	D	407	LHG	O7-C7-C8	2.13	116.09	111.50
24	D	404	BCR	C38-C26-C25	2.13	126.92	124.53
22	b	613	CLA	O2A-CGA-CBA	2.13	118.59	111.91
22	D	401	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
25	l	102	SQD	O47-C7-O49	-2.13	118.56	123.70
22	a	604	CLA	C1-O2A-CGA	2.13	122.03	116.44
22	c	512	CLA	CMC-C2C-C1C	2.13	128.28	125.04
22	B	610	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
22	b	607	CLA	C1-O2A-CGA	2.12	122.02	116.44
22	c	503	CLA	CED-O2D-CGD	2.12	120.74	115.94
22	C	509	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
32	d	405	LHG	O4-P-O5	2.12	122.74	112.24
22	B	617	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
24	K	102	BCR	C1-C6-C7	2.12	121.78	115.78
22	a	607	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
24	c	514	BCR	C2-C3-C4	2.12	116.12	111.38
22	d	402	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
25	l	102	SQD	O5-C1-C2	-2.12	105.86	110.35
22	d	401	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
32	D	405	LHG	O4-P-O5	2.12	122.72	112.24
22	B	617	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	b	613	CLA	C1D-CHD-C4C	2.12	125.35	122.56
22	B	609	CLA	O2A-CGA-O1A	-2.12	118.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	BCR	C2-C3-C4	2.12	116.11	111.38
24	T	102	BCR	C3-C2-C1	2.12	122.17	114.60
22	B	613	CLA	O2A-CGA-CBA	2.12	118.55	111.91
22	C	503	CLA	CED-O2D-CGD	2.12	120.72	115.94
24	k	102	BCR	C1-C6-C7	2.12	121.77	115.78
22	B	608	CLA	C4D-C3D-CAD	2.12	109.65	108.47
22	C	511	CLA	CMC-C2C-C1C	2.12	128.26	125.04
22	a	603	CLA	O2A-CGA-CBA	2.11	118.54	111.91
22	C	505	CLA	C1-O2A-CGA	2.11	121.99	116.44
22	B	606	CLA	C4D-C3D-CAD	2.11	109.65	108.47
24	t	101	BCR	C3-C2-C1	2.11	122.16	114.60
22	b	617	CLA	C4-C3-C5	2.11	118.83	115.27
32	D	409	LHG	O8-C23-C24	2.11	118.54	111.91
22	C	504	CLA	C7-C6-C5	-2.11	107.62	113.36
22	c	505	CLA	C1-O2A-CGA	2.11	121.99	116.44
22	b	609	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
24	b	618	BCR	C28-C29-C30	2.11	122.15	114.60
24	B	619	BCR	C28-C29-C30	2.11	122.15	114.60
22	b	617	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
22	B	611	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
32	d	409	LHG	O8-C23-C24	2.11	118.53	111.91
22	c	510	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
31	c	518	DGD	O1G-C1A-O1A	-2.11	118.27	123.59
22	C	508	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
33	f	101	HEM	CMA-C3A-C4A	-2.11	125.23	128.46
25	b	621	SQD	O47-C7-O49	-2.11	118.61	123.70
22	b	614	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
22	b	605	CLA	CHD-C4C-NC	-2.11	120.89	124.20
25	b	621	SQD	O5-C1-C2	-2.11	105.89	110.35
22	b	606	CLA	CAC-C3C-C4C	2.10	127.54	124.81
22	A	603	CLA	O2A-CGA-CBA	2.10	118.51	111.91
22	b	605	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
22	c	508	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
22	B	617	CLA	C4-C3-C5	2.10	118.81	115.27
22	c	504	CLA	C7-C6-C5	-2.10	107.65	113.36
22	B	614	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
22	b	604	CLA	CAC-C3C-C4C	2.10	127.53	124.81
24	K	102	BCR	C29-C28-C27	-2.10	106.69	111.38
22	C	512	CLA	CMC-C2C-C1C	2.10	128.24	125.04
22	B	604	CLA	O2A-CGA-CBA	2.10	118.50	111.91
22	b	611	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	B	609	CLA	CHC-C1C-C2C	-2.10	120.92	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	b	604	CLA	CHD-C4C-C3C	-2.10	121.75	124.84
22	c	505	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
24	k	102	BCR	C29-C28-C27	-2.09	106.70	111.38
24	D	404	BCR	C24-C25-C26	2.09	126.53	121.46
31	C	518	DGD	O1G-C1A-O1A	-2.09	118.31	123.59
22	B	604	CLA	CHD-C4C-C3C	-2.09	121.76	124.84
25	d	411	SQD	C3-C4-C5	2.09	113.97	110.24
22	b	609	CLA	C11-C10-C8	-2.09	109.16	115.92
22	B	606	CLA	CAC-C3C-C4C	2.09	127.52	124.81
22	c	501	CLA	C1-C2-C3	-2.09	122.43	126.04
24	d	404	BCR	C24-C25-C26	2.09	126.53	121.46
22	C	505	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
22	b	604	CLA	O2A-CGA-CBA	2.09	118.46	111.91
28	A	613	PL9	C51-C49-C50	2.09	119.21	114.60
22	c	509	CLA	C4-C3-C5	2.09	118.78	115.27
22	B	604	CLA	CAC-C3C-C4C	2.09	127.52	124.81
22	B	616	CLA	C11-C10-C8	-2.09	109.18	115.92
22	B	613	CLA	C1D-CHD-C4C	2.09	125.31	122.56
28	d	408	PL9	C7-C3-C2	-2.09	120.56	123.30
22	C	510	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
22	c	511	CLA	CMC-C2C-C1C	2.08	128.21	125.04
22	b	615	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	B	609	CLA	C11-C10-C8	-2.08	109.19	115.92
22	C	509	CLA	C4-C3-C5	2.08	118.77	115.27
28	D	408	PL9	C7-C3-C2	-2.08	120.57	123.30
28	a	613	PL9	C51-C49-C50	2.08	119.19	114.60
24	A	608	BCR	C2-C1-C6	2.08	113.68	110.48
22	B	604	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
22	b	609	CLA	CMC-C2C-C1C	2.08	128.20	125.04
22	D	403	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
22	b	604	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
33	F	101	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
22	A	604	CLA	CHC-C1C-C2C	-2.07	120.99	126.72
25	D	411	SQD	C3-C4-C5	2.07	113.93	110.24
29	Z	101	LMG	C9-O8-C28	2.07	122.30	117.10
22	A	607	CLA	CHB-C4A-NA	2.07	127.37	124.51
28	D	408	PL9	C51-C49-C50	2.07	119.17	114.60
22	b	616	CLA	C11-C10-C8	-2.07	109.24	115.92
22	c	509	CLA	C1-O2A-CGA	2.07	121.86	116.44
28	d	408	PL9	C51-C49-C50	2.06	119.16	114.60
22	C	509	CLA	C1-O2A-CGA	2.06	121.86	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	CMC-C2C-C1C	2.06	128.18	125.04
22	B	616	CLA	CMC-C2C-C1C	2.06	128.18	125.04
22	a	607	CLA	CHB-C4A-NA	2.06	127.36	124.51
22	B	607	CLA	CMC-C2C-C1C	2.06	128.18	125.04
22	d	403	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
22	B	610	CLA	CMC-C2C-C1C	2.06	128.18	125.04
22	B	602	CLA	C1-O2A-CGA	2.06	121.85	116.44
22	C	501	CLA	C1-C2-C3	-2.06	122.48	126.04
22	B	615	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	a	608	BCR	C2-C1-C6	2.06	113.65	110.48
29	z	101	LMG	C9-O8-C28	2.06	122.27	117.10
22	B	609	CLA	CMC-C2C-C1C	2.06	128.17	125.04
22	a	604	CLA	CHC-C1C-C2C	-2.05	121.04	126.72
22	c	512	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
22	b	602	CLA	C1-O2A-CGA	2.05	121.83	116.44
22	c	507	CLA	OBD-CAD-C3D	-2.05	124.58	127.98
22	b	610	CLA	CMC-C2C-C1C	2.05	128.16	125.04
25	A	609	SQD	O5-C1-C2	-2.05	106.01	110.35
24	b	622	BCR	C2-C3-C4	2.05	115.96	111.38
29	a	614	LMG	C7-O1-C1	-2.05	109.74	113.74
22	b	607	CLA	CMC-C2C-C1C	2.05	128.16	125.04
22	B	606	CLA	CMB-C2B-C3B	2.05	128.51	124.68
25	L	101	SQD	O9-S-C6	2.05	109.37	106.94
25	a	609	SQD	O5-C1-C2	-2.05	106.02	110.35
24	B	622	BCR	C2-C3-C4	2.05	115.95	111.38
29	A	614	LMG	C7-O1-C1	-2.04	109.75	113.74
22	C	510	CLA	C4-C3-C5	2.04	118.71	115.27
22	b	616	CLA	CMC-C2C-C1C	2.04	128.15	125.04
22	C	507	CLA	OBD-CAD-C3D	-2.04	124.59	127.98
22	D	403	CLA	C6-C7-C8	-2.04	109.32	115.92
25	L	101	SQD	C4-C3-C2	2.04	114.39	110.82
22	c	510	CLA	C4-C3-C5	2.04	118.70	115.27
22	c	509	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
22	C	512	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
24	T	102	BCR	C40-C30-C25	2.04	113.60	110.30
22	b	607	CLA	CAC-C3C-C4C	2.03	127.45	124.81
22	A	603	CLA	CHC-C1C-C2C	-2.03	121.09	126.72
25	l	101	SQD	O9-S-C6	2.03	109.36	106.94
24	h	101	BCR	C40-C30-C29	-2.03	100.78	108.91
24	H	101	BCR	C40-C30-C29	-2.03	100.78	108.91
24	C	515	BCR	C4-C5-C6	2.03	125.68	122.73
22	C	509	CLA	CHC-C1C-C2C	-2.03	121.11	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	O2A-CGA-CBA	2.03	118.27	111.91
22	a	603	CLA	CHC-C1C-C2C	-2.03	121.12	126.72
22	c	507	CLA	C1-O2A-CGA	2.03	121.76	116.44
23	A	605	PHO	O1D-CGD-CBD	-2.03	120.34	124.48
22	B	607	CLA	CAC-C3C-C4C	2.02	127.44	124.81
24	H	101	BCR	C1-C6-C5	-2.02	119.76	122.61
25	l	101	SQD	C4-C3-C2	2.02	114.36	110.82
24	t	101	BCR	C40-C30-C25	2.02	113.58	110.30
22	C	507	CLA	C1-O2A-CGA	2.02	121.75	116.44
24	c	515	BCR	C4-C5-C6	2.02	125.67	122.73
22	c	506	CLA	O2A-CGA-CBA	2.02	118.24	111.91
22	c	513	CLA	CED-O2D-CGD	2.02	120.50	115.94
22	d	403	CLA	C6-C7-C8	-2.02	109.40	115.92
22	c	505	CLA	CHD-C4C-C3C	-2.01	121.88	124.84
22	C	506	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
23	a	605	PHO	O1D-CGD-CBD	-2.01	120.37	124.48
22	B	608	CLA	CHB-C4A-NA	2.01	127.30	124.51
22	b	606	CLA	CMC-C2C-C1C	2.01	128.10	125.04
32	l	103	LHG	O4-P-O5	2.01	122.17	112.24
22	b	608	CLA	CHB-C4A-NA	2.01	127.29	124.51
32	L	102	LHG	O4-P-O5	2.01	122.16	112.24
22	b	606	CLA	CMB-C2B-C3B	2.01	128.43	124.68
22	B	610	CLA	C4D-C3D-CAD	2.00	109.59	108.47
22	b	603	CLA	CMC-C2C-C1C	2.00	128.09	125.04
22	c	507	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
22	A	603	CLA	C7-C6-C5	-2.00	107.92	113.36
24	h	101	BCR	C1-C6-C5	-2.00	119.80	122.61
22	C	513	CLA	CED-O2D-CGD	2.00	120.46	115.94

All (166) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	617	CLA	NC
22	B	617	CLA	ND
22	B	617	CLA	NA
22	c	513	CLA	NC
22	c	513	CLA	NA
22	A	607	CLA	NC
22	d	402	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	NA
22	B	610	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	610	CLA	ND
22	c	502	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	602	CLA	ND
22	b	602	CLA	NA
22	D	403	CLA	NC
22	D	403	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	NA
22	B	609	CLA	NC
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	C	505	CLA	ND
22	A	603	CLA	NC
22	A	603	CLA	ND
22	A	603	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	b	613	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	608	CLA	NC
22	b	608	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	608	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	B	602	CLA	ND
22	B	602	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	B	616	CLA	NC
22	B	616	CLA	ND
22	B	616	CLA	NA
22	D	401	CLA	ND
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	d	401	CLA	ND
22	c	501	CLA	NC
22	c	501	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	608	CLA	NA
22	b	604	CLA	NC
22	b	604	CLA	ND
22	b	604	CLA	NA
22	C	513	CLA	NC
22	C	513	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	a	603	CLA	NC
22	a	603	CLA	ND
22	a	603	CLA	NA
22	D	402	CLA	NA
22	C	502	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	NA
22	a	604	CLA	NC
22	a	604	CLA	NA
22	c	505	CLA	ND
22	b	603	CLA	NC
22	b	603	CLA	ND
22	b	603	CLA	NA
22	b	609	CLA	NC
22	A	604	CLA	NC
22	A	604	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	NA
22	C	512	CLA	ND
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	B	613	CLA	NA
22	B	613	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	613	CLA	ND
22	c	512	CLA	NC
22	c	512	CLA	NA
22	c	512	CLA	ND
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	d	403	CLA	NC
22	d	403	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	a	607	CLA	NC
22	C	511	CLA	NC
22	C	511	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA

All (1546) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	E	101	LHG	O9-C7-O7-C5
32	E	101	LHG	C8-C7-O7-C5
29	Z	101	LMG	O6-C1-O1-C7
29	Z	101	LMG	O1-C7-C8-O7
29	Z	101	LMG	O9-C10-O7-C8
22	c	502	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
24	K	102	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	K	102	BCR	C17-C18-C19-C20
24	K	102	BCR	C36-C18-C19-C20
24	K	102	BCR	C18-C19-C20-C21
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	C4-O6-P-O4
28	a	613	PL9	C9-C11-C12-C13
28	a	613	PL9	C18-C19-C21-C22
28	a	613	PL9	C20-C19-C21-C22
28	a	613	PL9	C19-C21-C22-C23
28	a	613	PL9	C24-C26-C27-C28
22	b	602	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
24	C	515	BCR	C14-C15-C16-C17
24	C	515	BCR	C18-C19-C20-C21
22	B	606	CLA	C2-C3-C5-C6
22	B	606	CLA	C4-C3-C5-C6
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	C4-O6-P-O4
24	h	101	BCR	C10-C11-C12-C13
24	h	101	BCR	C18-C19-C20-C21
31	D	410	DGD	C2B-C1B-O2G-C2G
31	D	410	DGD	C2D-C1D-O3G-C3G
31	D	410	DGD	C2E-C1E-O5D-C6D
31	D	410	DGD	O6E-C1E-O5D-C6D
25	D	411	SQD	C2-C1-O6-C44
25	D	411	SQD	O5-C1-O6-C44
22	b	606	CLA	C2-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
25	d	411	SQD	C2-C1-O6-C44
25	d	411	SQD	O5-C1-O6-C44
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
22	B	602	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	z	101	LMG	O6-C1-O1-C7
29	z	101	LMG	O1-C7-C8-O7
29	z	101	LMG	O9-C10-O7-C8
25	B	601	SQD	O6-C44-C45-O47
24	c	514	BCR	C14-C15-C16-C17
24	c	514	BCR	C18-C19-C20-C21
25	L	101	SQD	C8-C7-O47-C45
25	L	101	SQD	O5-C5-C6-S
28	A	613	PL9	C9-C11-C12-C13
28	A	613	PL9	C18-C19-C21-C22
28	A	613	PL9	C20-C19-C21-C22
28	A	613	PL9	C19-C21-C22-C23
28	A	613	PL9	C24-C26-C27-C28
24	C	514	BCR	C14-C15-C16-C17
24	C	514	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
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
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
24	H	101	BCR	C18-C19-C20-C21
31	d	410	DGD	C2B-C1B-O2G-C2G
31	d	410	DGD	C2D-C1D-O3G-C3G
31	d	410	DGD	C2E-C1E-O5D-C6D
31	d	410	DGD	O6E-C1E-O5D-C6D
24	T	101	BCR	C10-C11-C12-C13
24	T	101	BCR	C11-C12-C13-C14
24	T	101	BCR	C11-C12-C13-C35
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
25	b	621	SQD	O5-C1-O6-C44
25	b	621	SQD	C8-C7-O47-C45
25	b	621	SQD	O5-C5-C6-S
24	c	515	BCR	C14-C15-C16-C17
24	c	515	BCR	C18-C19-C20-C21
32	L	102	LHG	C4-O6-P-O4
32	L	102	LHG	C4-O6-P-O5
22	b	615	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	b	615	CLA	CAD-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
24	k	102	BCR	C10-C11-C12-C13
24	k	102	BCR	C17-C18-C19-C20
24	k	102	BCR	C36-C18-C19-C20
24	k	102	BCR	C18-C19-C20-C21
32	l	103	LHG	C4-O6-P-O4
32	l	103	LHG	C4-O6-P-O5
22	B	615	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D
24	B	618	BCR	C10-C11-C12-C13
24	B	618	BCR	C11-C12-C13-C14
24	B	618	BCR	C11-C12-C13-C35
32	e	101	LHG	O9-C7-O7-C5
32	e	101	LHG	C8-C7-O7-C5
25	b	601	SQD	O6-C44-C45-O47
29	Z	101	LMG	C29-C28-O8-C9
29	z	101	LMG	C29-C28-O8-C9
32	E	101	LHG	O10-C23-O8-C6
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	C24-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
29	Z	101	LMG	O10-C28-O8-C9
29	z	101	LMG	O10-C28-O8-C9
22	c	513	CLA	CBD-CGD-O2D-CED
22	C	513	CLA	CBD-CGD-O2D-CED
31	D	410	DGD	O1B-C1B-O2G-C2G
25	l	102	SQD	O49-C7-O47-C45
31	d	410	DGD	O1B-C1B-O2G-C2G
25	b	621	SQD	O49-C7-O47-C45
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
29	Z	101	LMG	C11-C10-O7-C8
29	z	101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
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
25	l	101	SQD	O49-C7-O47-C45
25	L	101	SQD	O49-C7-O47-C45
24	D	404	BCR	C15-C16-C17-C18
24	d	404	BCR	C15-C16-C17-C18
22	c	508	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
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
22	B	607	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
29	c	520	LMG	O6-C5-C6-O5
29	C	520	LMG	O6-C5-C6-O5
28	a	613	PL9	C14-C16-C17-C18
28	A	613	PL9	C14-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
24	C	515	BCR	C15-C16-C17-C18
24	c	515	BCR	C15-C16-C17-C18
29	c	520	LMG	C4-C5-C6-O5
29	C	520	LMG	C4-C5-C6-O5
22	c	502	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9
22	C	501	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C12-C13-C14
22	B	602	CLA	C11-C10-C8-C9
22	c	509	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C12-C13-C14
22	c	501	CLA	C11-C12-C13-C14
22	C	502	CLA	C14-C13-C15-C16
22	C	509	CLA	C6-C7-C8-C9
24	T	102	BCR	C37-C22-C23-C24
24	K	102	BCR	C7-C8-C9-C34
24	t	101	BCR	C37-C22-C23-C24
24	k	102	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
31	D	410	DGD	C4E-C5E-C6E-O5E
31	d	410	DGD	C4E-C5E-C6E-O5E
31	D	410	DGD	C1A-C2A-C3A-C4A
29	C	519	LMG	C28-C29-C30-C31
31	d	410	DGD	C1A-C2A-C3A-C4A
29	c	519	LMG	C28-C29-C30-C31
25	l	101	SQD	O10-C23-O48-C46
25	L	101	SQD	O10-C23-O48-C46
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	C10-C11-C12-C13
22	A	607	CLA	C13-C15-C16-C17
22	b	602	CLA	C10-C11-C12-C13
22	B	602	CLA	C10-C11-C12-C13
22	a	607	CLA	C13-C15-C16-C17
32	D	405	LHG	C23-C24-C25-C26
32	d	405	LHG	C23-C24-C25-C26
22	c	509	CLA	C8-C10-C11-C12
22	b	615	CLA	C5-C6-C7-C8
22	b	615	CLA	C10-C11-C12-C13
22	B	615	CLA	C5-C6-C7-C8
22	B	615	CLA	C10-C11-C12-C13
22	C	509	CLA	C8-C10-C11-C12
32	d	407	LHG	O1-C1-C2-O2
32	D	407	LHG	O1-C1-C2-O2
31	c	517	DGD	C1B-C2B-C3B-C4B
25	l	102	SQD	C7-C8-C9-C10
31	C	517	DGD	C1B-C2B-C3B-C4B
29	c	520	LMG	C28-C29-C30-C31
25	b	621	SQD	C7-C8-C9-C10
29	C	520	LMG	C28-C29-C30-C31
22	B	607	CLA	C13-C15-C16-C17
22	b	607	CLA	C13-C15-C16-C17
22	D	403	CLA	C8-C10-C11-C12
22	c	506	CLA	C5-C6-C7-C8
22	d	403	CLA	C8-C10-C11-C12
32	E	101	LHG	C7-C8-C9-C10
31	D	410	DGD	C1B-C2B-C3B-C4B
25	B	601	SQD	C23-C24-C25-C26
29	A	614	LMG	C28-C29-C30-C31
29	a	614	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
31	d	410	DGD	C1B-C2B-C3B-C4B
32	e	101	LHG	C7-C8-C9-C10
25	b	601	SQD	C23-C24-C25-C26
22	C	506	CLA	C5-C6-C7-C8
24	c	514	BCR	C19-C20-C21-C22
24	C	514	BCR	C19-C20-C21-C22
22	D	403	CLA	C10-C11-C12-C13
22	B	607	CLA	C15-C16-C17-C18
22	b	607	CLA	C15-C16-C17-C18
22	d	403	CLA	C10-C11-C12-C13
31	D	410	DGD	O6D-C1D-O3G-C3G
31	d	410	DGD	O6D-C1D-O3G-C3G
22	a	604	CLA	C13-C15-C16-C17
22	A	604	CLA	C13-C15-C16-C17
24	K	101	BCR	C10-C11-C12-C13
24	k	101	BCR	C10-C11-C12-C13
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	b	612	CLA	C15-C16-C17-C18
22	B	612	CLA	C15-C16-C17-C18
22	a	607	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	501	CLA	C15-C16-C17-C18
22	C	506	CLA	C10-C11-C12-C13
22	c	506	CLA	C10-C11-C12-C13
32	d	407	LHG	C3-O3-P-O6
32	D	407	LHG	C3-O3-P-O6
32	L	102	LHG	C4-O6-P-O3
32	l	103	LHG	C4-O6-P-O3
22	a	604	CLA	C16-C17-C18-C20
22	A	604	CLA	C16-C17-C18-C20
24	c	514	BCR	C15-C16-C17-C18
24	C	514	BCR	C15-C16-C17-C18
25	a	609	SQD	C11-C12-C13-C14
31	C	518	DGD	C9B-CAB-CBB-CCB
31	C	516	DGD	C4B-C5B-C6B-C7B
32	e	101	LHG	C24-C25-C26-C27
25	A	609	SQD	C11-C12-C13-C14
24	C	515	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
24	h	101	BCR	C20-C21-C22-C37
24	B	619	BCR	C20-C21-C22-C37
24	b	618	BCR	C20-C21-C22-C37
24	H	101	BCR	C20-C21-C22-C37
24	c	515	BCR	C20-C21-C22-C37
32	E	101	LHG	C14-C15-C16-C17
32	E	101	LHG	C24-C25-C26-C27
31	c	516	DGD	C4B-C5B-C6B-C7B
29	B	620	LMG	C32-C33-C34-C35
31	D	410	DGD	CCA-CDA-CEA-CFA
31	D	410	DGD	C7B-C8B-C9B-CAB
25	D	411	SQD	C26-C27-C28-C29
25	D	411	SQD	C29-C30-C31-C32
25	D	411	SQD	C34-C35-C36-C37
25	d	411	SQD	C26-C27-C28-C29
25	d	411	SQD	C29-C30-C31-C32
25	d	411	SQD	C34-C35-C36-C37
25	l	101	SQD	C11-C10-C9-C8
25	l	101	SQD	C10-C11-C12-C13
25	l	101	SQD	C15-C16-C17-C18
29	D	406	LMG	C14-C15-C16-C17
25	B	601	SQD	C15-C16-C17-C18
25	L	101	SQD	C10-C11-C12-C13
25	L	101	SQD	C15-C16-C17-C18
29	A	614	LMG	C12-C13-C14-C15
29	d	406	LMG	C14-C15-C16-C17
29	d	406	LMG	C16-C17-C18-C19
29	a	614	LMG	C12-C13-C14-C15
31	d	410	DGD	CCA-CDA-CEA-CFA
31	d	410	DGD	C7B-C8B-C9B-CAB
29	c	520	LMG	C29-C30-C31-C32
32	L	102	LHG	C12-C13-C14-C15
29	C	520	LMG	C29-C30-C31-C32
29	b	619	LMG	C32-C33-C34-C35
31	c	518	DGD	C9B-CAB-CBB-CCB
32	l	103	LHG	C12-C13-C14-C15
32	e	101	LHG	C14-C15-C16-C17
25	b	601	SQD	C15-C16-C17-C18
22	C	506	CLA	C16-C17-C18-C19
22	c	506	CLA	C16-C17-C18-C19
25	a	609	SQD	C28-C29-C30-C31
29	Z	101	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	Z	101	LMG	C19-C20-C21-C22
31	c	517	DGD	C9A-CAA-CBA-CCA
29	D	406	LMG	C16-C17-C18-C19
29	z	101	LMG	C12-C13-C14-C15
29	z	101	LMG	C19-C20-C21-C22
25	L	101	SQD	C11-C10-C9-C8
29	A	614	LMG	C13-C14-C15-C16
29	C	519	LMG	C15-C16-C17-C18
29	a	614	LMG	C13-C14-C15-C16
25	A	609	SQD	C28-C29-C30-C31
25	l	101	SQD	C46-C45-O47-C7
25	L	101	SQD	C46-C45-O47-C7
31	C	517	DGD	C1A-C2A-C3A-C4A
31	D	410	DGD	C2A-C3A-C4A-C5A
31	D	410	DGD	C9B-CAB-CBB-CCB
29	A	614	LMG	C34-C35-C36-C37
31	C	517	DGD	C9A-CAA-CBA-CCA
29	a	614	LMG	C34-C35-C36-C37
31	d	410	DGD	C2A-C3A-C4A-C5A
31	d	410	DGD	C9B-CAB-CBB-CCB
29	c	519	LMG	C15-C16-C17-C18
25	a	609	SQD	C12-C13-C14-C15
25	a	609	SQD	C15-C16-C17-C18
32	D	405	LHG	C32-C33-C34-C35
29	C	520	LMG	C30-C31-C32-C33
32	d	405	LHG	C32-C33-C34-C35
25	A	609	SQD	C12-C13-C14-C15
25	A	609	SQD	C15-C16-C17-C18
31	c	516	DGD	C5B-C6B-C7B-C8B
31	c	517	DGD	C9B-CAB-CBB-CCB
31	D	410	DGD	CBA-CCA-CDA-CEA
31	C	516	DGD	C5B-C6B-C7B-C8B
25	l	101	SQD	C12-C13-C14-C15
25	L	101	SQD	C12-C13-C14-C15
31	C	517	DGD	C9B-CAB-CBB-CCB
29	c	520	LMG	C30-C31-C32-C33
29	Z	101	LMG	C10-C11-C12-C13
31	c	517	DGD	C1A-C2A-C3A-C4A
29	z	101	LMG	C10-C11-C12-C13
24	K	102	BCR	C20-C21-C22-C23
24	h	101	BCR	C20-C21-C22-C23
24	B	619	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
24	c	514	BCR	C20-C21-C22-C23
24	C	514	BCR	C20-C21-C22-C23
24	b	618	BCR	C20-C21-C22-C23
24	H	101	BCR	C20-C21-C22-C23
24	k	102	BCR	C20-C21-C22-C23
31	c	517	DGD	CBB-CCB-CDB-CEB
25	l	101	SQD	C17-C18-C19-C20
25	l	101	SQD	C24-C25-C26-C27
25	L	101	SQD	C17-C18-C19-C20
25	L	101	SQD	C24-C25-C26-C27
31	C	517	DGD	CBB-CCB-CDB-CEB
29	C	519	LMG	C17-C18-C19-C20
31	d	410	DGD	CBA-CCA-CDA-CEA
29	c	519	LMG	C17-C18-C19-C20
22	B	614	CLA	C15-C16-C17-C18
22	b	614	CLA	C15-C16-C17-C18
22	D	403	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C19
25	d	411	SQD	C24-C25-C26-C27
25	l	101	SQD	C18-C19-C20-C21
25	L	101	SQD	C18-C19-C20-C21
29	C	520	LMG	C31-C32-C33-C34
29	b	619	LMG	C31-C32-C33-C34
31	H	102	DGD	C7A-C8A-C9A-CAA
22	b	604	CLA	C6-C7-C8-C9
22	B	604	CLA	C6-C7-C8-C9
32	E	101	LHG	C25-C26-C27-C28
29	B	620	LMG	C31-C32-C33-C34
31	h	102	DGD	C7A-C8A-C9A-CAA
31	C	518	DGD	C2A-C3A-C4A-C5A
25	D	411	SQD	C24-C25-C26-C27
25	l	101	SQD	C29-C30-C31-C32
25	l	102	SQD	C34-C35-C36-C37
29	D	406	LMG	C39-C40-C41-C42
31	C	517	DGD	C3A-C4A-C5A-C6A
29	d	406	LMG	C39-C40-C41-C42
29	c	520	LMG	C31-C32-C33-C34
25	b	621	SQD	C34-C35-C36-C37
31	c	518	DGD	C2A-C3A-C4A-C5A
32	e	101	LHG	C25-C26-C27-C28
22	B	617	CLA	C8-C10-C11-C12
22	b	617	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	a	609	SQD	C16-C17-C18-C19
31	c	517	DGD	C3A-C4A-C5A-C6A
31	c	517	DGD	C6B-C7B-C8B-C9B
29	D	406	LMG	C12-C13-C14-C15
29	D	406	LMG	C19-C20-C21-C22
25	L	101	SQD	C29-C30-C31-C32
29	A	614	LMG	C14-C15-C16-C17
31	C	517	DGD	C6B-C7B-C8B-C9B
29	d	406	LMG	C12-C13-C14-C15
29	d	406	LMG	C19-C20-C21-C22
29	a	614	LMG	C14-C15-C16-C17
25	b	621	SQD	C31-C32-C33-C34
25	A	609	SQD	C16-C17-C18-C19
32	D	405	LHG	O1-C1-C2-C3
32	d	405	LHG	O1-C1-C2-C3
29	A	614	LMG	C11-C10-O7-C8
29	a	614	LMG	C11-C10-O7-C8
31	c	516	DGD	C4A-C5A-C6A-C7A
31	c	516	DGD	C6A-C7A-C8A-C9A
31	D	410	DGD	CCB-CDB-CEB-CFB
32	D	405	LHG	C29-C30-C31-C32
31	C	516	DGD	C6A-C7A-C8A-C9A
25	l	101	SQD	C27-C28-C29-C30
25	l	102	SQD	C31-C32-C33-C34
25	L	101	SQD	C27-C28-C29-C30
29	A	614	LMG	C18-C19-C20-C21
29	a	614	LMG	C18-C19-C20-C21
31	d	410	DGD	CCB-CDB-CEB-CFB
25	b	621	SQD	C11-C12-C13-C14
32	d	405	LHG	C29-C30-C31-C32
29	C	519	LMG	C10-C11-C12-C13
29	c	519	LMG	C10-C11-C12-C13
31	c	516	DGD	CAB-CBB-CCB-CDB
29	B	620	LMG	C17-C18-C19-C20
31	C	516	DGD	C4A-C5A-C6A-C7A
31	C	516	DGD	CAB-CBB-CCB-CDB
25	l	101	SQD	C14-C15-C16-C17
25	l	101	SQD	C32-C33-C34-C35
25	l	102	SQD	C11-C10-C9-C8
25	l	102	SQD	C11-C12-C13-C14
25	B	601	SQD	C16-C17-C18-C19
25	L	101	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	L	101	SQD	C32-C33-C34-C35
25	b	621	SQD	C11-C10-C9-C8
32	L	102	LHG	C13-C14-C15-C16
29	b	619	LMG	C17-C18-C19-C20
32	l	103	LHG	C11-C12-C13-C14
32	l	103	LHG	C13-C14-C15-C16
25	b	601	SQD	C16-C17-C18-C19
32	E	101	LHG	C18-C19-C20-C21
25	a	609	SQD	C9-C10-C11-C12
31	h	102	DGD	CBA-CCA-CDA-CEA
31	c	517	DGD	CAA-CBA-CCA-CDA
31	c	517	DGD	CAB-CBB-CCB-CDB
31	D	410	DGD	C8B-C9B-CAB-CBB
25	l	102	SQD	C24-C25-C26-C27
25	B	601	SQD	C26-C27-C28-C29
31	C	517	DGD	CAA-CBA-CCA-CDA
31	C	517	DGD	CAB-CBB-CCB-CDB
29	C	519	LMG	C32-C33-C34-C35
31	d	410	DGD	C8B-C9B-CAB-CBB
25	b	621	SQD	C24-C25-C26-C27
32	L	102	LHG	C11-C12-C13-C14
29	c	519	LMG	C32-C33-C34-C35
31	H	102	DGD	CBA-CCA-CDA-CEA
32	e	101	LHG	C18-C19-C20-C21
25	A	609	SQD	C9-C10-C11-C12
25	b	601	SQD	C26-C27-C28-C29
22	c	506	CLA	O1D-CGD-O2D-CED
29	Z	101	LMG	C16-C17-C18-C19
29	B	620	LMG	C37-C38-C39-C40
29	z	101	LMG	C16-C17-C18-C19
29	A	614	LMG	C31-C32-C33-C34
29	A	614	LMG	C36-C37-C38-C39
29	d	406	LMG	C15-C16-C17-C18
29	a	614	LMG	C31-C32-C33-C34
29	a	614	LMG	C36-C37-C38-C39
29	b	619	LMG	C37-C38-C39-C40
25	b	601	SQD	C28-C29-C30-C31
32	E	101	LHG	C13-C14-C15-C16
31	c	516	DGD	C8B-C9B-CAB-CBB
29	D	406	LMG	C15-C16-C17-C18
29	D	406	LMG	C30-C31-C32-C33
25	B	601	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	d	406	LMG	C30-C31-C32-C33
32	e	101	LHG	C13-C14-C15-C16
31	C	516	DGD	C8B-C9B-CAB-CBB
29	D	406	LMG	C36-C37-C38-C39
22	C	506	CLA	O1D-CGD-O2D-CED
25	D	411	SQD	C31-C32-C33-C34
25	d	411	SQD	C31-C32-C33-C34
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
29	A	614	LMG	C15-C16-C17-C18
29	d	406	LMG	C36-C37-C38-C39
29	a	614	LMG	C15-C16-C17-C18
32	E	101	LHG	C26-C27-C28-C29
29	B	620	LMG	C15-C16-C17-C18
25	l	102	SQD	C10-C11-C12-C13
29	A	614	LMG	C29-C30-C31-C32
29	a	614	LMG	C29-C30-C31-C32
25	b	621	SQD	C10-C11-C12-C13
29	b	619	LMG	C15-C16-C17-C18
32	e	101	LHG	C26-C27-C28-C29
32	d	407	LHG	C16-C17-C18-C19
32	D	407	LHG	C16-C17-C18-C19
31	C	517	DGD	C4A-C5A-C6A-C7A
29	c	520	LMG	C11-C10-O7-C8
29	C	520	LMG	C11-C10-O7-C8
31	c	517	DGD	C4A-C5A-C6A-C7A
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
31	C	516	DGD	O6D-C5D-C6D-O5D
22	c	507	CLA	C16-C17-C18-C19
22	C	507	CLA	C16-C17-C18-C19
29	Z	101	LMG	C15-C16-C17-C18
32	D	405	LHG	C24-C25-C26-C27
29	z	101	LMG	C15-C16-C17-C18
32	d	405	LHG	C24-C25-C26-C27
22	b	605	CLA	C13-C15-C16-C17
23	A	606	PHO	C2C-C3C-CAC-CBC
23	a	606	PHO	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	A	609	SQD	C32-C33-C34-C35
22	B	605	CLA	C13-C15-C16-C17
25	a	609	SQD	C32-C33-C34-C35
29	D	406	LMG	C13-C14-C15-C16
29	d	406	LMG	C13-C14-C15-C16
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
22	B	617	CLA	C2-C1-O2A-CGA
31	c	516	DGD	O6D-C5D-C6D-O5D
22	b	617	CLA	C2-C1-O2A-CGA
32	d	409	LHG	C29-C30-C31-C32
29	C	519	LMG	C34-C35-C36-C37
29	c	519	LMG	C34-C35-C36-C37
32	D	409	LHG	C29-C30-C31-C32
32	E	101	LHG	C27-C28-C29-C30
29	C	519	LMG	C29-C30-C31-C32
29	C	519	LMG	C39-C40-C41-C42
29	c	519	LMG	C29-C30-C31-C32
32	e	101	LHG	C27-C28-C29-C30
24	h	101	BCR	C23-C24-C25-C26
24	H	101	BCR	C23-C24-C25-C26
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
24	B	618	BCR	C1-C6-C7-C8
24	B	618	BCR	C5-C6-C7-C8
32	d	407	LHG	C32-C33-C34-C35
32	D	407	LHG	C32-C33-C34-C35
29	D	406	LMG	C20-C21-C22-C23
29	d	406	LMG	C20-C21-C22-C23
29	c	519	LMG	C39-C40-C41-C42
25	B	601	SQD	C24-C23-O48-C46
25	b	601	SQD	C24-C23-O48-C46
22	C	506	CLA	C13-C15-C16-C17
22	c	506	CLA	C13-C15-C16-C17
25	D	411	SQD	C8-C7-O47-C45
25	d	411	SQD	C8-C7-O47-C45
31	h	102	DGD	C9B-CAB-CBB-CCB
31	c	517	DGD	C3B-C4B-C5B-C6B
25	l	102	SQD	C32-C33-C34-C35
31	C	517	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	C9B-CAB-CBB-CCB
25	b	621	SQD	C32-C33-C34-C35
31	c	518	DGD	C6B-C7B-C8B-C9B
32	d	409	LHG	C10-C11-C12-C13
31	C	518	DGD	C6B-C7B-C8B-C9B
32	D	409	LHG	C10-C11-C12-C13
22	B	617	CLA	C6-C7-C8-C10
22	b	617	CLA	C6-C7-C8-C10
22	c	504	CLA	C11-C12-C13-C15
22	b	611	CLA	C12-C13-C15-C16
22	c	510	CLA	C2-C3-C5-C6
22	C	504	CLA	C11-C12-C13-C15
22	b	604	CLA	C6-C7-C8-C10
22	a	604	CLA	C6-C7-C8-C10
22	A	604	CLA	C6-C7-C8-C10
22	B	611	CLA	C12-C13-C15-C16
22	B	604	CLA	C6-C7-C8-C10
22	C	510	CLA	C2-C3-C5-C6
25	l	102	SQD	C29-C30-C31-C32
25	b	621	SQD	C29-C30-C31-C32
22	c	504	CLA	C13-C15-C16-C17
22	C	504	CLA	C13-C15-C16-C17
24	H	101	BCR	C15-C16-C17-C18
25	l	101	SQD	C7-C8-C9-C10
25	L	101	SQD	C7-C8-C9-C10
29	B	620	LMG	C34-C35-C36-C37
29	b	619	LMG	C34-C35-C36-C37
25	l	102	SQD	C18-C19-C20-C21
25	b	621	SQD	C18-C19-C20-C21
31	h	102	DGD	C9A-CAA-CBA-CCA
31	H	102	DGD	C9A-CAA-CBA-CCA
32	E	101	LHG	C15-C16-C17-C18
25	a	609	SQD	C30-C31-C32-C33
29	c	519	LMG	C38-C39-C40-C41
24	K	102	BCR	C6-C7-C8-C9
24	k	102	BCR	C6-C7-C8-C9
22	C	501	CLA	C13-C15-C16-C17
22	c	501	CLA	C13-C15-C16-C17
31	D	410	DGD	C3A-C4A-C5A-C6A
31	C	516	DGD	C3B-C4B-C5B-C6B
29	C	519	LMG	C38-C39-C40-C41
31	d	410	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
32	e	101	LHG	C15-C16-C17-C18
25	A	609	SQD	C30-C31-C32-C33
32	L	102	LHG	C7-C8-C9-C10
32	l	103	LHG	C7-C8-C9-C10
24	D	404	BCR	C18-C19-C20-C21
24	d	404	BCR	C18-C19-C20-C21
31	c	516	DGD	C3B-C4B-C5B-C6B
29	A	614	LMG	C17-C18-C19-C20
25	D	411	SQD	O49-C7-O47-C45
25	d	411	SQD	O49-C7-O47-C45
31	D	410	DGD	C9A-CAA-CBA-CCA
29	a	614	LMG	C17-C18-C19-C20
29	Z	101	LMG	C2-C1-O1-C7
29	z	101	LMG	C2-C1-O1-C7
31	d	410	DGD	C9A-CAA-CBA-CCA
29	B	620	LMG	C38-C39-C40-C41
31	C	518	DGD	C6A-C7A-C8A-C9A
31	C	518	DGD	CBA-CCA-CDA-CEA
31	D	410	DGD	C4B-C5B-C6B-C7B
31	d	410	DGD	C4B-C5B-C6B-C7B
29	b	619	LMG	C38-C39-C40-C41
31	c	518	DGD	C6A-C7A-C8A-C9A
31	c	518	DGD	CBA-CCA-CDA-CEA
22	c	510	CLA	C4-C3-C5-C6
22	C	510	CLA	C4-C3-C5-C6
28	a	613	PL9	C4-C3-C7-C8
28	A	613	PL9	C4-C3-C7-C8
22	B	617	CLA	C6-C7-C8-C9
22	D	403	CLA	C11-C10-C8-C9
22	b	617	CLA	C6-C7-C8-C9
22	B	616	CLA	C14-C13-C15-C16
22	b	611	CLA	C14-C13-C15-C16
22	b	616	CLA	C14-C13-C15-C16
22	a	604	CLA	C6-C7-C8-C9
22	A	604	CLA	C6-C7-C8-C9
22	B	611	CLA	C14-C13-C15-C16
22	d	403	CLA	C11-C10-C8-C9
29	B	620	LMG	C14-C15-C16-C17
29	b	619	LMG	C14-C15-C16-C17
25	a	609	SQD	C34-C35-C36-C37
25	B	601	SQD	C18-C19-C20-C21
29	C	519	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
29	c	519	LMG	C20-C21-C22-C23
25	A	609	SQD	C34-C35-C36-C37
25	b	601	SQD	C18-C19-C20-C21
25	B	601	SQD	O10-C23-O48-C46
25	b	601	SQD	O10-C23-O48-C46
22	D	403	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C20
22	C	506	CLA	C16-C17-C18-C20
22	d	403	CLA	C16-C17-C18-C20
29	B	620	LMG	C18-C19-C20-C21
31	h	102	DGD	CBB-CCB-CDB-CEB
29	b	619	LMG	C18-C19-C20-C21
31	H	102	DGD	CBB-CCB-CDB-CEB
24	h	101	BCR	C15-C16-C17-C18
22	D	403	CLA	C13-C15-C16-C17
22	c	507	CLA	C5-C6-C7-C8
22	C	507	CLA	C5-C6-C7-C8
29	C	519	LMG	C21-C22-C23-C24
29	c	519	LMG	C21-C22-C23-C24
25	D	411	SQD	C23-C24-C25-C26
25	d	411	SQD	C23-C24-C25-C26
23	A	606	PHO	O1D-CGD-O2D-CED
23	a	606	PHO	O1D-CGD-O2D-CED
22	d	403	CLA	C13-C15-C16-C17
29	A	614	LMG	C21-C22-C23-C24
29	a	614	LMG	C21-C22-C23-C24
22	A	607	CLA	C16-C17-C18-C19
22	B	605	CLA	C16-C17-C18-C20
22	c	507	CLA	C16-C17-C18-C20
22	C	507	CLA	C16-C17-C18-C20
22	c	506	CLA	C16-C17-C18-C20
22	a	607	CLA	C16-C17-C18-C19
29	Z	101	LMG	C13-C14-C15-C16
25	l	102	SQD	C27-C28-C29-C30
29	c	520	LMG	C18-C19-C20-C21
25	b	621	SQD	C27-C28-C29-C30
29	C	520	LMG	C18-C19-C20-C21
29	z	101	LMG	C13-C14-C15-C16
29	c	519	LMG	C16-C17-C18-C19
29	B	620	LMG	C16-C17-C18-C19
31	c	517	DGD	C8B-C9B-CAB-CBB
31	C	517	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	C	519	LMG	C16-C17-C18-C19
25	b	621	SQD	C28-C29-C30-C31
31	c	516	DGD	C7B-C8B-C9B-CAB
31	C	516	DGD	C7B-C8B-C9B-CAB
25	l	102	SQD	C28-C29-C30-C31
29	D	406	LMG	C35-C36-C37-C38
29	d	406	LMG	C35-C36-C37-C38
29	b	619	LMG	C16-C17-C18-C19
25	a	609	SQD	C27-C28-C29-C30
25	A	609	SQD	C27-C28-C29-C30
31	D	410	DGD	CAA-CBA-CCA-CDA
31	d	410	DGD	CAA-CBA-CCA-CDA
22	a	604	CLA	C16-C17-C18-C19
22	A	604	CLA	C16-C17-C18-C19
32	E	101	LHG	C11-C10-C9-C8
29	Z	101	LMG	O1-C7-C8-C9
31	c	516	DGD	C8A-C9A-CAA-CBA
31	C	516	DGD	C8A-C9A-CAA-CBA
29	z	101	LMG	O1-C7-C8-C9
25	B	601	SQD	O6-C44-C45-C46
29	A	614	LMG	C7-C8-C9-O8
29	a	614	LMG	C7-C8-C9-O8
32	L	102	LHG	C32-C33-C34-C35
32	l	103	LHG	C32-C33-C34-C35
32	e	101	LHG	C11-C10-C9-C8
25	b	601	SQD	O6-C44-C45-C46
22	c	509	CLA	C10-C11-C12-C13
22	C	509	CLA	C10-C11-C12-C13
25	D	411	SQD	C35-C36-C37-C38
25	d	411	SQD	C35-C36-C37-C38
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
29	c	520	LMG	C8-C7-O1-C1
29	C	520	LMG	C8-C7-O1-C1
22	B	607	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
25	l	102	SQD	C35-C36-C37-C38
25	b	621	SQD	C13-C14-C15-C16
25	b	621	SQD	C35-C36-C37-C38
25	l	102	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	D	406	LMG	C38-C39-C40-C41
29	d	406	LMG	C38-C39-C40-C41
29	C	520	LMG	C17-C18-C19-C20
25	B	601	SQD	C19-C20-C21-C22
29	c	520	LMG	C17-C18-C19-C20
25	b	601	SQD	C19-C20-C21-C22
25	a	609	SQD	C35-C36-C37-C38
25	A	609	SQD	C35-C36-C37-C38
22	b	613	CLA	C13-C15-C16-C17
22	B	613	CLA	C13-C15-C16-C17
31	c	516	DGD	O6E-C5E-C6E-O5E
31	C	516	DGD	O6E-C5E-C6E-O5E
29	D	406	LMG	O6-C5-C6-O5
29	d	406	LMG	O6-C5-C6-O5
22	C	512	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
22	C	507	CLA	C2A-CAA-CBA-CGA
22	A	607	CLA	C5-C6-C7-C8
22	a	607	CLA	C5-C6-C7-C8
31	c	516	DGD	C6B-C7B-C8B-C9B
32	D	405	LHG	C27-C28-C29-C30
31	C	516	DGD	C6B-C7B-C8B-C9B
32	d	405	LHG	C27-C28-C29-C30
22	C	512	CLA	O1D-CGD-O2D-CED
31	h	102	DGD	CDB-CEB-CFB-CGB
31	c	517	DGD	C7B-C8B-C9B-CAB
31	C	517	DGD	C7B-C8B-C9B-CAB
22	c	512	CLA	O1D-CGD-O2D-CED
31	H	102	DGD	CDB-CEB-CFB-CGB
25	l	101	SQD	C19-C20-C21-C22
25	L	101	SQD	C19-C20-C21-C22
29	A	614	LMG	C32-C33-C34-C35
29	a	614	LMG	C32-C33-C34-C35
31	h	102	DGD	C6B-C7B-C8B-C9B
29	A	614	LMG	C22-C23-C24-C25
29	a	614	LMG	C22-C23-C24-C25
29	c	520	LMG	C15-C16-C17-C18
29	c	520	LMG	C40-C41-C42-C43
29	C	520	LMG	C40-C41-C42-C43
31	H	102	DGD	C6B-C7B-C8B-C9B
22	c	512	CLA	O1A-CGA-O2A-C1
22	a	607	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	C	520	LMG	C15-C16-C17-C18
22	B	617	CLA	C11-C12-C13-C15
22	c	513	CLA	C6-C7-C8-C10
22	A	607	CLA	C11-C10-C8-C7
22	b	602	CLA	C6-C7-C8-C10
22	b	602	CLA	C11-C10-C8-C7
22	D	403	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C10-C8-C7
22	b	617	CLA	C11-C12-C13-C15
22	C	501	CLA	C11-C12-C13-C15
22	B	602	CLA	C6-C7-C8-C10
22	B	602	CLA	C11-C10-C8-C7
22	B	616	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	c	501	CLA	C11-C12-C13-C15
22	C	513	CLA	C6-C7-C8-C10
22	b	616	CLA	C12-C13-C15-C16
22	C	512	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C12-C13-C15
22	c	512	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15
22	d	403	CLA	C11-C10-C8-C7
22	a	607	CLA	C11-C10-C8-C7
22	C	512	CLA	O1A-CGA-O2A-C1
22	B	617	CLA	C11-C12-C13-C14
22	c	513	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	b	617	CLA	C11-C12-C13-C14
22	C	501	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	c	501	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C12-C13-C14
22	C	506	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C12-C13-C14
25	a	609	SQD	C14-C15-C16-C17
31	D	410	DGD	C5A-C6A-C7A-C8A
31	d	410	DGD	C5A-C6A-C7A-C8A
25	A	609	SQD	C14-C15-C16-C17
22	c	507	CLA	C2A-CAA-CBA-CGA
32	e	101	LHG	C19-C20-C21-C22
29	Z	101	LMG	C4-C5-C6-O5
22	B	617	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	A	607	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C19
22	b	617	CLA	C16-C17-C18-C20
22	B	605	CLA	C16-C17-C18-C19
32	E	101	LHG	C19-C20-C21-C22
31	c	516	DGD	C5A-C6A-C7A-C8A
31	D	410	DGD	C6A-C7A-C8A-C9A
31	C	516	DGD	C5A-C6A-C7A-C8A
31	d	410	DGD	C6A-C7A-C8A-C9A
31	c	516	DGD	CAA-CBA-CCA-CDA
25	B	601	SQD	C25-C26-C27-C28
29	C	519	LMG	C11-C12-C13-C14
29	c	519	LMG	C11-C12-C13-C14
25	b	601	SQD	C25-C26-C27-C28
31	C	516	DGD	CAA-CBA-CCA-CDA
25	A	609	SQD	C19-C20-C21-C22
25	l	102	SQD	C24-C23-O48-C46
29	C	519	LMG	C29-C28-O8-C9
25	b	621	SQD	C24-C23-O48-C46
29	c	519	LMG	C29-C28-O8-C9
25	a	609	SQD	C19-C20-C21-C22
31	c	517	DGD	CDB-CEB-CFB-CGB
31	C	517	DGD	CDB-CEB-CFB-CGB
29	z	101	LMG	C4-C5-C6-O5
32	D	405	LHG	C25-C26-C27-C28
32	d	405	LHG	C25-C26-C27-C28
31	C	518	DGD	C8B-C9B-CAB-CBB
25	B	601	SQD	O5-C1-O6-C44
25	b	601	SQD	O5-C1-O6-C44
25	B	601	SQD	C31-C32-C33-C34
31	c	518	DGD	C8B-C9B-CAB-CBB
25	b	601	SQD	C31-C32-C33-C34
23	A	605	PHO	C4-C3-C5-C6
22	B	609	CLA	C13-C15-C16-C17
22	b	604	CLA	C16-C17-C18-C20
22	B	604	CLA	C16-C17-C18-C20
22	b	609	CLA	C13-C15-C16-C17
22	b	602	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	CBA-CGA-O2A-C1
22	b	602	CLA	CAA-CBA-CGA-O2A
32	d	409	LHG	C12-C13-C14-C15
25	l	101	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	D	409	LHG	C12-C13-C14-C15
22	c	508	CLA	C5-C6-C7-C8
22	b	616	CLA	C13-C15-C16-C17
31	C	518	DGD	C3B-C4B-C5B-C6B
25	B	601	SQD	C32-C33-C34-C35
25	L	101	SQD	C35-C36-C37-C38
31	c	518	DGD	C3B-C4B-C5B-C6B
22	B	602	CLA	CAA-CBA-CGA-O2A
25	b	601	SQD	C32-C33-C34-C35
22	C	508	CLA	C5-C6-C7-C8
31	D	410	DGD	O1G-C1G-C2G-C3G
25	l	101	SQD	C44-C45-C46-O48
25	l	102	SQD	C44-C45-C46-O48
25	L	101	SQD	C44-C45-C46-O48
31	d	410	DGD	O1G-C1G-C2G-C3G
29	c	520	LMG	C7-C8-C9-O8
25	b	621	SQD	C44-C45-C46-O48
29	C	520	LMG	C7-C8-C9-O8
31	D	410	DGD	CAB-CBB-CCB-CDB
31	d	410	DGD	CAB-CBB-CCB-CDB
22	B	616	CLA	C13-C15-C16-C17
23	a	605	PHO	C4-C3-C5-C6
31	c	516	DGD	C4D-C5D-C6D-O5D
31	C	516	DGD	C4D-C5D-C6D-O5D
31	D	410	DGD	C5B-C6B-C7B-C8B
31	d	410	DGD	C5B-C6B-C7B-C8B
29	A	614	LMG	C33-C34-C35-C36
29	a	614	LMG	C33-C34-C35-C36
25	B	601	SQD	C35-C36-C37-C38
29	A	614	LMG	C39-C40-C41-C42
29	a	614	LMG	C39-C40-C41-C42
25	b	601	SQD	C35-C36-C37-C38
22	B	616	CLA	C10-C11-C12-C13
22	b	616	CLA	C10-C11-C12-C13
29	C	519	LMG	O10-C28-O8-C9
29	c	519	LMG	O10-C28-O8-C9
25	l	101	SQD	O47-C45-C46-O48
25	l	102	SQD	O47-C45-C46-O48
25	L	101	SQD	O47-C45-C46-O48
29	A	614	LMG	O7-C8-C9-O8
29	a	614	LMG	O7-C8-C9-O8
25	b	621	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
22	b	602	CLA	C16-C17-C18-C20
22	B	602	CLA	C16-C17-C18-C20
25	l	101	SQD	C30-C31-C32-C33
25	L	101	SQD	C30-C31-C32-C33
22	D	401	CLA	C2-C1-O2A-CGA
22	d	401	CLA	C2-C1-O2A-CGA
23	A	605	PHO	C2-C3-C5-C6
23	a	605	PHO	C2-C3-C5-C6
22	c	507	CLA	C11-C10-C8-C9
22	b	615	CLA	C11-C12-C13-C14
22	b	615	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	B	615	CLA	C14-C13-C15-C16
32	L	102	LHG	C33-C34-C35-C36
32	l	103	LHG	C33-C34-C35-C36
29	D	406	LMG	C17-C18-C19-C20
29	d	406	LMG	C17-C18-C19-C20
22	b	602	CLA	C15-C16-C17-C18
22	B	602	CLA	C15-C16-C17-C18
22	B	607	CLA	C8-C10-C11-C12
22	b	607	CLA	C8-C10-C11-C12
22	d	402	CLA	C2C-C3C-CAC-CBC
24	D	404	BCR	C23-C24-C25-C30
24	d	404	BCR	C23-C24-C25-C30
22	D	402	CLA	C2C-C3C-CAC-CBC
32	l	103	LHG	C14-C15-C16-C17
32	D	409	LHG	C13-C14-C15-C16
32	d	409	LHG	C13-C14-C15-C16
25	l	102	SQD	C16-C17-C18-C19
22	C	508	CLA	O1D-CGD-O2D-CED
24	K	102	BCR	C7-C8-C9-C10
24	k	102	BCR	C7-C8-C9-C10
22	c	502	CLA	C15-C16-C17-C18
22	C	502	CLA	C15-C16-C17-C18
32	L	102	LHG	C14-C15-C16-C17
32	L	102	LHG	C34-C35-C36-C37
22	c	508	CLA	O1D-CGD-O2D-CED
24	A	608	BCR	C14-C15-C16-C17
24	a	608	BCR	C14-C15-C16-C17
32	D	405	LHG	C13-C14-C15-C16
25	b	621	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	CCB-CDB-CEB-CFB
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	c	502	CLA	C16-C17-C18-C20
22	C	501	CLA	C16-C17-C18-C19
22	c	501	CLA	C16-C17-C18-C19
22	C	502	CLA	C16-C17-C18-C20
23	A	606	PHO	C4C-C3C-CAC-CBC
23	a	606	PHO	C4C-C3C-CAC-CBC
25	l	102	SQD	O10-C23-O48-C46
31	c	517	DGD	C8A-C9A-CAA-CBA
29	b	619	LMG	C33-C34-C35-C36
22	B	617	CLA	C12-C13-C15-C16
22	c	513	CLA	C11-C12-C13-C15
22	D	403	CLA	C6-C7-C8-C10
22	b	612	CLA	C12-C13-C15-C16
22	B	612	CLA	C12-C13-C15-C16
22	b	617	CLA	C12-C13-C15-C16
22	C	501	CLA	C12-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C7
22	c	501	CLA	C12-C13-C15-C16
22	C	513	CLA	C11-C12-C13-C15
22	b	616	CLA	C11-C10-C8-C7
22	b	615	CLA	C11-C12-C13-C15
22	B	615	CLA	C11-C12-C13-C15
22	d	403	CLA	C6-C7-C8-C10
25	b	621	SQD	O10-C23-O48-C46
29	B	620	LMG	C33-C34-C35-C36
31	C	517	DGD	C8A-C9A-CAA-CBA
29	b	619	LMG	C30-C31-C32-C33
24	K	102	BCR	C19-C20-C21-C22
24	k	102	BCR	C19-C20-C21-C22
22	B	617	CLA	C16-C17-C18-C19
29	B	620	LMG	C30-C31-C32-C33
29	c	519	LMG	C14-C15-C16-C17
32	D	405	LHG	C15-C16-C17-C18
22	D	401	CLA	C2C-C3C-CAC-CBC
29	C	519	LMG	C14-C15-C16-C17
22	d	401	CLA	C2C-C3C-CAC-CBC
32	d	405	LHG	C15-C16-C17-C18
22	b	617	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	D	411	SQD	C11-C10-C9-C8
25	d	411	SQD	C11-C10-C9-C8
29	A	614	LMG	C38-C39-C40-C41
29	a	614	LMG	C38-C39-C40-C41
32	L	102	LHG	C24-C25-C26-C27
22	c	503	CLA	C8-C10-C11-C12
22	C	503	CLA	C8-C10-C11-C12
31	c	518	DGD	C4A-C5A-C6A-C7A
32	l	103	LHG	C24-C25-C26-C27
22	B	617	CLA	CAD-CBD-CGD-O2D
22	b	617	CLA	CAD-CBD-CGD-O2D
22	A	603	CLA	CAD-CBD-CGD-O2D
22	C	501	CLA	CAD-CBD-CGD-O2D
23	A	606	PHO	CAD-CBD-CGD-O2D
22	b	611	CLA	CAD-CBD-CGD-O2D
22	c	501	CLA	CAD-CBD-CGD-O2D
23	a	606	PHO	CAD-CBD-CGD-O2D
22	a	603	CLA	CAD-CBD-CGD-O2D
22	B	611	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	c	512	CLA	CAD-CBD-CGD-O2D
32	d	409	LHG	C16-C17-C18-C19
31	C	518	DGD	C4A-C5A-C6A-C7A
29	c	520	LMG	C38-C39-C40-C41
29	C	520	LMG	C38-C39-C40-C41
32	D	409	LHG	C16-C17-C18-C19
32	D	409	LHG	C17-C18-C19-C20
32	d	409	LHG	C17-C18-C19-C20
29	A	614	LMG	O6-C1-O1-C7
29	a	614	LMG	O6-C1-O1-C7
32	E	101	LHG	O6-C4-C5-O7
32	e	101	LHG	O6-C4-C5-O7
32	d	407	LHG	C11-C10-C9-C8
32	D	407	LHG	C11-C10-C9-C8
25	B	601	SQD	C24-C25-C26-C27
25	b	601	SQD	C24-C25-C26-C27
22	C	501	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C19
22	B	604	CLA	C16-C17-C18-C19
22	C	510	CLA	O1D-CGD-O2D-CED
22	b	602	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	b	606	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	O1D-CGD-O2D-CED
22	b	602	CLA	O1A-CGA-O2A-C1
22	B	602	CLA	O1A-CGA-O2A-C1
31	h	102	DGD	CCA-CDA-CEA-CFA
31	H	102	DGD	CCA-CDA-CEA-CFA
25	B	601	SQD	C2-C1-O6-C44
29	A	614	LMG	C2-C1-O1-C7
29	a	614	LMG	C2-C1-O1-C7
25	b	601	SQD	C2-C1-O6-C44
29	A	614	LMG	O1-C7-C8-O7
29	a	614	LMG	O1-C7-C8-O7
25	B	601	SQD	C29-C30-C31-C32
25	b	601	SQD	C29-C30-C31-C32
22	b	602	CLA	C16-C17-C18-C19
22	B	602	CLA	C16-C17-C18-C19
22	c	501	CLA	C16-C17-C18-C20
22	D	403	CLA	O1D-CGD-O2D-CED
22	d	403	CLA	O1D-CGD-O2D-CED
25	B	601	SQD	C27-C28-C29-C30
31	D	410	DGD	CDB-CEB-CFB-CGB
25	b	601	SQD	C27-C28-C29-C30
22	A	607	CLA	C11-C12-C13-C14
22	D	403	CLA	C6-C7-C8-C9
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	a	607	CLA	C11-C12-C13-C14
31	d	410	DGD	CDB-CEB-CFB-CGB
24	A	608	BCR	C36-C18-C19-C20
24	a	608	BCR	C36-C18-C19-C20
31	c	517	DGD	C5A-C6A-C7A-C8A
32	d	409	LHG	C27-C28-C29-C30
31	C	517	DGD	C5A-C6A-C7A-C8A
29	C	519	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
29	c	519	LMG	C19-C20-C21-C22
32	D	409	LHG	C27-C28-C29-C30
22	C	506	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
29	B	620	LMG	C10-C11-C12-C13
29	C	520	LMG	C10-C11-C12-C13
29	b	619	LMG	C10-C11-C12-C13
31	H	102	DGD	C5B-C6B-C7B-C8B
31	h	102	DGD	C5B-C6B-C7B-C8B
24	B	619	BCR	C19-C20-C21-C22
24	b	618	BCR	C19-C20-C21-C22
22	b	611	CLA	C8-C10-C11-C12
32	d	407	LHG	C26-C27-C28-C29
32	D	407	LHG	C26-C27-C28-C29
29	c	520	LMG	C16-C17-C18-C19
22	A	607	CLA	O1D-CGD-O2D-CED
22	a	607	CLA	O1D-CGD-O2D-CED
29	C	520	LMG	C16-C17-C18-C19
32	d	409	LHG	C2-C3-O3-P
32	D	409	LHG	C2-C3-O3-P
32	E	101	LHG	C10-C11-C12-C13
31	c	517	DGD	CBA-CCA-CDA-CEA
31	C	517	DGD	CBA-CCA-CDA-CEA
32	e	101	LHG	C10-C11-C12-C13
32	d	407	LHG	C3-O3-P-O4
32	D	407	LHG	C3-O3-P-O4
22	b	611	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
29	c	520	LMG	C10-C11-C12-C13
31	C	518	DGD	C9A-CAA-CBA-CCA
32	L	102	LHG	C31-C32-C33-C34
31	c	518	DGD	C9A-CAA-CBA-CCA
22	B	614	CLA	C13-C15-C16-C17
22	B	611	CLA	C8-C10-C11-C12
22	b	614	CLA	C13-C15-C16-C17
32	l	103	LHG	C31-C32-C33-C34
29	c	519	LMG	C12-C13-C14-C15
25	b	601	SQD	C9-C10-C11-C12
22	b	605	CLA	C3-C5-C6-C7
25	B	601	SQD	C9-C10-C11-C12
29	C	519	LMG	C12-C13-C14-C15
31	c	517	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
31	C	517	DGD	CDA-CEA-CFA-CGA
22	b	602	CLA	CAD-CBD-CGD-O1D
22	B	606	CLA	CAD-CBD-CGD-O1D
22	b	606	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	B	602	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
25	a	609	SQD	C23-C24-C25-C26
25	A	609	SQD	C23-C24-C25-C26
25	l	102	SQD	C19-C20-C21-C22
31	d	410	DGD	CBB-CCB-CDB-CEB
25	b	621	SQD	C19-C20-C21-C22
22	B	605	CLA	C3-C5-C6-C7
31	D	410	DGD	CBB-CCB-CDB-CEB
25	D	411	SQD	C28-C29-C30-C31
29	C	520	LMG	C33-C34-C35-C36
25	d	411	SQD	C28-C29-C30-C31
29	c	520	LMG	C33-C34-C35-C36
22	b	616	CLA	C16-C17-C18-C20
22	D	403	CLA	C12-C13-C15-C16
22	c	504	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	509	CLA	C6-C7-C8-C10
22	C	504	CLA	C12-C13-C15-C16
22	a	604	CLA	C11-C10-C8-C7
22	A	604	CLA	C11-C10-C8-C7
22	b	615	CLA	C12-C13-C15-C16
22	C	506	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C10-C8-C7
22	B	615	CLA	C12-C13-C15-C16
22	c	506	CLA	C6-C7-C8-C10
22	d	403	CLA	C11-C12-C13-C15
22	d	403	CLA	C12-C13-C15-C16
22	C	509	CLA	C6-C7-C8-C10
29	z	101	LMG	C17-C18-C19-C20
22	B	616	CLA	C16-C17-C18-C20
29	Z	101	LMG	C17-C18-C19-C20
31	c	516	DGD	CBA-CCA-CDA-CEA
31	C	516	DGD	CBA-CCA-CDA-CEA
29	A	614	LMG	O1-C7-C8-C9
29	a	614	LMG	O1-C7-C8-C9
32	E	101	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
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	D	405	LHG	C33-C34-C35-C36
32	d	405	LHG	C33-C34-C35-C36
29	C	519	LMG	C13-C14-C15-C16
32	L	102	LHG	C26-C27-C28-C29
29	c	519	LMG	C13-C14-C15-C16
31	c	516	DGD	CDA-CEA-CFA-CGA
31	h	102	DGD	CDA-CEA-CFA-CGA
31	H	102	DGD	CDA-CEA-CFA-CGA
32	l	103	LHG	C26-C27-C28-C29
31	C	516	DGD	CDA-CEA-CFA-CGA
31	h	102	DGD	O2G-C1B-C2B-C3B
31	H	102	DGD	O2G-C1B-C2B-C3B
25	L	101	SQD	C13-C14-C15-C16
22	B	617	CLA	C14-C13-C15-C16
22	b	617	CLA	C14-C13-C15-C16
22	c	504	CLA	C14-C13-C15-C16
22	C	504	CLA	C14-C13-C15-C16
22	a	604	CLA	C11-C10-C8-C9
22	A	604	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C10-C8-C9
29	B	620	LMG	C28-C29-C30-C31
29	B	620	LMG	O9-C10-O7-C8
22	c	513	CLA	C3-C5-C6-C7
22	C	513	CLA	C3-C5-C6-C7
25	l	101	SQD	C13-C14-C15-C16
29	b	619	LMG	C28-C29-C30-C31
29	a	614	LMG	O10-C28-O8-C9
32	L	102	LHG	C25-C26-C27-C28
29	Z	101	LMG	C14-C15-C16-C17
29	z	101	LMG	C14-C15-C16-C17
29	A	614	LMG	O10-C28-O8-C9
29	b	619	LMG	O9-C10-O7-C8
29	a	614	LMG	C30-C31-C32-C33
32	l	103	LHG	C25-C26-C27-C28
29	A	614	LMG	C30-C31-C32-C33
25	b	621	SQD	C14-C15-C16-C17
25	l	102	SQD	C14-C15-C16-C17
25	l	102	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
25	b	621	SQD	C46-C45-O47-C7
22	b	602	CLA	C2-C1-O2A-CGA
22	B	602	CLA	C2-C1-O2A-CGA
22	c	509	CLA	C2-C1-O2A-CGA
22	C	509	CLA	C2-C1-O2A-CGA
31	c	516	DGD	C1B-C2B-C3B-C4B
31	C	516	DGD	C1B-C2B-C3B-C4B
24	h	101	BCR	C23-C24-C25-C30
24	H	101	BCR	C23-C24-C25-C30
22	C	512	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C19
31	c	516	DGD	O6E-C1E-O5D-C6D
31	c	517	DGD	O6E-C1E-O5D-C6D
31	C	516	DGD	O6E-C1E-O5D-C6D
31	c	517	DGD	C2E-C1E-O5D-C6D
31	C	517	DGD	C2E-C1E-O5D-C6D
32	E	101	LHG	C4-O6-P-O3
32	e	101	LHG	C4-O6-P-O3
29	D	406	LMG	C32-C33-C34-C35
29	d	406	LMG	C32-C33-C34-C35
32	L	102	LHG	C11-C10-C9-C8
32	l	103	LHG	C11-C10-C9-C8
29	c	520	LMG	C39-C40-C41-C42
29	C	520	LMG	C39-C40-C41-C42
22	D	403	CLA	C11-C12-C13-C15
22	C	506	CLA	C12-C13-C15-C16
22	c	506	CLA	C12-C13-C15-C16
22	c	513	CLA	C6-C7-C8-C9
22	A	607	CLA	C11-C10-C8-C9
22	b	602	CLA	C6-C7-C8-C9
22	B	602	CLA	C6-C7-C8-C9
22	B	616	CLA	C11-C10-C8-C9
22	C	513	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	a	607	CLA	C11-C10-C8-C9
29	B	620	LMG	C11-C10-O7-C8
29	b	619	LMG	C11-C10-O7-C8
22	b	611	CLA	C16-C17-C18-C20
22	B	611	CLA	C16-C17-C18-C20
29	A	614	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
29	a	614	LMG	C29-C28-O8-C9
31	C	518	DGD	C7A-C8A-C9A-CAA
31	c	518	DGD	C7A-C8A-C9A-CAA
22	c	502	CLA	C16-C17-C18-C19
22	C	502	CLA	C16-C17-C18-C19
29	C	519	LMG	C30-C31-C32-C33
29	c	519	LMG	C30-C31-C32-C33
29	D	406	LMG	C34-C35-C36-C37
22	B	616	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C19
29	c	520	LMG	C29-C28-O8-C9
29	C	520	LMG	C29-C28-O8-C9
29	d	406	LMG	C34-C35-C36-C37
22	B	606	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
31	C	517	DGD	O6E-C1E-O5D-C6D
28	d	408	PL9	C39-C41-C42-C43
28	D	408	PL9	C39-C41-C42-C43
29	C	520	LMG	O10-C28-O8-C9
32	E	101	LHG	C17-C18-C19-C20
32	e	101	LHG	C17-C18-C19-C20
24	A	608	BCR	C18-C19-C20-C21
24	a	608	BCR	C18-C19-C20-C21
29	c	520	LMG	O10-C28-O8-C9
31	C	518	DGD	CAB-CBB-CCB-CDB
22	c	510	CLA	O1A-CGA-O2A-C1
22	C	510	CLA	O1A-CGA-O2A-C1
31	c	518	DGD	CAB-CBB-CCB-CDB
22	b	611	CLA	C13-C15-C16-C17
22	B	611	CLA	C13-C15-C16-C17
31	C	517	DGD	C4B-C5B-C6B-C7B
22	A	603	CLA	C2C-C3C-CAC-CBC
25	B	601	SQD	C10-C11-C12-C13
31	c	517	DGD	C4B-C5B-C6B-C7B
22	a	603	CLA	C2C-C3C-CAC-CBC
25	b	601	SQD	C10-C11-C12-C13
29	Z	101	LMG	O6-C5-C6-O5
29	c	520	LMG	O1-C7-C8-O7
29	C	520	LMG	O1-C7-C8-O7
31	c	516	DGD	C2B-C3B-C4B-C5B
31	C	516	DGD	C2B-C3B-C4B-C5B
29	z	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
32	e	101	LHG	C9-C10-C11-C12
32	E	101	LHG	C9-C10-C11-C12
31	c	516	DGD	CBB-CCB-CDB-CEB
31	C	516	DGD	CBB-CCB-CDB-CEB
32	D	409	LHG	C28-C29-C30-C31
32	d	409	LHG	C28-C29-C30-C31
29	c	520	LMG	C36-C37-C38-C39
29	C	520	LMG	C36-C37-C38-C39
31	h	102	DGD	O1G-C1G-C2G-C3G
31	H	102	DGD	O1G-C1G-C2G-C3G
22	c	510	CLA	C8-C10-C11-C12
29	B	620	LMG	C36-C37-C38-C39
29	b	619	LMG	C36-C37-C38-C39
22	C	512	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C20
22	C	510	CLA	CBA-CGA-O2A-C1
22	C	510	CLA	C8-C10-C11-C12
28	a	613	PL9	C2-C3-C7-C8
28	A	613	PL9	C2-C3-C7-C8
22	B	617	CLA	C13-C15-C16-C17
24	A	608	BCR	C17-C18-C19-C20
24	a	608	BCR	C17-C18-C19-C20
22	b	617	CLA	C13-C15-C16-C17
22	c	510	CLA	CBA-CGA-O2A-C1
22	A	607	CLA	C12-C13-C15-C16
22	c	502	CLA	C12-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C7
22	C	504	CLA	C11-C10-C8-C7
22	C	502	CLA	C12-C13-C15-C16
22	a	607	CLA	C12-C13-C15-C16
31	H	102	DGD	CAA-CBA-CCA-CDA
31	h	102	DGD	CAA-CBA-CCA-CDA
22	C	501	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
29	C	519	LMG	C22-C23-C24-C25
29	c	519	LMG	C22-C23-C24-C25
32	E	101	LHG	O6-C4-C5-C6
32	e	101	LHG	O6-C4-C5-C6
22	c	513	CLA	C16-C17-C18-C19
22	C	513	CLA	C16-C17-C18-C19
25	a	609	SQD	O6-C44-C45-O47
31	h	102	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	O1G-C1G-C2G-O2G
25	A	609	SQD	O6-C44-C45-O47
24	K	101	BCR	C15-C16-C17-C18
24	k	101	BCR	C15-C16-C17-C18
24	T	102	BCR	C23-C24-C25-C30
24	t	101	BCR	C23-C24-C25-C30
24	B	622	BCR	C13-C14-C15-C16
29	C	520	LMG	C19-C20-C21-C22
22	c	513	CLA	C4-C3-C5-C6
22	C	513	CLA	C4-C3-C5-C6
32	D	405	LHG	C31-C32-C33-C34
22	B	610	CLA	C2-C3-C5-C6
22	b	610	CLA	C2-C3-C5-C6
29	c	520	LMG	C19-C20-C21-C22
32	d	405	LHG	C31-C32-C33-C34
22	c	507	CLA	C4-C3-C5-C6
22	C	507	CLA	C4-C3-C5-C6
31	C	518	DGD	C2A-C1A-O1G-C1G
31	c	518	DGD	C2A-C1A-O1G-C1G
24	b	622	BCR	C13-C14-C15-C16
29	C	519	LMG	C31-C32-C33-C34
29	b	619	LMG	C35-C36-C37-C38
31	C	518	DGD	O1A-C1A-O1G-C1G
29	B	620	LMG	C35-C36-C37-C38
29	c	519	LMG	C31-C32-C33-C34
32	D	407	LHG	C13-C14-C15-C16
22	C	512	CLA	CAA-CBA-CGA-O2A
31	c	518	DGD	O1A-C1A-O1G-C1G
32	d	407	LHG	C13-C14-C15-C16
22	c	512	CLA	CAA-CBA-CGA-O2A
22	b	602	CLA	CAA-CBA-CGA-O1A
22	B	602	CLA	CAA-CBA-CGA-O1A
25	l	102	SQD	C33-C34-C35-C36
22	D	403	CLA	C11-C12-C13-C14
22	c	510	CLA	C6-C7-C8-C9
22	B	607	CLA	C11-C12-C13-C14
22	b	607	CLA	C11-C12-C13-C14
22	d	403	CLA	C11-C12-C13-C14
22	C	510	CLA	C6-C7-C8-C9
22	b	604	CLA	C13-C15-C16-C17
25	b	621	SQD	C33-C34-C35-C36
22	B	604	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	A	614	LMG	O8-C28-C29-C30
29	a	614	LMG	O8-C28-C29-C30
22	B	610	CLA	CAD-CBD-CGD-O2D
22	D	403	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
23	A	605	PHO	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
23	a	605	PHO	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	b	610	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
22	c	505	CLA	CAD-CBD-CGD-O2D
22	B	613	CLA	CAD-CBD-CGD-O2D
22	d	403	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	CAD-CBD-CGD-O2D
22	C	510	CLA	CAD-CBD-CGD-O2D
22	D	402	CLA	C4C-C3C-CAC-CBC
22	d	402	CLA	C4C-C3C-CAC-CBC
22	a	607	CLA	C4-C3-C5-C6
25	l	102	SQD	C17-C18-C19-C20
25	l	101	SQD	O48-C23-C24-C25
25	b	621	SQD	C17-C18-C19-C20
32	E	101	LHG	C4-C5-C6-O8
32	e	101	LHG	C4-C5-C6-O8
22	a	607	CLA	O1A-CGA-O2A-C1
25	L	101	SQD	O48-C23-C24-C25
32	e	101	LHG	O7-C7-C8-C9
22	b	605	CLA	O2A-C1-C2-C3
22	B	605	CLA	O2A-C1-C2-C3
23	A	605	PHO	O2A-C1-C2-C3
23	a	605	PHO	O2A-C1-C2-C3
22	B	603	CLA	O2A-C1-C2-C3
22	D	401	CLA	O2A-C1-C2-C3
22	c	509	CLA	O2A-C1-C2-C3
22	d	401	CLA	O2A-C1-C2-C3
22	b	603	CLA	O2A-C1-C2-C3
22	C	509	CLA	O2A-C1-C2-C3
22	A	607	CLA	O1A-CGA-O2A-C1
29	B	620	LMG	C12-C13-C14-C15
29	b	619	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
32	E	101	LHG	O7-C7-C8-C9
22	B	617	CLA	CHA-CBD-CGD-O1D
22	d	402	CLA	CHA-CBD-CGD-O1D
22	d	402	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	CHA-CBD-CGD-O2D
22	b	617	CLA	CHA-CBD-CGD-O1D
22	b	608	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O1D
22	B	603	CLA	CHA-CBD-CGD-O2D
23	A	606	PHO	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	b	611	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O2D
23	a	606	PHO	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	D	402	CLA	CHA-CBD-CGD-O1D
22	D	402	CLA	CHA-CBD-CGD-O2D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	a	604	CLA	CHA-CBD-CGD-O2D
22	b	603	CLA	CHA-CBD-CGD-O1D
22	b	603	CLA	CHA-CBD-CGD-O2D
22	A	604	CLA	CHA-CBD-CGD-O2D
22	B	611	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	C16-C17-C18-C20
22	b	607	CLA	C16-C17-C18-C20
31	D	410	DGD	O1G-C1A-C2A-C3A
32	D	405	LHG	C34-C35-C36-C37
31	D	410	DGD	O2G-C2G-C3G-O3G
31	d	410	DGD	O2G-C2G-C3G-O3G
31	C	518	DGD	O6D-C5D-C6D-O5D
31	c	518	DGD	O6D-C5D-C6D-O5D
31	C	518	DGD	O1G-C1A-C2A-C3A
31	d	410	DGD	O1G-C1A-C2A-C3A
31	c	518	DGD	O1G-C1A-C2A-C3A
32	d	405	LHG	C34-C35-C36-C37
22	A	607	CLA	C4-C3-C5-C6
22	A	607	CLA	C11-C12-C13-C15
22	a	607	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	D	403	CLA	C14-C13-C15-C16
22	b	605	CLA	C6-C7-C8-C9
22	B	605	CLA	C6-C7-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C9
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	506	CLA	C14-C13-C15-C16
22	d	403	CLA	C14-C13-C15-C16
24	h	101	BCR	C9-C10-C11-C12
24	B	619	BCR	C14-C15-C16-C17
24	b	618	BCR	C14-C15-C16-C17
25	A	609	SQD	C18-C19-C20-C21
25	a	609	SQD	C18-C19-C20-C21
22	a	603	CLA	C4C-C3C-CAC-CBC
22	c	512	CLA	CAA-CBA-CGA-O1A
22	c	513	CLA	C16-C17-C18-C20
22	C	513	CLA	C16-C17-C18-C20
22	B	610	CLA	C4-C3-C5-C6
22	b	610	CLA	C4-C3-C5-C6
22	C	512	CLA	CAA-CBA-CGA-O1A
22	A	603	CLA	C4C-C3C-CAC-CBC
32	D	409	LHG	C33-C34-C35-C36
32	d	409	LHG	C33-C34-C35-C36
28	a	613	PL9	C26-C27-C28-C29
28	A	613	PL9	C26-C27-C28-C29
22	A	607	CLA	CBA-CGA-O2A-C1
22	a	607	CLA	CBA-CGA-O2A-C1
25	b	601	SQD	C11-C12-C13-C14
25	B	601	SQD	C11-C12-C13-C14
22	B	606	CLA	C13-C15-C16-C17
22	b	606	CLA	C13-C15-C16-C17
31	c	516	DGD	C2E-C1E-O5D-C6D
31	C	516	DGD	C2E-C1E-O5D-C6D
32	D	409	LHG	C19-C20-C21-C22
32	d	407	LHG	C4-O6-P-O5
32	D	407	LHG	C4-O6-P-O5
29	c	520	LMG	O7-C8-C9-O8
29	C	520	LMG	O7-C8-C9-O8
32	d	409	LHG	C19-C20-C21-C22
31	C	518	DGD	O1A-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
31	D	410	DGD	O1A-C1A-C2A-C3A
25	l	101	SQD	O10-C23-C24-C25
25	L	101	SQD	O10-C23-C24-C25
29	A	614	LMG	O10-C28-C29-C30
31	d	410	DGD	O1A-C1A-C2A-C3A
29	a	614	LMG	O10-C28-C29-C30
31	c	518	DGD	O1A-C1A-C2A-C3A
29	C	520	LMG	C32-C33-C34-C35
29	c	520	LMG	C32-C33-C34-C35
24	b	622	BCR	C18-C19-C20-C21
24	B	622	BCR	C18-C19-C20-C21
24	H	101	BCR	C9-C10-C11-C12
22	B	610	CLA	CAD-CBD-CGD-O1D
22	b	608	CLA	CAD-CBD-CGD-O1D
22	B	603	CLA	CAD-CBD-CGD-O1D
22	b	610	CLA	CAD-CBD-CGD-O1D
22	B	608	CLA	CAD-CBD-CGD-O1D
22	b	603	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	O1A-CGA-O2A-C1
32	E	101	LHG	O9-C7-C8-C9
32	e	101	LHG	O9-C7-C8-C9
22	A	607	CLA	C14-C13-C15-C16
22	d	402	CLA	C11-C12-C13-C14
22	c	511	CLA	C6-C7-C8-C9
22	D	402	CLA	C11-C12-C13-C14
22	a	607	CLA	C14-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C9
32	D	405	LHG	C11-C10-C9-C8
32	d	405	LHG	C11-C10-C9-C8
25	l	102	SQD	C45-C46-O48-C23
25	b	621	SQD	C45-C46-O48-C23
31	c	516	DGD	C3A-C4A-C5A-C6A
22	b	616	CLA	C15-C16-C17-C18
31	c	516	DGD	C9A-CAA-CBA-CCA
31	c	517	DGD	C6A-C7A-C8A-C9A
31	C	516	DGD	C3A-C4A-C5A-C6A
31	C	516	DGD	C9A-CAA-CBA-CCA
31	C	517	DGD	C6A-C7A-C8A-C9A
32	L	102	LHG	C5-C6-O8-C23
32	l	103	LHG	C5-C6-O8-C23
22	B	616	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C12-C13-C15
22	D	401	CLA	C12-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C10
22	d	401	CLA	C12-C13-C15-C16
22	c	505	CLA	C12-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C7
22	C	507	CLA	C11-C12-C13-C15
22	B	615	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	C	510	CLA	C6-C7-C8-C10
31	c	517	DGD	O2G-C1B-C2B-C3B
31	C	517	DGD	O2G-C1B-C2B-C3B
24	K	102	BCR	C9-C10-C11-C12
24	k	102	BCR	C9-C10-C11-C12
29	A	614	LMG	C35-C36-C37-C38
29	a	614	LMG	C35-C36-C37-C38
22	B	613	CLA	C8-C10-C11-C12
22	b	613	CLA	C8-C10-C11-C12
22	C	505	CLA	CAA-CBA-CGA-O2A
22	C	501	CLA	CAA-CBA-CGA-O2A
22	c	501	CLA	CAA-CBA-CGA-O2A
31	c	518	DGD	C1B-C2B-C3B-C4B
22	C	506	CLA	C15-C16-C17-C18
22	c	506	CLA	C15-C16-C17-C18

There are no ring outliers.

62 monomers are involved in 148 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	E	101	LHG	2	0
22	B	617	CLA	4	0
22	A	607	CLA	2	0
29	Z	101	LMG	1	0
22	B	614	CLA	5	0
24	T	102	BCR	2	0
24	K	102	BCR	1	0
29	B	620	LMG	3	0
22	D	403	CLA	3	0
22	B	609	CLA	2	0
31	C	518	DGD	1	0

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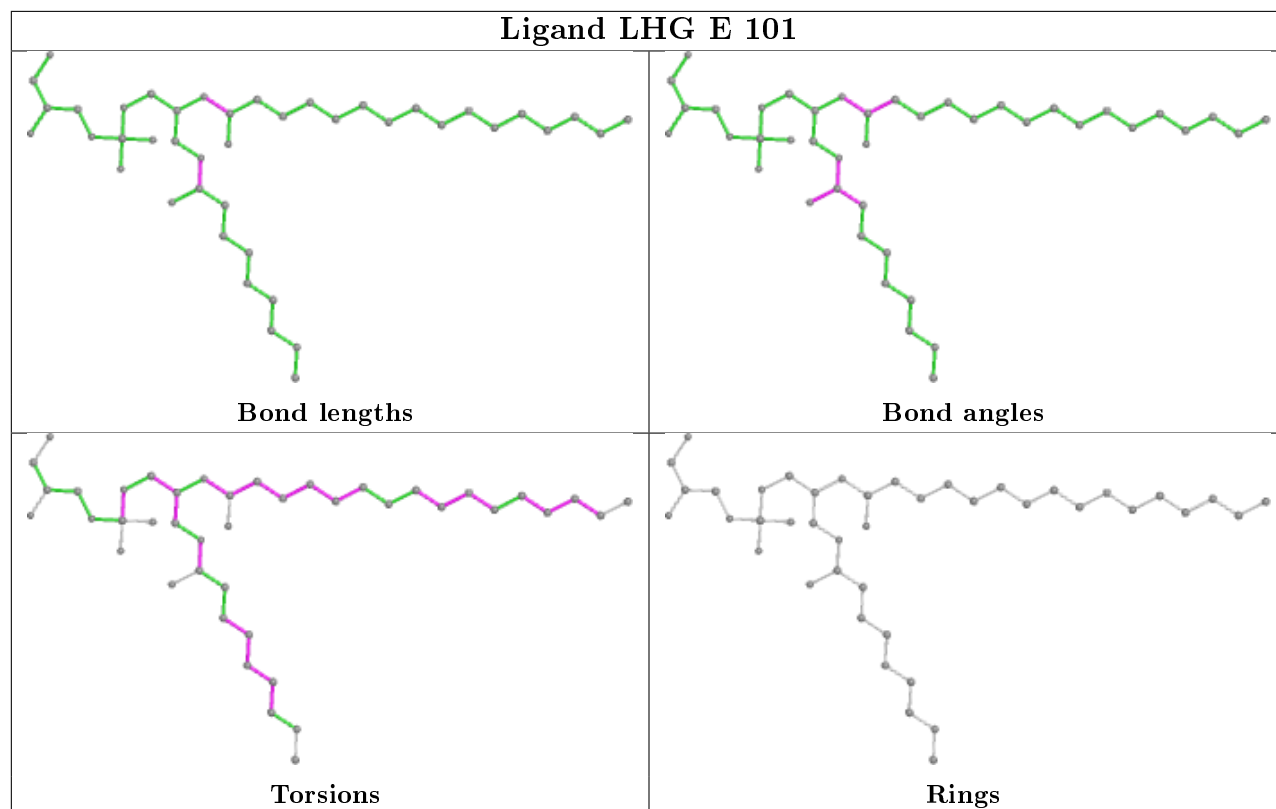
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	606	CLA	5	0
22	B	612	CLA	2	0
22	B	605	CLA	2	0
23	A	605	PHO	2	0
22	C	505	CLA	2	0
33	F	101	HEM	1	0
22	A	603	CLA	5	0
22	C	501	CLA	2	0
31	D	410	DGD	3	0
24	B	619	BCR	1	0
24	B	622	BCR	4	0
31	C	516	DGD	2	0
22	B	603	CLA	1	0
24	A	608	BCR	1	0
22	C	508	CLA	3	0
29	D	406	LMG	2	0
25	B	601	SQD	4	0
25	L	101	SQD	5	0
28	A	613	PL9	8	0
22	B	616	CLA	2	0
22	D	401	CLA	1	0
24	D	404	BCR	3	0
29	A	614	LMG	3	0
31	C	517	DGD	2	0
22	B	607	CLA	2	0
23	A	606	PHO	4	0
22	C	504	CLA	1	0
29	C	519	LMG	1	0
24	H	101	BCR	1	0
22	C	513	CLA	1	0
22	D	402	CLA	4	0
24	T	101	BCR	7	0
22	C	502	CLA	3	0
32	L	102	LHG	1	0
31	H	102	DGD	1	0
22	A	604	CLA	3	0
22	B	611	CLA	4	0
22	C	512	CLA	3	0
22	C	506	CLA	4	0
22	C	507	CLA	1	0
22	B	613	CLA	3	0
22	B	615	CLA	3	0

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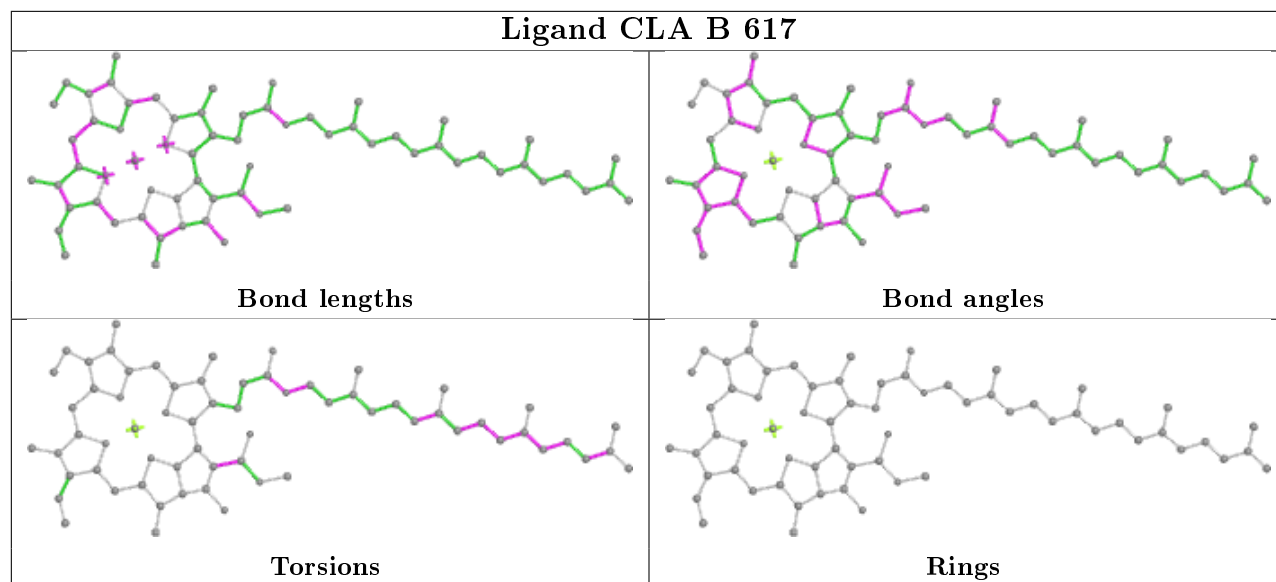
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	618	BCR	3	0
22	B	604	CLA	2	0
25	A	609	SQD	2	0
22	C	509	CLA	2	0
32	D	409	LHG	13	0
33	V	201	HEM	9	0
22	C	511	CLA	2	0
22	C	510	CLA	6	0
22	C	503	CLA	3	0

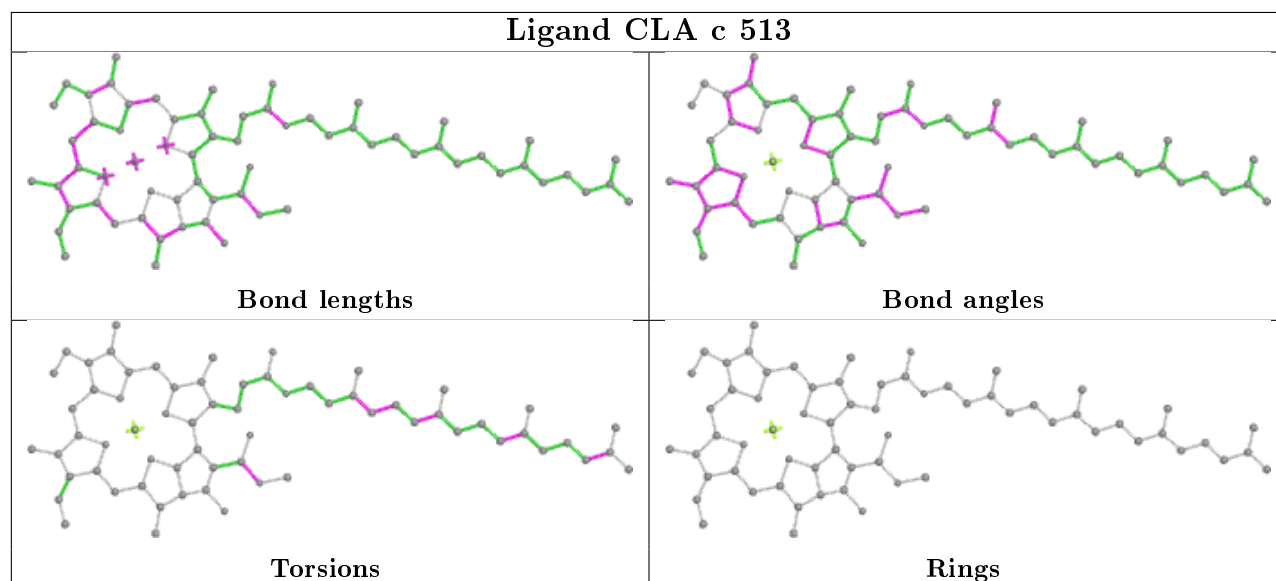
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

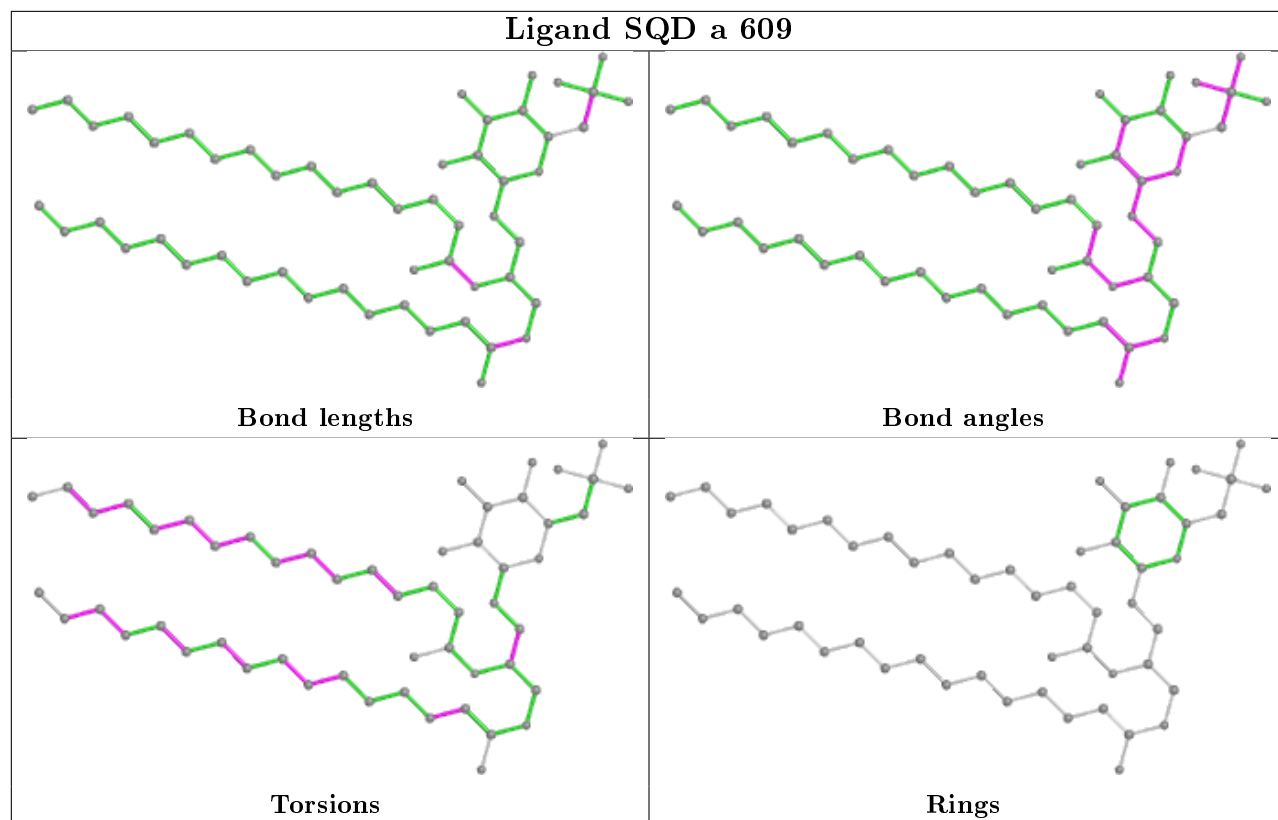


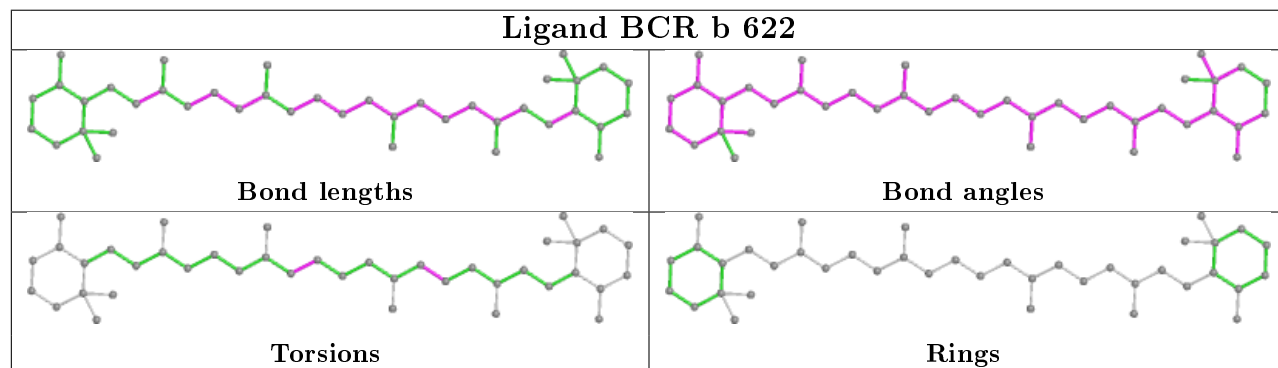
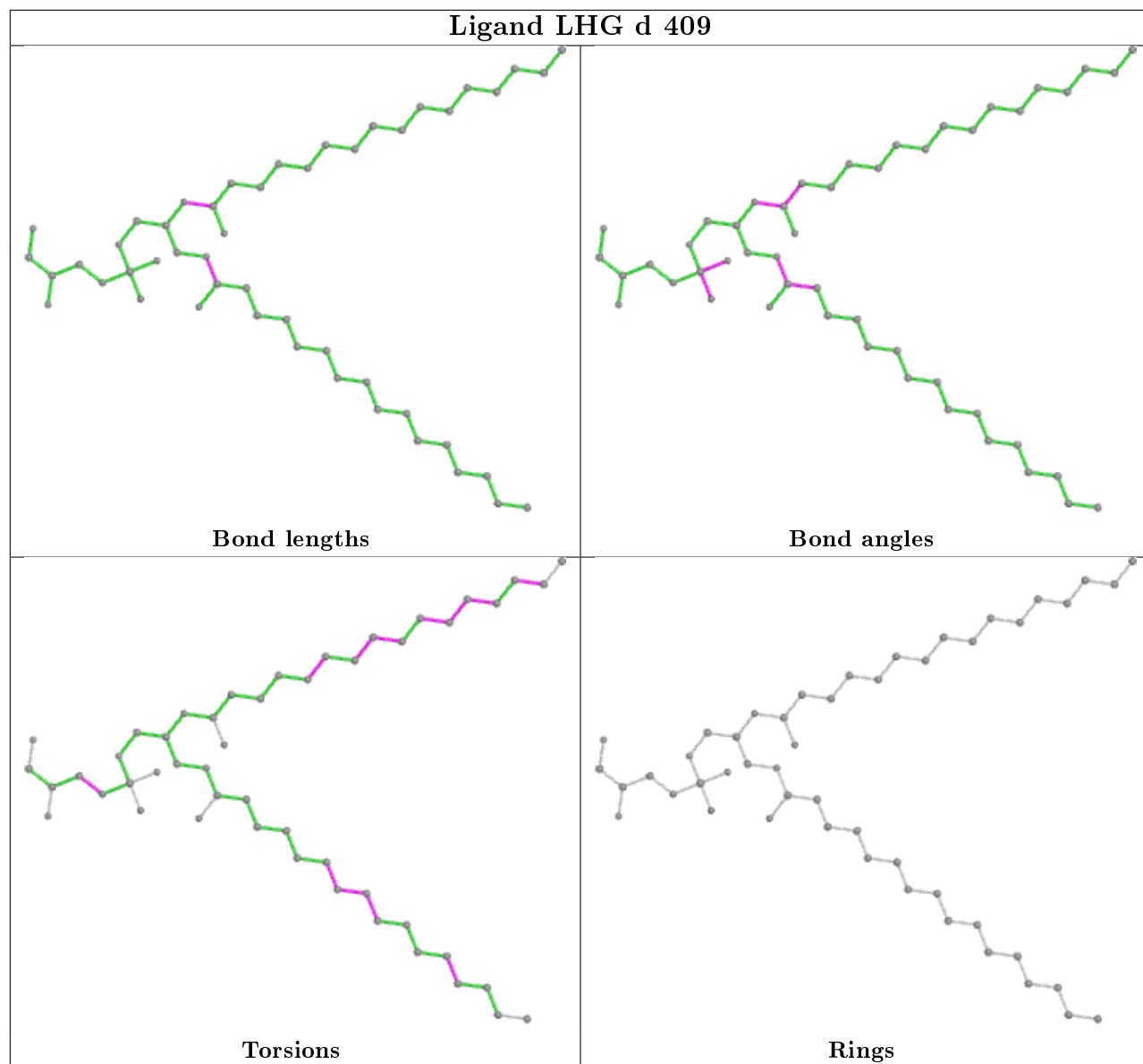
Ligand CLA B 617



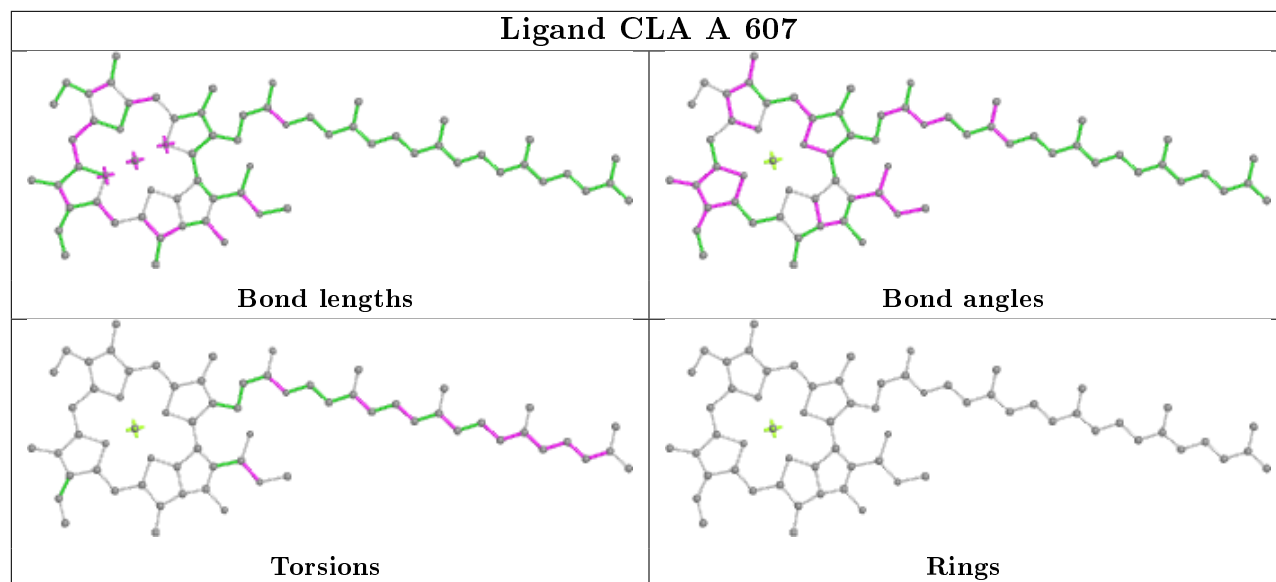
Ligand CLA c 513



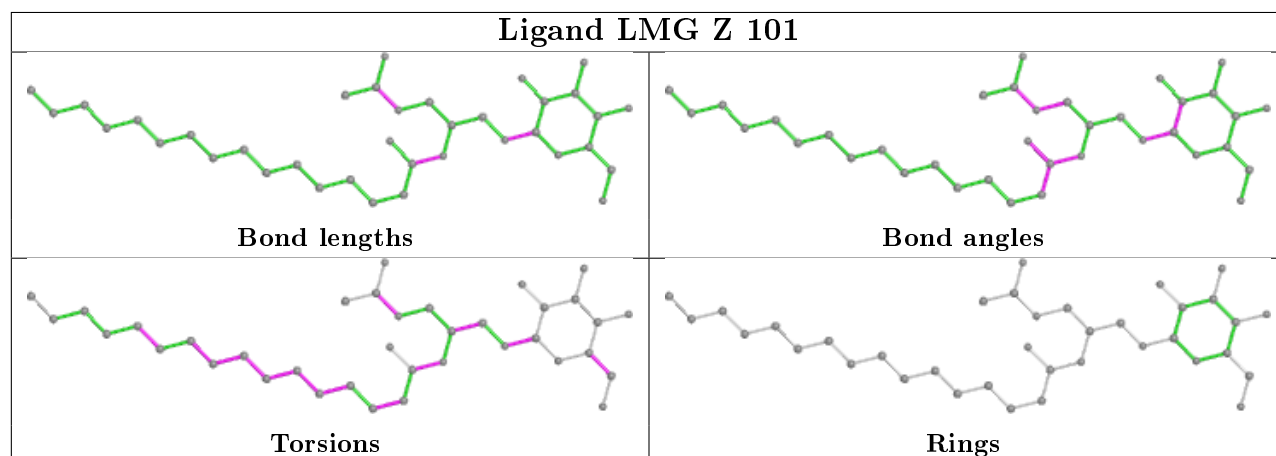




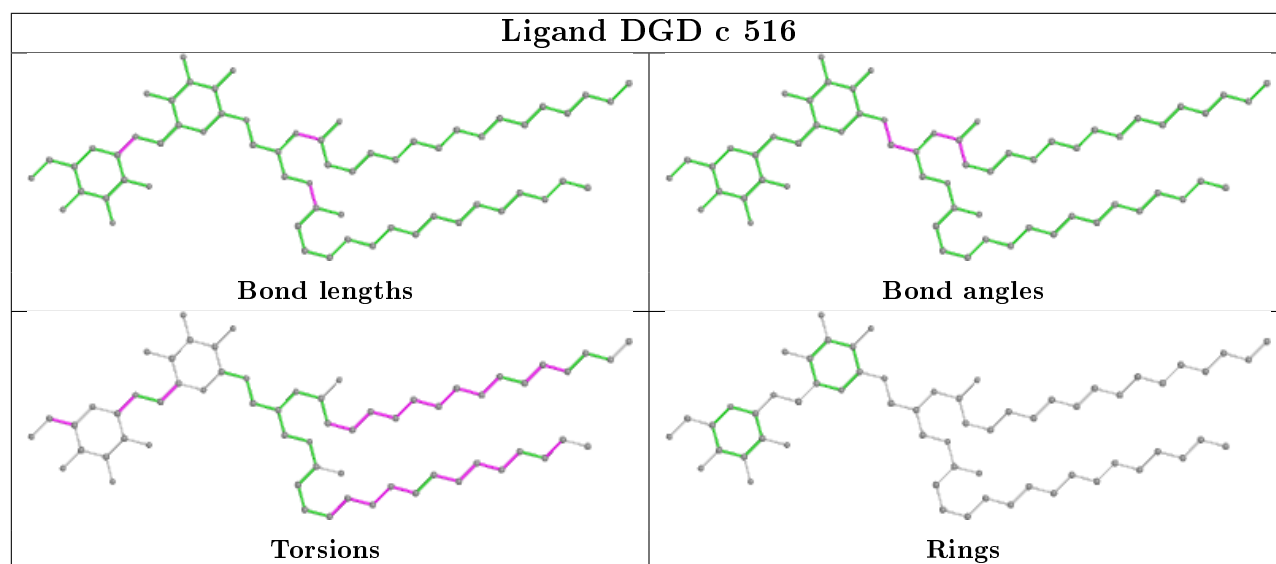
Ligand CLA A 607

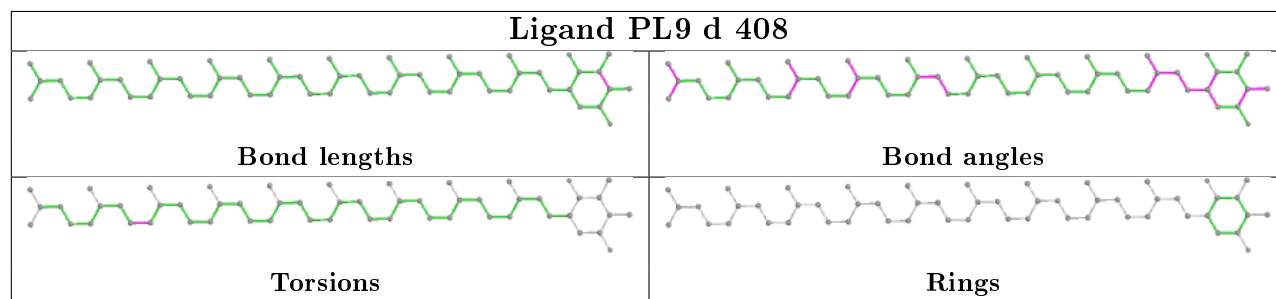
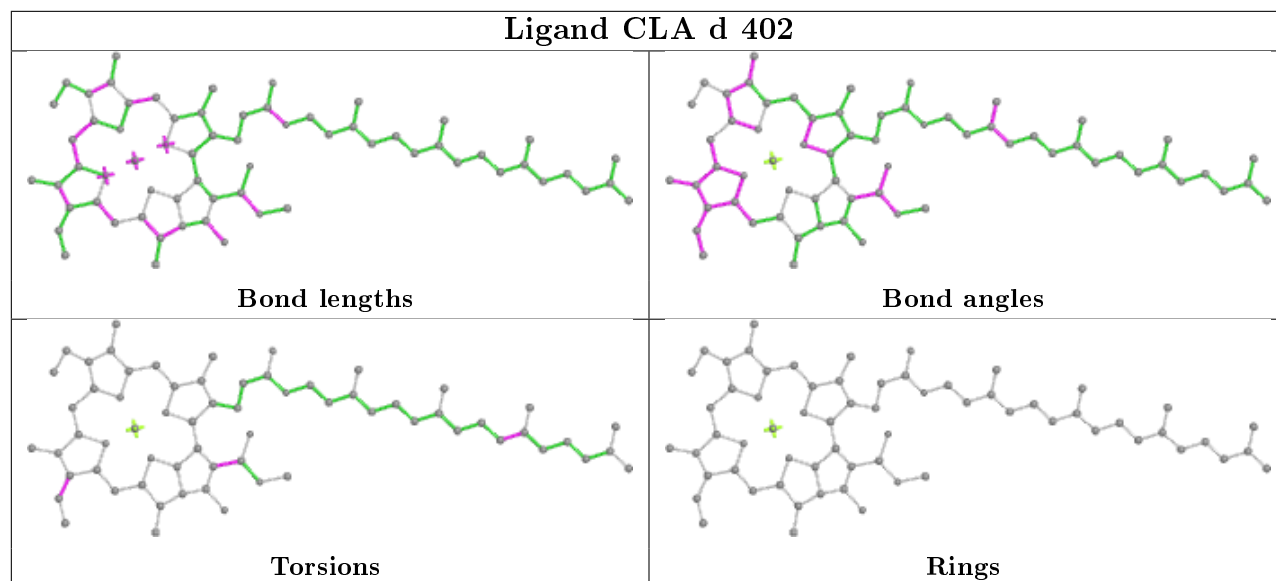
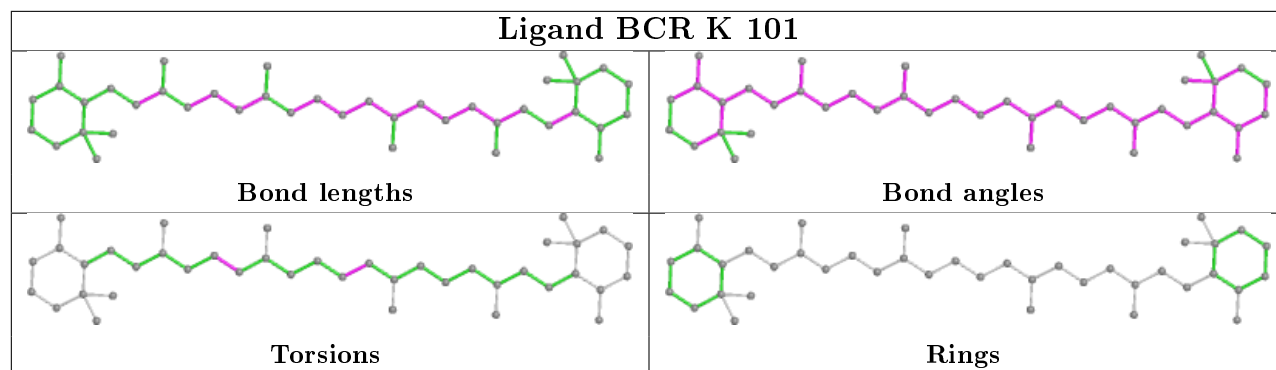


Ligand LMG Z 101

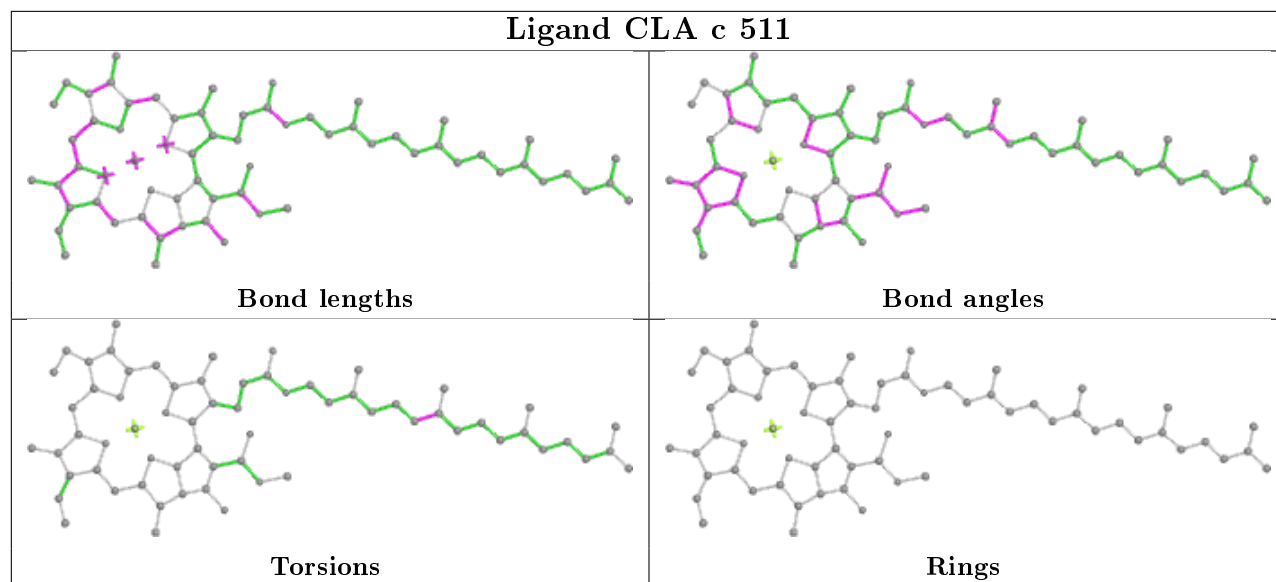


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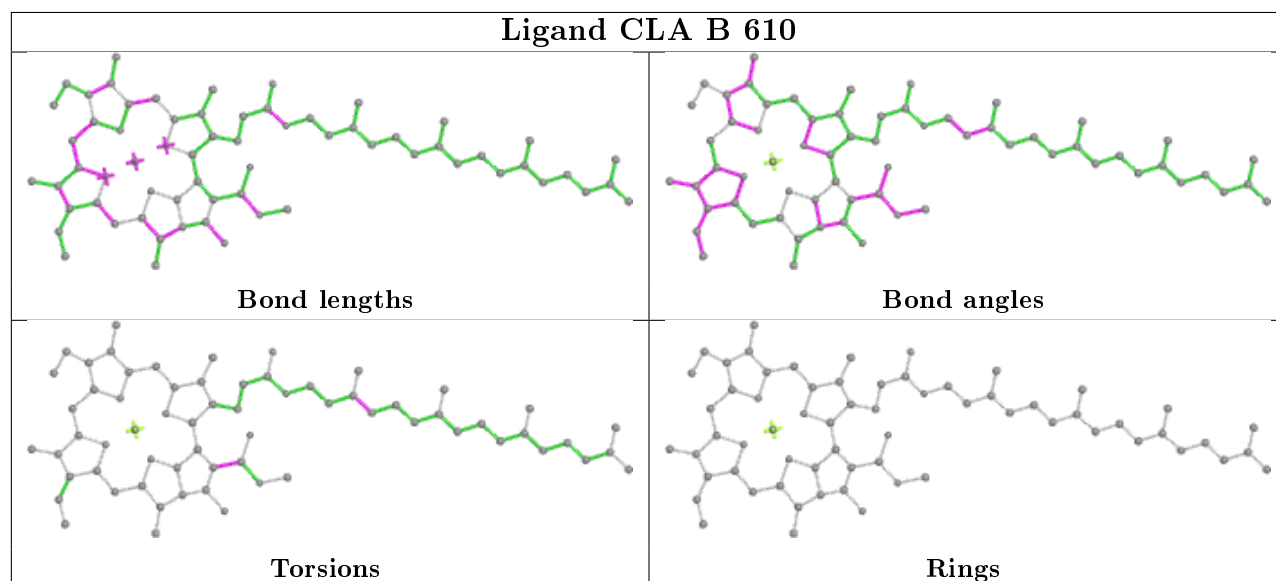




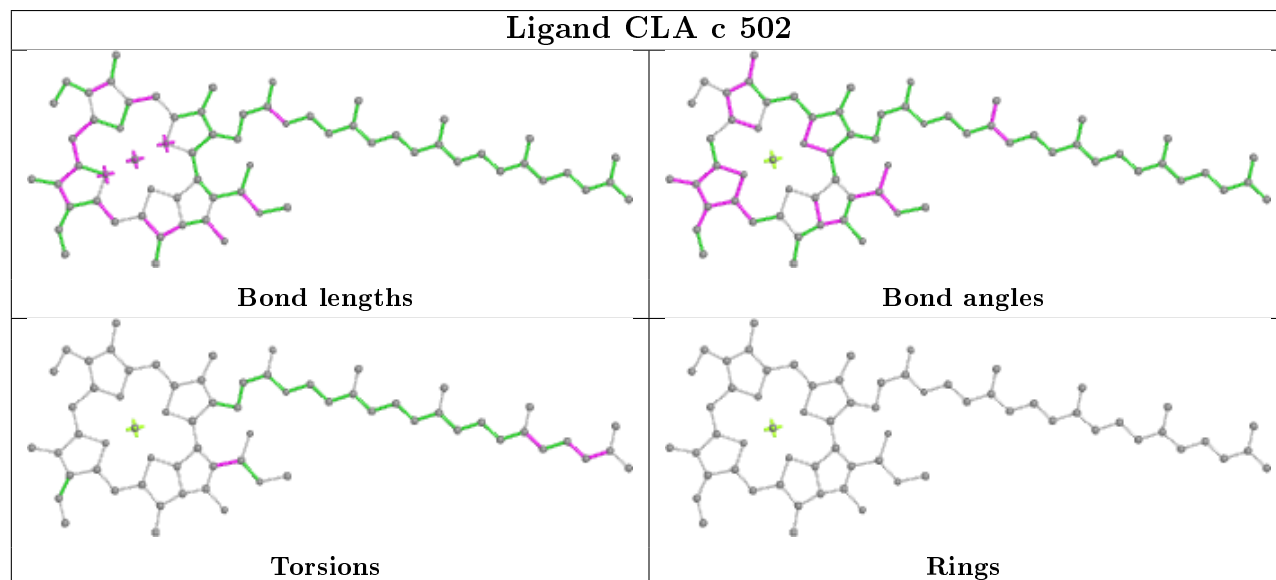
Ligand CLA c 511

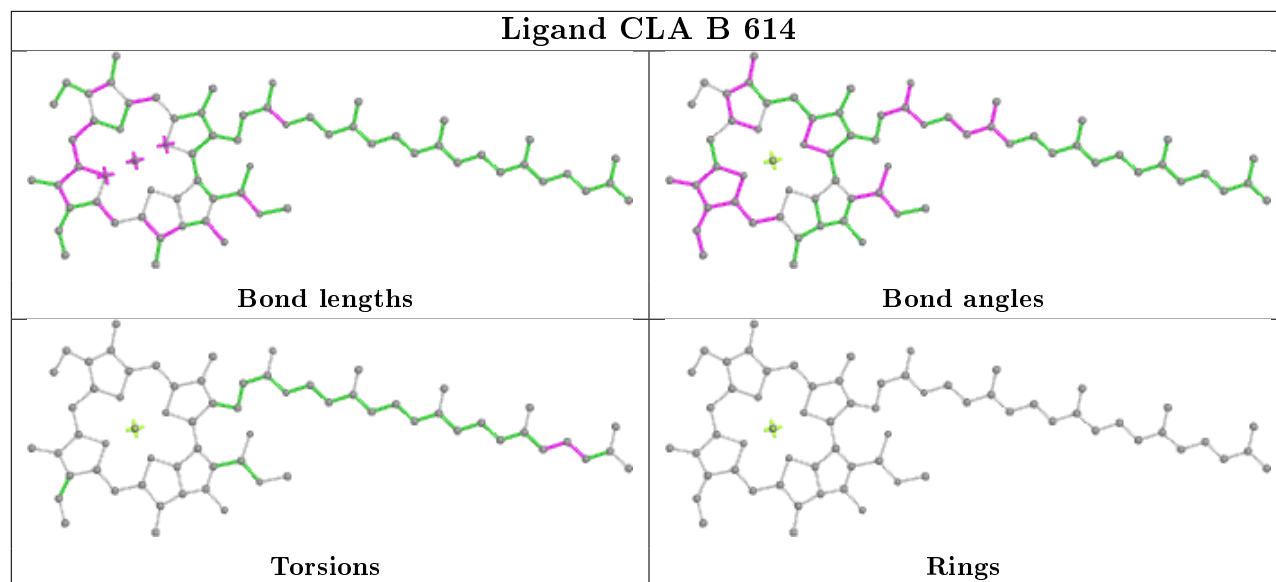
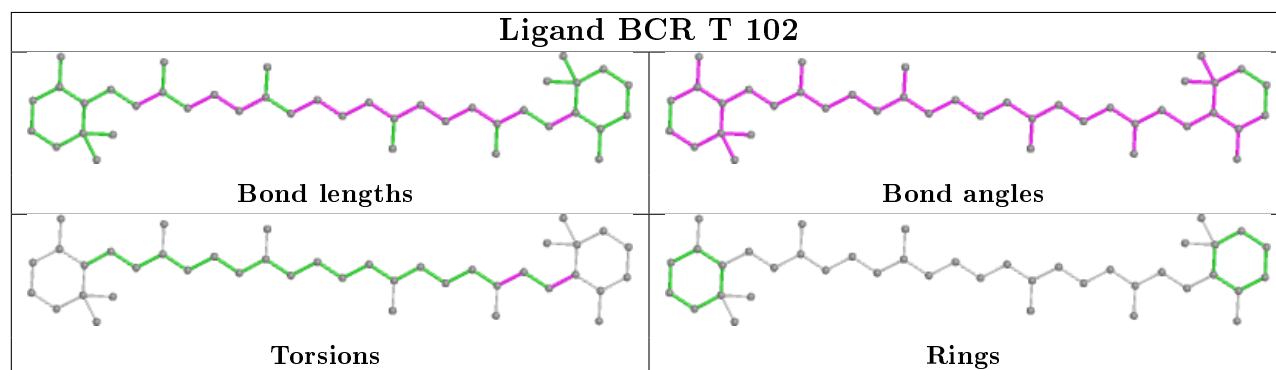
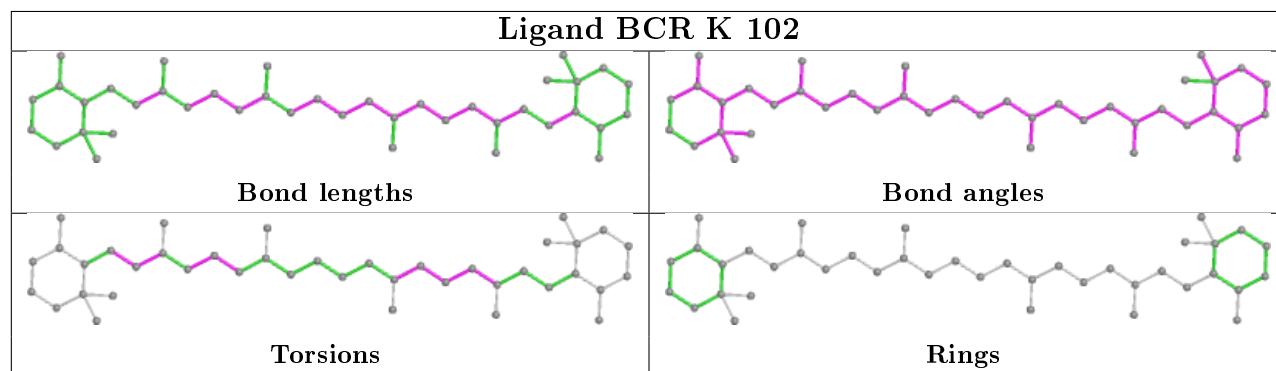


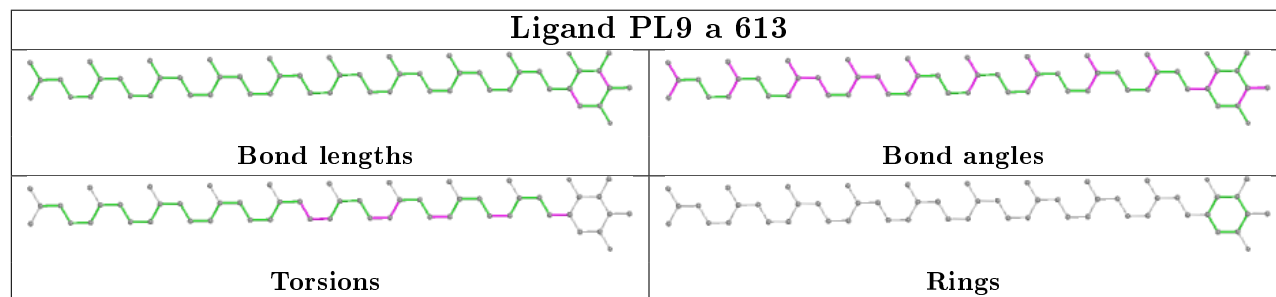
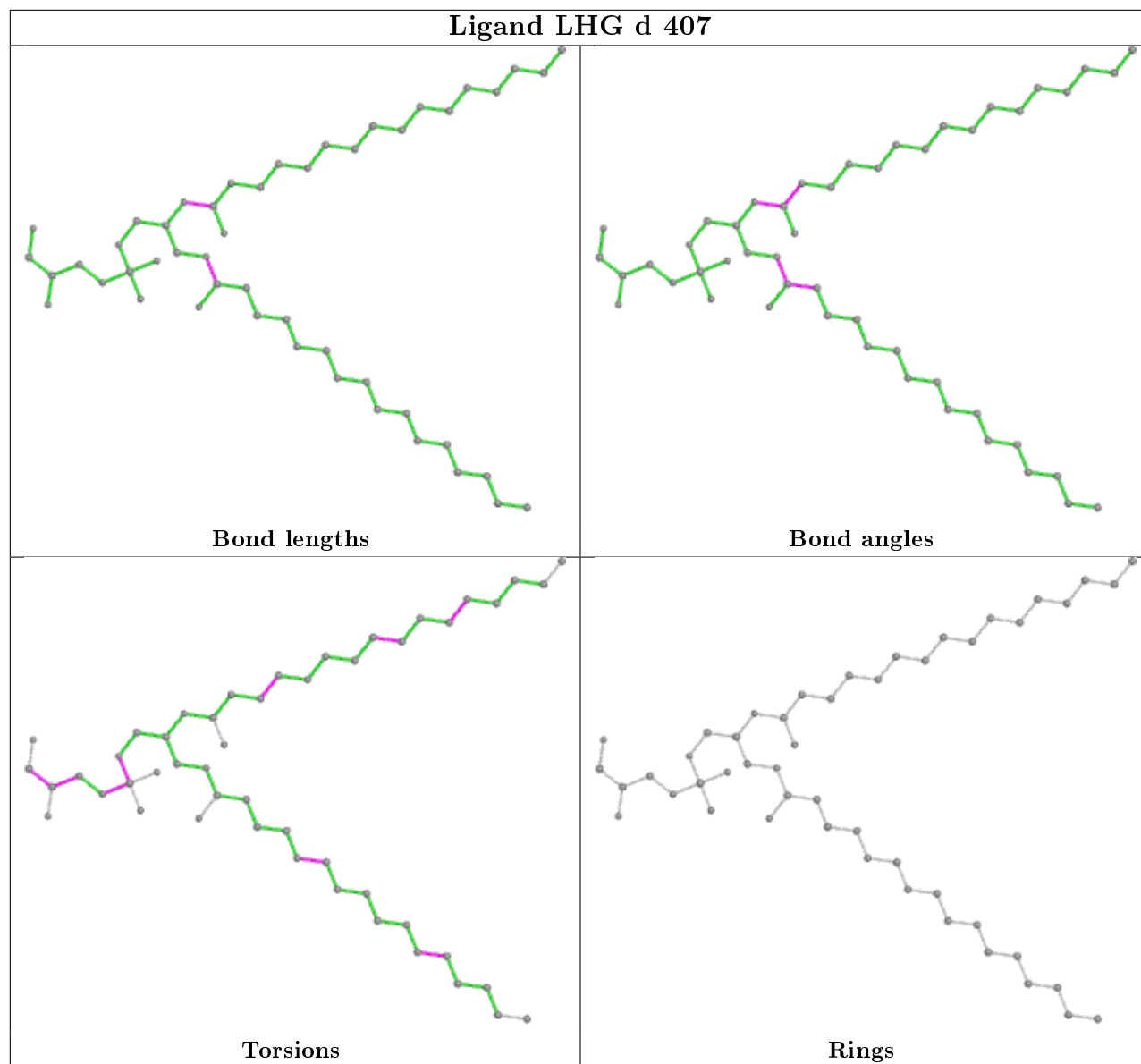
Ligand CLA B 610

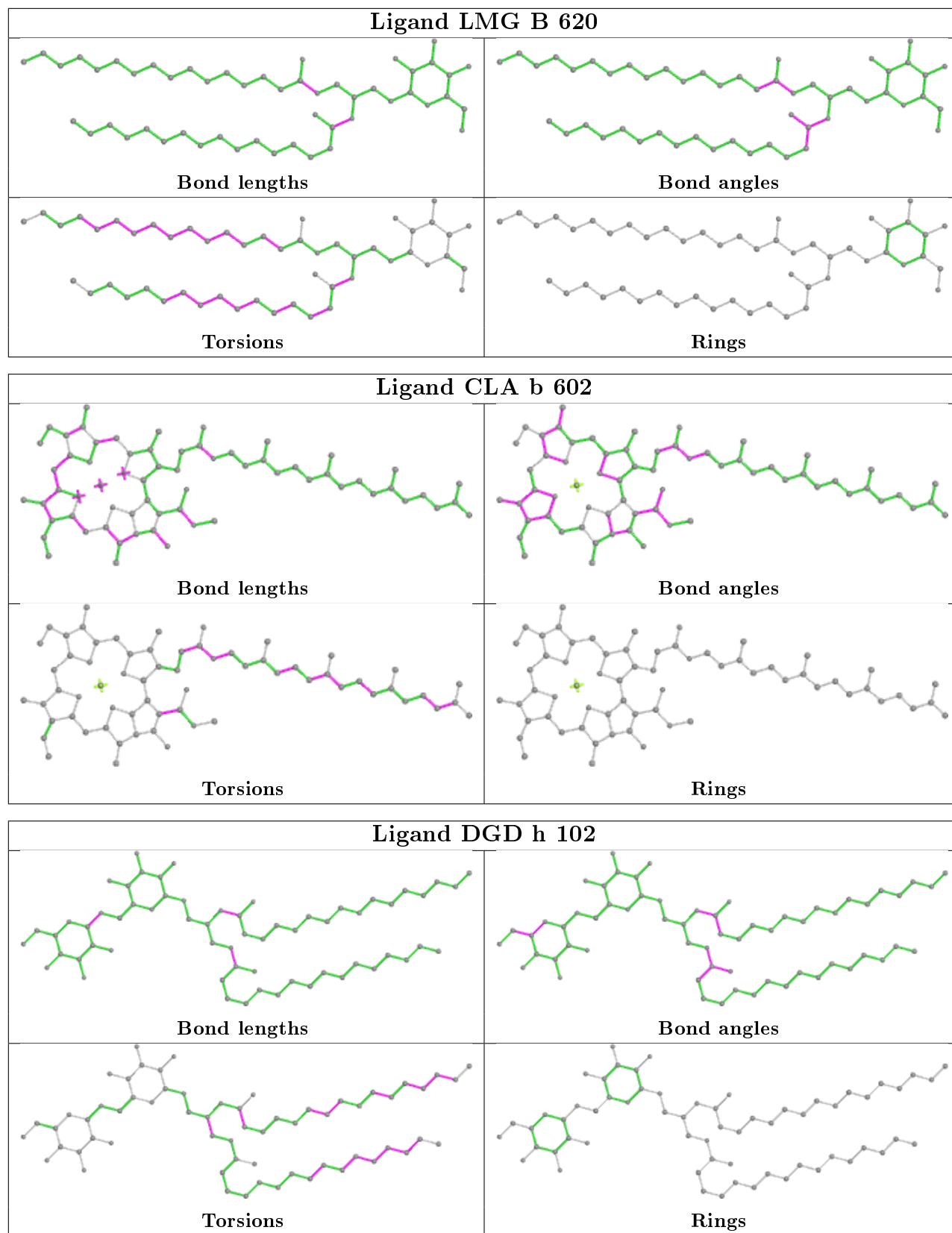


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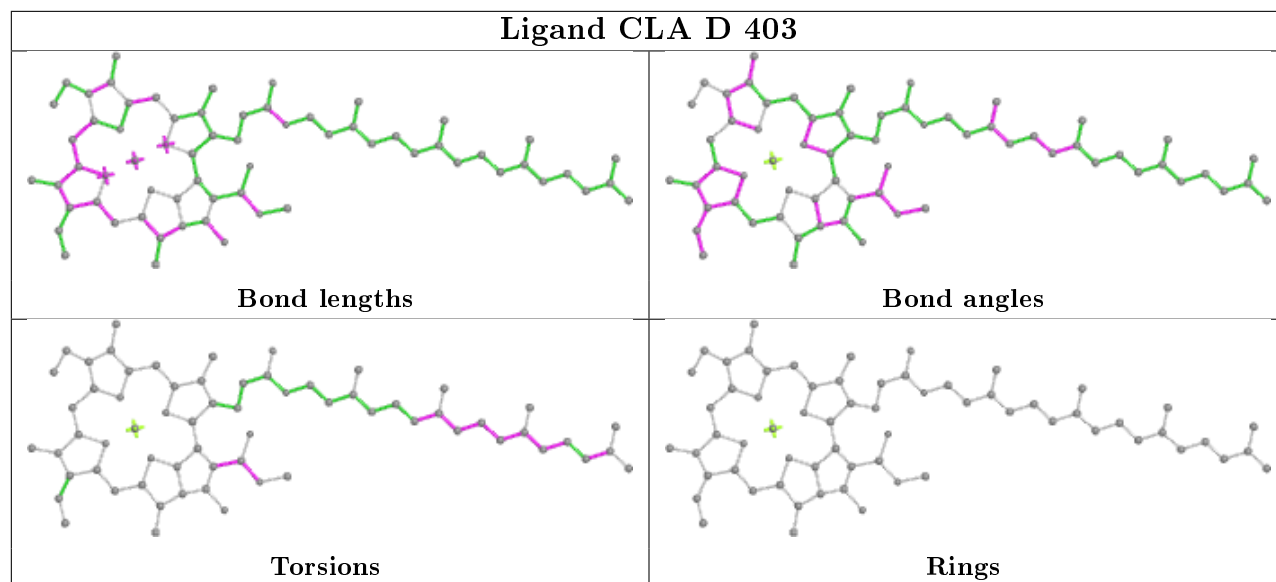


Ligand CLA B 614**Ligand BCR T 102****Ligand BCR K 102**

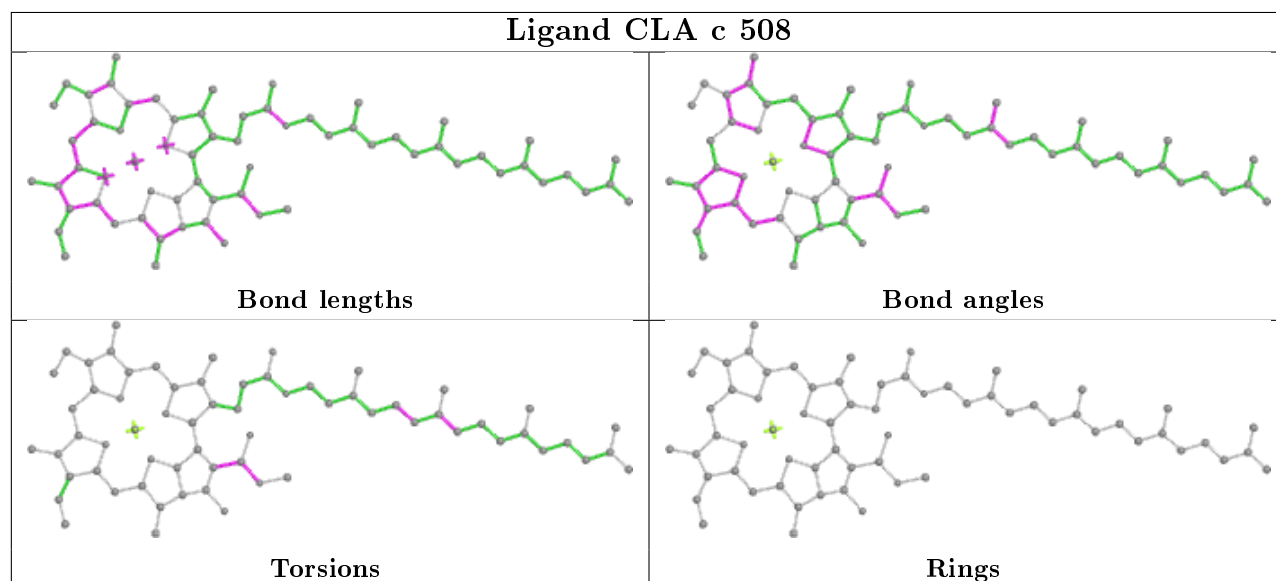




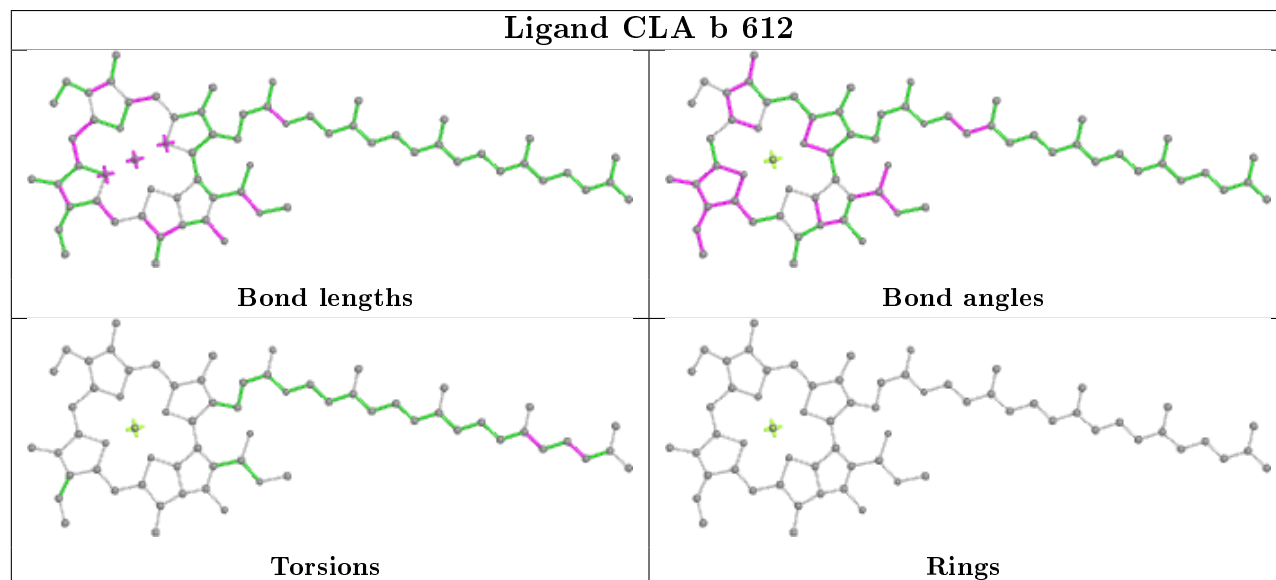
Ligand CLA D 403



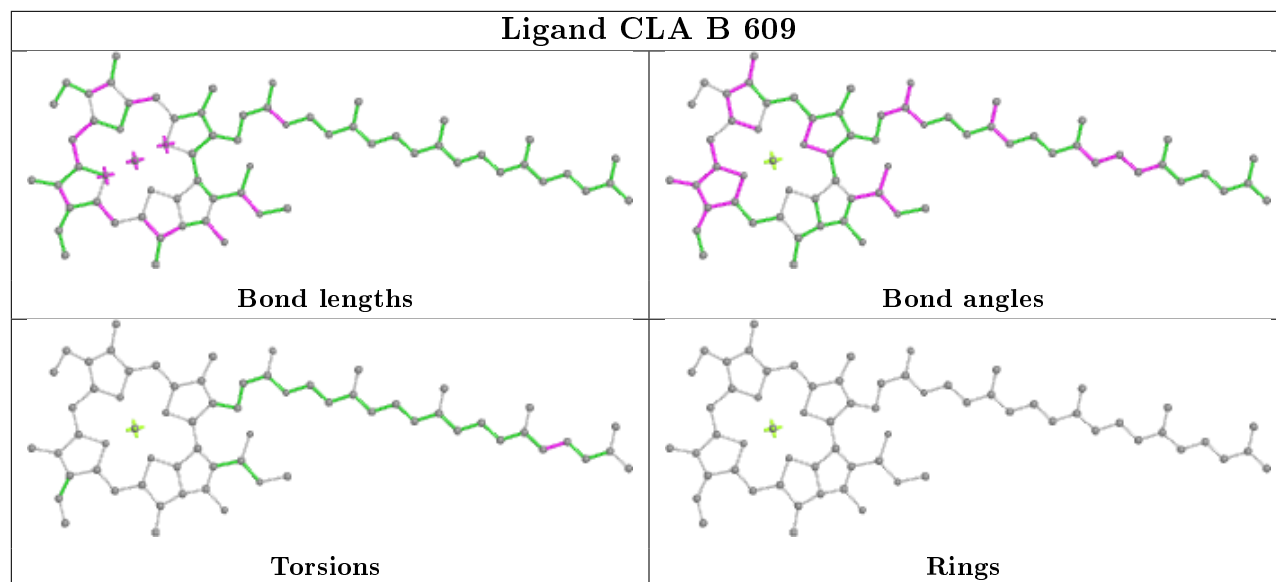
Ligand CLA c 508



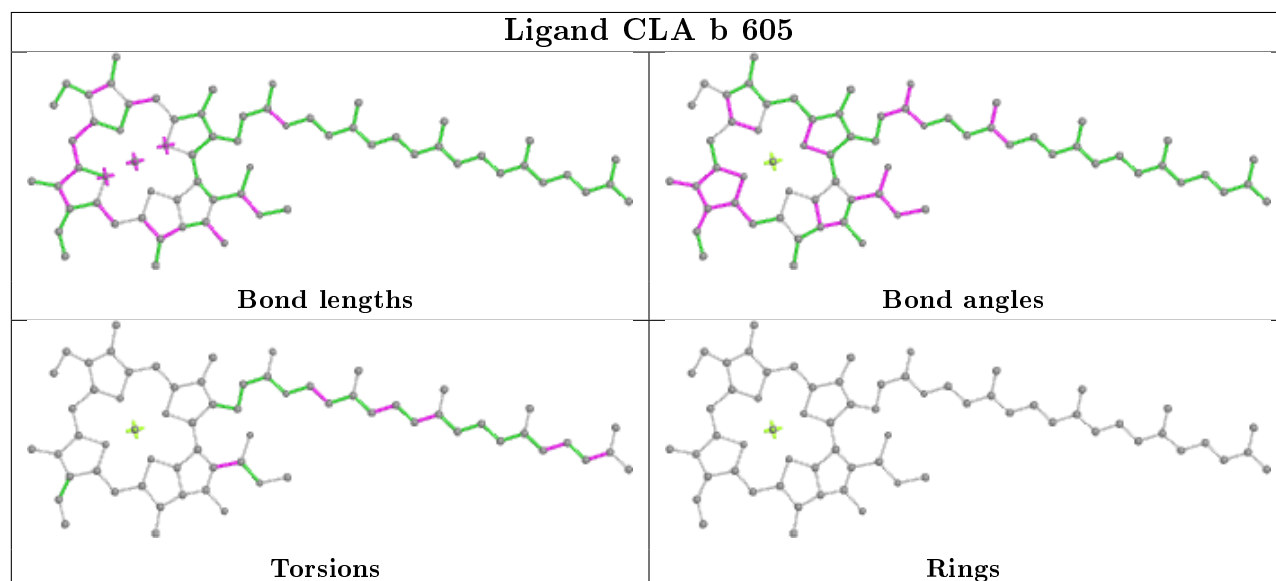
Ligand CLA b 612



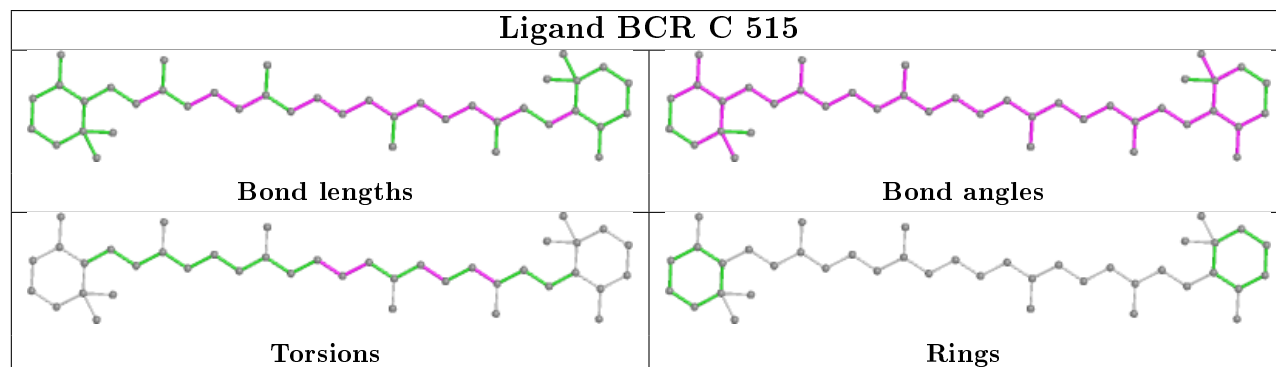
Ligand CLA B 609

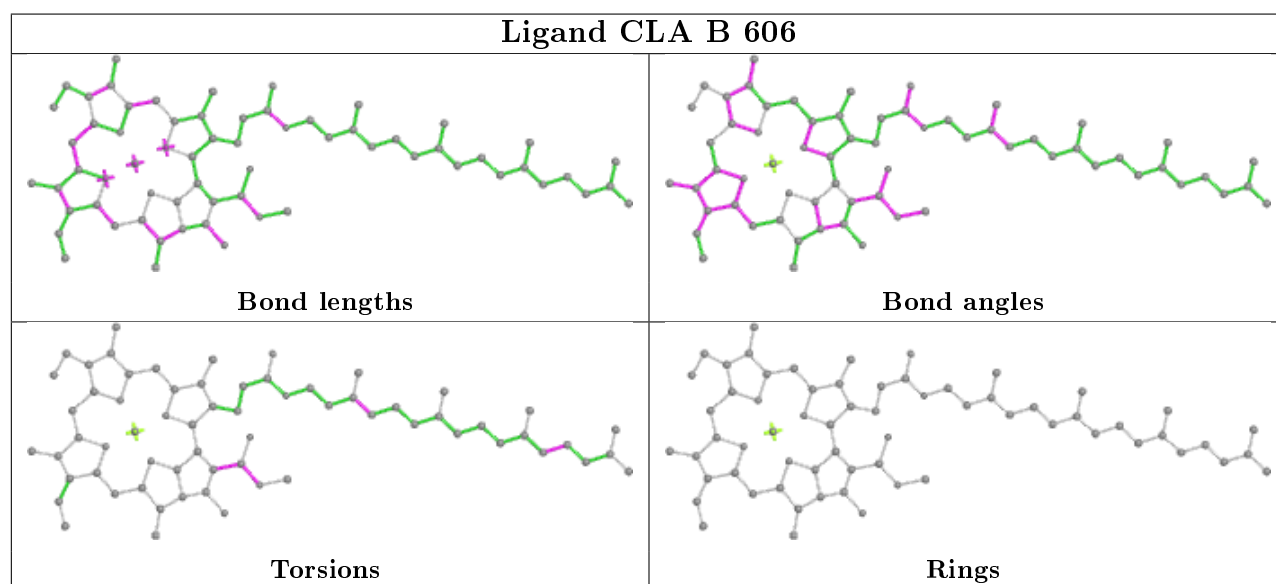
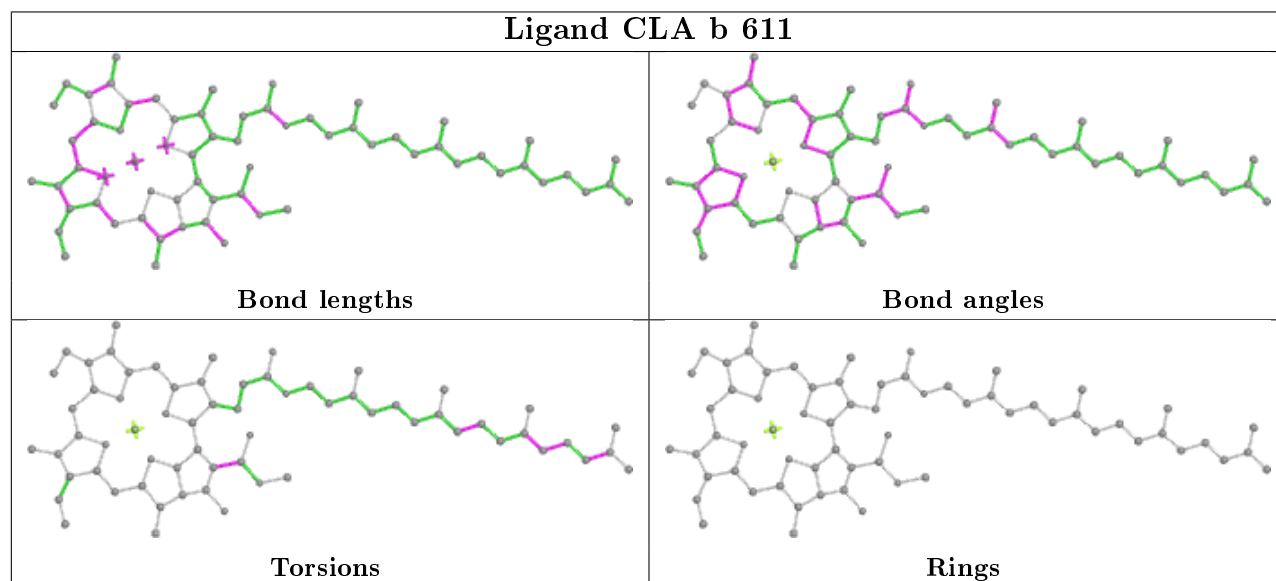
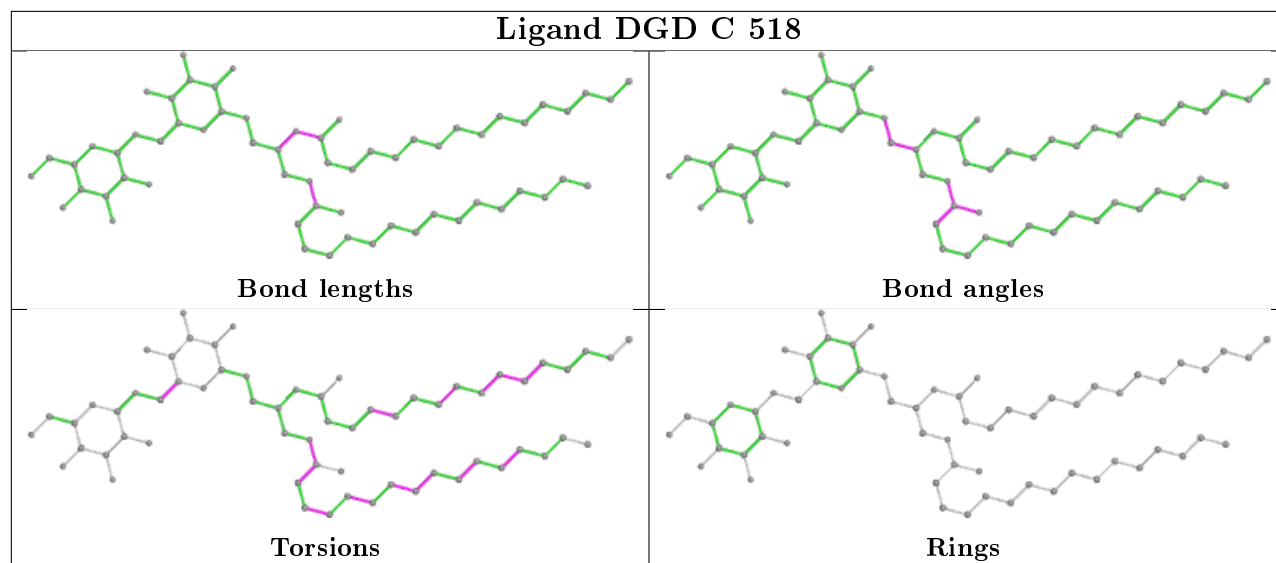


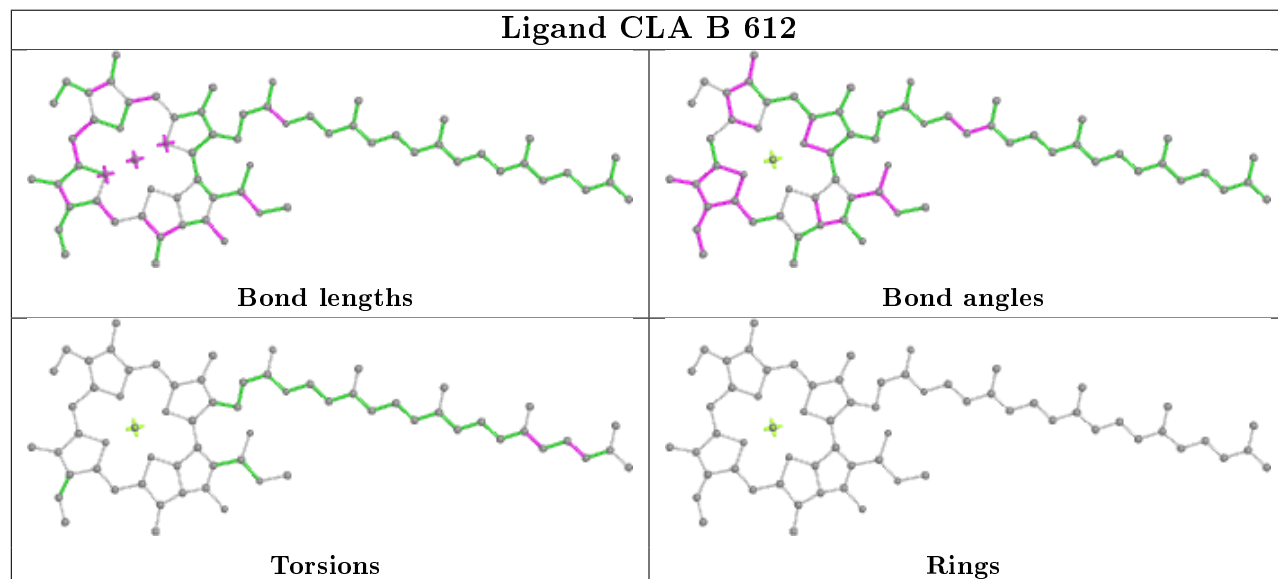
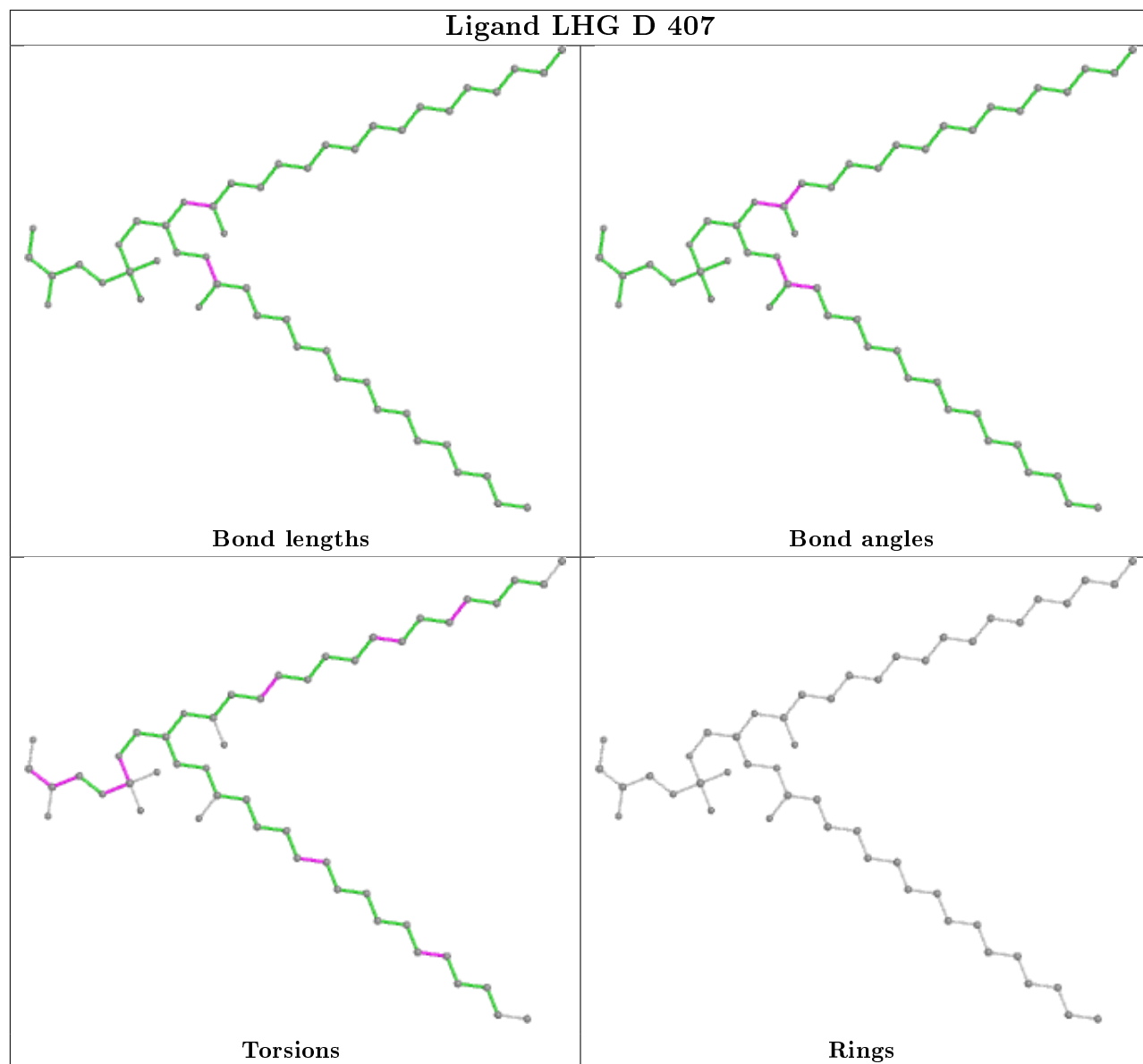
Ligand CLA b 605



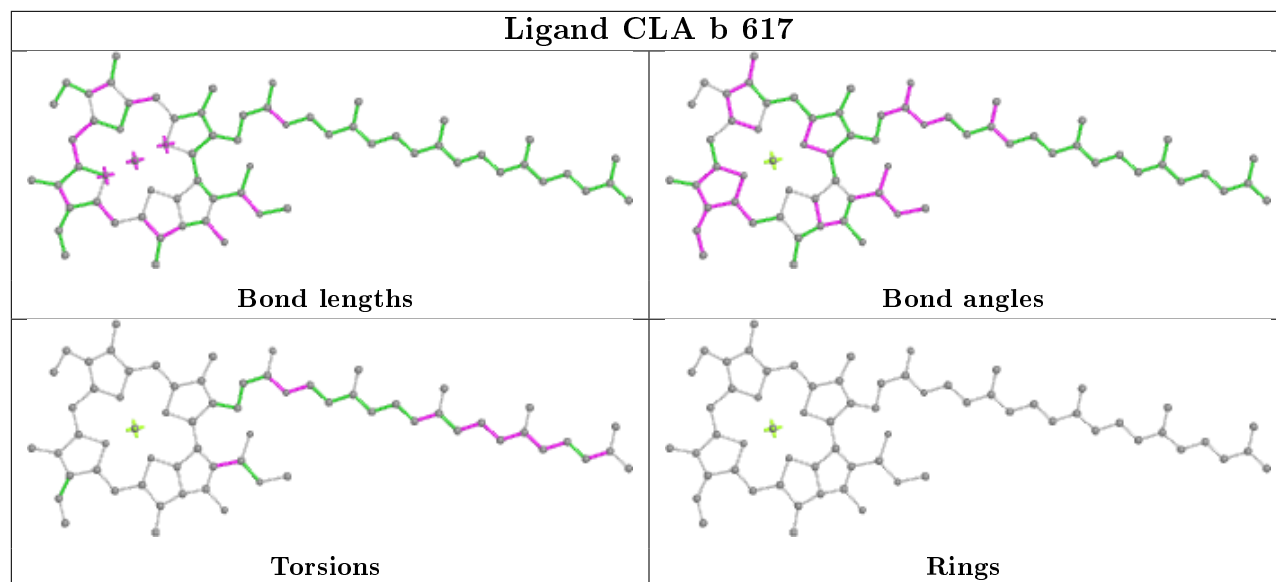
Ligand BCR C 515



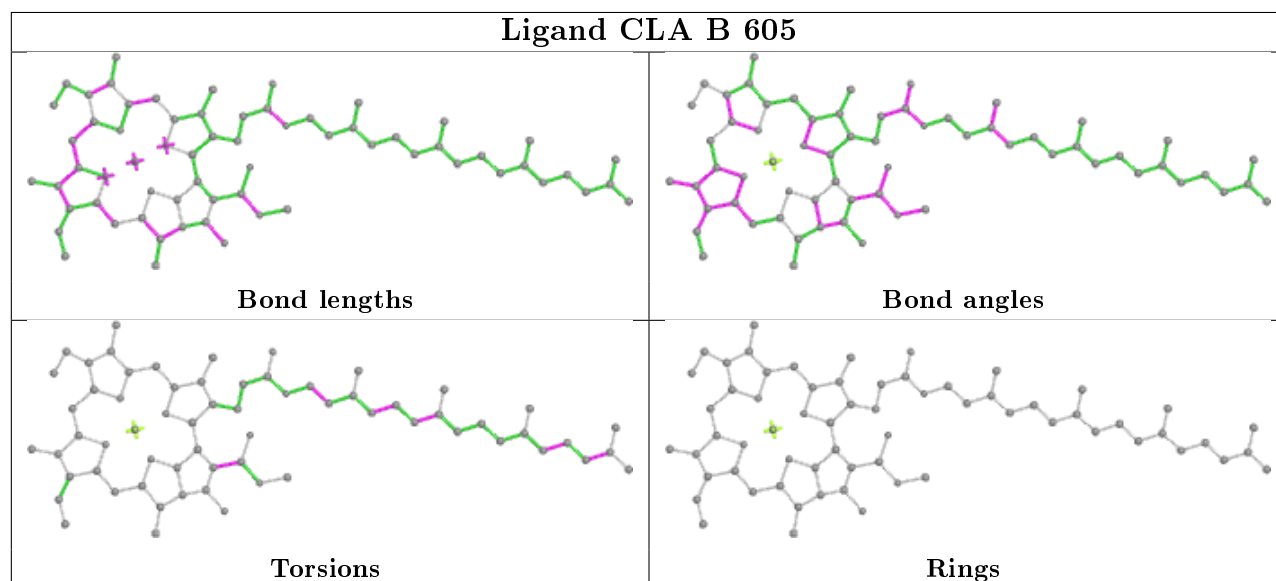




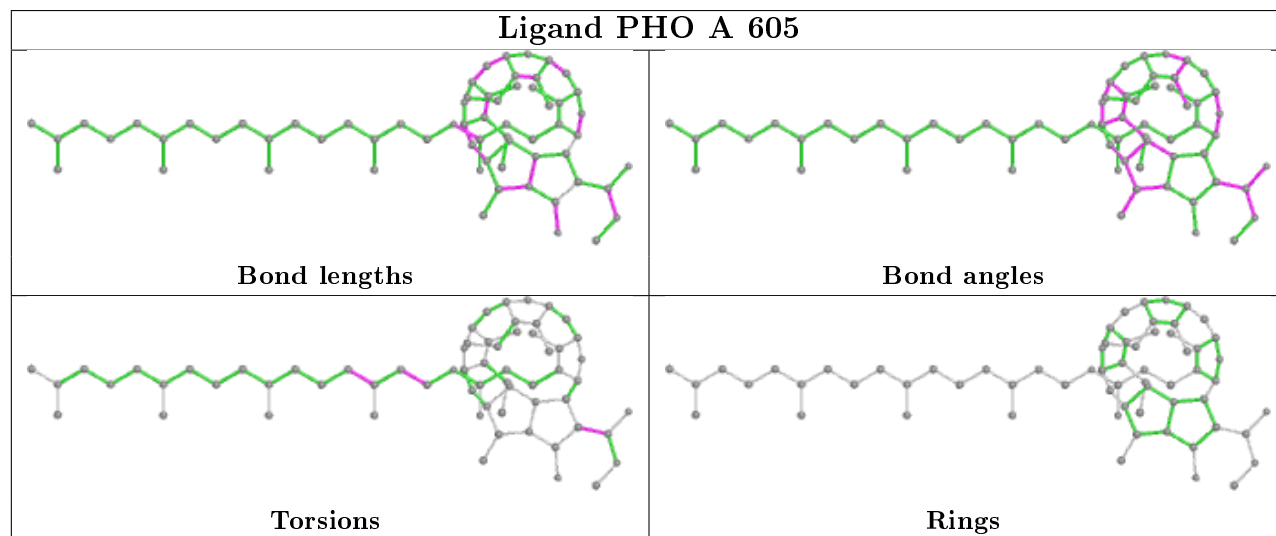
Ligand CLA b 617



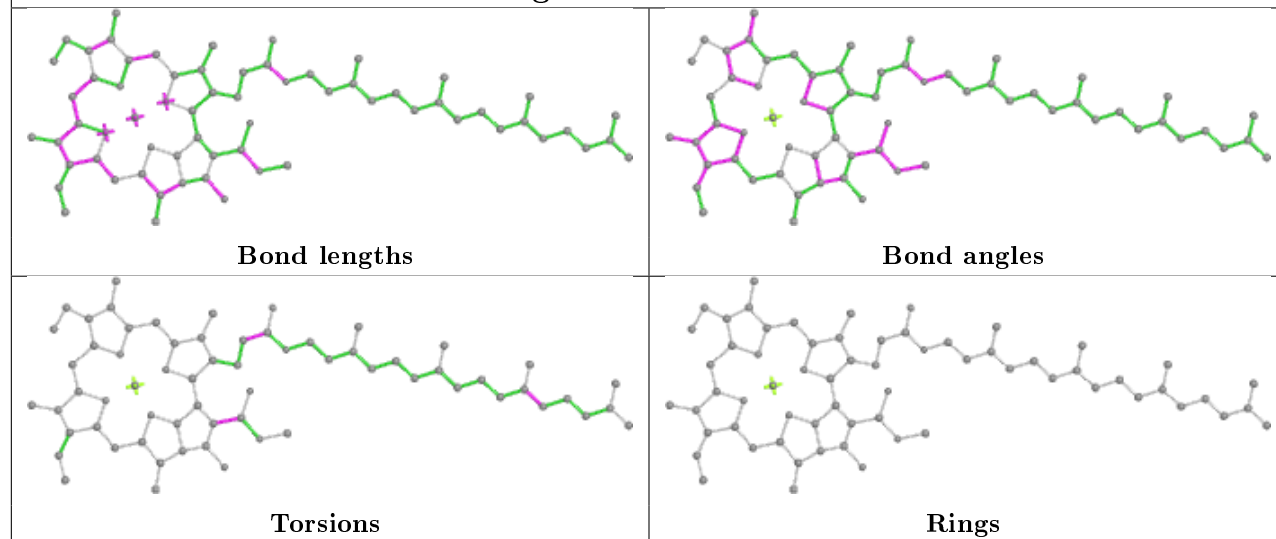
Ligand CLA B 605



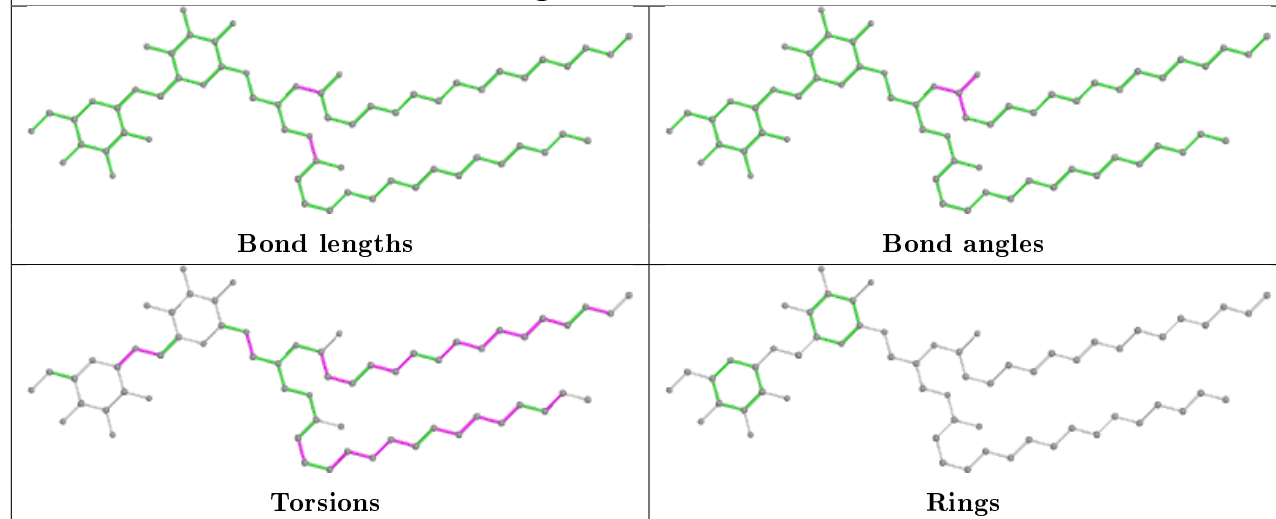
Ligand PHO A 605

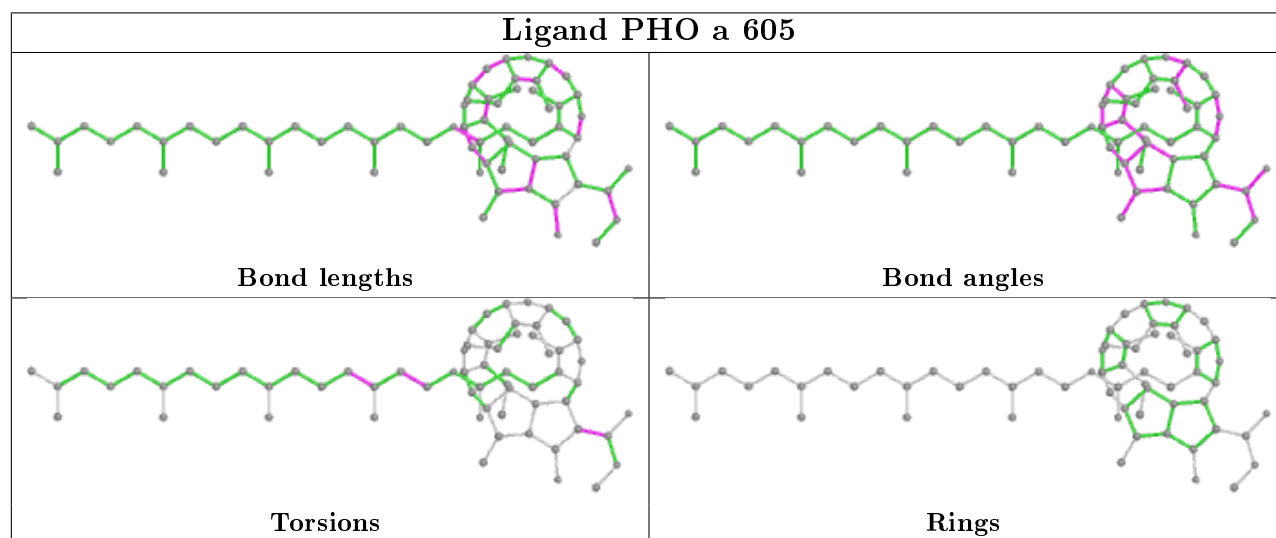
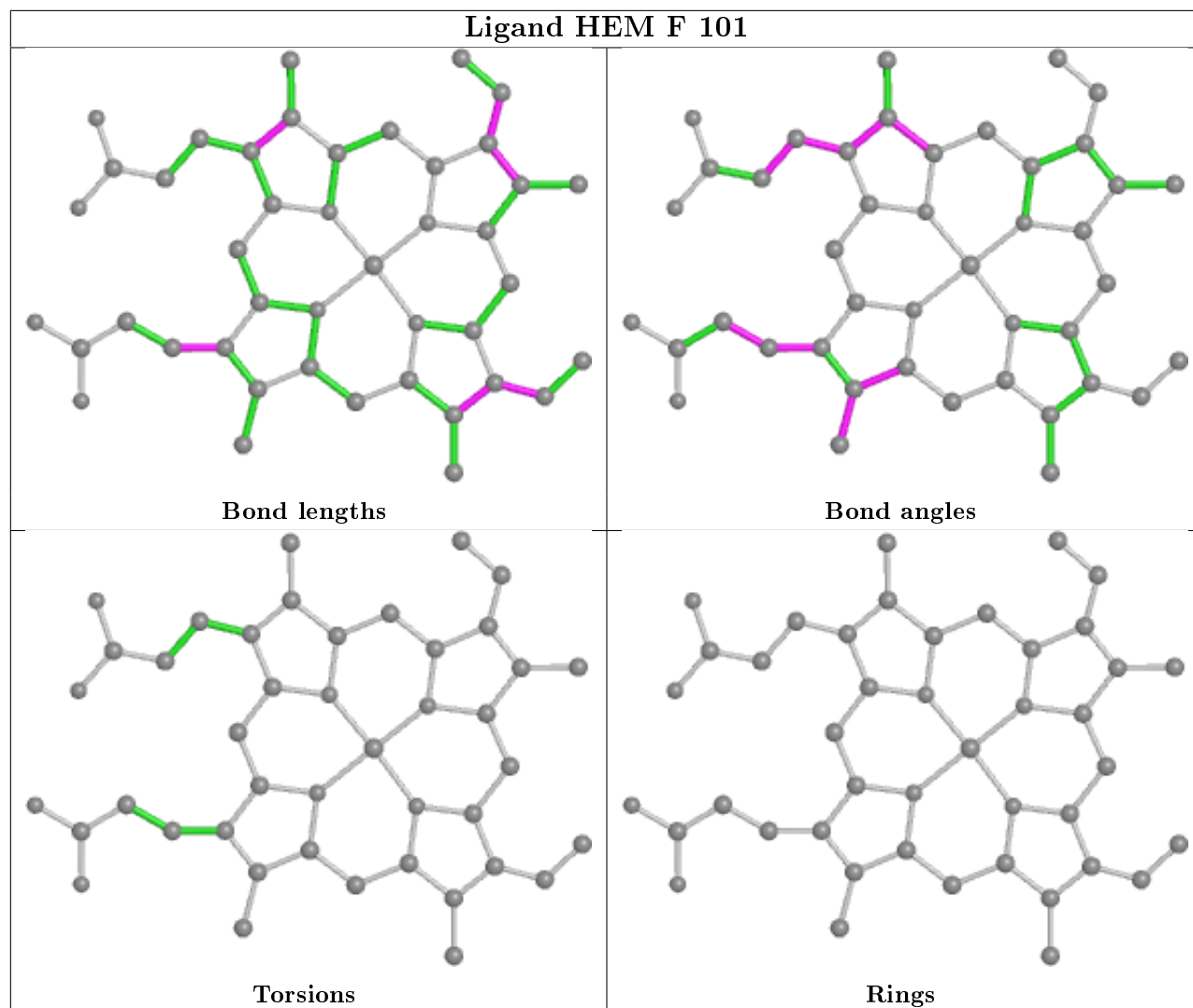


Ligand CLA C 505

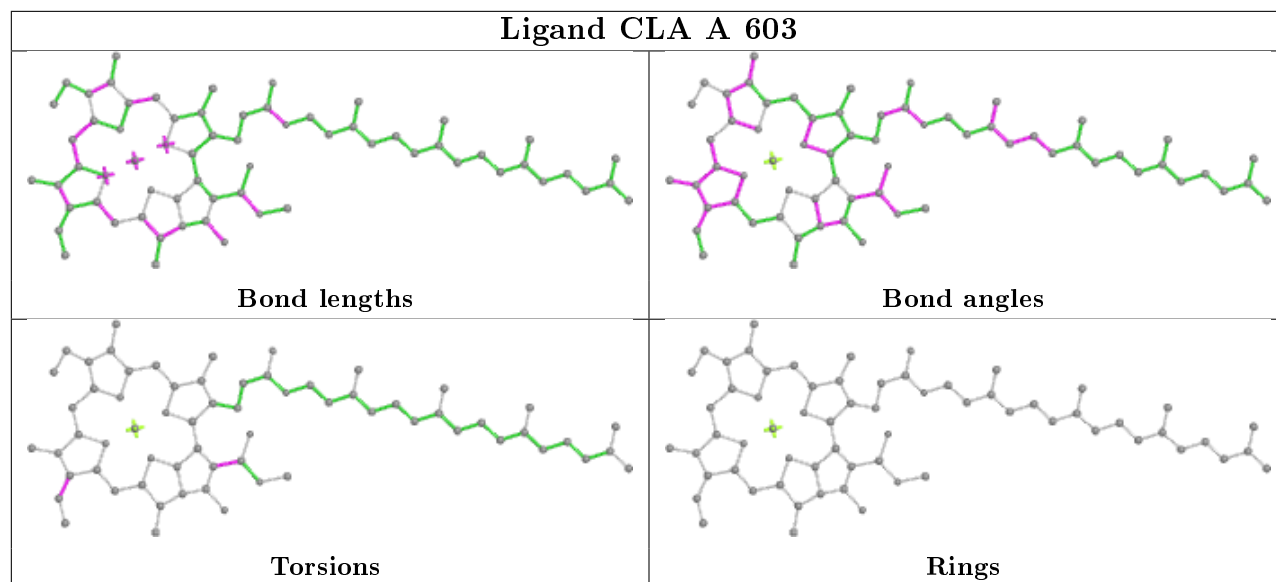


Ligand DGD c 517

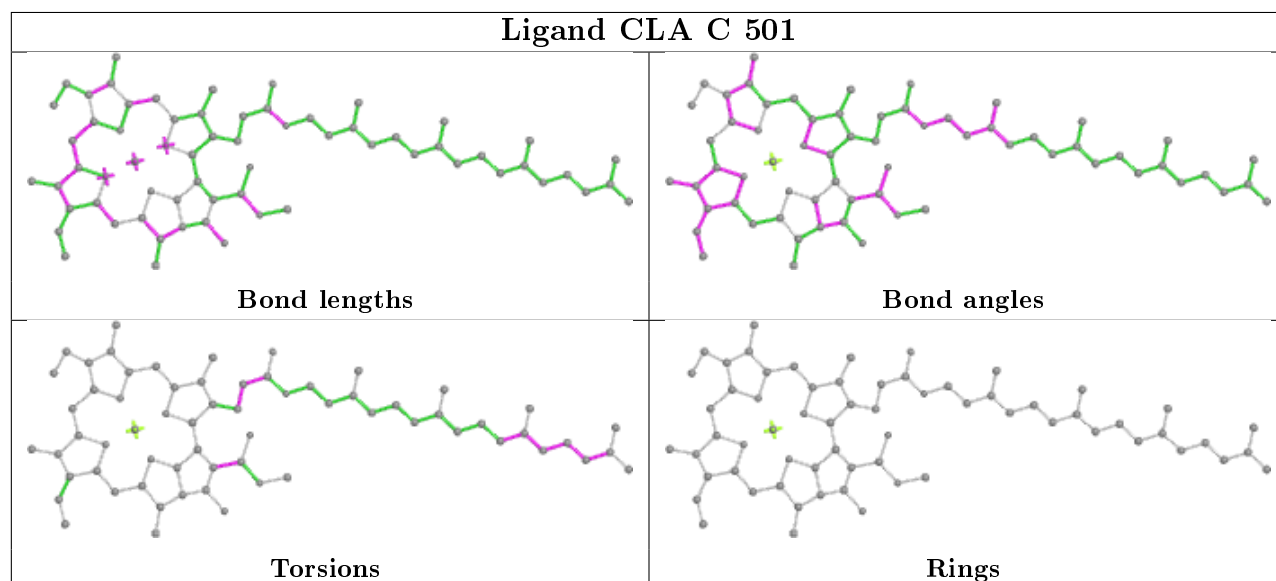




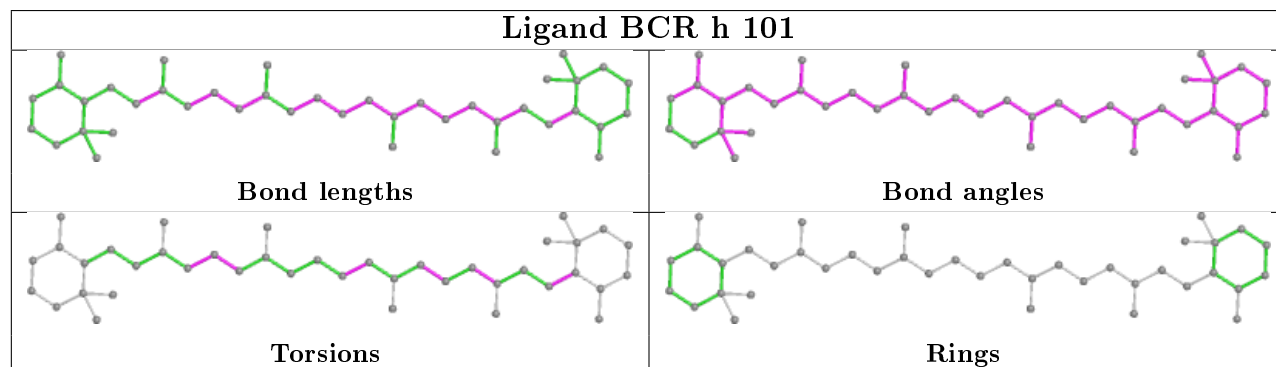
Ligand CLA A 603

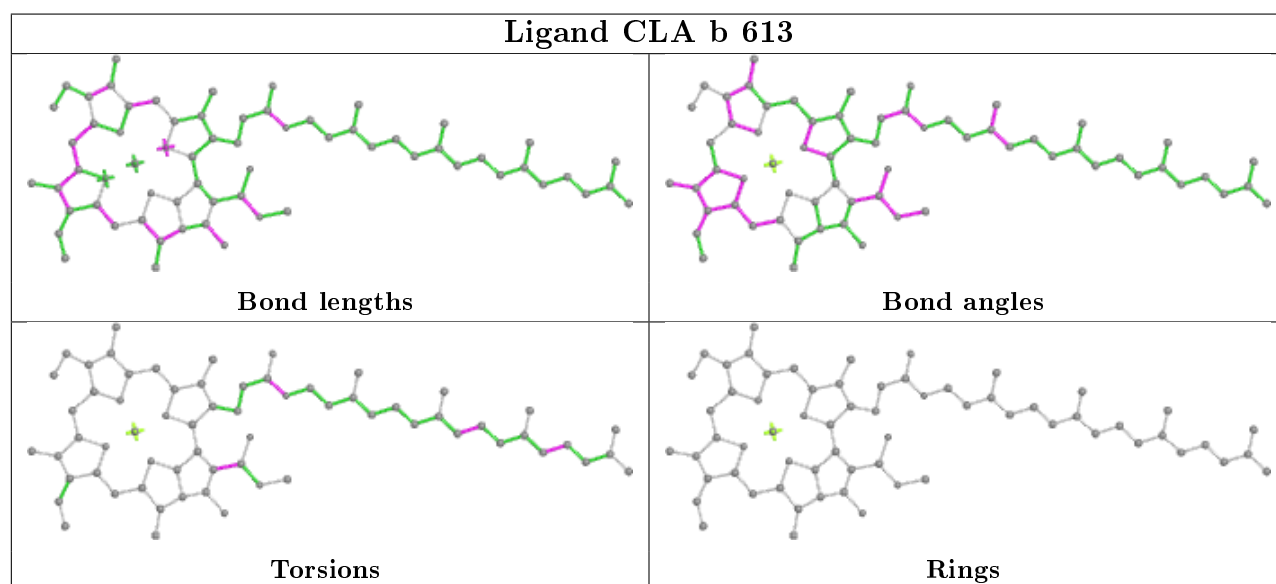
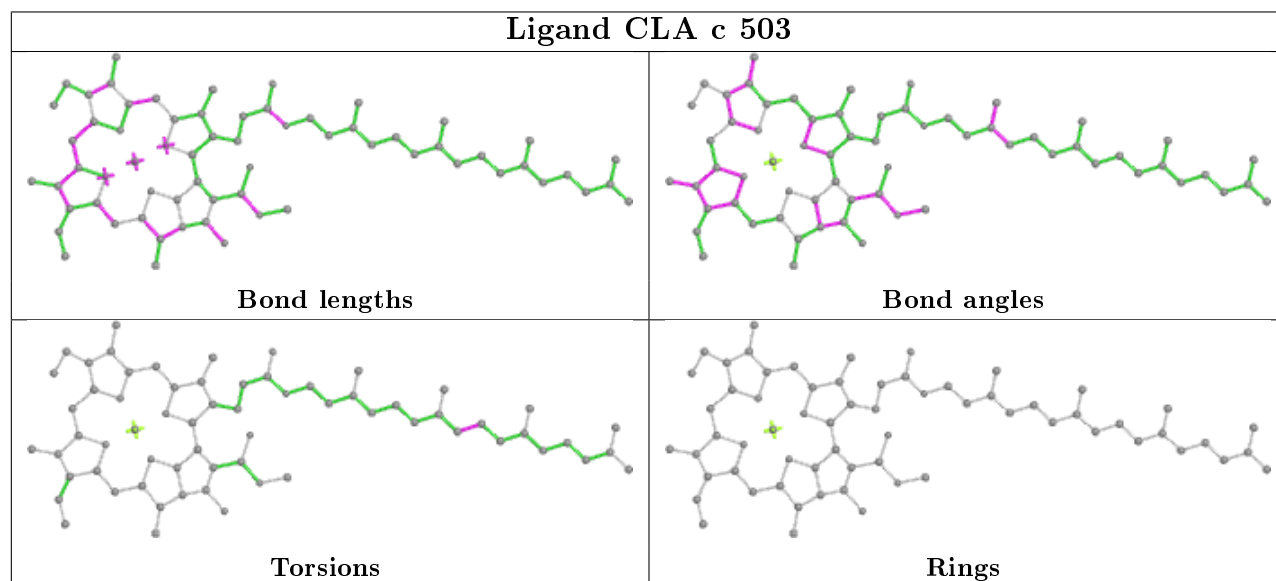
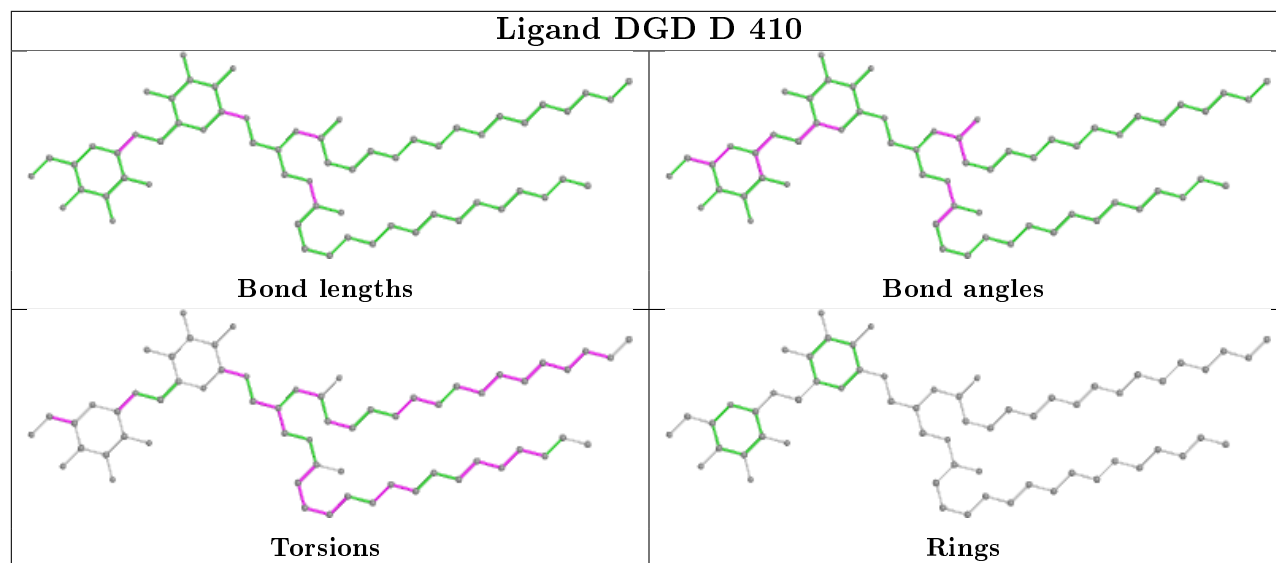


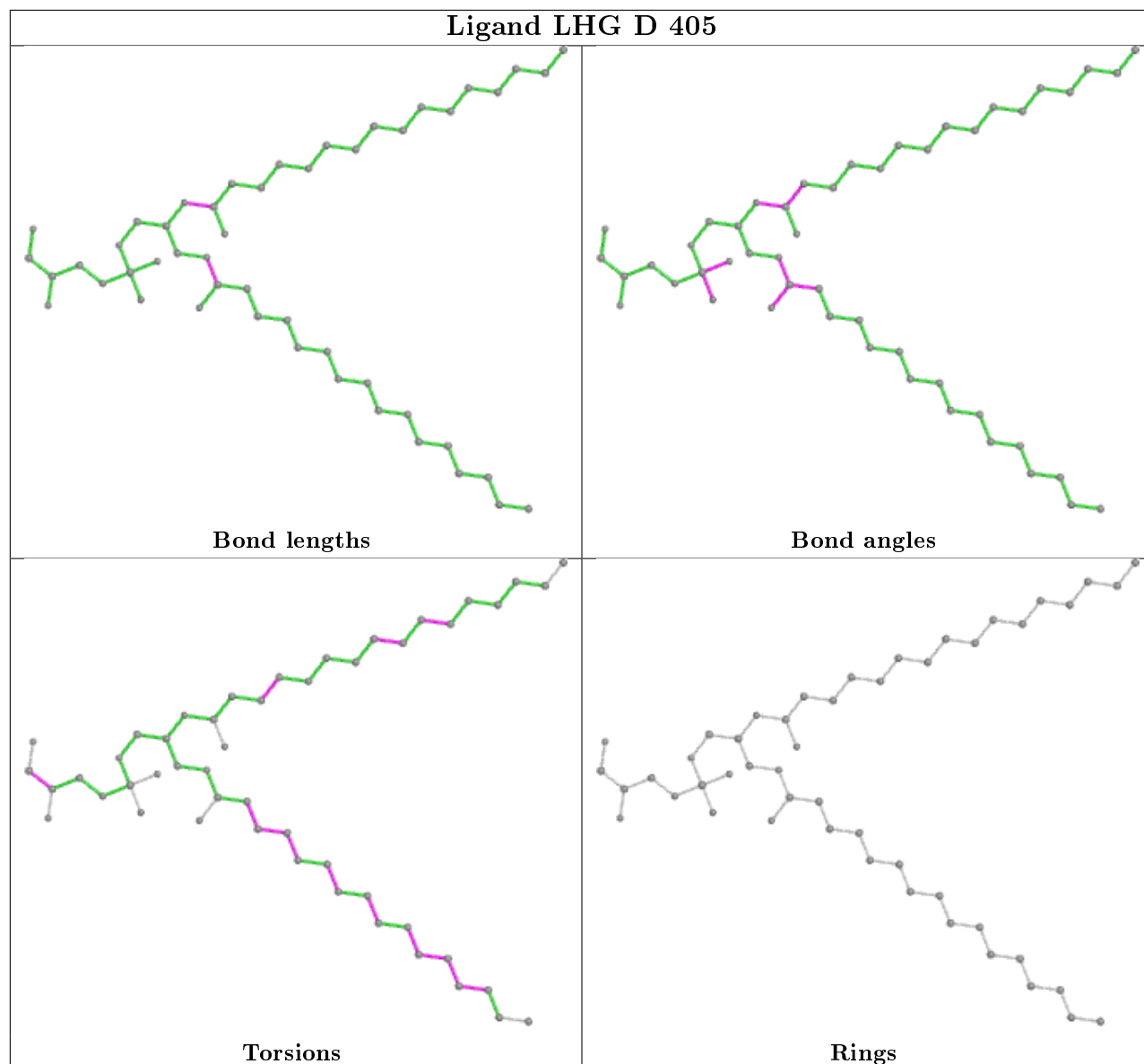
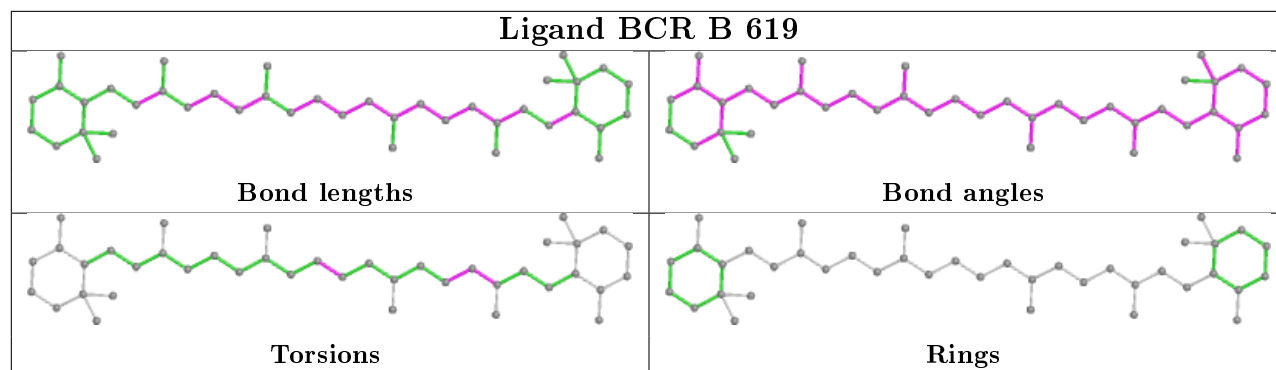
Ligand CLA C 501

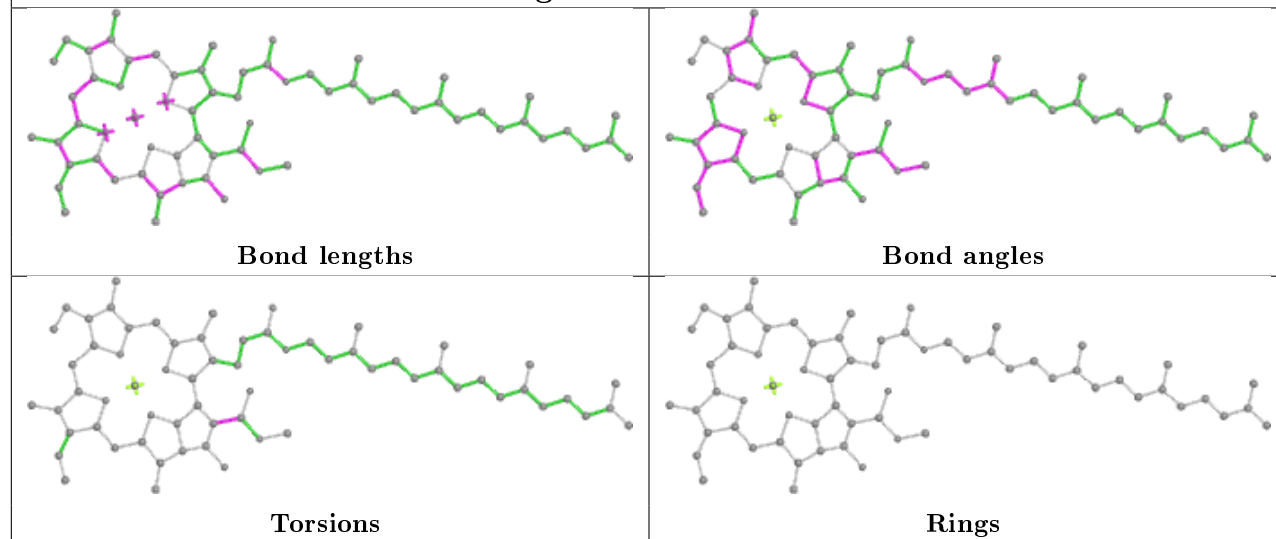
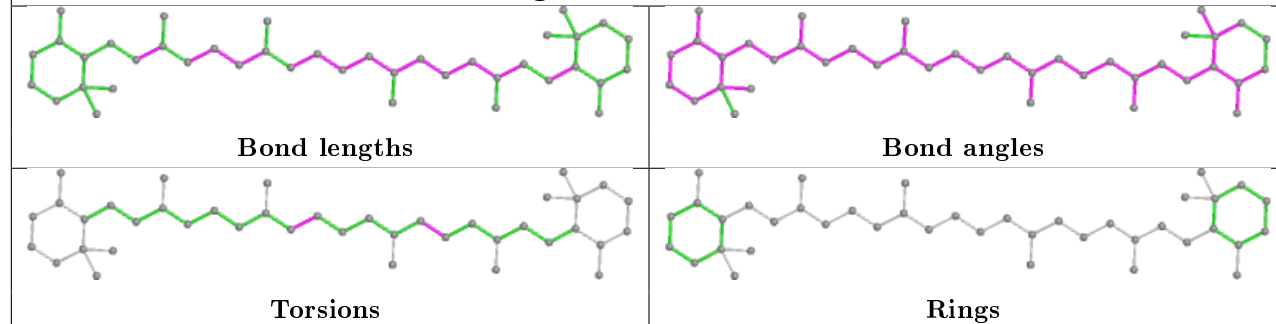
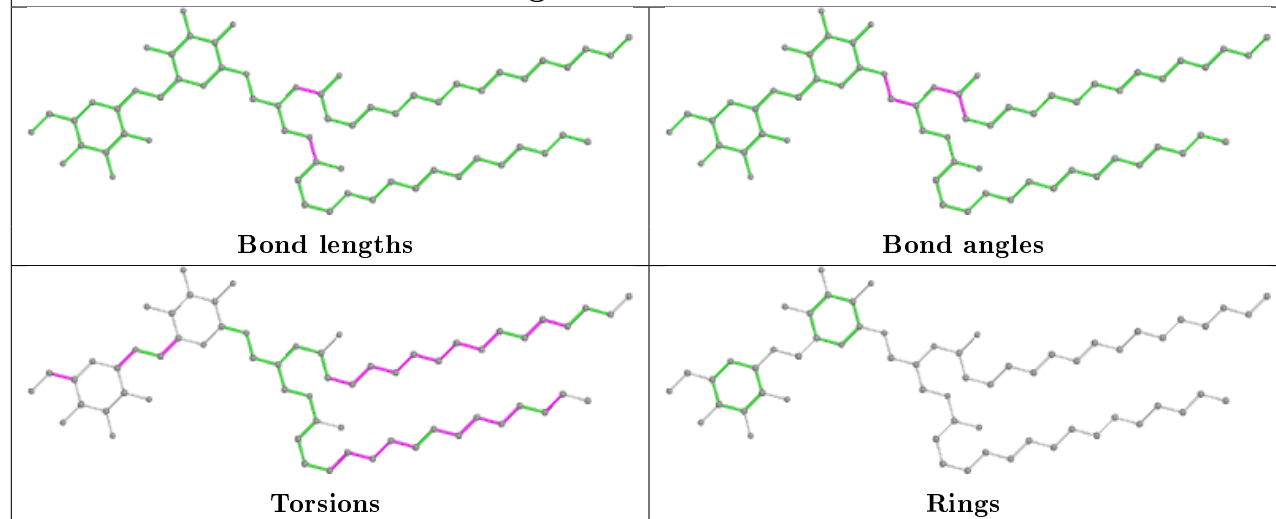


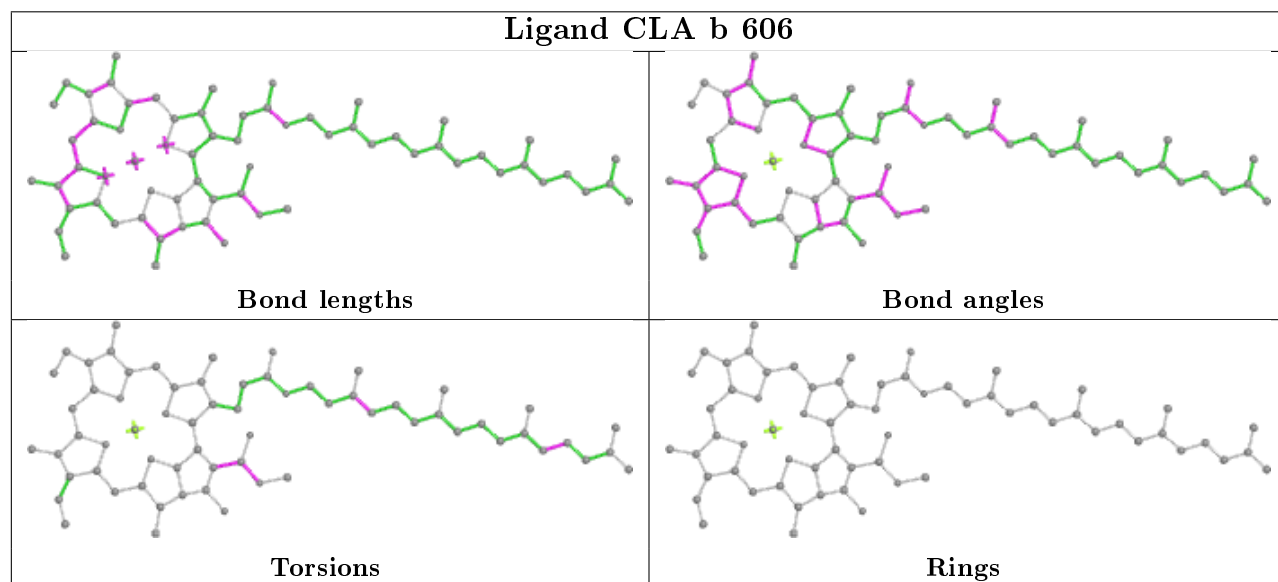
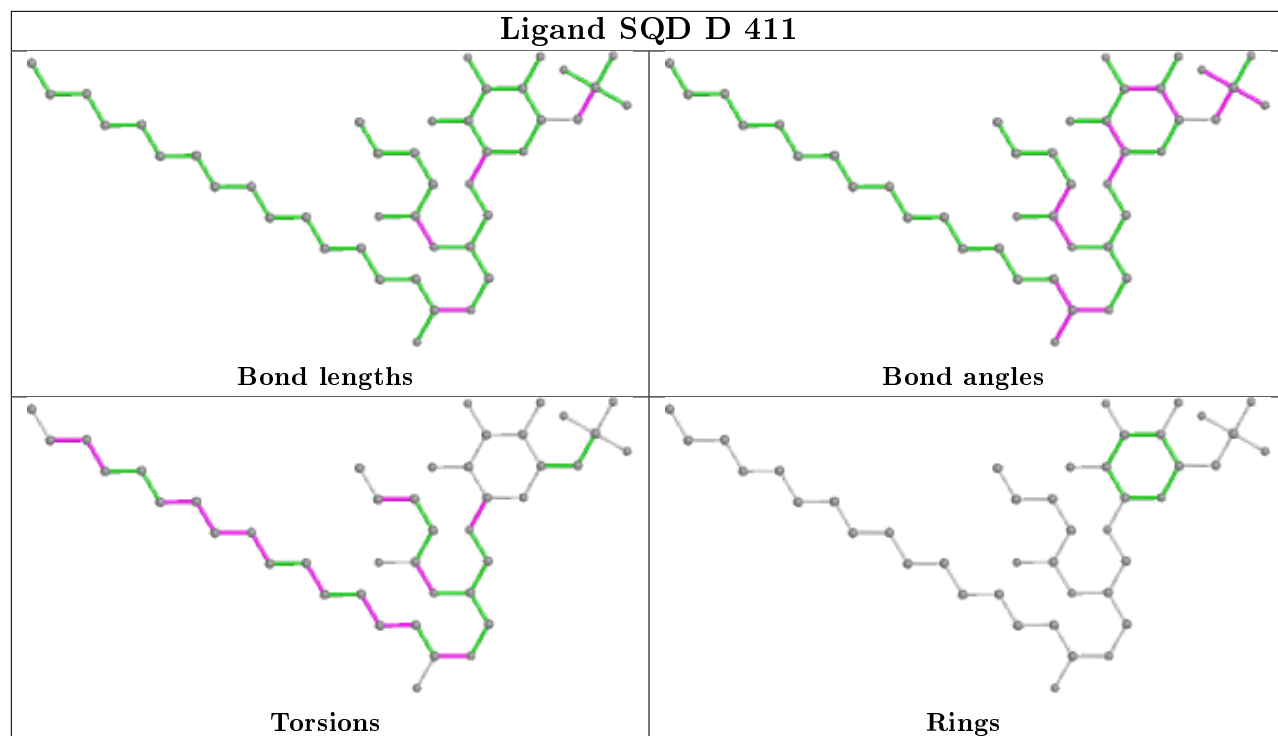
Ligand BCR h 101

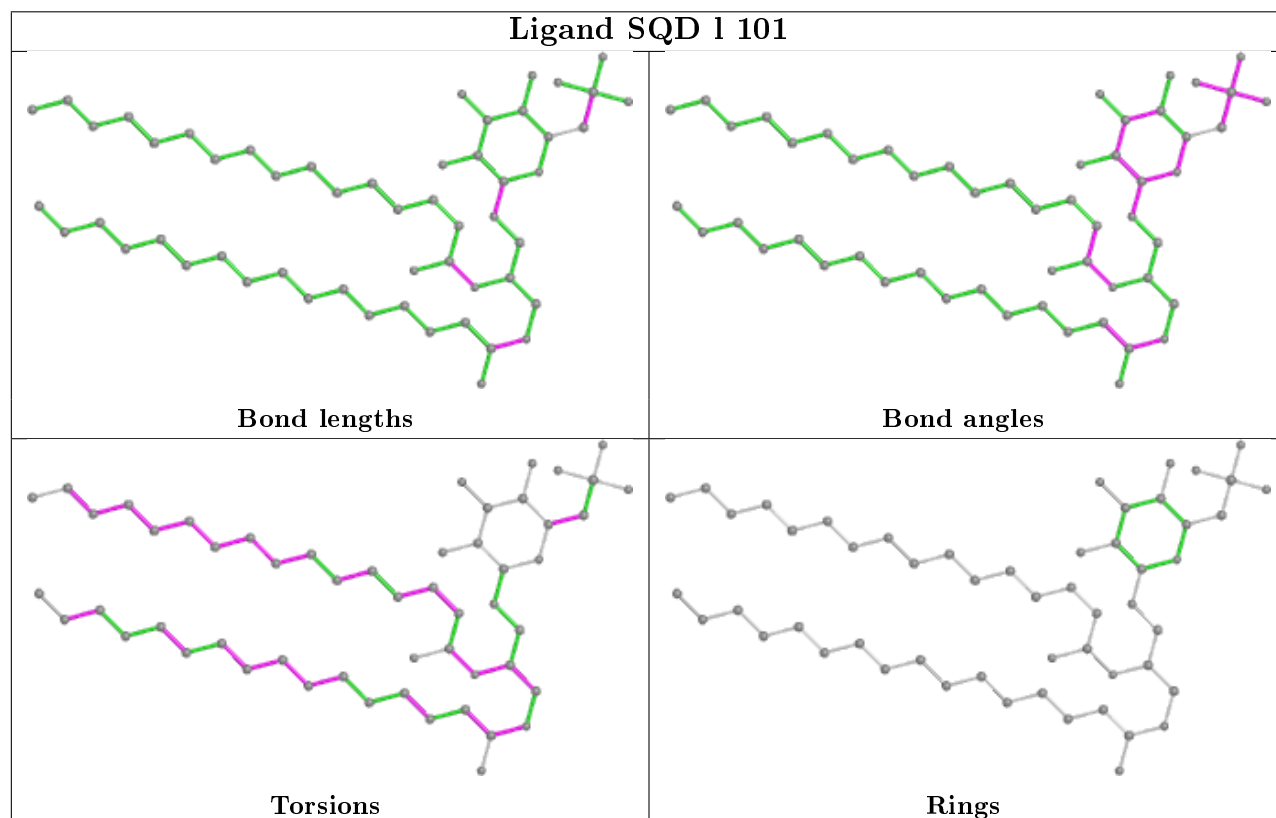
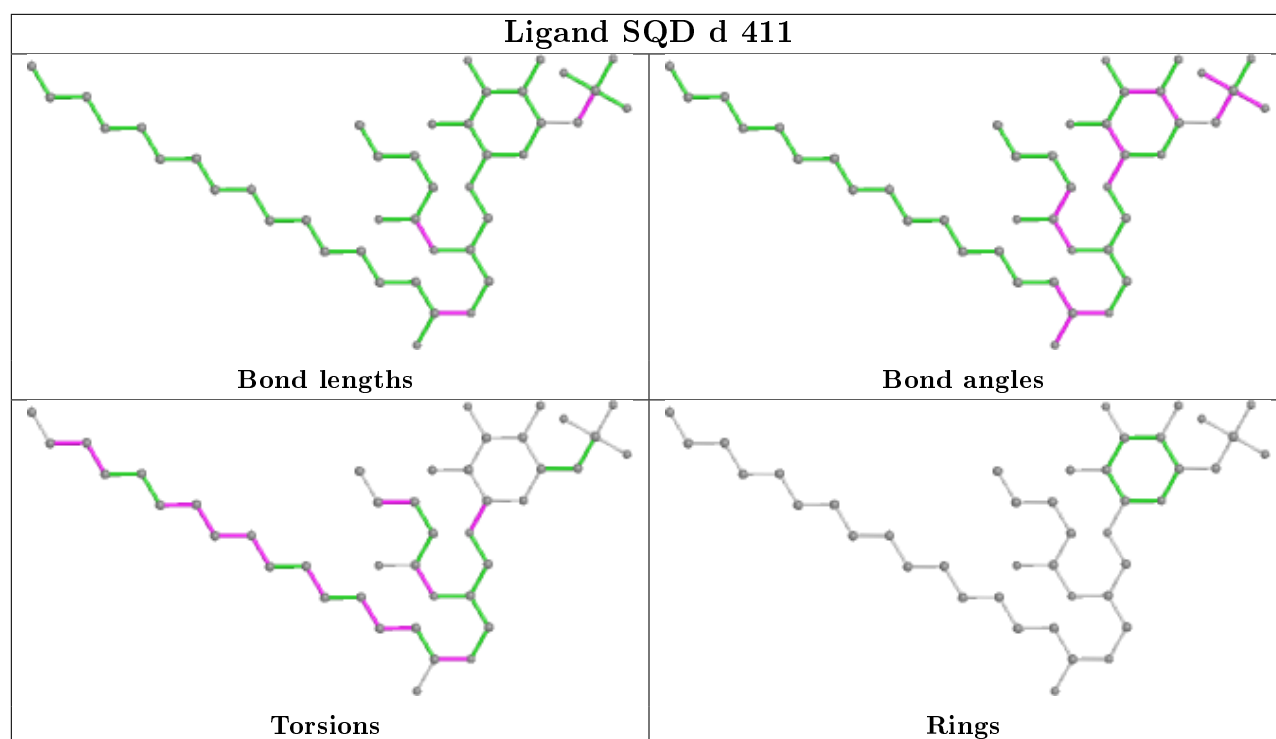


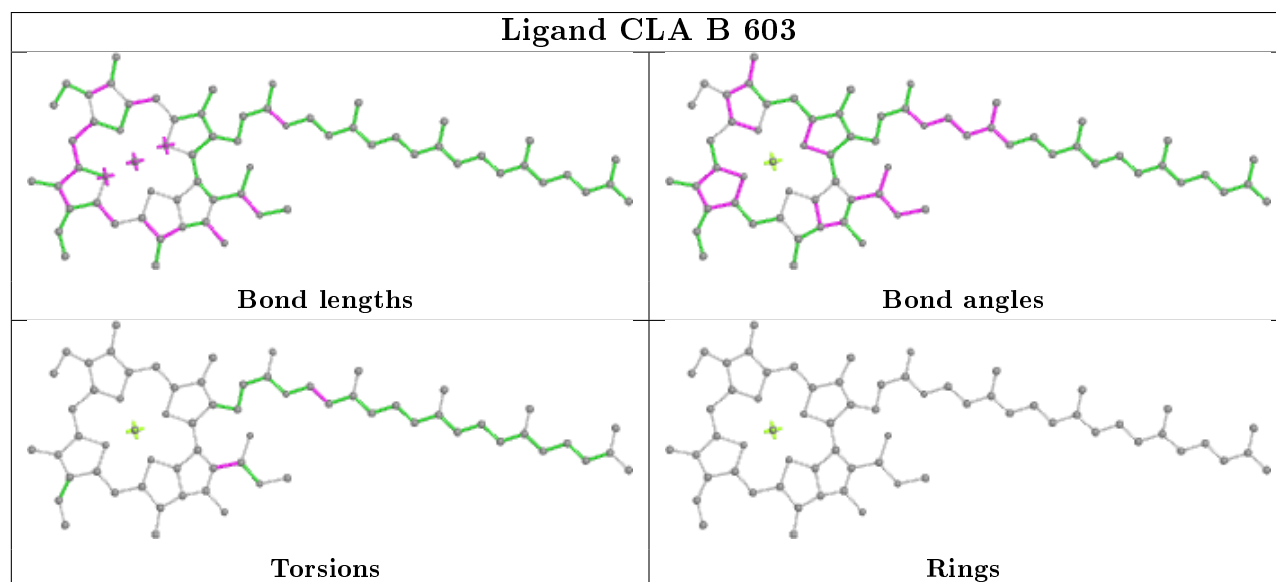
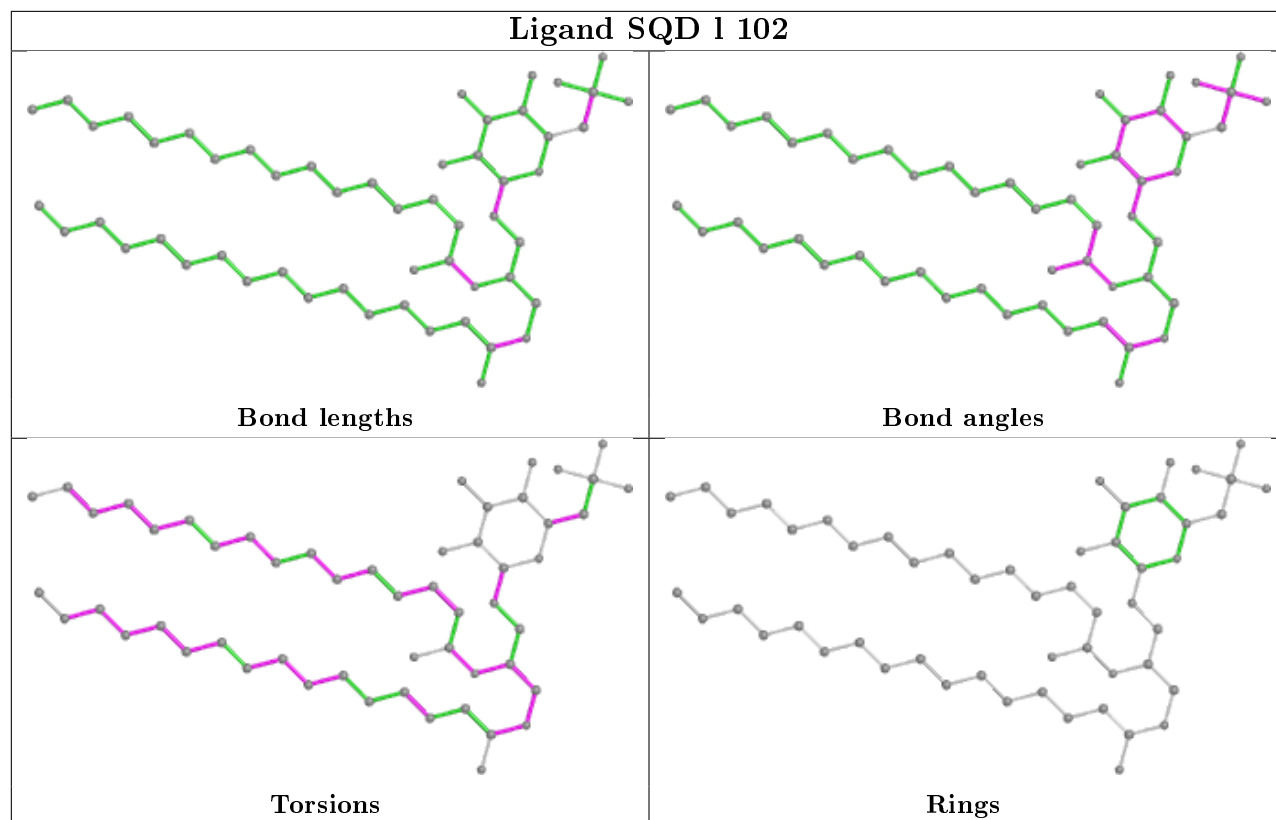




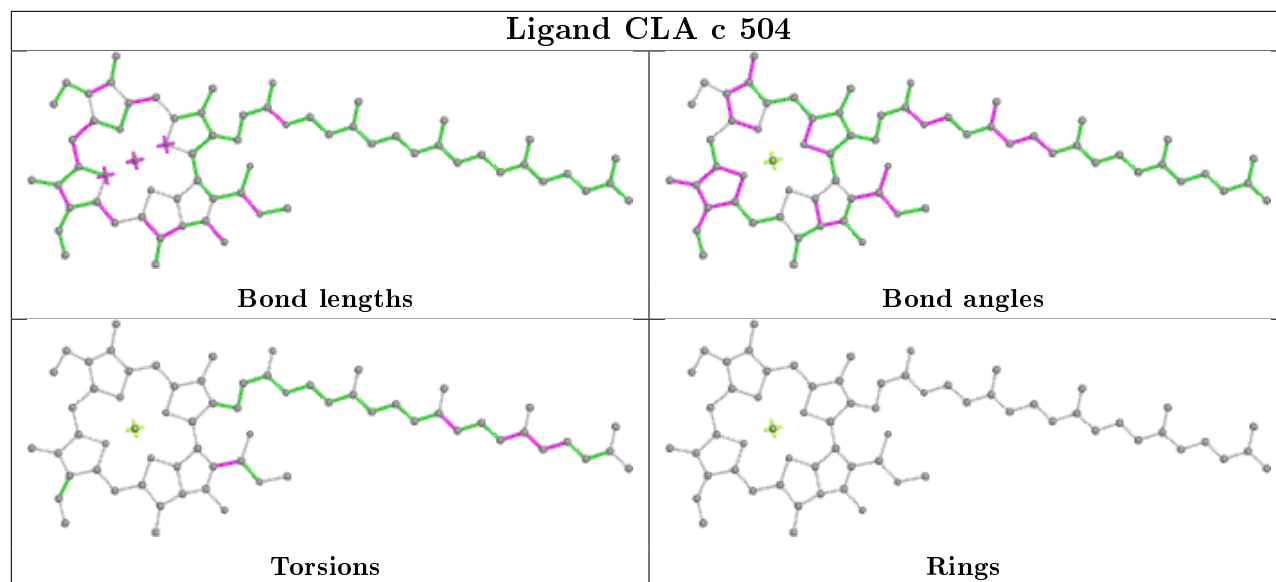
Ligand CLA b 608**Ligand BCR B 622****Ligand DGD C 516**



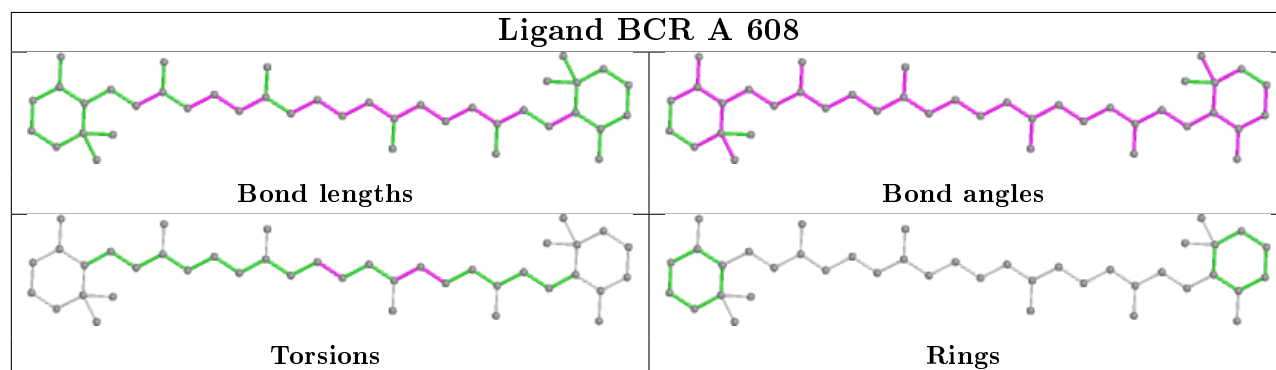




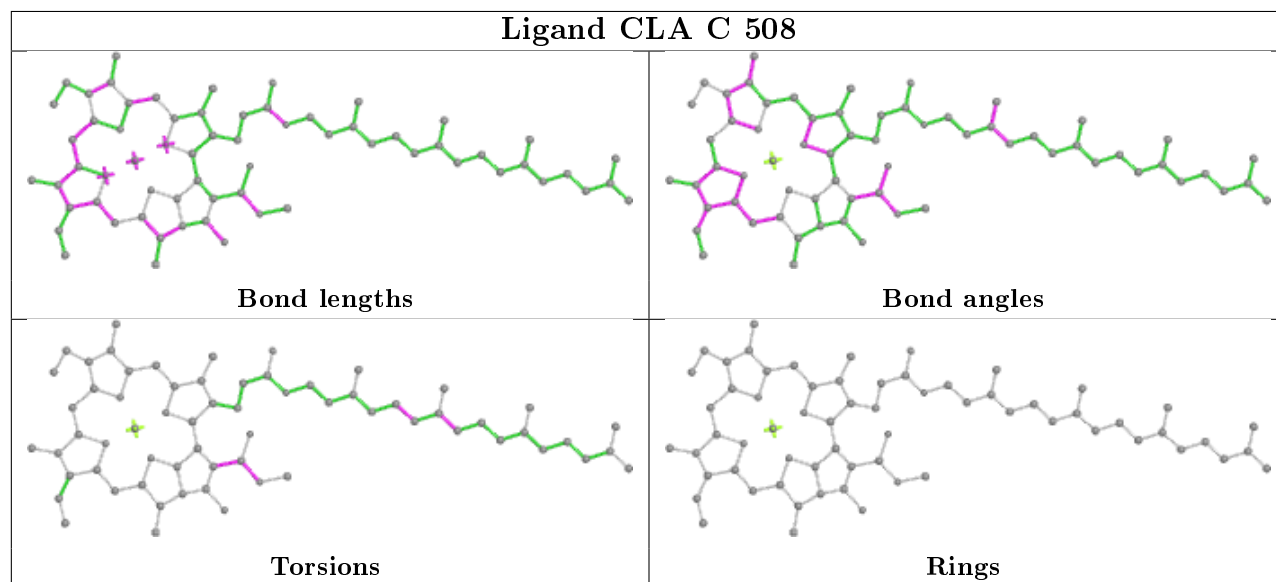
Ligand CLA c 504

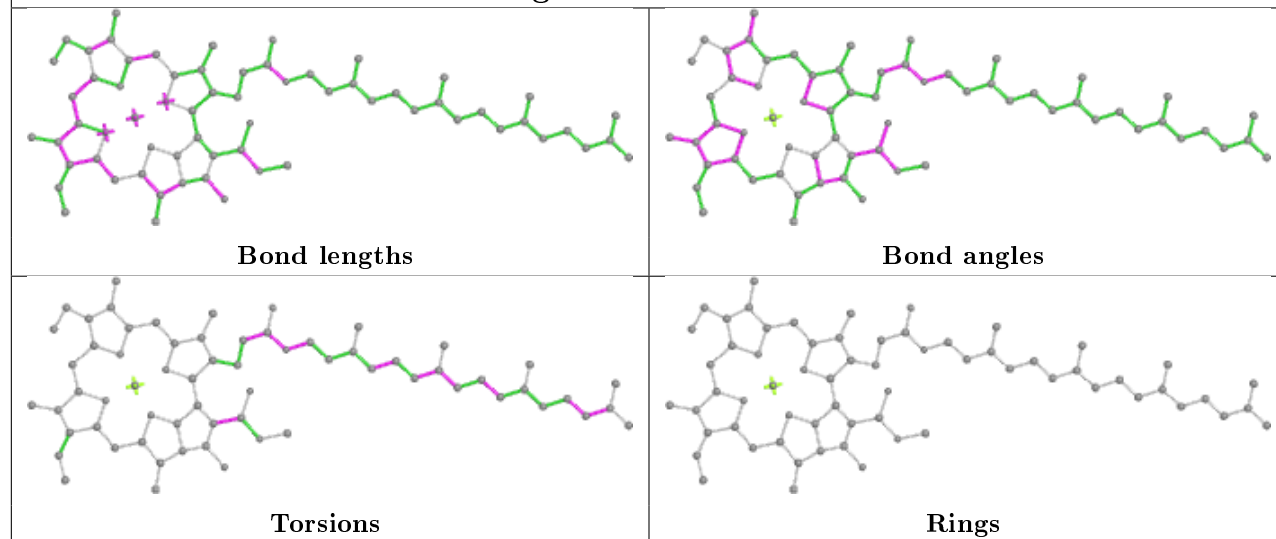
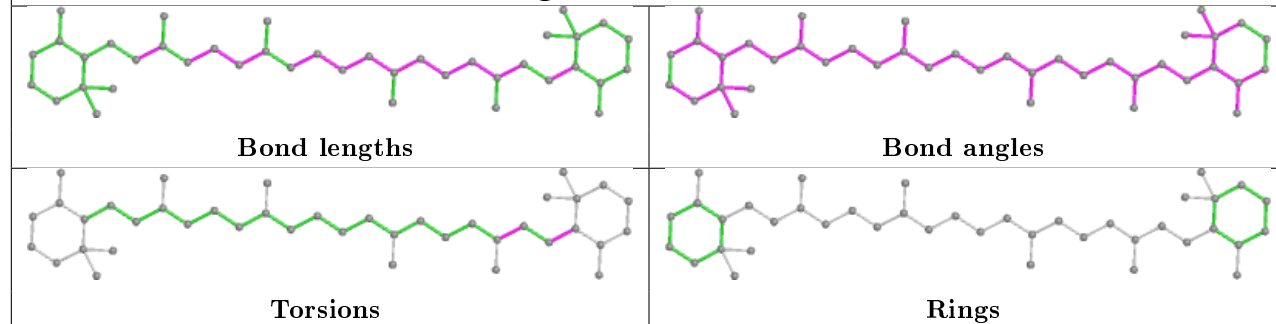
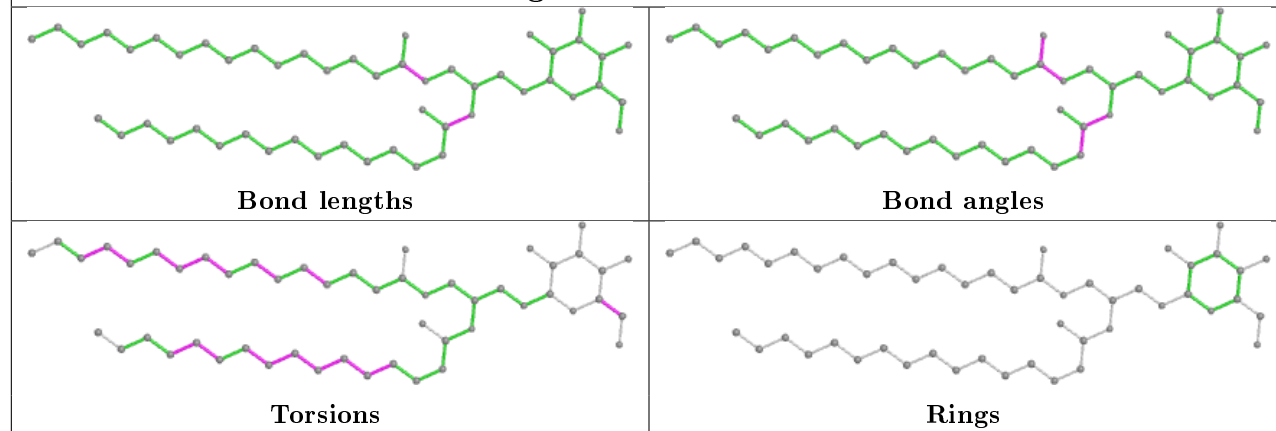


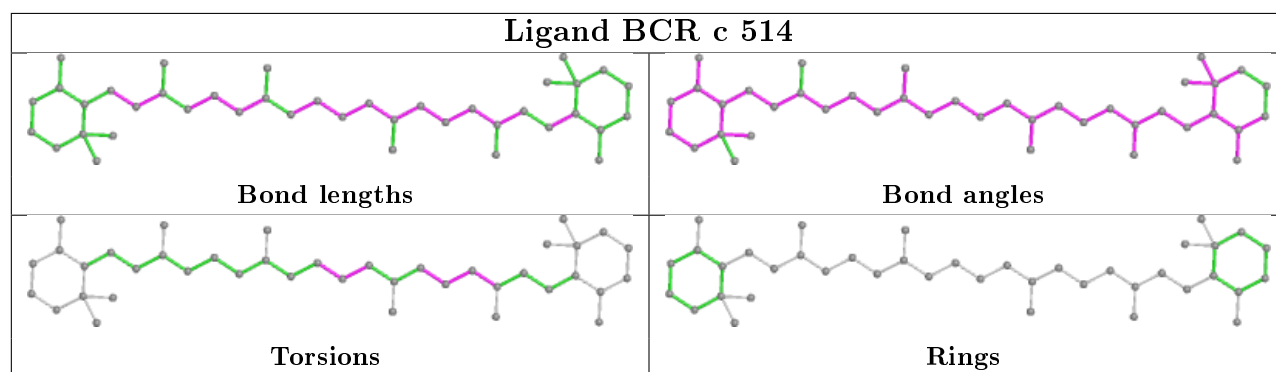
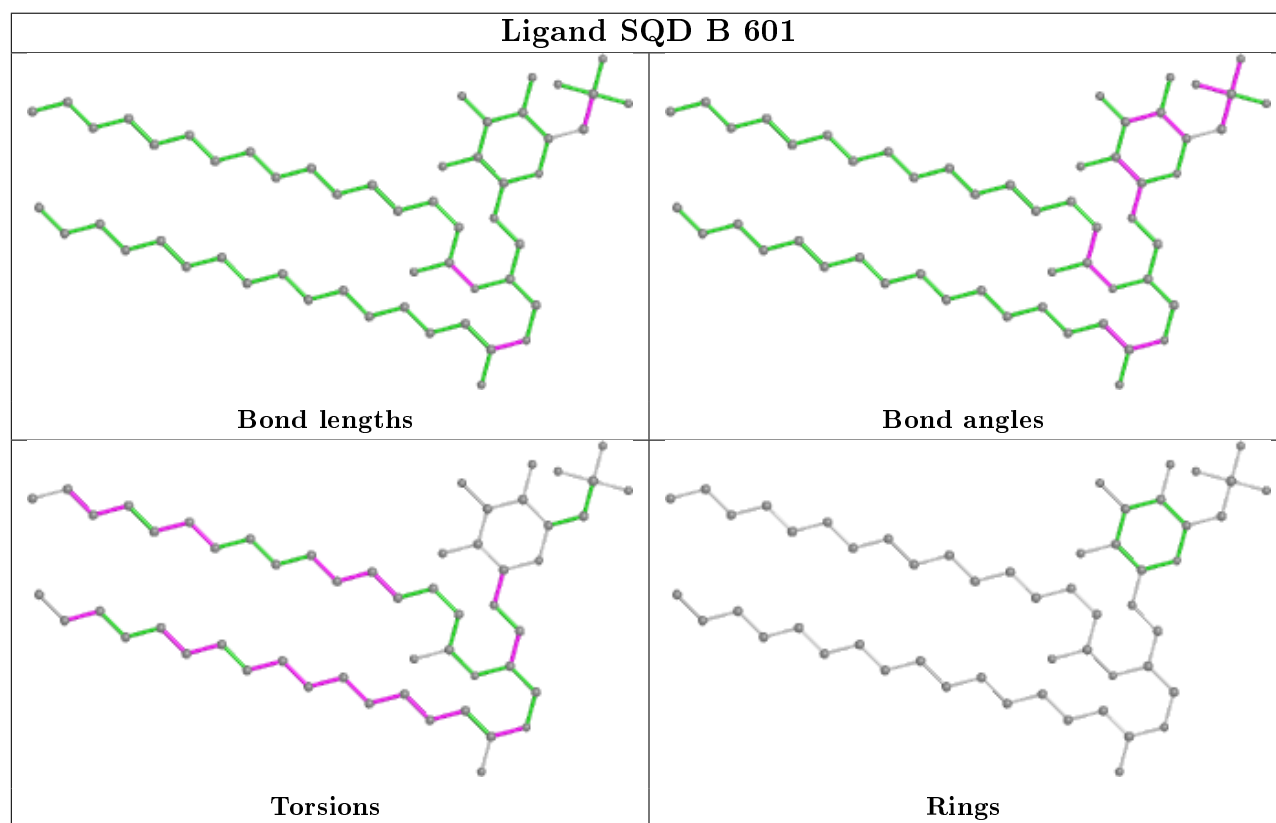
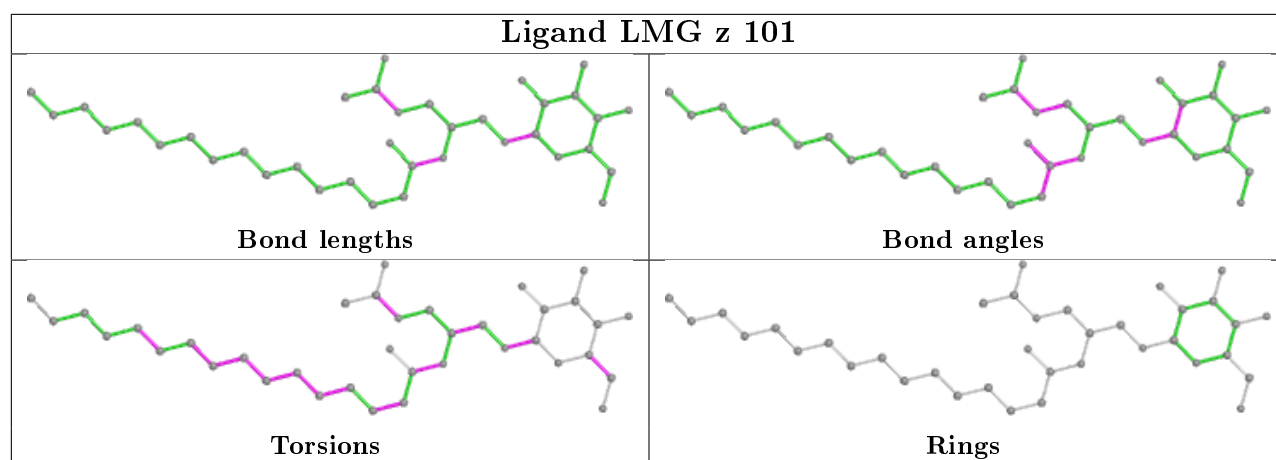
Ligand BCR A 608



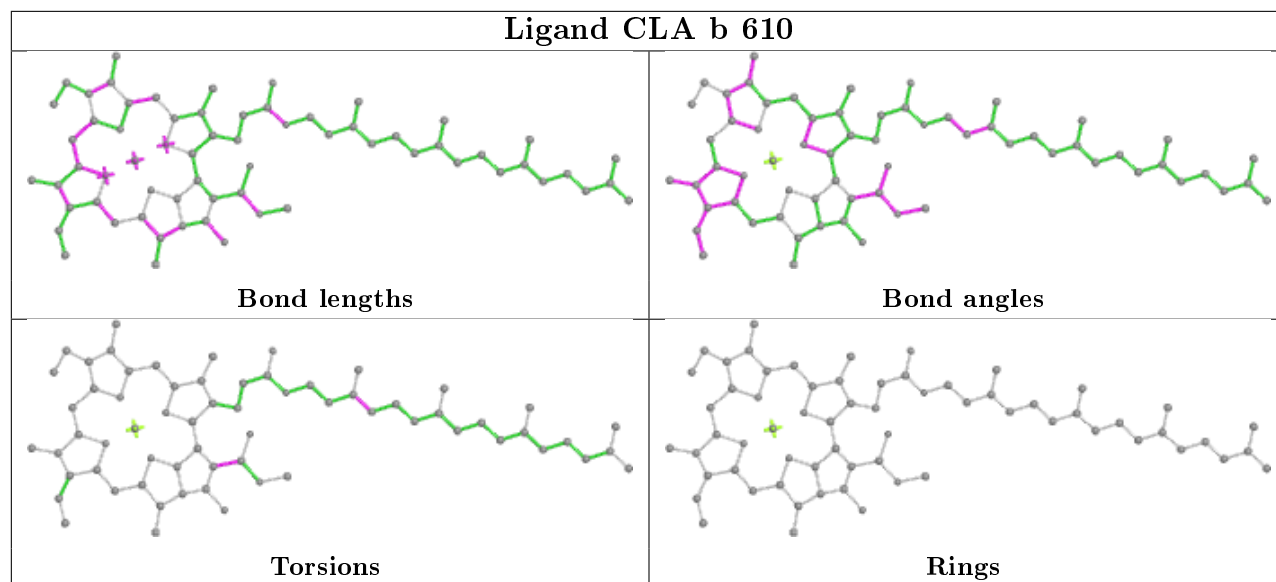
Ligand CLA C 508



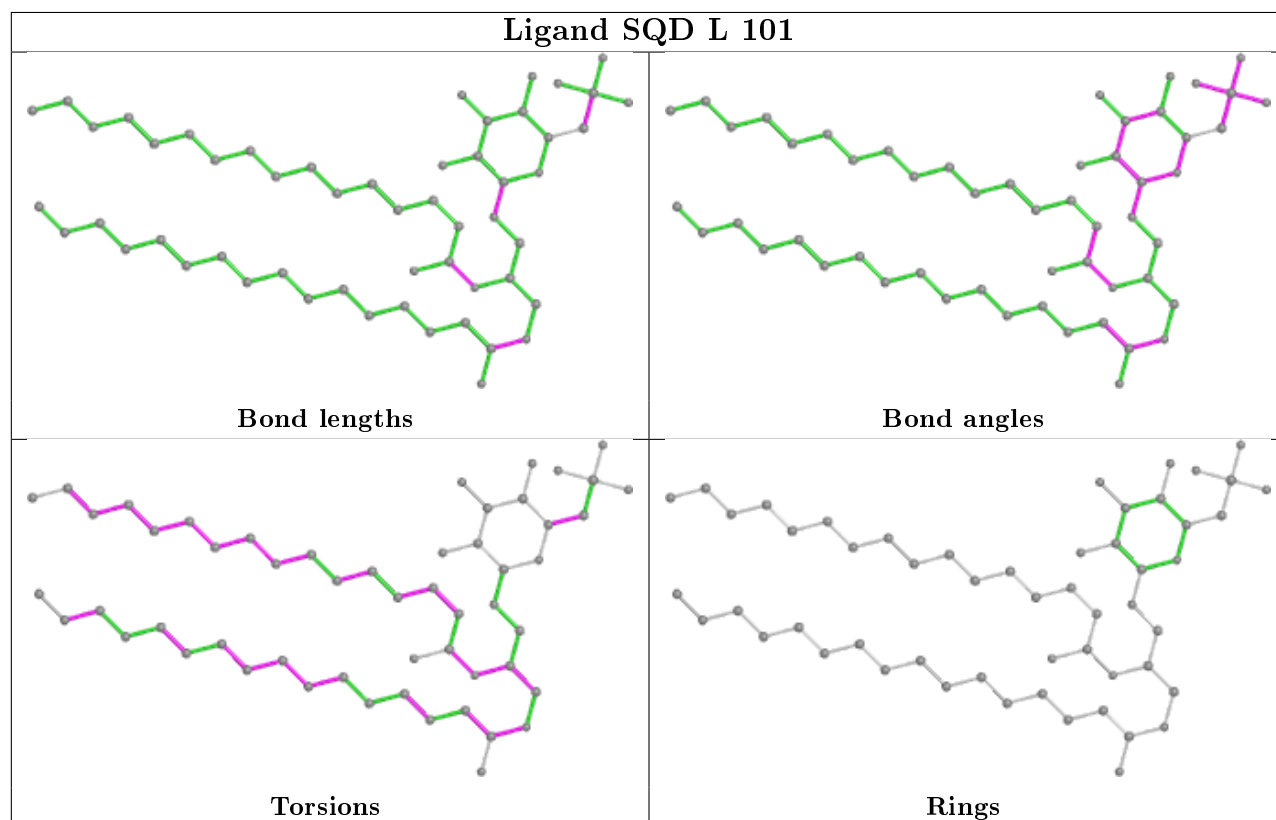
Ligand CLA B 602**Ligand BCR t 101****Ligand LMG D 406**



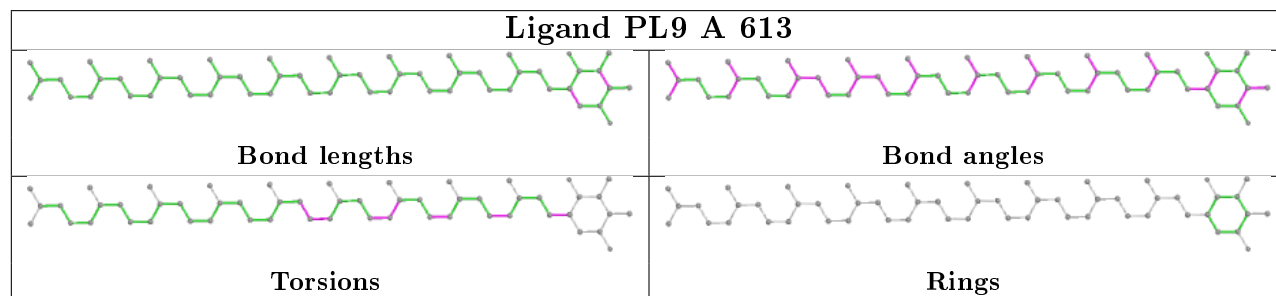
Ligand CLA b 610

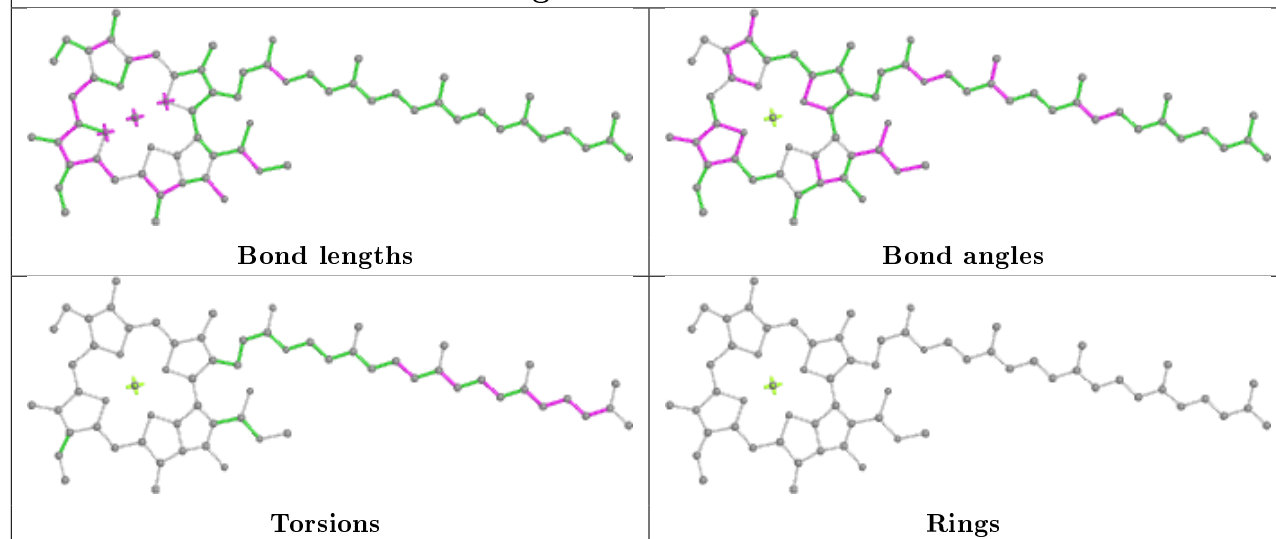
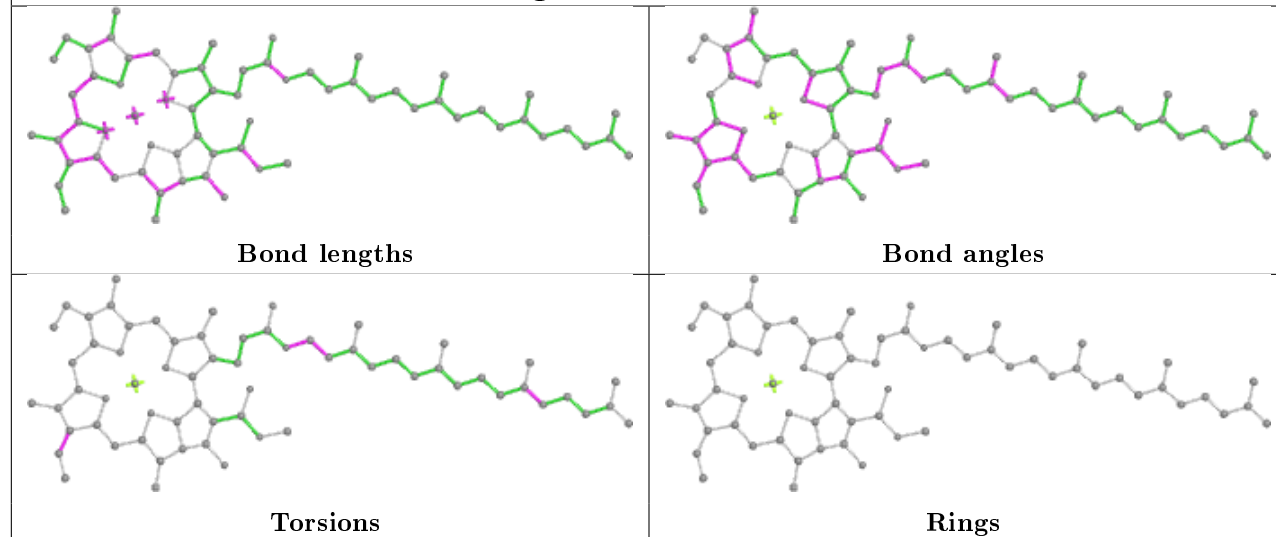
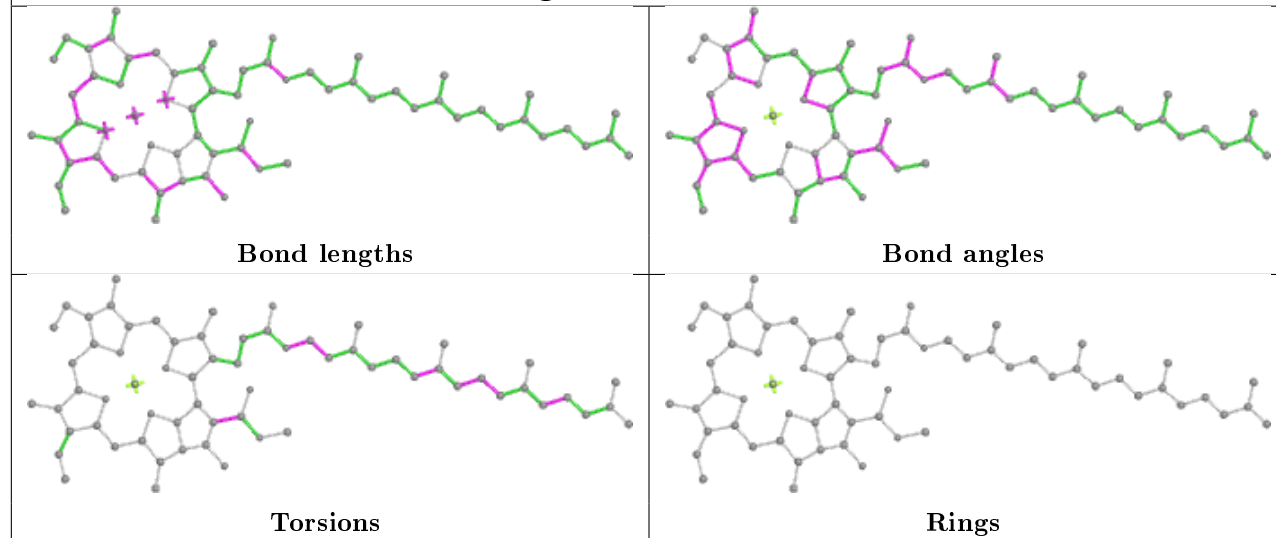


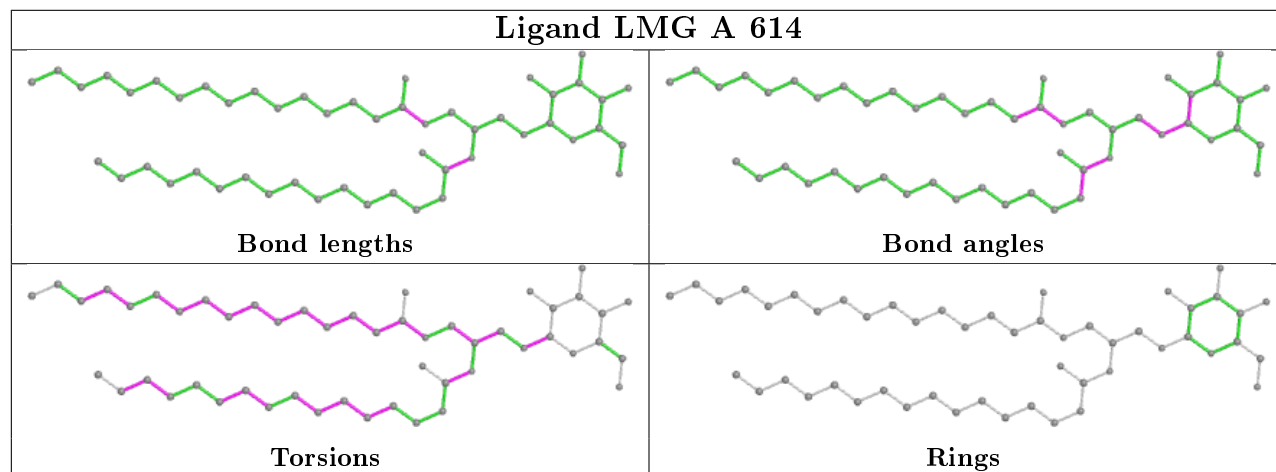
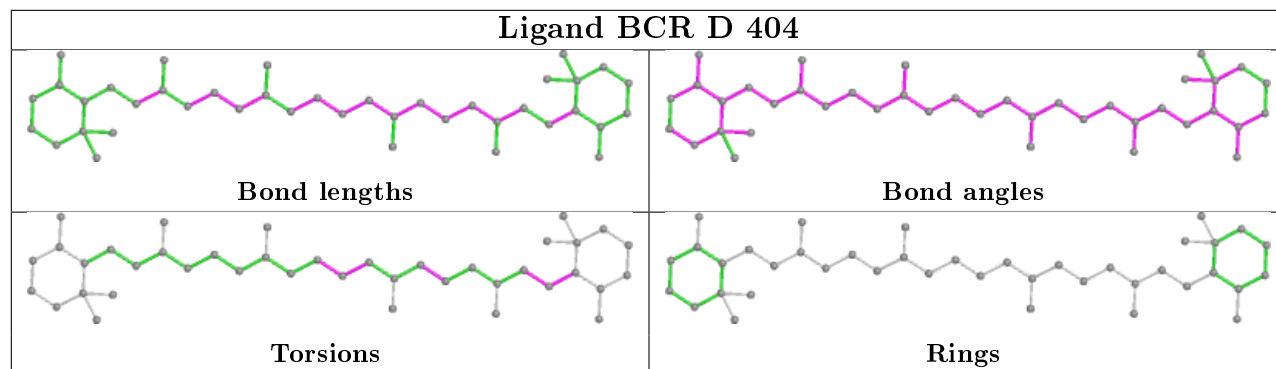
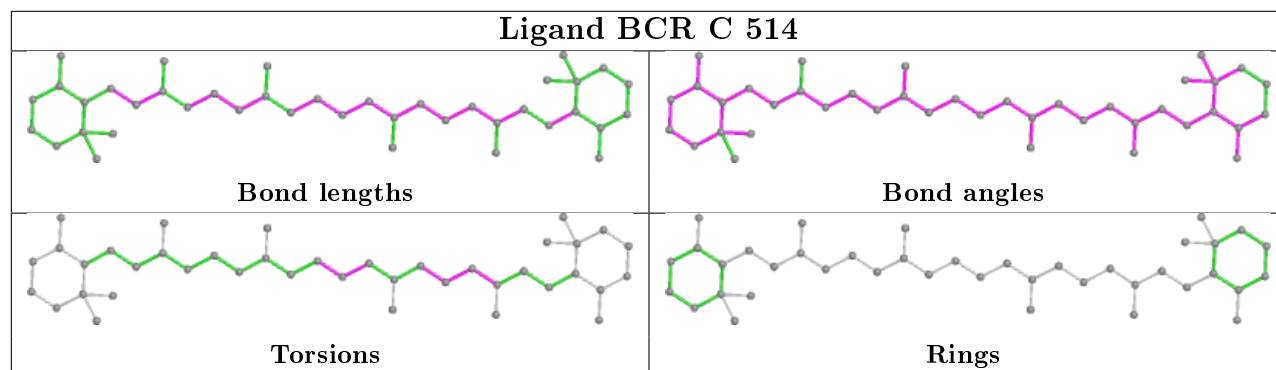
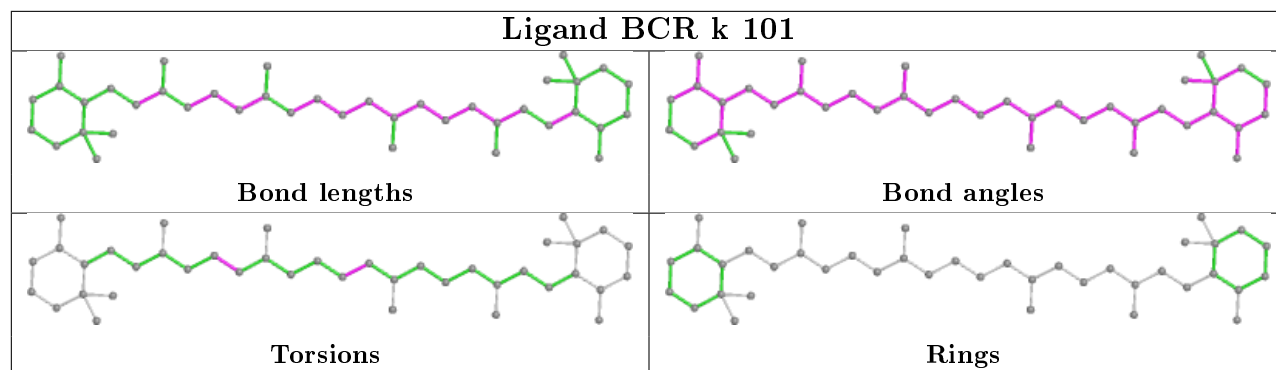
Ligand SQD L 101



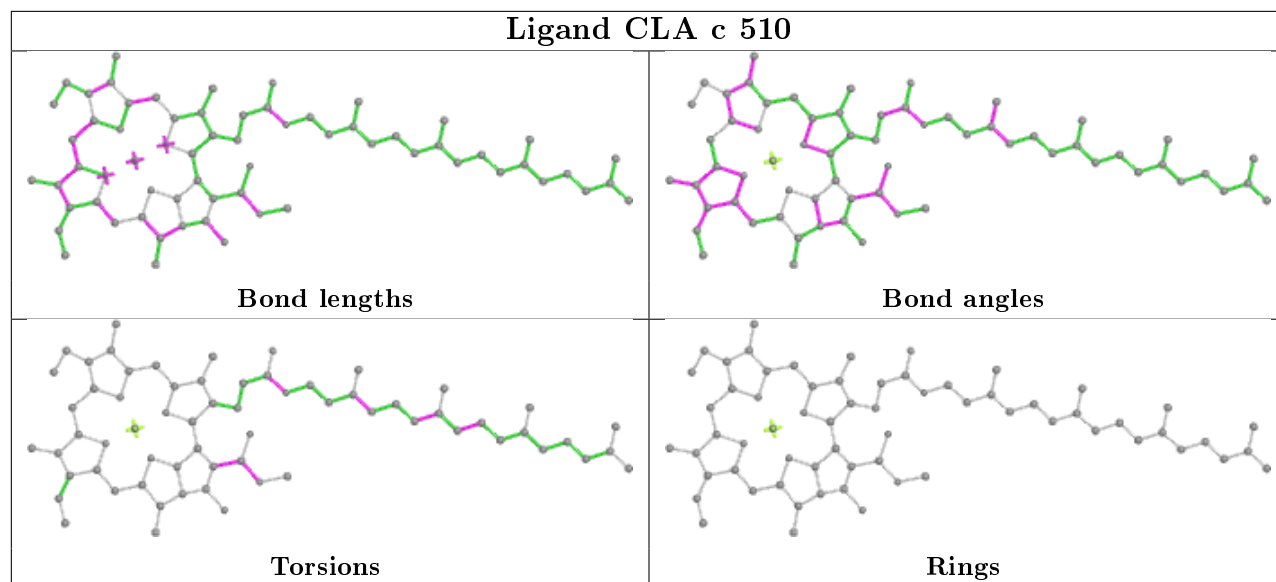
Ligand PL9 A 613



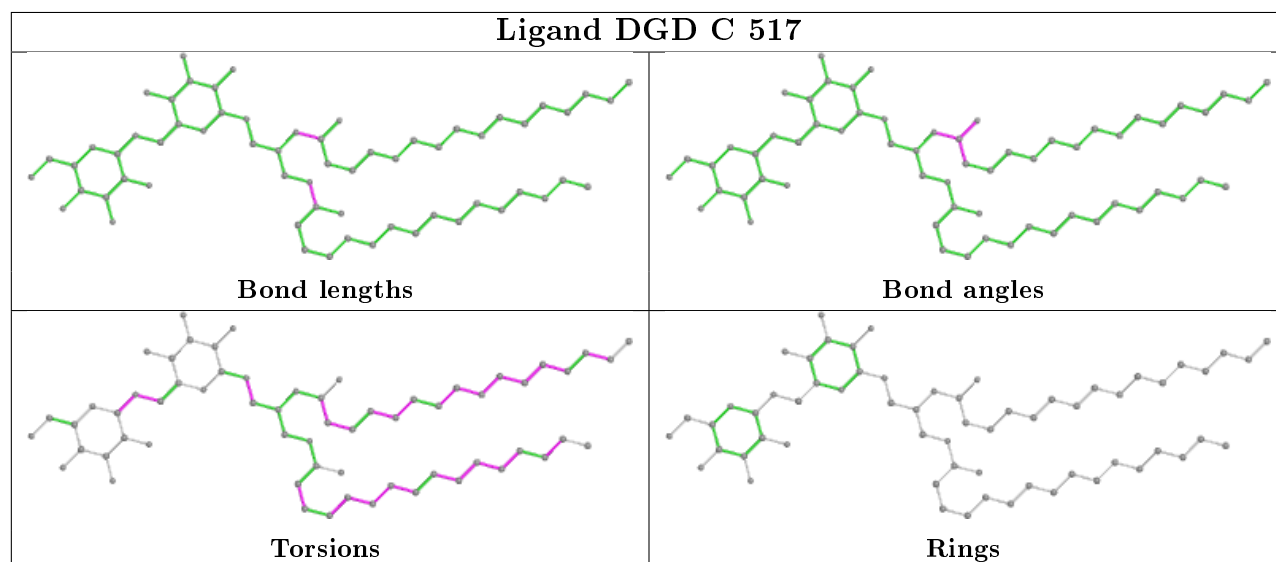
Ligand CLA B 616**Ligand CLA D 401****Ligand CLA c 509**



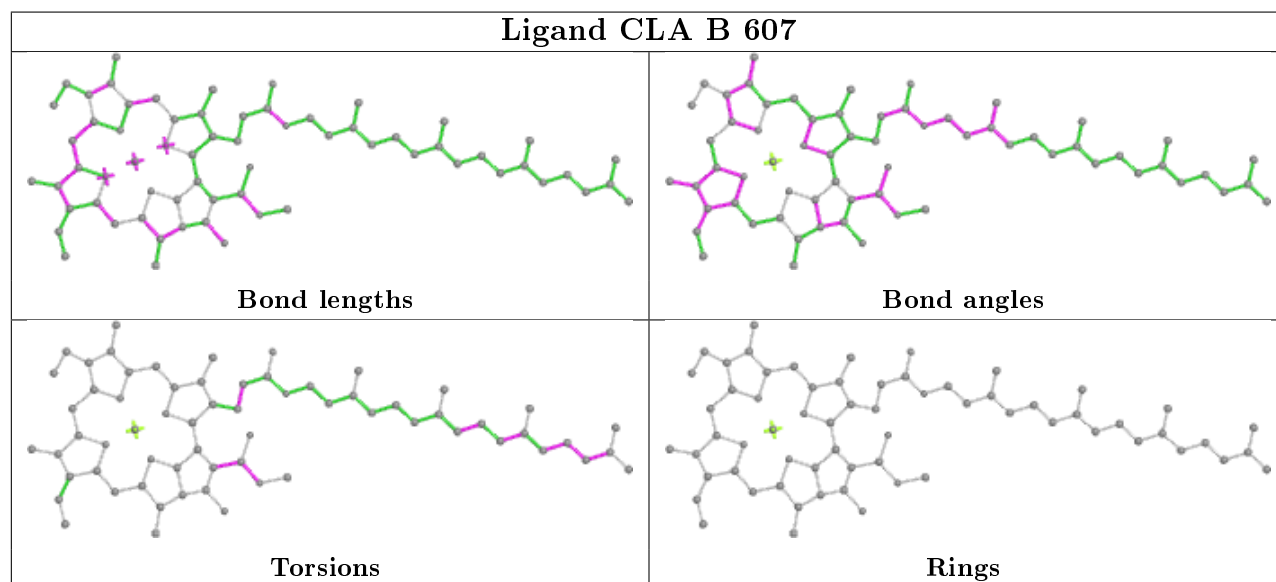
Ligand CLA c 510

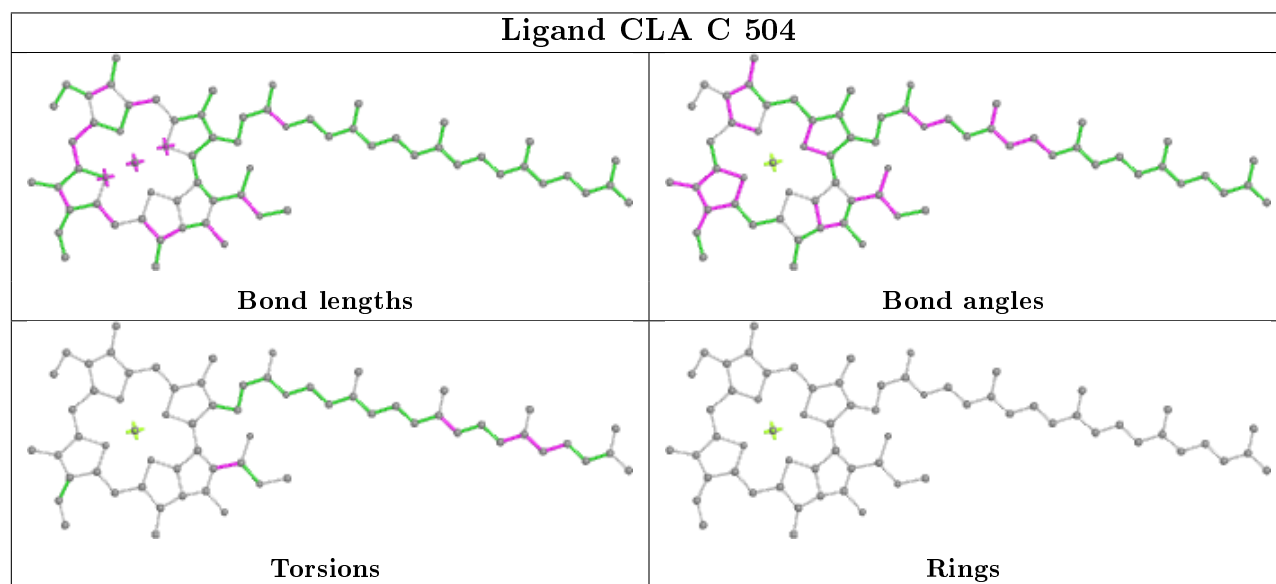
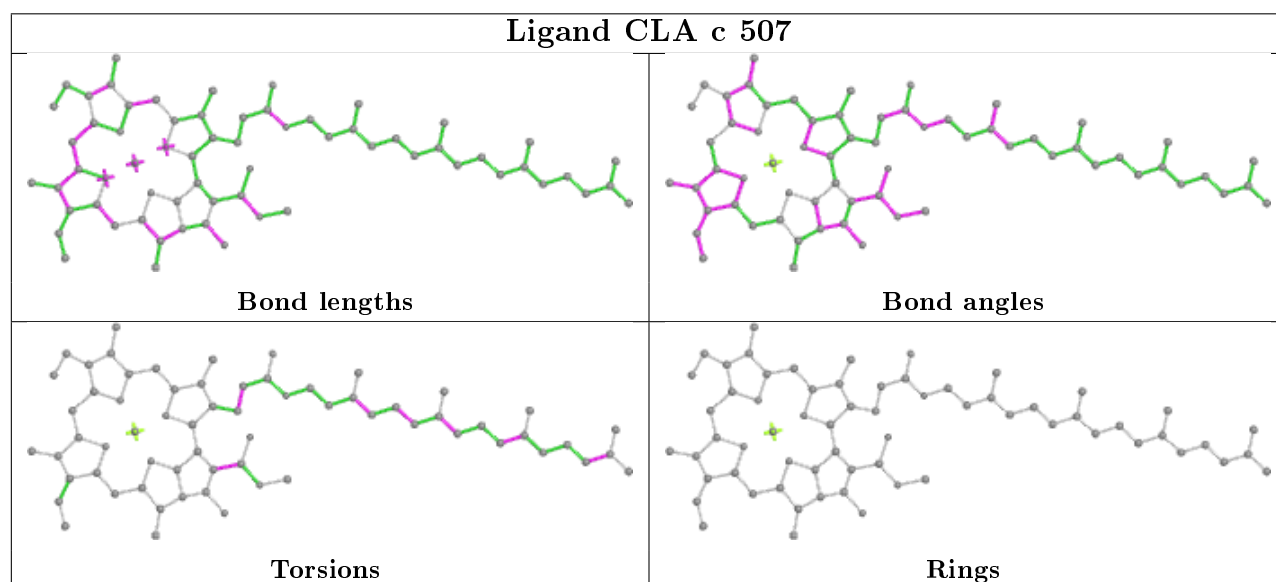
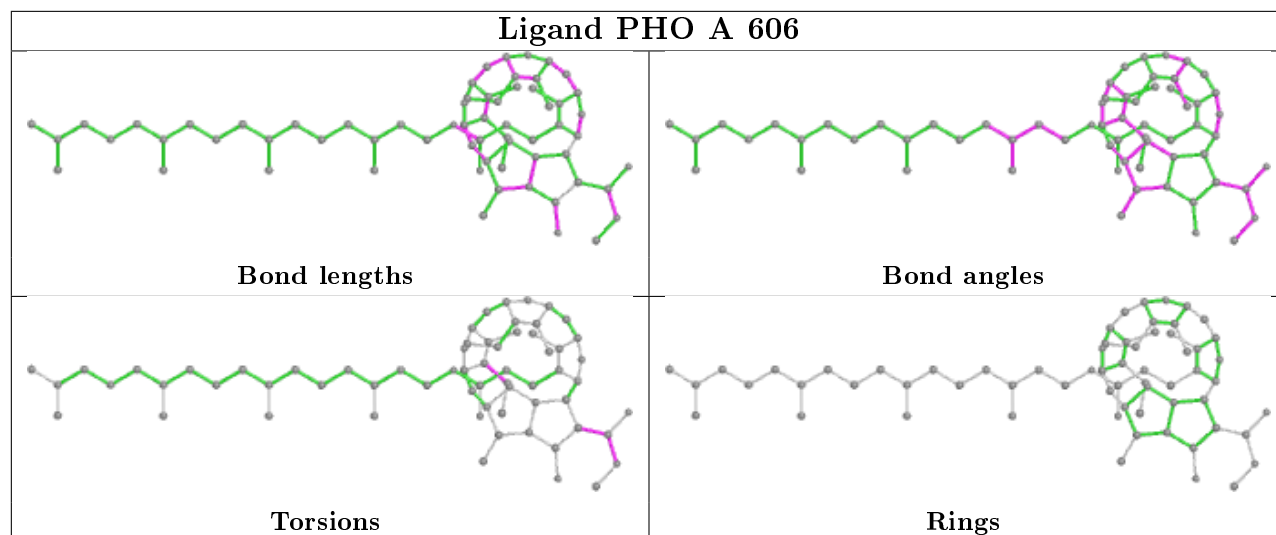


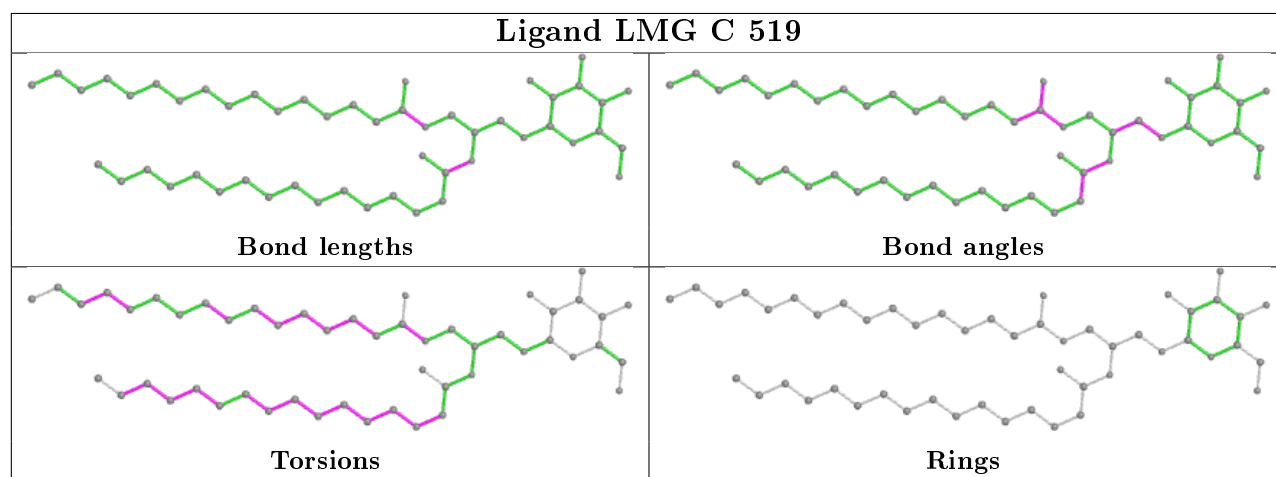
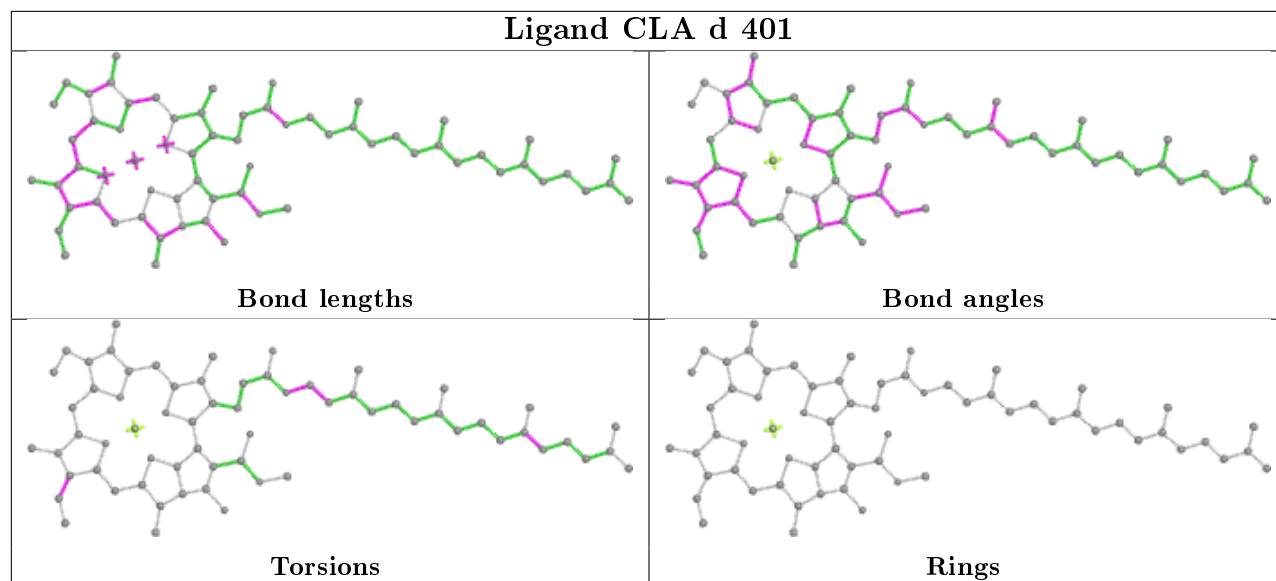
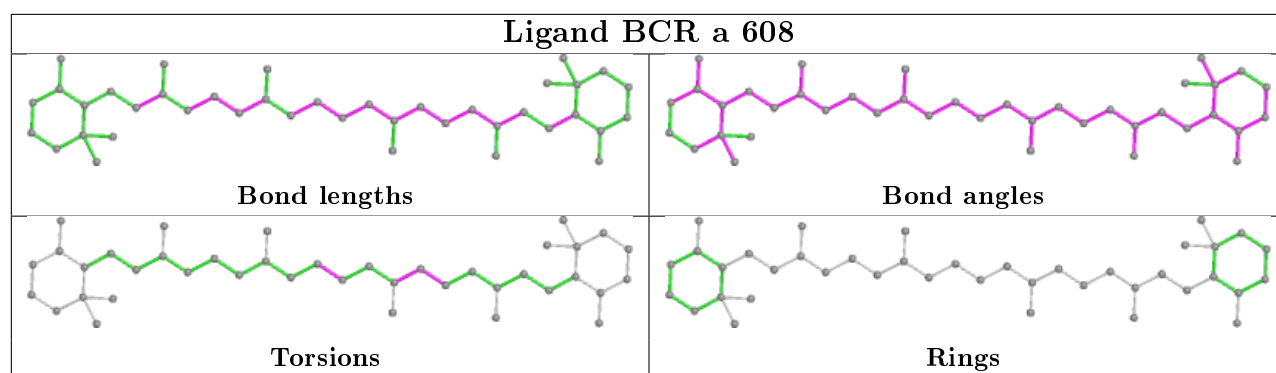
Ligand DGD C 517

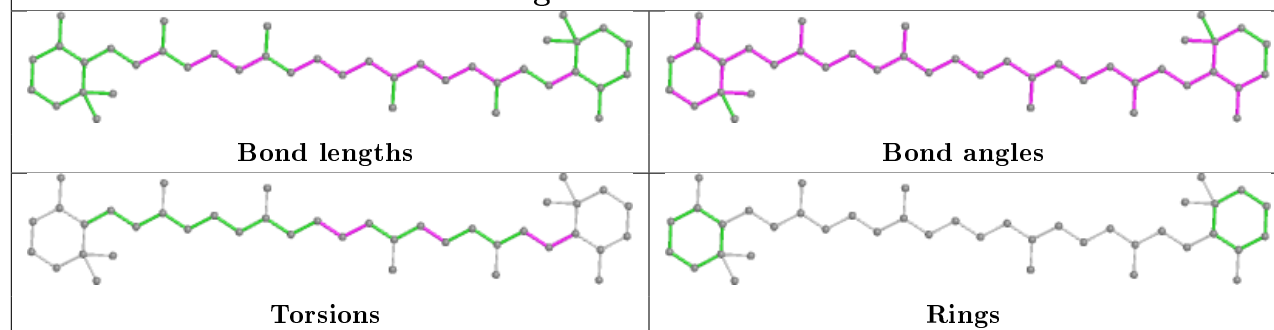
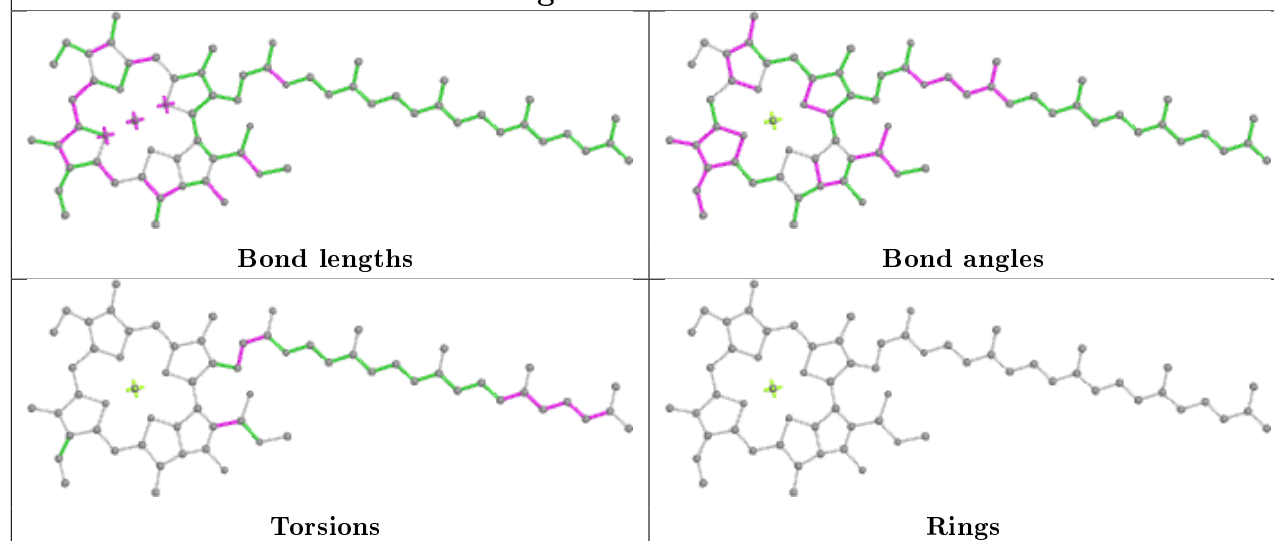
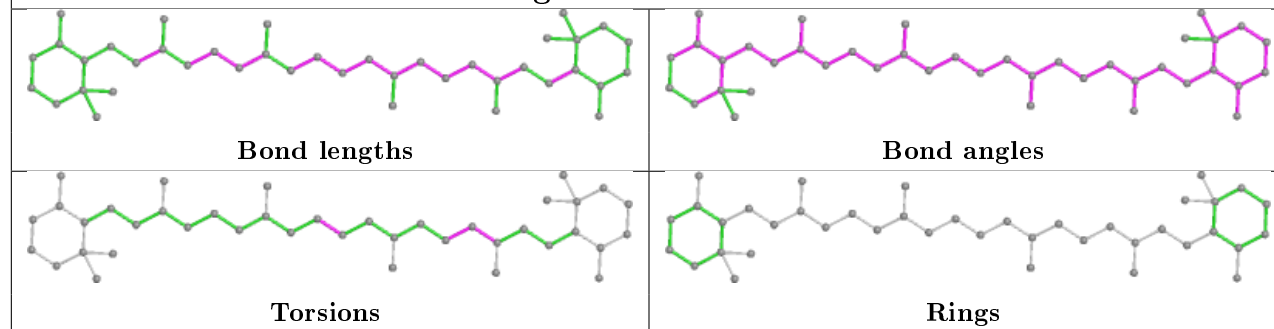


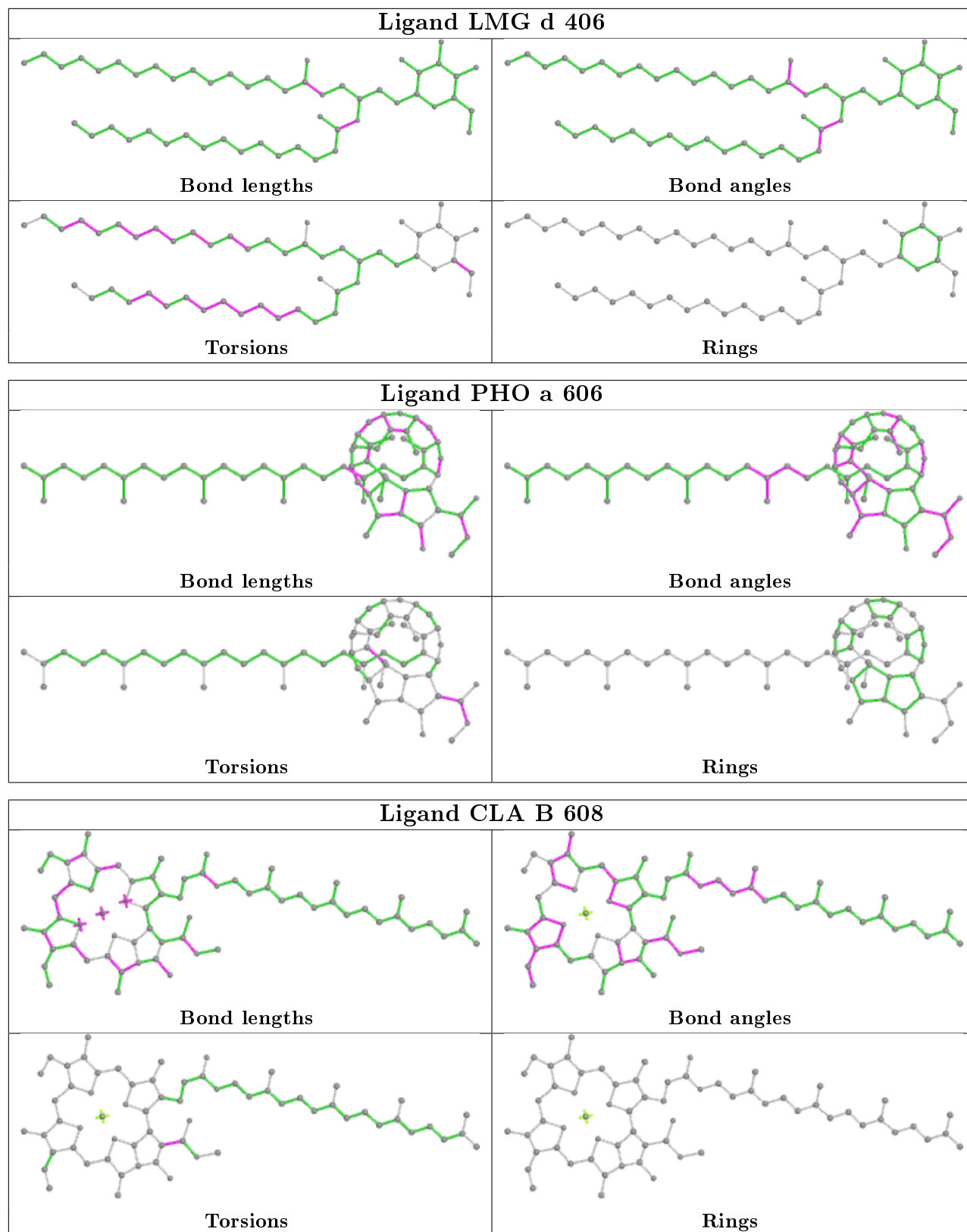
Ligand CLA B 607

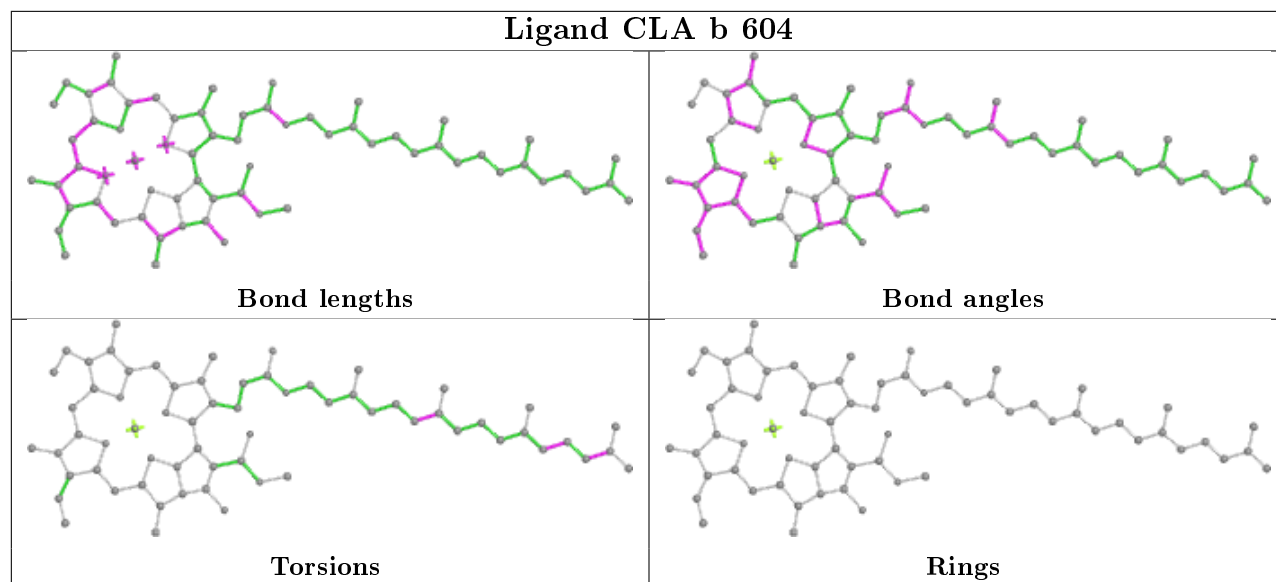
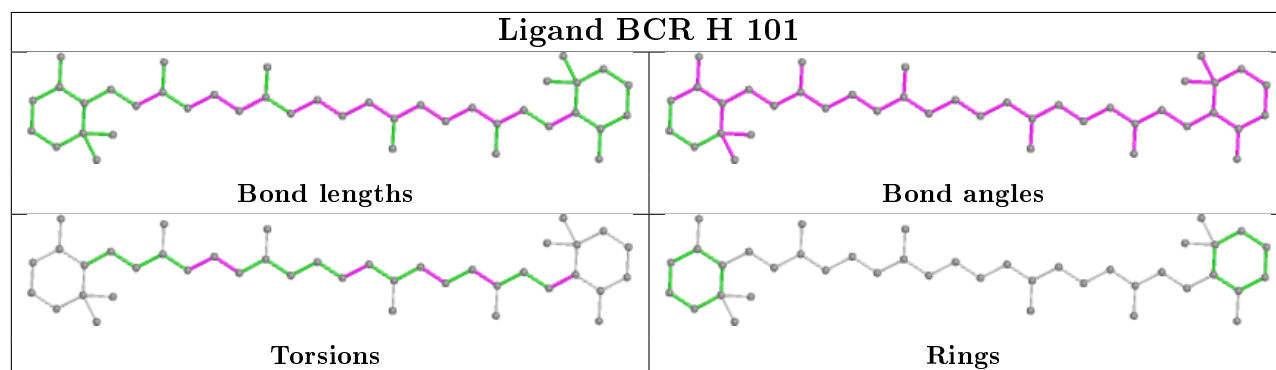
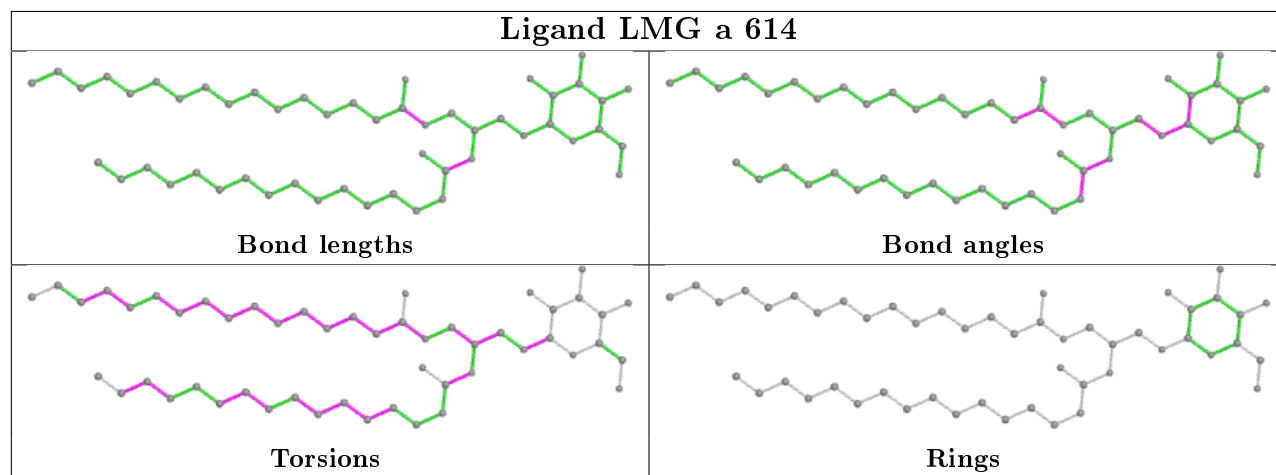


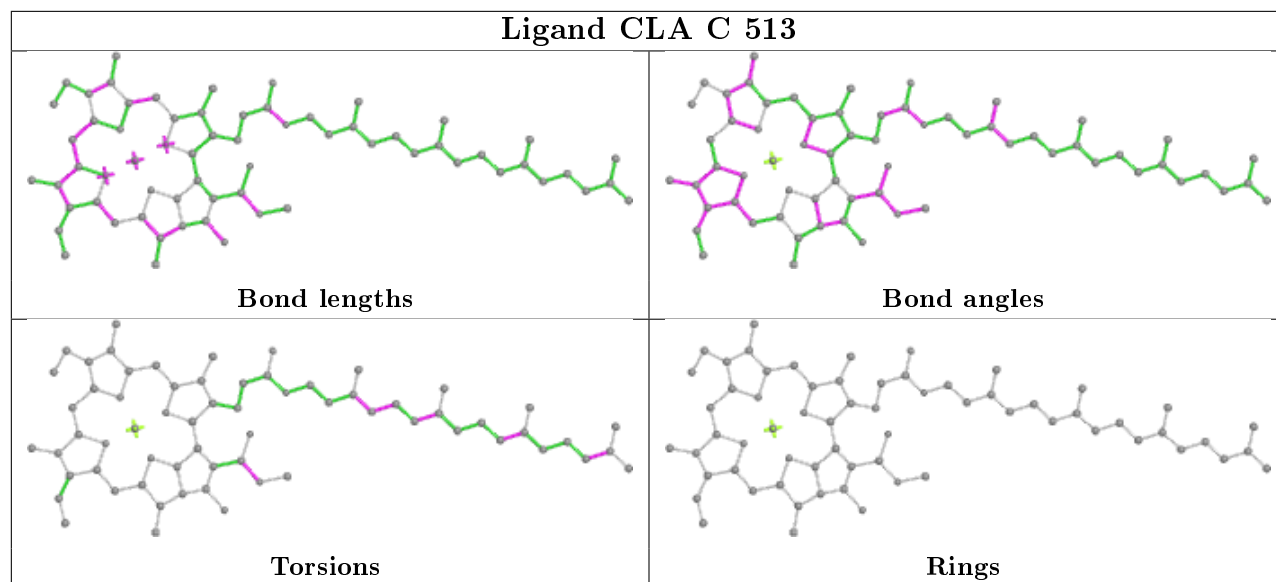
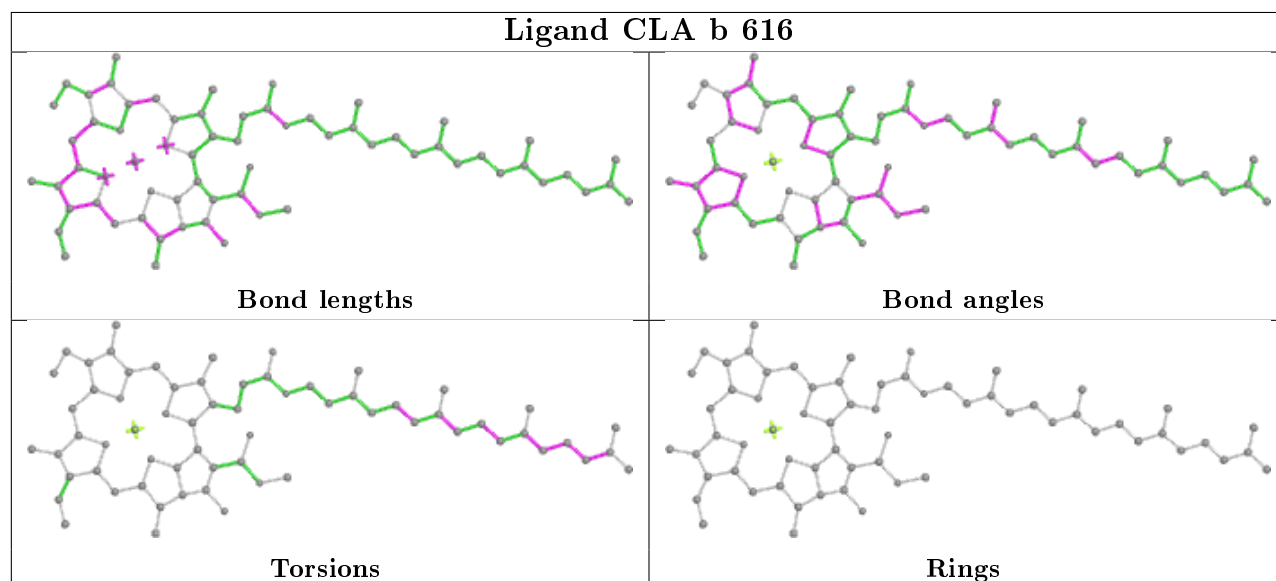
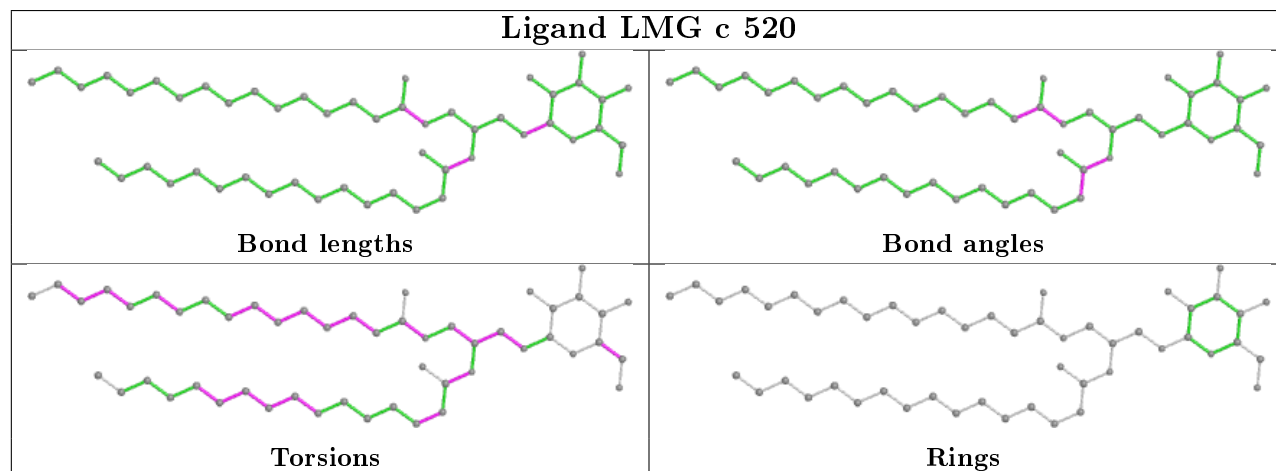




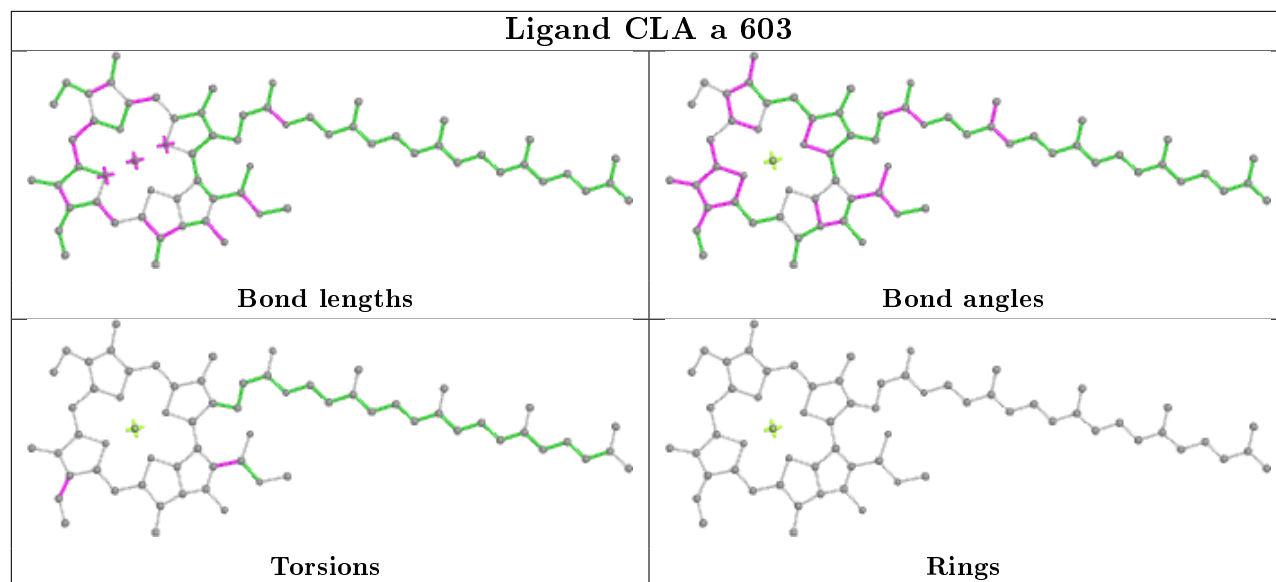
Ligand BCR d 404**Ligand CLA c 501****Ligand BCR b 618**



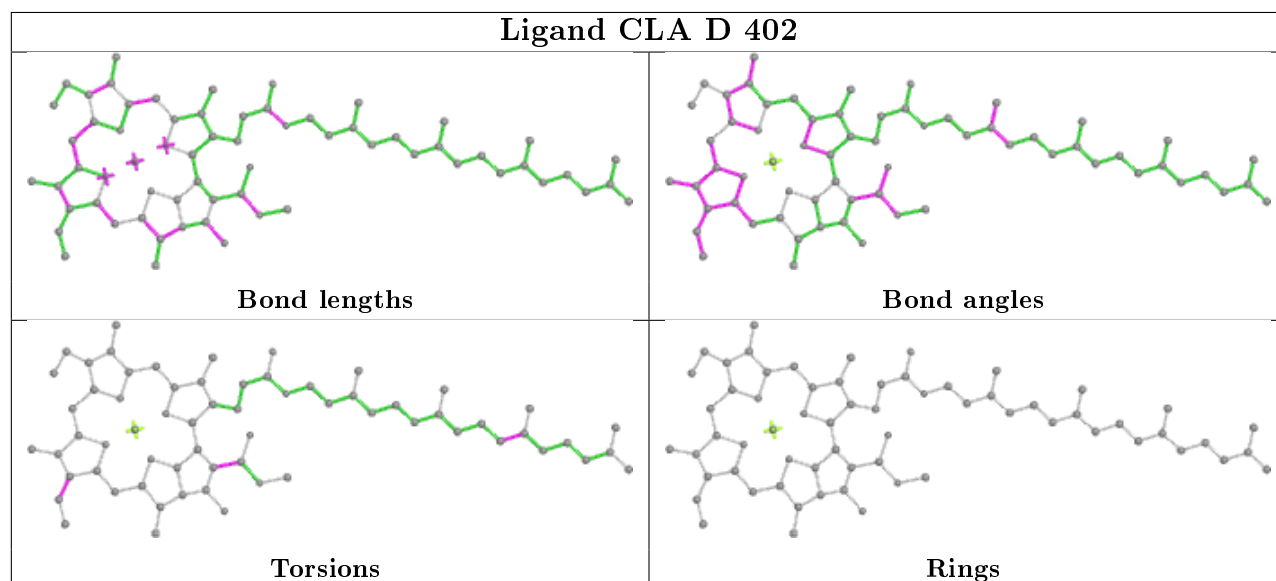
Ligand CLA b 604**Ligand BCR H 101****Ligand LMG a 614**

Ligand CLA C 513**Ligand CLA b 616****Ligand LMG c 520**

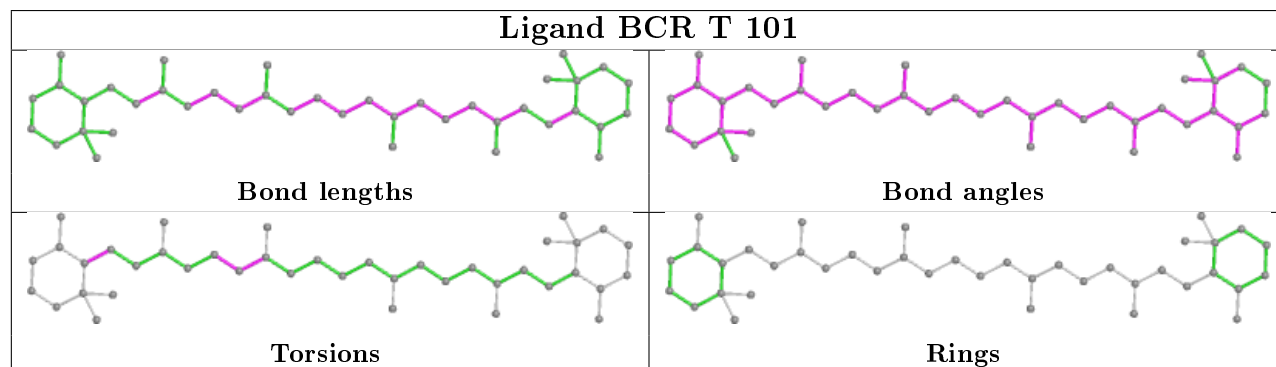
Ligand CLA a 603

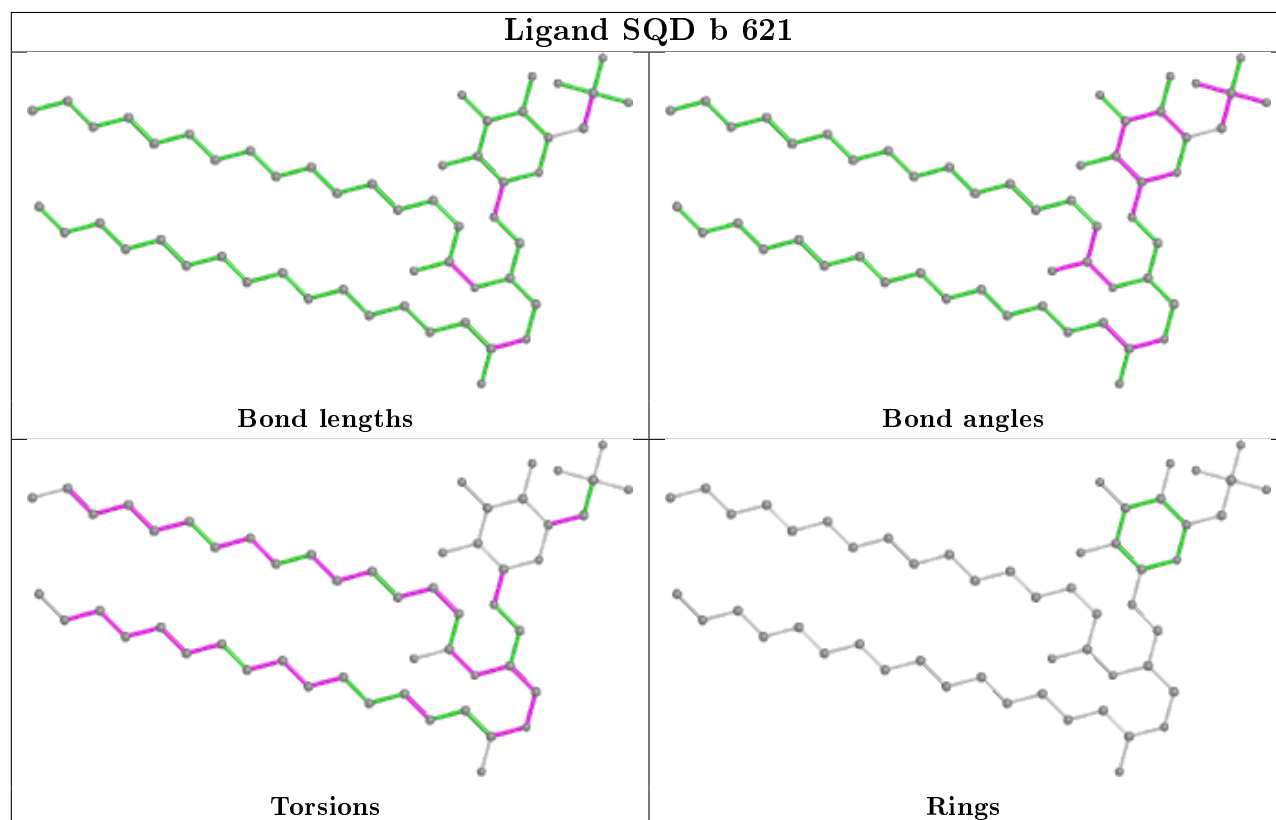
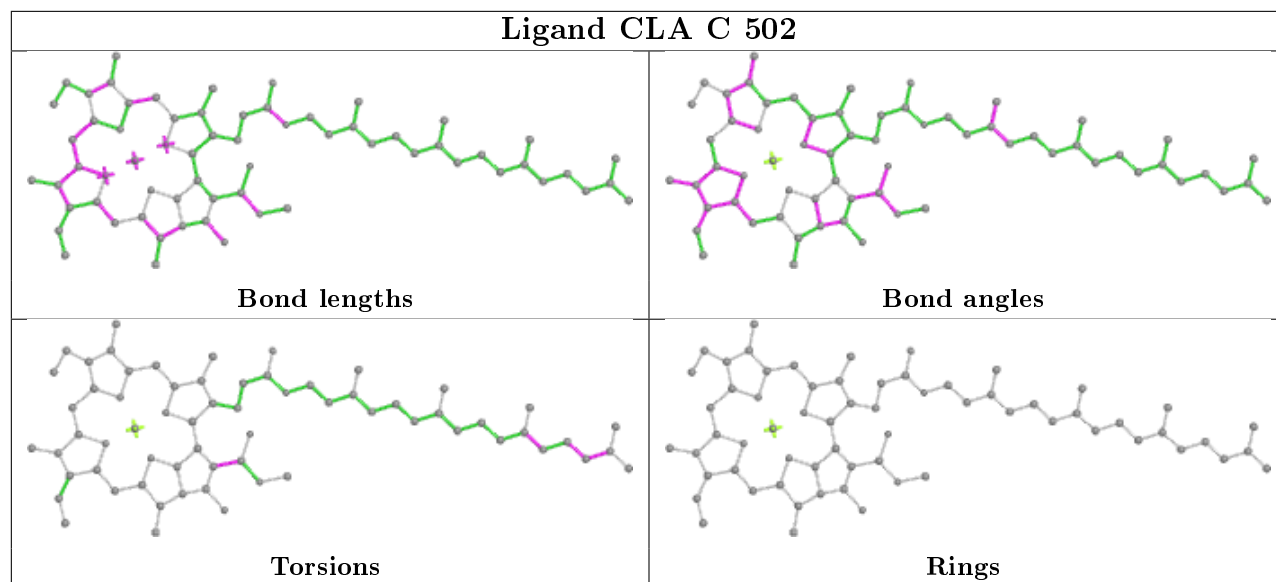


Ligand CLA D 402

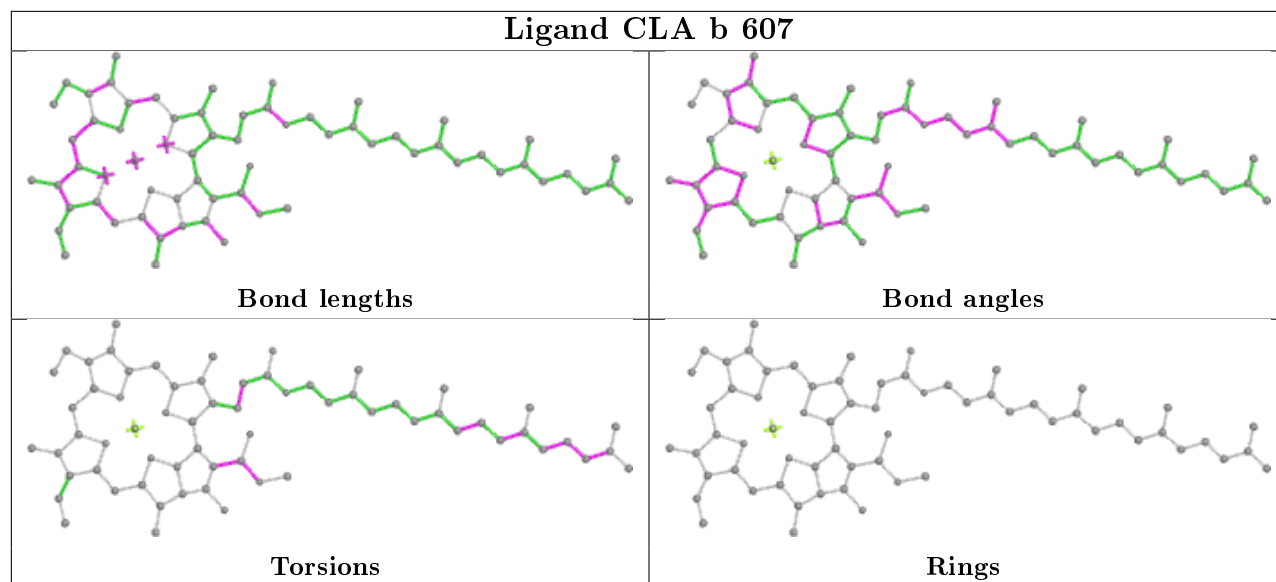


Ligand BCR T 101

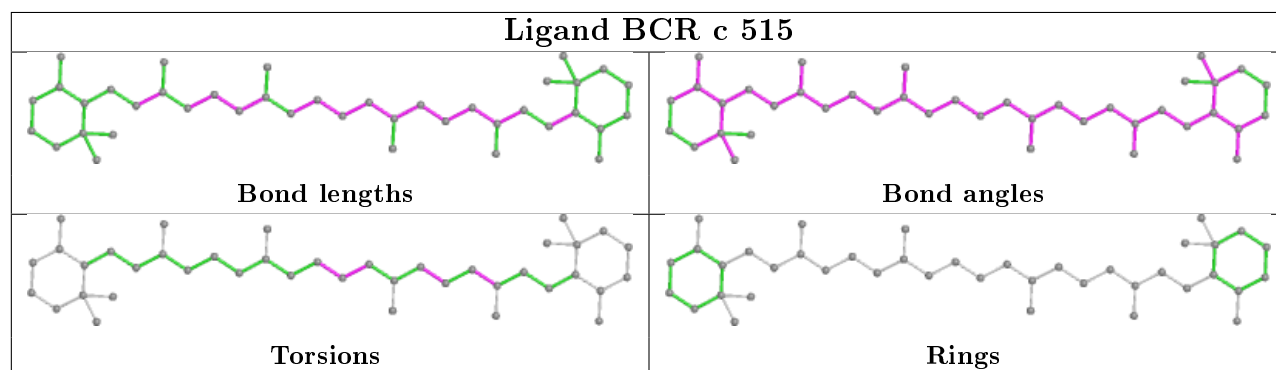


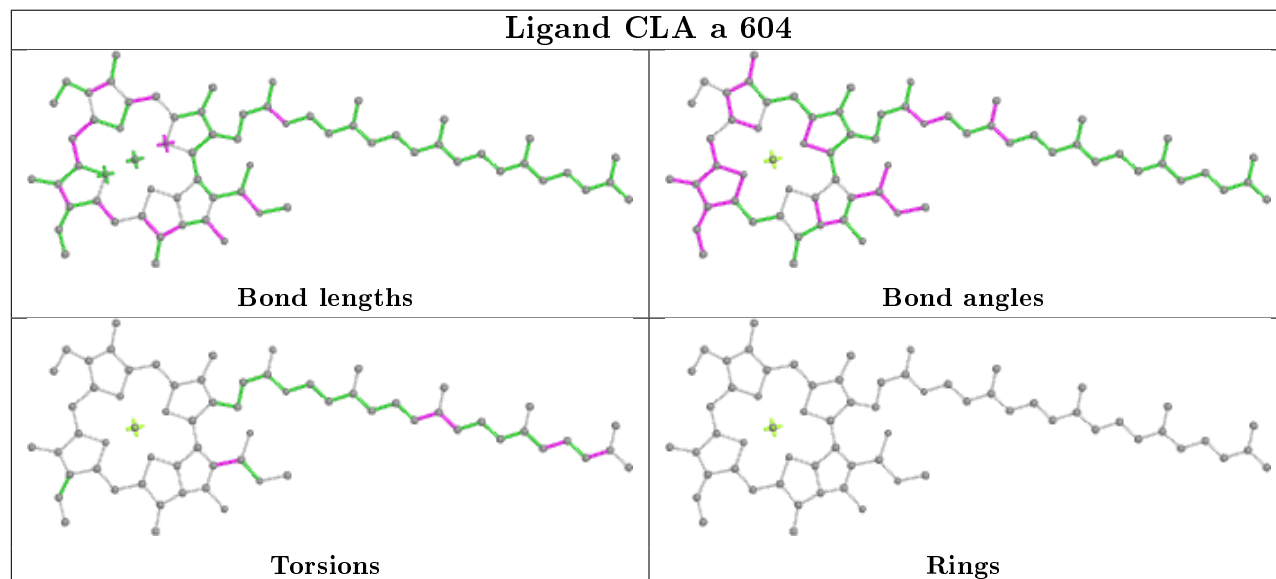
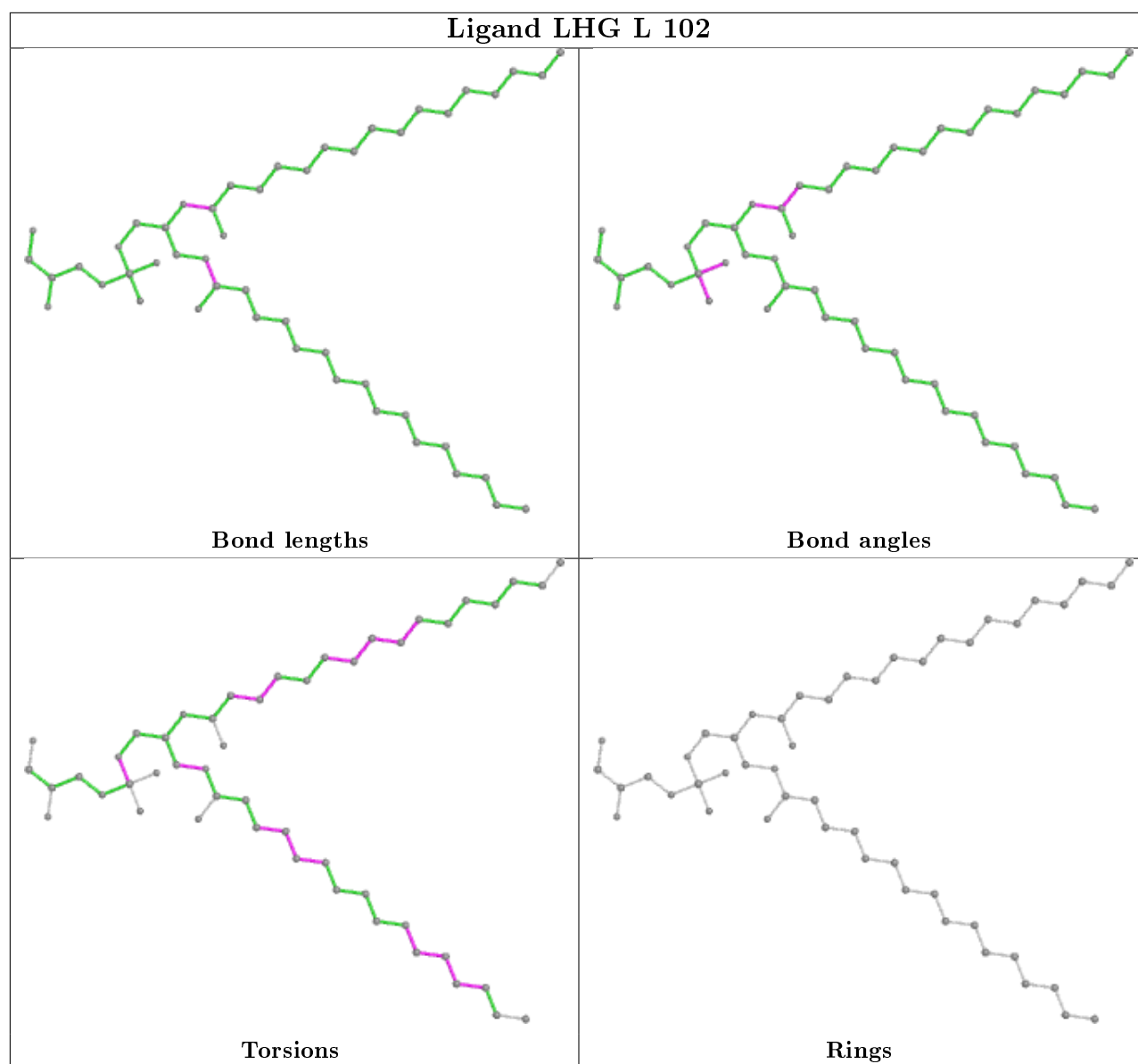


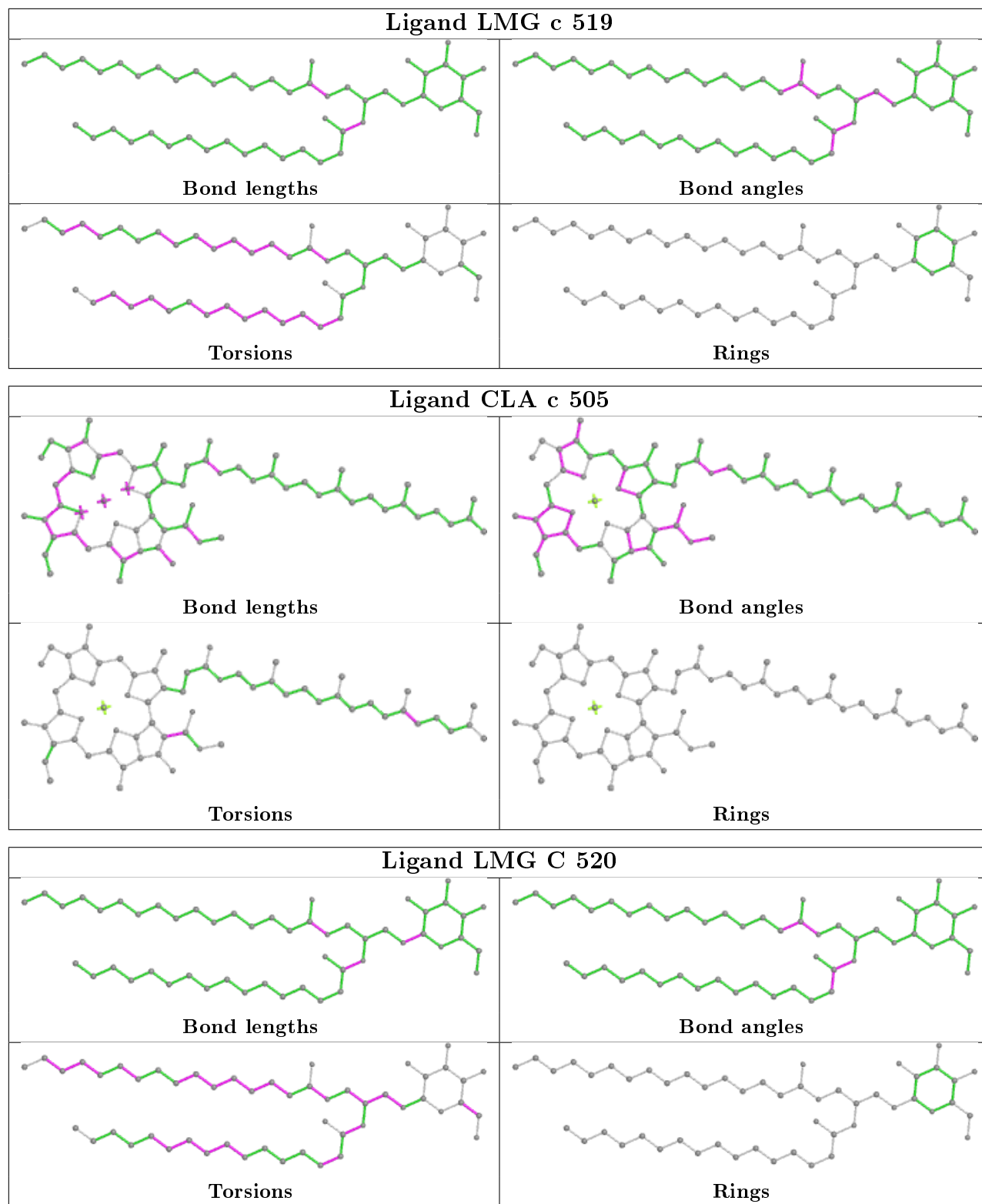
Ligand CLA b 607



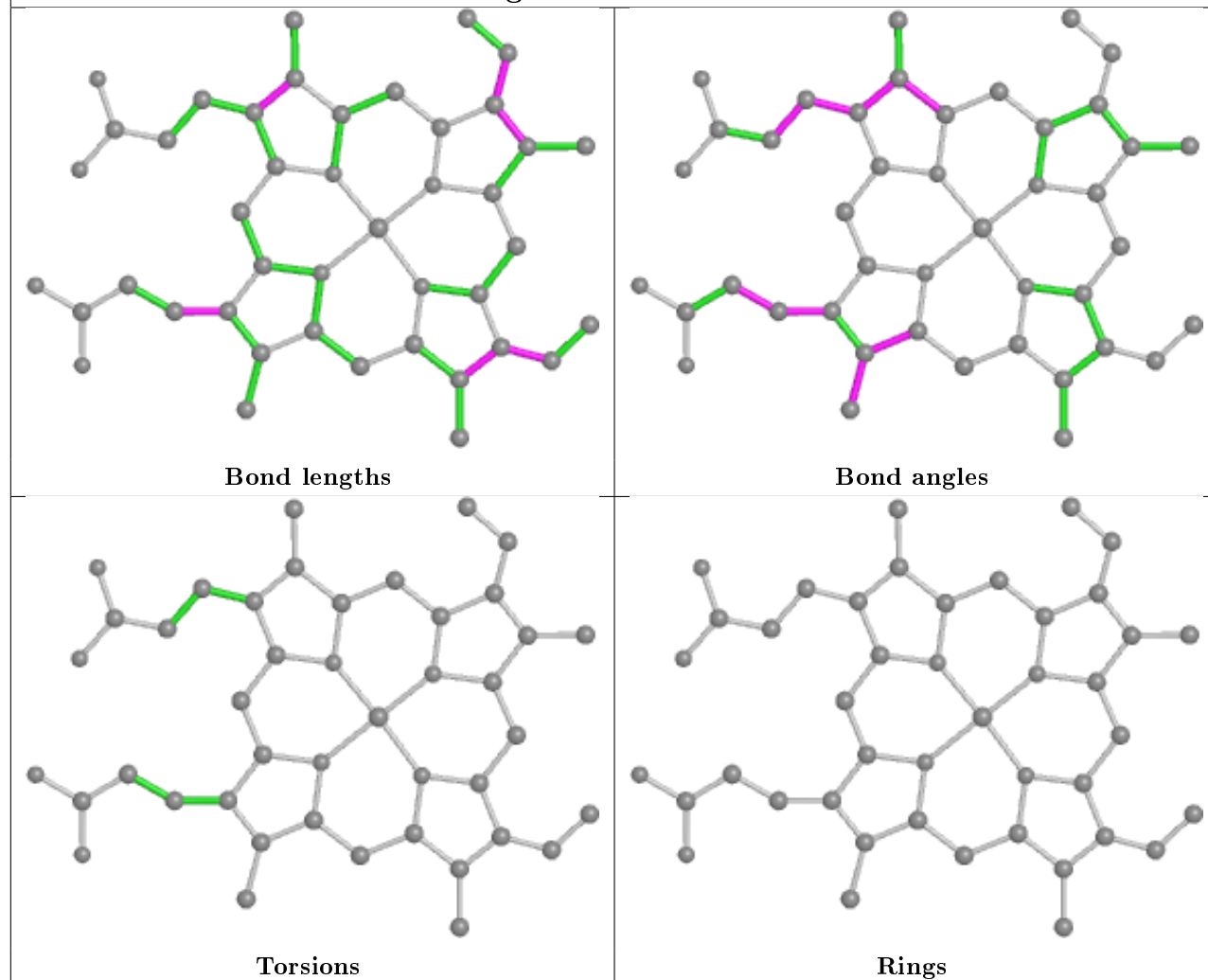
Ligand BCR c 515



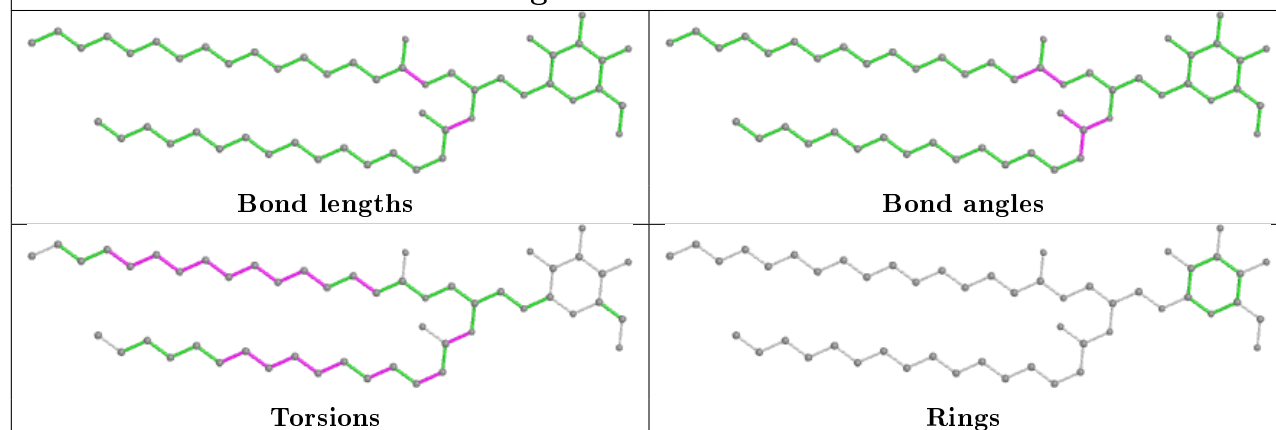


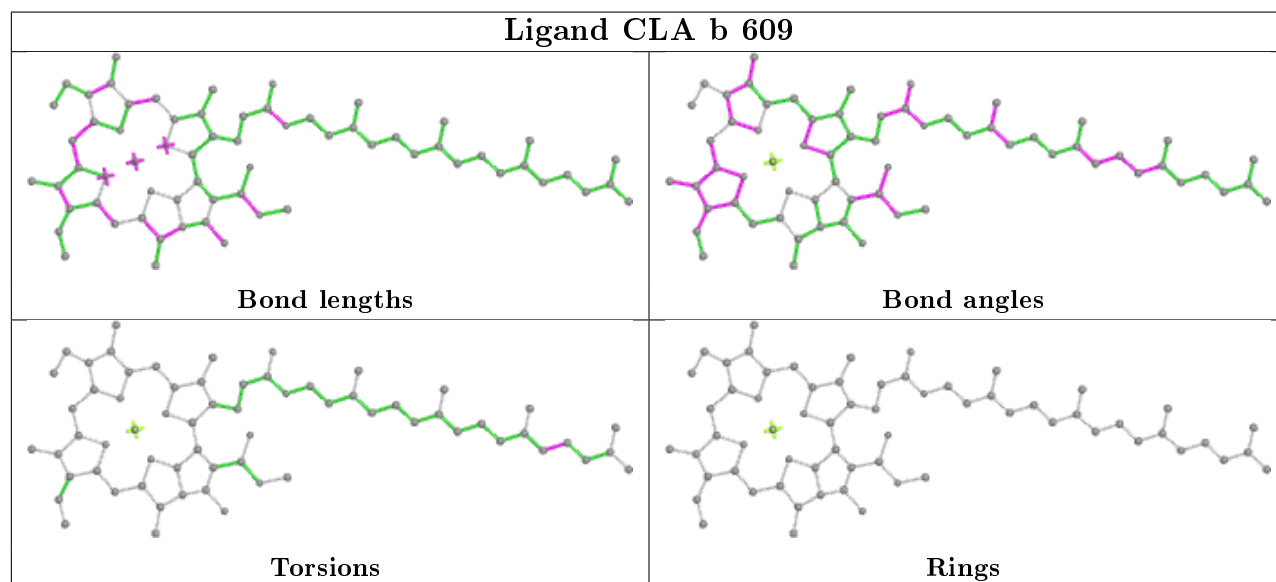
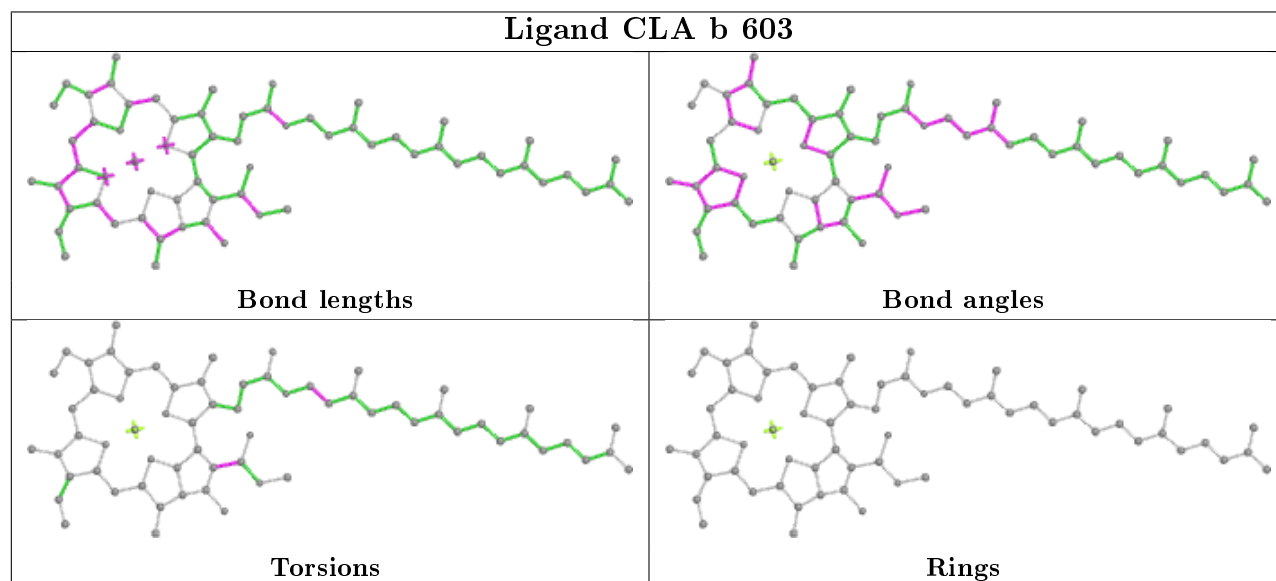
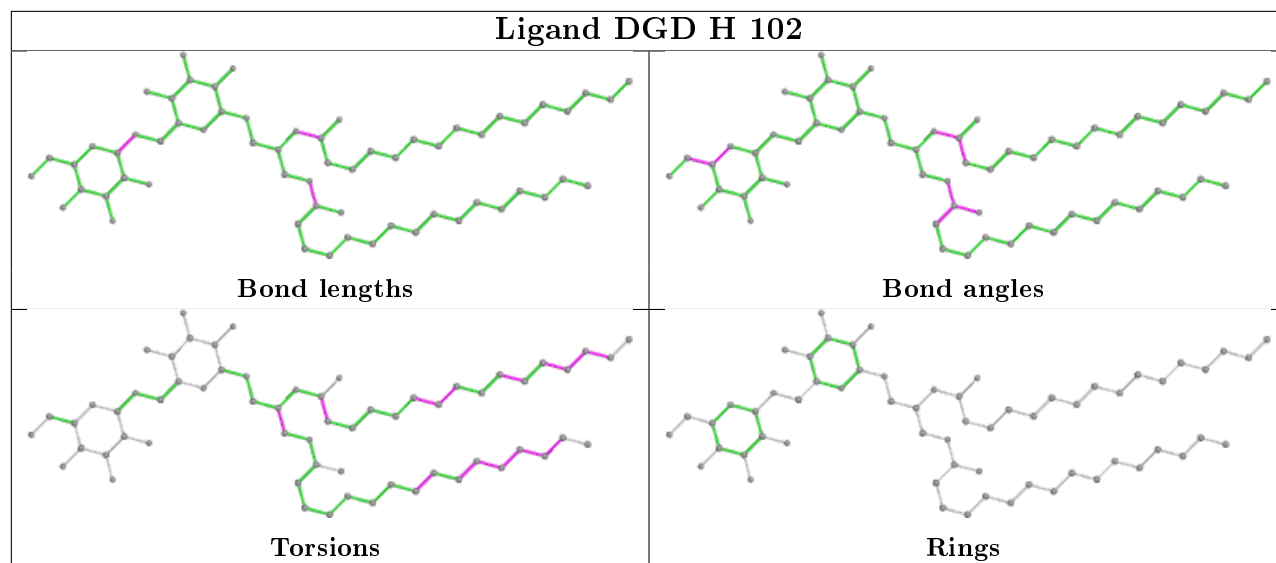


Ligand HEM f 101

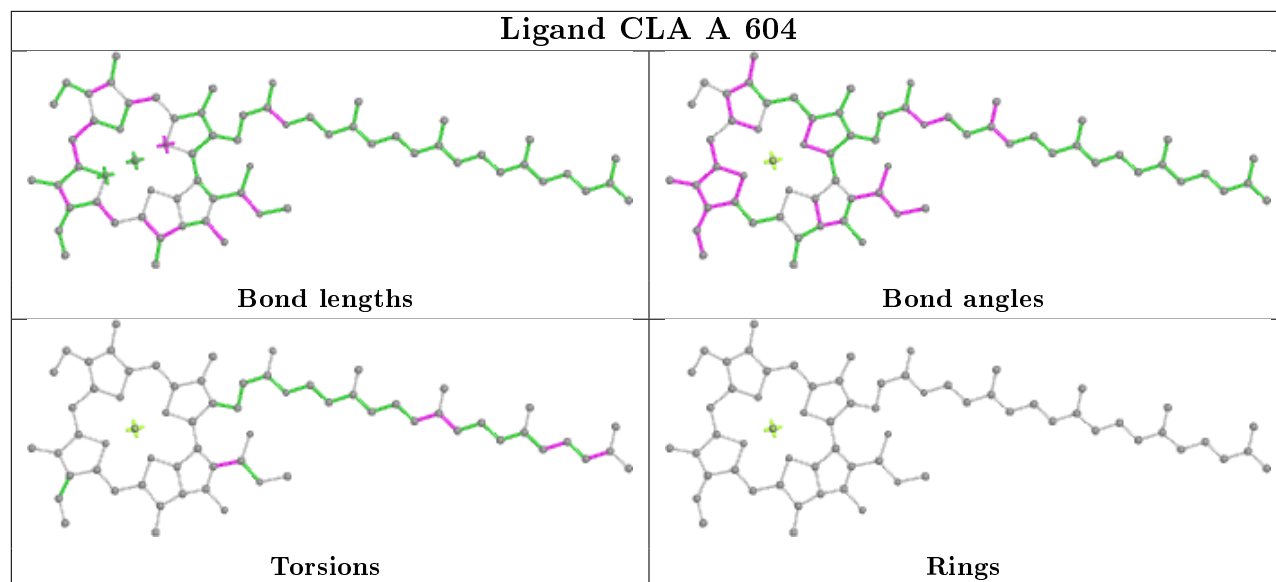


Ligand LMG b 619

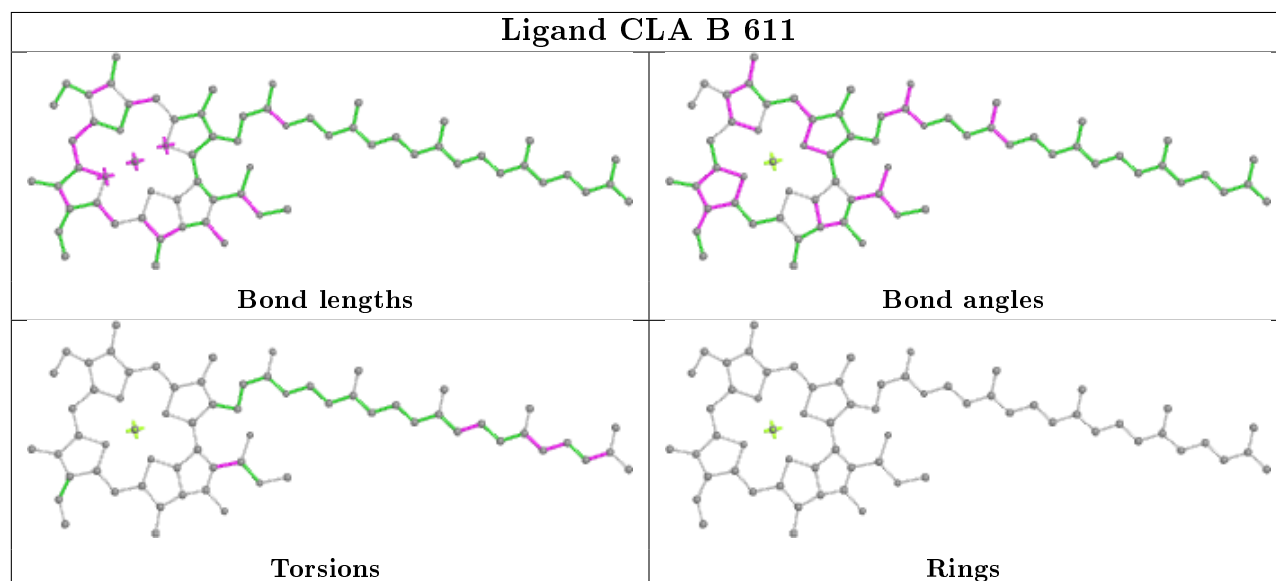




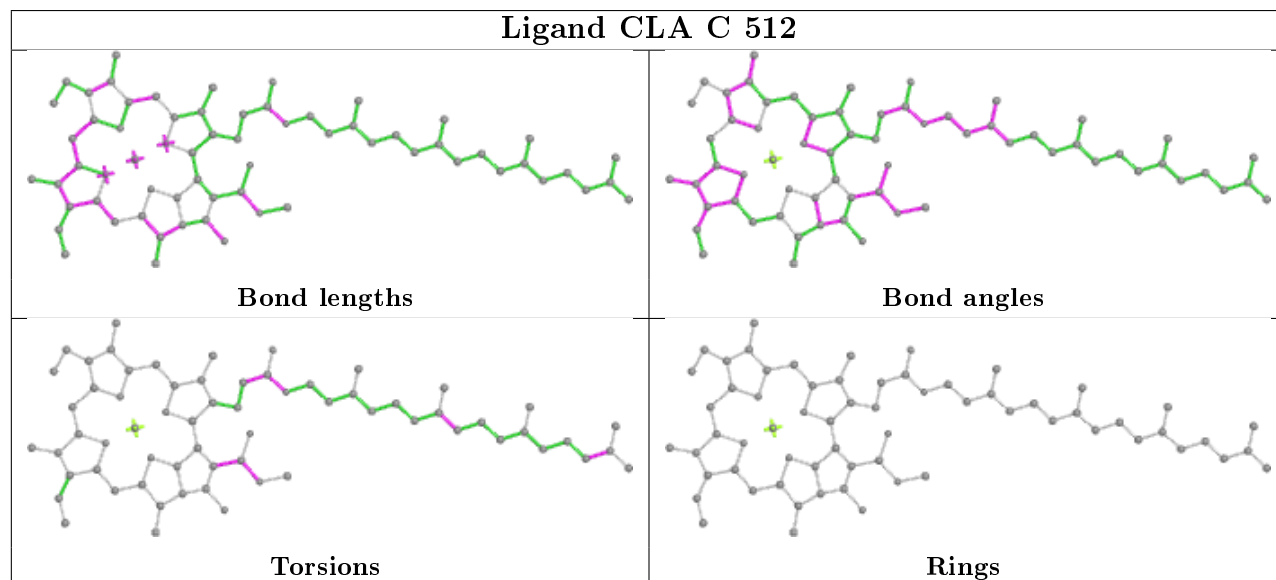
Ligand CLA A 604



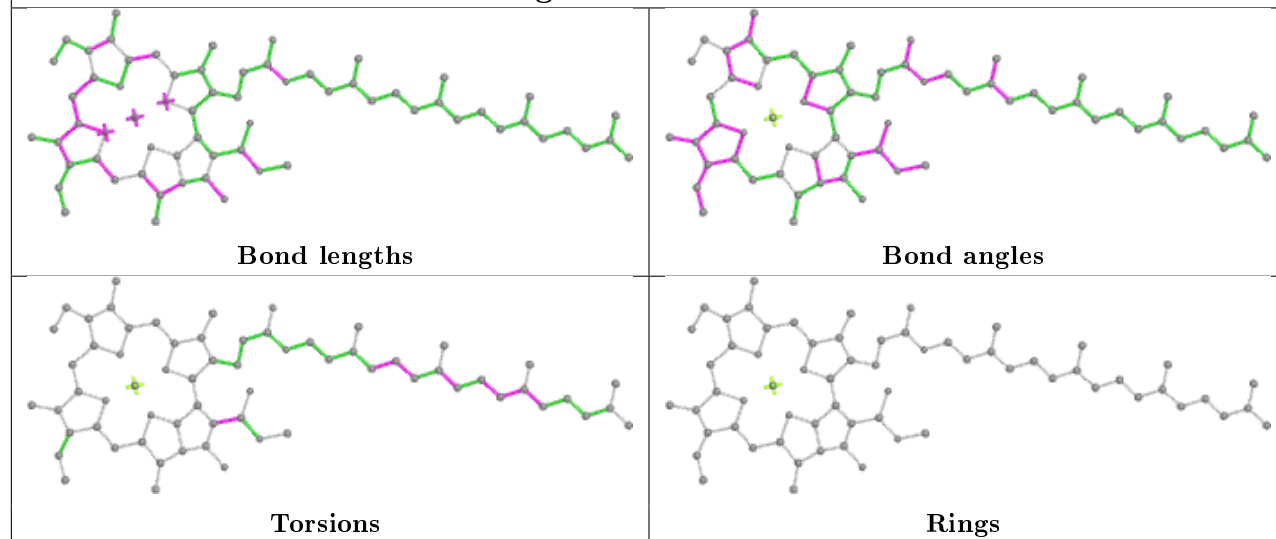
Ligand CLA B 611



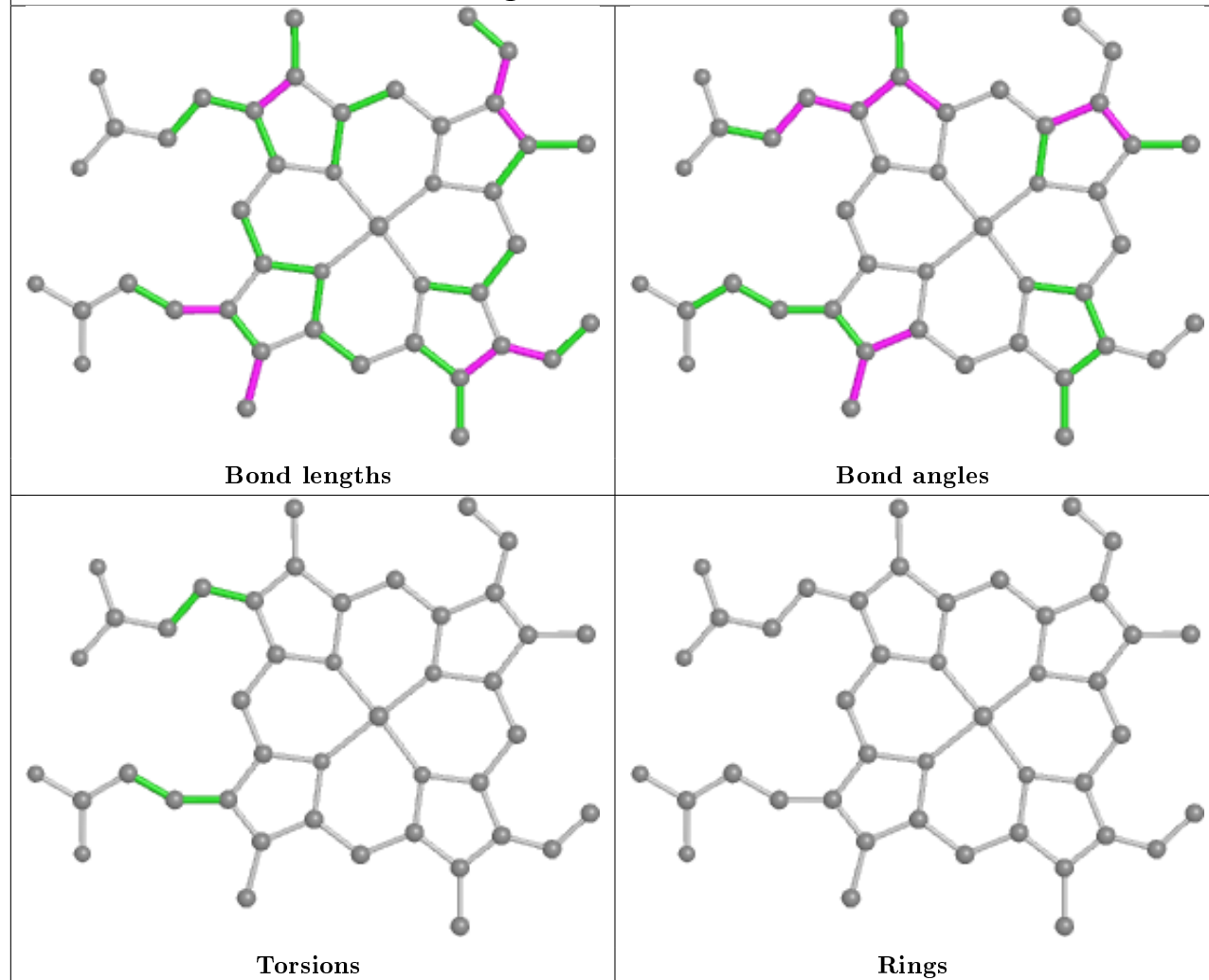
Ligand CLA C 512



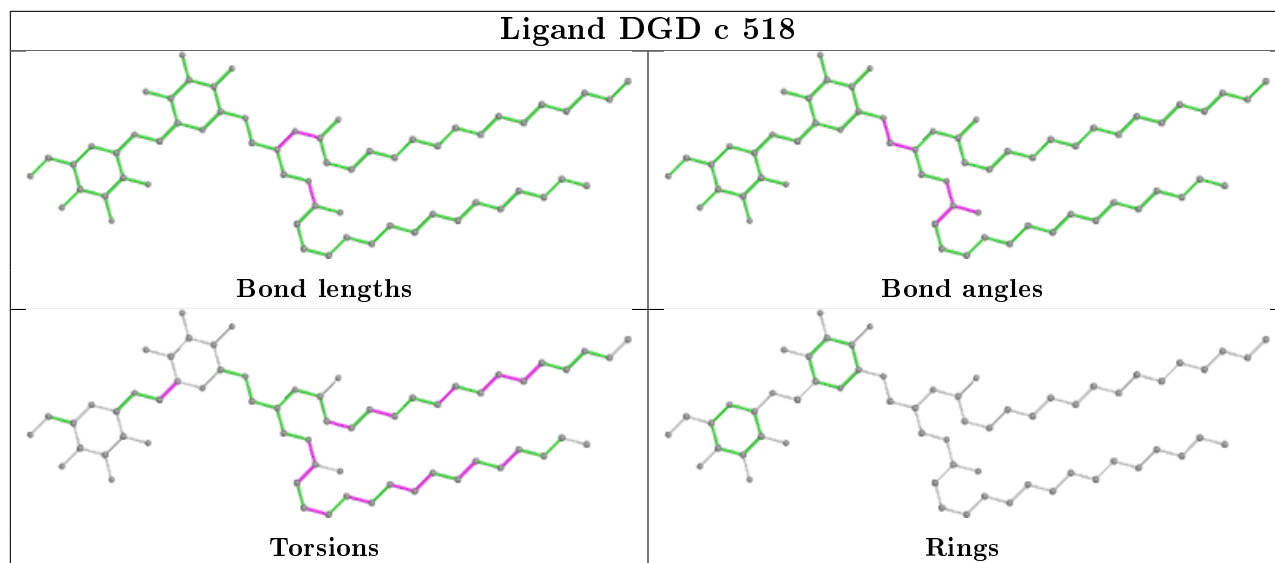
Ligand CLA b 615



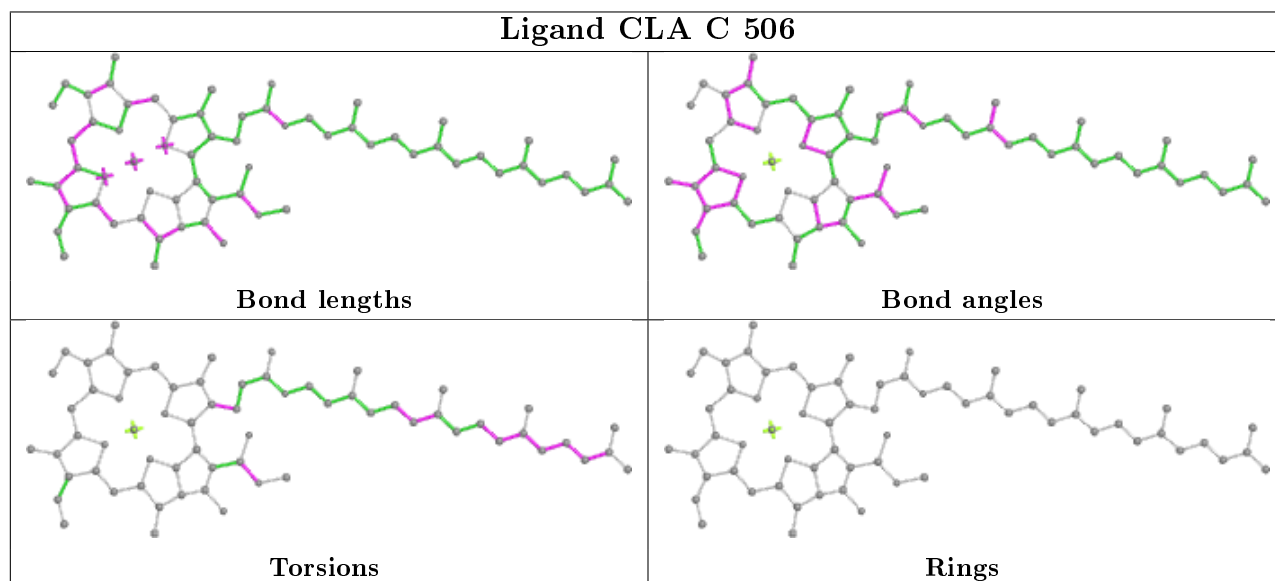
Ligand HEM v 201



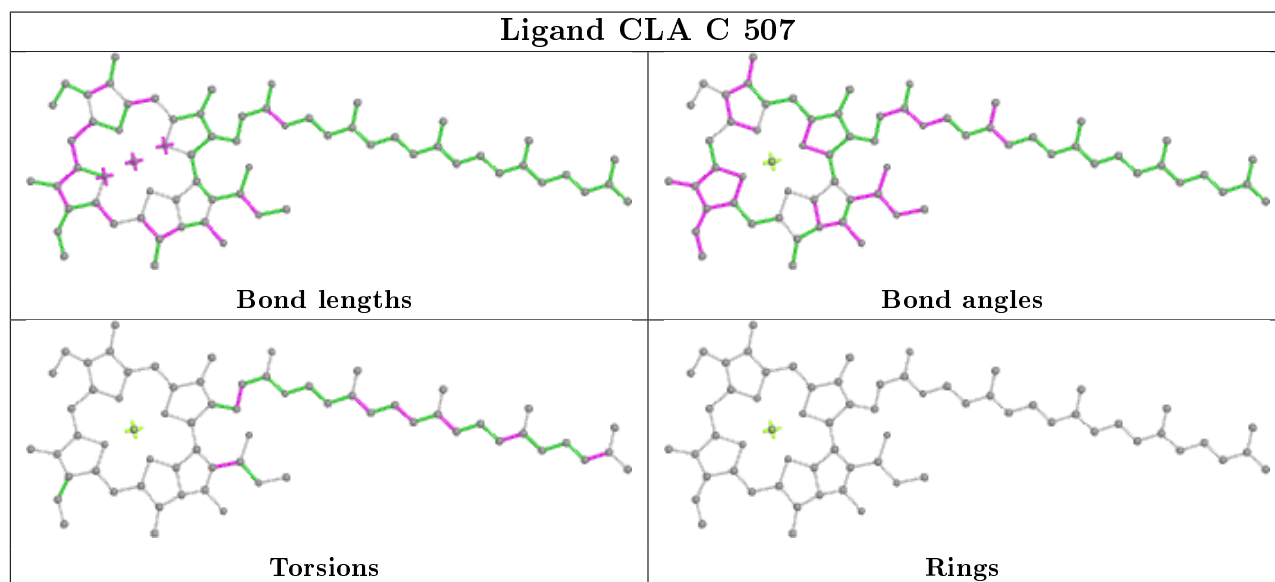
Ligand DGD c 518



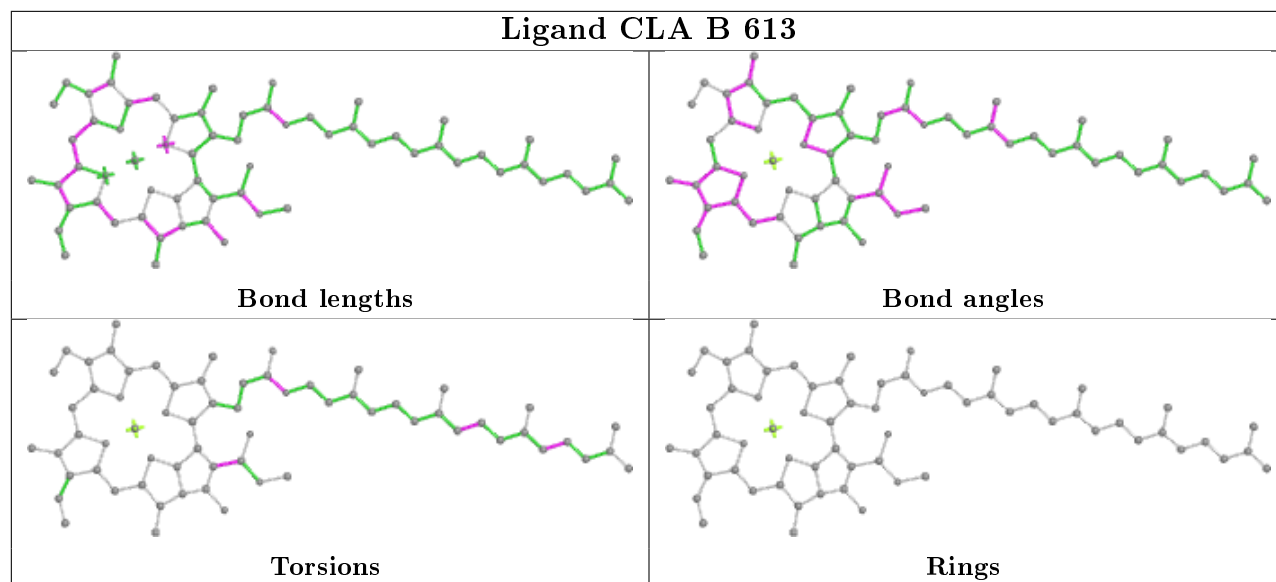
Ligand CLA C 506



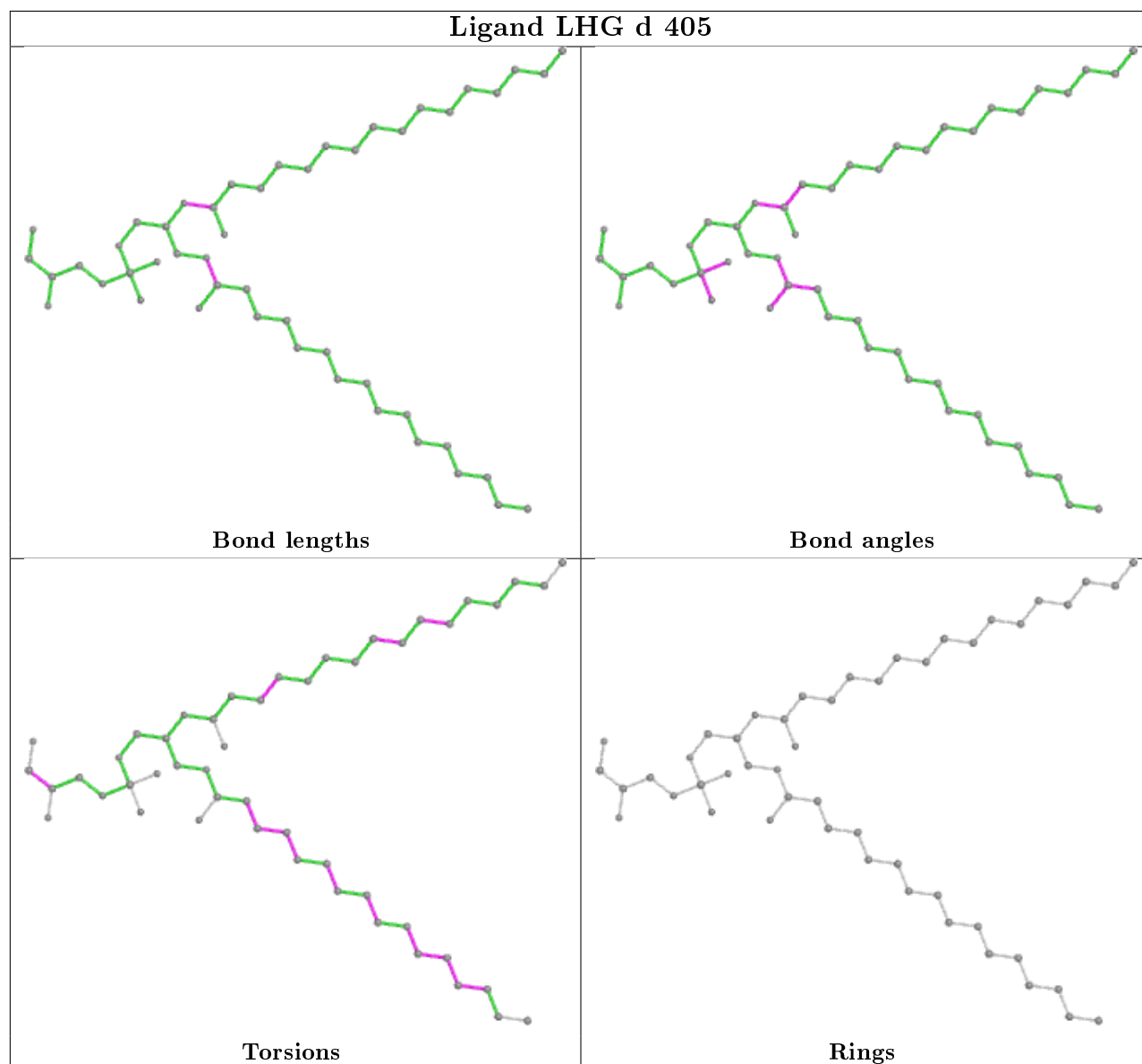
Ligand CLA C 507

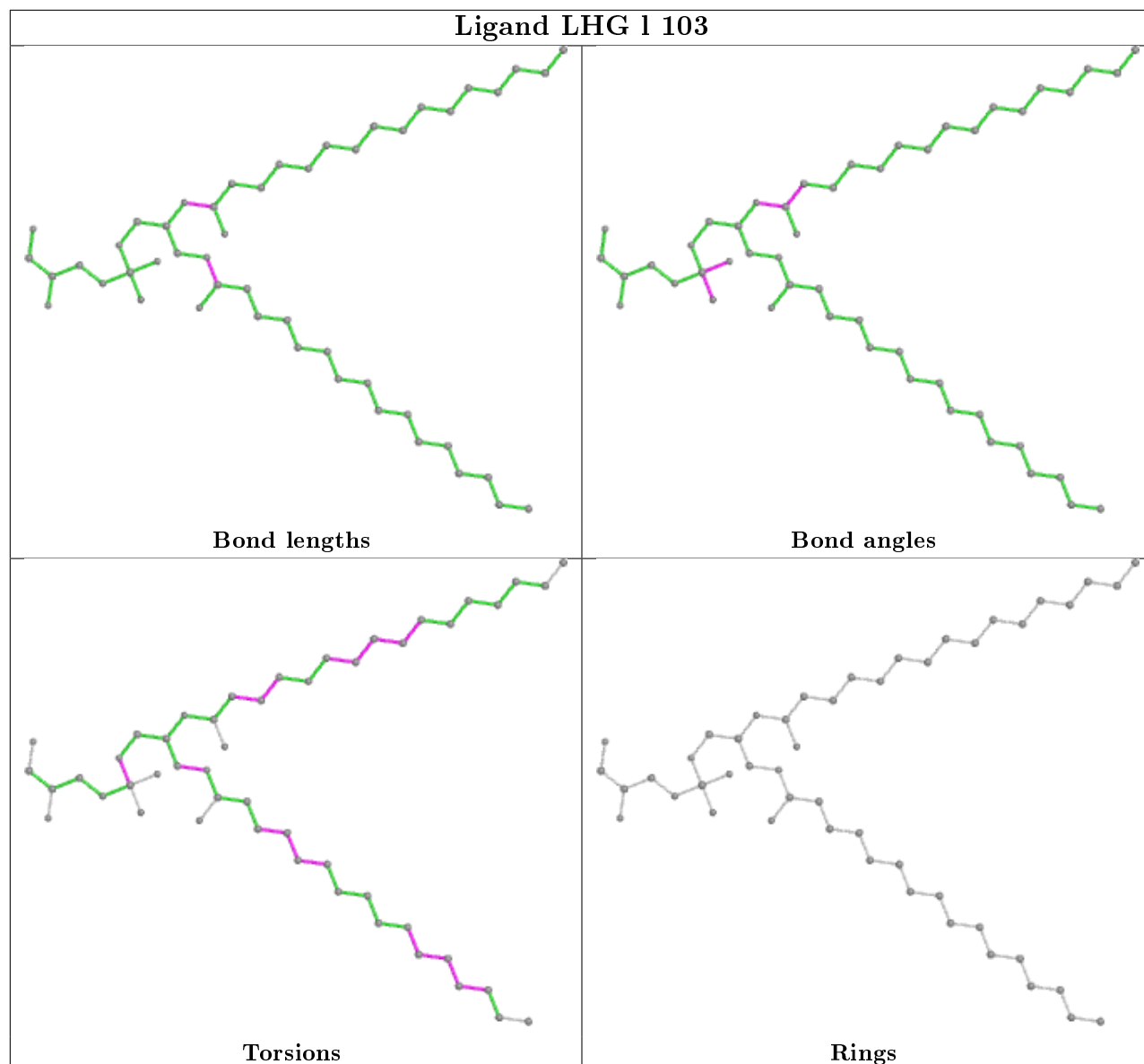
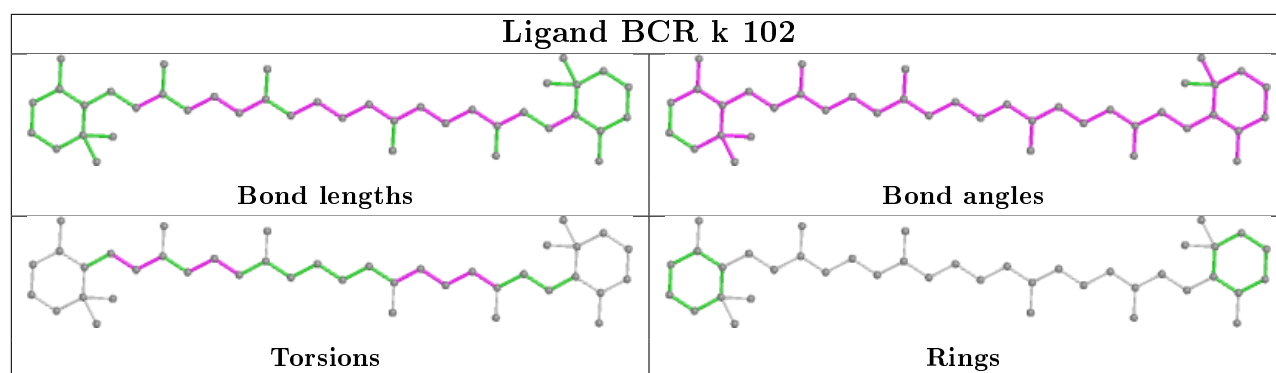


Ligand CLA B 613

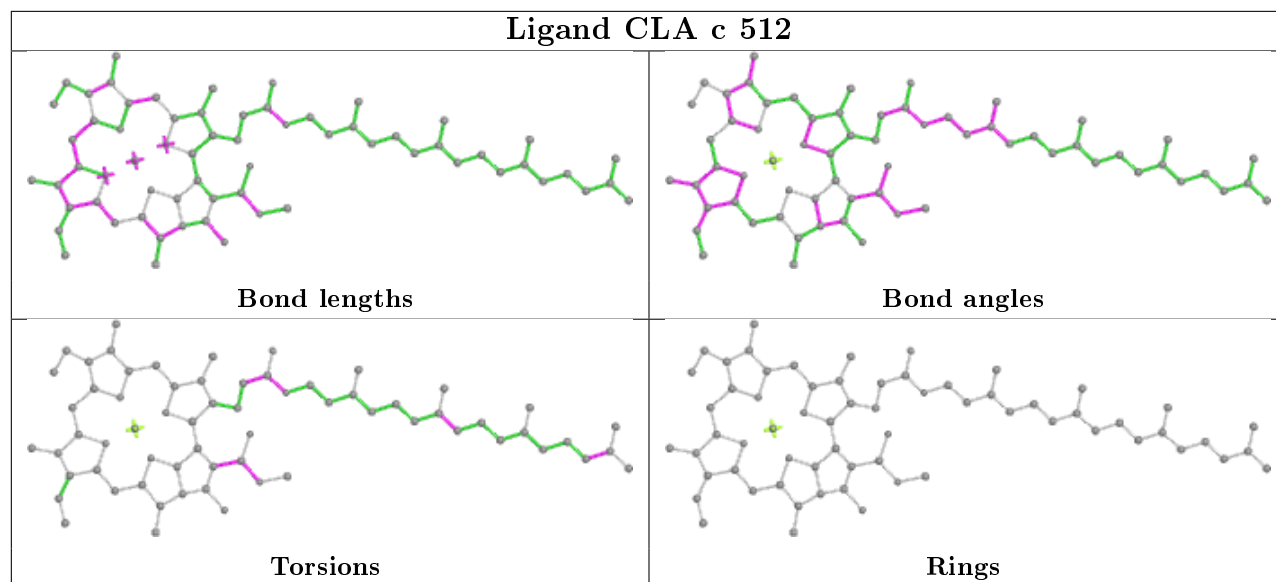


Ligand LHG d 405

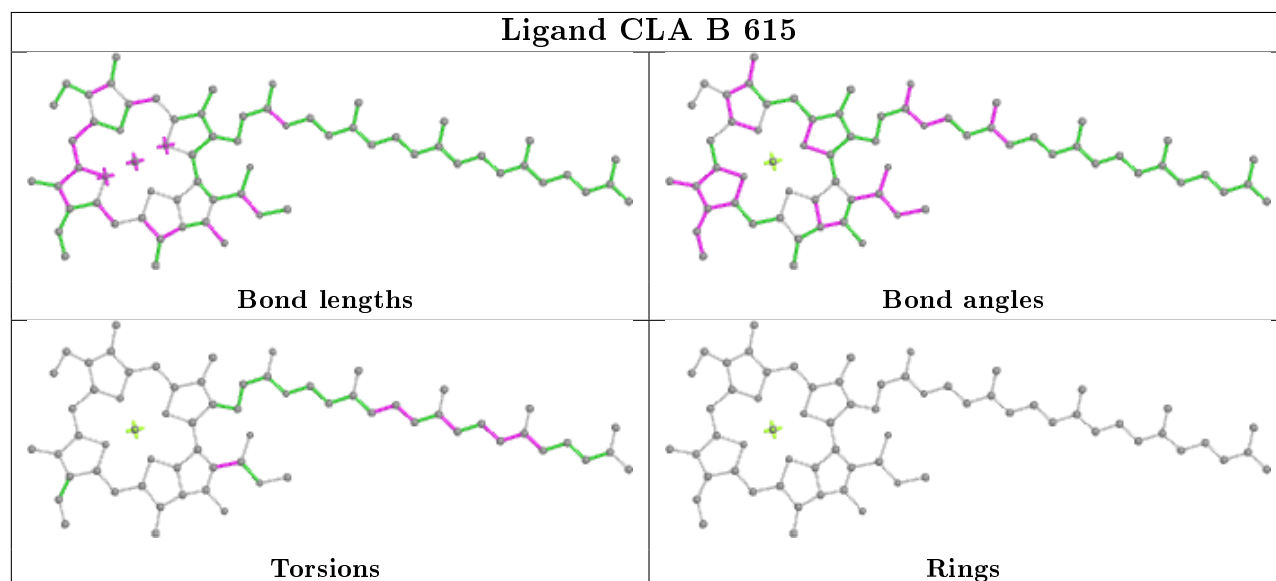




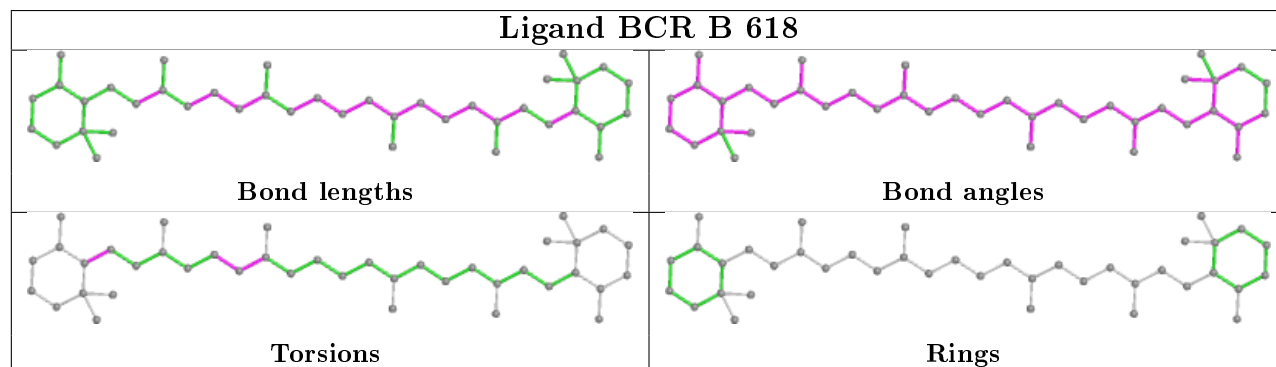
Ligand CLA c 512



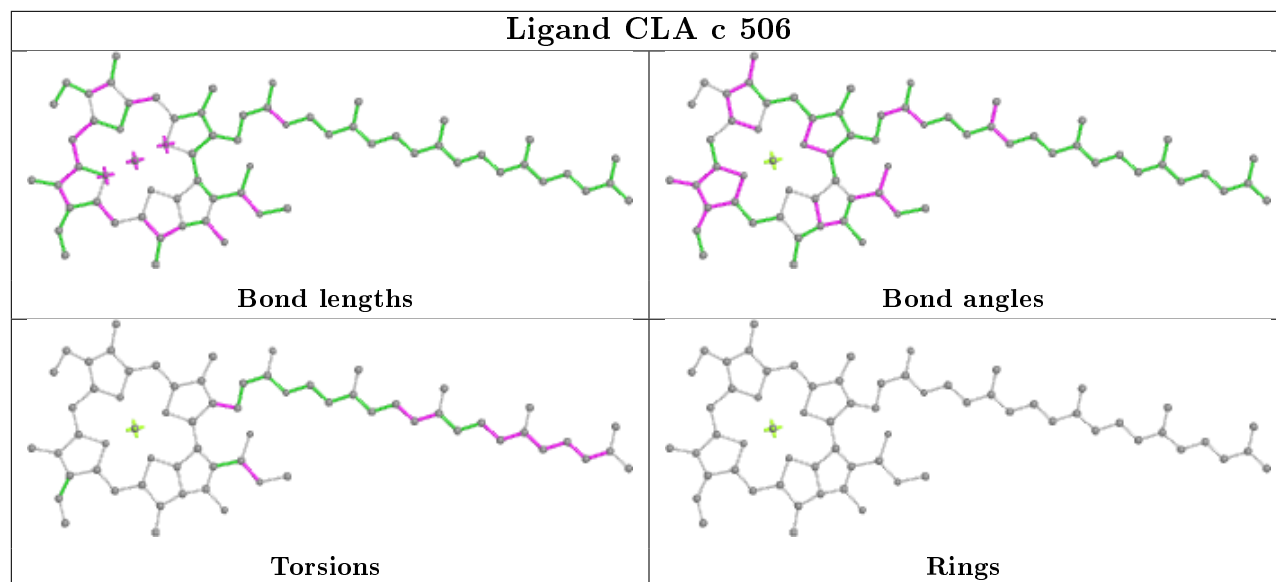
Ligand CLA B 615



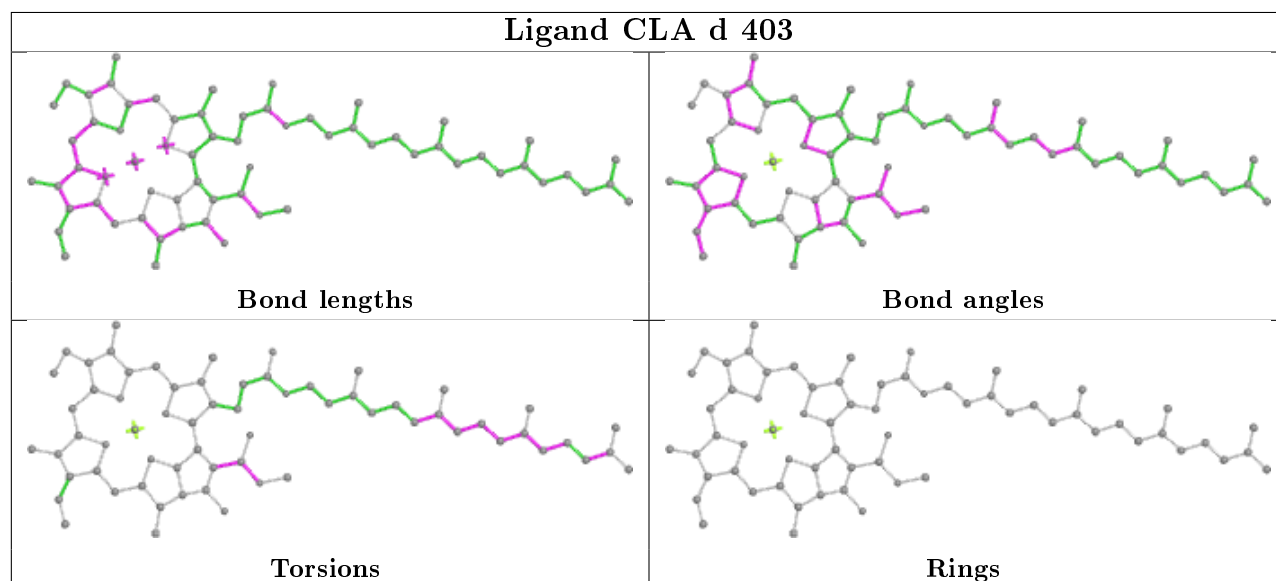
Ligand BCR B 618

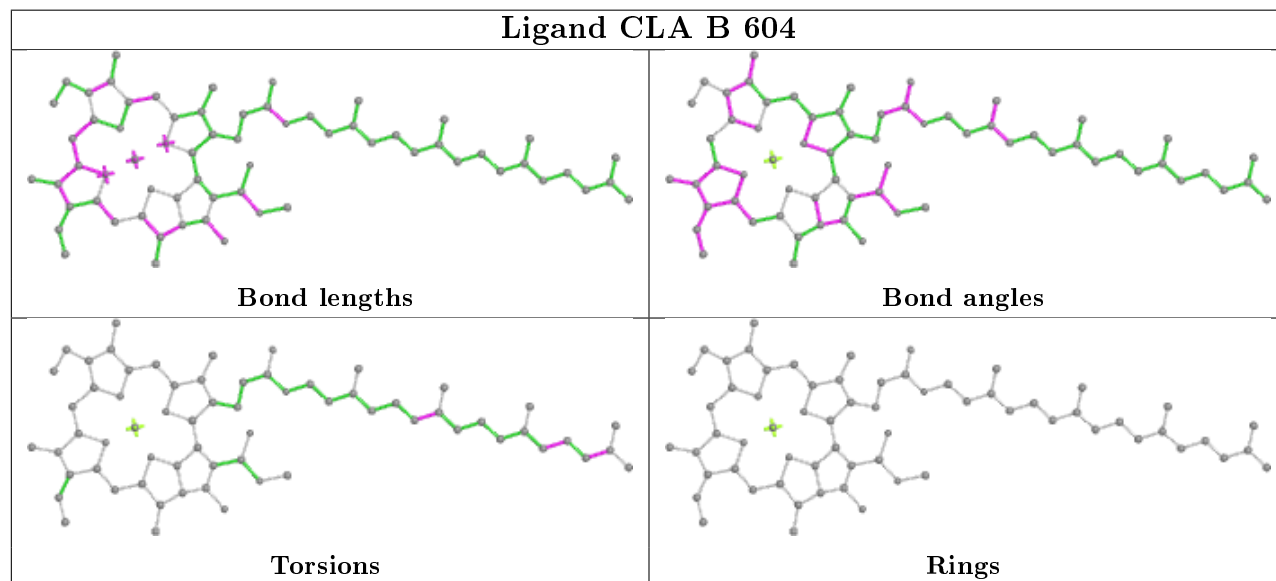
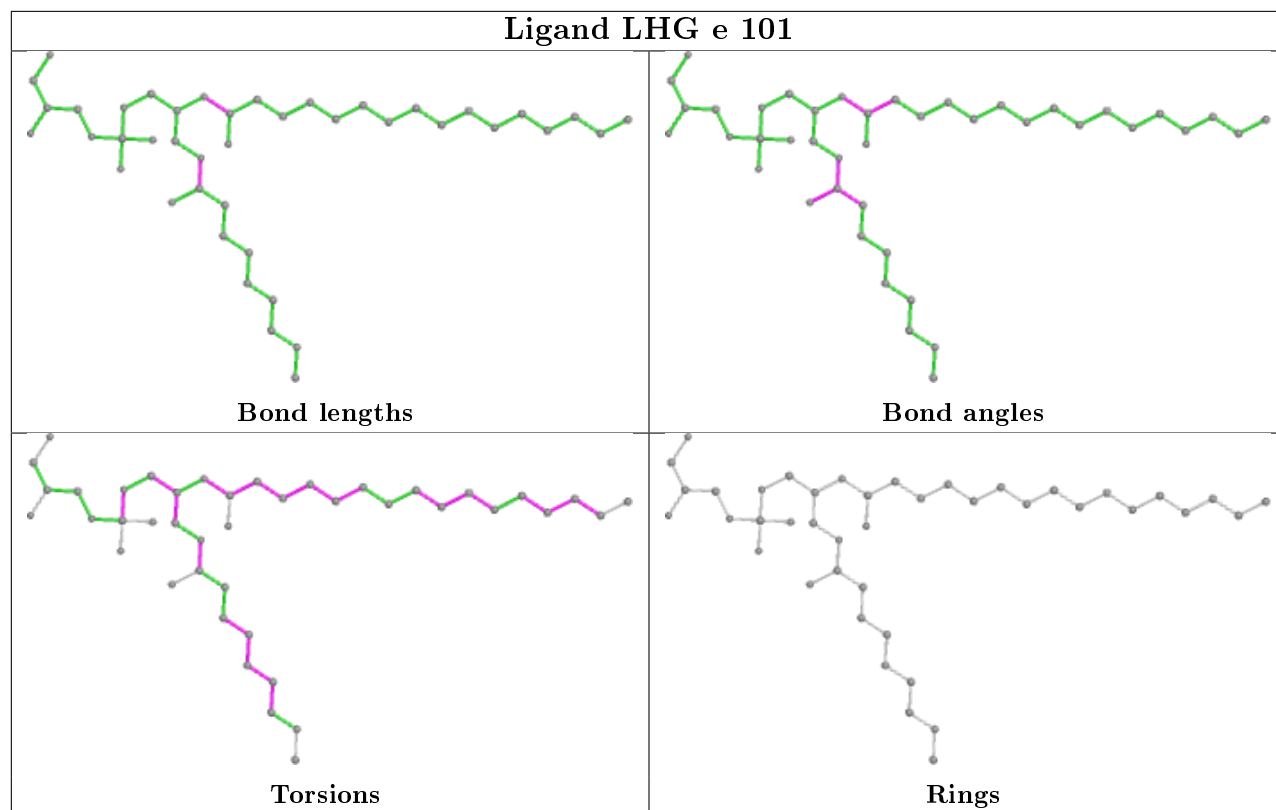


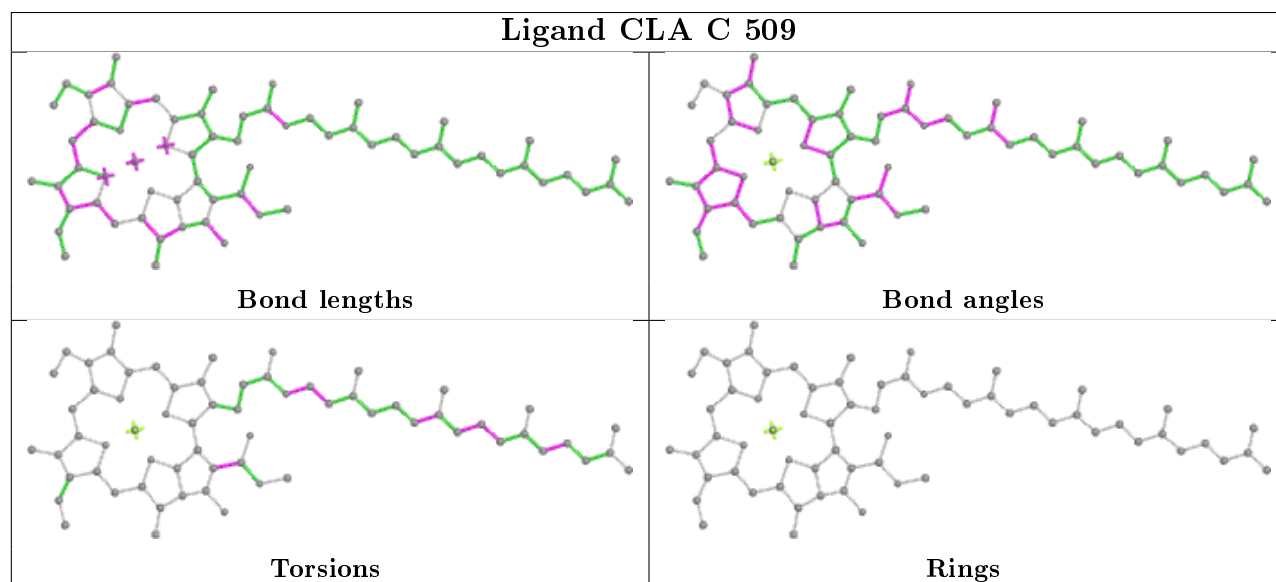
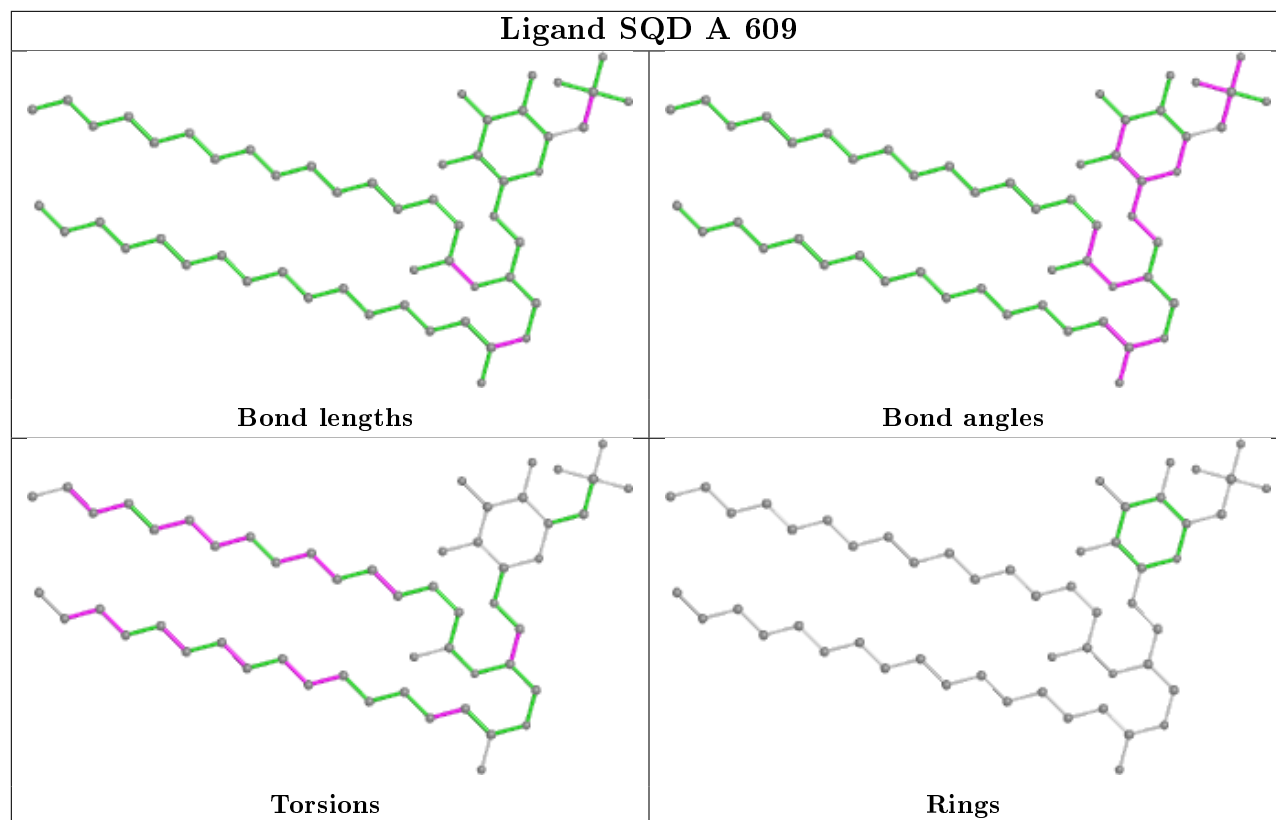
Ligand CLA c 506

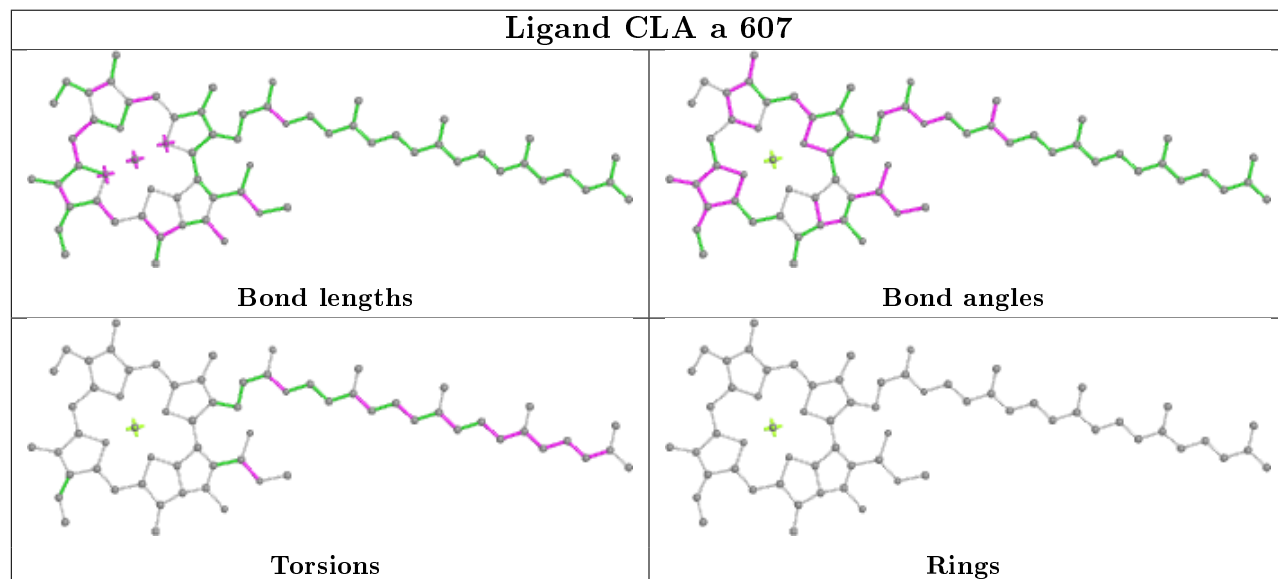
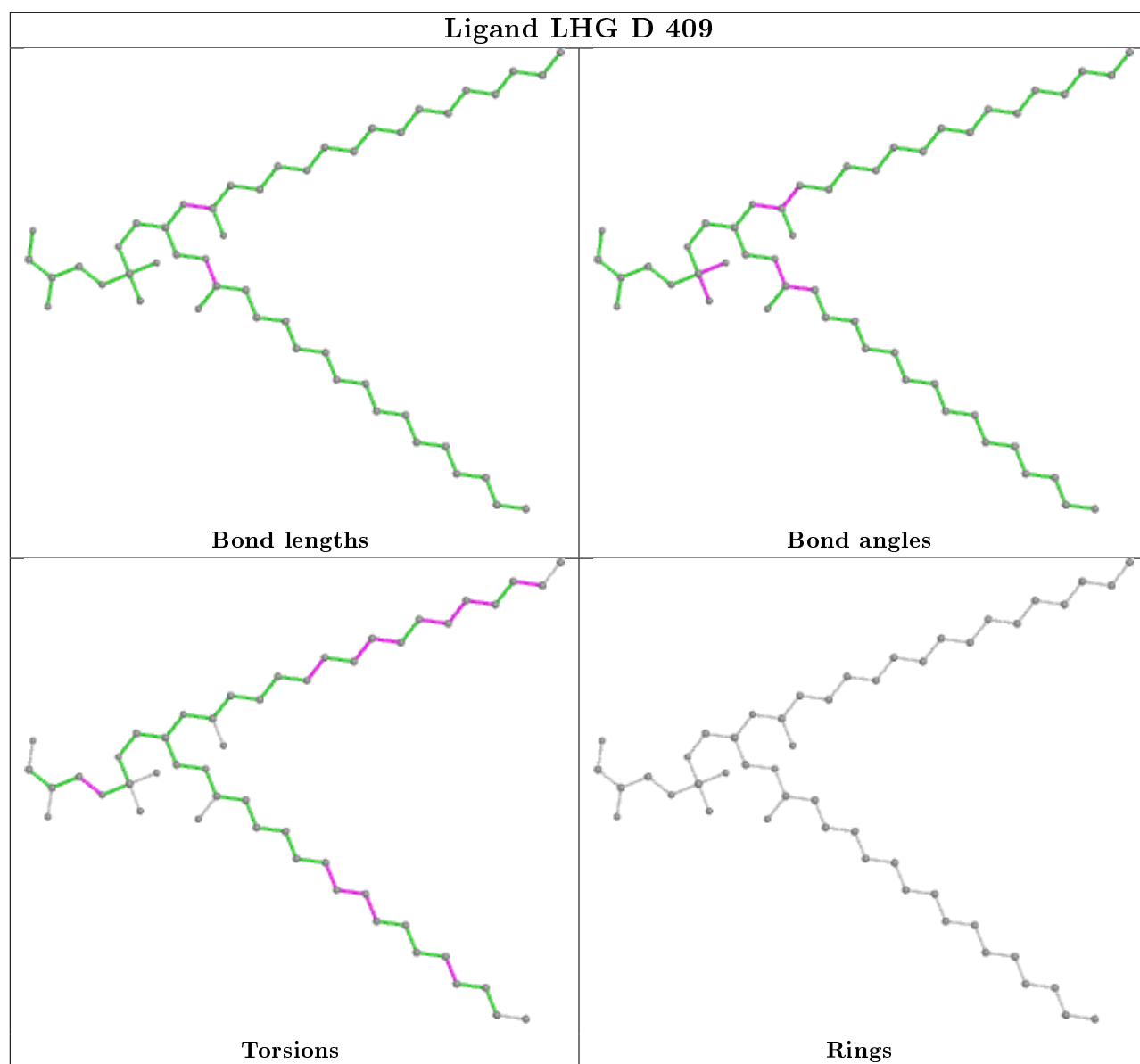


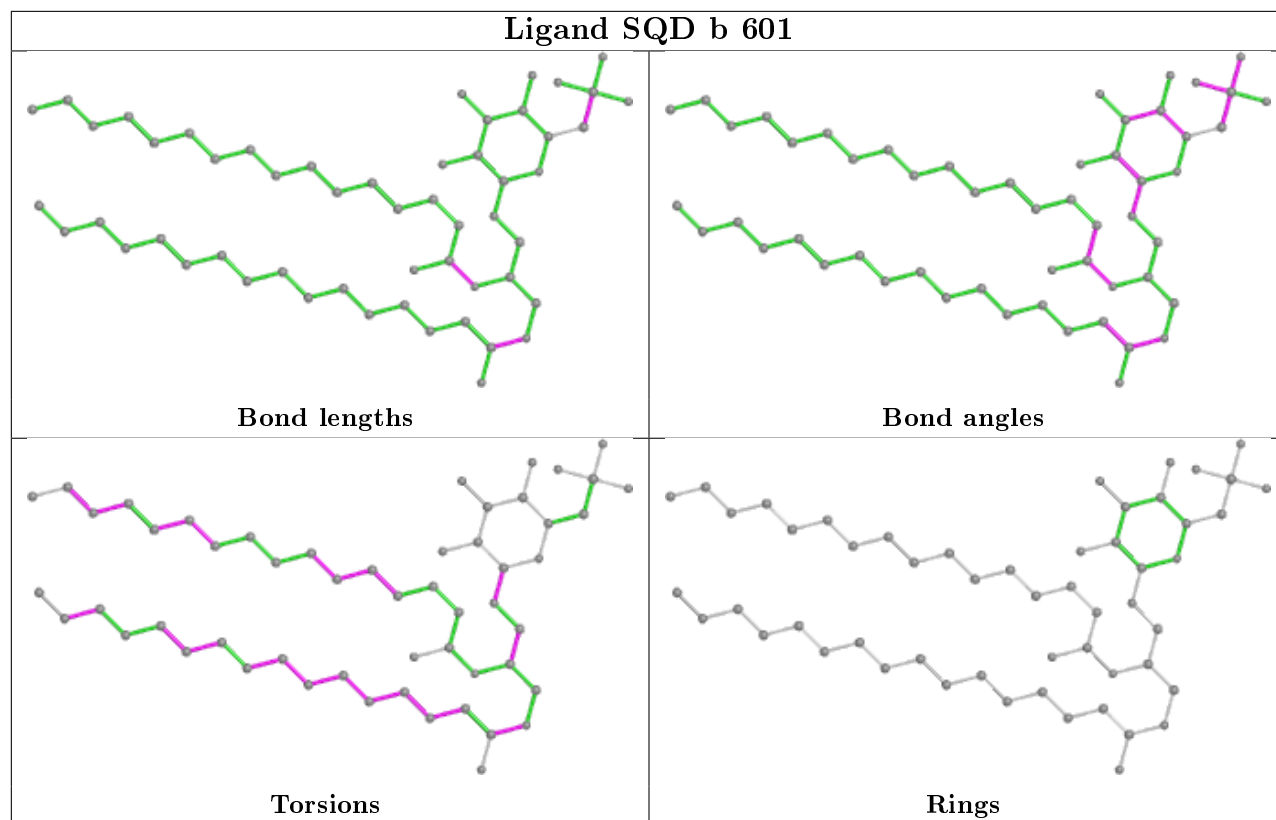
Ligand CLA d 403

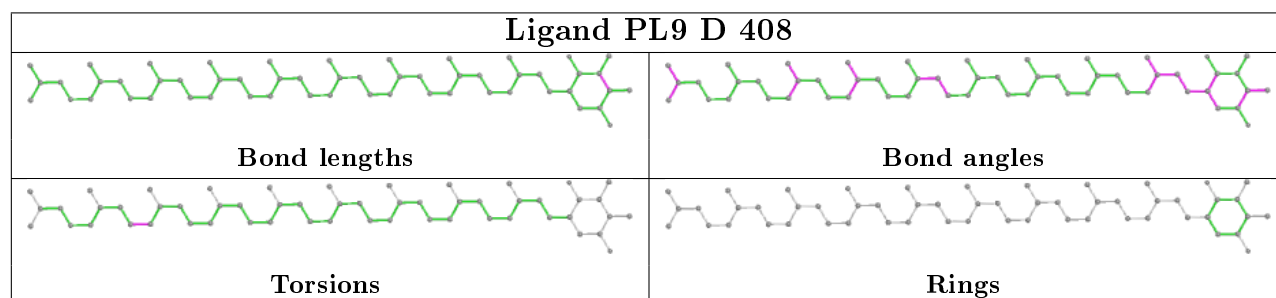
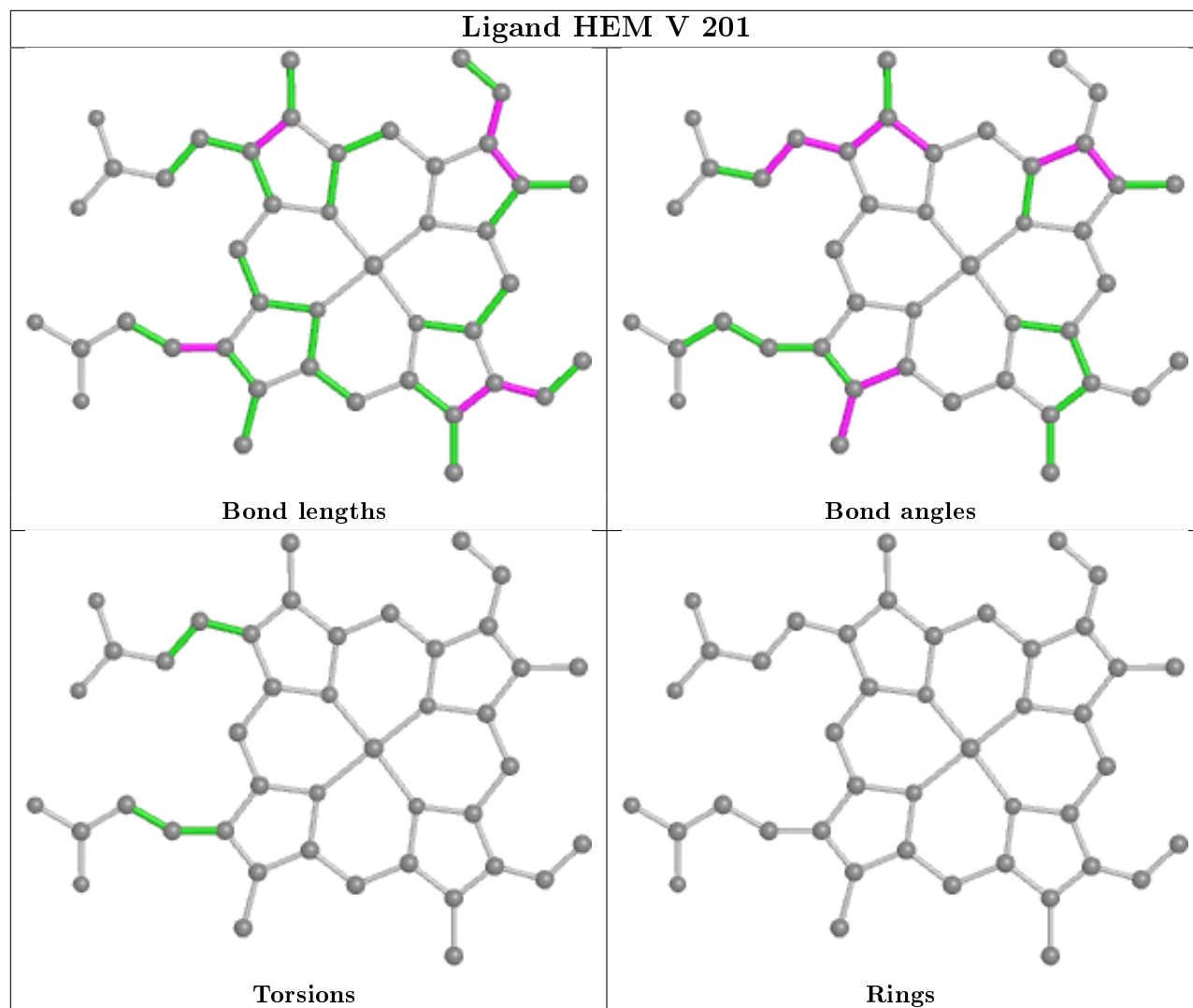




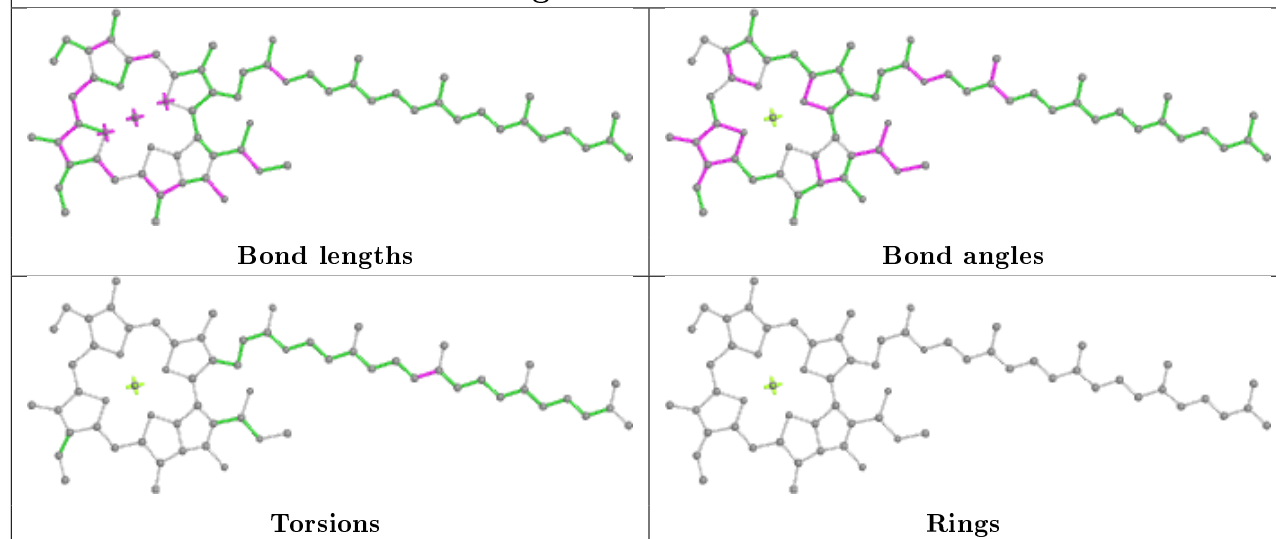




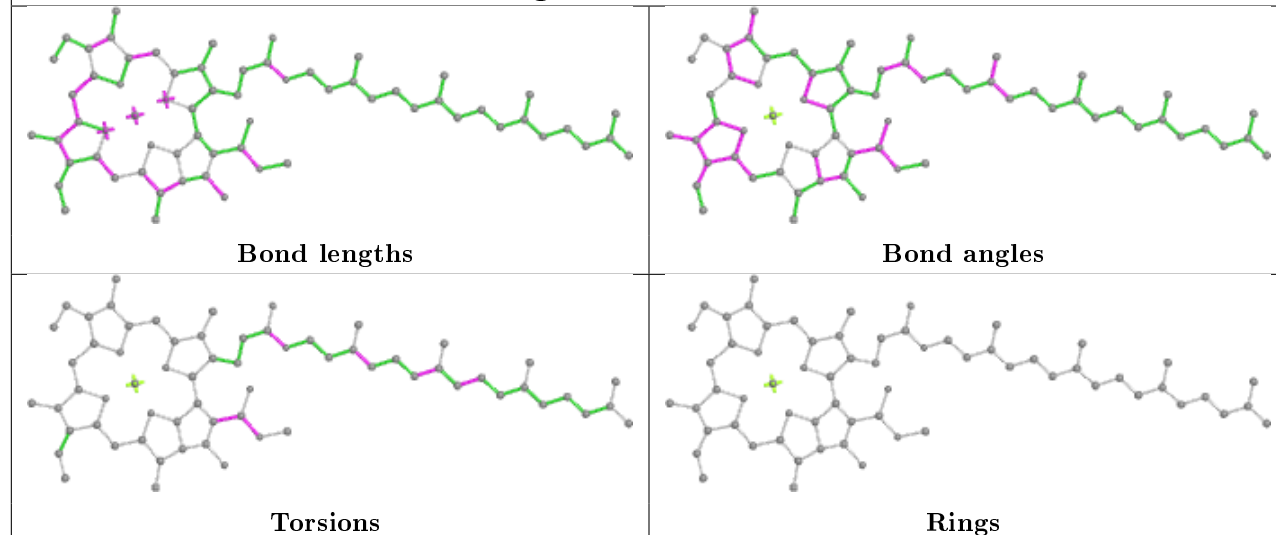




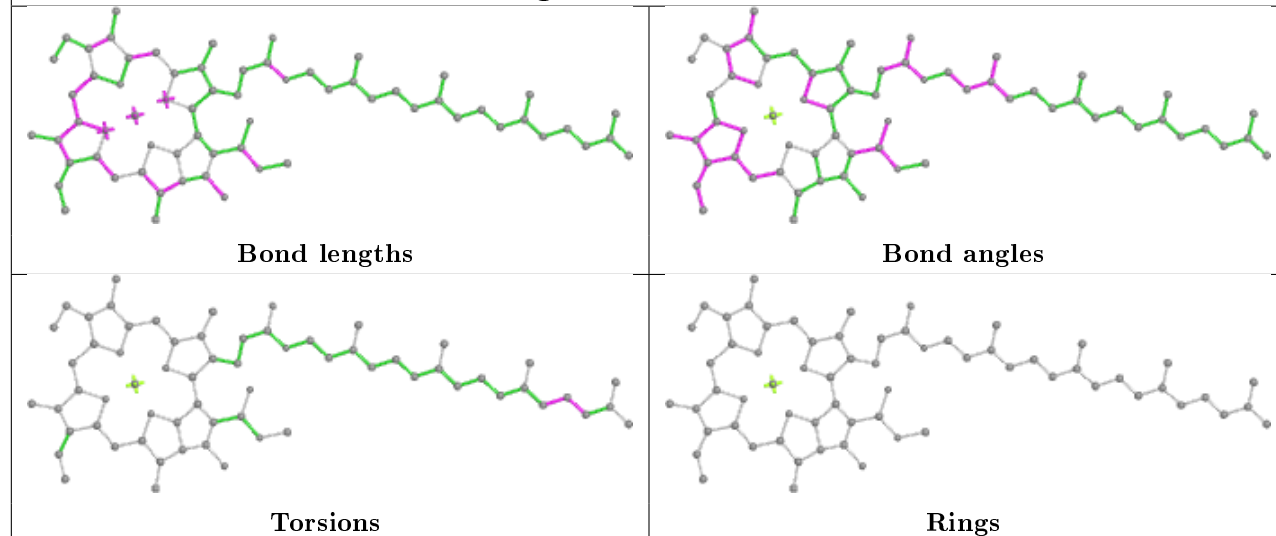
Ligand CLA C 511

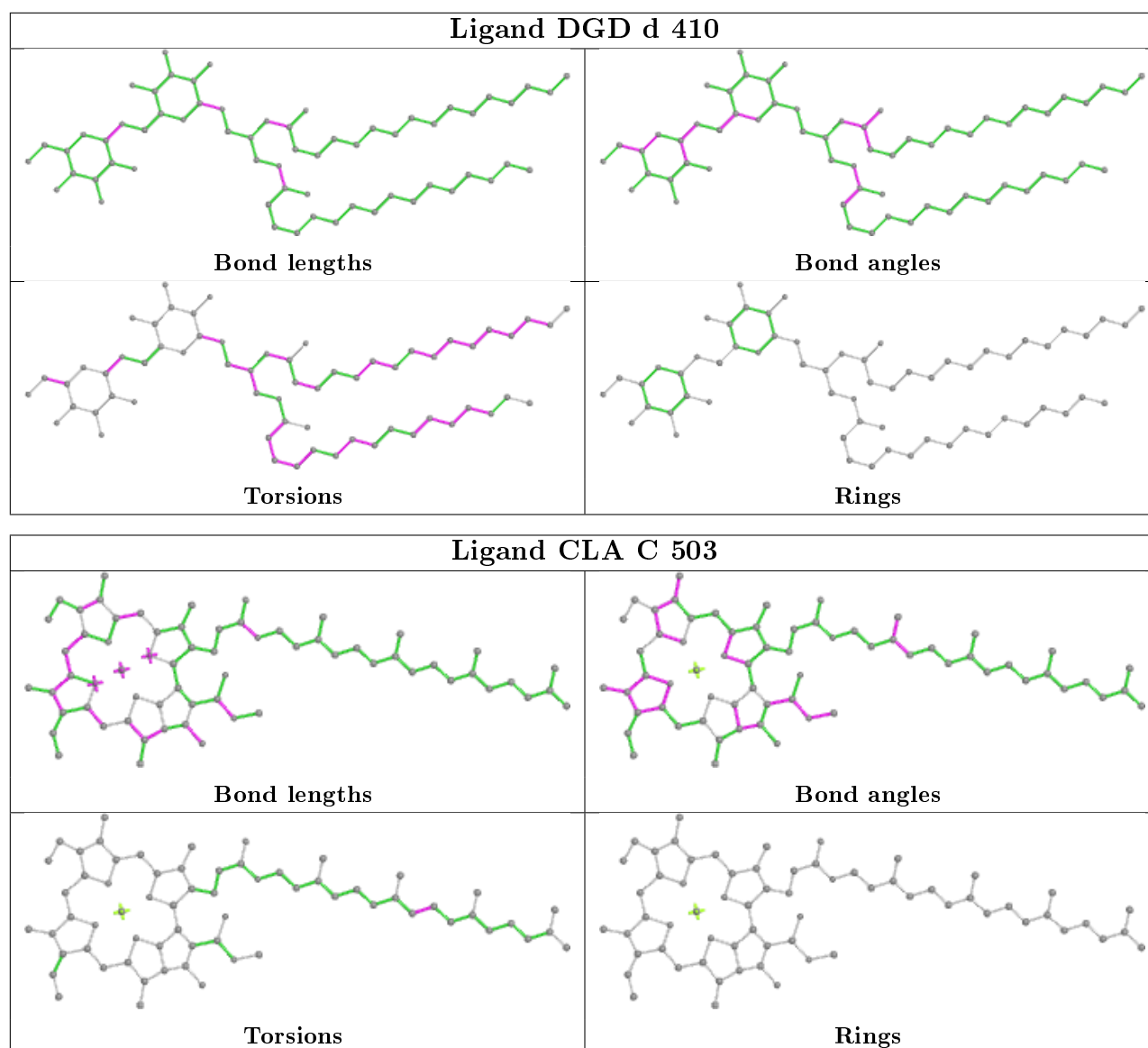


Ligand CLA C 510



Ligand CLA b 614





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	19 (5%) 23 22	16, 22, 43, 53	0
1	a	334/334 (100%)	0.60	26 (7%) 13 13	16, 22, 43, 53	0
2	B	504/504 (100%)	0.48	33 (6%) 18 17	18, 27, 49, 70	0
2	b	504/504 (100%)	0.76	72 (14%) 2 5	18, 27, 49, 70	0
3	C	451/461 (97%)	0.64	44 (9%) 7 9	21, 31, 44, 56	0
3	c	451/461 (97%)	0.52	37 (8%) 11 12	21, 31, 44, 56	0
4	D	342/342 (100%)	0.78	32 (9%) 8 10	17, 23, 39, 61	0
4	d	342/342 (100%)	0.70	24 (7%) 16 15	17, 23, 39, 61	0
5	E	81/81 (100%)	0.83	10 (12%) 4 7	27, 40, 57, 63	0
5	e	81/81 (100%)	0.42	9 (11%) 5 8	27, 40, 57, 63	0
6	F	34/34 (100%)	0.36	1 (2%) 51 43	28, 33, 58, 61	0
6	f	34/34 (100%)	-0.00	0 100 100	28, 33, 58, 61	0
7	H	65/65 (100%)	0.66	10 (15%) 2 4	23, 34, 40, 58	0
7	h	65/65 (100%)	1.42	19 (29%) 0 1	23, 34, 40, 58	0
8	I	38/38 (100%)	0.54	4 (10%) 6 8	30, 34, 65, 68	0
8	i	38/38 (100%)	0.08	4 (10%) 6 8	30, 34, 65, 68	0
9	J	38/40 (95%)	0.56	3 (7%) 12 13	26, 37, 68, 72	0
9	j	38/40 (95%)	-0.14	0 100 100	26, 37, 68, 72	0
10	K	37/37 (100%)	0.51	2 (5%) 25 24	33, 38, 45, 47	0
10	k	37/37 (100%)	0.60	4 (10%) 5 8	33, 38, 45, 47	0
11	L	37/37 (100%)	0.59	1 (2%) 54 46	17, 22, 50, 59	0
11	l	37/37 (100%)	0.59	3 (8%) 12 12	17, 22, 50, 59	0
12	M	34/34 (100%)	1.02	6 (17%) 1 3	21, 23, 36, 52	0
12	m	34/34 (100%)	0.74	3 (8%) 10 11	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%)	0.38	8 (3%) 46 39	18, 32, 55, 71	0
13	o	243/243 (100%)	0.56	15 (6%) 20 18	18, 32, 55, 71	0
14	T	30/30 (100%)	0.86	3 (10%) 7 9	19, 23, 44, 52	0
14	t	30/30 (100%)	0.84	1 (3%) 46 39	19, 23, 44, 52	0
15	U	97/97 (100%)	0.30	2 (2%) 63 55	23, 30, 48, 50	0
15	u	97/97 (100%)	0.55	6 (6%) 20 18	23, 30, 48, 50	0
16	V	137/137 (100%)	0.22	2 (1%) 73 64	23, 28, 39, 48	0
16	v	137/137 (100%)	0.38	6 (4%) 34 30	23, 28, 39, 48	0
17	X	39/39 (100%)	0.99	7 (17%) 1 3	33, 40, 66, 68	0
17	x	39/39 (100%)	1.00	7 (17%) 1 3	33, 40, 66, 68	0
18	Y	29/29 (100%)	0.68	3 (10%) 6 8	42, 48, 75, 77	0
18	y	29/29 (100%)	0.29	0 100 100	42, 48, 75, 77	0
19	Z	62/62 (100%)	0.48	2 (3%) 47 39	39, 48, 68, 72	0
19	z	62/62 (100%)	0.69	7 (11%) 5 8	39, 48, 68, 72	0
All	All	5264/5288 (99%)	0.59	435 (8%) 11 12	16, 29, 51, 77	0

All (435) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	X	2	THR	7.3
4	D	59	TYR	6.8
9	J	3	SER	6.6
4	D	56	THR	5.7
4	d	136	VAL	5.5
1	a	140	ARG	5.4
4	D	136	VAL	5.4
2	b	270	PRO	5.3
1	a	138	GLY	5.2
3	C	24	THR	5.2
4	d	59	TYR	5.1
2	b	499	VAL	5.0
17	x	2	THR	5.0
2	b	262	THR	5.0
3	C	256	PRO	5.0
4	d	135	LEU	4.9
1	a	139	MET	4.8
7	H	56	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
3	C	265	ILE	4.8
3	c	146	PHE	4.7
4	d	107	LEU	4.7
3	c	198	VAL	4.7
2	b	187	PRO	4.6
4	d	106	GLN	4.6
2	b	435	GLU	4.5
3	C	137	PRO	4.5
1	a	245	THR	4.5
2	b	131	PRO	4.4
4	D	106	GLN	4.4
3	C	264	PHE	4.4
2	b	500	GLY	4.4
12	M	2	GLU	4.3
7	h	23	PRO	4.3
3	C	138	GLU	4.3
3	c	228	ASN	4.2
3	C	97	TRP	4.2
3	c	86	LEU	4.1
2	B	136	PRO	4.1
4	D	135	LEU	4.1
5	E	49	THR	4.1
6	F	12	SER	4.1
4	D	55	VAL	4.1
7	H	55	LEU	4.1
17	X	40	SER	4.1
2	b	71	VAL	4.1
1	A	245	THR	4.1
2	b	261	ALA	4.0
3	c	197	ARG	4.0
7	h	55	LEU	4.0
3	C	266	TRP	3.9
4	d	137	GLY	3.9
19	z	62	VAL	3.9
2	b	361	ALA	3.9
19	Z	1	MET	3.9
4	D	137	GLY	3.9
17	x	40	SER	3.9
2	b	188	ASP	3.8
3	C	25	ASN	3.8
4	d	264	LYS	3.8
2	b	267	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
16	v	21	LEU	3.7
1	a	246	TYR	3.7
3	c	127	PHE	3.7
3	C	400	PRO	3.7
1	A	11	ALA	3.7
3	C	146	PHE	3.6
1	A	262	TYR	3.6
1	A	317	TRP	3.6
17	x	3	ILE	3.6
2	b	70	GLY	3.6
2	b	190	PHE	3.5
15	U	8	GLU	3.5
4	d	29	PHE	3.5
4	D	107	LEU	3.5
3	C	263	ALA	3.5
4	d	221	THR	3.5
2	b	218	LEU	3.5
7	h	54	ILE	3.5
19	z	23	VAL	3.5
19	z	61	VAL	3.5
2	b	229	LEU	3.5
4	D	27	PHE	3.5
2	B	43	ALA	3.5
19	z	1	MET	3.5
3	c	373	ASN	3.4
3	C	457	LYS	3.4
13	o	243	ILE	3.4
5	e	84	LYS	3.4
2	B	499	VAL	3.4
1	A	137	LEU	3.4
1	A	139	MET	3.4
4	d	54	PHE	3.3
18	Y	46	LEU	3.3
7	h	56	ASP	3.3
2	B	367	PRO	3.3
2	B	362	PHE	3.3
4	D	93	TRP	3.3
7	h	27	THR	3.3
7	h	53	LEU	3.3
2	B	183	PRO	3.3
13	O	243	ILE	3.2
7	H	65	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	a	137	LEU	3.2
2	b	133	LEU	3.2
4	D	32	TRP	3.2
18	Y	43	ARG	3.2
3	c	264	PHE	3.2
17	x	38	GLN	3.2
4	D	54	PHE	3.2
17	X	3	ILE	3.1
3	c	457	LYS	3.1
10	k	18	PHE	3.1
2	b	123	PHE	3.1
2	b	219	VAL	3.1
5	e	55	TYR	3.1
8	i	38	GLU	3.1
13	O	169	ASP	3.1
2	b	305	ILE	3.1
3	C	127	PHE	3.1
2	b	87	ASP	3.1
2	b	119	ASP	3.1
2	b	72	THR	3.1
8	I	25	SER	3.1
4	D	264	LYS	3.1
1	A	306	VAL	3.1
4	d	11	GLU	3.0
2	B	44	THR	3.0
7	h	2	ALA	3.0
3	C	452	ALA	3.0
3	c	422	PRO	3.0
2	b	217	ILE	3.0
2	B	187	PRO	3.0
4	d	28	VAL	3.0
2	B	378	LYS	3.0
2	B	368	VAL	3.0
1	A	246	TYR	3.0
1	A	12	ASN	3.0
2	B	262	THR	3.0
15	u	66	GLY	3.0
2	b	356	VAL	3.0
2	B	69	LEU	3.0
4	D	12	ARG	3.0
8	i	37	LEU	3.0
4	d	98	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
4	d	138	VAL	3.0
2	b	497	GLN	3.0
2	B	309	LEU	3.0
2	B	500	GLY	3.0
3	C	147	PHE	3.0
1	a	257	ARG	2.9
13	o	129	THR	2.9
3	c	400	PRO	2.9
1	a	268	SER	2.9
2	b	302	TRP	2.9
16	v	3	LEU	2.9
17	X	38	GLN	2.9
7	h	26	GLY	2.9
16	v	120	LEU	2.9
1	A	265	PHE	2.9
3	C	399	ALA	2.9
3	c	291	TRP	2.9
1	A	257	ARG	2.9
3	c	336	GLY	2.9
2	b	343	HIS	2.9
15	u	56	GLU	2.9
12	M	1	MET	2.9
5	E	70	PHE	2.9
3	C	255	THR	2.9
3	c	69	LEU	2.9
1	a	240	GLY	2.9
4	D	96	GLU	2.8
2	b	264	PRO	2.8
19	z	24	PRO	2.8
2	B	347	ARG	2.8
3	c	112	PHE	2.8
4	D	333	ASP	2.8
5	E	47	PHE	2.8
7	h	47	GLU	2.8
8	I	30	ARG	2.8
3	c	200	THR	2.8
3	C	199	ILE	2.8
15	u	103	TYR	2.8
13	o	181	GLU	2.8
10	K	32	PHE	2.8
1	a	244	GLU	2.8
2	B	306	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
5	e	56	TYR	2.8
4	d	56	THR	2.7
2	B	70	GLY	2.7
19	z	27	TYR	2.7
2	B	366	PHE	2.7
3	C	268	GLY	2.7
7	H	66	GLY	2.7
9	J	5	GLY	2.7
3	c	134	ILE	2.7
4	D	95	PRO	2.7
7	h	14	LEU	2.7
1	A	261	GLN	2.7
12	M	3	VAL	2.7
4	d	108	GLY	2.7
8	I	32	PRO	2.7
3	C	139	THR	2.7
2	b	16	PRO	2.7
4	D	103	ARG	2.7
19	Z	35	ARG	2.7
2	B	305	ILE	2.7
2	b	490	GLN	2.7
3	c	181	PHE	2.7
15	U	32	ILE	2.7
19	z	40	ILE	2.7
4	d	262	SER	2.7
13	o	190	PHE	2.6
5	e	66	VAL	2.6
2	B	229	LEU	2.6
2	B	166	MET	2.6
2	B	498	LYS	2.6
3	C	99	VAL	2.6
3	C	202	PRO	2.6
3	c	296	VAL	2.6
3	C	204	LEU	2.6
3	c	147	PHE	2.6
2	B	87	ASP	2.6
2	b	491	VAL	2.6
15	u	8	GLU	2.6
2	b	268	PHE	2.6
2	b	494	GLY	2.6
13	o	87	VAL	2.6
17	x	39	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	a	74	GLY	2.6
3	C	81	MET	2.6
3	c	199	ILE	2.6
4	d	23	LYS	2.6
2	b	234	ILE	2.6
3	c	458	GLY	2.6
3	c	81	MET	2.6
2	b	318	ASN	2.6
8	i	36	ASP	2.6
3	C	365	TRP	2.5
14	T	30	THR	2.5
1	a	223	LEU	2.5
2	B	185	TRP	2.5
3	c	143	TYR	2.5
4	D	110	LEU	2.5
2	b	220	ARG	2.5
17	X	34	ILE	2.5
3	c	227	VAL	2.5
2	b	317	ASN	2.5
3	C	267	SER	2.5
13	O	164	LEU	2.5
1	A	268	SER	2.5
13	o	184	ARG	2.5
2	b	438	ASN	2.5
1	a	250	ALA	2.5
11	l	33	SER	2.5
4	D	180	ARG	2.5
2	b	392	PHE	2.5
3	c	238	ILE	2.5
2	b	443	PHE	2.5
2	b	120	LEU	2.4
1	a	222	SER	2.4
5	e	54	SER	2.4
1	a	239	PHE	2.4
1	a	317	TRP	2.4
4	d	32	TRP	2.4
2	B	195	PRO	2.4
12	m	7	GLY	2.4
5	e	64	PRO	2.4
1	A	244	GLU	2.4
4	D	60	THR	2.4
1	A	219	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	497	GLN	2.4
2	b	362	PHE	2.4
2	b	447	PRO	2.4
2	b	353	GLU	2.4
2	B	71	VAL	2.4
7	h	22	ALA	2.4
5	E	84	LYS	2.4
5	E	64	PRO	2.4
2	b	195	PRO	2.4
8	I	24	LEU	2.4
2	B	77	GLY	2.4
1	a	224	ILE	2.4
2	b	183	PRO	2.4
15	u	101	GLY	2.4
13	O	120	PHE	2.3
13	o	211	ILE	2.3
16	v	116	ALA	2.3
2	b	189	GLY	2.3
7	H	57	GLY	2.3
4	D	138	VAL	2.3
2	B	490	GLN	2.3
7	h	3	ARG	2.3
4	D	25	ASP	2.3
5	e	57	ALA	2.3
17	X	39	ARG	2.3
7	h	65	LEU	2.3
3	c	456	GLU	2.3
2	b	274	GLN	2.3
4	d	60	THR	2.3
4	D	28	VAL	2.3
17	x	37	VAL	2.3
2	b	122	LEU	2.3
1	a	76	ASN	2.3
3	C	296	VAL	2.3
3	C	203	THR	2.3
1	A	85	SER	2.3
3	C	23	ALA	2.3
13	O	20	PRO	2.3
5	e	60	GLN	2.3
12	m	33	GLN	2.3
7	H	53	LEU	2.3
10	K	11	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
7	H	64	ALA	2.3
1	a	306	VAL	2.3
1	a	141	PRO	2.3
2	b	306	PRO	2.3
3	c	82	TYR	2.3
4	D	300	SER	2.3
5	E	17	VAL	2.3
5	E	18	ARG	2.3
1	A	143	ILE	2.2
7	h	24	GLY	2.2
13	o	42	ARG	2.2
3	C	234	VAL	2.2
2	B	505	ARG	2.2
3	C	238	ILE	2.2
3	C	336	GLY	2.2
7	H	47	GLU	2.2
2	b	309	LEU	2.2
3	c	149	TYR	2.2
5	E	5	THR	2.2
7	h	20	LYS	2.2
3	C	200	THR	2.2
3	c	203	THR	2.2
2	b	182	ALA	2.2
2	b	369	ILE	2.2
3	c	263	ALA	2.2
5	E	22	ILE	2.2
12	M	4	ASN	2.2
11	l	8	GLN	2.2
2	b	185	TRP	2.2
4	d	292	ASN	2.2
5	E	12	ASP	2.2
11	L	33	SER	2.2
13	O	87	VAL	2.2
1	a	80	GLY	2.2
2	b	84	THR	2.2
12	M	5	GLN	2.2
14	T	2	GLU	2.2
4	d	308	ASP	2.2
13	O	154	ALA	2.2
2	b	436	THR	2.2
1	A	304	HIS	2.2
3	C	72	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	132	ALA	2.2
3	c	249	ILE	2.2
7	H	54	ILE	2.2
7	h	48	ILE	2.2
13	o	40	ILE	2.2
3	C	213	LEU	2.2
10	k	21	LEU	2.2
14	t	3	THR	2.2
1	a	247	ASN	2.2
3	C	291	TRP	2.2
2	b	367	PRO	2.1
4	d	341	PHE	2.1
7	h	28	THR	2.1
3	C	124	VAL	2.1
4	D	350	ASN	2.1
17	x	36	LYS	2.1
18	Y	45	ASN	2.1
3	C	466	VAL	2.1
4	D	79	SER	2.1
13	o	150	SER	2.1
1	a	75	ASN	2.1
9	J	4	GLU	2.1
1	a	340	PRO	2.1
16	v	90	GLU	2.1
12	M	7	GLY	2.1
3	C	86	LEU	2.1
15	u	77	GLU	2.1
13	O	76	THR	2.1
11	l	1	MET	2.1
2	b	445	THR	2.1
3	C	95	LEU	2.1
4	D	89	LEU	2.1
14	T	3	THR	2.1
4	D	307	GLU	2.1
4	d	35	ILE	2.1
2	b	420	TYR	2.1
4	D	308	ASP	2.1
7	h	66	GLY	2.1
2	b	344	ALA	2.1
13	o	140	THR	2.1
2	b	192	PRO	2.1
10	k	15	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
12	m	4	ASN	2.1
2	b	284	ILE	2.1
3	C	111	PHE	2.1
3	c	292	PHE	2.1
17	X	36	LYS	2.1
3	c	230	LEU	2.1
16	V	125	ILE	2.1
4	D	23	LYS	2.1
3	C	269	GLU	2.1
1	a	79	THR	2.1
13	o	176	GLN	2.1
2	b	428	GLU	2.1
13	o	101	ILE	2.1
3	c	256	PRO	2.0
3	c	447	ARG	2.0
1	a	236	GLY	2.0
3	c	243	ILE	2.0
13	o	112	GLY	2.0
7	H	63	LYS	2.0
4	D	85	MET	2.0
2	B	379	ALA	2.0
2	b	304	ALA	2.0
2	b	311	PHE	2.0
5	e	37	PHE	2.0
1	A	194	MET	2.0
13	o	20	PRO	2.0
2	B	503	THR	2.0
2	b	136	PRO	2.0
2	b	194	ASN	2.0
8	i	32	PRO	2.0
2	b	85	GLY	2.0
10	k	14	ALA	2.0
2	b	231	MET	2.0
2	B	421	ALA	2.0
2	b	421	ALA	2.0
16	V	120	LEU	2.0
3	C	364	PRO	2.0
16	v	10	VAL	2.0
7	h	46	LEU	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 carbohydrates 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
26	CL	U	201	1/1	0.01	0.17	50,50,50,50	0
26	CL	u	201	1/1	0.03	0.36	50,50,50,50	0
29	LMG	c	520	51/55	0.21	1.84	43,76,81,82	0
30	CA	B	621	1/1	0.26	0.72	76,76,76,76	0
28	PL9	a	613	55/55	0.26	1.48	52,69,78,78	0
29	LMG	z	101	37/55	0.27	1.47	55,84,88,88	0
30	CA	f	102	1/1	0.28	0.74	56,56,56,56	0
24	BCR	k	101	40/40	0.29	1.14	34,38,39,39	0
29	LMG	C	520	51/55	0.31	1.34	43,76,81,82	0
29	LMG	Z	101	37/55	0.33	1.65	55,84,88,88	0
24	BCR	d	404	40/40	0.34	1.17	25,30,48,49	0
28	PL9	A	613	55/55	0.34	1.95	52,69,78,78	0
24	BCR	a	608	40/40	0.39	0.47	22,27,32,32	0
24	BCR	D	404	40/40	0.40	1.52	25,30,48,49	0
24	BCR	T	102	40/40	0.41	1.10	27,33,39,39	0
29	LMG	C	519	51/55	0.42	0.86	31,57,72,73	0
24	BCR	A	608	40/40	0.45	0.70	22,27,32,32	0
24	BCR	t	101	40/40	0.47	0.63	27,33,39,39	0
31	DGD	D	410	62/66	0.48	1.24	77,89,103,103	0
22	CLA	b	607	65/65	0.51	0.88	24,28,40,41	0
32	LHG	e	101	42/49	0.52	0.61	69,83,86,86	0
31	DGD	d	410	62/66	0.53	0.76	77,89,103,103	0
30	CA	b	620	1/1	0.53	1.25	76,76,76,76	0
32	LHG	E	101	42/49	0.55	1.29	69,83,86,86	0
26	CL	a	610	1/1	0.57	0.55	24,24,24,24	0
22	CLA	a	604	65/65	0.57	0.86	19,21,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	LMG	B	620	51/55	0.58	0.38	29,39,51,54	0
24	BCR	K	101	40/40	0.61	1.40	34,38,39,39	0
25	SQD	d	411	43/54	0.61	0.91	67,74,78,79	0
22	CLA	B	607	65/65	0.61	0.62	24,28,40,41	0
22	CLA	b	602	65/65	0.61	1.48	32,41,66,66	0
22	CLA	B	602	65/65	0.62	1.02	32,41,66,66	0
29	LMG	A	614	51/55	0.63	0.85	53,59,64,65	0
25	SQD	a	609	54/54	0.64	0.53	49,57,66,67	0
25	SQD	A	609	54/54	0.65	0.63	49,57,66,67	0
25	SQD	D	411	43/54	0.66	1.27	67,74,78,79	0
22	CLA	C	513	65/65	0.66	1.10	39,45,64,64	0
22	CLA	c	512	65/65	0.66	1.57	37,41,62,63	0
22	CLA	b	615	65/65	0.67	0.44	20,24,60,61	0
24	BCR	B	622	40/40	0.67	0.43	25,37,44,45	0
24	BCR	H	101	40/40	0.67	1.33	26,33,42,42	0
22	CLA	b	617	65/65	0.67	0.91	22,29,77,78	0
29	LMG	b	619	51/55	0.67	0.38	29,39,51,54	0
22	CLA	c	502	65/65	0.68	0.96	24,26,39,42	0
29	LMG	a	614	51/55	0.68	0.80	53,59,64,65	0
22	CLA	c	513	65/65	0.68	1.01	39,45,64,64	0
24	BCR	b	622	40/40	0.69	0.48	25,37,44,45	0
22	CLA	B	617	65/65	0.69	0.51	22,29,77,78	0
22	CLA	C	507	65/65	0.70	1.34	29,33,52,53	0
24	BCR	k	102	40/40	0.70	2.16	29,33,37,37	0
30	CA	F	102	1/1	0.70	0.49	56,56,56,56	0
34	MG	j	101	1/1	0.70	0.29	27,27,27,27	0
22	CLA	C	512	65/65	0.70	1.32	37,41,62,63	0
22	CLA	D	403	65/65	0.70	1.20	24,27,65,67	0
28	PL9	D	408	55/55	0.70	0.51	19,23,29,32	0
24	BCR	c	514	40/40	0.72	1.69	37,43,47,47	0
22	CLA	c	501	65/65	0.72	1.66	29,32,44,46	0
22	CLA	C	508	65/65	0.73	0.74	25,29,54,58	0
24	BCR	C	515	40/40	0.73	1.99	30,37,40,41	0
25	SQD	B	601	54/54	0.73	0.35	50,63,68,68	0
25	SQD	b	601	54/54	0.73	0.49	50,63,68,68	0
24	BCR	B	619	40/40	0.73	0.31	21,28,40,40	0
22	CLA	a	603	65/65	0.73	0.60	15,19,25,34	0
22	CLA	b	614	65/65	0.73	0.45	19,22,45,47	0
22	CLA	B	615	65/65	0.74	0.38	20,24,60,61	0
22	CLA	d	403	65/65	0.74	1.19	24,27,65,67	0
31	DGD	C	518	62/66	0.75	0.64	22,31,52,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	b	618	40/40	0.75	0.42	21,28,40,40	0
22	CLA	A	604	65/65	0.75	1.02	19,21,63,65	0
32	LHG	D	409	49/49	0.75	0.75	26,33,62,64	0
22	CLA	c	507	65/65	0.76	1.38	29,33,52,53	0
22	CLA	a	607	65/65	0.76	0.81	21,24,71,72	0
32	LHG	D	405	49/49	0.76	0.38	29,34,41,41	0
22	CLA	C	506	65/65	0.76	0.96	31,38,74,75	0
29	LMG	d	406	51/55	0.76	0.50	26,35,65,67	0
24	BCR	C	514	40/40	0.76	1.48	37,43,47,47	0
25	SQD	b	621	54/54	0.77	0.40	58,66,80,80	0
28	PL9	d	408	55/55	0.77	0.40	19,23,29,32	0
25	SQD	L	101	54/54	0.77	0.41	57,69,84,85	0
23	PHO	A	605	64/64	0.77	0.59	16,21,25,26	0
22	CLA	A	603	65/65	0.77	0.67	15,19,25,34	0
22	CLA	b	612	65/65	0.77	0.43	19,21,32,34	0
32	LHG	d	409	49/49	0.77	0.71	26,33,62,64	0
22	CLA	D	402	65/65	0.77	0.53	14,18,29,35	0
29	LMG	D	406	51/55	0.78	0.80	26,35,65,67	0
22	CLA	d	402	65/65	0.78	0.47	14,18,29,35	0
24	BCR	c	515	40/40	0.78	1.59	30,37,40,41	0
22	CLA	B	616	65/65	0.78	0.74	25,27,45,46	0
22	CLA	b	606	65/65	0.78	0.84	19,23,34,35	0
24	BCR	T	101	40/40	0.79	0.40	23,27,28,29	0
22	CLA	C	501	65/65	0.79	1.23	29,32,44,46	0
32	LHG	d	407	49/49	0.80	0.37	24,28,37,40	0
26	CL	A	610	1/1	0.80	0.45	24,24,24,24	0
23	PHO	a	605	64/64	0.81	0.52	16,21,25,26	0
22	CLA	C	504	65/65	0.81	0.70	25,28,54,54	0
31	DGD	c	518	62/66	0.81	0.53	22,31,52,56	0
24	BCR	K	102	40/40	0.81	2.31	29,33,37,37	0
22	CLA	B	609	65/65	0.81	0.88	20,24,31,31	0
32	LHG	d	405	49/49	0.81	0.44	29,34,41,41	0
24	BCR	h	101	40/40	0.81	1.31	26,33,42,42	0
22	CLA	c	509	65/65	0.81	1.18	29,32,46,47	0
22	CLA	b	616	65/65	0.81	1.25	25,27,45,46	0
24	BCR	B	618	40/40	0.81	0.31	23,27,28,29	0
25	SQD	l	102	54/54	0.82	0.32	58,66,80,80	0
22	CLA	A	607	65/65	0.82	0.78	21,24,71,72	0
23	PHO	A	606	64/64	0.82	1.13	19,22,28,32	0
22	CLA	b	605	65/65	0.82	0.78	19,22,50,51	0
31	DGD	h	102	62/66	0.82	0.90	26,32,38,40	0

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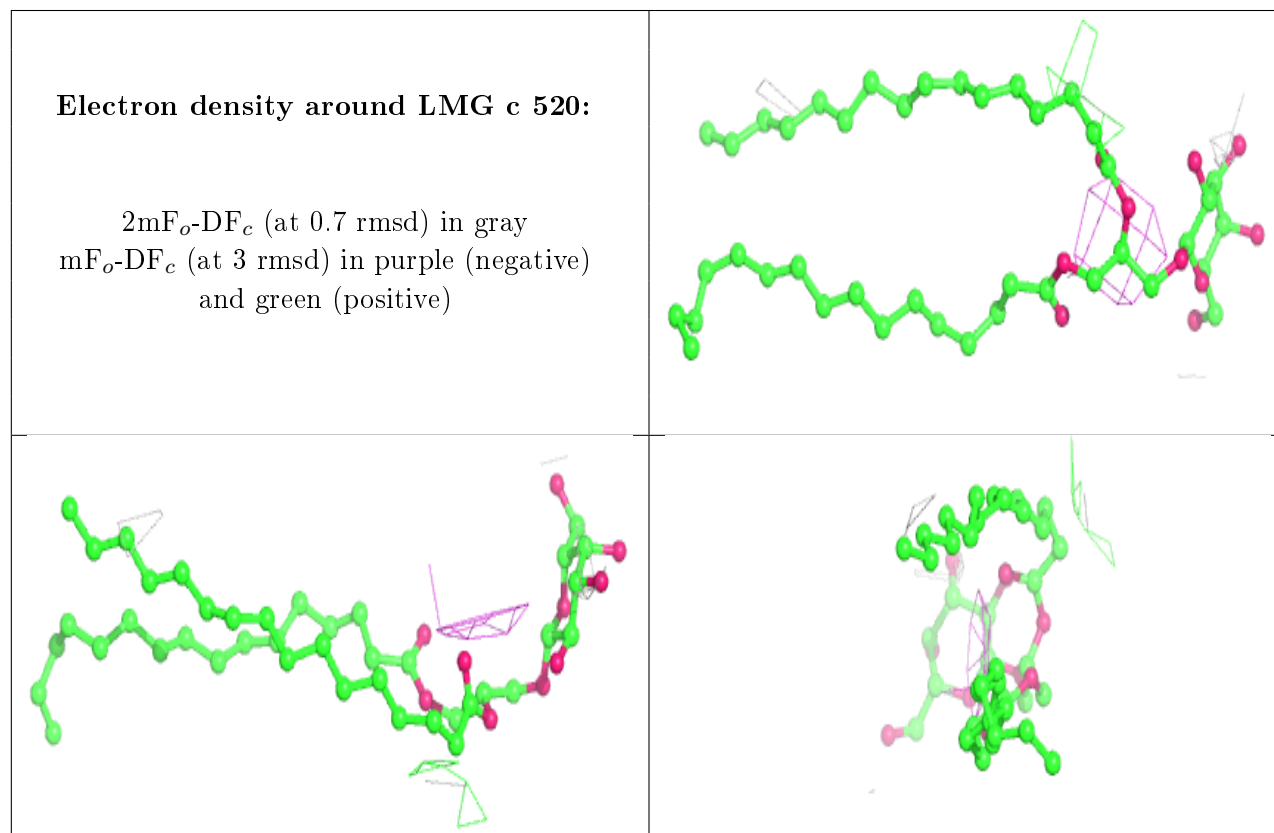
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	c	503	65/65	0.82	1.11	27,31,35,36	0
23	PHO	a	606	64/64	0.82	0.79	19,22,28,32	0
32	LHG	D	407	49/49	0.82	0.49	24,28,37,40	0
25	SQD	l	101	54/54	0.82	0.32	57,69,84,85	0
29	LMG	c	519	51/55	0.83	0.67	31,57,72,73	0
21	FE2	a	602	1/1	0.83	0.35	26,26,26,26	0
22	CLA	c	511	65/65	0.83	0.89	29,34,37,38	0
22	CLA	B	606	65/65	0.83	0.84	19,23,34,35	0
22	CLA	b	603	65/65	0.83	1.17	23,26,32,32	0
22	CLA	b	609	65/65	0.83	1.02	20,24,31,31	0
31	DGD	C	517	62/66	0.83	0.53	23,35,62,63	0
22	CLA	D	401	65/65	0.83	0.95	13,18,34,35	0
22	CLA	B	603	65/65	0.83	1.15	23,26,32,32	0
32	LHG	L	102	49/49	0.84	0.35	23,31,43,44	0
22	CLA	C	510	65/65	0.84	0.81	24,28,35,37	0
22	CLA	B	612	65/65	0.84	0.44	19,21,32,34	0
22	CLA	b	611	65/65	0.84	0.94	21,25,32,37	0
26	CL	A	611	1/1	0.85	0.35	21,21,21,21	0
31	DGD	H	102	62/66	0.85	1.00	26,32,38,40	0
31	DGD	C	516	62/66	0.85	0.58	23,33,61,62	0
22	CLA	c	506	65/65	0.85	0.93	31,38,74,75	0
32	LHG	l	103	49/49	0.85	0.33	23,31,43,44	0
22	CLA	b	610	65/65	0.86	1.10	23,28,31,32	0
22	CLA	c	510	65/65	0.86	0.85	24,28,35,37	0
34	MG	J	101	1/1	0.86	0.11	27,27,27,27	0
22	CLA	b	613	65/65	0.86	0.75	20,24,30,31	0
22	CLA	C	502	65/65	0.86	0.79	24,26,39,42	0
22	CLA	B	613	65/65	0.87	0.73	20,24,30,31	0
22	CLA	c	508	65/65	0.87	0.60	25,29,54,58	0
22	CLA	b	608	65/65	0.87	0.43	17,20,32,34	0
31	DGD	c	516	62/66	0.87	0.55	23,33,61,62	0
22	CLA	c	505	65/65	0.87	0.82	28,30,44,45	0
22	CLA	b	604	65/65	0.88	1.31	18,22,31,35	0
22	CLA	B	604	65/65	0.88	1.04	18,22,31,35	0
22	CLA	B	605	65/65	0.89	0.57	19,22,50,51	0
33	HEM	F	101	43/43	0.89	0.80	39,42,45,47	0
27	BCT	A	612	4/4	0.89	1.01	39,39,40,42	0
31	DGD	c	517	62/66	0.89	0.40	23,35,62,63	0
22	CLA	d	401	65/65	0.90	0.84	13,18,34,35	0
22	CLA	B	611	65/65	0.90	1.00	21,25,32,37	0
22	CLA	B	610	65/65	0.90	0.83	23,28,31,32	0
22	CLA	C	505	65/65	0.90	0.90	28,30,44,45	0

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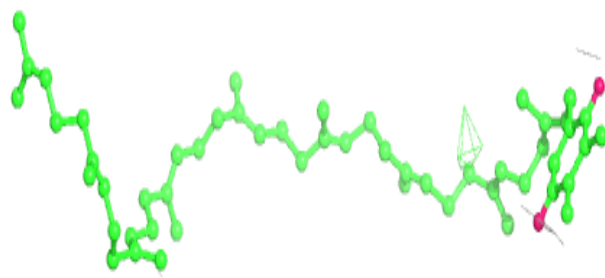
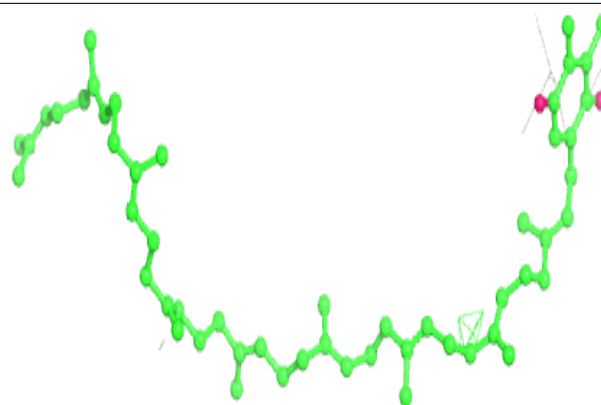
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	C	503	65/65	0.90	0.81	27,31,35,36	0
26	CL	a	611	1/1	0.91	0.37	21,21,21,21	0
33	HEM	f	101	43/43	0.91	0.69	39,42,45,47	0
22	CLA	C	511	65/65	0.91	1.24	29,34,37,38	0
22	CLA	B	608	65/65	0.91	0.41	17,20,32,34	0
22	CLA	c	504	65/65	0.91	0.51	25,28,54,54	0
22	CLA	B	614	65/65	0.91	0.38	19,22,45,47	0
33	HEM	V	201	43/43	0.91	0.69	23,24,27,29	0
33	HEM	v	201	43/43	0.92	0.72	23,24,27,29	0
20	OEX	A	601	10/10	0.92	0.40	22,23,26,26	0
30	CA	O	301	1/1	0.93	0.14	49,49,49,49	0
27	BCT	a	612	4/4	0.93	1.21	39,39,40,42	0
22	CLA	C	509	65/65	0.93	1.30	29,32,46,47	0
20	OEX	a	601	10/10	0.94	0.41	22,23,26,26	0
30	CA	o	301	1/1	0.95	0.28	49,49,49,49	0
21	FE2	A	602	1/1	0.96	0.16	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.

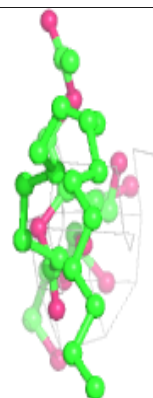
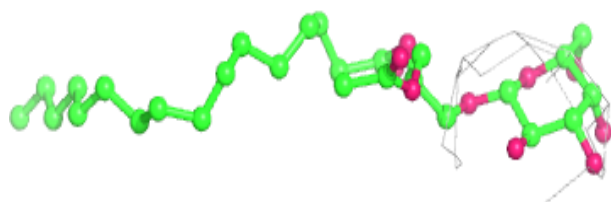
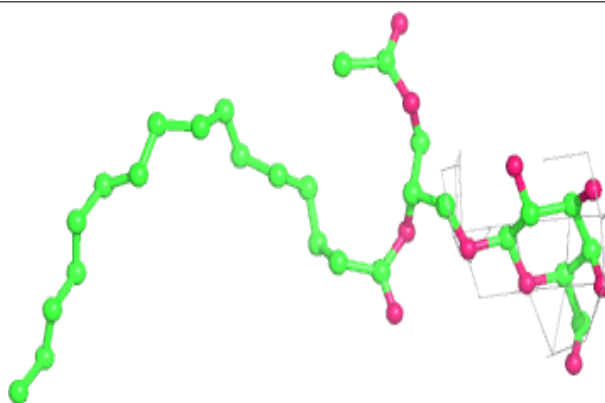


Electron density around PL9 a 613:

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

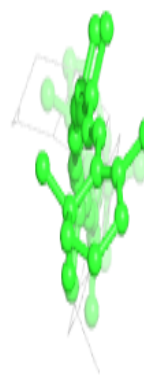
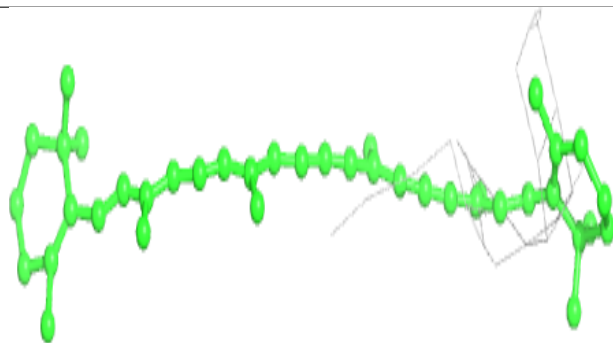
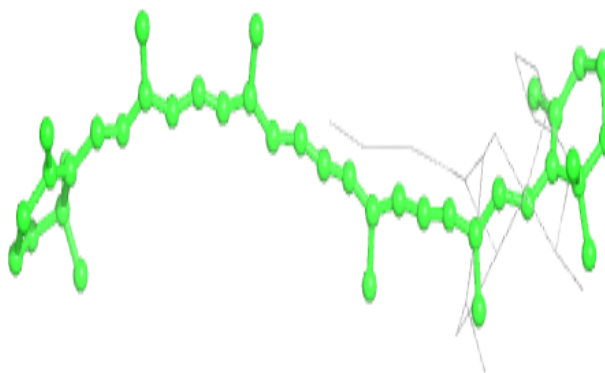
**Electron density around LMG z 101:**

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

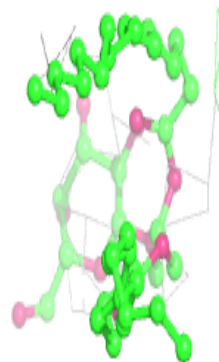
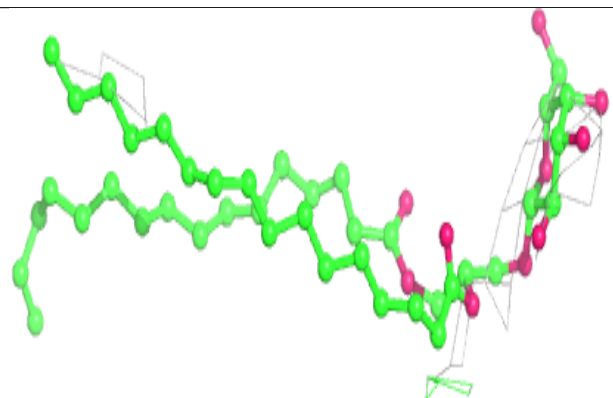
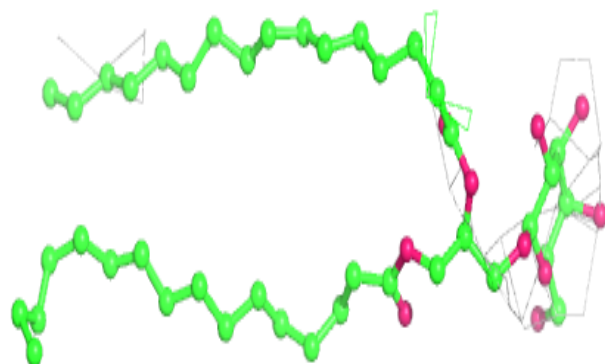


Electron density around BCR k 101:

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

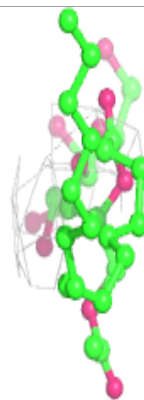
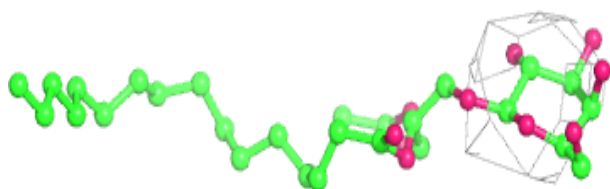
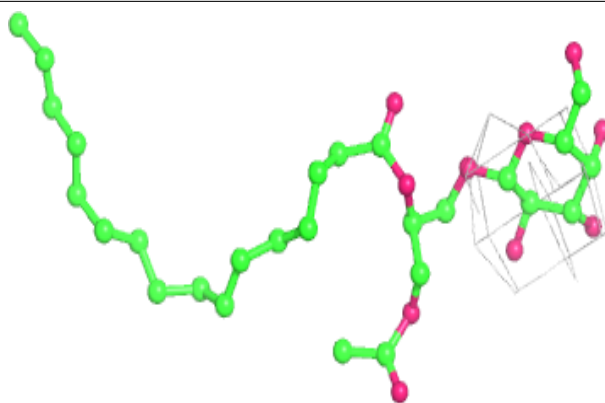
**Electron density around LMG C 520:**

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

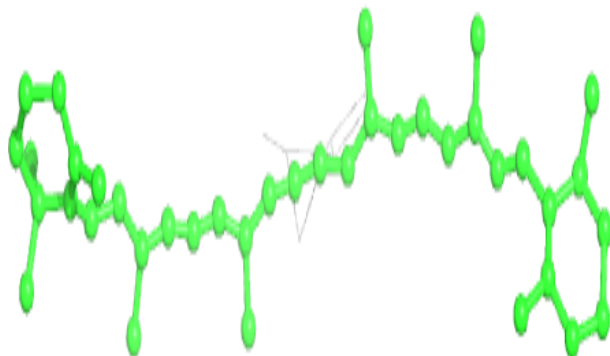
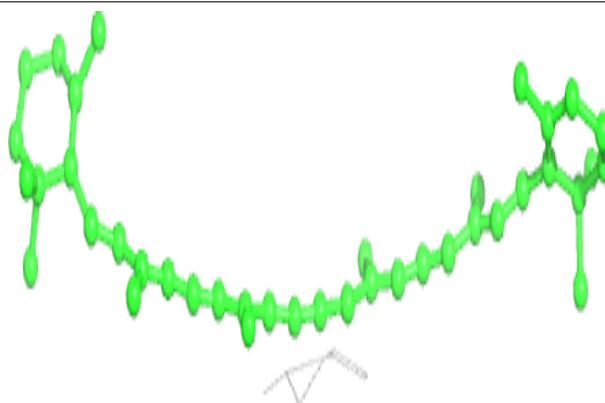


Electron density around LMG Z 101:

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

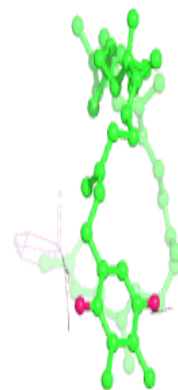
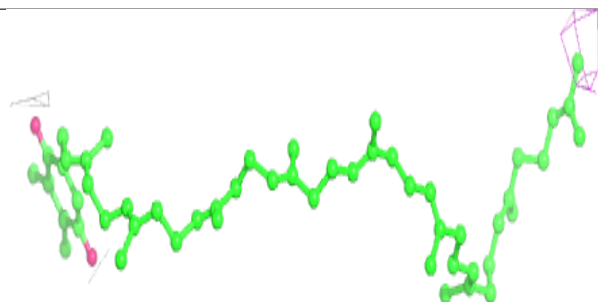
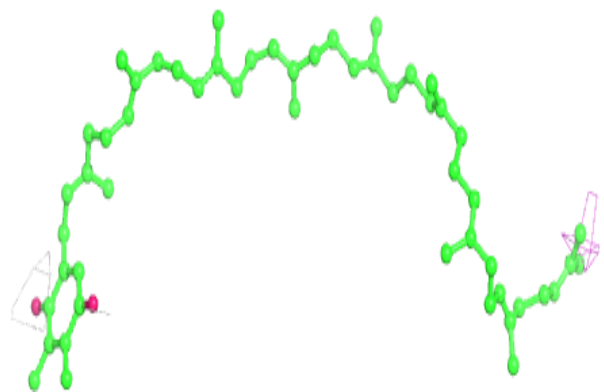
**Electron density around BCR d 404:**

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

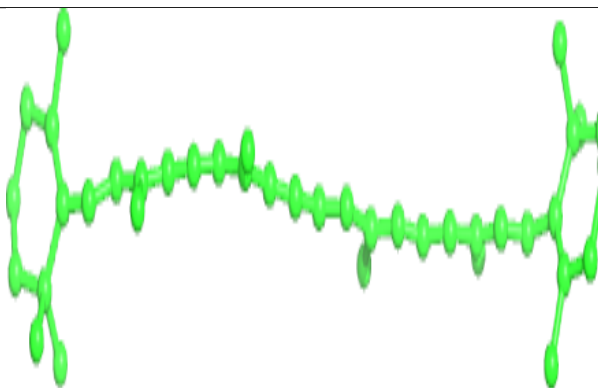
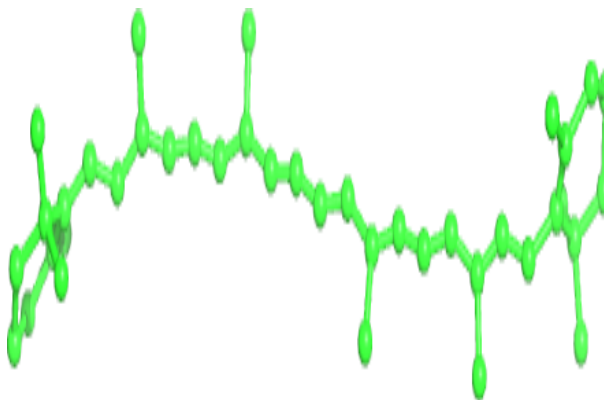


Electron density around PL9 A 613:

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

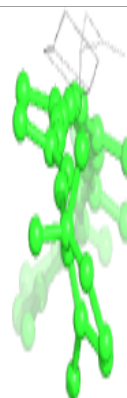
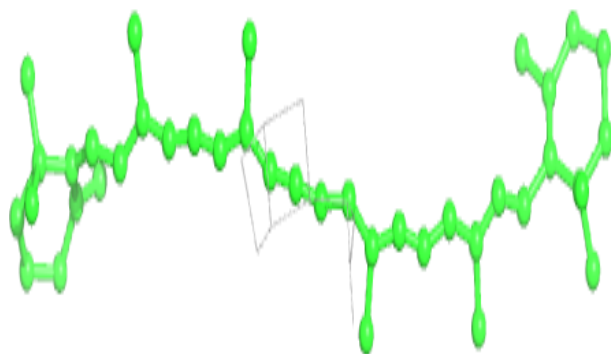
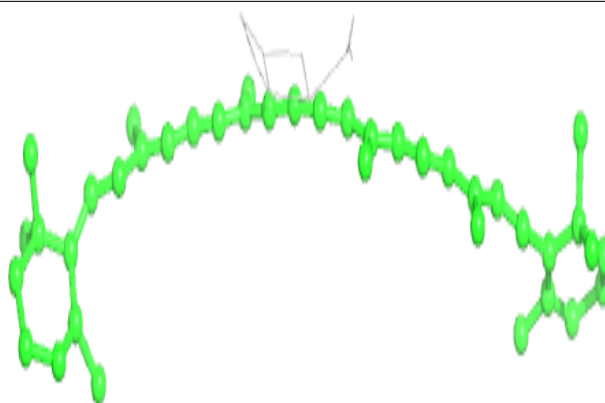
**Electron density around BCR a 608:**

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

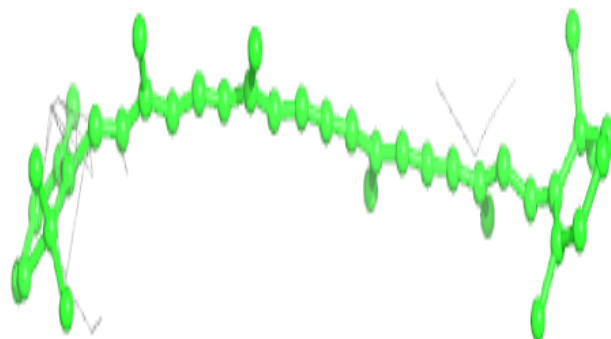
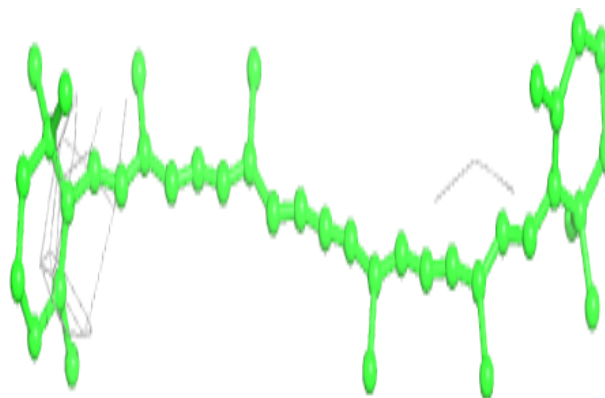


Electron density around BCR D 404:

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

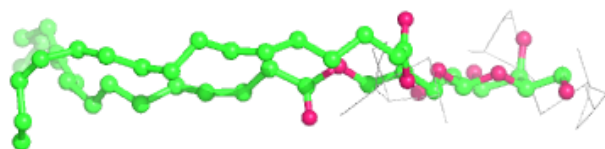
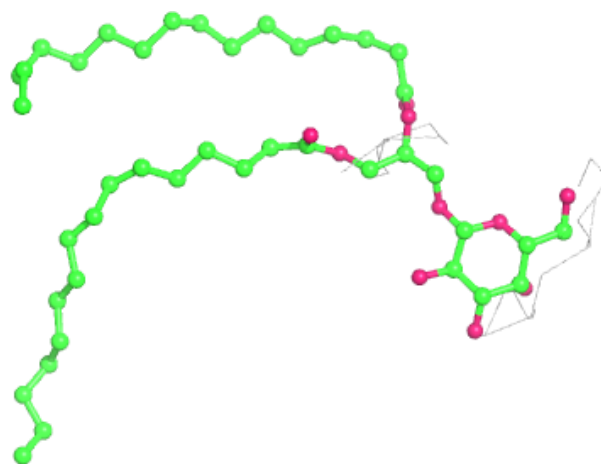
**Electron density around BCR T 102:**

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



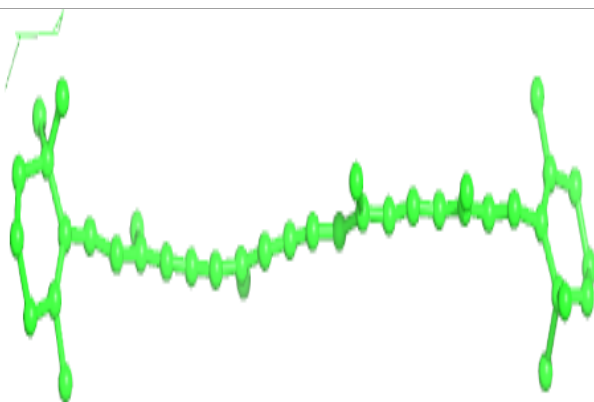
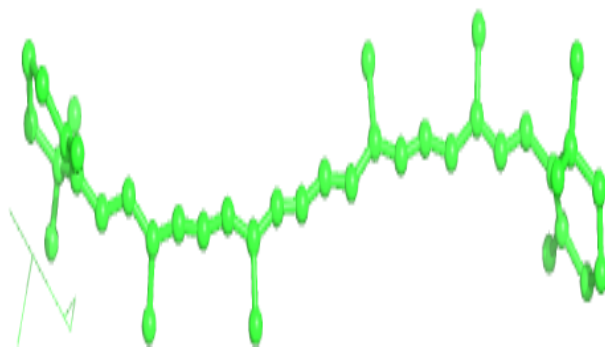
Electron density around LMG C 519:

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

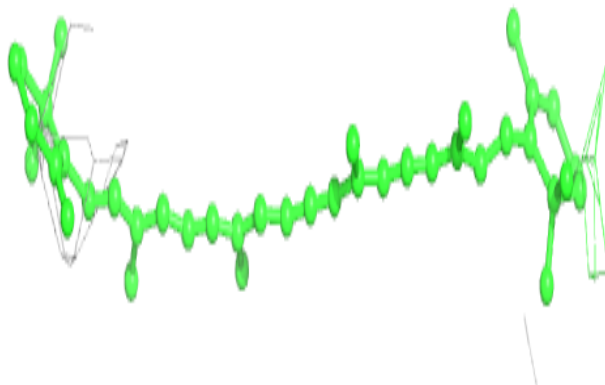
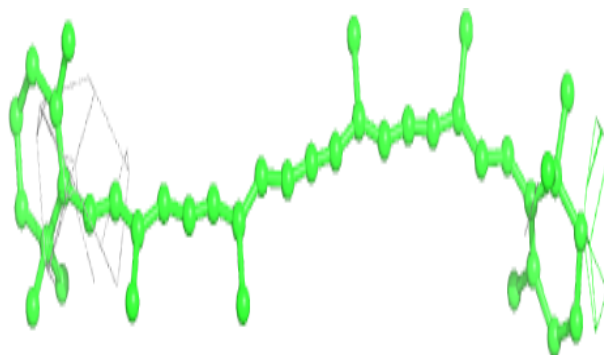


Electron density around BCR A 608:

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

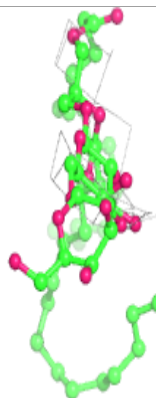
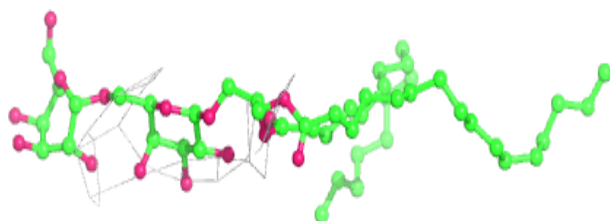
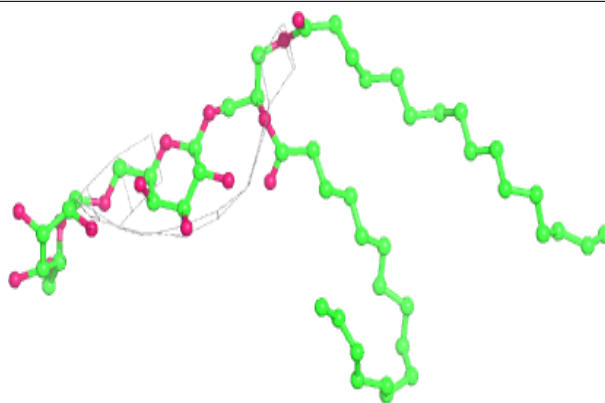
**Electron density around BCR t 101:**

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

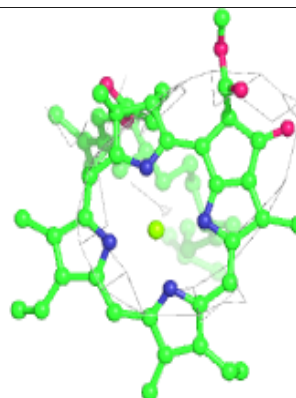
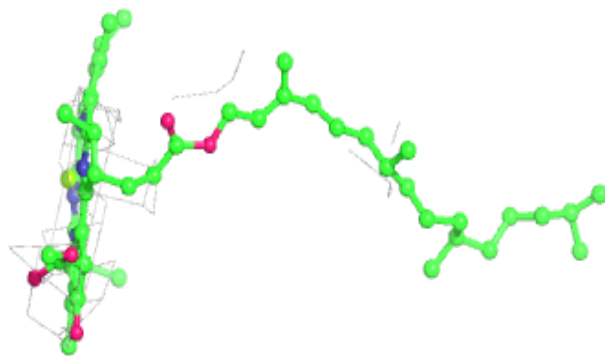
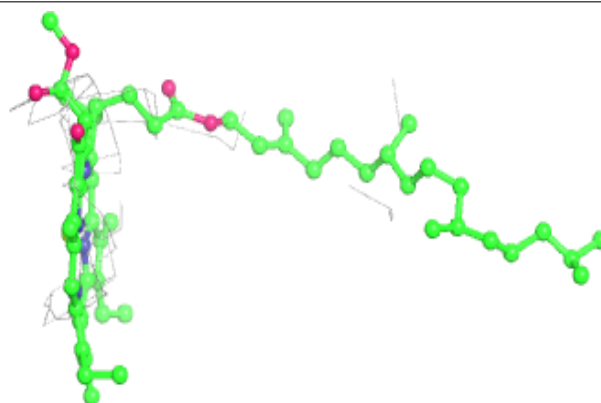


Electron density around DGD D 410:

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

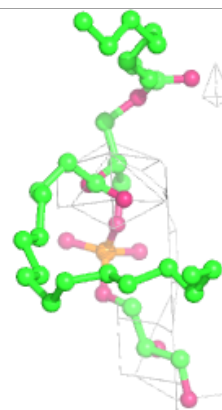
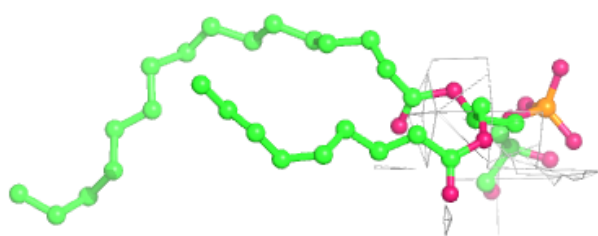
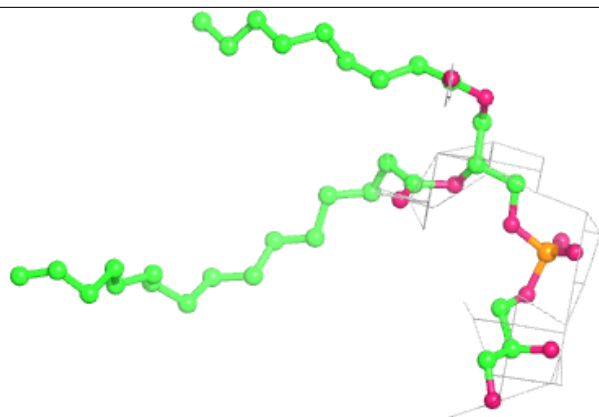
**Electron density around CLA b 607:**

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

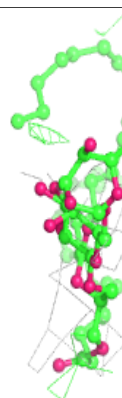
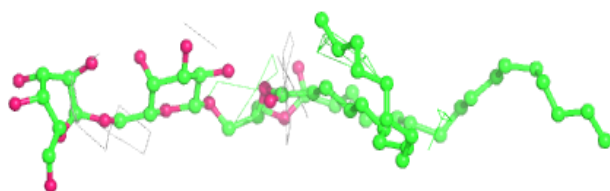
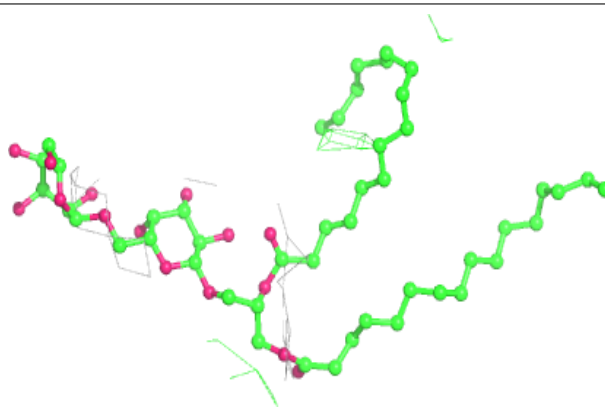


Electron density around LHG e 101:

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

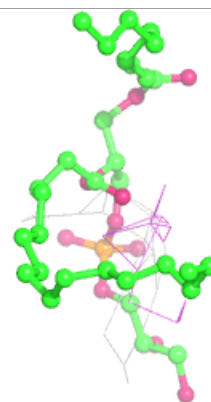
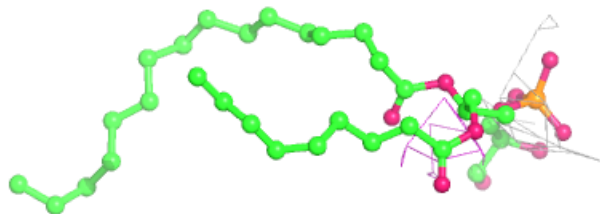
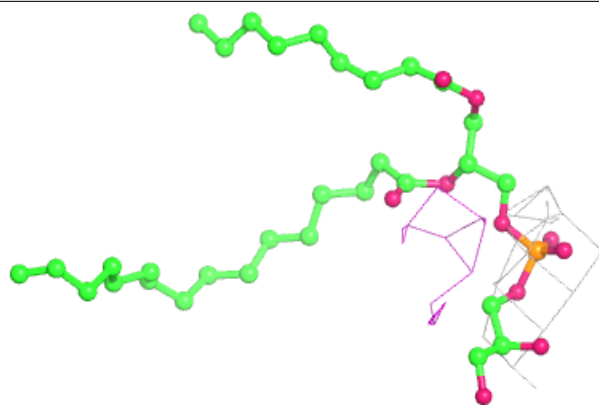
**Electron density around DGD d 410:**

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

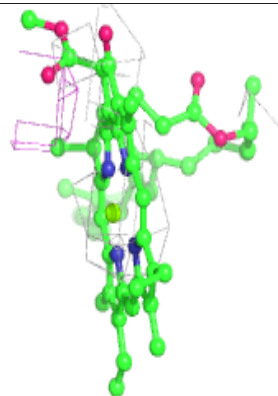
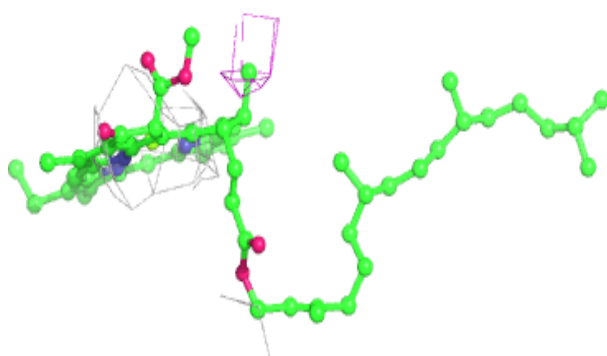
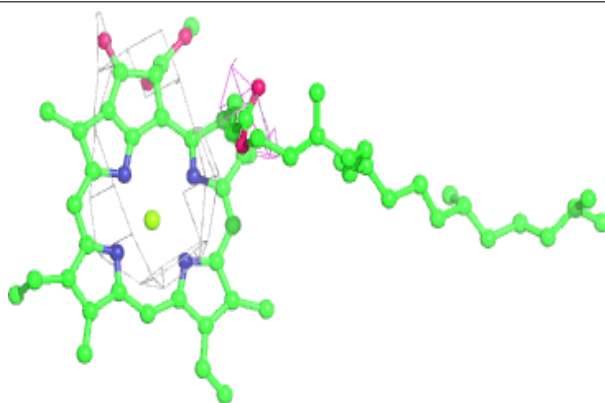


Electron density around LHG E 101:

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

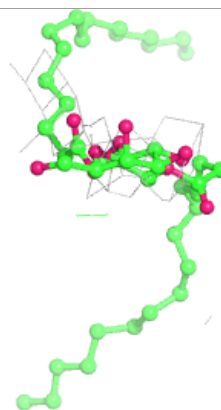
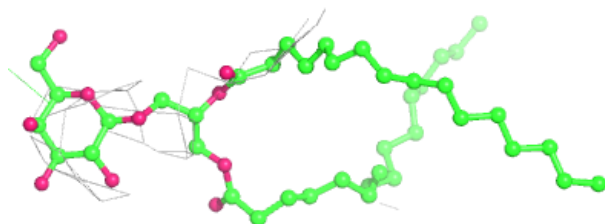
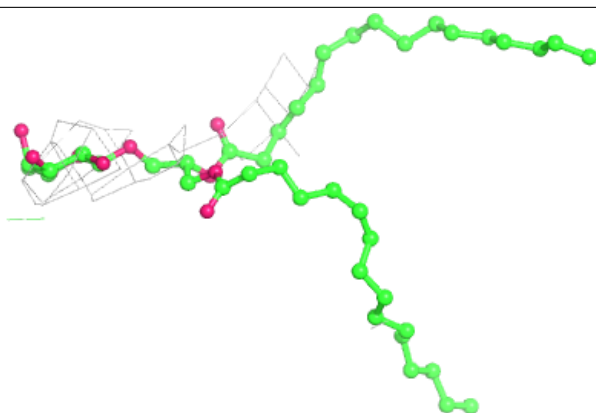
**Electron density around CLA a 604:**

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

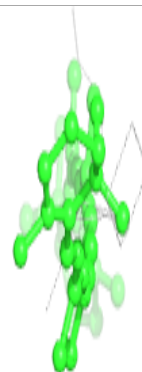
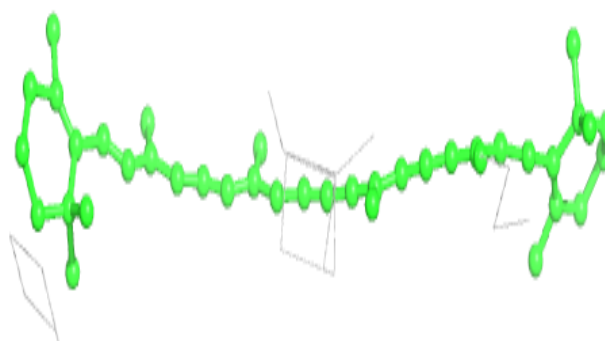
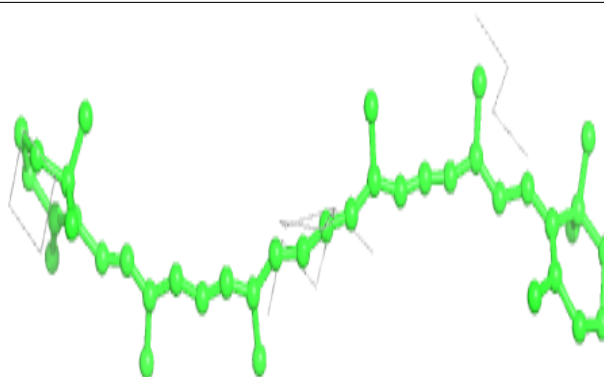


Electron density around LMG B 620:

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

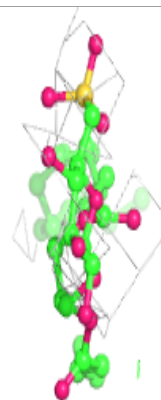
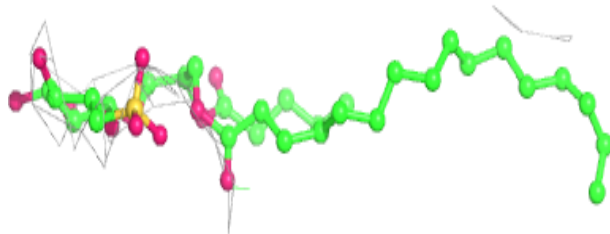
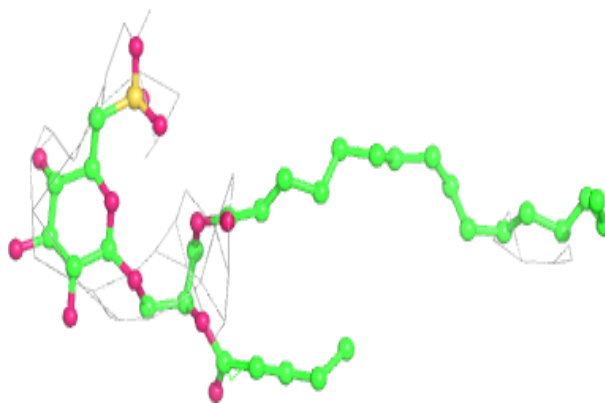
**Electron density around BCR K 101:**

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

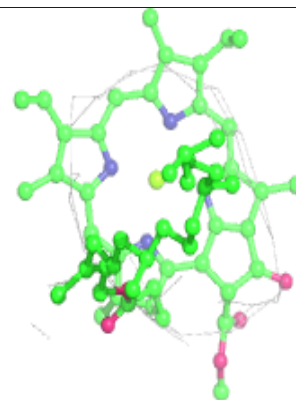
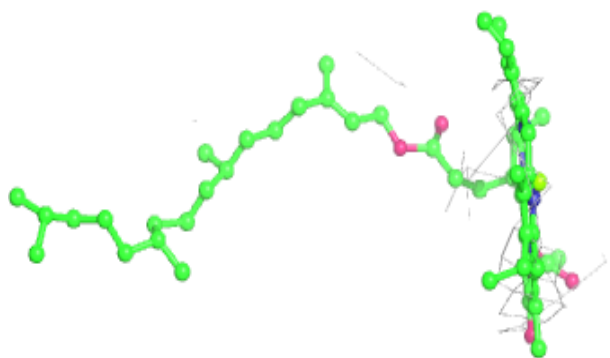
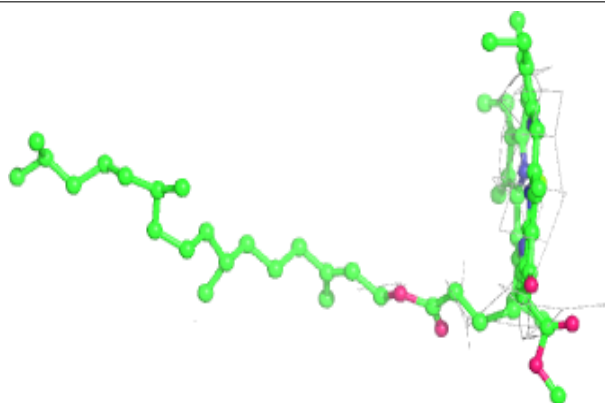


Electron density around SQD d 411:

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

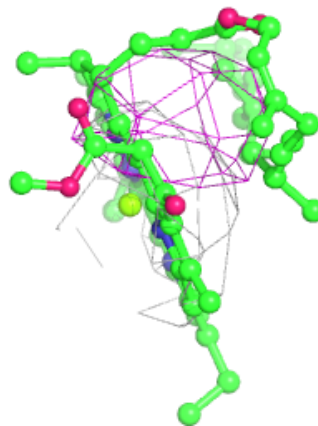
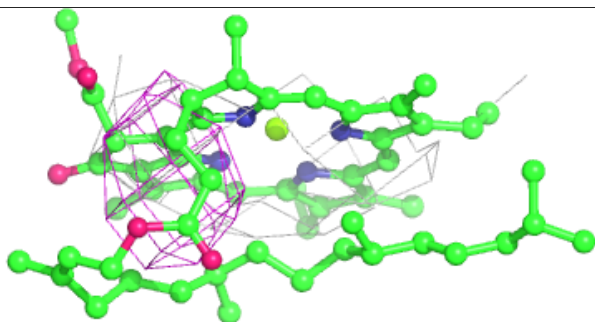
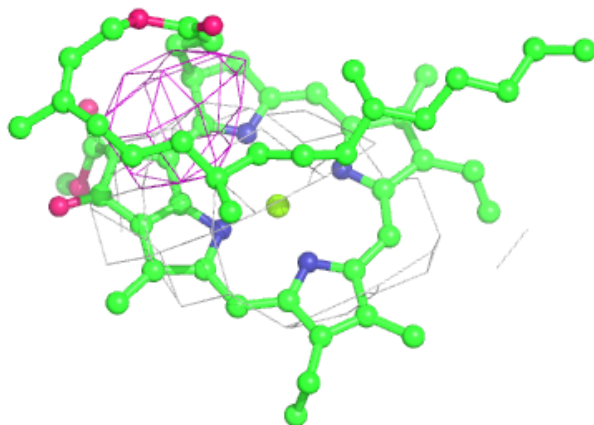
**Electron density around CLA B 607:**

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

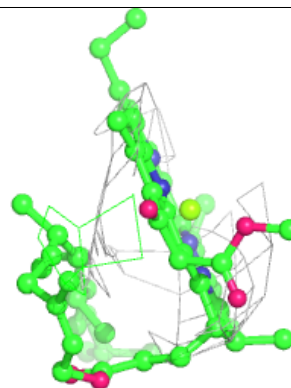
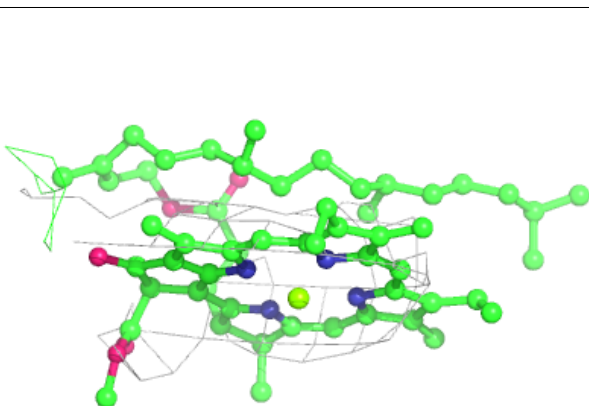
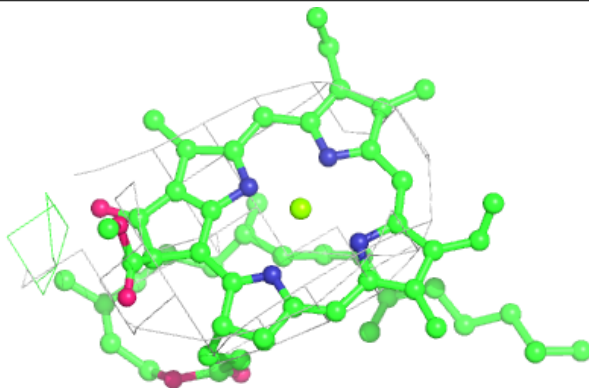


Electron density around CLA b 602:

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

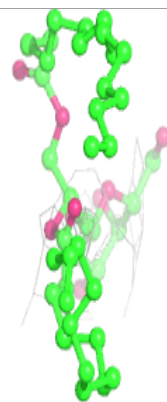
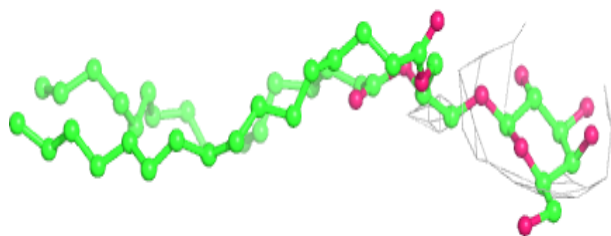
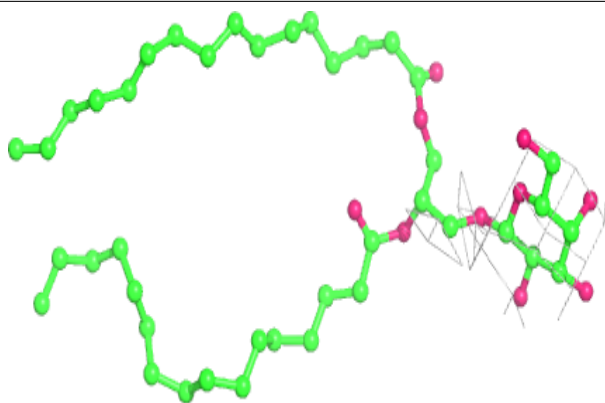
**Electron density around CLA B 602:**

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



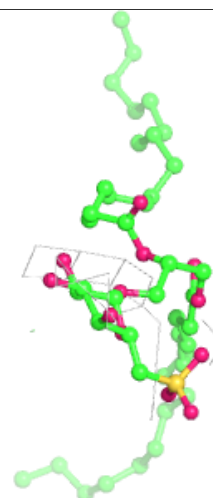
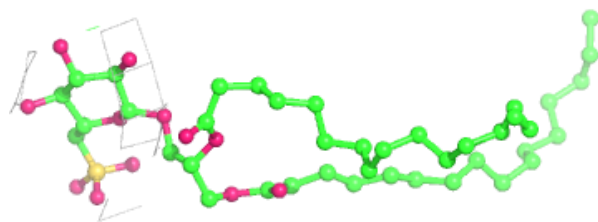
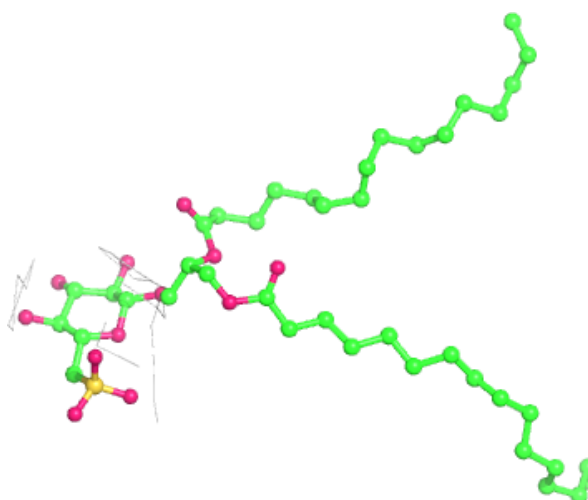
Electron density around LMG A 614:

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



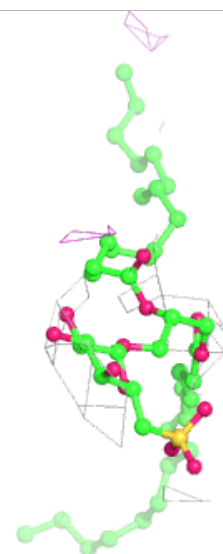
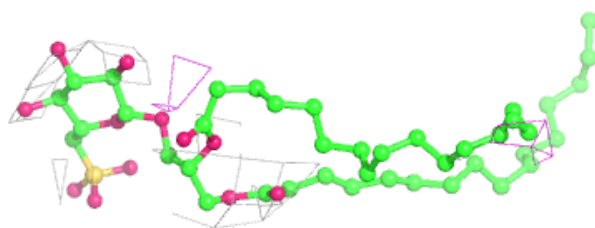
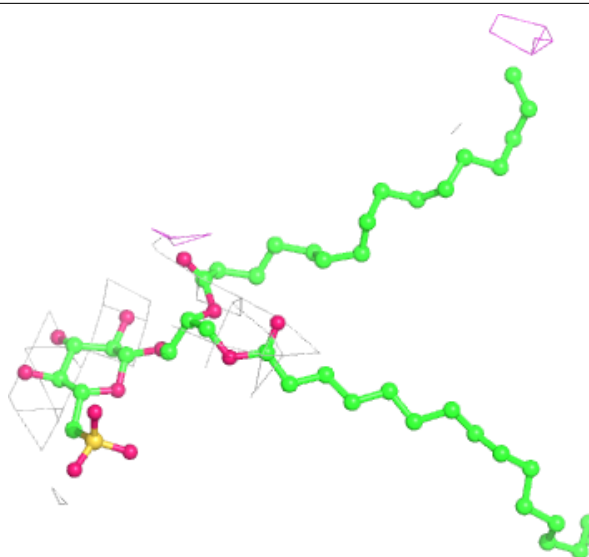
Electron density around SQD a 609:

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



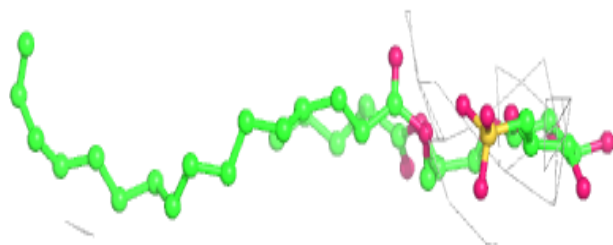
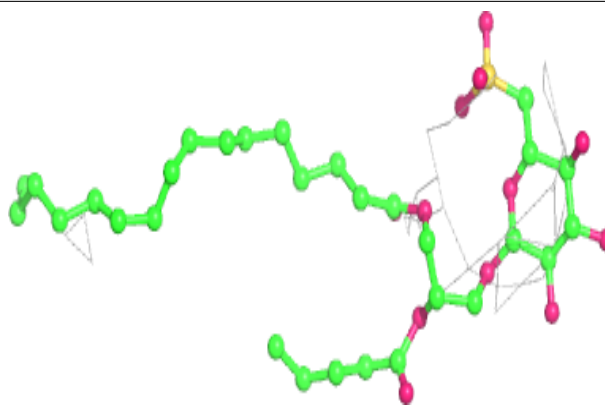
Electron density around SQD A 609:

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

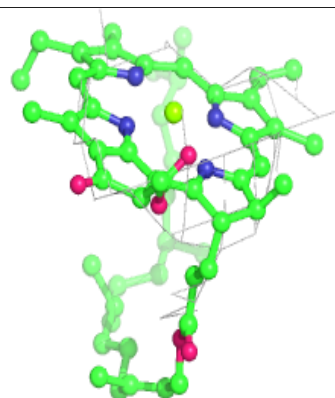
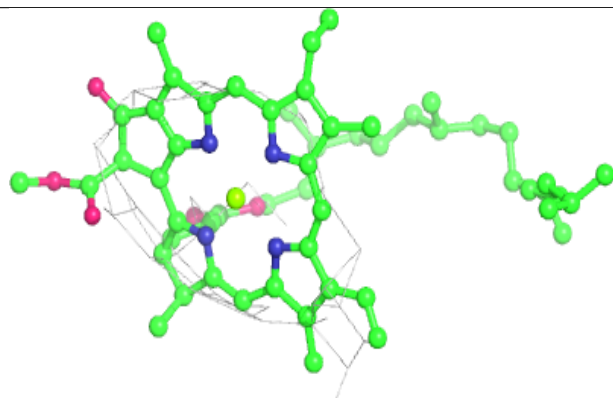
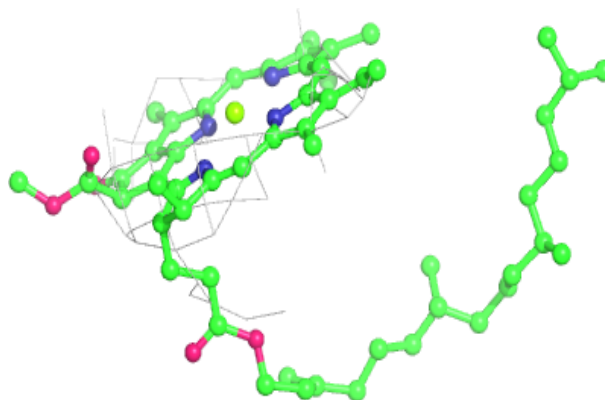


Electron density around SQD D 411:

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

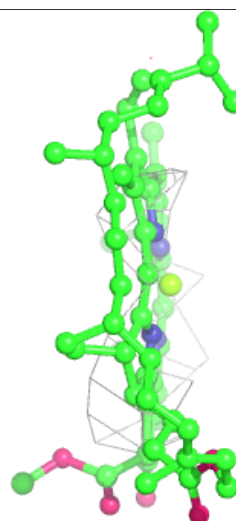
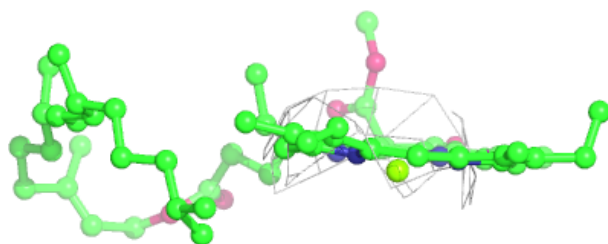
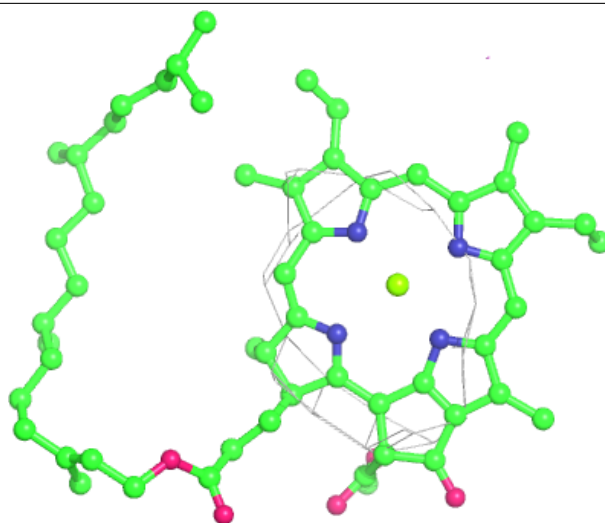
**Electron density around CLA C 513:**

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



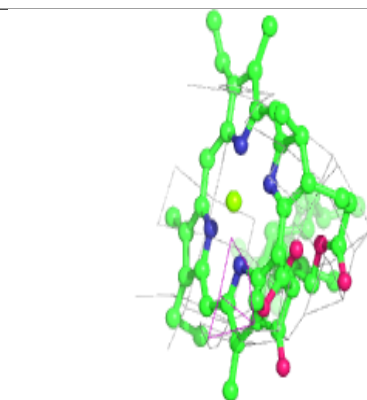
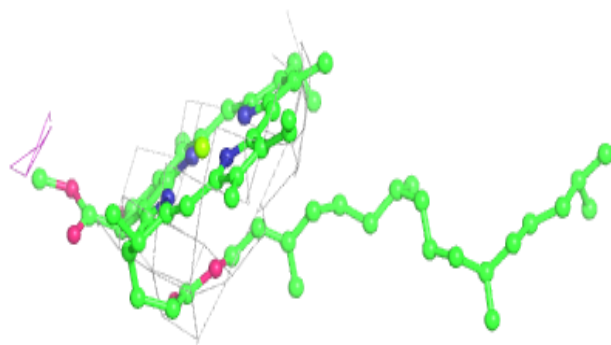
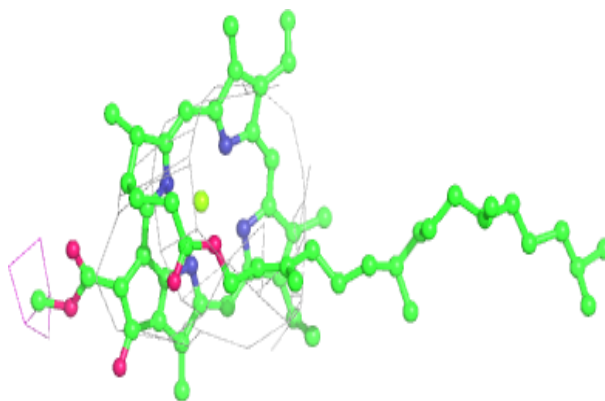
Electron density around CLA c 512:

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

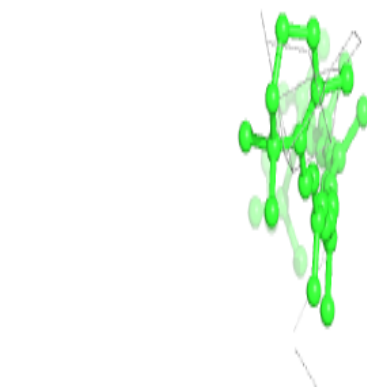
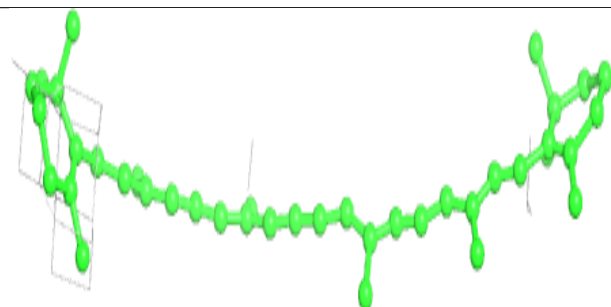
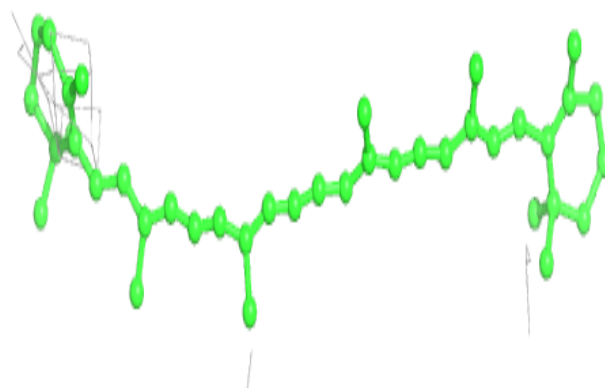


Electron density around CLA b 615:

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

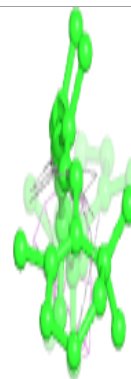
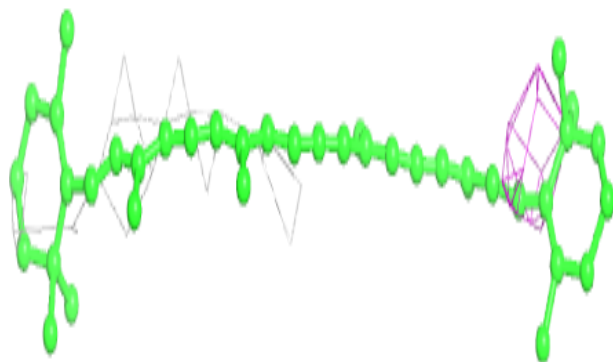
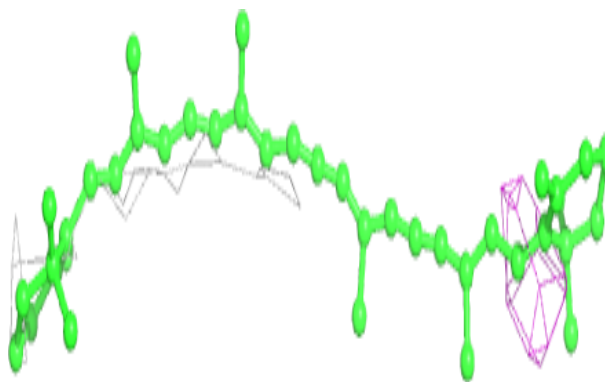
**Electron density around BCR B 622:**

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



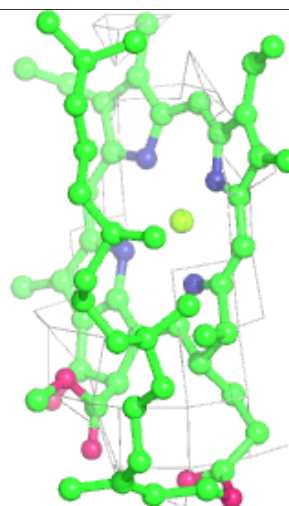
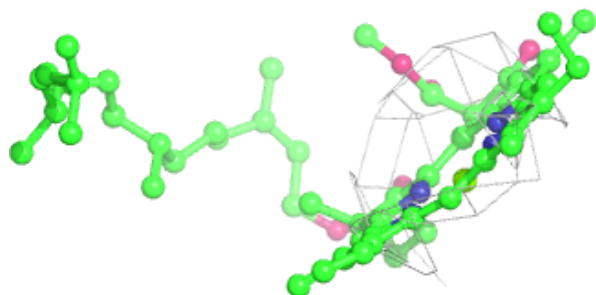
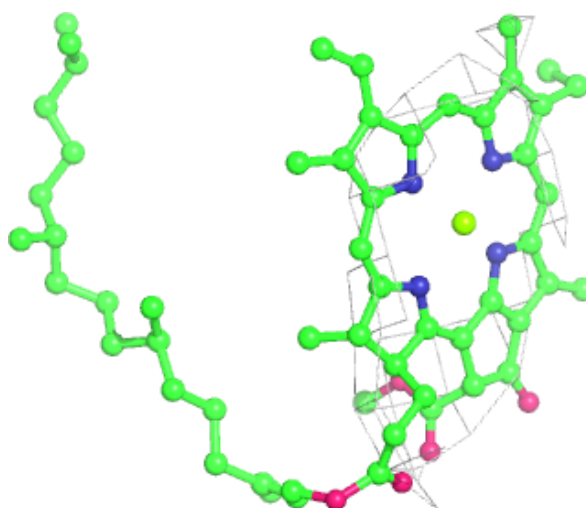
Electron density around BCR H 101:

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



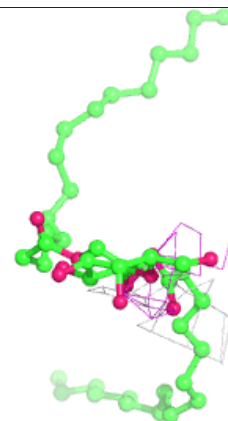
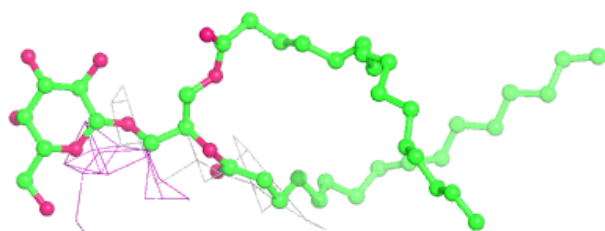
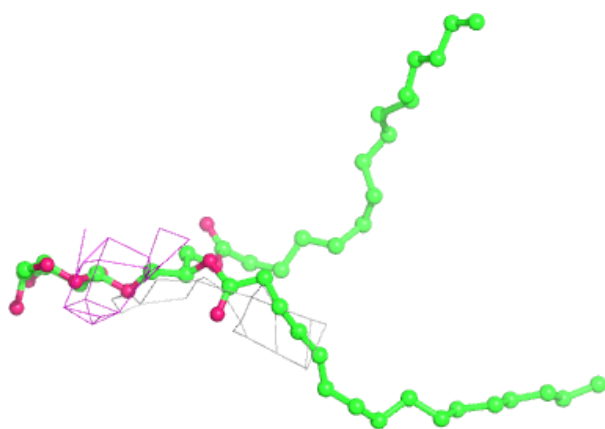
Electron density around CLA b 617:

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

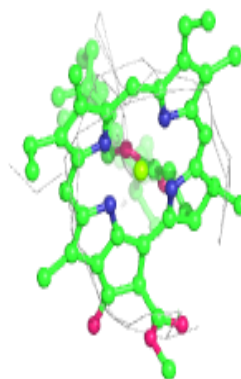
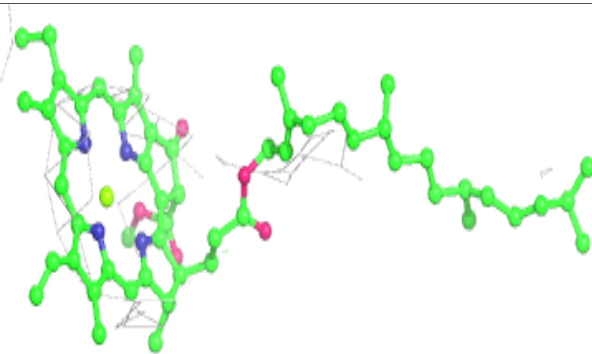
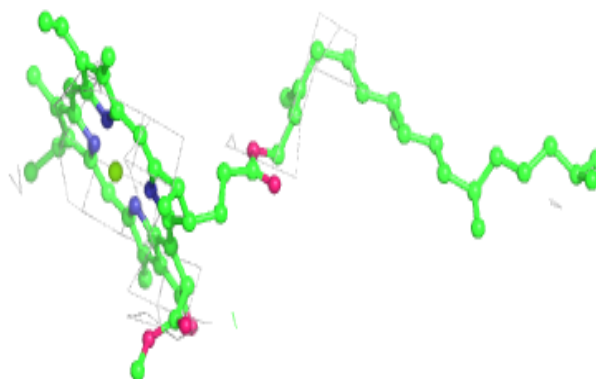


Electron density around LMG b 619:

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

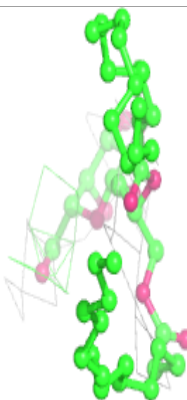
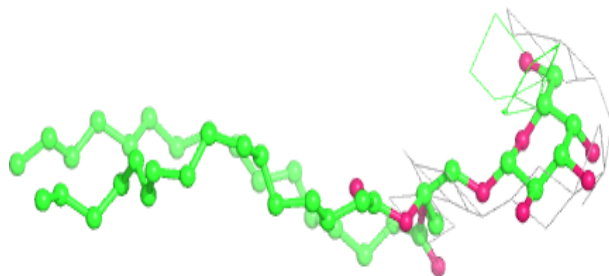
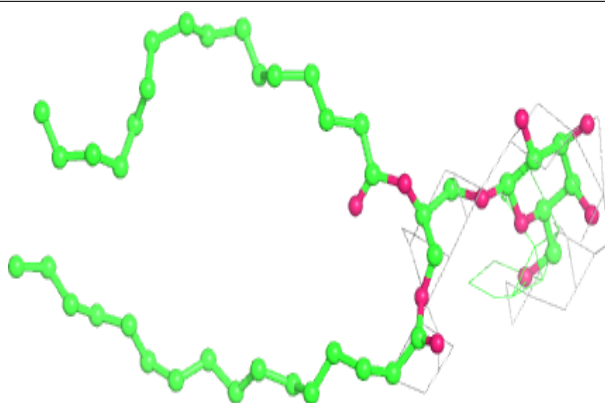
**Electron density around CLA c 502:**

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

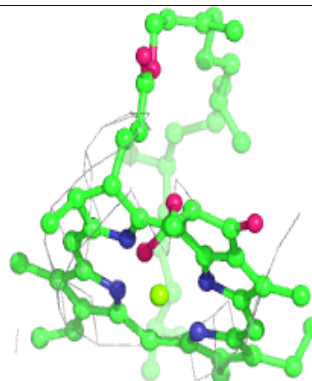
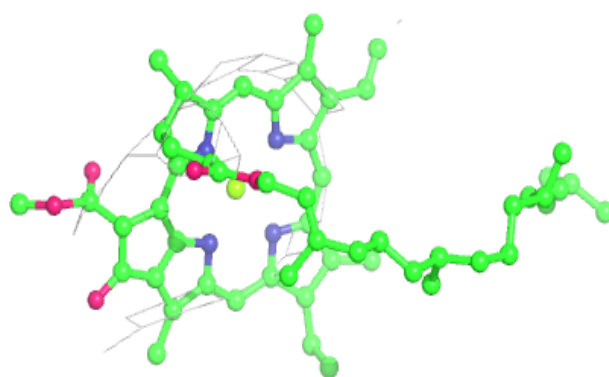
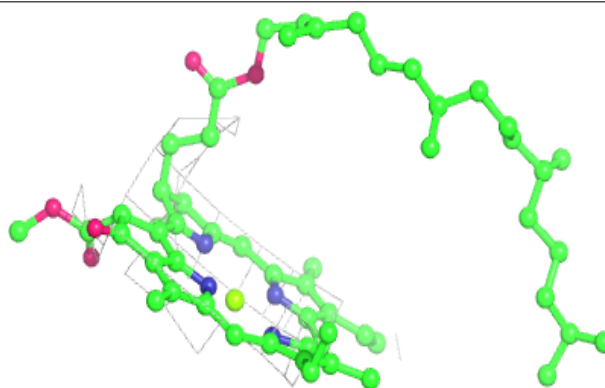


Electron density around LMG a 614:

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

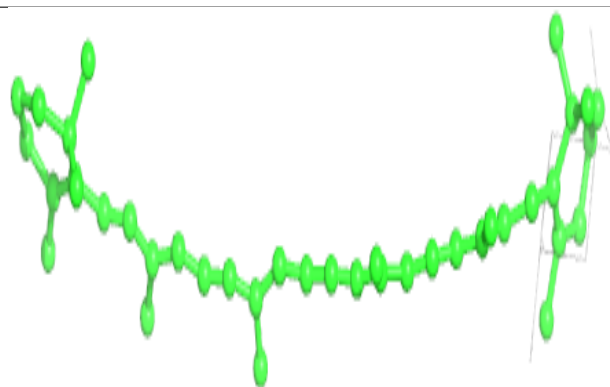
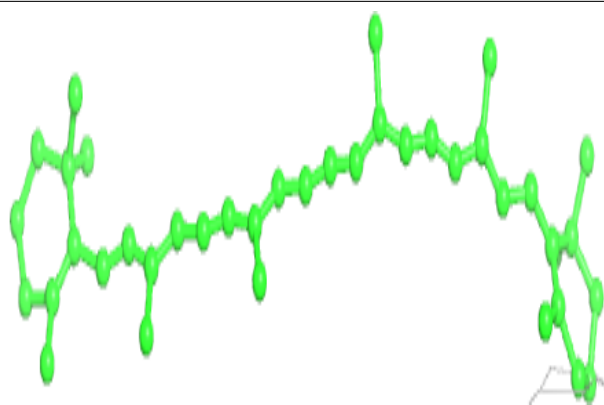
**Electron density around CLA c 513:**

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



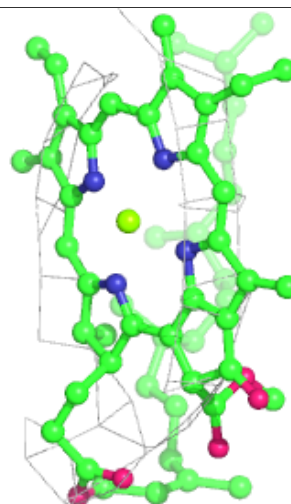
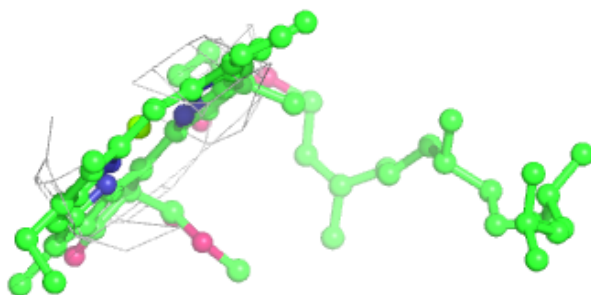
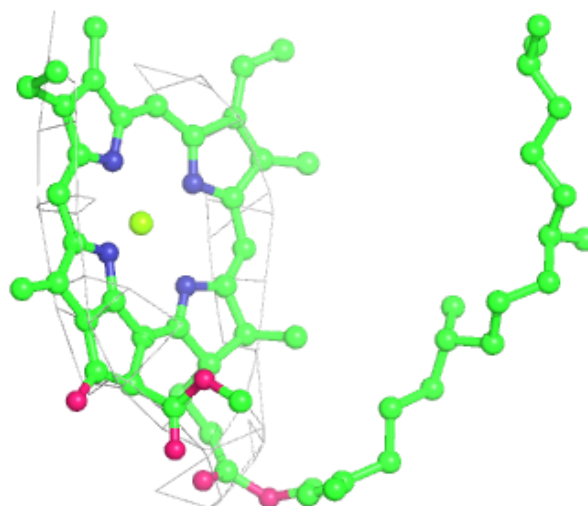
Electron density around BCR b 622:

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



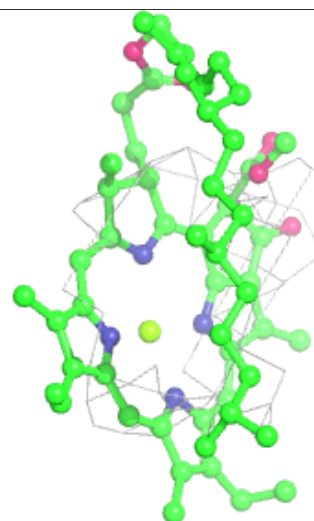
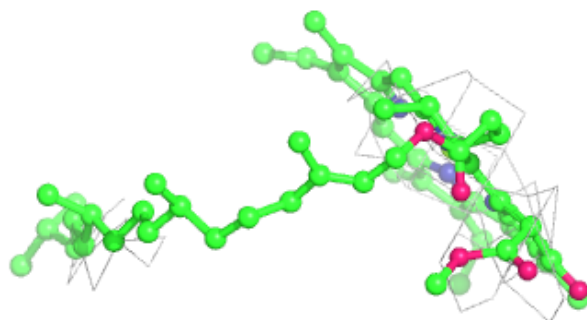
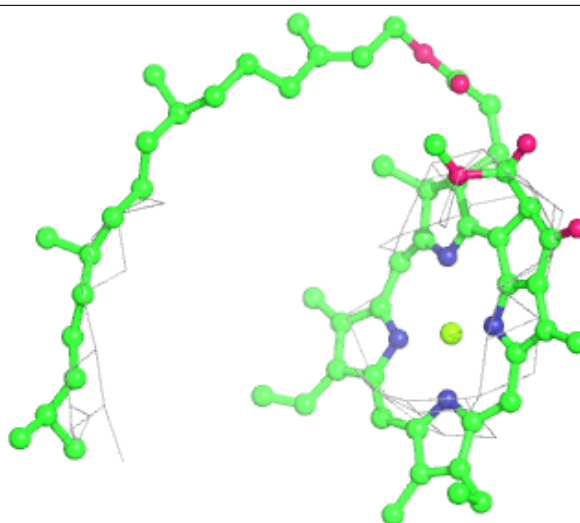
Electron density around CLA B 617:

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



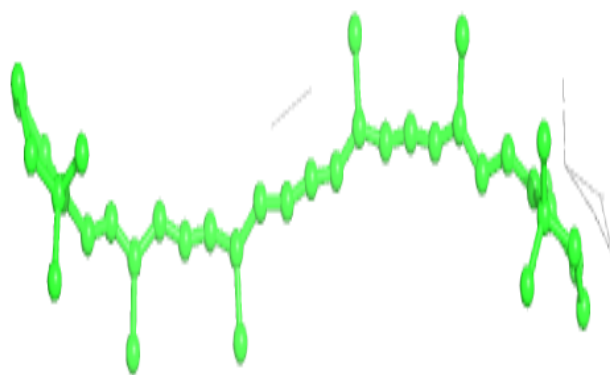
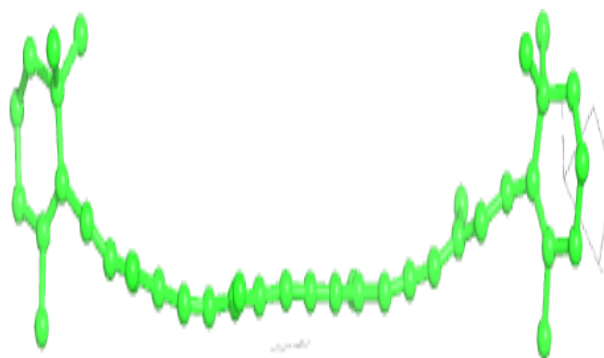
Electron density around CLA C 507:

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



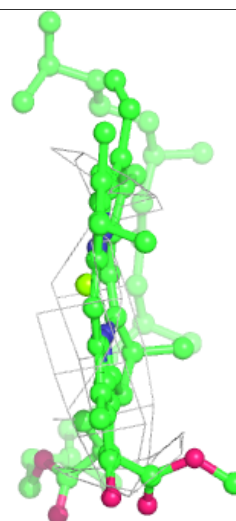
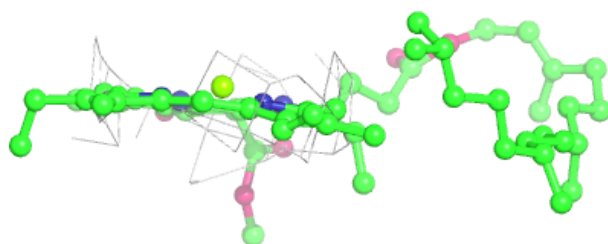
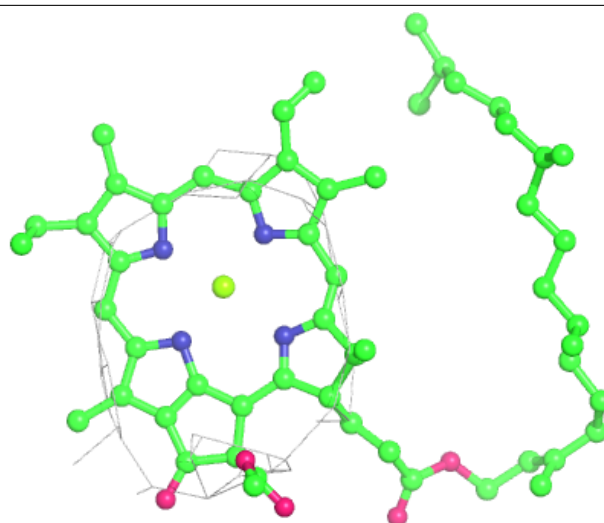
Electron density around BCR k 102:

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



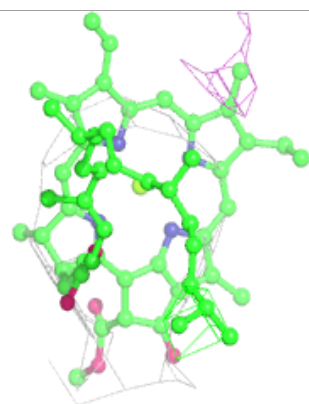
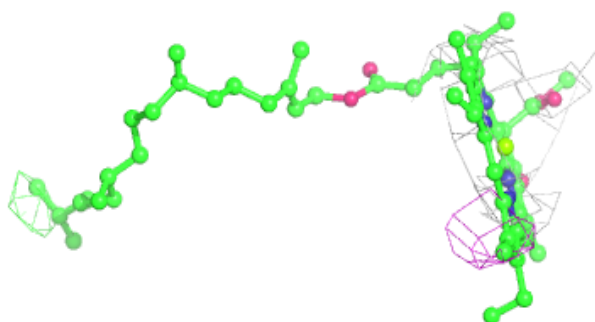
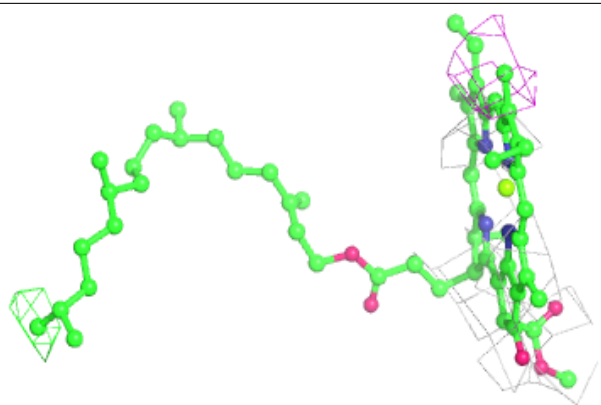
Electron density around CLA C 512:

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

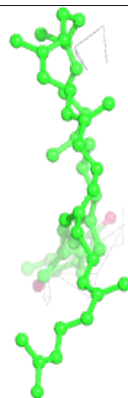
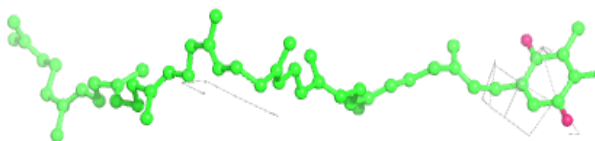
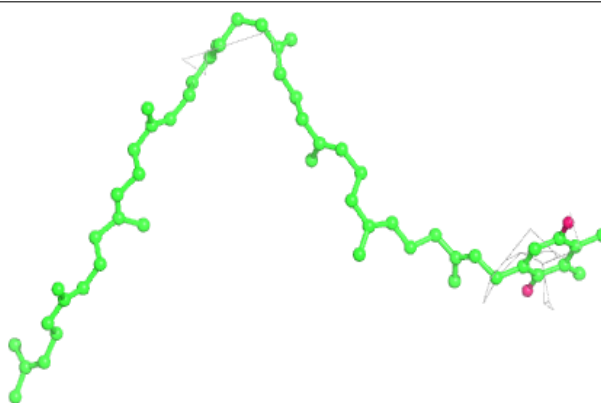


Electron density around CLA D 403:

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

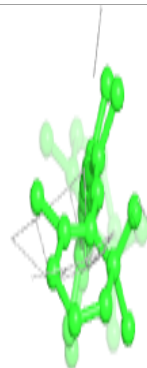
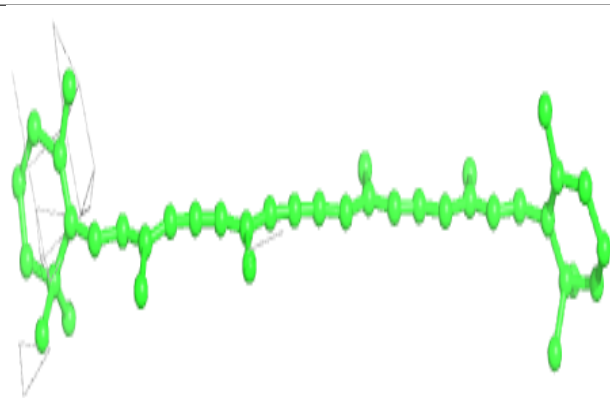
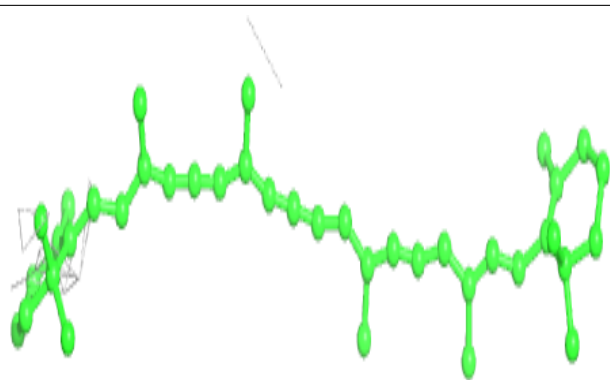
**Electron density around PL9 D 408:**

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

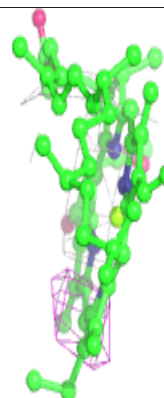
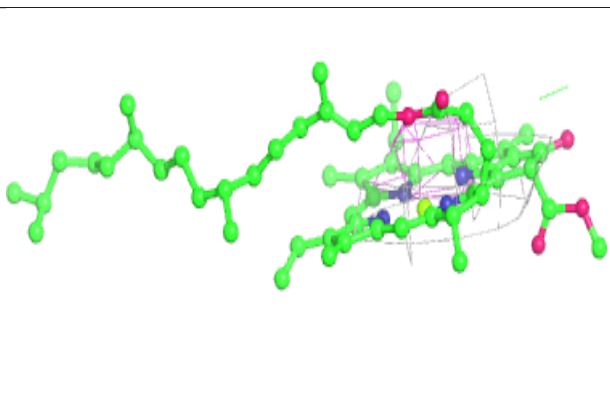
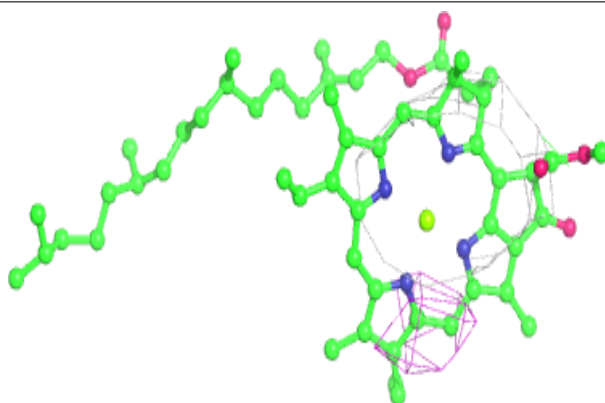


Electron density around BCR c 514:

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

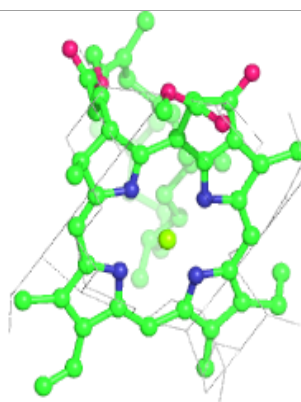
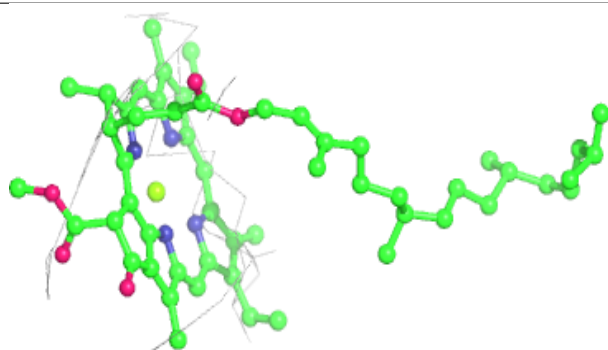
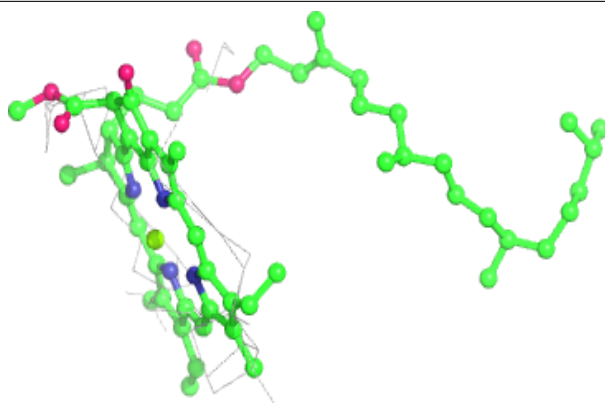
**Electron density around CLA c 501:**

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

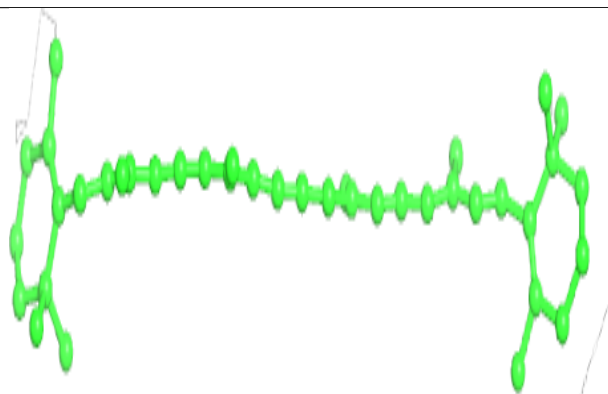
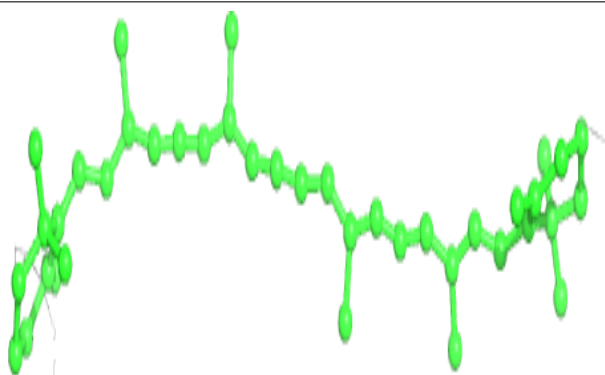


Electron density around CLA C 508:

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

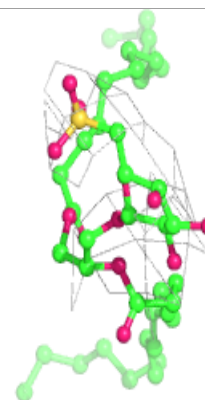
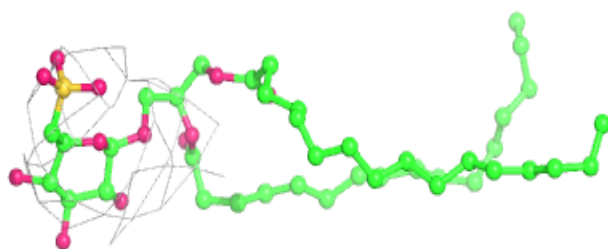
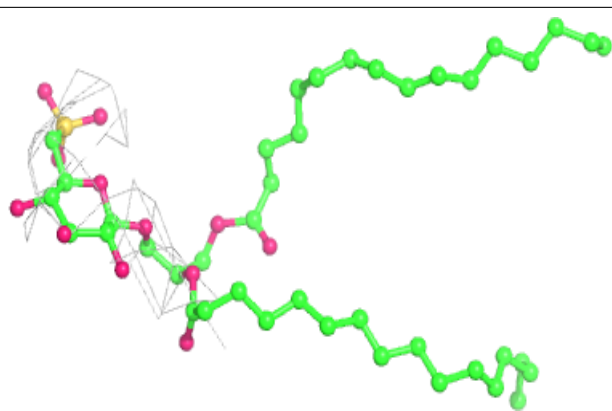
**Electron density around BCR C 515:**

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

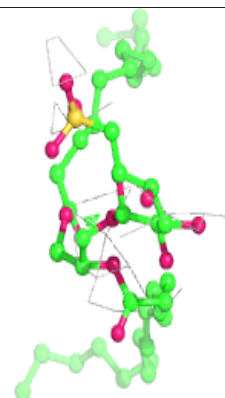
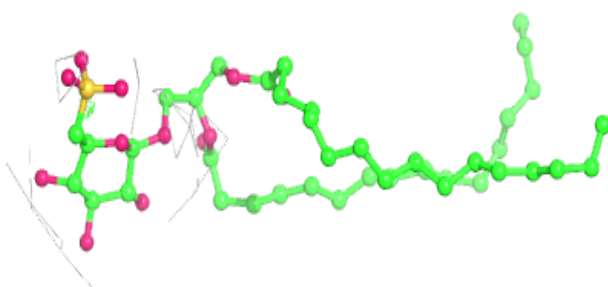
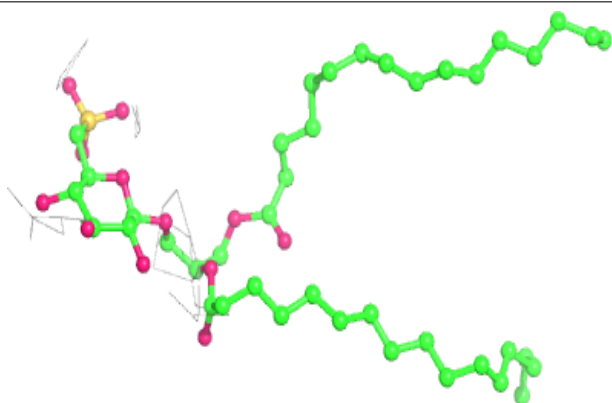


Electron density around SQD B 601:

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

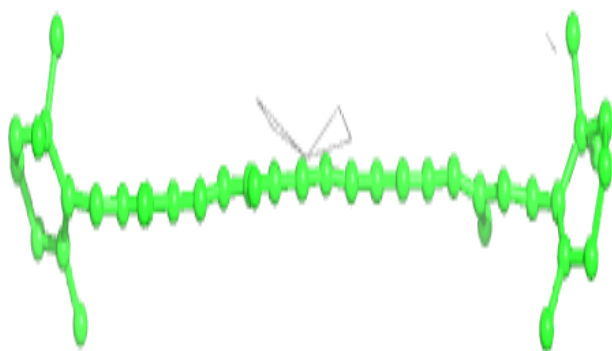
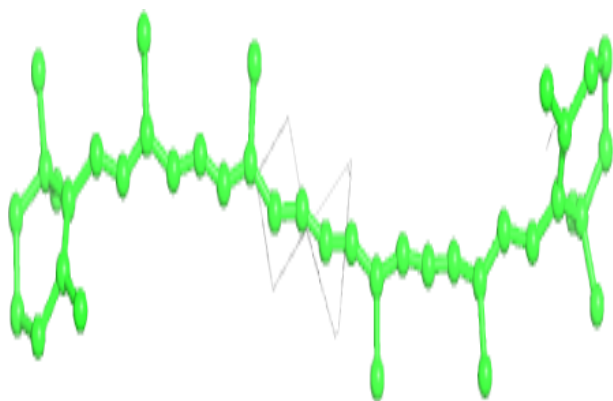
**Electron density around SQD b 601:**

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

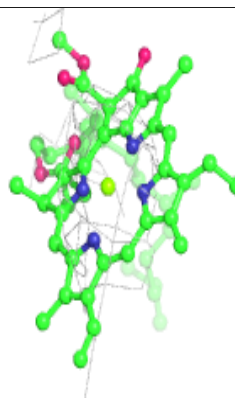
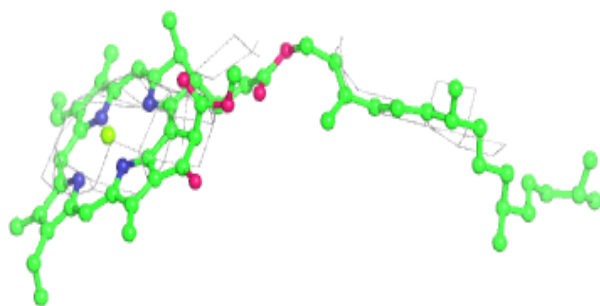
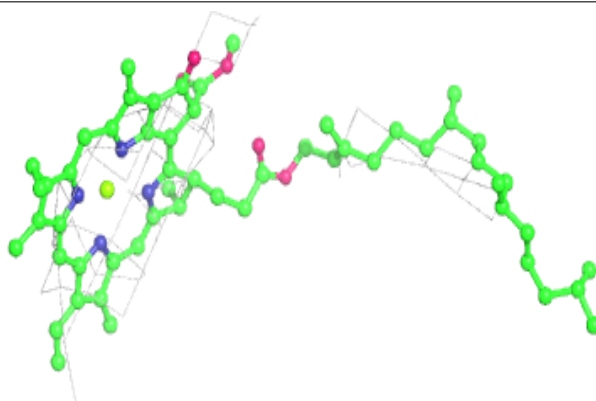


Electron density around BCR B 619:

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

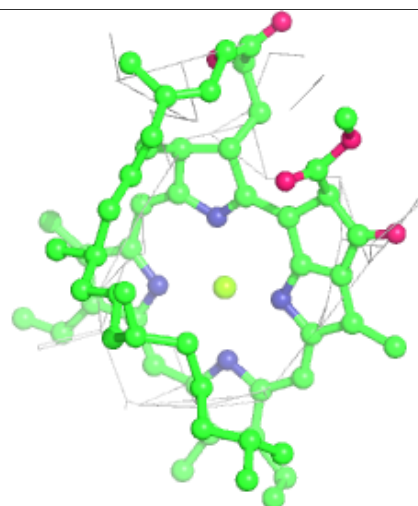
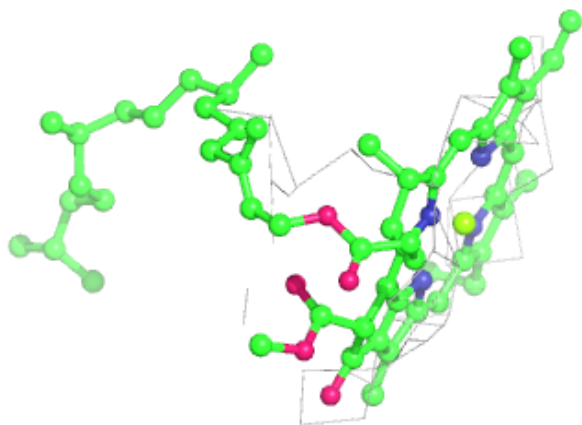
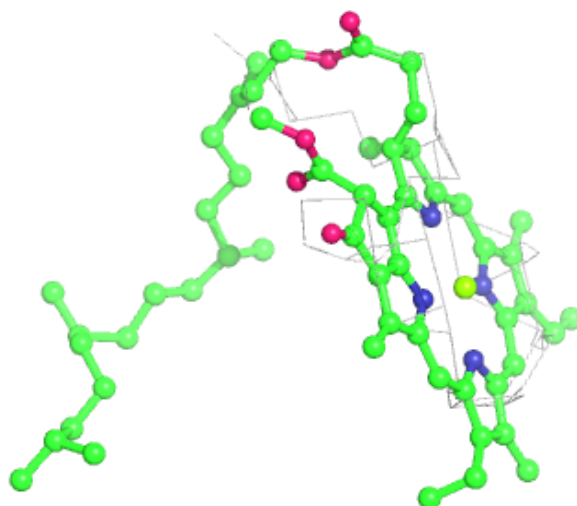
**Electron density around CLA a 603:**

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



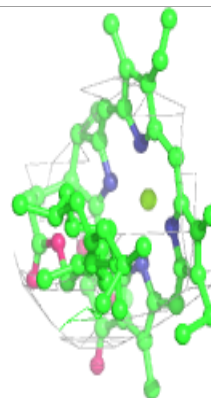
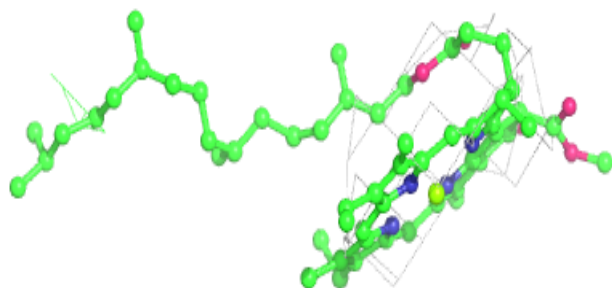
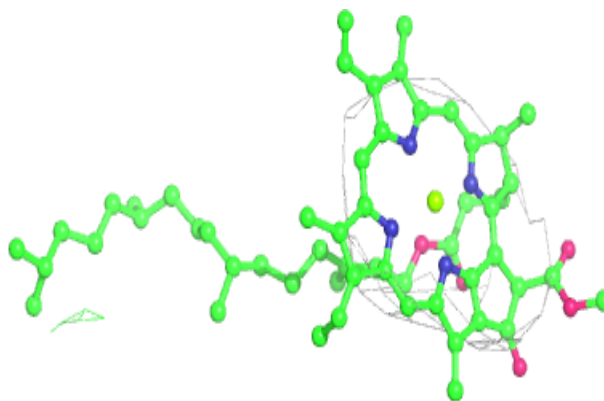
Electron density around CLA b 614:

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

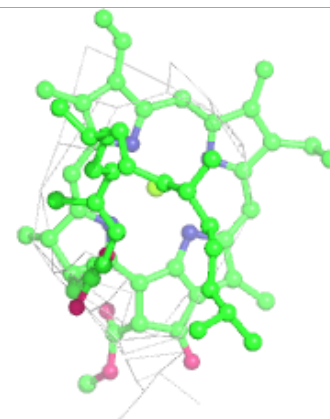
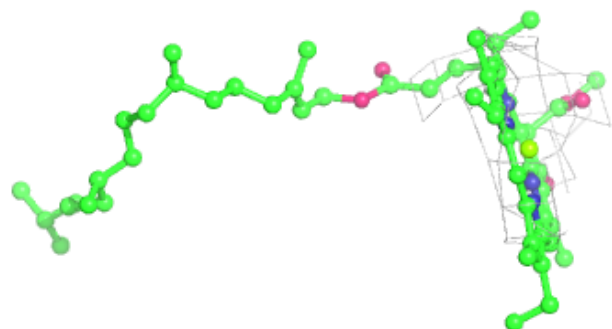
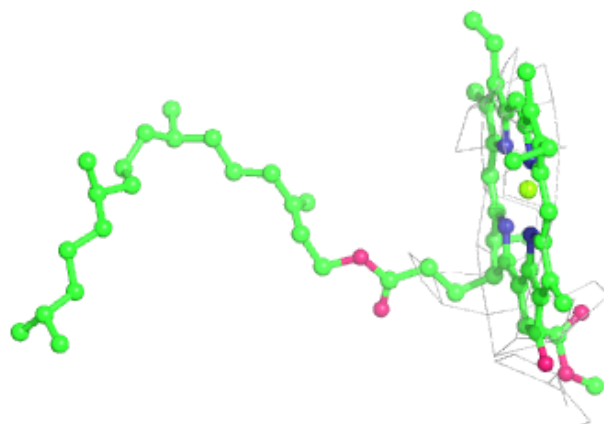


Electron density around CLA B 615:

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

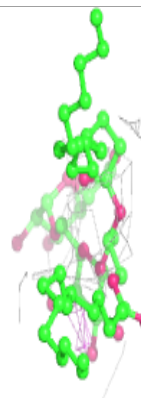
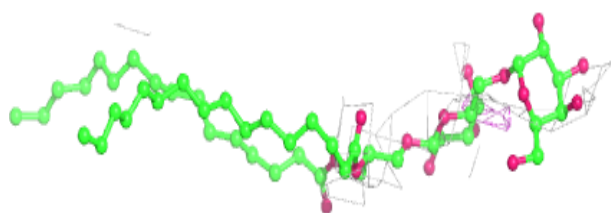
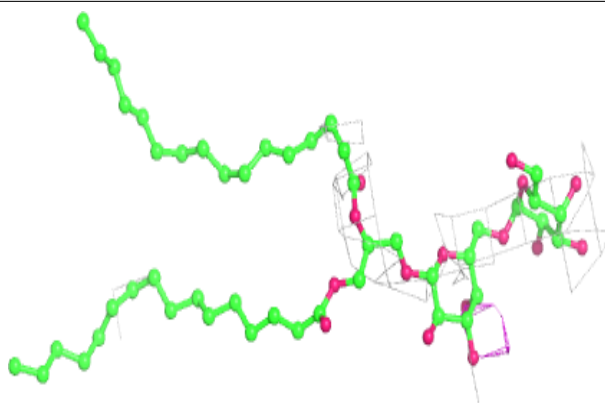
**Electron density around CLA d 403:**

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

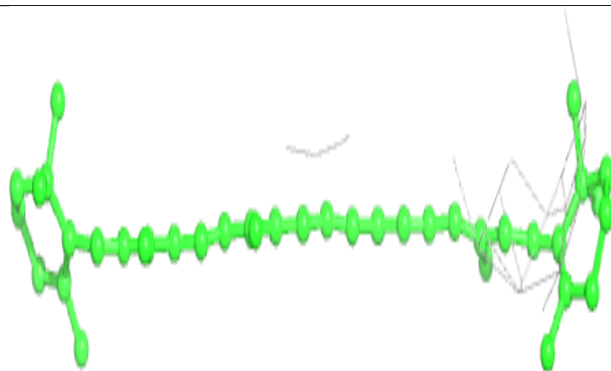
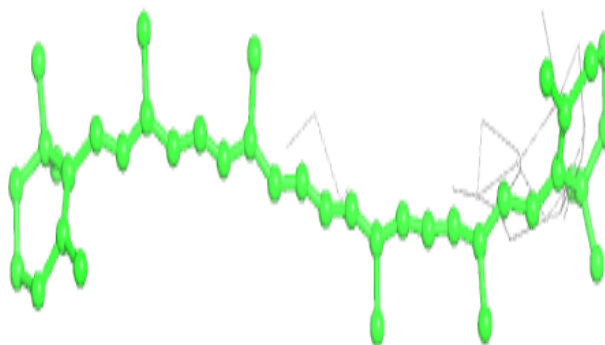


Electron density around DGD C 518:

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

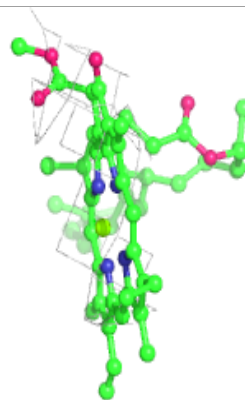
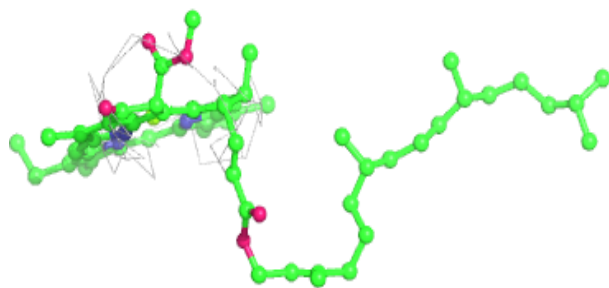
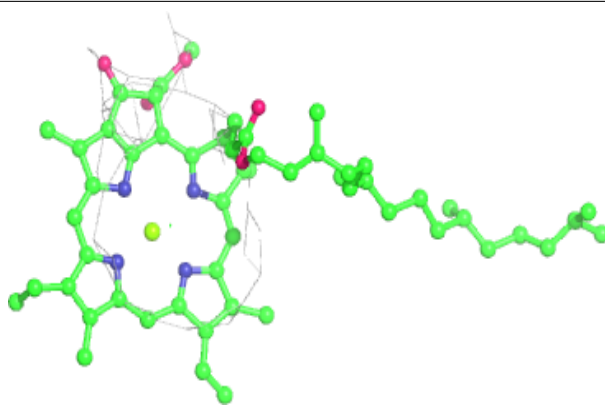
**Electron density around BCR b 618:**

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

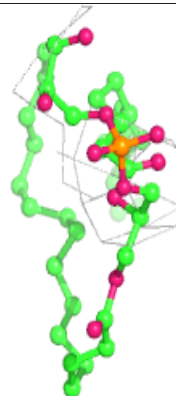
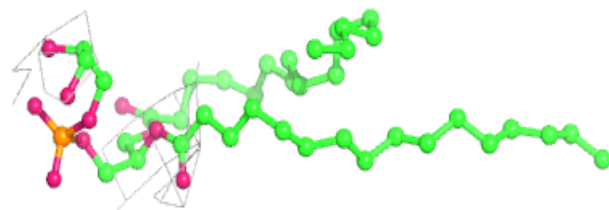
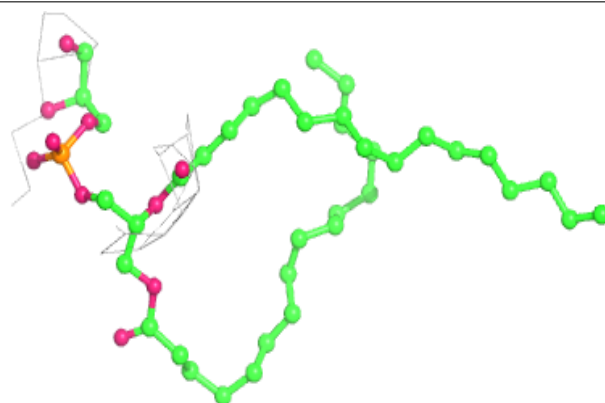


Electron density around CLA A 604:

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

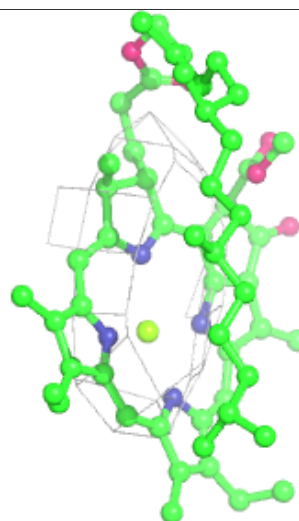
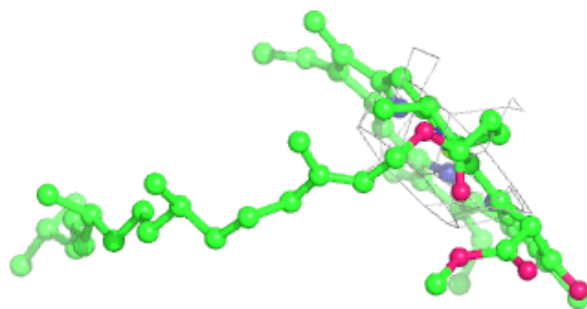
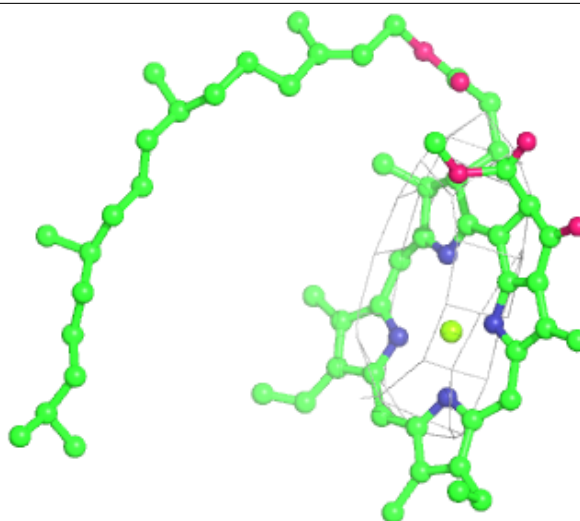
**Electron density around LHG D 409:**

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



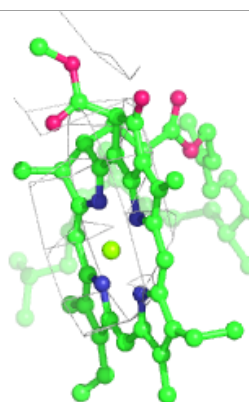
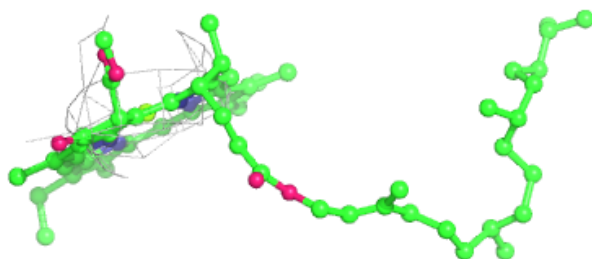
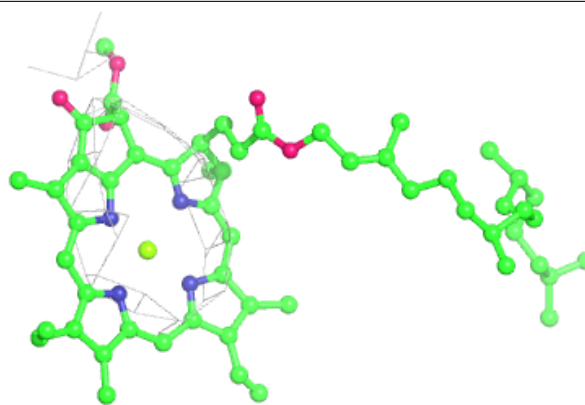
Electron density around CLA c 507:

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

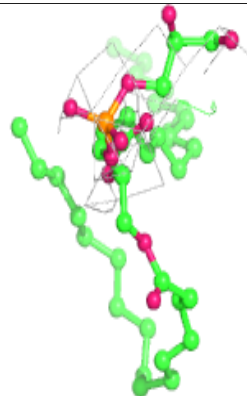
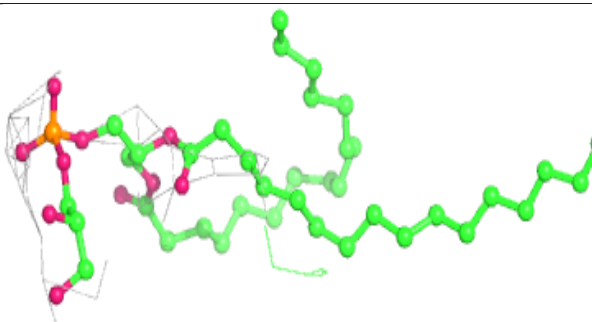
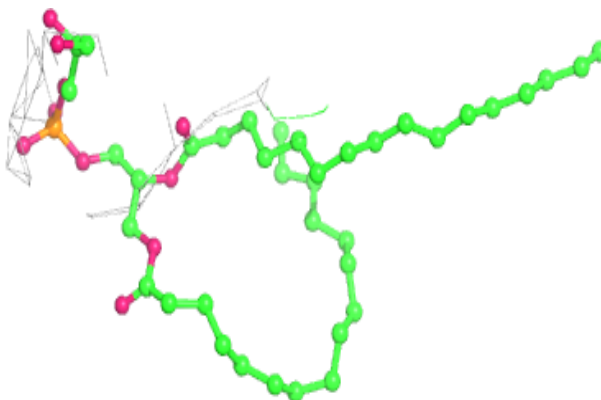


Electron density around CLA a 607:

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

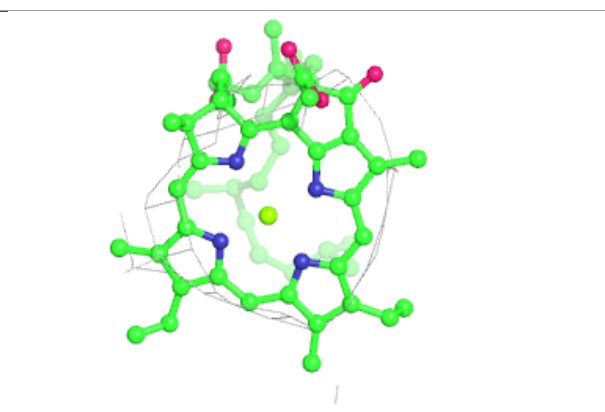
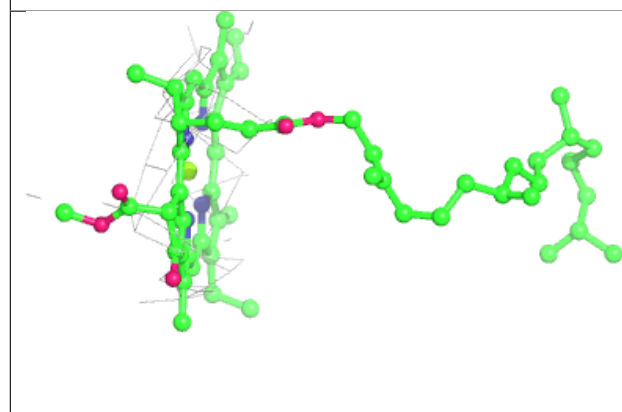
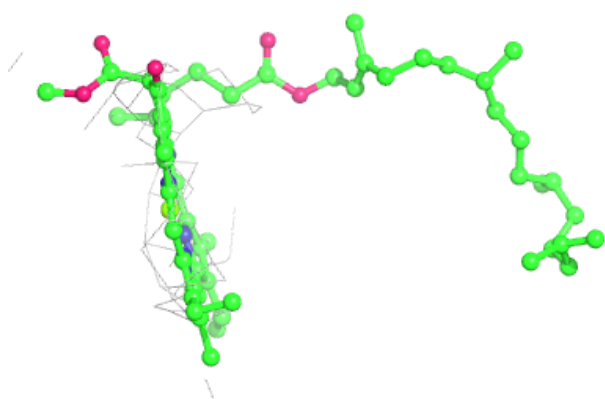
**Electron density around LHG D 405:**

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

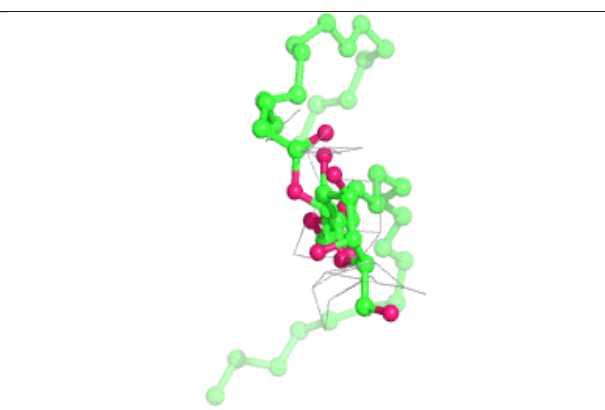
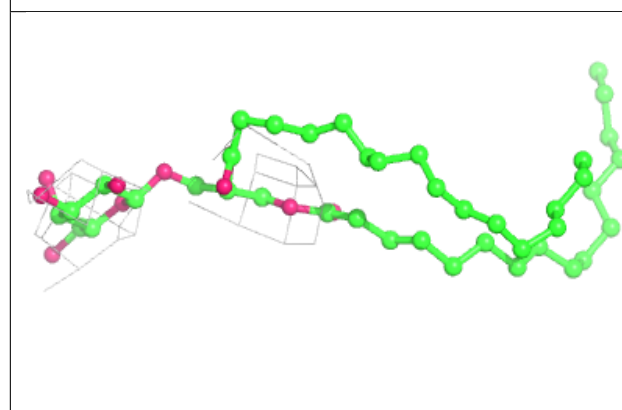
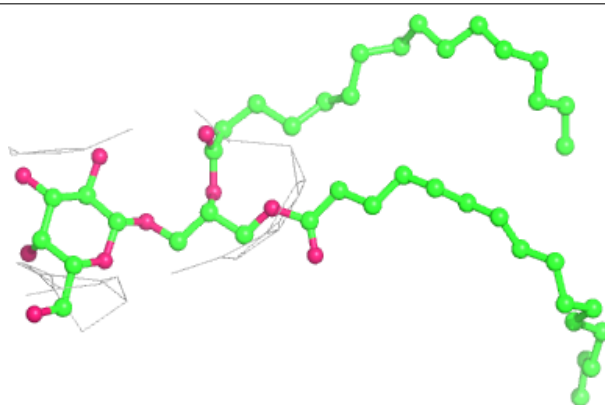


Electron density around CLA C 506:

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

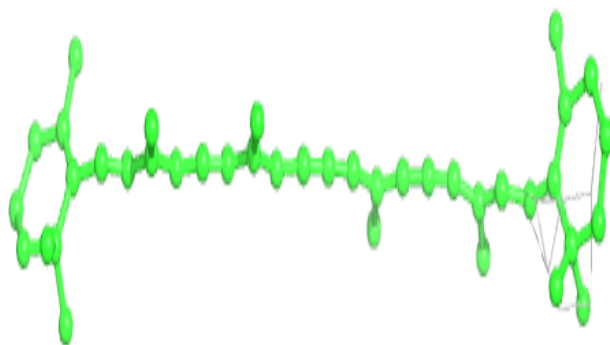
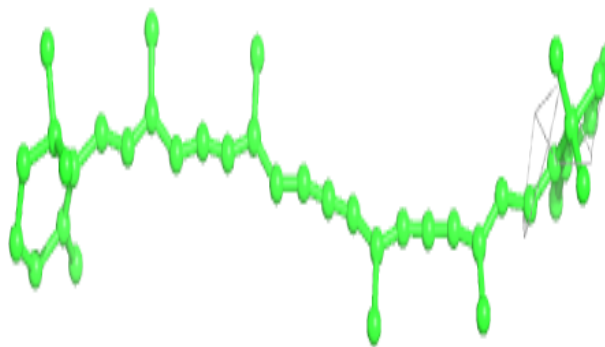
**Electron density around LMG d 406:**

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

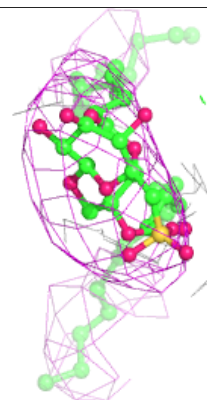
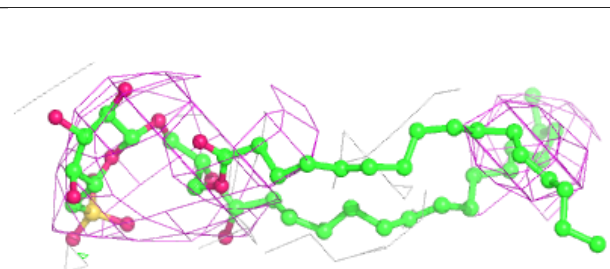
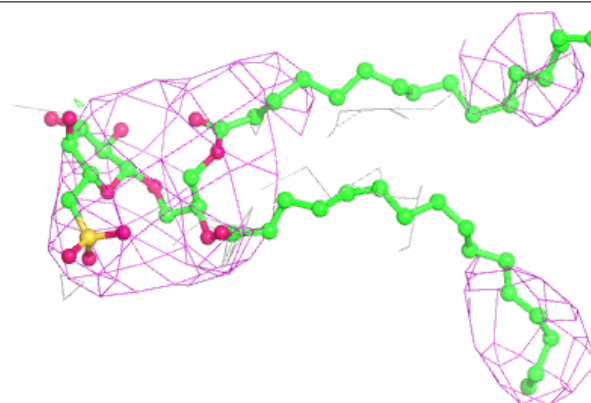


Electron density around BCR C 514:

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

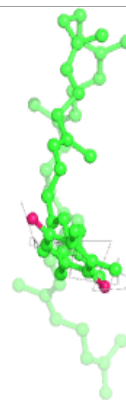
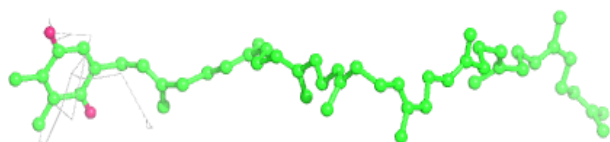
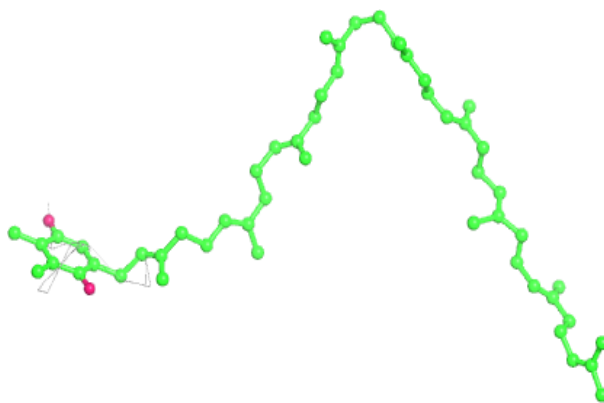
**Electron density around SQD b 621:**

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

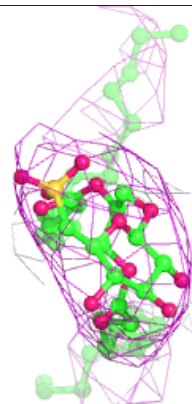
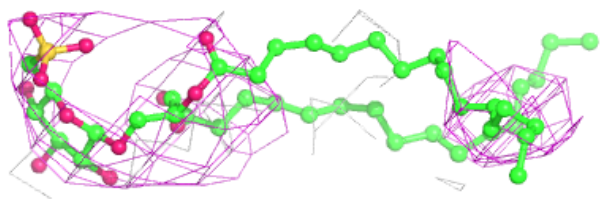
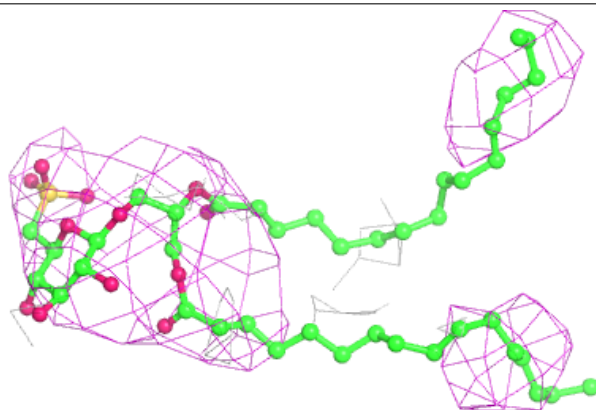


Electron density around PL9 d 408:

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

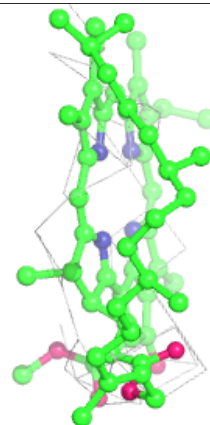
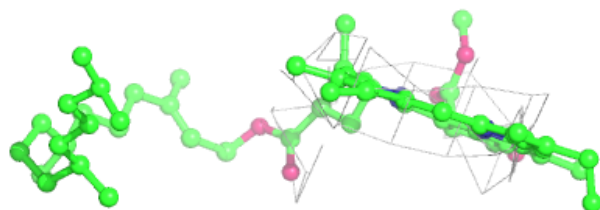
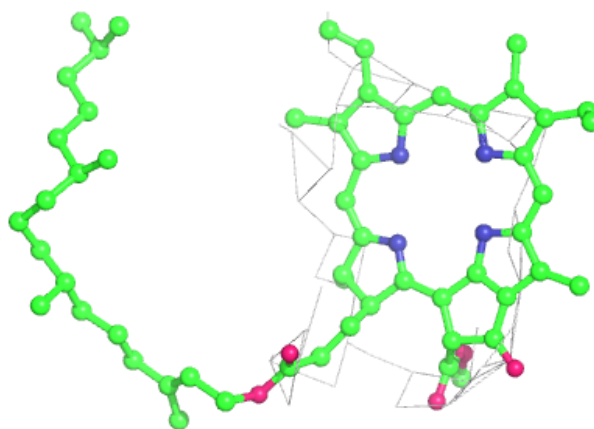
**Electron density around SQD L 101:**

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

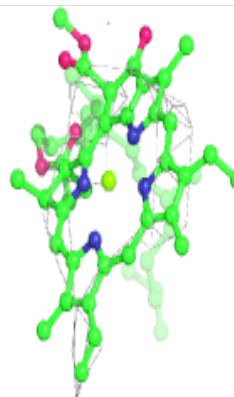
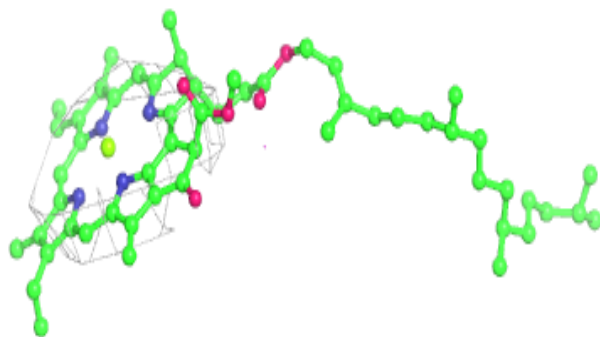
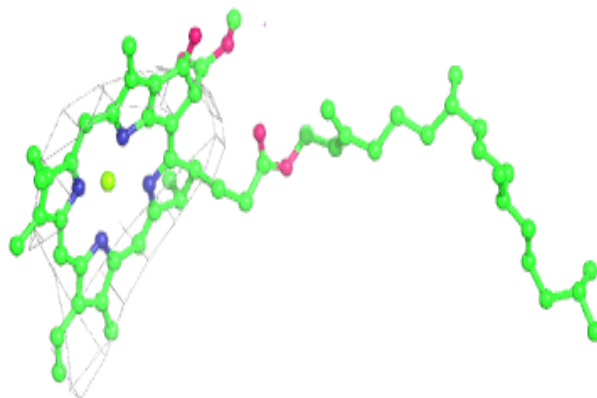


Electron density around PHO A 605:

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

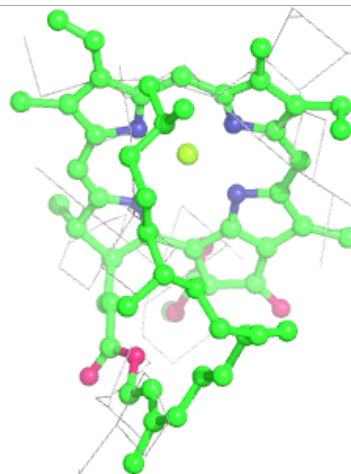
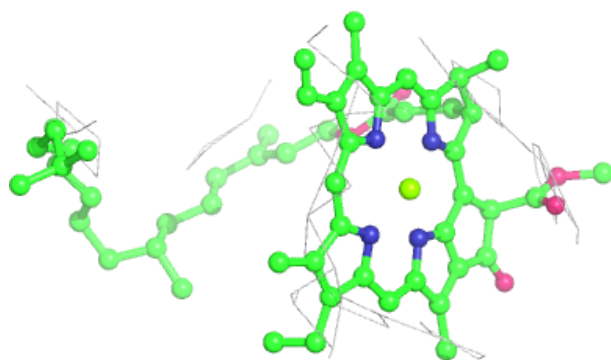
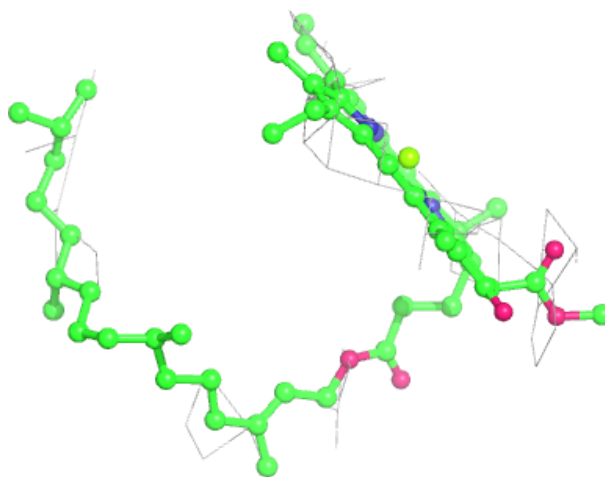
**Electron density around CLA A 603:**

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



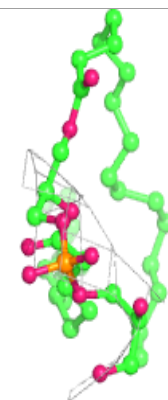
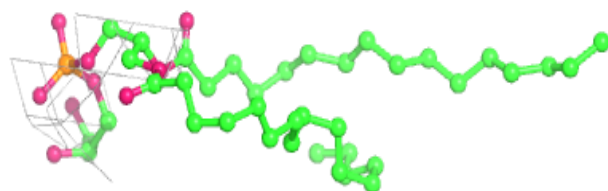
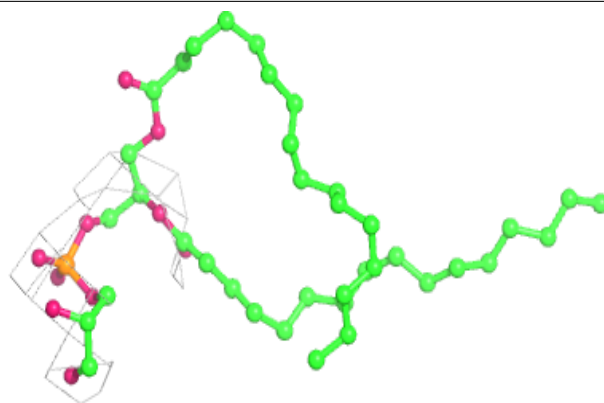
Electron density around CLA b 612:

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

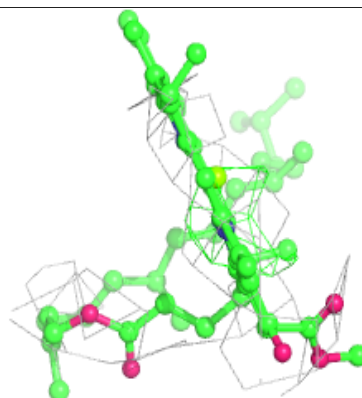
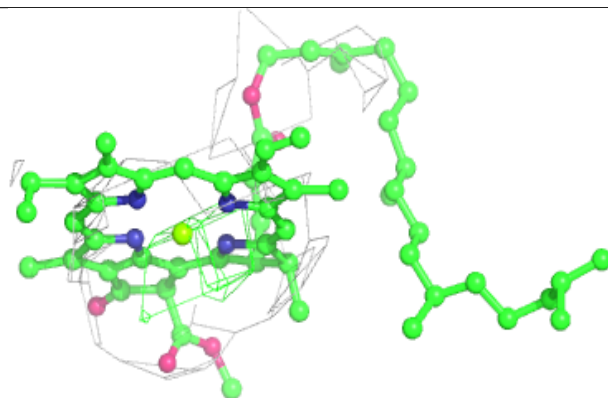
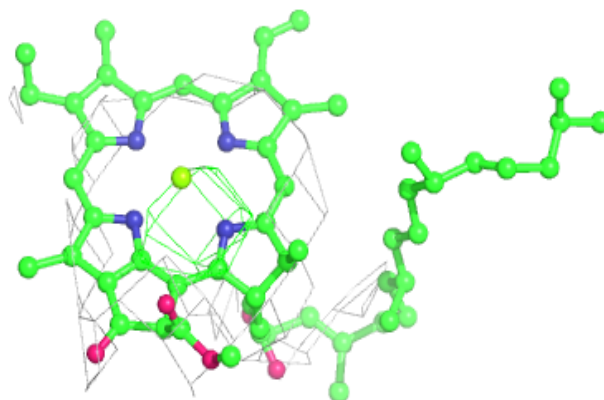


Electron density around LHG d 409:

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

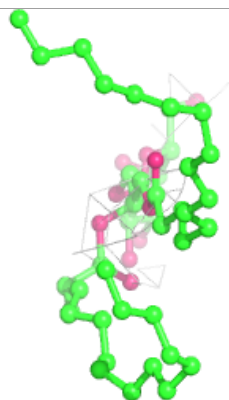
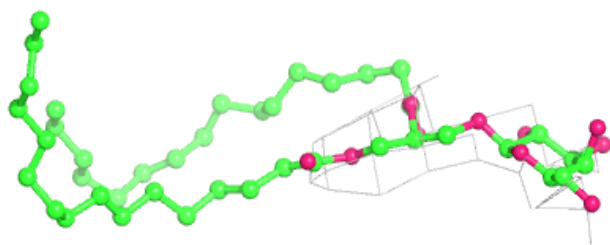
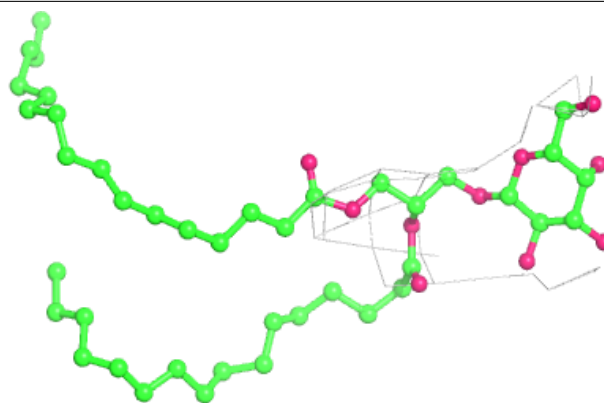
**Electron density around CLA D 402:**

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

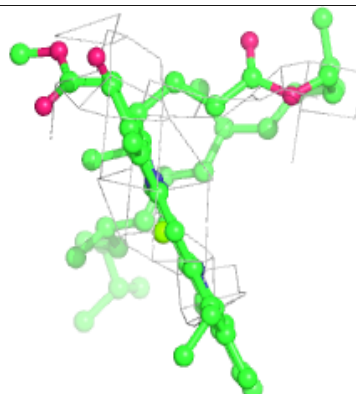
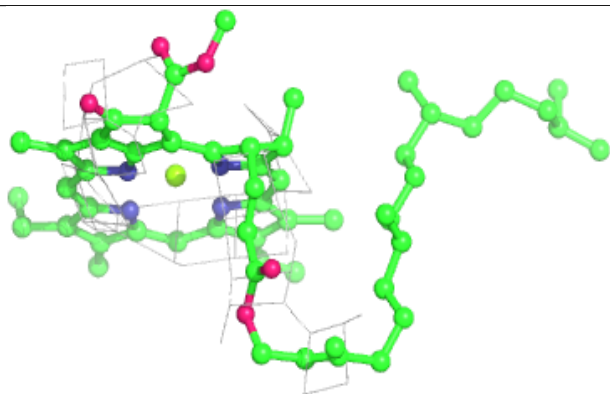
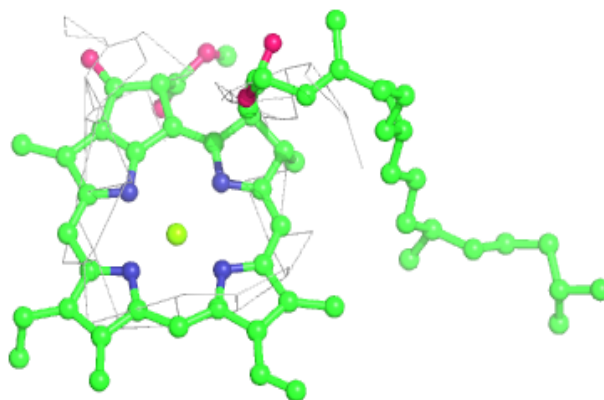


Electron density around LMG D 406:

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

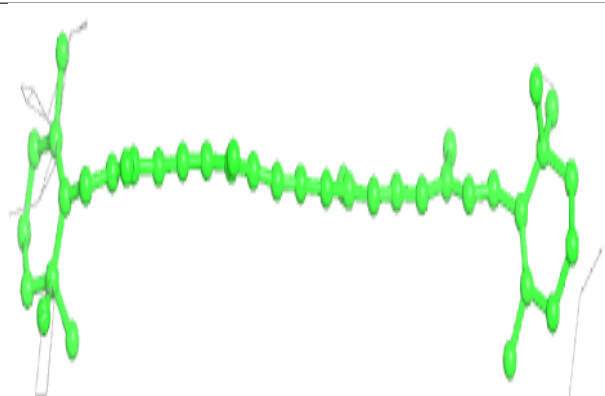
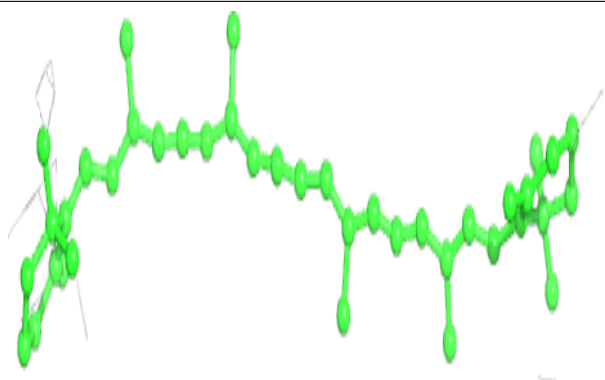
**Electron density around CLA d 402:**

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



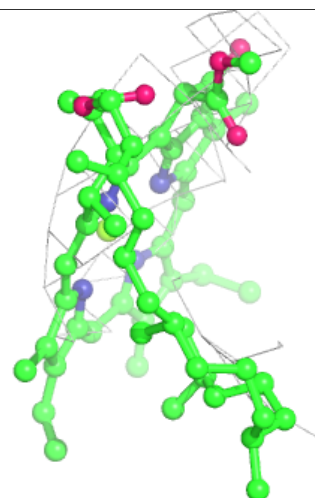
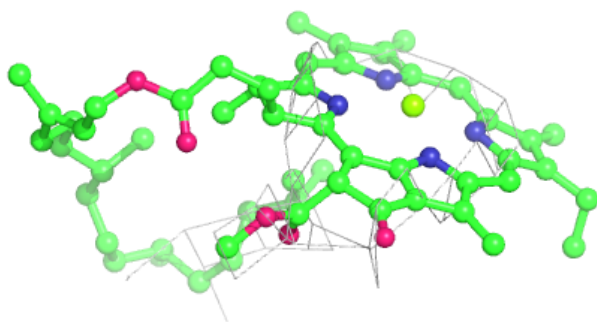
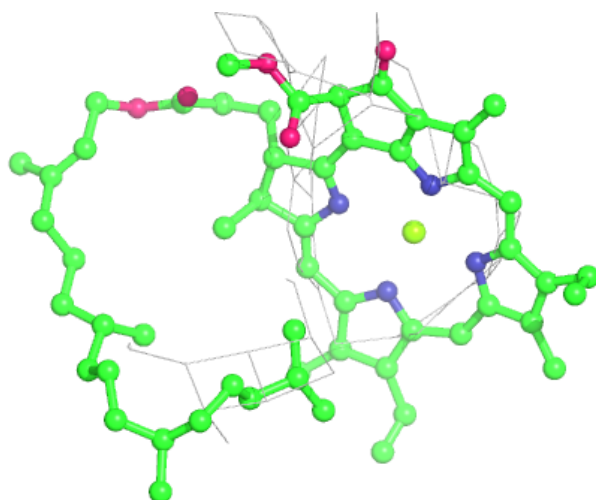
Electron density around BCR c 515:

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



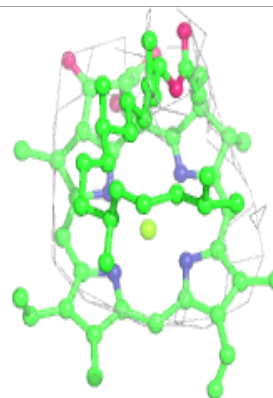
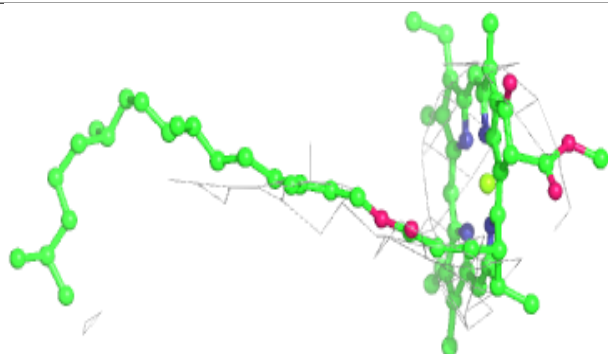
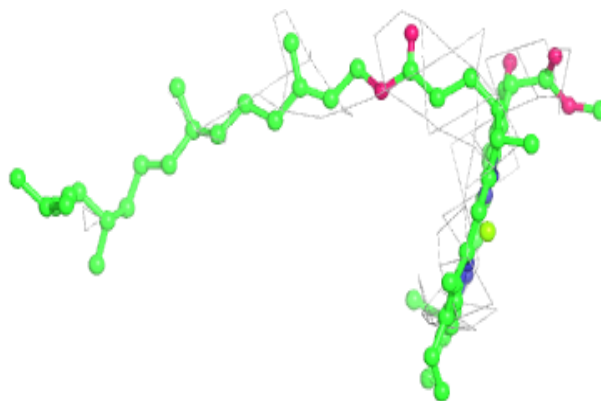
Electron density around CLA B 616:

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

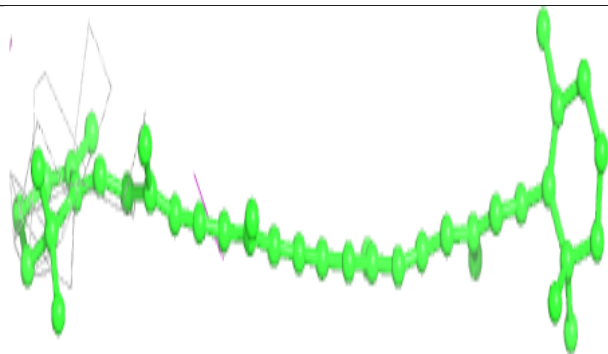
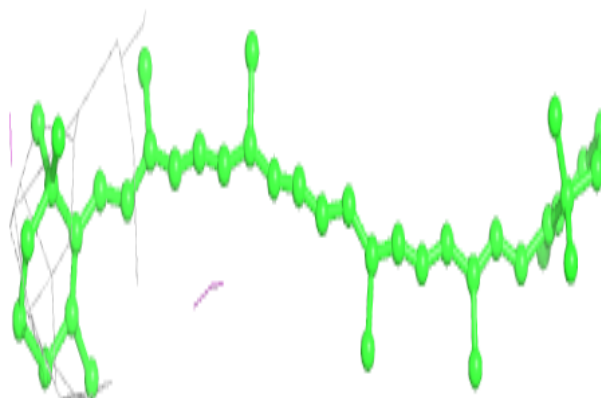


Electron density around CLA b 606:

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

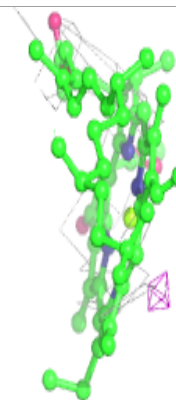
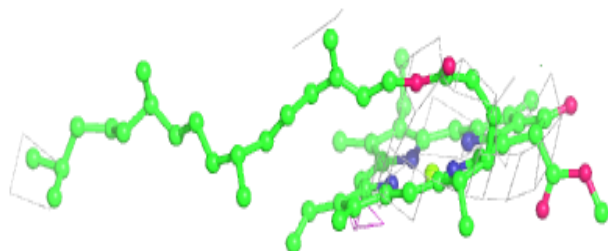
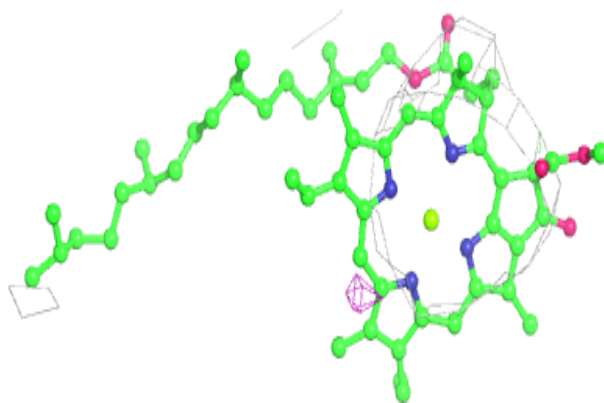
**Electron density around BCR T 101:**

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

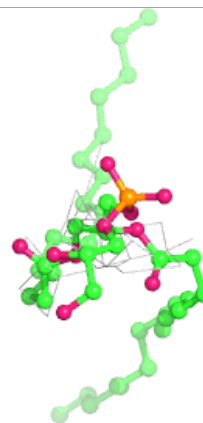
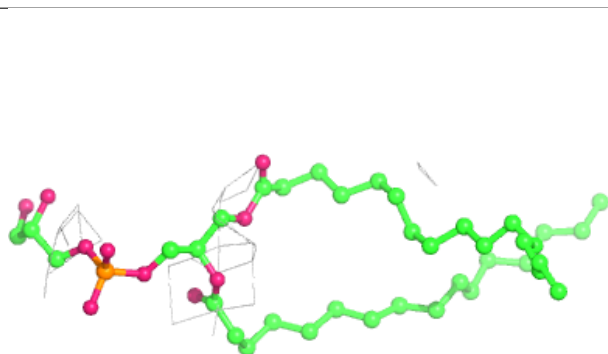
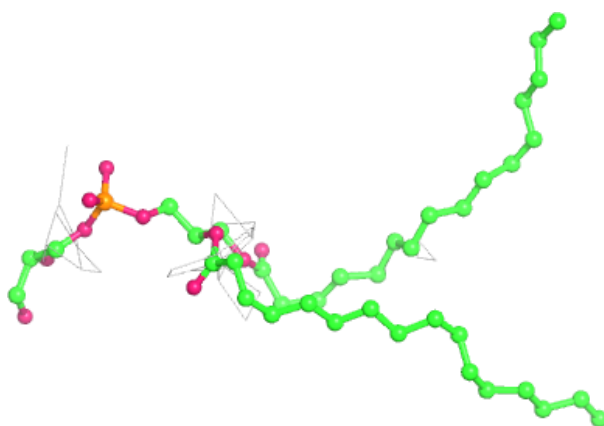


Electron density around CLA C 501:

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

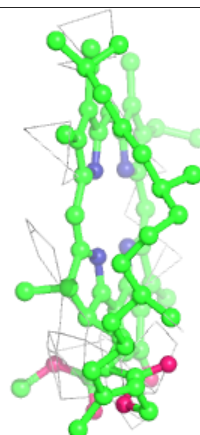
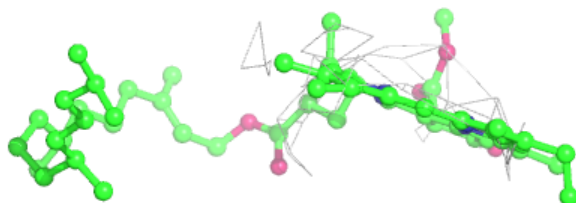
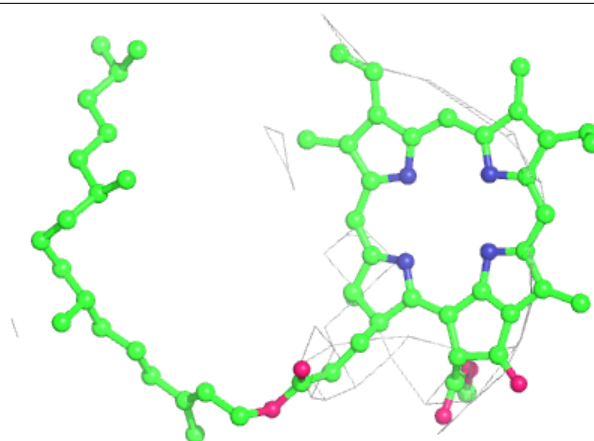
**Electron density around LHG d 407:**

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

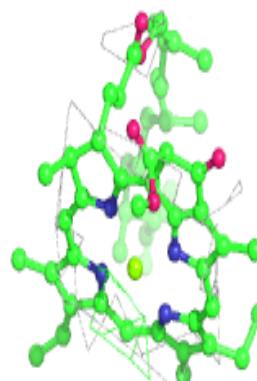
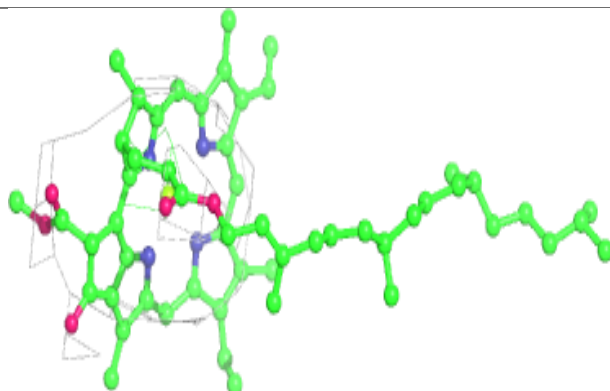
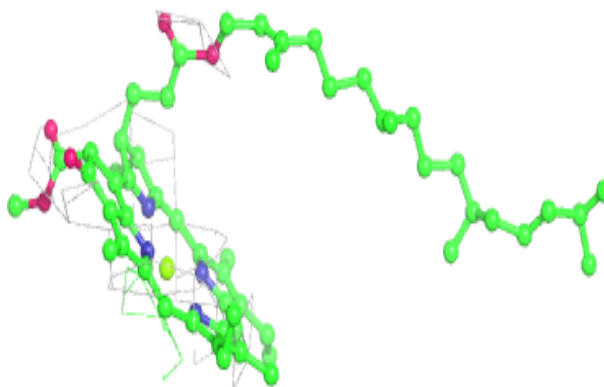


Electron density around PHO a 605:

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

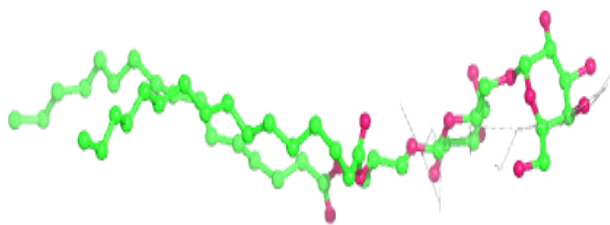
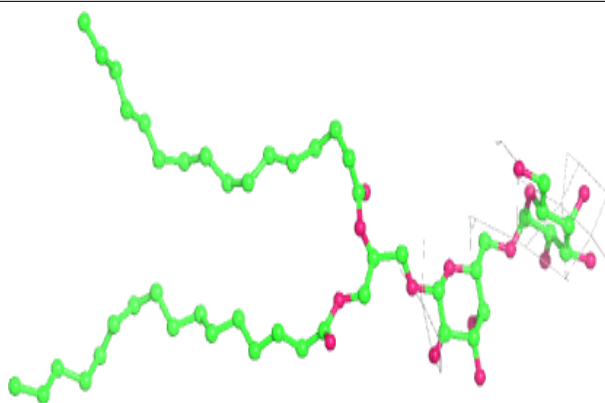
**Electron density around CLA C 504:**

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

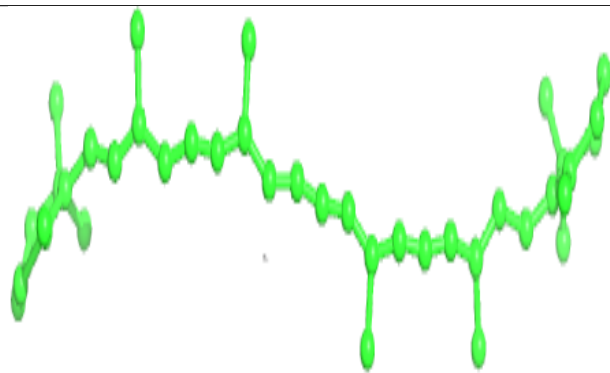
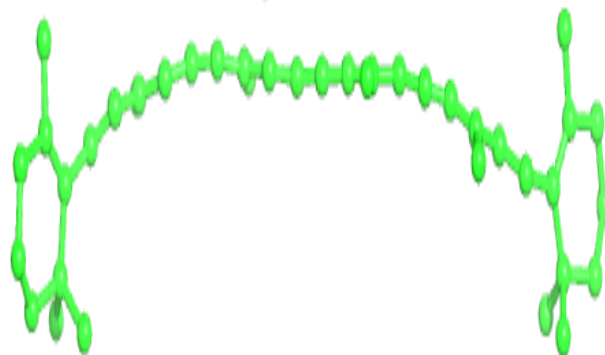


Electron density around DGD c 518:

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

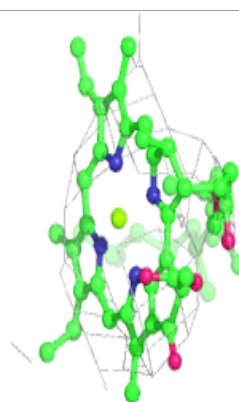
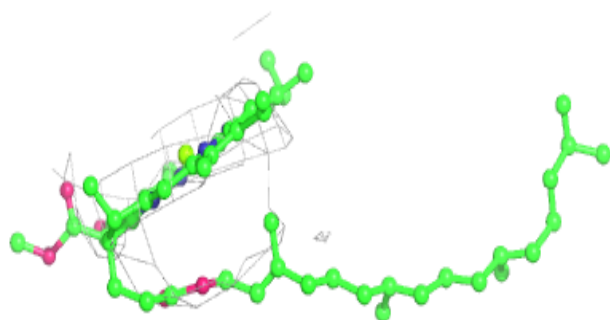
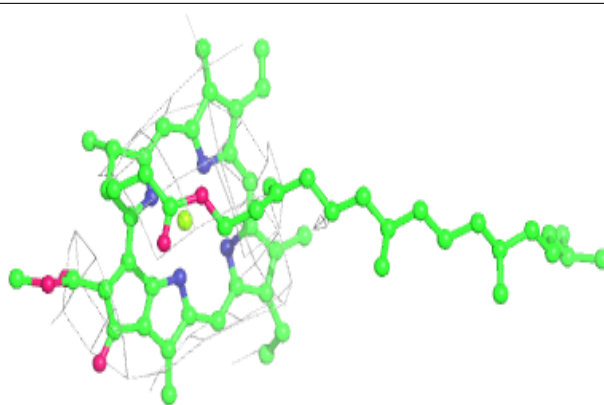
**Electron density around BCR K 102:**

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

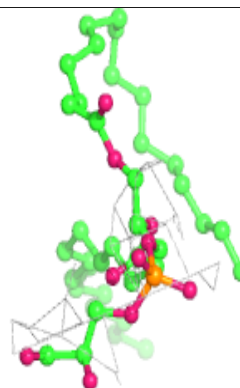
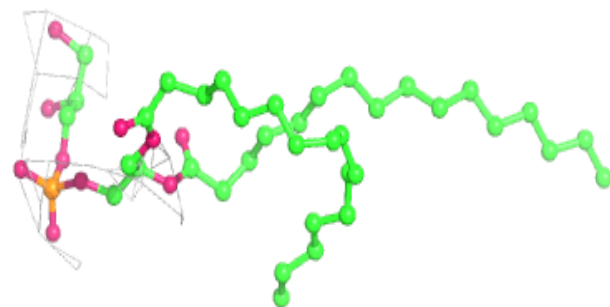
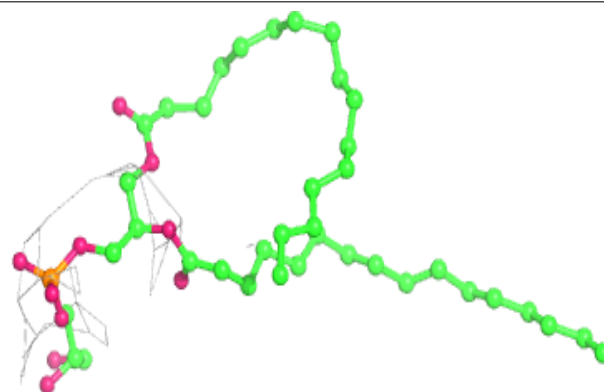


Electron density around CLA B 609:

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

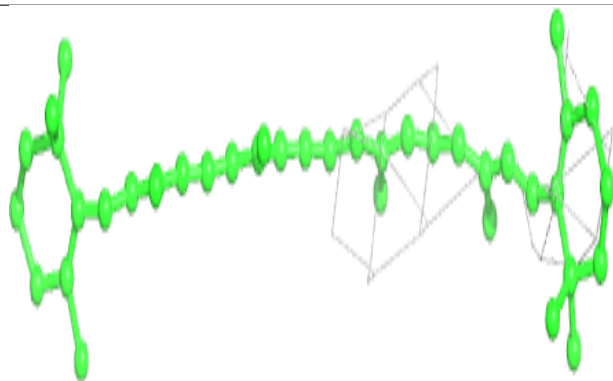
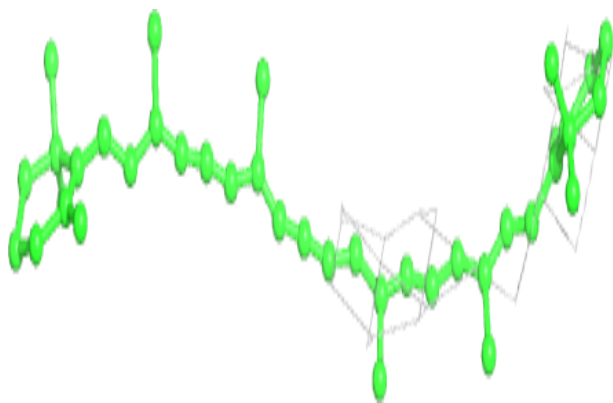
**Electron density around LHG d 405:**

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



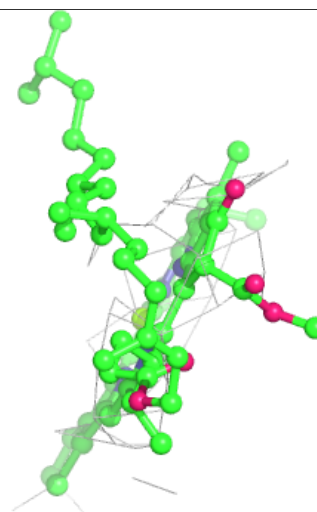
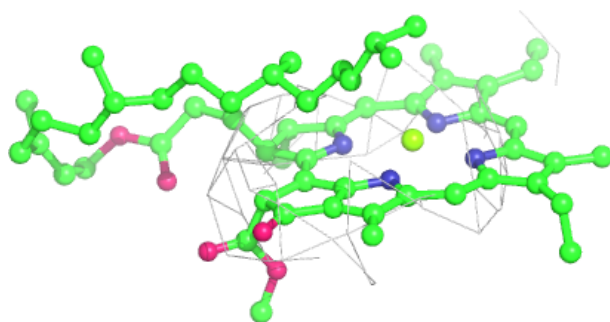
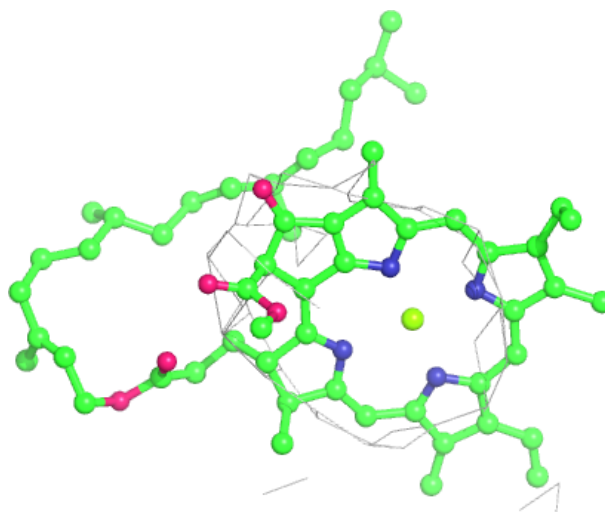
Electron density around BCR h 101:

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



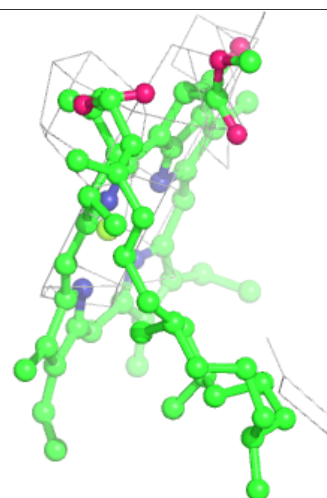
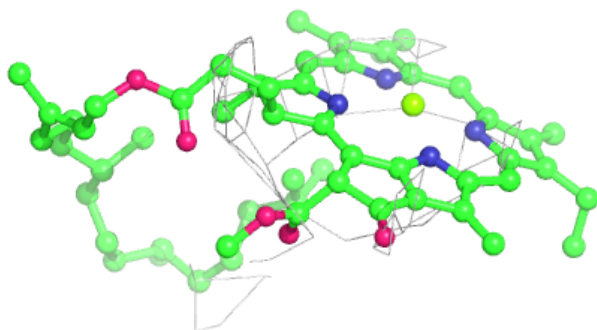
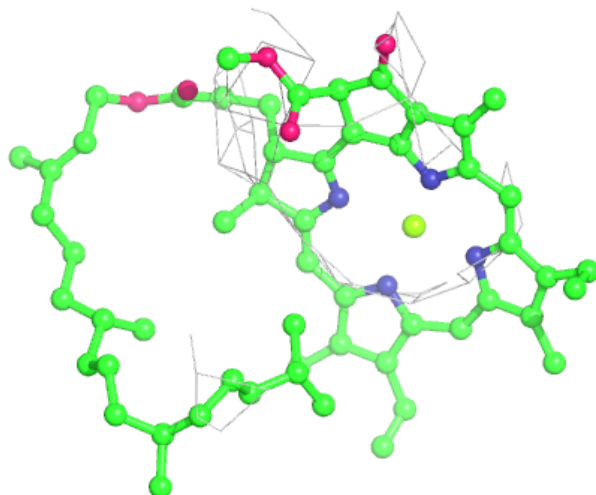
Electron density around CLA c 509:

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



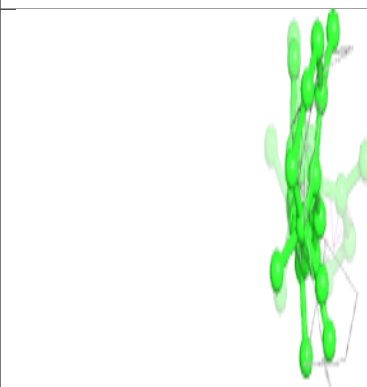
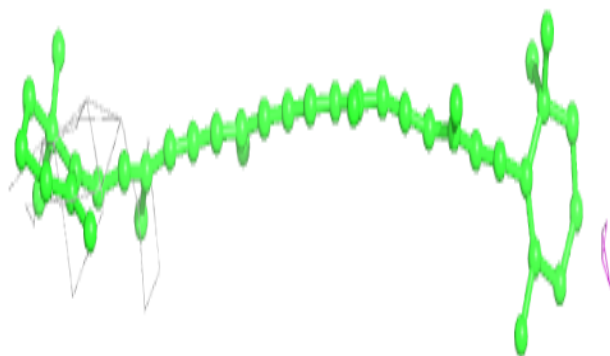
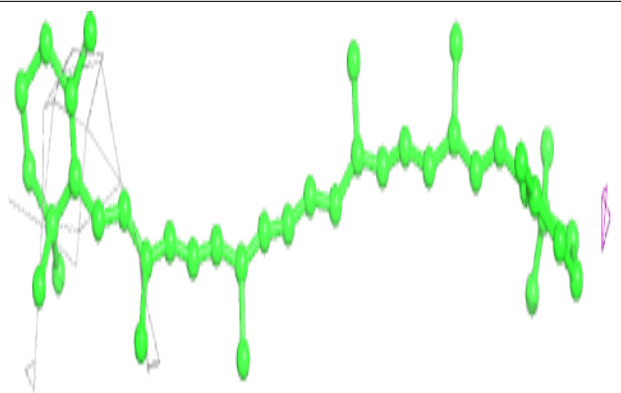
Electron density around CLA b 616:

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

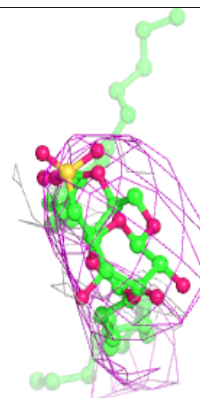
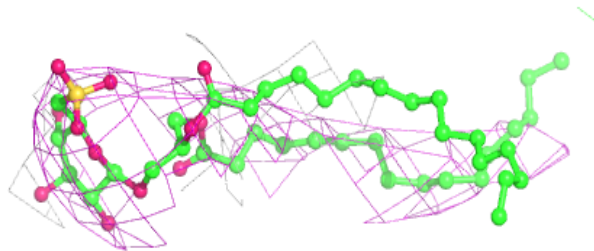
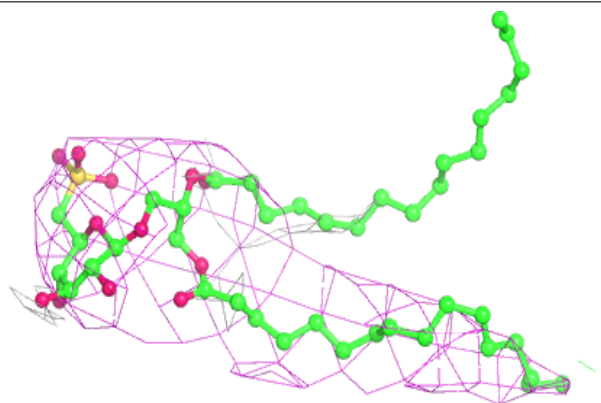


Electron density around BCR B 618:

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

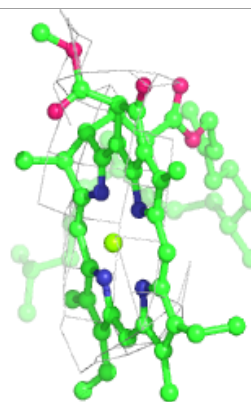
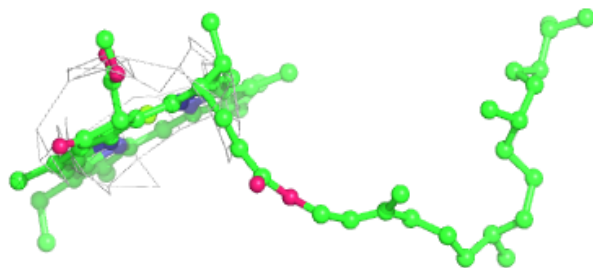
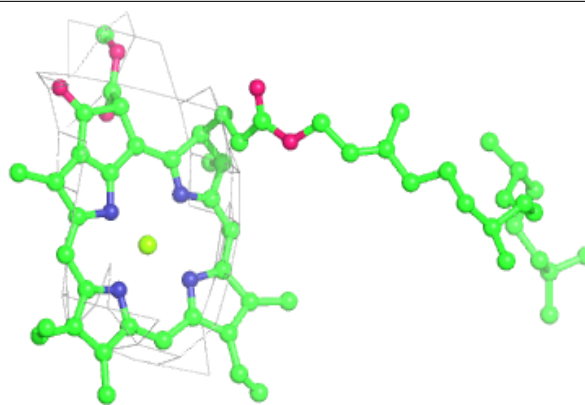
**Electron density around SQD 1 102:**

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



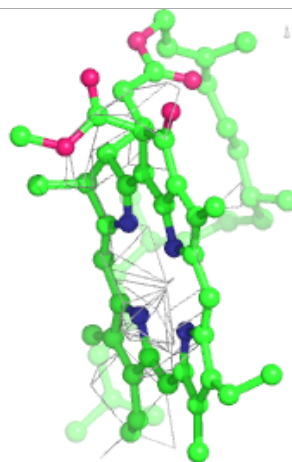
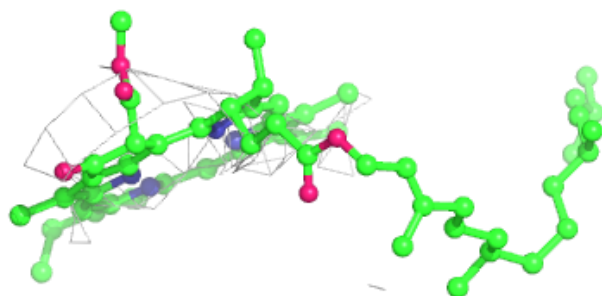
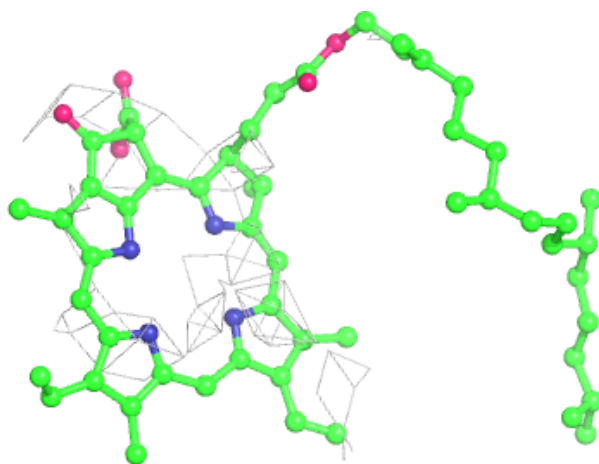
Electron density around CLA A 607:

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



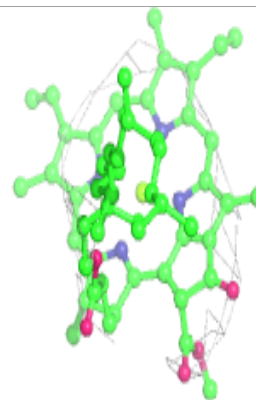
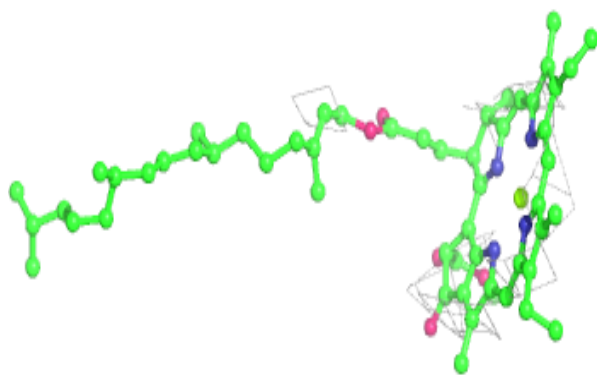
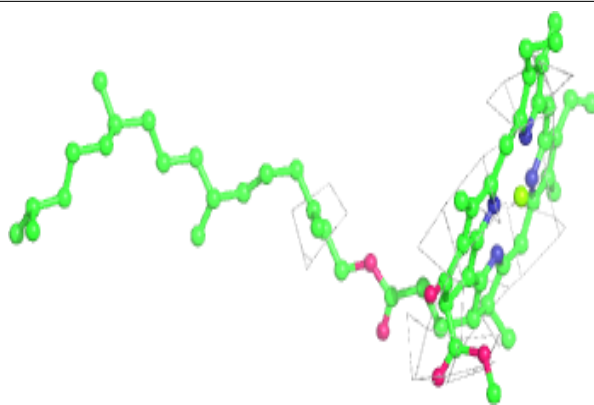
Electron density around PHO A 606:

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

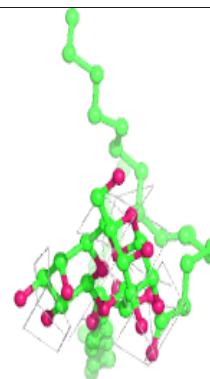
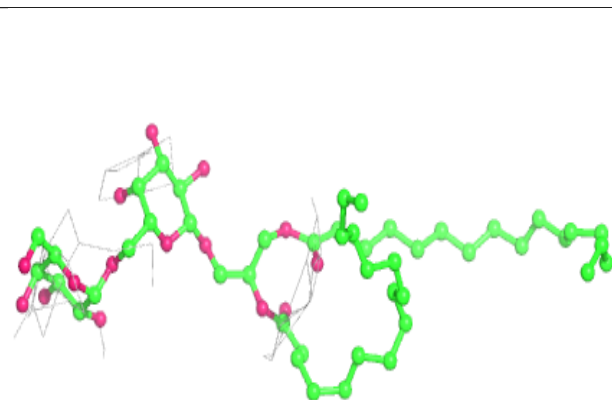
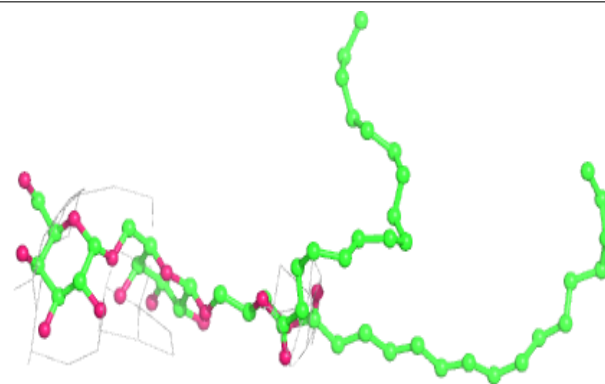


Electron density around CLA b 605:

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

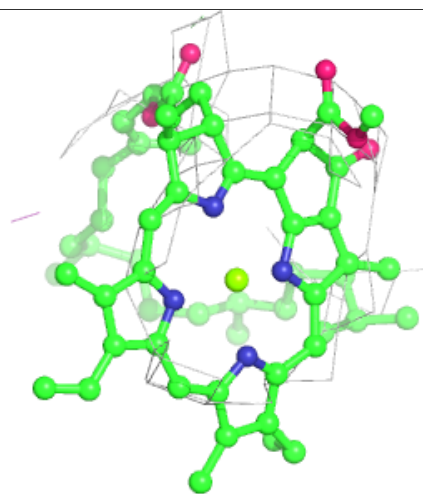
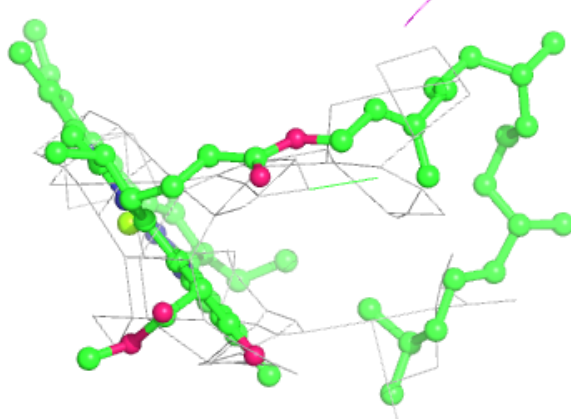
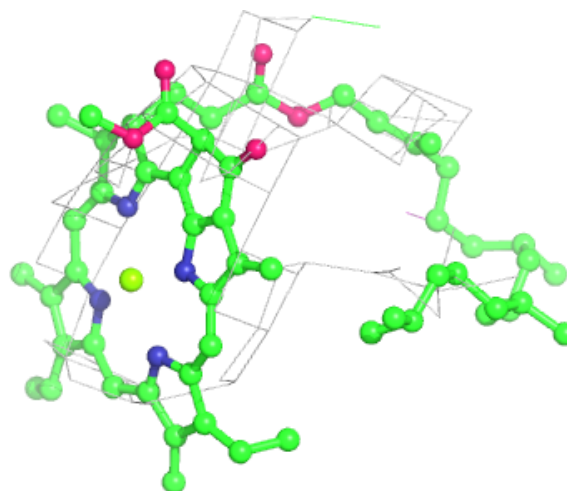
**Electron density around DGD h 102:**

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



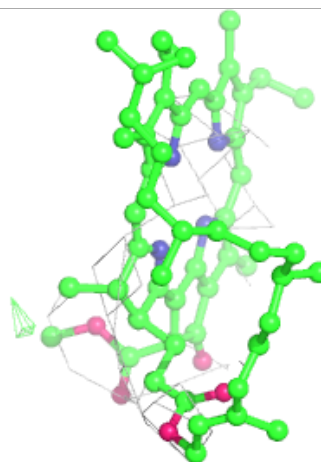
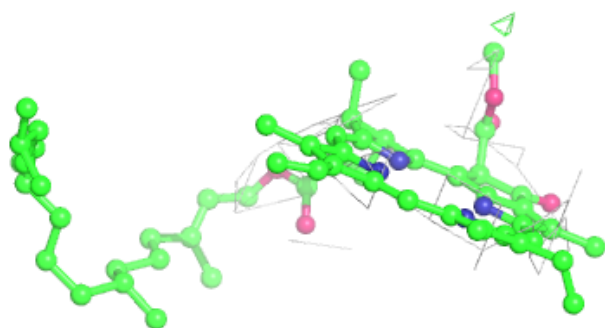
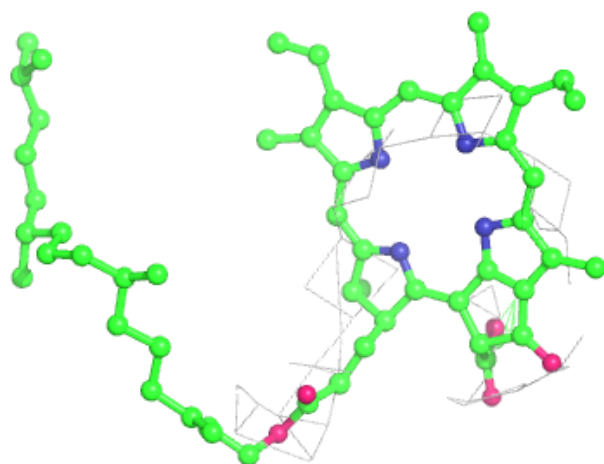
Electron density around CLA c 503:

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



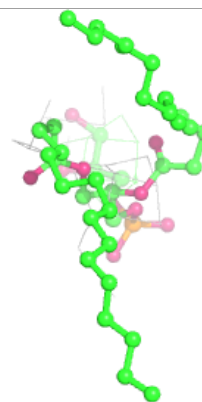
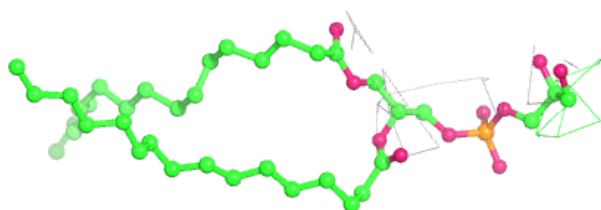
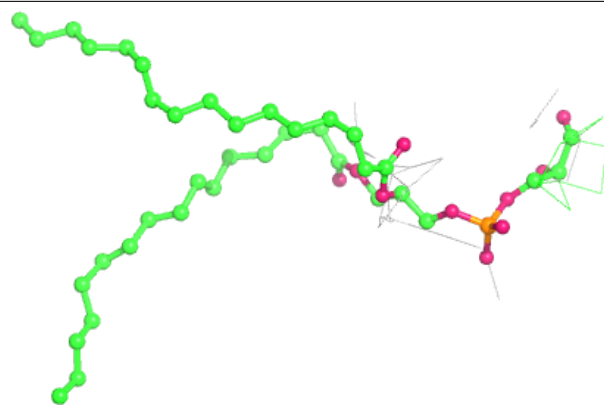
Electron density around PHO a 606:

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

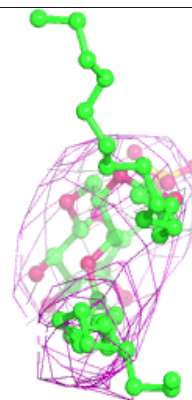
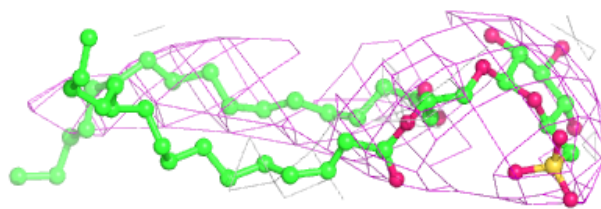
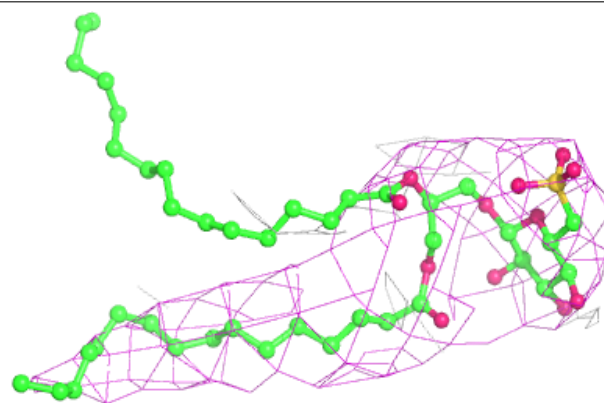


Electron density around LHG D 407:

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

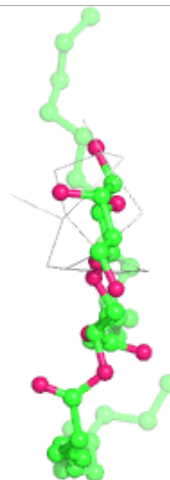
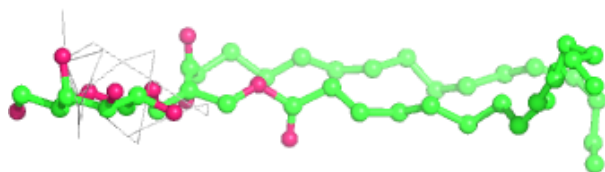
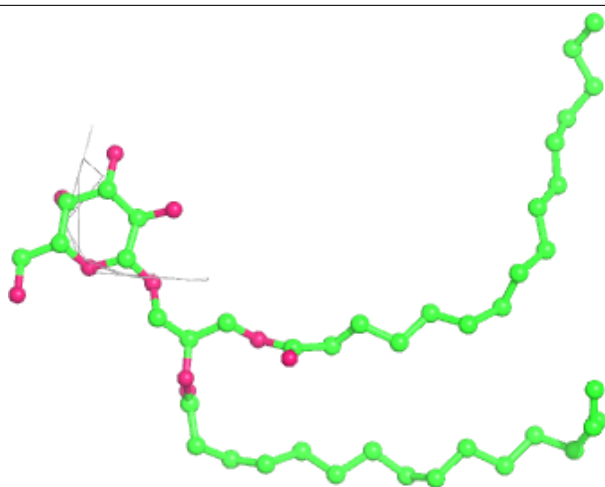
**Electron density around SQD I 101:**

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



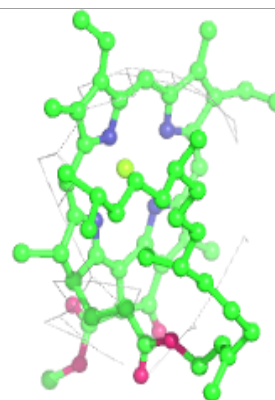
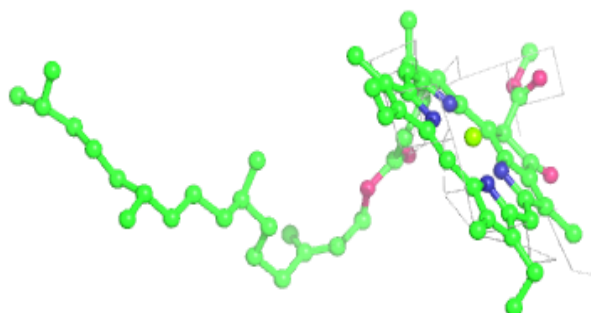
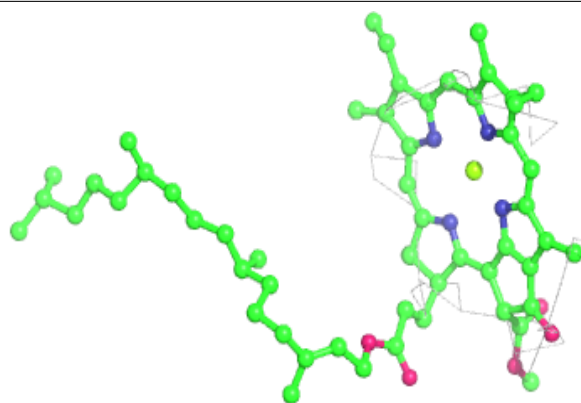
Electron density around LMG c 519:

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

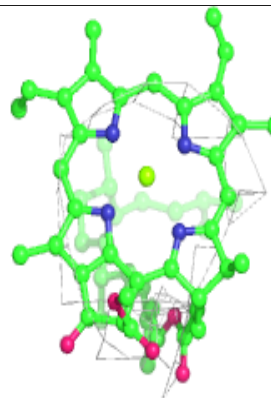
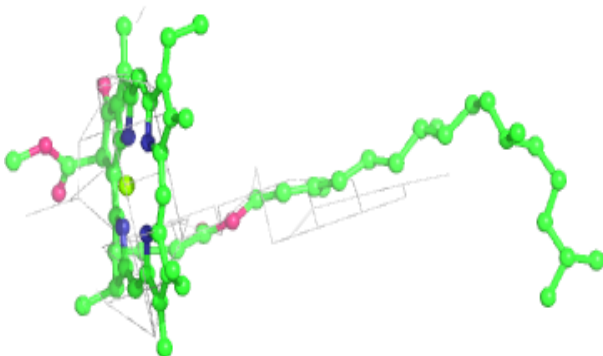
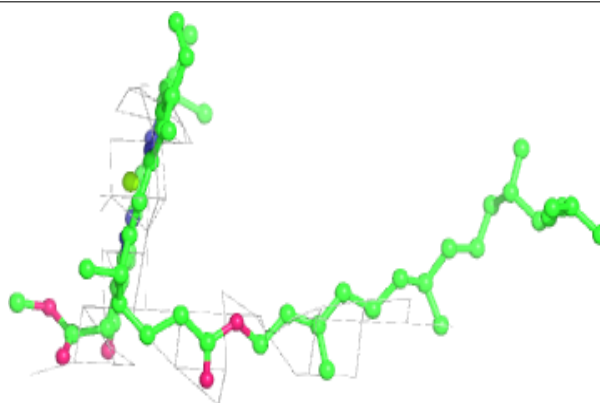


Electron density around CLA c 511:

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

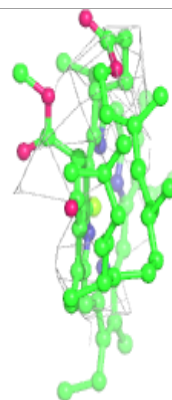
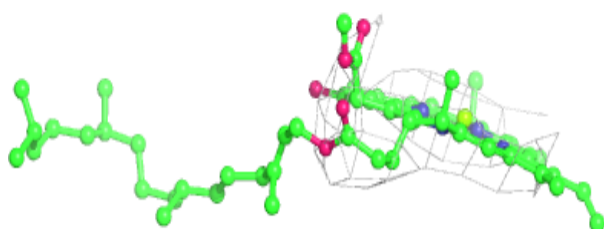
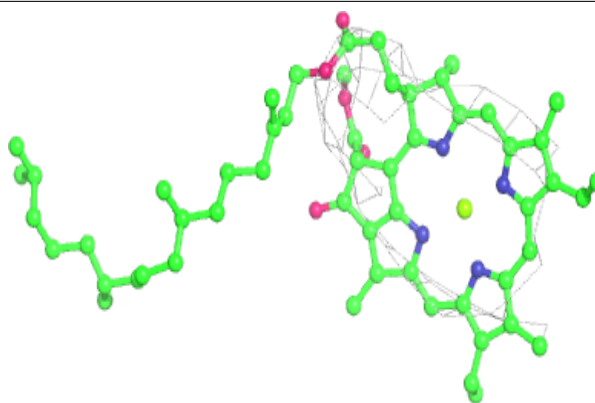
**Electron density around CLA B 606:**

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

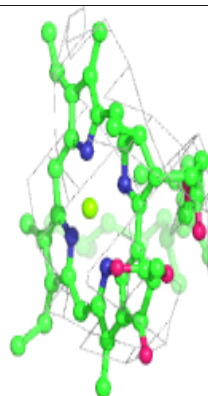
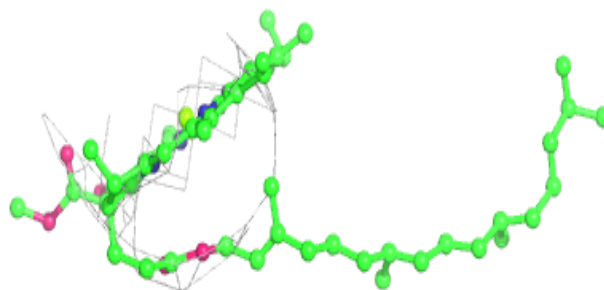
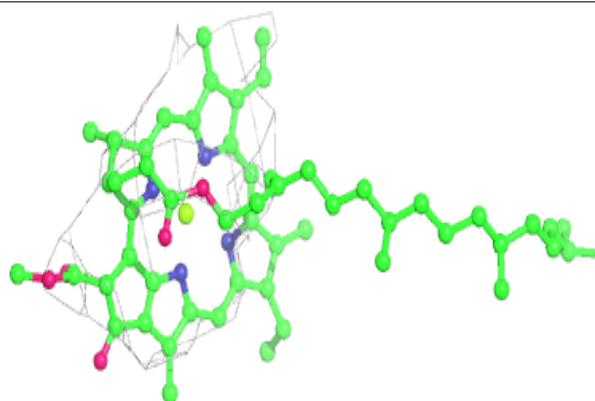


Electron density around CLA b 603:

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

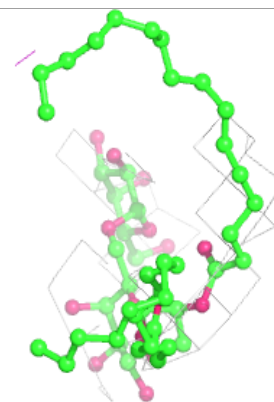
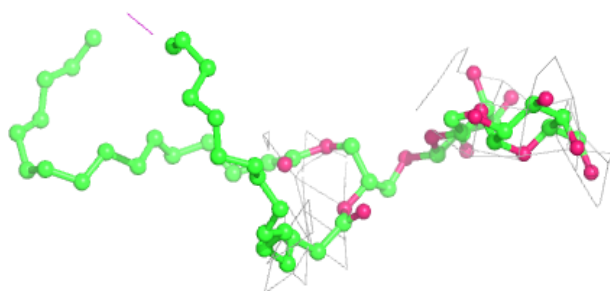
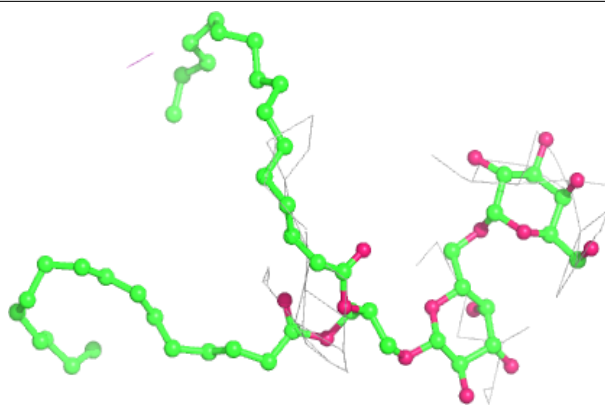
**Electron density around CLA b 609:**

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

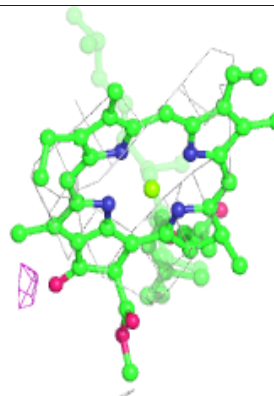
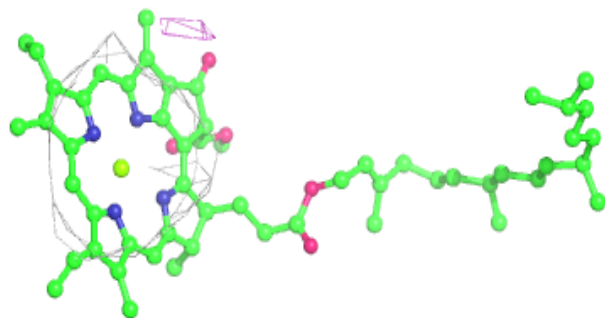
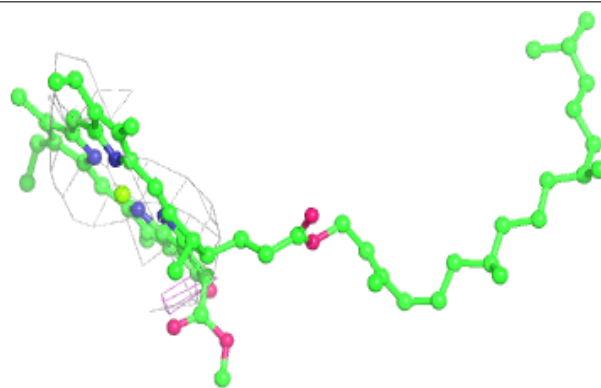


Electron density around DGD C 517:

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

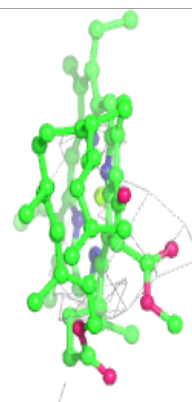
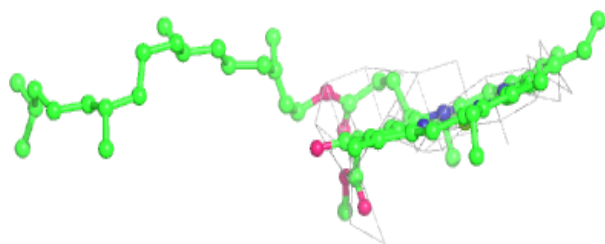
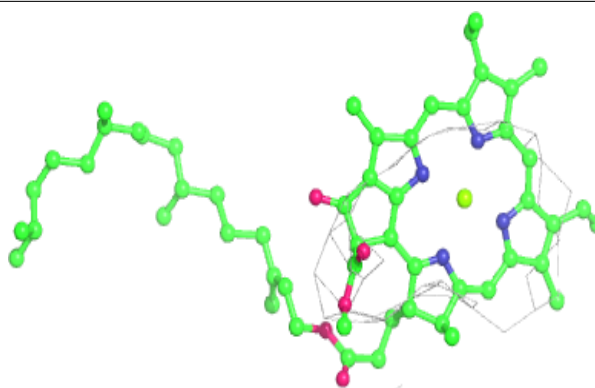
**Electron density around CLA D 401:**

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



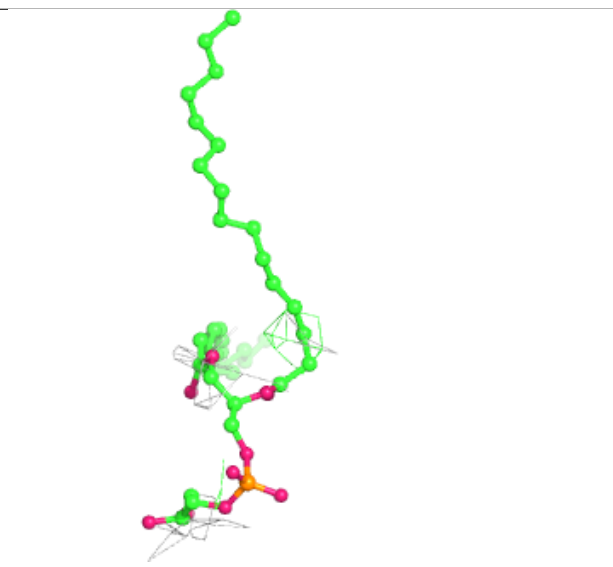
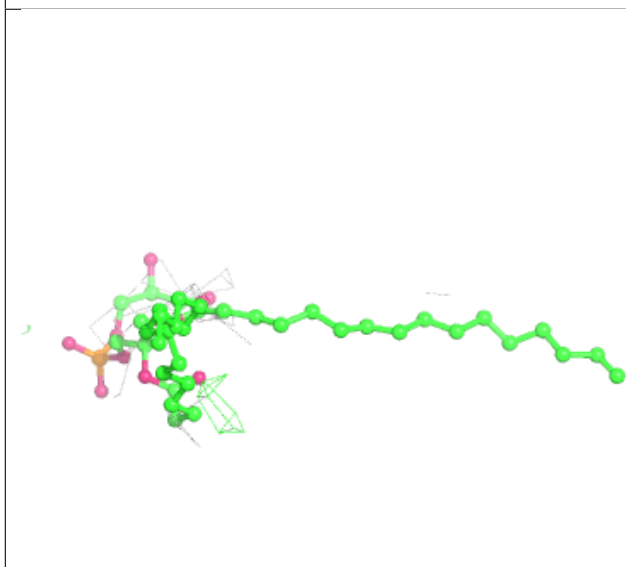
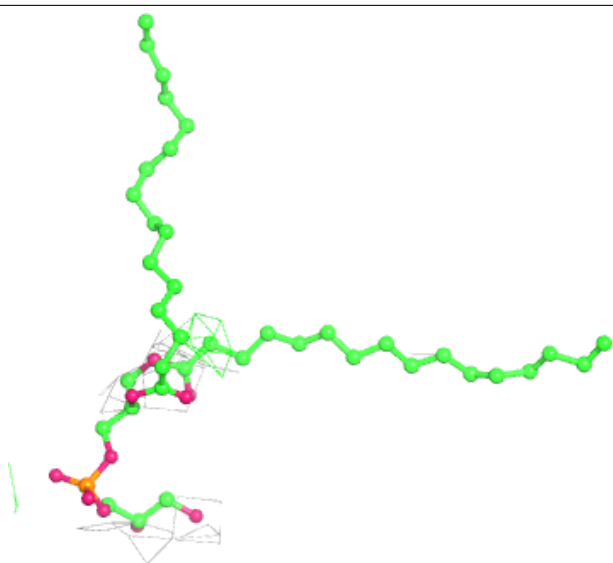
Electron density around CLA B 603:

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



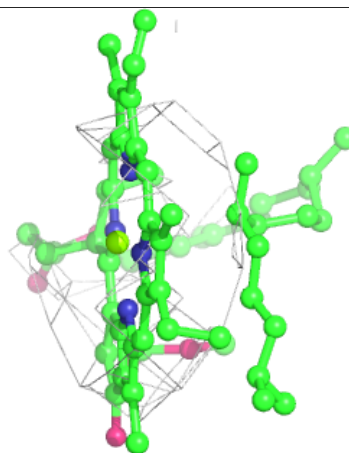
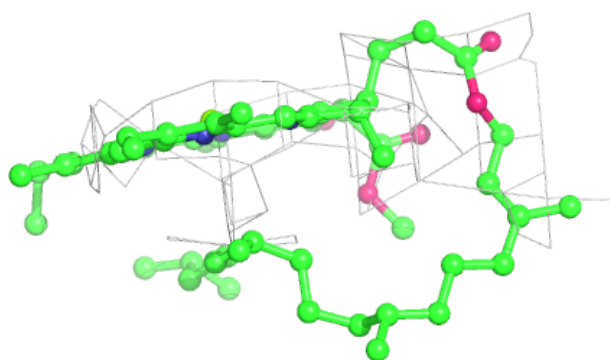
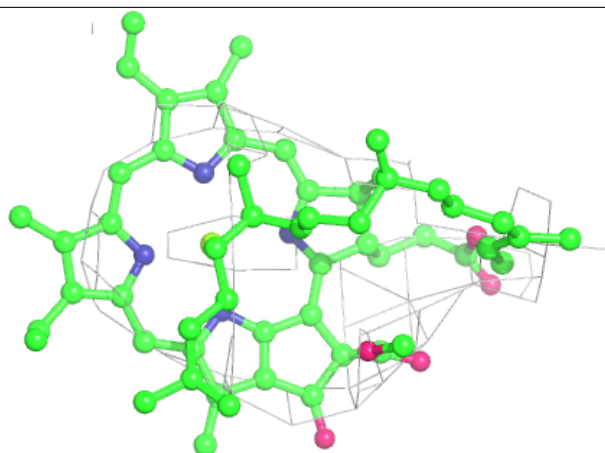
Electron density around LHG L 102:

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



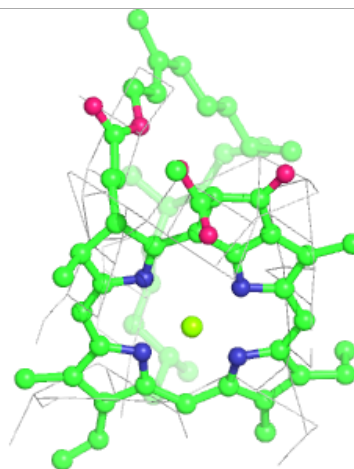
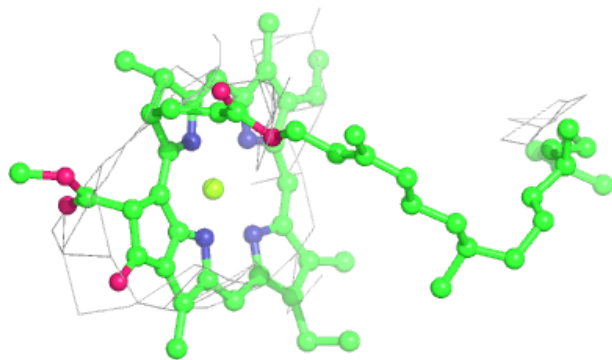
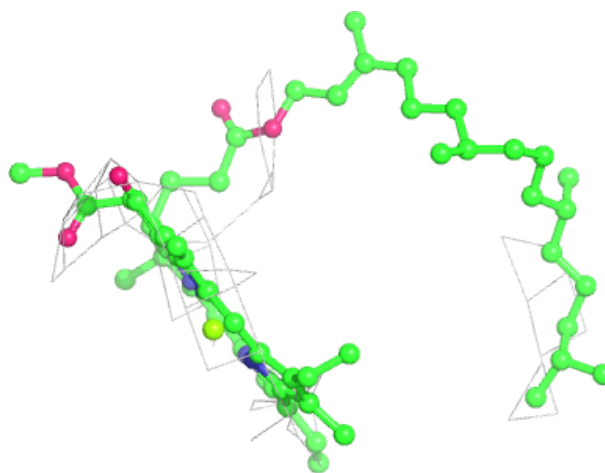
Electron density around CLA C 510:

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



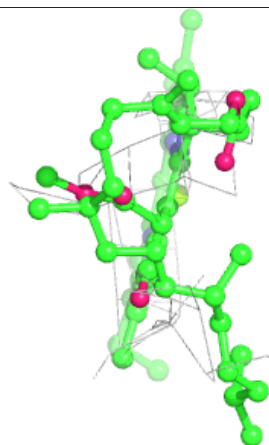
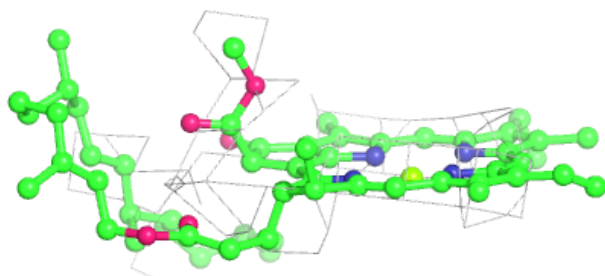
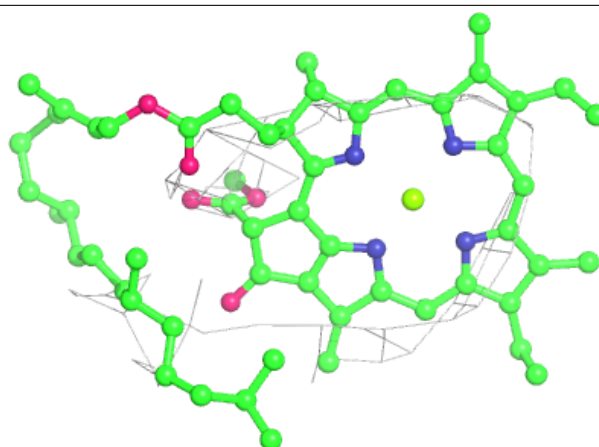
Electron density around CLA B 612:

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

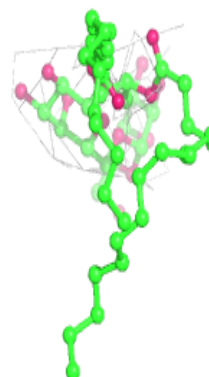
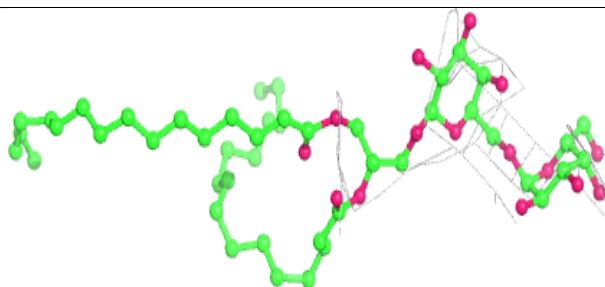
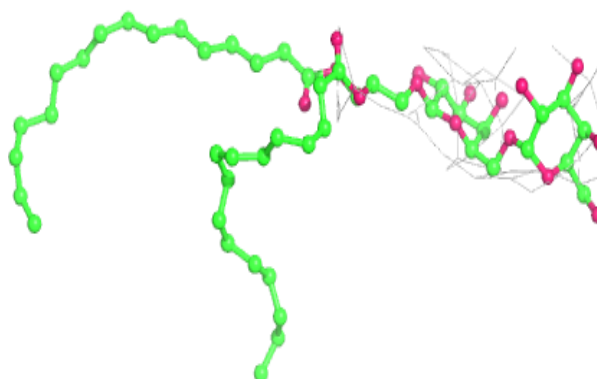


Electron density around CLA b 611:

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

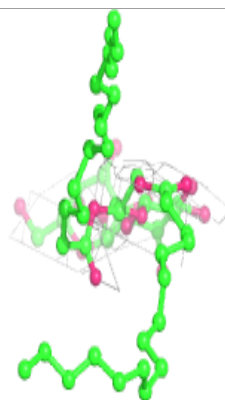
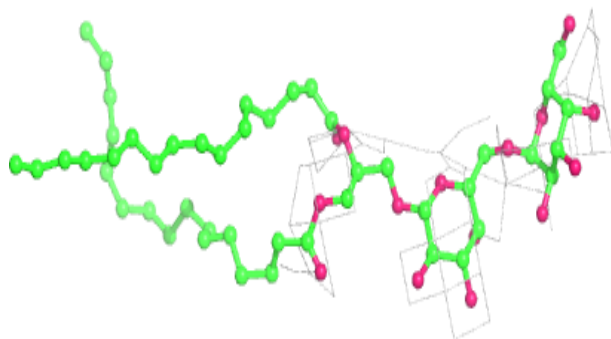
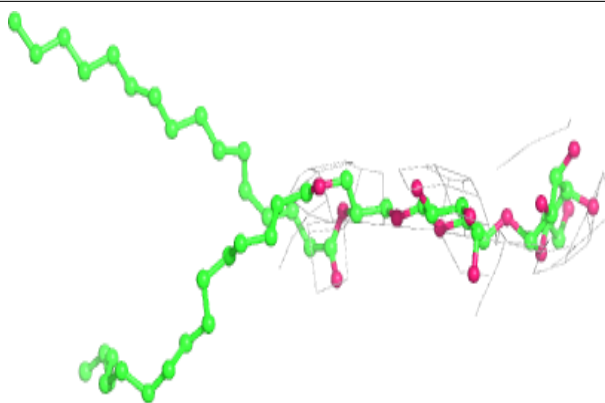
**Electron density around DGD H 102:**

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

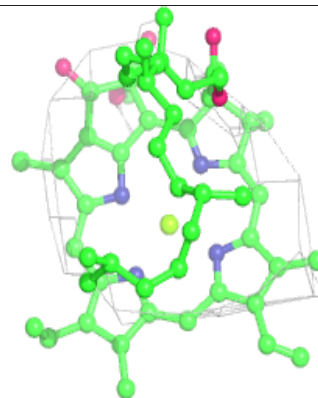
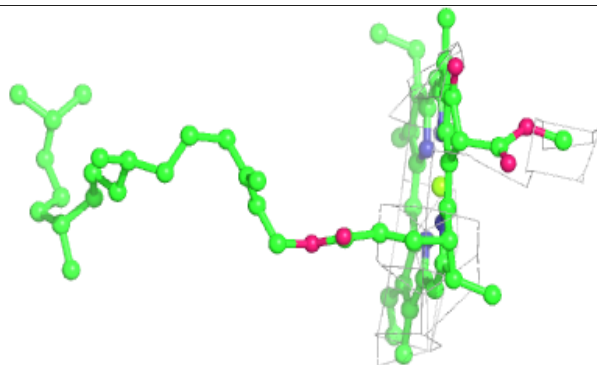
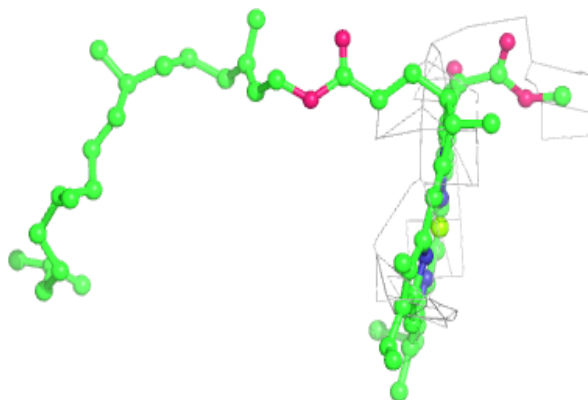


Electron density around DGD C 516:

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

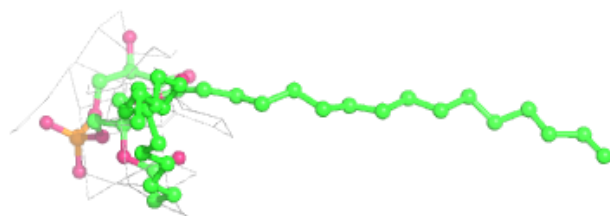
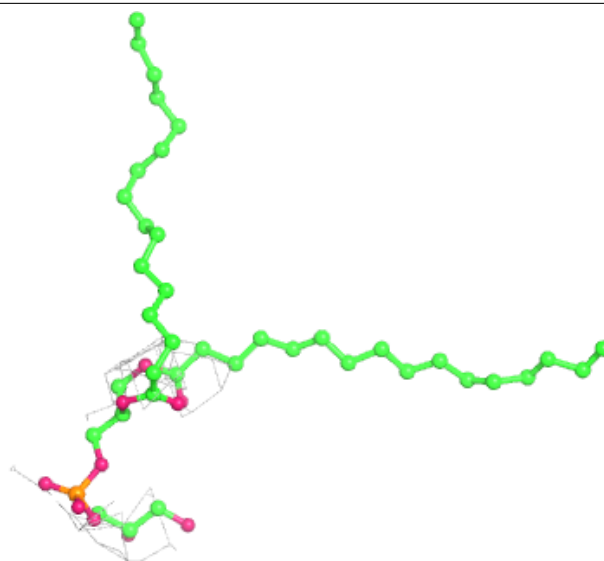
**Electron density around CLA c 506:**

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



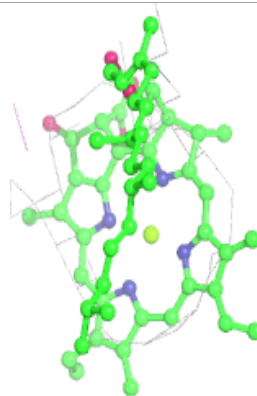
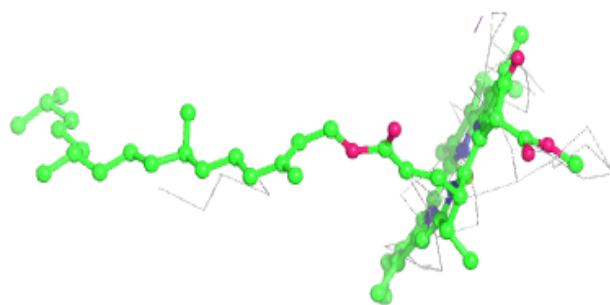
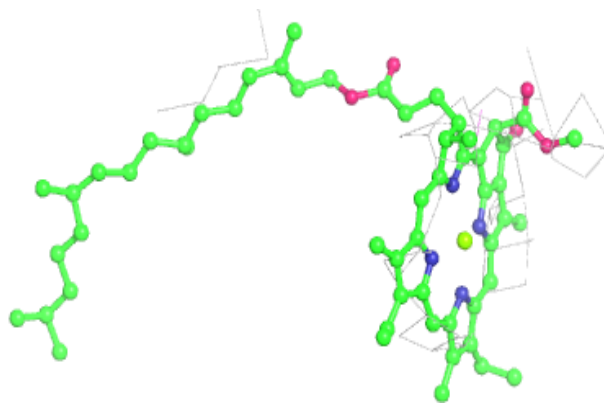
Electron density around LHG 1 103:

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



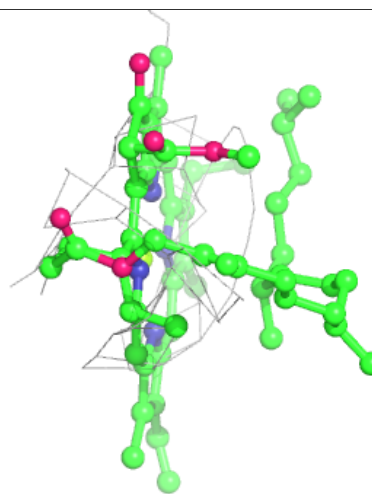
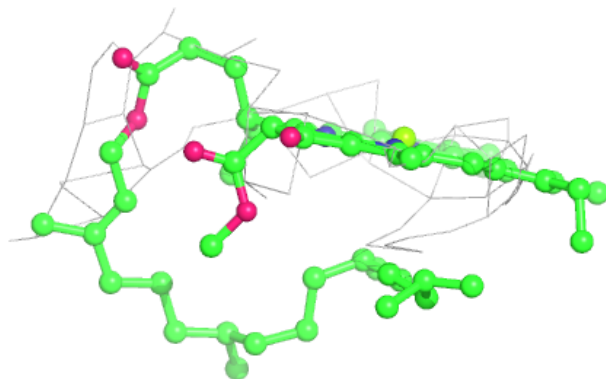
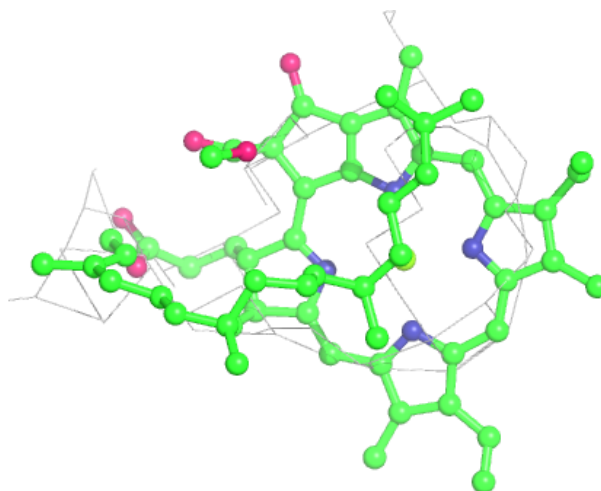
Electron density around CLA b 610:

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



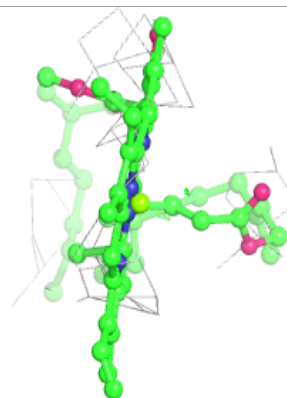
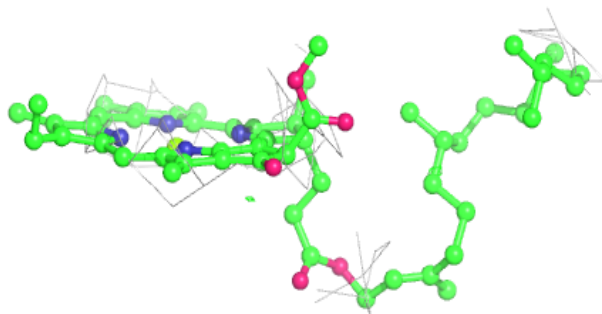
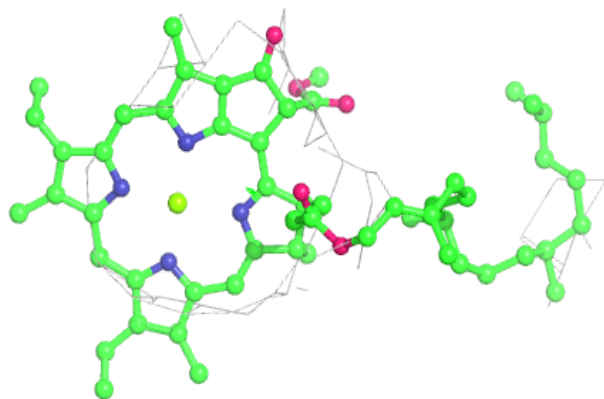
Electron density around CLA c 510:

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

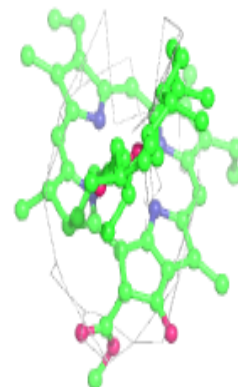
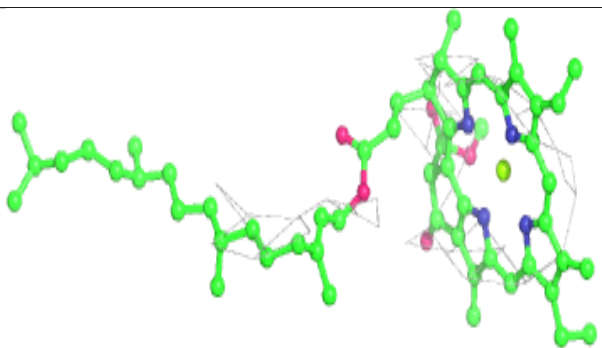
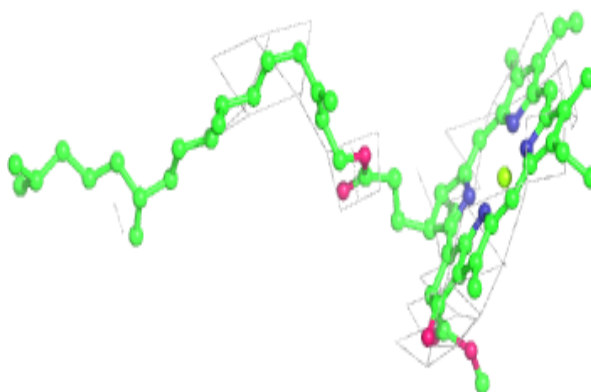


Electron density around CLA b 613:

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

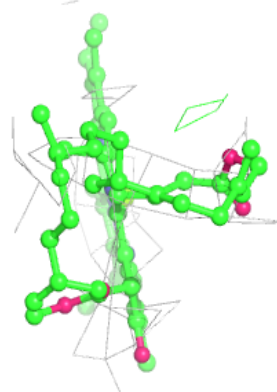
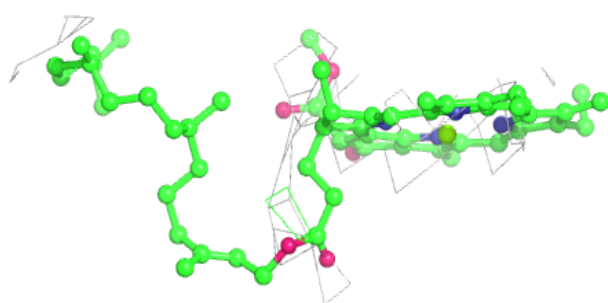
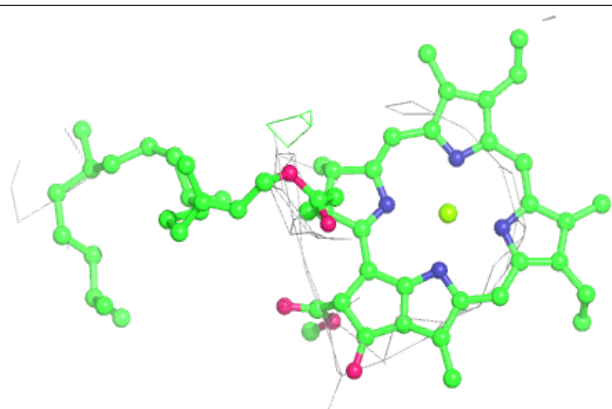
**Electron density around CLA C 502:**

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

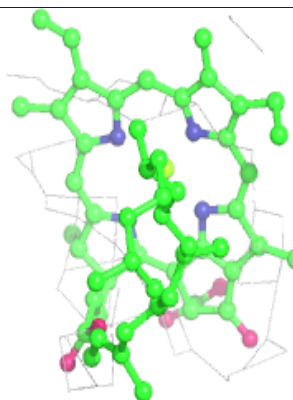
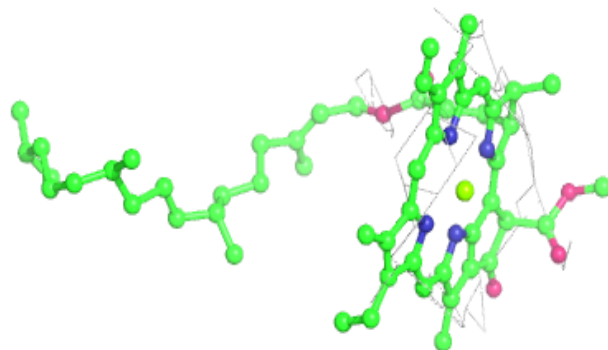
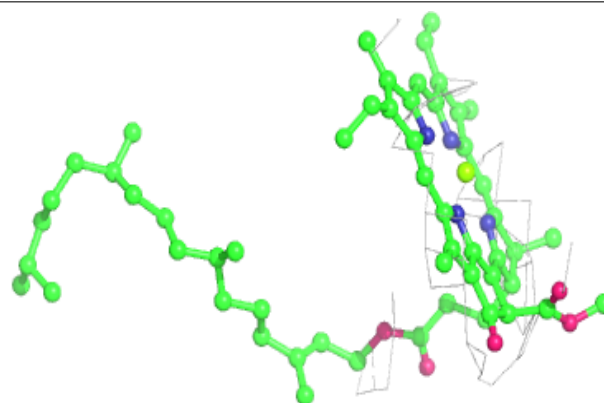


Electron density around CLA B 613:

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

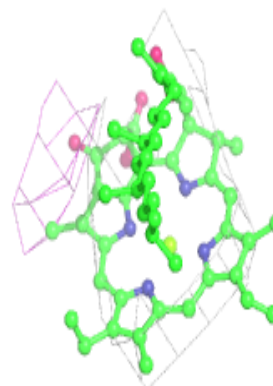
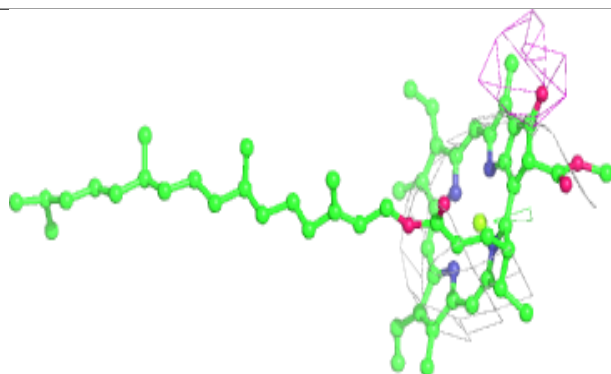
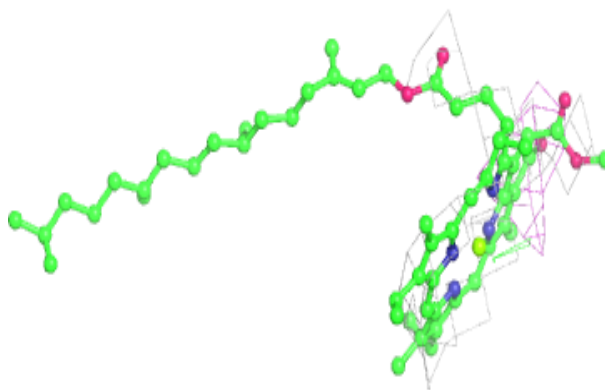
**Electron density around CLA c 508:**

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

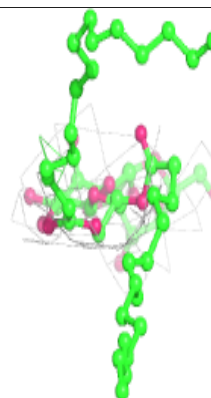
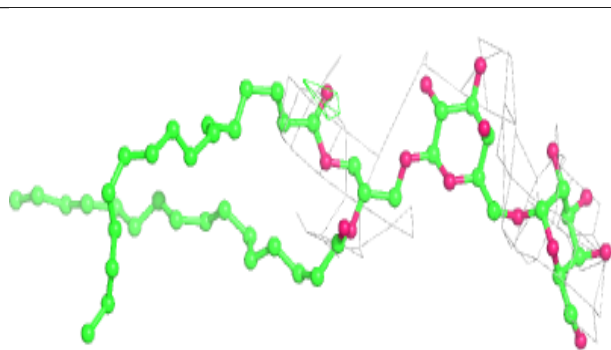
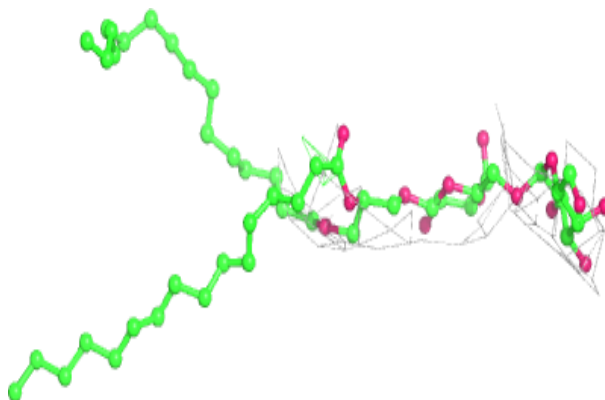


Electron density around CLA b 608:

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

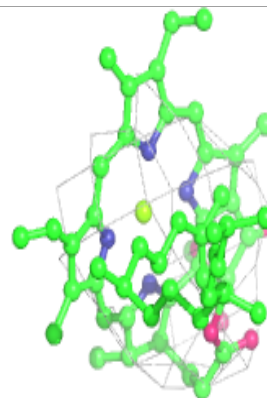
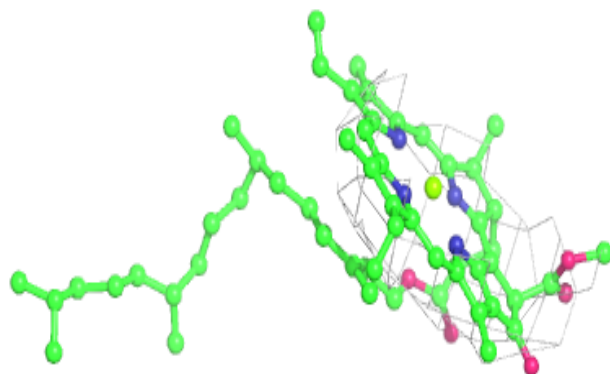
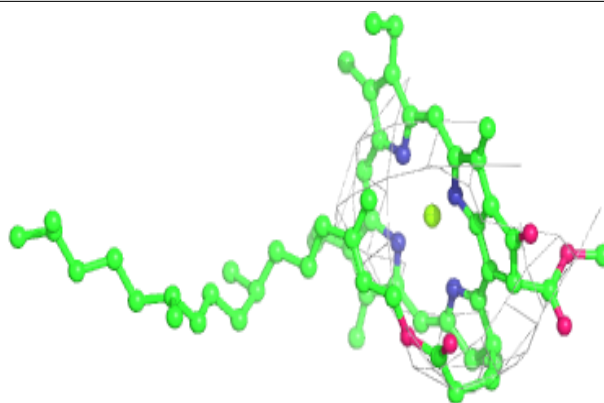
**Electron density around DGD c 516:**

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

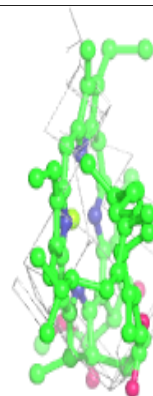
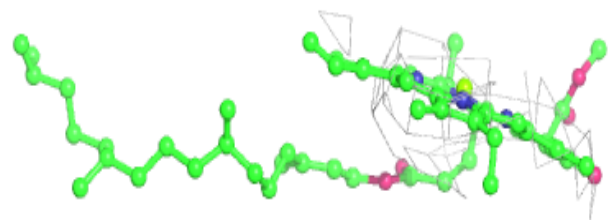
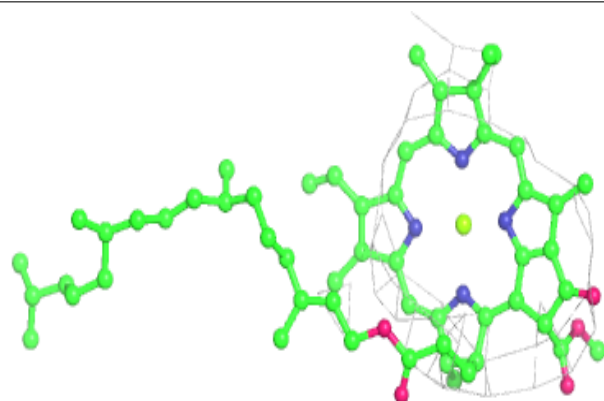


Electron density around CLA c 505:

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

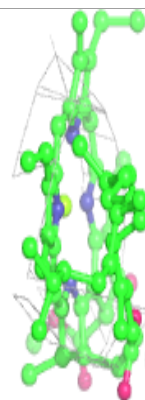
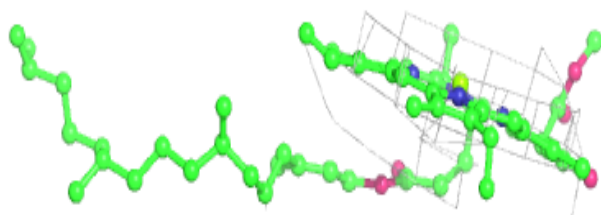
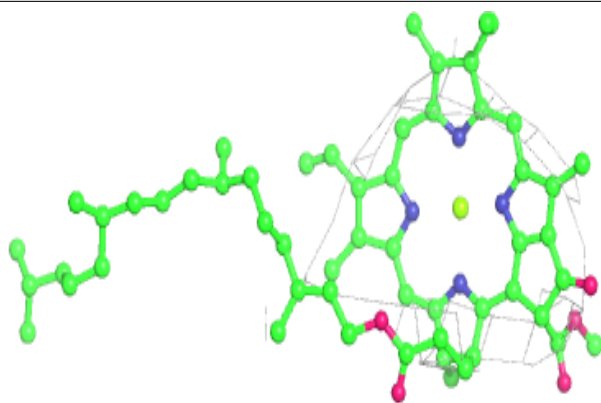
**Electron density around CLA b 604:**

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

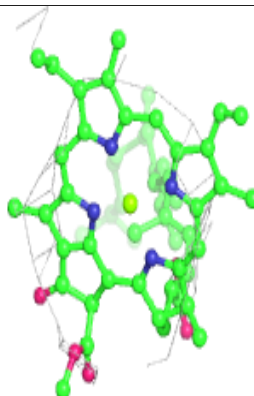
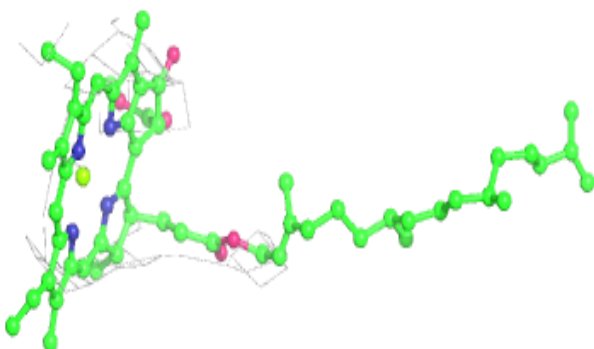
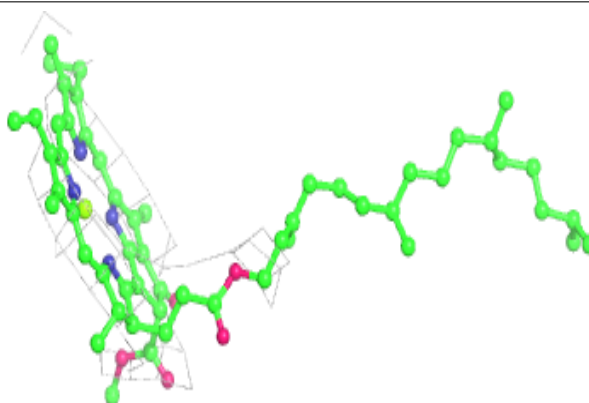


Electron density around CLA B 604:

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

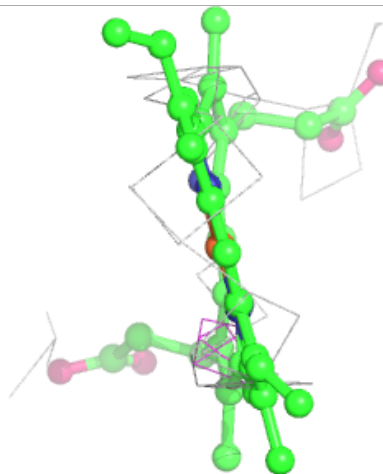
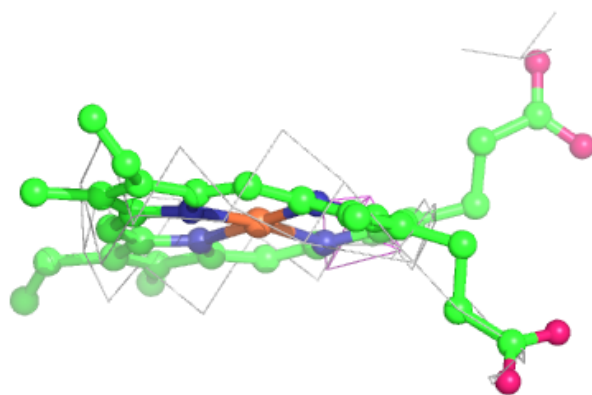
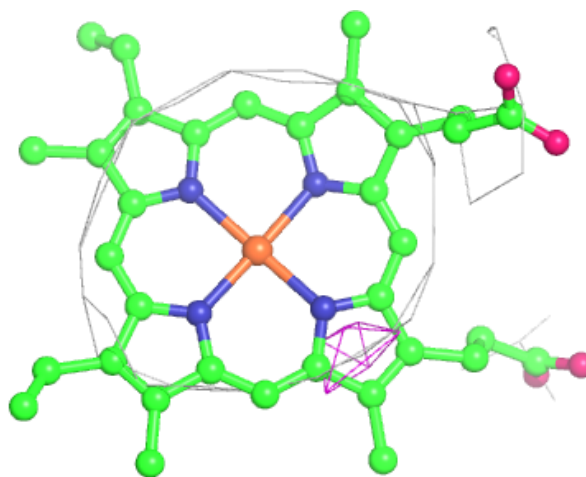
**Electron density around CLA B 605:**

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



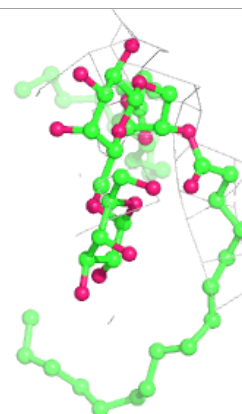
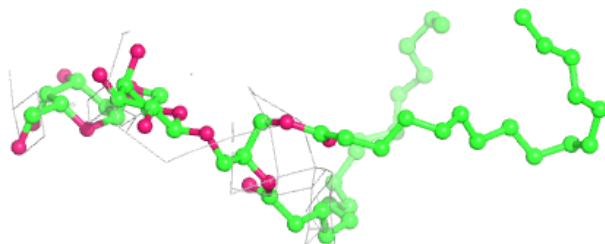
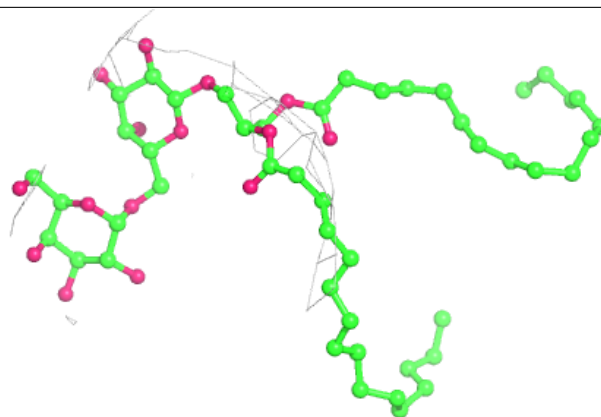
Electron density around HEM F 101:

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

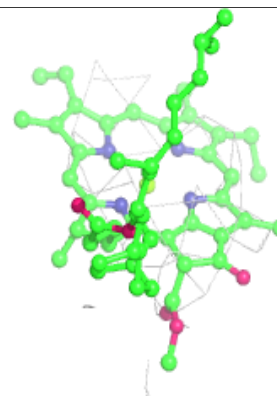
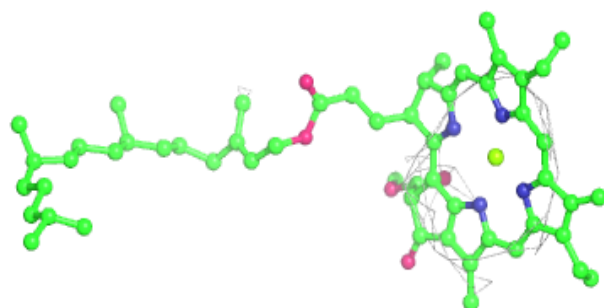
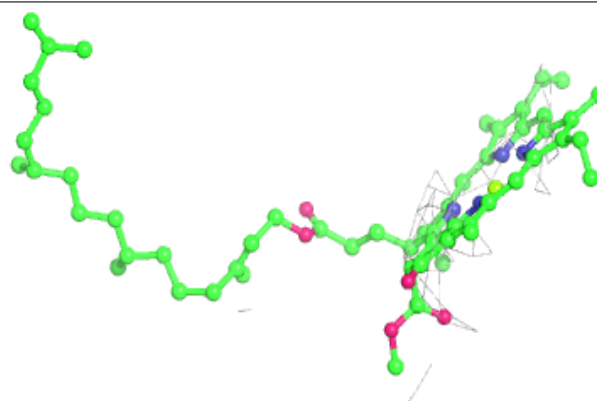


Electron density around DGD c 517:

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

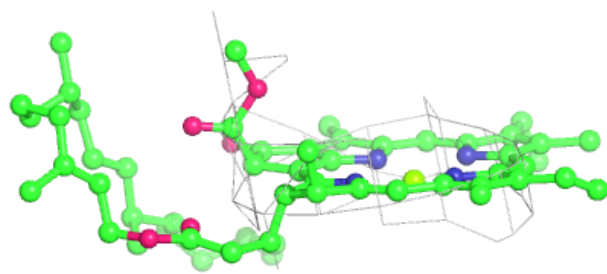
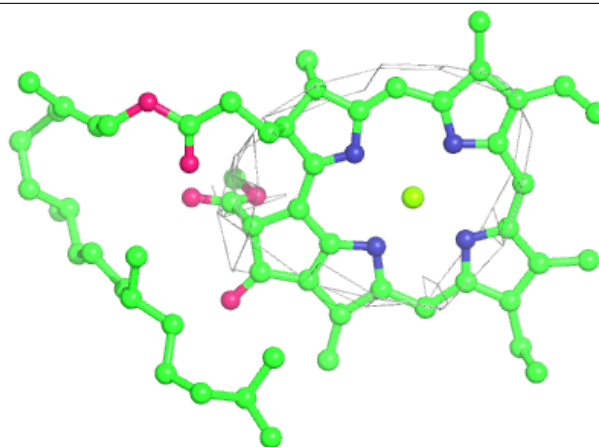
**Electron density around CLA d 401:**

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

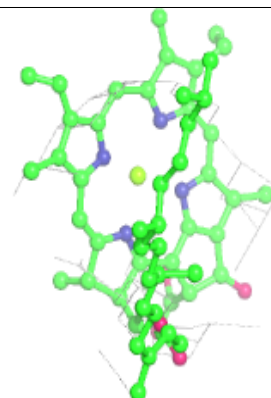
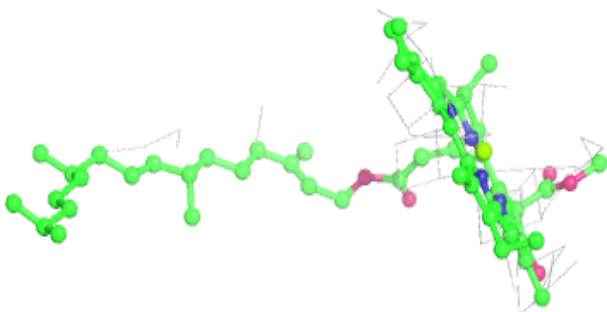
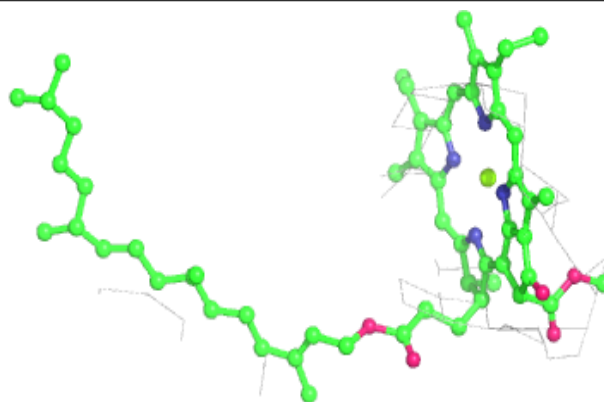


Electron density around CLA B 611:

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

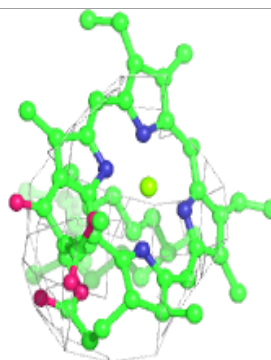
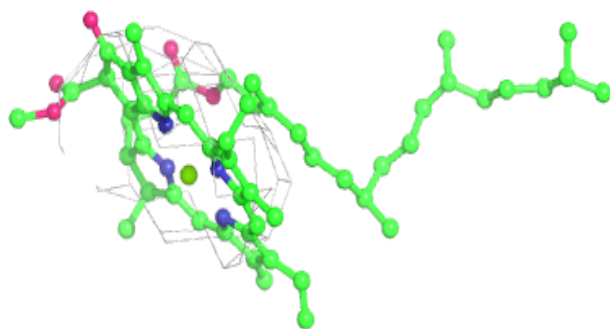
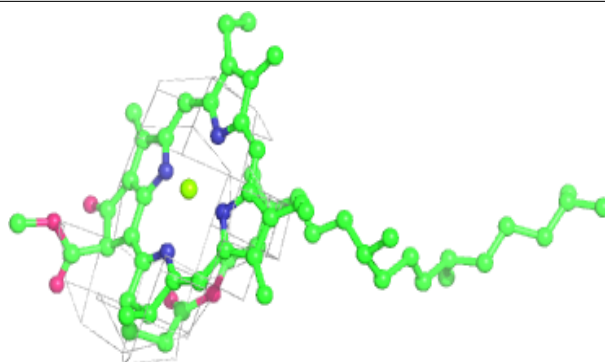
**Electron density around CLA B 610:**

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



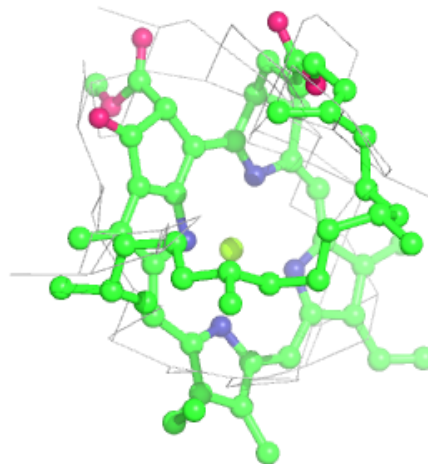
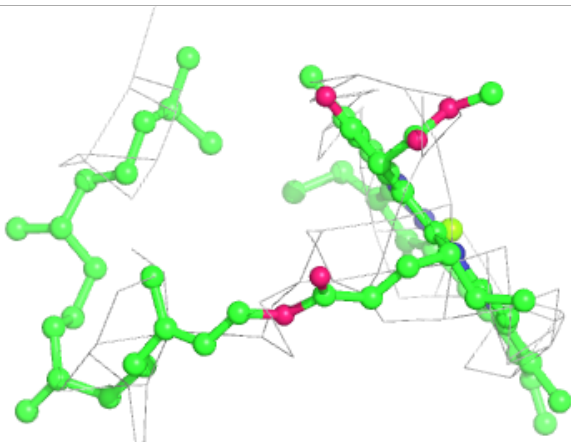
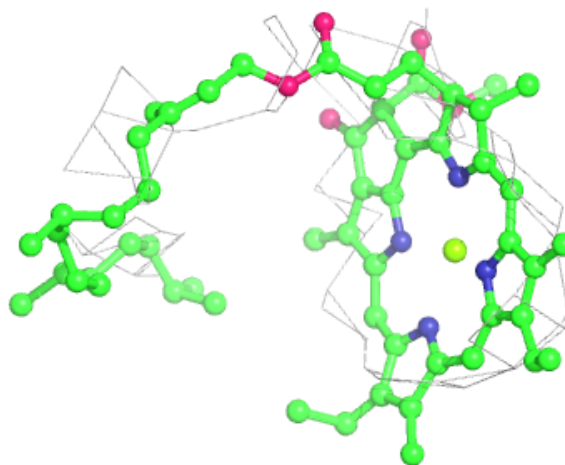
Electron density around CLA C 505:

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



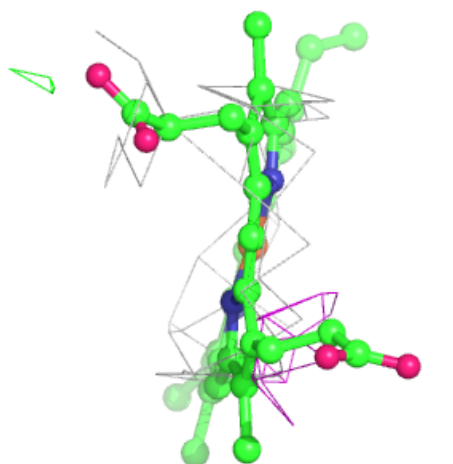
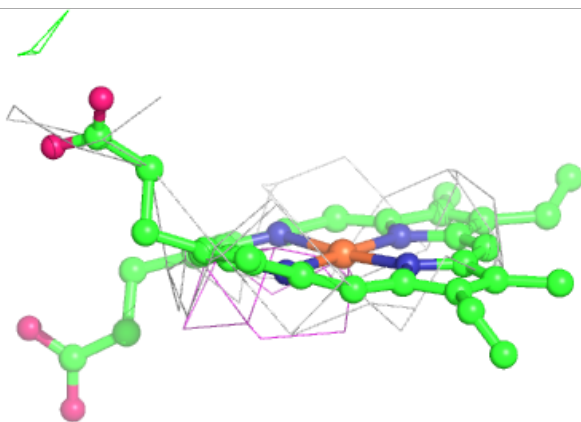
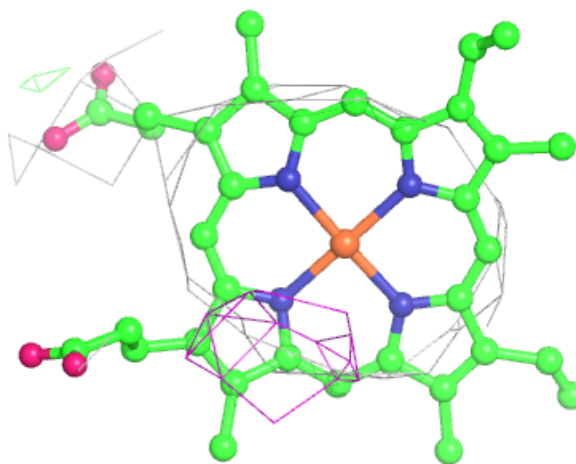
Electron density around CLA C 503:

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



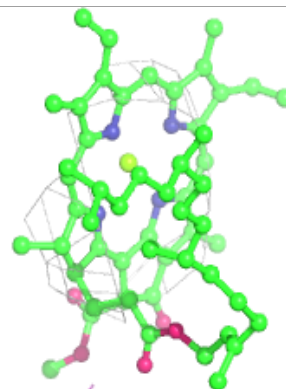
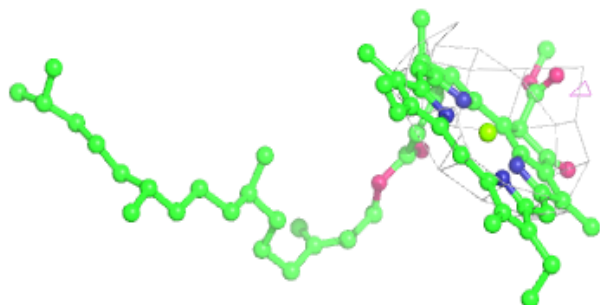
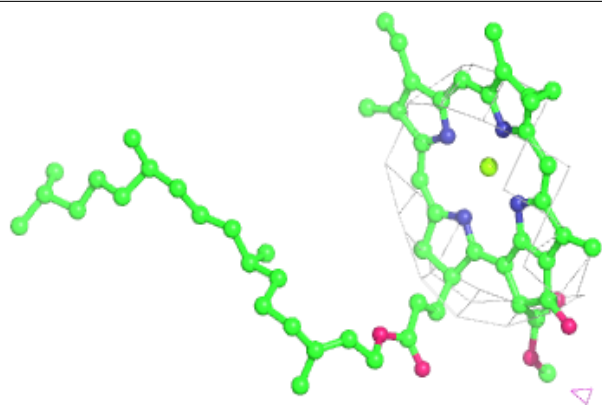
Electron density around HEM f 101:

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

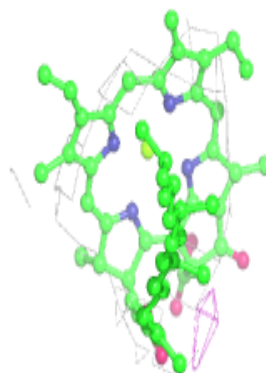
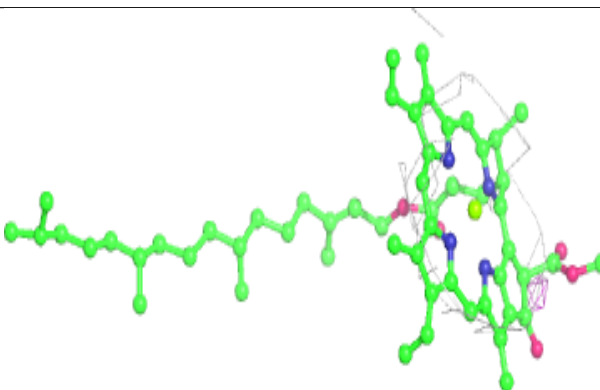
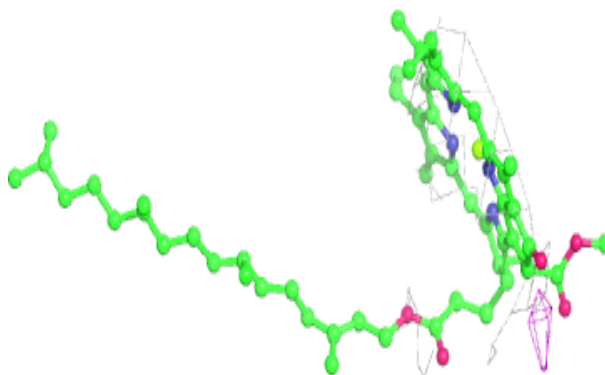


Electron density around CLA C 511:

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

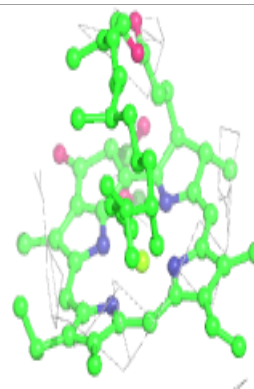
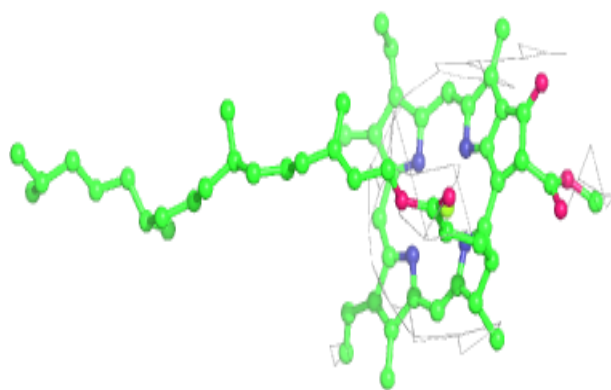
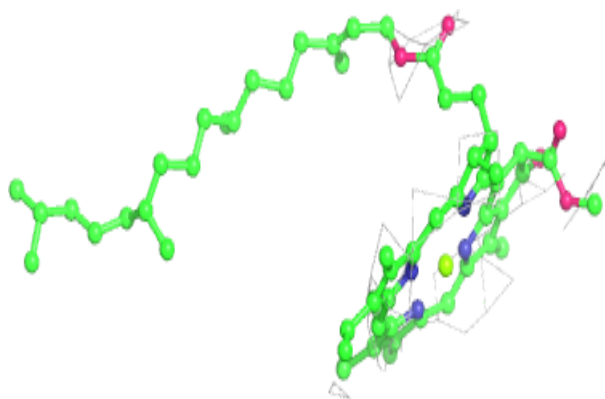
**Electron density around CLA B 608:**

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



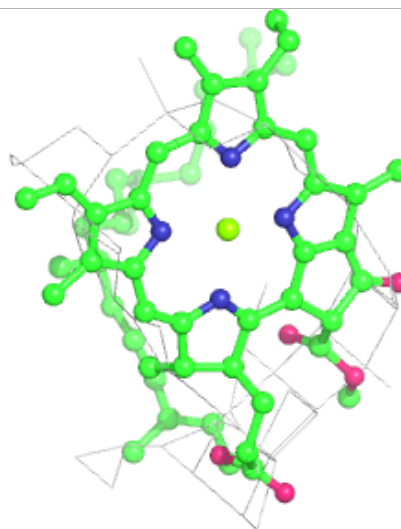
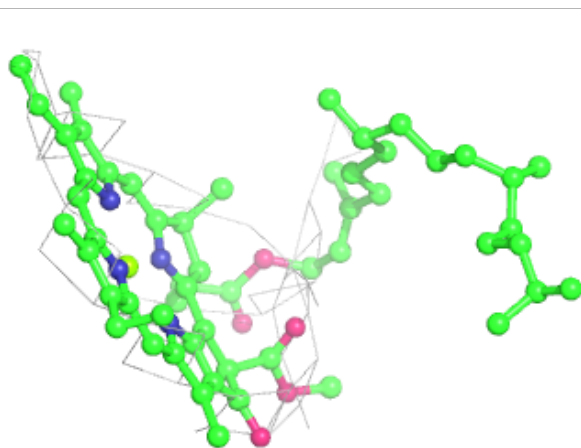
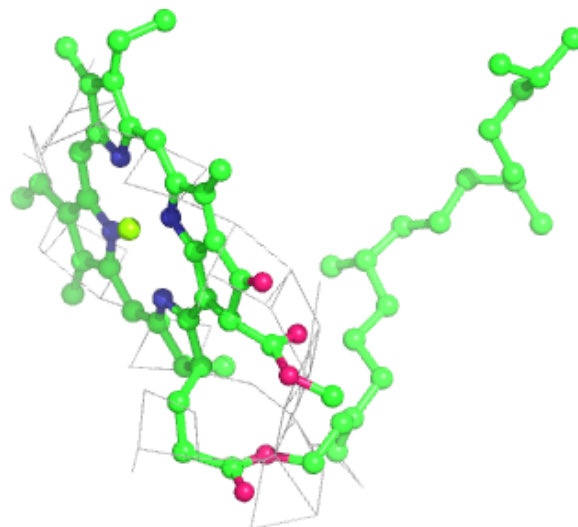
Electron density around CLA c 504:

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



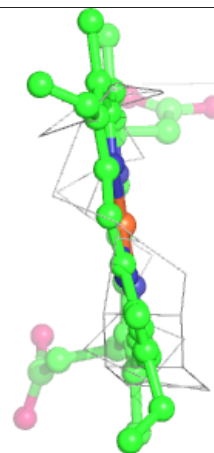
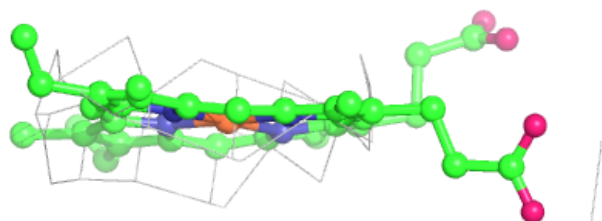
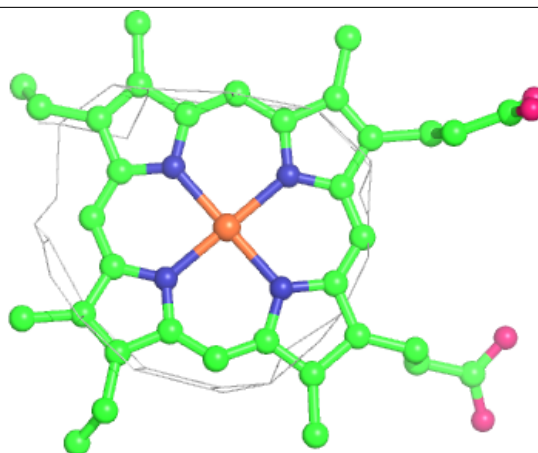
Electron density around CLA B 614:

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



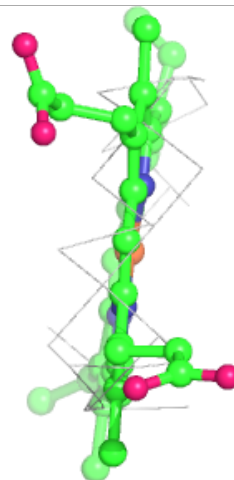
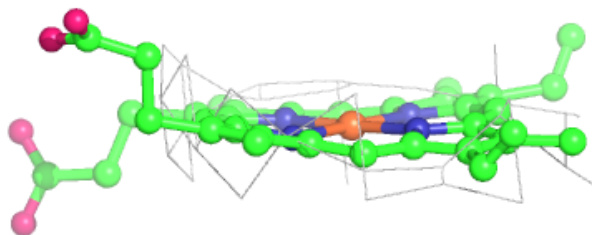
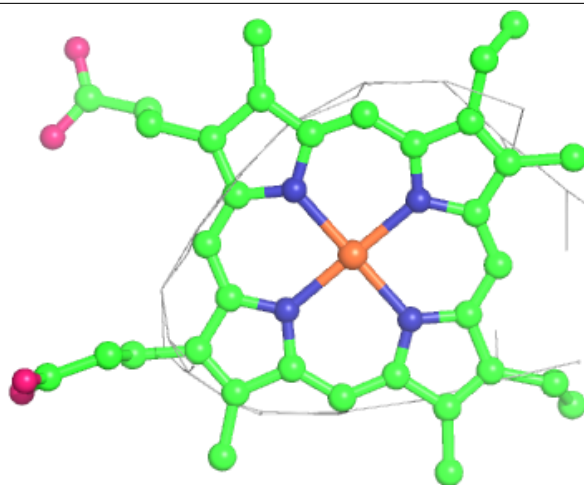
Electron density around HEM V 201:

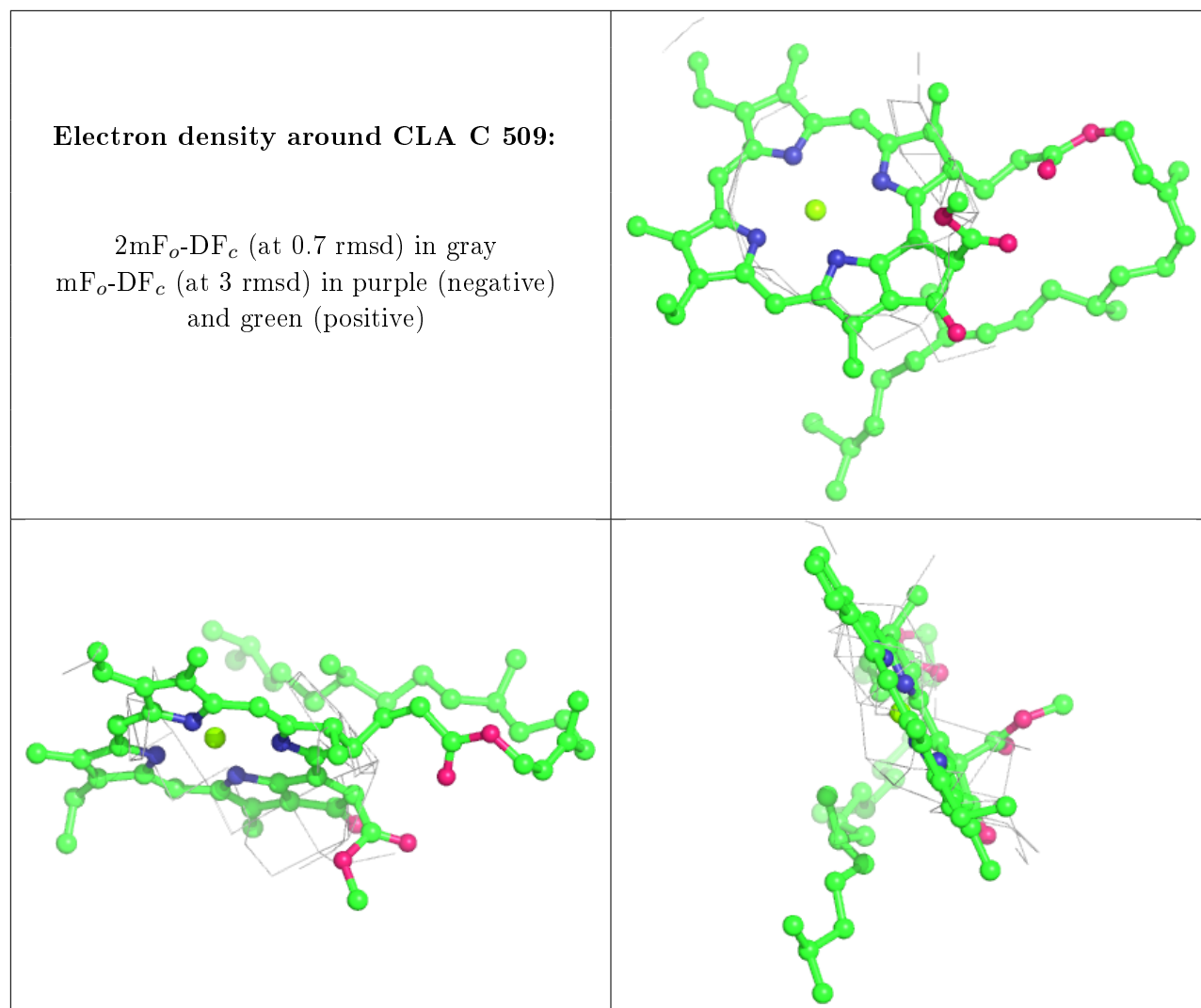
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM v 201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.