



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 10:22 am GMT

PDB ID : 5E79
Title : Macromolecular diffractive imaging using imperfect crystals
Authors : Ayer, K.; Yefanov, O.; Oberthur, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffer, A.; Dorner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on : 2015-10-12
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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)

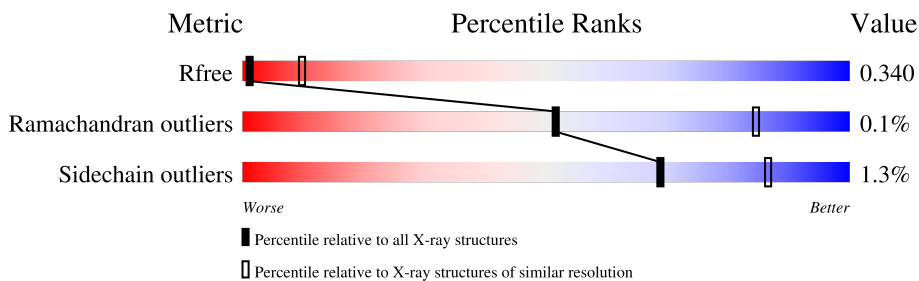
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

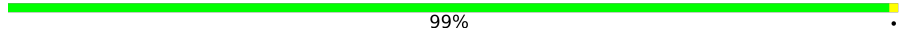
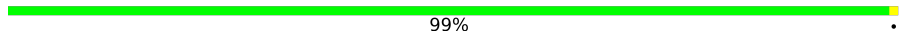
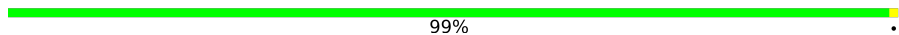

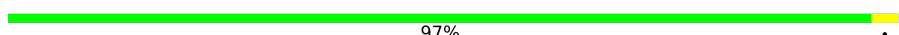
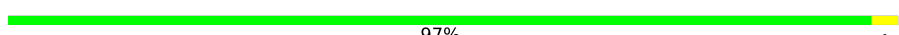
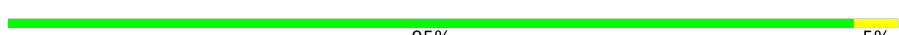




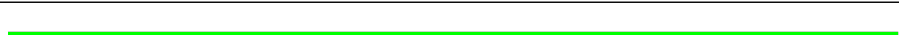

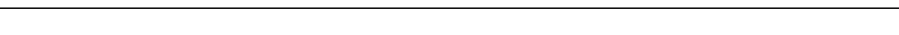
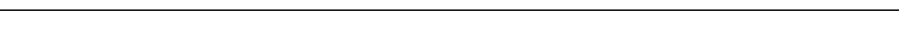
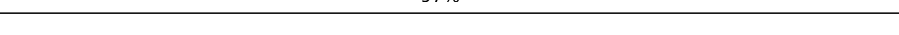
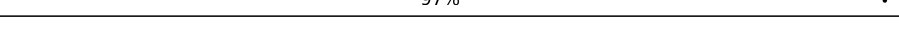
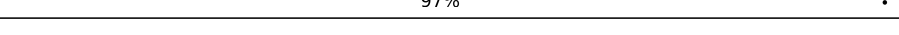
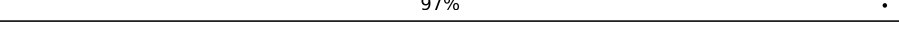
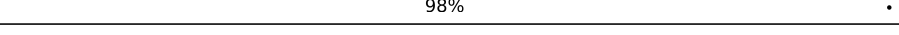
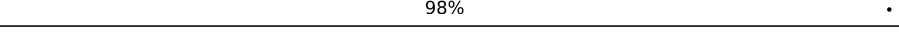
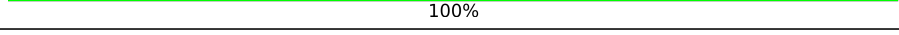
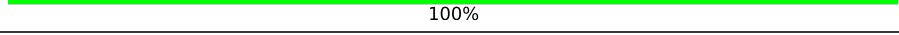
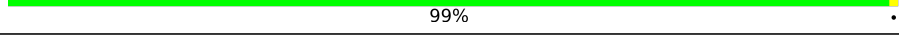
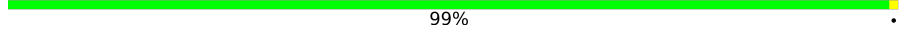
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	334	
1	a	334	
2	B	504	
2	b	504	
3	C	451	
3	c	451	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
4	D	342	 99%
4	d	342	 99%
5	E	81	 99%
5	e	81	 99%
6	F	34	 97%
6	f	34	 97%
7	H	65	 95% 5%
7	h	65	 95% 5%
8	I	38	 100%
8	i	38	 100%
9	J	38	 100%
9	j	38	 100%
10	K	37	 95% 5%
10	k	37	 92% 8%
11	L	37	 97%
11	l	37	 97%
12	M	34	 97%
12	m	34	 97%
13	O	243	 98%
13	o	243	 98%
14	T	30	 100%
14	t	30	 100%
15	U	97	 99%
15	u	97	 99%
16	V	137	 99%

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Mol	Chain	Length	Quality of chain
16	v	137	99%
17	Y	29	97%
17	y	29	97%
18	X	39	100%
18	x	39	100%
19	Z	62	98%
19	z	62	98%

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
24	CLA	A	606	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	609	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607[A]	X	-	-	-
24	CLA	B	607[B]	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	606	X	-	-	-
24	CLA	a	607	X	-	-	-
24	CLA	a	609	X	-	-	-
24	CLA	a	615	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608[A]	X	-	-	-
24	CLA	b	608[B]	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
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24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	A	610	-	X	-	-
26	BCR	B	618	-	X	-	-
26	BCR	B	619	-	X	-	-
26	BCR	B	620	-	X	-	-
26	BCR	C	514	-	X	-	-
26	BCR	F	101	-	X	-	-
26	BCR	H	101	-	X	-	-
26	BCR	I	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	K	102	-	X	-	-
26	BCR	T	101	-	X	-	-
26	BCR	a	610	-	X	-	-
26	BCR	b	619	-	X	-	-
26	BCR	b	620	-	X	-	-
26	BCR	b	621	-	X	-	-
26	BCR	c	514	-	X	-	-
26	BCR	c	515	-	X	-	-
26	BCR	c	521	-	X	-	-
26	BCR	f	101	-	X	-	-
26	BCR	h	101	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	t	101	-	X	-	-
27	PL9	D	405	-	X	-	-
27	PL9	d	404	-	X	-	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 50074 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
			Total	C	N	O	S			
1	A	334	2637	1730	432	460	15	0	4	0
1	a	334	2637	1730	432	460	15	3	4	0

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
			Total	C	N	O	S			
2	B	504	4024	2641	668	702	13	0	10	0
2	b	504	4024	2641	668	702	13	0	10	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3506	2296	584	613	13	0	5	0
3	c	451	3506	2296	584	613	13	0	5	0

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			668	436	107	125			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	5	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			

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

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

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

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

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

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

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

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

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

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

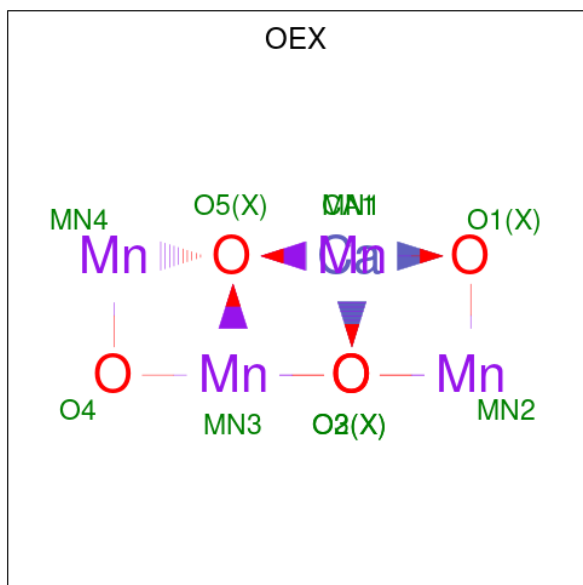
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	1	0
			292	196	46	50			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

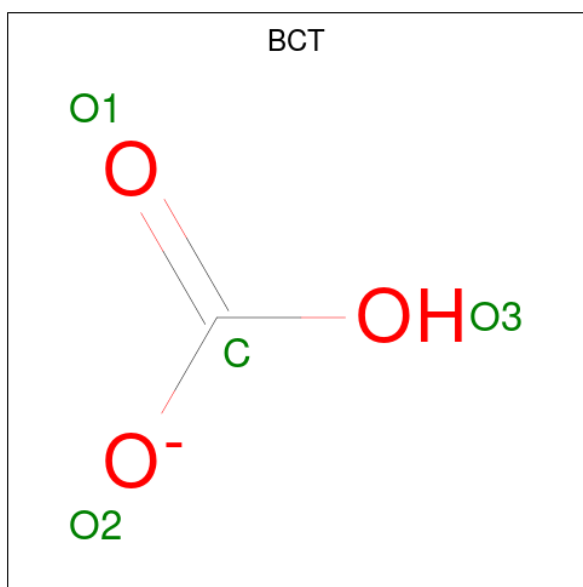
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

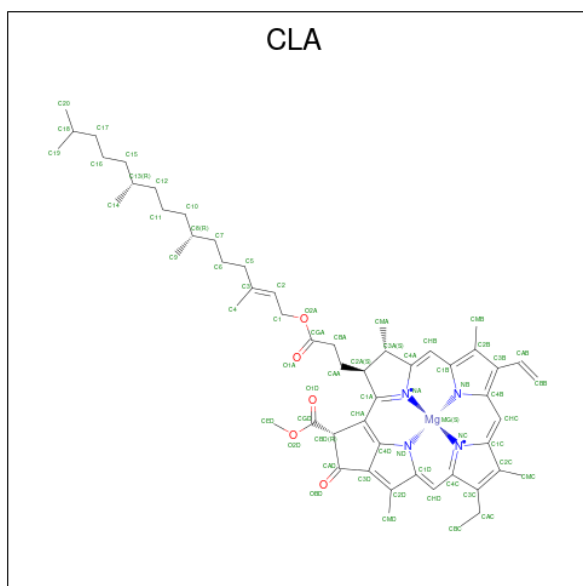
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
22	A	2	2	2	0	0
22	U	1	1	1	0	0
22	a	2	2	2	0	0
22	u	1	1	1	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

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



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

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

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

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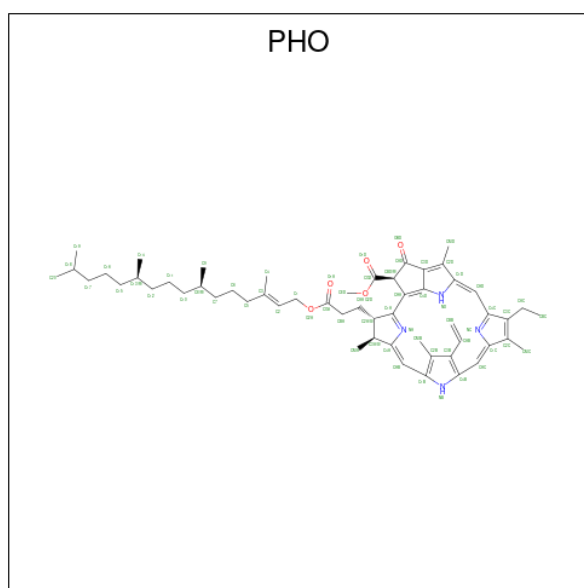
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
24	b	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b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

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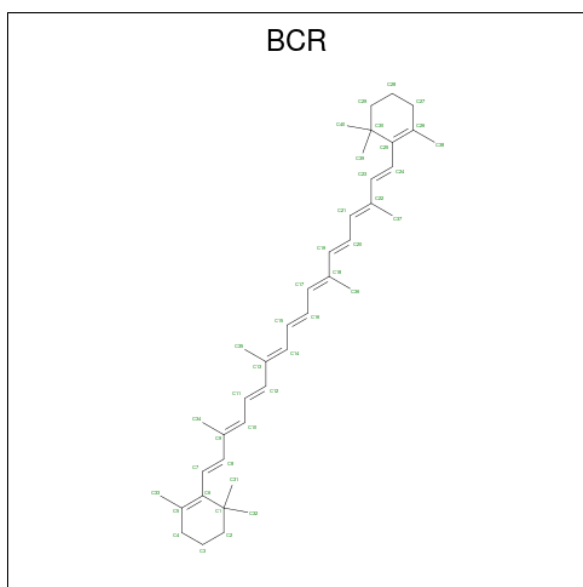
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



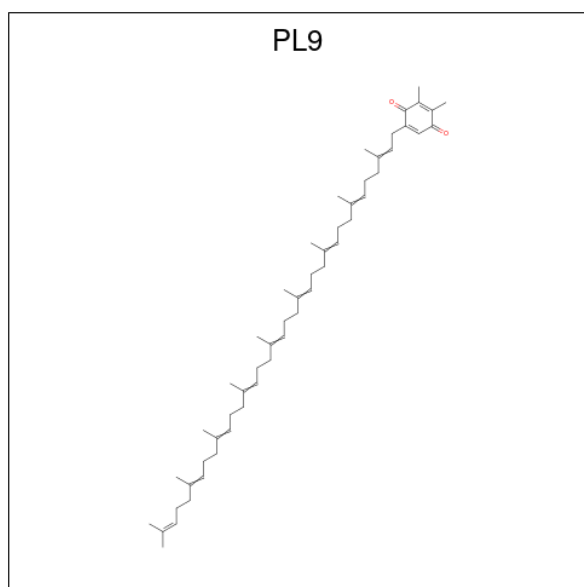
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	F	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	I	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

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

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



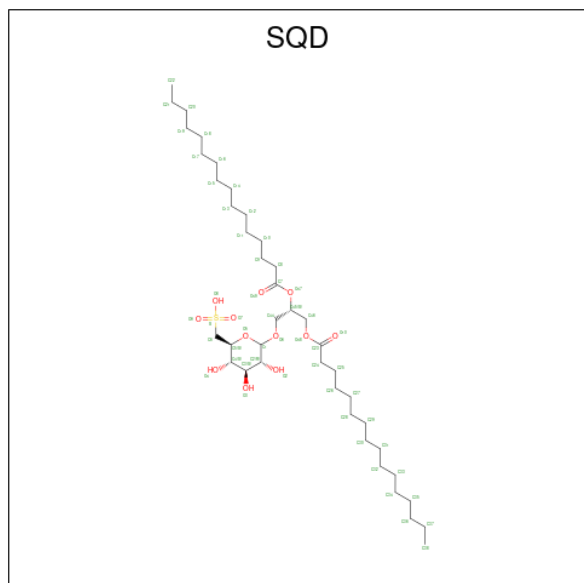
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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

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



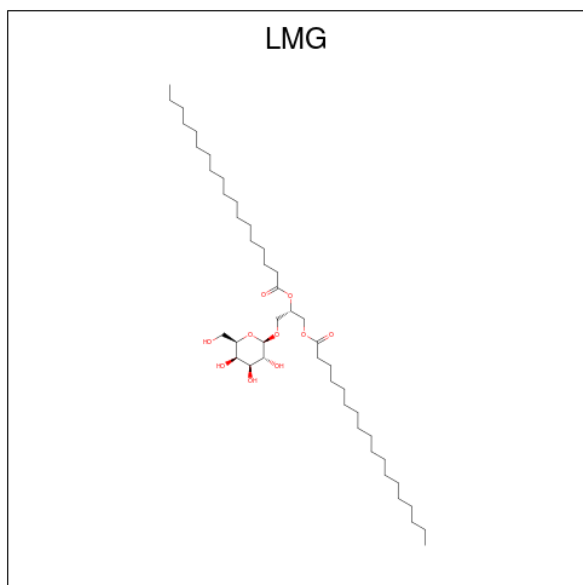
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	B	1	Total	C	O	S	0	0
			54	41	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	X	1	Total	C	O	S	0	0
			43	30	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
28	x	1	43	30	12	1	0	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



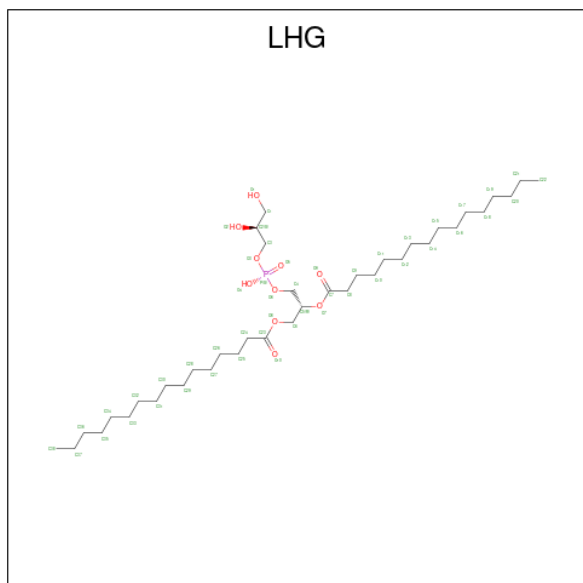
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	A	1	51	41	10	0	0
29	B	1	51	41	10	0	0
29	C	1	51	41	10	0	0
29	C	1	51	41	10	0	0
29	D	1	51	41	10	0	0
29	Z	1	37	27	10	0	0
29	a	1	51	41	10	0	0
29	b	1	51	41	10	0	0
29	c	1	51	41	10	0	0
29	c	1	51	41	10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	j	1	Total	C	O	0	0
			51	41	10		
29	z	1	Total	C	O	0	0
			37	27	10		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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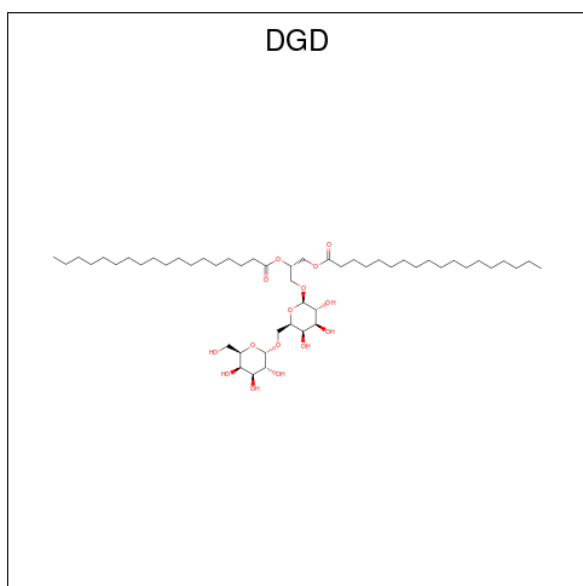
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



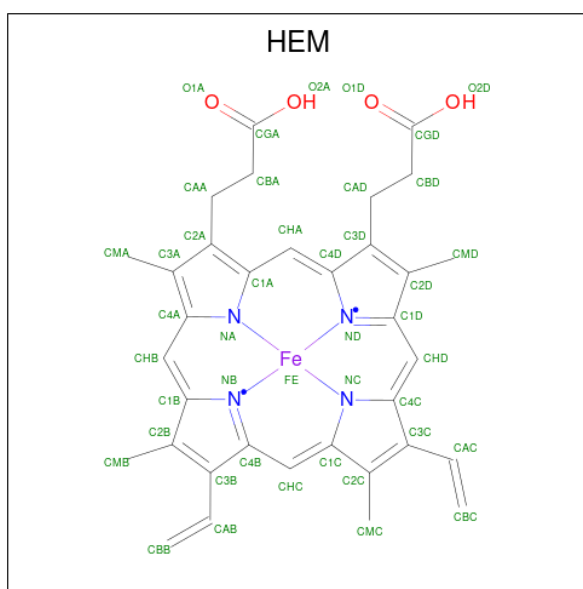
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		

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

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



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

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

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

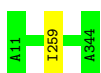
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem II protein D1 1

Chain A:  100%



- Molecule 1: Photosystem II protein D1 1

Chain a:  100%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  99%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  99%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  99%



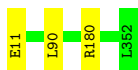
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  99%



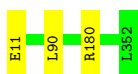
- Molecule 4: Photosystem II D2 protein

Chain D: 99%



- Molecule 4: Photosystem II D2 protein

Chain d: 99%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 99%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 99%



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 97%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 97%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 95% 5%



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein I



There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein J



There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein J



There are no outlier residues recorded for this chain.

- 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

Chain l: 97%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 97%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 97%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 98%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 98%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 100%

There are no outlier residues recorded for this chain.

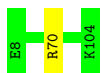
- Molecule 14: Photosystem II reaction center protein T

Chain t: 100%

There are no outlier residues recorded for this chain.

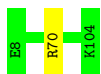
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  99%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  99%



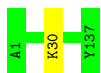
- Molecule 16: Cytochrome c-550

Chain V:  99%



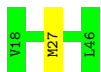
- Molecule 16: Cytochrome c-550

Chain v:  99%



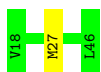
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  97%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  97%



- Molecule 18: Photosystem II reaction center X protein

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: Photosystem II reaction center X protein

Chain x:  100%

There are no outlier residues recorded for this chain.

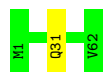
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  98% .



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  98% .



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	250.80Å 250.80Å 250.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 250.80 – 3.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.98-3.50) 100.0 (250.80-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.324 , 0.331 0.343 , 0.340	Depositor DCC
R_{free} test set	45921 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50074	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	0/2734	0.68	0/3727
1	a	0.49	0/2734	0.64	0/3727
2	B	0.51	0/4194	0.65	1/5713 (0.0%)
2	b	0.48	0/4194	0.63	1/5713 (0.0%)
3	C	0.51	0/3634	0.64	0/4947
3	c	0.47	0/3634	0.60	0/4947
4	D	0.53	0/2821	0.65	0/3844
4	d	0.48	0/2821	0.60	0/3844
5	E	0.46	0/693	0.63	0/944
5	e	0.43	0/693	0.58	0/944
6	F	0.51	0/284	0.61	0/387
6	f	0.41	0/284	0.56	0/387
7	H	0.47	0/544	0.64	0/739
7	h	0.46	0/544	0.66	0/739
8	I	0.52	0/327	0.68	0/439
8	i	0.46	0/327	0.60	0/439
9	J	0.46	0/278	0.59	0/376
9	j	0.43	0/278	0.53	0/376
10	K	0.48	0/303	0.70	0/416
10	k	0.55	0/303	0.79	0/416
11	L	0.55	0/319	0.70	0/433
11	l	0.48	0/319	0.62	0/433
12	M	0.52	0/278	0.74	0/378
12	m	0.49	0/278	0.69	0/378
13	O	0.46	0/1926	0.65	0/2611
13	o	0.41	0/1926	0.61	0/2611
14	T	0.60	0/282	0.68	0/382
14	t	0.49	0/282	0.60	0/382
15	U	0.48	0/785	0.64	0/1064
15	u	0.46	0/785	0.63	0/1064
16	V	0.52	1/1096 (0.1%)	0.66	0/1487
16	v	0.42	0/1096	0.62	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.44	0/216	0.61	0/289
17	y	0.44	0/216	0.59	0/289
18	X	0.43	0/298	0.53	0/403
18	x	0.44	0/298	0.54	0/403
19	Z	0.44	0/490	0.58	0/669
19	z	0.46	0/490	0.56	0/669
All	All	0.49	1/43004 (0.0%)	0.63	2/58496 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	37	CYS	CB-SG	-5.25	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	127	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	39	LEU	CA-CB-CG	-5.25	103.23	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	41 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	41	75
2	B	512/504 (102%)	506 (99%)	6 (1%)	0	100	100
2	b	512/504 (102%)	505 (99%)	7 (1%)	0	100	100
3	C	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	34	72
3	c	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	34	72
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	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	4	31
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	34	72
13	o	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	34	72
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	28 (97%)	1 (3%)	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	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5139 (98%)	104 (2%)	9 (0%)	51	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
10	k	11	LEU
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	412/402 (102%)	408 (99%)	4 (1%)	76	88
2	b	412/402 (102%)	410 (100%)	2 (0%)	88	94
3	C	357/352 (101%)	351 (98%)	6 (2%)	60	82
3	c	357/352 (101%)	353 (99%)	4 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	88
4	d	277/277 (100%)	274 (99%)	3 (1%)	73	88
5	E	74/72 (103%)	73 (99%)	1 (1%)	67	85
5	e	74/72 (103%)	73 (99%)	1 (1%)	67	85
6	F	28/28 (100%)	27 (96%)	1 (4%)	35	66
6	f	28/28 (100%)	27 (96%)	1 (4%)	35	66
7	H	56/54 (104%)	52 (93%)	4 (7%)	14	46
7	h	56/54 (104%)	52 (93%)	4 (7%)	14	46
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	48
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	48
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	72
11	l	36/35 (103%)	35 (97%)	1 (3%)	43	72
12	M	32/31 (103%)	31 (97%)	1 (3%)	40	70
12	m	32/31 (103%)	31 (97%)	1 (3%)	40	70
13	O	210/206 (102%)	206 (98%)	4 (2%)	57	80
13	o	210/206 (102%)	206 (98%)	4 (2%)	57	80
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	71	87
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	87
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	91
16	v	118/117 (101%)	117 (99%)	1 (1%)	81	91
17	Y	22/22 (100%)	21 (96%)	1 (4%)	27	61
17	y	22/22 (100%)	21 (96%)	1 (4%)	27	61
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	80
All	All	4370/4302 (102%)	4312 (99%)	58 (1%)	69	86

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	76[A]	SER
2	B	76[B]	SER
2	B	246	PHE
2	B	472	ARG
3	C	24	THR
3	C	289	PHE
3	C	315	MET
3	C	416[A]	SER
3	C	416[B]	SER
3	C	418	ASN
4	D	11	GLU
4	D	90	LEU
4	D	180	ARG
5	E	71	GLU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
7	H	65	LEU
10	K	13	GLU
10	K	17	ILE
11	L	1	MET
12	M	9	ILE
13	O	61	GLN
13	O	118	LEU
13	O	181	GLU
13	O	234	LYS
15	U	70	ARG
16	V	30	LYS
17	Y	27	MET
19	Z	31	GLN
2	b	246	PHE
2	b	472	ARG
3	c	24	THR
3	c	289	PHE
3	c	315	MET

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Mol	Chain	Res	Type
3	c	418	ASN
4	d	11	GLU
4	d	90	LEU
4	d	180	ARG
5	e	71	GLU
6	f	44	GLN
7	h	12[A]	ARG
7	h	12[B]	ARG
7	h	49	TYR
7	h	65	LEU
10	k	13	GLU
10	k	17	ILE
11	l	1	MET
12	m	9	ILE
13	o	61	GLN
13	o	118	LEU
13	o	181	GLU
13	o	234	LYS
15	u	70	ARG
16	v	30	LYS
17	y	27	MET
19	z	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	216	HIS
2	B	409	GLN
4	d	197	HIS
15	u	78	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 168 ligands modelled in this entry, 16 are monoatomic - leaving 152 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	z	101	-	37,37,55	1.40	4 (10%)	45,45,63	1.22	4 (8%)
32	DGD	H	102	-	63,63,67	1.69	14 (22%)	77,77,81	1.02	4 (5%)
26	BCR	B	618	-	41,41,41	8.92	29 (70%)	56,56,56	5.95	31 (55%)
27	PL9	A	611	-	55,55,55	4.17	20 (36%)	68,69,69	3.92	34 (50%)
26	BCR	B	620	-	41,41,41	9.12	29 (70%)	56,56,56	5.77	33 (58%)
24	CLA	A	606	-	65,73,73	3.71	30 (46%)	76,113,113	1.97	18 (23%)
24	CLA	c	509	-	65,73,73	3.53	30 (46%)	76,113,113	1.82	16 (21%)
24	CLA	B	615	-	65,73,73	3.58	29 (44%)	76,113,113	1.85	15 (19%)
24	CLA	D	404	-	65,73,73	3.59	30 (46%)	76,113,113	2.00	18 (23%)
24	CLA	b	606	-	65,73,73	3.63	27 (41%)	76,113,113	1.94	16 (21%)
30	LHG	e	101	-	41,41,48	1.23	3 (7%)	44,47,54	1.05	2 (4%)
24	CLA	c	506	-	65,73,73	3.54	27 (41%)	76,113,113	1.86	14 (18%)
24	CLA	D	402	-	65,73,73	3.71	32 (49%)	76,113,113	1.83	20 (26%)
24	CLA	b	608[A]	-	65,73,73	3.57	29 (44%)	76,113,113	1.86	18 (23%)
29	LMG	j	101	34	51,51,55	1.31	5 (9%)	59,59,63	0.87	4 (6%)
32	DGD	E	101	-	63,63,67	1.73	15 (23%)	77,77,81	1.23	10 (12%)
30	LHG	D	406	-	48,48,48	1.13	2 (4%)	51,54,54	0.97	4 (7%)
25	PHO	A	608	-	51,69,69	0.99	2 (3%)	47,99,99	1.21	6 (12%)
24	CLA	b	610	-	65,73,73	3.52	29 (44%)	76,113,113	1.86	17 (22%)
24	CLA	B	603	-	65,73,73	3.59	31 (47%)	76,113,113	1.87	19 (25%)
26	BCR	t	101	-	41,41,41	9.01	30 (73%)	56,56,56	5.95	34 (60%)
24	CLA	A	609	-	65,73,73	3.66	30 (46%)	76,113,113	1.80	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	604	-	65,73,73	3.59	30 (46%)	76,113,113	1.80	17 (22%)
24	CLA	C	507	-	65,73,73	3.49	29 (44%)	76,113,113	2.03	17 (22%)
27	PL9	D	405	-	55,55,55	4.19	20 (36%)	68,69,69	3.80	36 (52%)
30	LHG	L	101	-	48,48,48	1.10	2 (4%)	51,54,54	0.90	3 (5%)
32	DGD	h	102	-	63,63,67	1.68	15 (23%)	77,77,81	1.21	8 (10%)
30	LHG	d	407	-	48,48,48	1.15	3 (6%)	51,54,54	1.09	3 (5%)
27	PL9	a	611	-	55,55,55	4.18	21 (38%)	68,69,69	3.89	34 (50%)
26	BCR	c	514	-	41,41,41	8.98	30 (73%)	56,56,56	5.91	34 (60%)
24	CLA	a	607	-	65,73,73	3.60	27 (41%)	76,113,113	1.86	18 (23%)
28	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	1.45	7 (13%)
33	HEM	E	103	5,6	41,50,50	2.02	7 (17%)	45,82,82	1.42	6 (13%)
26	BCR	b	620	-	41,41,41	8.87	29 (70%)	56,56,56	5.73	31 (55%)
26	BCR	C	514	-	41,41,41	8.98	30 (73%)	56,56,56	5.93	33 (58%)
28	SQD	a	612	-	53,54,54	0.99	3 (5%)	62,65,65	1.53	11 (17%)
24	CLA	c	505	-	65,73,73	3.59	27 (41%)	76,113,113	1.84	14 (18%)
26	BCR	H	101	-	41,41,41	9.06	30 (73%)	56,56,56	5.72	30 (53%)
24	CLA	c	510	-	65,73,73	3.58	29 (44%)	76,113,113	1.81	16 (21%)
24	CLA	B	608	-	65,73,73	3.66	28 (43%)	76,113,113	1.90	19 (25%)
26	BCR	K	101	-	41,41,41	9.12	31 (75%)	56,56,56	5.42	29 (51%)
29	LMG	b	622	-	51,51,55	1.32	4 (7%)	59,59,63	1.06	5 (8%)
24	CLA	C	510	-	65,73,73	3.57	30 (46%)	76,113,113	1.85	16 (21%)
24	CLA	a	615	-	65,73,73	3.70	29 (44%)	76,113,113	1.94	20 (26%)
24	CLA	c	503	-	65,73,73	3.58	30 (46%)	76,113,113	1.74	14 (18%)
28	SQD	A	612	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
24	CLA	c	502	-	65,73,73	3.56	28 (43%)	76,113,113	1.81	16 (21%)
23	BCT	a	605	21	2,3,3	0.96	0	2,3,3	3.74	2 (100%)
30	LHG	l	102	-	48,48,48	1.18	2 (4%)	51,54,54	0.92	2 (3%)
24	CLA	b	609	-	65,73,73	3.63	28 (43%)	76,113,113	1.90	17 (22%)
33	HEM	e	102	5,6	41,50,50	1.99	8 (19%)	45,82,82	1.49	5 (11%)
33	HEM	v	201	16	41,50,50	2.05	6 (14%)	45,82,82	1.70	8 (17%)
24	CLA	c	507	-	65,73,73	3.52	28 (43%)	76,113,113	2.01	16 (21%)
28	SQD	L	102	-	53,54,54	1.04	4 (7%)	62,65,65	1.36	9 (14%)
29	LMG	c	519	-	51,51,55	1.38	5 (9%)	59,59,63	1.06	5 (8%)
30	LHG	a	616	-	48,48,48	1.10	2 (4%)	51,54,54	1.17	6 (11%)
24	CLA	b	612	-	65,73,73	3.60	28 (43%)	76,113,113	1.88	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	OEX	A	601	3,1	0,15,15	-	-	-		
26	BCR	F	101	-	41,41,41	9.04	26 (63%)	56,56,56	6.08	27 (48%)
24	CLA	B	613	-	65,73,73	3.68	28 (43%)	76,113,113	1.96	19 (25%)
26	BCR	c	515	-	41,41,41	9.15	31 (75%)	56,56,56	5.57	27 (48%)
26	BCR	h	101	-	41,41,41	9.16	30 (73%)	56,56,56	5.68	33 (58%)
24	CLA	b	603	-	65,73,73	3.60	28 (43%)	76,113,113	1.82	16 (21%)
26	BCR	k	101	-	41,41,41	9.22	31 (75%)	56,56,56	5.67	28 (50%)
32	DGD	C	517	-	63,63,67	1.66	15 (23%)	77,77,81	1.14	6 (7%)
24	CLA	c	513	-	65,73,73	3.48	30 (46%)	76,113,113	1.80	16 (21%)
24	CLA	c	512	-	65,73,73	3.60	29 (44%)	76,113,113	1.82	18 (23%)
24	CLA	C	504	-	65,73,73	3.57	29 (44%)	76,113,113	1.91	18 (23%)
33	HEM	V	201	16	41,50,50	2.01	8 (19%)	45,82,82	1.58	7 (15%)
26	BCR	K	102	-	41,41,41	9.13	29 (70%)	56,56,56	5.63	25 (44%)
24	CLA	B	616	-	65,73,73	3.55	29 (44%)	76,113,113	1.73	18 (23%)
30	LHG	D	407	-	48,48,48	1.11	3 (6%)	51,54,54	0.89	3 (5%)
30	LHG	A	615	-	48,48,48	1.11	3 (6%)	51,54,54	1.30	5 (9%)
28	SQD	x	101	-	42,43,54	1.20	4 (9%)	51,54,65	1.46	7 (13%)
24	CLA	b	618	-	65,73,73	3.64	28 (43%)	76,113,113	1.81	18 (23%)
24	CLA	B	612	-	65,73,73	3.66	29 (44%)	76,113,113	1.86	18 (23%)
24	CLA	b	611	-	65,73,73	3.57	26 (40%)	76,113,113	1.78	16 (21%)
24	CLA	B	611	-	65,73,73	3.55	31 (47%)	76,113,113	1.81	19 (25%)
24	CLA	B	607[B]	-	65,73,73	3.60	28 (43%)	76,113,113	1.88	18 (23%)
25	PHO	d	401	-	51,69,69	0.97	0	47,99,99	1.40	6 (12%)
24	CLA	B	610	-	65,73,73	3.69	27 (41%)	76,113,113	1.81	19 (25%)
26	BCR	T	101	-	41,41,41	9.04	30 (73%)	56,56,56	6.12	32 (57%)
24	CLA	B	606	-	65,73,73	3.56	28 (43%)	76,113,113	1.78	14 (18%)
24	CLA	b	613	-	65,73,73	3.71	29 (44%)	76,113,113	1.91	19 (25%)
32	DGD	c	516	-	63,63,67	1.70	15 (23%)	77,77,81	1.09	7 (9%)
24	CLA	b	615	-	65,73,73	3.63	29 (44%)	76,113,113	1.75	16 (21%)
24	CLA	b	617	-	65,73,73	3.54	30 (46%)	76,113,113	1.77	15 (19%)
24	CLA	a	606	-	65,73,73	3.64	28 (43%)	76,113,113	1.90	19 (25%)
24	CLA	b	605	-	65,73,73	3.70	29 (44%)	76,113,113	1.90	19 (25%)
32	DGD	c	517	-	63,63,67	1.62	16 (25%)	77,77,81	1.11	9 (11%)
24	CLA	c	508	-	65,73,73	3.60	28 (43%)	76,113,113	1.94	17 (22%)
24	CLA	A	607	-	65,73,73	3.59	29 (44%)	76,113,113	1.99	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PL9	d	404	-	55,55,55	4.15	20 (36%)	68,69,69	3.85	34 (50%)
24	CLA	C	509	-	65,73,73	3.58	30 (46%)	76,113,113	1.86	16 (21%)
24	CLA	C	511	3	65,73,73	3.63	29 (44%)	76,113,113	1.93	20 (26%)
24	CLA	b	607	-	65,73,73	3.57	29 (44%)	76,113,113	1.80	14 (18%)
24	CLA	B	605	-	65,73,73	3.59	27 (41%)	76,113,113	1.91	17 (22%)
26	BCR	A	610	-	41,41,41	9.17	30 (73%)	56,56,56	5.54	27 (48%)
24	CLA	c	501	-	65,73,73	3.56	30 (46%)	76,113,113	1.87	20 (26%)
24	CLA	c	504	-	65,73,73	3.63	31 (47%)	76,113,113	1.96	22 (28%)
26	BCR	f	101	-	41,41,41	8.99	29 (70%)	56,56,56	5.59	26 (46%)
24	CLA	C	505	-	65,73,73	3.53	27 (41%)	76,113,113	1.86	15 (19%)
24	CLA	D	403	-	65,73,73	3.65	28 (43%)	76,113,113	1.73	18 (23%)
26	BCR	b	621	-	41,41,41	9.05	31 (75%)	56,56,56	6.43	31 (55%)
29	LMG	A	613	-	51,51,55	1.33	4 (7%)	59,59,63	0.91	4 (6%)
28	SQD	B	622	-	53,54,54	1.07	4 (7%)	62,65,65	1.44	9 (14%)
32	DGD	c	518	-	63,63,67	1.68	15 (23%)	77,77,81	1.25	8 (10%)
20	OEX	a	601	3,1	0,15,15	-	-	-	-	-
24	CLA	C	502	-	65,73,73	3.55	28 (43%)	76,113,113	1.85	16 (21%)
24	CLA	B	609	-	65,73,73	3.52	27 (41%)	76,113,113	1.97	23 (30%)
24	CLA	B	617	-	65,73,73	3.57	28 (43%)	76,113,113	1.79	16 (21%)
25	PHO	D	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.48	8 (17%)
30	LHG	d	406	-	48,48,48	1.11	2 (4%)	51,54,54	1.02	3 (5%)
29	LMG	C	518	-	51,51,55	1.42	6 (11%)	59,59,63	1.29	10 (16%)
32	DGD	d	405	-	63,63,67	1.71	16 (25%)	77,77,81	1.16	9 (11%)
24	CLA	d	403	-	65,73,73	3.53	29 (44%)	76,113,113	1.87	19 (25%)
28	SQD	l	101	-	53,54,54	1.04	4 (7%)	62,65,65	1.36	8 (12%)
24	CLA	B	602	-	65,73,73	3.52	29 (44%)	76,113,113	1.77	13 (17%)
26	BCR	b	619	-	41,41,41	9.23	29 (70%)	56,56,56	5.80	28 (50%)
29	LMG	C	519	-	51,51,55	1.33	5 (9%)	59,59,63	1.02	4 (6%)
29	LMG	c	520	-	51,51,55	1.37	5 (9%)	59,59,63	1.12	4 (6%)
24	CLA	B	607[A]	-	65,73,73	3.59	27 (41%)	76,113,113	1.90	19 (25%)
24	CLA	a	609	-	65,73,73	3.61	28 (43%)	76,113,113	1.83	17 (22%)
30	LHG	E	102	-	41,41,48	1.22	3 (7%)	44,47,54	0.99	3 (6%)
24	CLA	C	506	-	65,73,73	3.53	28 (43%)	76,113,113	1.90	16 (21%)
24	CLA	b	608[B]	-	65,73,73	3.58	28 (43%)	76,113,113	1.84	19 (25%)
29	LMG	Z	101	-	37,37,55	1.44	4 (10%)	45,45,63	1.34	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	508	-	65,73,73	3.70	30 (46%)	76,113,113	1.81	16 (21%)
24	CLA	B	614	-	65,73,73	3.63	29 (44%)	76,113,113	1.78	15 (19%)
24	CLA	d	402	-	65,73,73	3.61	30 (46%)	76,113,113	1.83	18 (23%)
24	CLA	C	503	-	65,73,73	3.60	30 (46%)	76,113,113	1.72	14 (18%)
29	LMG	B	621	-	51,51,55	1.29	4 (7%)	59,59,63	1.01	3 (5%)
26	BCR	c	521	-	41,41,41	9.34	29 (70%)	56,56,56	5.62	26 (46%)
26	BCR	I	101	-	41,41,41	9.05	31 (75%)	56,56,56	5.91	30 (53%)
29	LMG	D	408	-	51,51,55	1.34	5 (9%)	59,59,63	1.10	7 (11%)
28	SQD	a	614	-	53,54,54	1.04	3 (5%)	62,65,65	1.22	6 (9%)
24	CLA	c	511	3	65,73,73	3.57	28 (43%)	76,113,113	1.85	16 (21%)
25	PHO	a	608	-	51,69,69	1.01	3 (5%)	47,99,99	1.21	5 (10%)
29	LMG	a	613	-	51,51,55	1.33	5 (9%)	59,59,63	0.99	3 (5%)
32	DGD	C	515	-	63,63,67	1.70	15 (23%)	77,77,81	1.03	5 (6%)
26	BCR	B	619	-	41,41,41	8.94	30 (73%)	56,56,56	5.62	29 (51%)
24	CLA	b	616	-	65,73,73	3.58	29 (44%)	76,113,113	1.85	16 (21%)
32	DGD	C	516	-	63,63,67	1.67	15 (23%)	77,77,81	1.21	10 (12%)
24	CLA	C	512	-	65,73,73	3.53	30 (46%)	76,113,113	1.88	20 (26%)
24	CLA	b	604	-	65,73,73	3.64	28 (43%)	76,113,113	1.92	16 (21%)
23	BCT	A	605	21	2,3,3	0.95	0	2,3,3	2.68	2 (100%)
28	SQD	A	614	-	53,54,54	1.04	3 (5%)	62,65,65	1.22	6 (9%)
24	CLA	b	614	-	65,73,73	3.68	28 (43%)	76,113,113	1.88	18 (23%)
24	CLA	C	513	-	65,73,73	3.51	27 (41%)	76,113,113	1.88	19 (25%)
24	CLA	C	501	-	65,73,73	3.54	28 (43%)	76,113,113	1.90	20 (26%)
28	SQD	b	601	-	53,54,54	1.08	4 (7%)	62,65,65	1.44	9 (14%)
26	BCR	a	610	-	41,41,41	8.98	30 (73%)	56,56,56	5.53	24 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	z	101	-	-	18/31/51/70	0/1/1/1
32	DGD	H	102	-	-	20/51/91/95	0/2/2/2
26	BCR	B	618	-	-	23/29/63/63	0/2/2/2
27	PL9	A	611	-	-	25/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	620	-	-	19/29/63/63	0/2/2/2
24	CLA	A	606	-	1/1/15/20	1/37/115/115	-
24	CLA	c	509	-	1/1/15/20	11/37/115/115	-
24	CLA	B	615	-	1/1/15/20	15/37/115/115	-
24	CLA	D	404	-	1/1/15/20	13/37/115/115	-
24	CLA	b	606	-	1/1/15/20	10/37/115/115	-
30	LHG	e	101	-	-	24/46/46/53	-
24	CLA	c	506	-	1/1/15/20	13/37/115/115	-
24	CLA	D	402	-	1/1/15/20	6/37/115/115	-
24	CLA	b	608[A]	-	1/1/15/20	8/37/115/115	-
29	LMG	j	101	34	-	17/46/66/70	0/1/1/1
32	DGD	E	101	-	-	35/51/91/95	0/2/2/2
30	LHG	D	406	-	-	19/53/53/53	-
25	PHO	A	608	-	-	4/37/103/103	0/5/6/6
24	CLA	b	610	-	1/1/15/20	5/37/115/115	-
24	CLA	B	603	-	1/1/15/20	4/37/115/115	-
26	BCR	t	101	-	-	26/29/63/63	0/2/2/2
24	CLA	A	609	-	1/1/15/20	19/37/115/115	-
24	CLA	B	604	-	1/1/15/20	6/37/115/115	-
24	CLA	C	507	-	1/1/15/20	9/37/115/115	-
27	PL9	D	405	-	-	26/53/73/73	0/1/1/1
30	LHG	L	101	-	-	19/53/53/53	-
32	DGD	h	102	-	-	17/51/91/95	0/2/2/2
30	LHG	d	407	-	-	18/53/53/53	-
27	PL9	a	611	-	-	24/53/73/73	0/1/1/1
26	BCR	c	514	-	-	24/29/63/63	0/2/2/2
24	CLA	a	607	-	1/1/15/20	11/37/115/115	-
28	SQD	X	101	-	-	16/38/58/69	0/1/1/1
33	HEM	E	103	5,6	-	3/12/54/54	-
26	BCR	b	620	-	-	19/29/63/63	0/2/2/2
26	BCR	C	514	-	-	25/29/63/63	0/2/2/2
28	SQD	a	612	-	-	16/49/69/69	0/1/1/1
24	CLA	c	505	-	1/1/15/20	8/37/115/115	-
26	BCR	H	101	-	-	21/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	510	-	1/1/15/20	11/37/115/115	-
24	CLA	B	608	-	1/1/15/20	7/37/115/115	-
26	BCR	K	101	-	-	19/29/63/63	0/2/2/2
29	LMG	b	622	-	-	19/46/66/70	0/1/1/1
24	CLA	C	510	-	1/1/15/20	12/37/115/115	-
24	CLA	a	615	-	1/1/15/20	7/37/115/115	-
24	CLA	c	503	-	1/1/15/20	3/37/115/115	-
28	SQD	A	612	-	-	16/49/69/69	0/1/1/1
24	CLA	c	502	-	1/1/15/20	10/37/115/115	-
30	LHG	l	102	-	-	23/53/53/53	-
24	CLA	b	609	-	1/1/15/20	4/37/115/115	-
33	HEM	e	102	5,6	-	3/12/54/54	-
33	HEM	v	201	16	-	2/12/54/54	-
24	CLA	c	507	-	1/1/15/20	9/37/115/115	-
28	SQD	L	102	-	-	28/49/69/69	0/1/1/1
29	LMG	c	519	-	-	21/46/66/70	0/1/1/1
30	LHG	a	616	-	-	17/53/53/53	-
24	CLA	b	612	-	1/1/15/20	10/37/115/115	-
26	BCR	F	101	-	-	21/29/63/63	0/2/2/2
26	BCR	h	101	-	-	25/29/63/63	0/2/2/2
24	CLA	B	613	-	1/1/15/20	7/37/115/115	-
26	BCR	c	515	-	-	20/29/63/63	0/2/2/2
26	BCR	k	101	-	-	20/29/63/63	0/2/2/2
24	CLA	b	603	-	1/1/15/20	19/37/115/115	-
32	DGD	C	517	-	-	17/51/91/95	0/2/2/2
24	CLA	c	513	-	1/1/15/20	10/37/115/115	-
24	CLA	c	512	-	1/1/15/20	7/37/115/115	-
24	CLA	C	504	-	1/1/15/20	12/37/115/115	-
33	HEM	V	201	16	-	2/12/54/54	-
26	BCR	K	102	-	-	20/29/63/63	0/2/2/2
24	CLA	B	616	-	1/1/15/20	13/37/115/115	-
30	LHG	D	407	-	-	19/53/53/53	-
30	LHG	A	615	-	-	16/53/53/53	-
28	SQD	x	101	-	-	16/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	618	-	1/1/15/20	14/37/115/115	-
24	CLA	B	612	-	1/1/15/20	5/37/115/115	-
24	CLA	b	611	-	1/1/15/20	5/37/115/115	-
24	CLA	B	611	-	1/1/15/20	9/37/115/115	-
24	CLA	B	607[B]	-	1/1/15/20	10/37/115/115	-
25	PHO	d	401	-	-	2/37/103/103	0/5/6/6
24	CLA	B	610	-	1/1/15/20	6/37/115/115	-
26	BCR	T	101	-	-	25/29/63/63	0/2/2/2
24	CLA	B	606	-	1/1/15/20	7/37/115/115	-
24	CLA	b	613	-	1/1/15/20	4/37/115/115	-
32	DGD	c	516	-	-	22/51/91/95	0/2/2/2
24	CLA	b	615	-	1/1/15/20	5/37/115/115	-
24	CLA	b	617	-	1/1/15/20	11/37/115/115	-
24	CLA	a	606	-	1/1/15/20	3/37/115/115	-
24	CLA	b	605	-	1/1/15/20	7/37/115/115	-
32	DGD	c	517	-	-	26/51/91/95	0/2/2/2
24	CLA	c	508	-	1/1/15/20	4/37/115/115	-
24	CLA	A	607	-	1/1/15/20	11/37/115/115	-
27	PL9	d	404	-	-	26/53/73/73	0/1/1/1
24	CLA	C	509	-	1/1/15/20	7/37/115/115	-
24	CLA	C	511	3	1/1/15/20	6/37/115/115	-
24	CLA	b	607	-	1/1/15/20	6/37/115/115	-
24	CLA	B	605	-	1/1/15/20	9/37/115/115	-
26	BCR	A	610	-	-	23/29/63/63	0/2/2/2
24	CLA	c	501	-	1/1/15/20	11/37/115/115	-
24	CLA	c	504	-	1/1/15/20	11/37/115/115	-
26	BCR	f	101	-	-	18/29/63/63	0/2/2/2
24	CLA	C	505	-	1/1/15/20	7/37/115/115	-
24	CLA	D	403	-	1/1/15/20	6/37/115/115	-
26	BCR	b	621	-	-	20/29/63/63	0/2/2/2
29	LMG	A	613	-	-	32/46/66/70	0/1/1/1
28	SQD	B	622	-	-	29/49/69/69	0/1/1/1
32	DGD	c	518	-	-	21/51/91/95	0/2/2/2
24	CLA	C	502	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	609	-	1/1/15/20	4/37/115/115	-
24	CLA	B	617	-	1/1/15/20	14/37/115/115	-
25	PHO	D	401	-	-	4/37/103/103	0/5/6/6
30	LHG	d	406	-	-	15/53/53/53	-
29	LMG	C	518	-	-	22/46/66/70	0/1/1/1
32	DGD	d	405	-	-	34/51/91/95	0/2/2/2
24	CLA	d	403	-	1/1/15/20	14/37/115/115	-
28	SQD	l	101	-	-	28/49/69/69	0/1/1/1
24	CLA	B	602	-	1/1/15/20	21/37/115/115	-
26	BCR	b	619	-	-	21/29/63/63	0/2/2/2
29	LMG	C	519	-	-	20/46/66/70	0/1/1/1
29	LMG	c	520	-	-	22/46/66/70	0/1/1/1
24	CLA	B	607[A]	-	1/1/15/20	9/37/115/115	-
24	CLA	a	609	-	1/1/15/20	14/37/115/115	-
30	LHG	E	102	-	-	26/46/46/53	-
24	CLA	C	506	-	1/1/15/20	17/37/115/115	-
24	CLA	b	608[B]	-	1/1/15/20	10/37/115/115	-
29	LMG	Z	101	-	-	17/31/51/70	0/1/1/1
24	CLA	C	508	-	1/1/15/20	6/37/115/115	-
24	CLA	B	614	-	1/1/15/20	3/37/115/115	-
24	CLA	d	402	-	1/1/15/20	3/37/115/115	-
24	CLA	C	503	-	1/1/15/20	6/37/115/115	-
29	LMG	B	621	-	-	21/46/66/70	0/1/1/1
26	BCR	c	521	-	-	22/29/63/63	0/2/2/2
26	BCR	I	101	-	-	21/29/63/63	0/2/2/2
29	LMG	D	408	-	-	20/46/66/70	0/1/1/1
28	SQD	a	614	-	-	23/49/69/69	0/1/1/1
24	CLA	c	511	3	1/1/15/20	4/37/115/115	-
25	PHO	a	608	-	-	3/37/103/103	0/5/6/6
29	LMG	a	613	-	-	30/46/66/70	0/1/1/1
32	DGD	C	515	-	-	23/51/91/95	0/2/2/2
26	BCR	B	619	-	-	23/29/63/63	0/2/2/2
24	CLA	b	616	-	1/1/15/20	13/37/115/115	-
32	DGD	C	516	-	-	31/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	512	-	1/1/15/20	9/37/115/115	-
24	CLA	b	604	-	1/1/15/20	5/37/115/115	-
28	SQD	A	614	-	-	23/49/69/69	0/1/1/1
24	CLA	b	614	-	1/1/15/20	7/37/115/115	-
24	CLA	C	513	-	1/1/15/20	12/37/115/115	-
24	CLA	C	501	-	1/1/15/20	12/37/115/115	-
28	SQD	b	601	-	-	29/49/69/69	0/1/1/1
26	BCR	a	610	-	-	22/29/63/63	0/2/2/2

All (3107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	619	BCR	C14-C13	28.80	1.74	1.35
26	F	101	BCR	C14-C13	27.15	1.71	1.35
26	c	515	BCR	C14-C13	27.13	1.71	1.35
26	K	102	BCR	C14-C13	26.70	1.71	1.35
26	B	620	BCR	C14-C13	26.66	1.71	1.35
26	A	610	BCR	C14-C13	26.48	1.70	1.35
26	k	101	BCR	C14-C13	26.33	1.70	1.35
26	I	101	BCR	C14-C13	26.33	1.70	1.35
26	f	101	BCR	C14-C13	26.28	1.70	1.35
26	B	618	BCR	C14-C13	26.13	1.70	1.35
26	H	101	BCR	C14-C13	26.09	1.70	1.35
26	K	101	BCR	C14-C13	26.04	1.70	1.35
26	B	619	BCR	C14-C13	25.81	1.70	1.35
26	h	101	BCR	C14-C13	25.67	1.69	1.35
26	a	610	BCR	C14-C13	25.65	1.69	1.35
26	b	621	BCR	C14-C13	25.45	1.69	1.35
26	t	101	BCR	C14-C13	25.38	1.69	1.35
26	c	521	BCR	C14-C13	25.31	1.69	1.35
26	C	514	BCR	C14-C13	24.44	1.68	1.35
26	c	514	BCR	C14-C13	24.44	1.68	1.35
26	T	101	BCR	C14-C13	24.31	1.68	1.35
26	b	620	BCR	C14-C13	24.21	1.67	1.35
26	b	620	BCR	C21-C22	-22.39	1.06	1.35
26	T	101	BCR	C21-C22	-22.21	1.06	1.35
26	H	101	BCR	C21-C22	-21.75	1.06	1.35
26	h	101	BCR	C21-C22	-21.74	1.07	1.35
26	h	101	BCR	C10-C9	21.48	1.64	1.35
26	b	619	BCR	C21-C22	-21.35	1.07	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	610	BCR	C10-C9	21.31	1.64	1.35
26	c	514	BCR	C21-C22	-21.25	1.07	1.35
26	c	515	BCR	C10-C9	21.20	1.63	1.35
26	k	101	BCR	C10-C9	21.19	1.63	1.35
26	H	101	BCR	C10-C9	21.17	1.63	1.35
26	A	610	BCR	C21-C22	-21.11	1.07	1.35
26	B	620	BCR	C21-C22	-21.08	1.07	1.35
26	k	101	BCR	C21-C22	-21.05	1.07	1.35
26	I	101	BCR	C10-C9	21.03	1.63	1.35
26	b	621	BCR	C10-C9	21.02	1.63	1.35
26	T	101	BCR	C10-C9	20.99	1.63	1.35
26	K	101	BCR	C21-C22	-20.99	1.08	1.35
26	A	610	BCR	C10-C9	20.87	1.63	1.35
26	t	101	BCR	C21-C22	-20.84	1.08	1.35
26	t	101	BCR	C10-C9	20.70	1.63	1.35
26	F	101	BCR	C10-C9	20.69	1.63	1.35
26	I	101	BCR	C21-C22	-20.65	1.08	1.35
26	K	102	BCR	C10-C9	20.65	1.63	1.35
26	c	521	BCR	C10-C9	20.61	1.63	1.35
26	f	101	BCR	C10-C9	20.55	1.63	1.35
26	B	618	BCR	C10-C9	20.54	1.63	1.35
26	K	102	BCR	C21-C22	-20.44	1.08	1.35
26	a	610	BCR	C21-C22	-20.34	1.08	1.35
26	C	514	BCR	C10-C9	20.33	1.62	1.35
26	B	620	BCR	C10-C9	20.33	1.62	1.35
26	c	514	BCR	C10-C9	20.28	1.62	1.35
26	B	619	BCR	C10-C9	20.20	1.62	1.35
26	K	101	BCR	C10-C9	20.10	1.62	1.35
26	B	618	BCR	C21-C22	-20.10	1.09	1.35
26	c	515	BCR	C21-C22	-20.08	1.09	1.35
26	f	101	BCR	C21-C22	-19.90	1.09	1.35
26	c	521	BCR	C21-C22	-19.84	1.09	1.35
26	b	619	BCR	C10-C9	19.75	1.62	1.35
26	b	620	BCR	C10-C9	19.53	1.61	1.35
26	C	514	BCR	C21-C22	-19.53	1.09	1.35
26	B	619	BCR	C21-C22	-19.49	1.09	1.35
26	F	101	BCR	C21-C22	-19.13	1.10	1.35
26	b	621	BCR	C20-C19	18.76	1.82	1.34
24	c	510	CLA	C4B-NB	18.31	1.51	1.35
24	C	505	CLA	C4B-NB	18.27	1.51	1.35
24	C	502	CLA	C4B-NB	18.27	1.51	1.35
24	B	602	CLA	C4B-NB	18.22	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	609	CLA	C4B-NB	18.20	1.51	1.35
24	c	512	CLA	C4B-NB	18.18	1.51	1.35
24	b	603	CLA	C4B-NB	18.17	1.51	1.35
24	B	616	CLA	C4B-NB	18.14	1.51	1.35
24	b	615	CLA	C4B-NB	18.14	1.51	1.35
24	c	503	CLA	C4B-NB	18.13	1.51	1.35
24	c	505	CLA	C4B-NB	18.06	1.51	1.35
24	c	508	CLA	C4B-NB	18.04	1.51	1.35
24	B	617	CLA	C4B-NB	18.01	1.51	1.35
24	B	609	CLA	C4B-NB	17.98	1.51	1.35
24	B	610	CLA	C4B-NB	17.96	1.51	1.35
24	b	612	CLA	C4B-NB	17.96	1.51	1.35
24	b	605	CLA	C4B-NB	17.92	1.51	1.35
24	B	606	CLA	C4B-NB	17.85	1.51	1.35
24	c	502	CLA	C4B-NB	17.82	1.51	1.35
24	b	611	CLA	C4B-NB	17.82	1.51	1.35
24	B	611	CLA	C4B-NB	17.81	1.51	1.35
24	b	617	CLA	C4B-NB	17.80	1.51	1.35
24	b	613	CLA	C4B-NB	17.80	1.51	1.35
24	B	603	CLA	C4B-NB	17.80	1.51	1.35
24	c	501	CLA	C4B-NB	17.79	1.51	1.35
24	c	511	CLA	C4B-NB	17.77	1.51	1.35
24	C	511	CLA	C4B-NB	17.76	1.51	1.35
24	c	513	CLA	C4B-NB	17.76	1.51	1.35
26	c	521	BCR	C20-C19	17.73	1.80	1.34
24	b	608[A]	CLA	C4B-NB	17.72	1.51	1.35
24	B	607[A]	CLA	C4B-NB	17.68	1.51	1.35
24	D	402	CLA	C4B-NB	17.66	1.51	1.35
24	c	506	CLA	C4B-NB	17.61	1.50	1.35
24	b	608[B]	CLA	C4B-NB	17.59	1.50	1.35
24	a	607	CLA	C4B-NB	17.57	1.50	1.35
24	c	507	CLA	C4B-NB	17.54	1.50	1.35
24	b	618	CLA	C4B-NB	17.54	1.50	1.35
24	c	504	CLA	C4B-NB	17.47	1.50	1.35
24	B	607[B]	CLA	C4B-NB	17.46	1.50	1.35
24	B	608	CLA	C4B-NB	17.46	1.50	1.35
24	B	614	CLA	C4B-NB	17.40	1.50	1.35
24	b	610	CLA	C4B-NB	17.39	1.50	1.35
24	b	606	CLA	C4B-NB	17.33	1.50	1.35
24	C	503	CLA	C4B-NB	17.32	1.50	1.35
24	b	614	CLA	C4B-NB	17.31	1.50	1.35
24	c	509	CLA	C4B-NB	17.29	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C4B-NB	17.29	1.50	1.35
24	d	403	CLA	C4B-NB	17.27	1.50	1.35
24	C	504	CLA	C4B-NB	17.22	1.50	1.35
24	B	612	CLA	C4B-NB	17.20	1.50	1.35
24	C	501	CLA	C4B-NB	17.18	1.50	1.35
24	A	606	CLA	C4B-NB	17.18	1.50	1.35
24	B	605	CLA	C4B-NB	17.14	1.50	1.35
24	b	607	CLA	C4B-NB	17.14	1.50	1.35
24	C	512	CLA	C4B-NB	17.10	1.50	1.35
24	b	609	CLA	C4B-NB	17.06	1.50	1.35
24	D	404	CLA	C4B-NB	17.05	1.50	1.35
24	B	615	CLA	C4B-NB	17.03	1.50	1.35
24	b	604	CLA	C4B-NB	17.01	1.50	1.35
24	C	506	CLA	C4B-NB	16.94	1.50	1.35
24	C	513	CLA	C4B-NB	16.72	1.50	1.35
24	A	609	CLA	C4B-NB	16.70	1.50	1.35
24	C	507	CLA	C4B-NB	16.70	1.50	1.35
24	d	402	CLA	C4B-NB	16.61	1.50	1.35
24	a	615	CLA	C4B-NB	16.58	1.50	1.35
24	C	509	CLA	C4B-NB	16.54	1.50	1.35
26	b	621	BCR	C21-C22	-16.52	1.13	1.35
24	A	607	CLA	C4B-NB	16.51	1.49	1.35
24	B	613	CLA	C4B-NB	16.48	1.49	1.35
24	B	604	CLA	C4B-NB	16.44	1.49	1.35
24	a	606	CLA	C4B-NB	16.39	1.49	1.35
24	b	616	CLA	C4B-NB	16.22	1.49	1.35
26	t	101	BCR	C20-C19	16.18	1.76	1.34
24	C	510	CLA	C4B-NB	16.13	1.49	1.35
26	B	619	BCR	C20-C19	16.10	1.76	1.34
26	T	101	BCR	C20-C19	15.98	1.75	1.34
26	b	619	BCR	C20-C19	15.92	1.75	1.34
26	B	618	BCR	C20-C19	15.85	1.75	1.34
26	h	101	BCR	C20-C19	15.82	1.75	1.34
24	D	403	CLA	C4B-NB	15.82	1.49	1.35
26	F	101	BCR	C20-C19	15.66	1.74	1.34
26	c	515	BCR	C20-C19	15.59	1.74	1.34
26	c	521	BCR	C37-C22	15.56	1.83	1.50
26	c	514	BCR	C20-C19	15.48	1.74	1.34
26	A	610	BCR	C20-C19	15.42	1.74	1.34
26	B	620	BCR	C20-C19	15.35	1.74	1.34
26	K	102	BCR	C20-C19	15.34	1.74	1.34
26	b	620	BCR	C20-C19	15.28	1.74	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	521	BCR	C36-C18	15.27	1.82	1.50
26	k	101	BCR	C20-C19	15.16	1.73	1.34
26	a	610	BCR	C20-C19	15.12	1.73	1.34
26	b	621	BCR	C20-C21	15.11	1.90	1.43
26	f	101	BCR	C20-C19	15.05	1.73	1.34
26	C	514	BCR	C20-C19	14.97	1.73	1.34
26	K	101	BCR	C20-C19	14.93	1.73	1.34
26	I	101	BCR	C20-C19	14.87	1.72	1.34
26	c	514	BCR	C5-C6	14.78	1.60	1.34
26	h	101	BCR	C36-C18	14.59	1.81	1.50
26	T	101	BCR	C5-C6	14.51	1.59	1.34
26	c	514	BCR	C36-C18	14.45	1.80	1.50
26	c	515	BCR	C5-C6	14.45	1.59	1.34
26	C	514	BCR	C5-C6	14.45	1.59	1.34
26	b	621	BCR	C5-C6	14.40	1.59	1.34
26	B	620	BCR	C36-C18	14.32	1.80	1.50
26	c	521	BCR	C5-C6	14.31	1.59	1.34
26	K	102	BCR	C36-C18	14.28	1.80	1.50
26	H	101	BCR	C20-C19	14.28	1.71	1.34
26	c	515	BCR	C36-C18	14.28	1.80	1.50
26	k	101	BCR	C5-C6	14.25	1.59	1.34
26	C	514	BCR	C36-C18	14.21	1.80	1.50
26	T	101	BCR	C16-C15	14.14	1.72	1.36
26	K	101	BCR	C16-C15	14.11	1.72	1.36
26	t	101	BCR	C16-C15	14.08	1.72	1.36
26	k	101	BCR	C36-C18	14.07	1.80	1.50
26	H	101	BCR	C36-C18	14.05	1.79	1.50
26	K	101	BCR	C5-C6	14.05	1.58	1.34
26	B	620	BCR	C16-C15	14.00	1.72	1.36
26	k	101	BCR	C16-C15	13.98	1.72	1.36
26	I	101	BCR	C36-C18	13.97	1.79	1.50
26	K	102	BCR	C5-C6	13.95	1.58	1.34
26	B	620	BCR	C5-C6	13.90	1.58	1.34
26	C	514	BCR	C16-C15	13.89	1.72	1.36
26	t	101	BCR	C5-C6	13.83	1.58	1.34
26	F	101	BCR	C16-C15	13.79	1.71	1.36
26	b	620	BCR	C36-C18	13.77	1.79	1.50
26	a	610	BCR	C16-C15	13.74	1.71	1.36
26	I	101	BCR	C5-C6	13.74	1.58	1.34
26	A	610	BCR	C36-C18	13.71	1.79	1.50
26	b	619	BCR	C36-C18	13.70	1.79	1.50
26	b	619	BCR	C16-C15	13.70	1.71	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	BCR	C36-C18	13.70	1.79	1.50
26	A	610	BCR	C16-C15	13.68	1.71	1.36
26	K	102	BCR	C16-C15	13.66	1.71	1.36
26	A	610	BCR	C5-C6	13.60	1.58	1.34
26	H	101	BCR	C16-C15	13.58	1.71	1.36
26	c	514	BCR	C16-C15	13.54	1.71	1.36
26	h	101	BCR	C16-C15	13.48	1.71	1.36
26	a	610	BCR	C36-C18	13.48	1.78	1.50
26	b	620	BCR	C16-C15	13.47	1.71	1.36
26	F	101	BCR	C5-C6	13.47	1.57	1.34
26	K	101	BCR	C36-C18	13.45	1.78	1.50
26	a	610	BCR	C5-C6	13.43	1.57	1.34
26	f	101	BCR	C5-C6	13.42	1.57	1.34
26	t	101	BCR	C36-C18	13.30	1.78	1.50
26	f	101	BCR	C36-C18	13.24	1.78	1.50
26	b	621	BCR	C36-C18	13.20	1.78	1.50
26	h	101	BCR	C5-C6	13.18	1.57	1.34
26	K	101	BCR	C19-C18	-13.18	1.17	1.45
26	b	621	BCR	C16-C15	13.13	1.70	1.36
26	I	101	BCR	C16-C15	13.12	1.70	1.36
26	c	515	BCR	C16-C15	13.07	1.70	1.36
26	c	521	BCR	C20-C21	13.06	1.83	1.43
26	f	101	BCR	C16-C15	13.06	1.70	1.36
26	b	621	BCR	C37-C22	13.03	1.77	1.50
26	B	618	BCR	C36-C18	13.00	1.77	1.50
26	B	619	BCR	C16-C15	13.00	1.69	1.36
26	B	618	BCR	C19-C18	-12.93	1.18	1.45
26	B	619	BCR	C5-C6	12.86	1.56	1.34
26	b	619	BCR	C5-C6	12.82	1.56	1.34
26	F	101	BCR	C36-C18	12.78	1.77	1.50
26	B	618	BCR	C5-C6	12.78	1.56	1.34
26	H	101	BCR	C5-C6	12.52	1.56	1.34
26	k	101	BCR	C19-C18	-12.46	1.19	1.45
26	a	610	BCR	C19-C18	-12.44	1.19	1.45
26	B	620	BCR	C37-C22	12.43	1.76	1.50
26	B	618	BCR	C16-C15	12.36	1.68	1.36
26	C	514	BCR	C37-C22	12.36	1.76	1.50
26	b	620	BCR	C5-C6	12.34	1.55	1.34
26	B	619	BCR	C36-C18	12.34	1.76	1.50
26	H	101	BCR	C19-C18	-12.27	1.19	1.45
26	c	515	BCR	C19-C18	-12.22	1.19	1.45
26	K	102	BCR	C37-C22	12.22	1.76	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	521	BCR	C16-C15	12.12	1.67	1.36
26	K	102	BCR	C19-C18	-12.10	1.19	1.45
26	A	610	BCR	C37-C22	12.09	1.75	1.50
26	a	610	BCR	C37-C22	12.06	1.75	1.50
26	B	619	BCR	C20-C21	12.01	1.80	1.43
26	C	514	BCR	C19-C18	-11.98	1.20	1.45
26	F	101	BCR	C20-C21	11.96	1.80	1.43
26	A	610	BCR	C19-C18	-11.90	1.20	1.45
26	t	101	BCR	C37-C22	11.87	1.75	1.50
26	b	619	BCR	C19-C18	-11.87	1.20	1.45
26	K	101	BCR	C37-C22	11.85	1.75	1.50
26	B	618	BCR	C20-C21	11.84	1.80	1.43
26	f	101	BCR	C19-C18	-11.79	1.20	1.45
26	f	101	BCR	C37-C22	11.79	1.75	1.50
26	K	102	BCR	C20-C21	11.77	1.79	1.43
26	I	101	BCR	C19-C18	-11.76	1.20	1.45
26	b	619	BCR	C20-C21	11.74	1.79	1.43
26	c	514	BCR	C19-C18	-11.74	1.20	1.45
26	B	618	BCR	C37-C22	11.74	1.75	1.50
26	k	101	BCR	C37-C22	11.70	1.75	1.50
26	B	620	BCR	C19-C18	-11.68	1.20	1.45
26	b	619	BCR	C37-C22	11.65	1.75	1.50
26	b	620	BCR	C19-C18	-11.65	1.20	1.45
26	B	619	BCR	C19-C18	-11.54	1.21	1.45
26	h	101	BCR	C19-C18	-11.53	1.21	1.45
26	k	101	BCR	C8-C7	11.53	1.67	1.33
26	t	101	BCR	C20-C21	11.49	1.79	1.43
26	t	101	BCR	C19-C18	-11.47	1.21	1.45
26	T	101	BCR	C37-C22	11.44	1.74	1.50
26	c	515	BCR	C20-C21	11.44	1.78	1.43
26	K	101	BCR	C20-C21	11.43	1.78	1.43
26	K	101	BCR	C8-C7	11.42	1.67	1.33
26	k	101	BCR	C20-C21	11.41	1.78	1.43
26	B	620	BCR	C20-C21	11.40	1.78	1.43
26	f	101	BCR	C20-C21	11.40	1.78	1.43
26	B	619	BCR	C37-C22	11.37	1.74	1.50
26	h	101	BCR	C20-C21	11.37	1.78	1.43
26	c	514	BCR	C37-C22	11.35	1.74	1.50
26	c	521	BCR	C19-C18	-11.34	1.21	1.45
26	c	515	BCR	C37-C22	11.34	1.74	1.50
26	c	521	BCR	C8-C7	11.33	1.67	1.33
26	F	101	BCR	C19-C18	-11.30	1.21	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	BCR	C20-C21	11.29	1.78	1.43
26	C	514	BCR	C20-C21	11.29	1.78	1.43
26	T	101	BCR	C19-C18	-11.29	1.21	1.45
26	c	514	BCR	C8-C7	11.22	1.67	1.33
26	F	101	BCR	C37-C22	11.20	1.74	1.50
26	I	101	BCR	C20-C21	11.17	1.78	1.43
26	b	620	BCR	C37-C22	11.12	1.73	1.50
26	I	101	BCR	C37-C22	11.11	1.73	1.50
26	A	610	BCR	C20-C21	11.09	1.77	1.43
26	C	514	BCR	C8-C7	11.06	1.66	1.33
26	h	101	BCR	C37-C22	11.05	1.73	1.50
26	b	621	BCR	C8-C7	11.03	1.66	1.33
26	A	610	BCR	C8-C7	11.03	1.66	1.33
26	H	101	BCR	C8-C7	11.00	1.66	1.33
26	b	620	BCR	C20-C21	10.95	1.77	1.43
26	a	610	BCR	C8-C7	10.92	1.66	1.33
26	f	101	BCR	C8-C7	10.89	1.66	1.33
26	T	101	BCR	C8-C7	10.88	1.66	1.33
26	c	515	BCR	C8-C7	10.87	1.66	1.33
26	I	101	BCR	C8-C7	10.86	1.65	1.33
26	K	102	BCR	C8-C7	10.86	1.65	1.33
26	b	619	BCR	C8-C7	10.86	1.65	1.33
26	t	101	BCR	C8-C7	10.84	1.65	1.33
26	F	101	BCR	C8-C7	10.83	1.65	1.33
26	a	610	BCR	C20-C21	10.82	1.77	1.43
26	h	101	BCR	C8-C7	10.79	1.65	1.33
26	B	618	BCR	C8-C7	10.76	1.65	1.33
26	B	619	BCR	C8-C7	10.72	1.65	1.33
26	c	514	BCR	C20-C21	10.71	1.76	1.43
26	b	620	BCR	C8-C7	10.68	1.65	1.33
26	H	101	BCR	C20-C21	10.59	1.76	1.43
27	a	611	PL9	C18-C19	10.55	1.58	1.33
27	A	611	PL9	C18-C19	10.54	1.58	1.33
27	D	405	PL9	C18-C19	10.50	1.58	1.33
26	B	620	BCR	C8-C7	10.39	1.64	1.33
27	d	404	PL9	C18-C19	10.38	1.57	1.33
27	D	405	PL9	C38-C39	9.94	1.56	1.33
26	C	514	BCR	C16-C17	9.90	1.74	1.43
27	d	404	PL9	C38-C39	9.83	1.56	1.33
27	a	611	PL9	C38-C39	9.82	1.56	1.33
27	D	405	PL9	C23-C24	9.78	1.56	1.33
26	T	101	BCR	C16-C17	9.70	1.73	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	619	BCR	C26-C25	9.69	1.51	1.34
26	H	101	BCR	C16-C17	9.68	1.73	1.43
26	K	101	BCR	C16-C17	9.68	1.73	1.43
27	A	611	PL9	C23-C24	9.68	1.56	1.33
26	t	101	BCR	C16-C17	9.63	1.73	1.43
26	f	101	BCR	C26-C25	9.58	1.51	1.34
26	h	101	BCR	C16-C17	9.53	1.73	1.43
27	a	611	PL9	C23-C24	9.53	1.55	1.33
26	k	101	BCR	C16-C17	9.51	1.72	1.43
26	b	621	BCR	C19-C18	-9.51	1.25	1.45
26	b	620	BCR	C26-C25	9.50	1.50	1.34
26	F	101	BCR	C26-C25	9.49	1.50	1.34
27	A	611	PL9	C38-C39	9.48	1.55	1.33
26	K	102	BCR	C16-C17	9.46	1.72	1.43
26	c	514	BCR	C16-C17	9.46	1.72	1.43
26	B	620	BCR	C16-C17	9.45	1.72	1.43
27	d	404	PL9	C23-C24	9.45	1.55	1.33
26	H	101	BCR	C37-C22	9.44	1.70	1.50
26	b	619	BCR	C16-C17	9.44	1.72	1.43
26	A	610	BCR	C16-C17	9.31	1.72	1.43
26	b	621	BCR	C16-C17	9.23	1.72	1.43
26	I	101	BCR	C16-C17	9.20	1.71	1.43
26	F	101	BCR	C16-C17	9.13	1.71	1.43
26	a	610	BCR	C16-C17	9.10	1.71	1.43
26	b	620	BCR	C16-C17	9.04	1.71	1.43
26	c	521	BCR	C16-C17	8.97	1.71	1.43
27	d	404	PL9	C28-C29	8.97	1.54	1.33
26	f	101	BCR	C16-C17	8.93	1.71	1.43
24	C	508	CLA	C4D-ND	-8.92	1.25	1.37
26	c	515	BCR	C16-C17	8.85	1.70	1.43
27	a	611	PL9	C48-C49	8.83	1.57	1.32
27	D	405	PL9	C28-C29	8.81	1.54	1.33
26	B	619	BCR	C16-C17	8.78	1.70	1.43
27	A	611	PL9	C48-C49	8.77	1.57	1.32
27	d	404	PL9	C13-C14	8.75	1.54	1.33
27	D	405	PL9	C13-C14	8.75	1.54	1.33
26	B	618	BCR	C16-C17	8.70	1.70	1.43
26	A	610	BCR	C26-C25	8.65	1.49	1.34
26	h	101	BCR	C26-C25	8.64	1.49	1.34
26	H	101	BCR	C26-C25	8.58	1.49	1.34
24	a	615	CLA	C4D-ND	-8.55	1.26	1.37
27	a	611	PL9	C28-C29	8.52	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	405	PL9	C48-C49	8.50	1.56	1.32
27	A	611	PL9	C13-C14	8.50	1.53	1.33
27	D	405	PL9	C43-C44	8.50	1.53	1.33
24	D	402	CLA	C4D-ND	-8.49	1.26	1.37
27	d	404	PL9	C48-C49	8.47	1.56	1.32
24	b	604	CLA	C4D-ND	-8.45	1.26	1.37
27	A	611	PL9	C28-C29	8.44	1.53	1.33
26	I	101	BCR	C26-C25	8.42	1.49	1.34
27	a	611	PL9	C8-C9	8.41	1.53	1.33
24	b	613	CLA	C4D-ND	-8.41	1.26	1.37
24	B	610	CLA	C4D-ND	-8.39	1.26	1.37
26	b	619	BCR	C26-C25	8.39	1.49	1.34
24	D	403	CLA	C1B-NB	-8.38	1.27	1.35
24	a	615	CLA	MG-ND	-8.37	1.89	2.05
27	d	404	PL9	C43-C44	8.34	1.53	1.33
24	B	613	CLA	C4D-ND	-8.33	1.26	1.37
27	D	405	PL9	C8-C9	8.30	1.52	1.33
24	B	606	CLA	C4D-ND	-8.30	1.26	1.37
27	A	611	PL9	C8-C9	8.29	1.52	1.33
27	a	611	PL9	C13-C14	8.29	1.52	1.33
24	A	606	CLA	MG-ND	-8.28	1.89	2.05
24	B	604	CLA	C4D-ND	-8.26	1.26	1.37
24	c	508	CLA	C4D-ND	-8.26	1.26	1.37
24	A	607	CLA	MG-ND	-8.26	1.89	2.05
26	k	101	BCR	C26-C25	8.26	1.48	1.34
24	A	609	CLA	C4D-ND	-8.24	1.26	1.37
27	A	611	PL9	C43-C44	8.23	1.52	1.33
24	b	606	CLA	C4D-ND	-8.22	1.26	1.37
27	a	611	PL9	C43-C44	8.21	1.52	1.33
33	v	201	HEM	C3D-C2D	8.18	1.54	1.36
24	a	606	CLA	C4D-ND	-8.17	1.26	1.37
24	D	403	CLA	C4D-ND	-8.17	1.26	1.37
24	B	615	CLA	C4D-ND	-8.14	1.26	1.37
26	A	610	BCR	C8-C9	8.13	1.63	1.45
27	d	404	PL9	O1-C4	8.12	1.41	1.23
24	b	605	CLA	C4D-ND	-8.08	1.26	1.37
27	d	404	PL9	C8-C9	8.08	1.52	1.33
24	a	606	CLA	MG-ND	-8.08	1.89	2.05
24	b	616	CLA	C4D-ND	-8.07	1.26	1.37
26	k	101	BCR	C8-C9	8.07	1.63	1.45
27	a	611	PL9	C33-C34	8.06	1.52	1.33
24	c	504	CLA	C4D-ND	-8.02	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C4D-ND	-7.99	1.26	1.37
24	B	612	CLA	MG-ND	-7.97	1.90	2.05
24	b	609	CLA	C4D-ND	-7.97	1.26	1.37
24	A	606	CLA	C4D-ND	-7.96	1.26	1.37
24	C	506	CLA	C4D-ND	-7.95	1.26	1.37
24	B	612	CLA	C4D-ND	-7.95	1.26	1.37
24	b	614	CLA	C4D-ND	-7.94	1.26	1.37
27	A	611	PL9	C33-C34	7.93	1.52	1.33
24	B	613	CLA	MG-ND	-7.91	1.90	2.05
24	C	510	CLA	C4D-ND	-7.90	1.26	1.37
24	b	616	CLA	MG-ND	-7.89	1.90	2.05
26	K	102	BCR	C26-C25	7.89	1.48	1.34
26	c	515	BCR	C26-C25	7.89	1.48	1.34
24	D	404	CLA	MG-ND	-7.89	1.90	2.05
24	B	608	CLA	C4D-ND	-7.88	1.26	1.37
26	K	101	BCR	C8-C9	7.88	1.62	1.45
24	A	606	CLA	C3A-C2A	-7.88	1.32	1.54
24	A	609	CLA	MG-ND	-7.86	1.90	2.05
26	K	101	BCR	C26-C25	7.86	1.48	1.34
24	C	509	CLA	C4D-ND	-7.85	1.26	1.37
26	C	514	BCR	C26-C25	7.84	1.48	1.34
24	B	608	CLA	MG-ND	-7.81	1.90	2.05
27	A	611	PL9	O1-C4	7.81	1.40	1.23
24	a	606	CLA	C3A-C2A	-7.79	1.32	1.54
26	c	521	BCR	C8-C9	7.78	1.62	1.45
24	a	607	CLA	C4D-ND	-7.78	1.27	1.37
24	b	607	CLA	C4D-ND	-7.78	1.27	1.37
26	c	514	BCR	C8-C9	7.75	1.62	1.45
26	c	521	BCR	C26-C25	7.74	1.47	1.34
26	c	521	BCR	C17-C18	7.74	1.46	1.35
27	D	405	PL9	C33-C34	7.70	1.51	1.33
26	C	514	BCR	C8-C9	7.70	1.62	1.45
24	B	603	CLA	C4D-ND	-7.70	1.27	1.37
24	C	511	CLA	C4D-ND	-7.70	1.27	1.37
26	a	610	BCR	C8-C9	7.69	1.62	1.45
24	B	613	CLA	C1B-NB	-7.68	1.28	1.35
27	d	404	PL9	C33-C34	7.67	1.51	1.33
24	b	609	CLA	MG-ND	-7.66	1.90	2.05
24	B	613	CLA	C3A-C2A	-7.66	1.33	1.54
33	V	201	HEM	C3D-C2D	7.64	1.53	1.36
24	C	507	CLA	MG-ND	-7.63	1.90	2.05
24	D	402	CLA	C3A-C2A	-7.62	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I	101	BCR	C8-C9	7.62	1.62	1.45
24	b	614	CLA	C3A-C2A	-7.62	1.33	1.54
24	B	608	CLA	C3A-C2A	-7.62	1.33	1.54
24	d	402	CLA	C4D-ND	-7.61	1.27	1.37
24	C	501	CLA	C4D-ND	-7.61	1.27	1.37
33	e	102	HEM	C3D-C2D	7.61	1.52	1.36
24	D	403	CLA	C3A-C2A	-7.60	1.33	1.54
24	C	503	CLA	C4D-ND	-7.60	1.27	1.37
24	b	610	CLA	C3A-C2A	-7.60	1.33	1.54
24	B	605	CLA	C4D-ND	-7.60	1.27	1.37
24	C	509	CLA	C1B-NB	-7.60	1.28	1.35
24	B	607[B]	CLA	C4D-ND	-7.59	1.27	1.37
24	C	511	CLA	MG-ND	-7.58	1.90	2.05
24	c	502	CLA	C4D-ND	-7.58	1.27	1.37
24	b	614	CLA	MG-ND	-7.58	1.90	2.05
24	B	604	CLA	C1B-NB	-7.58	1.28	1.35
24	b	605	CLA	C3A-C2A	-7.57	1.33	1.54
24	D	402	CLA	MG-ND	-7.57	1.90	2.05
24	c	505	CLA	C4D-ND	-7.56	1.27	1.37
24	c	503	CLA	C4D-ND	-7.56	1.27	1.37
24	C	504	CLA	C4D-ND	-7.56	1.27	1.37
24	a	609	CLA	MG-ND	-7.55	1.90	2.05
26	c	515	BCR	C8-C9	7.55	1.62	1.45
24	b	618	CLA	C3A-C2A	-7.55	1.33	1.54
24	B	611	CLA	C4D-ND	-7.54	1.27	1.37
24	b	613	CLA	MG-ND	-7.54	1.90	2.05
24	b	604	CLA	C3A-C2A	-7.53	1.33	1.54
24	B	607[A]	CLA	C3A-C2A	-7.53	1.33	1.54
24	B	607[B]	CLA	C3A-C2A	-7.53	1.33	1.54
24	B	609	CLA	C3A-C2A	-7.52	1.33	1.54
24	b	608[B]	CLA	C4D-ND	-7.52	1.27	1.37
24	D	404	CLA	C3A-C2A	-7.52	1.33	1.54
24	C	510	CLA	C3A-C2A	-7.51	1.33	1.54
24	c	506	CLA	C3A-C2A	-7.51	1.33	1.54
26	B	618	BCR	C26-C25	7.51	1.47	1.34
24	b	608[A]	CLA	C3A-C2A	-7.51	1.33	1.54
24	b	608[B]	CLA	C3A-C2A	-7.50	1.33	1.54
24	B	612	CLA	C1B-NB	-7.49	1.28	1.35
24	b	609	CLA	C3A-C2A	-7.49	1.33	1.54
24	C	509	CLA	MG-ND	-7.48	1.91	2.05
24	b	618	CLA	MG-ND	-7.48	1.91	2.05
26	b	621	BCR	C8-C9	7.48	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C1B-NB	-7.47	1.28	1.35
24	b	612	CLA	C3A-C2A	-7.46	1.33	1.54
24	c	506	CLA	C4D-ND	-7.46	1.27	1.37
24	C	504	CLA	C3A-C2A	-7.46	1.33	1.54
24	b	611	CLA	C4D-ND	-7.44	1.27	1.37
24	C	501	CLA	C3A-C2A	-7.44	1.33	1.54
24	B	614	CLA	C3A-C2A	-7.44	1.33	1.54
24	B	615	CLA	C3A-C2A	-7.44	1.33	1.54
24	b	603	CLA	C4D-ND	-7.43	1.27	1.37
24	C	513	CLA	C4D-ND	-7.43	1.27	1.37
26	t	101	BCR	C8-C9	7.43	1.61	1.45
24	B	607[A]	CLA	C4D-ND	-7.41	1.27	1.37
24	C	509	CLA	C3A-C2A	-7.41	1.33	1.54
24	a	609	CLA	C3A-C2A	-7.41	1.33	1.54
24	C	513	CLA	MG-ND	-7.41	1.91	2.05
26	B	620	BCR	C26-C25	7.40	1.47	1.34
24	A	609	CLA	C3A-C2A	-7.40	1.33	1.54
24	a	609	CLA	C4D-ND	-7.40	1.27	1.37
24	a	607	CLA	MG-ND	-7.40	1.91	2.05
24	c	507	CLA	MG-ND	-7.40	1.91	2.05
24	c	512	CLA	C3A-C2A	-7.39	1.33	1.54
27	D	405	PL9	O1-C4	7.38	1.39	1.23
26	b	621	BCR	C26-C25	7.38	1.47	1.34
26	H	101	BCR	C8-C9	7.37	1.61	1.45
24	B	604	CLA	MG-ND	-7.37	1.91	2.05
26	f	101	BCR	C8-C9	7.37	1.61	1.45
24	c	511	CLA	C3A-C2A	-7.37	1.33	1.54
27	a	611	PL9	O1-C4	7.37	1.39	1.23
24	b	610	CLA	C4D-ND	-7.36	1.27	1.37
24	b	617	CLA	C4D-ND	-7.36	1.27	1.37
24	b	615	CLA	C3A-C2A	-7.35	1.33	1.54
24	b	608[A]	CLA	C4D-ND	-7.35	1.27	1.37
33	E	103	HEM	C3D-C2D	7.35	1.52	1.36
24	C	505	CLA	C4D-ND	-7.35	1.27	1.37
24	B	610	CLA	MG-ND	-7.35	1.91	2.05
26	T	101	BCR	C8-C9	7.35	1.61	1.45
24	B	603	CLA	C3A-C2A	-7.34	1.34	1.54
24	b	612	CLA	MG-ND	-7.34	1.91	2.05
24	a	615	CLA	C3A-C2A	-7.34	1.34	1.54
24	C	511	CLA	C3A-C2A	-7.33	1.34	1.54
24	c	504	CLA	C3A-C2A	-7.32	1.34	1.54
24	b	612	CLA	C4D-ND	-7.31	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C3A-C2A	-7.31	1.34	1.54
24	C	502	CLA	C3A-C2A	-7.30	1.34	1.54
24	c	509	CLA	C3A-C2A	-7.30	1.34	1.54
24	C	508	CLA	C3A-C2A	-7.30	1.34	1.54
24	b	607	CLA	C3A-C2A	-7.30	1.34	1.54
24	c	502	CLA	C3A-C2A	-7.29	1.34	1.54
24	b	613	CLA	C3A-C2A	-7.29	1.34	1.54
24	D	403	CLA	MG-ND	-7.29	1.91	2.05
24	C	503	CLA	MG-ND	-7.29	1.91	2.05
24	d	402	CLA	C3A-C2A	-7.27	1.34	1.54
26	c	514	BCR	C26-C25	7.27	1.47	1.34
24	B	607[B]	CLA	MG-ND	-7.27	1.91	2.05
26	h	101	BCR	C8-C9	7.26	1.61	1.45
24	B	615	CLA	MG-ND	-7.25	1.91	2.05
26	b	619	BCR	C8-C9	7.25	1.61	1.45
24	b	606	CLA	C3A-C2A	-7.25	1.34	1.54
24	c	510	CLA	C3A-C2A	-7.25	1.34	1.54
24	C	510	CLA	C1B-NB	-7.25	1.28	1.35
24	d	402	CLA	MG-ND	-7.24	1.91	2.05
24	B	616	CLA	C4D-ND	-7.24	1.27	1.37
24	d	403	CLA	C3A-C2A	-7.23	1.34	1.54
24	b	615	CLA	MG-ND	-7.23	1.91	2.05
24	b	617	CLA	C3A-C2A	-7.22	1.34	1.54
26	f	101	BCR	C38-C26	7.22	1.62	1.50
24	b	616	CLA	C3A-C2A	-7.22	1.34	1.54
24	B	610	CLA	C3A-C2A	-7.22	1.34	1.54
24	b	611	CLA	C3A-C2A	-7.21	1.34	1.54
24	a	606	CLA	C1B-NB	-7.21	1.28	1.35
26	a	610	BCR	C26-C25	7.21	1.46	1.34
24	C	503	CLA	C3A-C2A	-7.20	1.34	1.54
26	b	620	BCR	C8-C9	7.20	1.61	1.45
24	d	402	CLA	C1B-NB	-7.19	1.28	1.35
24	b	603	CLA	MG-ND	-7.19	1.91	2.05
24	A	607	CLA	C3A-C2A	-7.17	1.34	1.54
24	c	508	CLA	C3A-C2A	-7.16	1.34	1.54
24	B	612	CLA	C3A-C2A	-7.16	1.34	1.54
24	C	505	CLA	C3A-C2A	-7.15	1.34	1.54
26	K	102	BCR	C8-C9	7.15	1.61	1.45
24	C	508	CLA	MG-ND	-7.14	1.91	2.05
24	c	505	CLA	C3A-C2A	-7.13	1.34	1.54
24	b	604	CLA	MG-ND	-7.13	1.91	2.05
24	B	614	CLA	MG-ND	-7.13	1.91	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C3A-C2A	-7.12	1.34	1.54
24	B	617	CLA	C3A-C2A	-7.12	1.34	1.54
24	b	608[B]	CLA	MG-ND	-7.11	1.91	2.05
24	D	404	CLA	C4D-ND	-7.11	1.28	1.37
24	B	617	CLA	C4D-ND	-7.10	1.28	1.37
24	C	506	CLA	C3A-C2A	-7.10	1.34	1.54
24	a	607	CLA	C3A-C2A	-7.10	1.34	1.54
24	c	503	CLA	C3A-C2A	-7.10	1.34	1.54
24	C	507	CLA	C3A-C2A	-7.08	1.34	1.54
24	c	501	CLA	C3A-C2A	-7.08	1.34	1.54
24	c	512	CLA	C4D-ND	-7.07	1.28	1.37
24	b	606	CLA	MG-ND	-7.06	1.91	2.05
24	B	614	CLA	C4D-ND	-7.06	1.28	1.37
26	B	619	BCR	C8-C9	7.05	1.61	1.45
24	A	607	CLA	C4D-ND	-7.04	1.28	1.37
24	B	609	CLA	C4D-ND	-7.04	1.28	1.37
24	B	616	CLA	C3A-C2A	-7.03	1.34	1.54
24	b	605	CLA	MG-ND	-7.03	1.91	2.05
24	c	513	CLA	C3A-C2A	-7.03	1.34	1.54
24	B	604	CLA	C3A-C2A	-7.02	1.34	1.54
24	c	509	CLA	C4D-ND	-7.02	1.28	1.37
24	B	605	CLA	MG-ND	-7.02	1.91	2.05
24	B	611	CLA	C3A-C2A	-7.00	1.34	1.54
24	a	615	CLA	C1B-NB	-7.00	1.29	1.35
24	c	501	CLA	MG-ND	-6.99	1.91	2.05
26	B	618	BCR	C8-C9	6.99	1.61	1.45
24	C	512	CLA	MG-ND	-6.98	1.91	2.05
24	c	504	CLA	C1B-NB	-6.98	1.29	1.35
24	c	501	CLA	C4D-ND	-6.98	1.28	1.37
24	B	607[A]	CLA	MG-ND	-6.98	1.92	2.05
24	B	606	CLA	C3A-C2A	-6.97	1.35	1.54
24	b	603	CLA	C3A-C2A	-6.96	1.35	1.54
24	c	511	CLA	MG-ND	-6.96	1.92	2.05
24	c	507	CLA	C3A-C2A	-6.95	1.35	1.54
24	c	510	CLA	C4D-ND	-6.95	1.28	1.37
24	C	510	CLA	MG-ND	-6.95	1.92	2.05
24	C	506	CLA	MG-ND	-6.94	1.92	2.05
24	B	616	CLA	MG-ND	-6.90	1.92	2.05
24	B	602	CLA	C3A-C2A	-6.90	1.35	1.54
24	C	507	CLA	C4D-ND	-6.87	1.28	1.37
26	t	101	BCR	C26-C25	6.86	1.46	1.34
24	c	513	CLA	C4D-ND	-6.85	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	C3A-C2A	-6.85	1.35	1.54
26	F	101	BCR	C8-C9	6.84	1.60	1.45
24	b	605	CLA	C1B-NB	-6.84	1.29	1.35
24	b	615	CLA	C4D-ND	-6.82	1.28	1.37
24	c	503	CLA	MG-ND	-6.82	1.92	2.05
24	c	510	CLA	MG-ND	-6.81	1.92	2.05
24	C	508	CLA	C1B-NB	-6.80	1.29	1.35
24	B	605	CLA	C1B-NB	-6.79	1.29	1.35
26	K	101	BCR	C34-C9	-6.79	1.36	1.50
24	b	608[A]	CLA	MG-ND	-6.78	1.92	2.05
24	A	606	CLA	C1B-NB	-6.78	1.29	1.35
24	C	504	CLA	MG-ND	-6.78	1.92	2.05
24	C	502	CLA	C4D-ND	-6.77	1.28	1.37
24	b	613	CLA	C1B-NB	-6.76	1.29	1.35
24	B	602	CLA	C4D-ND	-6.76	1.28	1.37
24	B	611	CLA	MG-ND	-6.75	1.92	2.05
26	B	619	BCR	C34-C9	-6.73	1.37	1.50
24	C	501	CLA	MG-ND	-6.72	1.92	2.05
24	b	610	CLA	MG-ND	-6.72	1.92	2.05
26	T	101	BCR	C26-C25	6.71	1.46	1.34
24	c	507	CLA	C4D-ND	-6.70	1.28	1.37
24	c	504	CLA	MG-ND	-6.70	1.92	2.05
26	h	101	BCR	C38-C26	6.70	1.61	1.50
24	c	511	CLA	C4D-ND	-6.70	1.28	1.37
26	F	101	BCR	C38-C26	6.70	1.61	1.50
27	a	611	PL9	O2-C1	6.68	1.42	1.24
24	C	504	CLA	C1B-NB	-6.68	1.29	1.35
26	B	620	BCR	C8-C9	6.67	1.60	1.45
24	c	512	CLA	MG-ND	-6.66	1.92	2.05
26	b	620	BCR	C38-C26	6.65	1.61	1.50
26	H	101	BCR	C38-C26	6.63	1.61	1.50
24	D	404	CLA	C1B-NB	-6.62	1.29	1.35
24	b	607	CLA	MG-ND	-6.60	1.92	2.05
24	d	403	CLA	C4D-ND	-6.58	1.28	1.37
24	c	505	CLA	MG-ND	-6.58	1.92	2.05
24	d	403	CLA	MG-ND	-6.57	1.92	2.05
26	b	619	BCR	C34-C9	-6.55	1.37	1.50
27	A	611	PL9	O2-C1	6.55	1.42	1.24
24	B	614	CLA	C1B-NB	-6.54	1.29	1.35
26	B	618	BCR	C34-C9	-6.53	1.37	1.50
24	B	617	CLA	MG-ND	-6.53	1.92	2.05
26	b	621	BCR	C34-C9	-6.52	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I	101	BCR	C34-C9	-6.50	1.37	1.50
26	C	514	BCR	C34-C9	-6.49	1.37	1.50
24	b	611	CLA	MG-ND	-6.48	1.92	2.05
24	C	512	CLA	C4D-ND	-6.48	1.28	1.37
24	C	506	CLA	C1B-NB	-6.47	1.29	1.35
24	c	509	CLA	MG-ND	-6.47	1.93	2.05
24	b	618	CLA	C1B-NB	-6.46	1.29	1.35
24	B	609	CLA	MG-ND	-6.45	1.93	2.05
26	C	514	BCR	C17-C18	6.45	1.44	1.35
24	b	606	CLA	C1B-NB	-6.44	1.29	1.35
24	b	615	CLA	C1B-NB	-6.44	1.29	1.35
24	b	616	CLA	C1B-NB	-6.44	1.29	1.35
24	B	603	CLA	MG-ND	-6.44	1.93	2.05
24	c	506	CLA	C1B-NB	-6.43	1.29	1.35
26	c	514	BCR	C34-C9	-6.42	1.37	1.50
26	F	101	BCR	C34-C9	-6.42	1.37	1.50
24	c	501	CLA	C1B-NB	-6.41	1.29	1.35
26	b	620	BCR	C34-C9	-6.41	1.37	1.50
24	b	604	CLA	C1B-NB	-6.40	1.29	1.35
24	b	606	CLA	C1D-C2D	-6.37	1.32	1.45
24	c	508	CLA	MG-ND	-6.36	1.93	2.05
26	c	515	BCR	C34-C9	-6.35	1.37	1.50
24	C	512	CLA	C1B-NB	-6.34	1.29	1.35
24	A	607	CLA	C1B-NB	-6.34	1.29	1.35
24	b	617	CLA	MG-ND	-6.34	1.93	2.05
24	A	609	CLA	C1B-NB	-6.33	1.29	1.35
26	t	101	BCR	C34-C9	-6.32	1.37	1.50
26	I	101	BCR	C38-C26	6.31	1.61	1.50
24	B	602	CLA	MG-ND	-6.31	1.93	2.05
24	C	502	CLA	MG-ND	-6.30	1.93	2.05
24	C	503	CLA	C1B-NB	-6.29	1.29	1.35
24	c	506	CLA	MG-ND	-6.29	1.93	2.05
24	B	615	CLA	C1B-NB	-6.28	1.29	1.35
24	b	609	CLA	C1B-NB	-6.27	1.29	1.35
24	D	402	CLA	C1B-NB	-6.26	1.29	1.35
26	c	521	BCR	C34-C9	-6.26	1.37	1.50
24	B	606	CLA	MG-ND	-6.26	1.93	2.05
26	A	610	BCR	C38-C26	6.24	1.61	1.50
26	B	620	BCR	C34-C9	-6.24	1.38	1.50
27	d	404	PL9	O2-C1	6.23	1.41	1.24
27	D	405	PL9	O2-C1	6.23	1.41	1.24
26	f	101	BCR	C34-C9	-6.23	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	619	BCR	C24-C23	6.22	1.51	1.33
26	B	619	BCR	C38-C26	6.21	1.61	1.50
24	A	606	CLA	C1D-C2D	-6.21	1.33	1.45
24	b	607	CLA	C1B-NB	-6.18	1.29	1.35
26	c	521	BCR	C38-C26	6.17	1.61	1.50
26	K	102	BCR	C38-C26	6.16	1.61	1.50
24	c	502	CLA	MG-ND	-6.14	1.93	2.05
26	c	521	BCR	C11-C12	6.14	1.50	1.34
26	H	101	BCR	C34-C9	-6.13	1.38	1.50
26	K	102	BCR	C34-C9	-6.13	1.38	1.50
26	c	514	BCR	C38-C26	6.13	1.61	1.50
24	b	608[B]	CLA	C1B-NB	-6.11	1.29	1.35
24	B	617	CLA	C1B-NB	-6.11	1.29	1.35
26	A	610	BCR	C34-C9	-6.10	1.38	1.50
26	k	101	BCR	C38-C26	6.10	1.60	1.50
26	k	101	BCR	C34-C9	-6.09	1.38	1.50
24	C	513	CLA	C1B-NB	-6.08	1.29	1.35
26	B	620	BCR	C38-C26	6.07	1.60	1.50
26	T	101	BCR	C34-C9	-6.07	1.38	1.50
26	F	101	BCR	C23-C22	6.07	1.59	1.45
24	c	502	CLA	C1B-NB	-6.06	1.29	1.35
24	B	603	CLA	C1B-NB	-6.05	1.29	1.35
24	B	605	CLA	C1D-C2D	-6.05	1.33	1.45
26	b	621	BCR	C38-C26	6.04	1.60	1.50
26	F	101	BCR	C24-C23	6.04	1.51	1.33
26	I	101	BCR	C11-C12	6.04	1.50	1.34
24	B	604	CLA	C1D-C2D	-6.03	1.33	1.45
26	h	101	BCR	C34-C9	-6.03	1.38	1.50
24	c	509	CLA	C1B-NB	-6.00	1.29	1.35
24	c	513	CLA	MG-ND	-6.00	1.93	2.05
24	B	613	CLA	C1D-C2D	-5.99	1.33	1.45
26	I	101	BCR	C17-C18	5.98	1.43	1.35
24	B	608	CLA	C1D-C2D	-5.97	1.33	1.45
24	C	505	CLA	MG-ND	-5.97	1.94	2.05
24	b	608[A]	CLA	C1B-NB	-5.95	1.29	1.35
24	b	605	CLA	C1D-C2D	-5.95	1.33	1.45
24	a	606	CLA	C1D-C2D	-5.95	1.33	1.45
24	B	607[B]	CLA	C1B-NB	-5.94	1.29	1.35
24	C	508	CLA	C1D-C2D	-5.94	1.33	1.45
26	b	619	BCR	C38-C26	5.93	1.60	1.50
26	B	618	BCR	C38-C26	5.92	1.60	1.50
26	c	515	BCR	C38-C26	5.92	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C1B-NB	-5.92	1.29	1.35
26	a	610	BCR	C34-C9	-5.90	1.38	1.50
26	A	610	BCR	C11-C12	5.90	1.49	1.34
24	B	610	CLA	C1D-C2D	-5.89	1.33	1.45
24	C	502	CLA	C1B-NB	-5.88	1.30	1.35
24	a	607	CLA	C1B-NB	-5.86	1.30	1.35
24	b	613	CLA	C1D-C2D	-5.85	1.33	1.45
26	b	621	BCR	C11-C12	5.85	1.49	1.34
24	C	511	CLA	C1D-C2D	-5.85	1.33	1.45
24	C	506	CLA	C1D-C2D	-5.85	1.33	1.45
26	C	514	BCR	C38-C26	5.84	1.60	1.50
24	b	612	CLA	C1B-NB	-5.83	1.30	1.35
24	b	610	CLA	C1B-NB	-5.81	1.30	1.35
26	K	101	BCR	C38-C26	5.81	1.60	1.50
26	B	619	BCR	C23-C22	5.81	1.58	1.45
24	c	507	CLA	C1B-NB	-5.80	1.30	1.35
24	c	504	CLA	C1D-C2D	-5.80	1.33	1.45
24	d	403	CLA	C1B-NB	-5.80	1.30	1.35
24	c	508	CLA	C1B-NB	-5.79	1.30	1.35
24	C	507	CLA	C1B-NB	-5.79	1.30	1.35
26	h	101	BCR	C11-C12	5.79	1.49	1.34
26	t	101	BCR	C38-C26	5.79	1.60	1.50
24	c	505	CLA	C1D-C2D	-5.78	1.33	1.45
26	K	102	BCR	C11-C12	5.77	1.49	1.34
24	B	611	CLA	C1D-C2D	-5.77	1.33	1.45
24	b	616	CLA	C1D-C2D	-5.76	1.34	1.45
26	c	515	BCR	C11-C12	5.75	1.49	1.34
24	B	607[A]	CLA	C1B-NB	-5.75	1.30	1.35
26	H	101	BCR	C24-C23	5.74	1.50	1.33
26	B	619	BCR	C11-C12	5.74	1.49	1.34
26	H	101	BCR	C11-C12	5.73	1.49	1.34
24	c	512	CLA	C1B-NB	-5.73	1.30	1.35
24	B	612	CLA	C1D-C2D	-5.73	1.34	1.45
24	a	615	CLA	C1D-C2D	-5.72	1.34	1.45
26	B	618	BCR	C23-C22	5.72	1.58	1.45
24	A	609	CLA	C1D-C2D	-5.72	1.34	1.45
24	d	402	CLA	C1D-C2D	-5.71	1.34	1.45
26	b	621	BCR	C17-C18	5.70	1.43	1.35
26	C	514	BCR	C11-C12	5.70	1.49	1.34
24	b	604	CLA	C1D-C2D	-5.69	1.34	1.45
26	t	101	BCR	C11-C12	5.69	1.49	1.34
26	T	101	BCR	C11-C12	5.67	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	609	CLA	C1D-C2D	-5.66	1.34	1.45
24	C	507	CLA	C1D-C2D	-5.66	1.34	1.45
24	B	607[B]	CLA	C1D-C2D	-5.63	1.34	1.45
26	t	101	BCR	C23-C22	5.61	1.58	1.45
26	H	101	BCR	C17-C18	5.61	1.43	1.35
24	c	505	CLA	C1B-NB	-5.61	1.30	1.35
24	C	512	CLA	C1D-C2D	-5.61	1.34	1.45
26	a	610	BCR	C11-C12	5.60	1.49	1.34
26	c	521	BCR	C23-C22	5.60	1.58	1.45
26	c	514	BCR	C11-C12	5.60	1.49	1.34
24	c	513	CLA	C1B-NB	-5.60	1.30	1.35
24	D	403	CLA	C1D-C2D	-5.60	1.34	1.45
26	C	514	BCR	C23-C22	5.59	1.58	1.45
24	c	508	CLA	C1D-C2D	-5.59	1.34	1.45
24	C	502	CLA	CHD-C1D	5.57	1.49	1.38
26	A	610	BCR	C24-C23	5.57	1.49	1.33
26	a	610	BCR	C38-C26	5.57	1.60	1.50
24	C	501	CLA	C1B-NB	-5.56	1.30	1.35
26	a	610	BCR	C23-C22	5.55	1.57	1.45
24	b	603	CLA	C1D-C2D	-5.55	1.34	1.45
24	B	610	CLA	C1B-NB	-5.54	1.30	1.35
26	k	101	BCR	C11-C12	5.53	1.48	1.34
24	b	618	CLA	C1D-C2D	-5.53	1.34	1.45
24	b	614	CLA	C1D-C2D	-5.53	1.34	1.45
24	B	609	CLA	CHD-C1D	5.53	1.49	1.38
24	D	402	CLA	C1D-C2D	-5.53	1.34	1.45
26	K	101	BCR	C17-C18	5.53	1.43	1.35
24	C	503	CLA	C1D-C2D	-5.51	1.34	1.45
24	B	616	CLA	C1B-NB	-5.50	1.30	1.35
26	b	620	BCR	C24-C23	5.50	1.49	1.33
24	B	607[A]	CLA	C1D-C2D	-5.50	1.34	1.45
24	B	603	CLA	C1D-C2D	-5.49	1.34	1.45
24	B	606	CLA	C1D-C2D	-5.48	1.34	1.45
26	T	101	BCR	C23-C22	5.47	1.57	1.45
27	D	405	PL9	C3-C4	-5.47	1.40	1.49
24	C	505	CLA	CHD-C1D	5.46	1.49	1.38
26	A	610	BCR	C23-C22	5.46	1.57	1.45
26	f	101	BCR	C24-C23	5.45	1.49	1.33
24	b	611	CLA	C1D-C2D	-5.45	1.34	1.45
24	B	603	CLA	CHC-C1C	5.44	1.48	1.35
24	c	507	CLA	C1D-C2D	-5.44	1.34	1.45
26	B	619	BCR	C24-C25	5.44	1.64	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C1D-C2D	-5.43	1.34	1.45
24	b	608[B]	CLA	C1D-C2D	-5.42	1.34	1.45
24	C	509	CLA	C1D-C2D	-5.42	1.34	1.45
26	B	620	BCR	C11-C12	5.38	1.48	1.34
26	h	101	BCR	C24-C23	5.37	1.49	1.33
24	C	513	CLA	C1D-C2D	-5.37	1.34	1.45
24	b	607	CLA	C1D-C2D	-5.36	1.34	1.45
26	B	618	BCR	C11-C12	5.36	1.48	1.34
24	C	511	CLA	C1B-NB	-5.36	1.30	1.35
24	b	617	CLA	C1B-NB	-5.34	1.30	1.35
26	T	101	BCR	C38-C26	5.33	1.59	1.50
24	D	403	CLA	C4B-CHC	-5.33	1.26	1.41
24	B	611	CLA	C1B-NB	-5.32	1.30	1.35
24	b	603	CLA	CHD-C4C	-5.31	1.27	1.39
26	f	101	BCR	C23-C22	5.31	1.57	1.45
26	F	101	BCR	C11-C12	5.30	1.48	1.34
24	b	617	CLA	C1D-C2D	-5.30	1.34	1.45
26	H	101	BCR	C23-C22	5.29	1.57	1.45
24	c	510	CLA	C1B-NB	-5.29	1.30	1.35
24	b	608[A]	CLA	C1D-C2D	-5.29	1.34	1.45
26	h	101	BCR	C17-C18	5.27	1.42	1.35
26	B	618	BCR	C24-C23	5.27	1.49	1.33
26	a	610	BCR	C24-C23	5.26	1.49	1.33
24	c	501	CLA	C1D-C2D	-5.26	1.34	1.45
24	c	503	CLA	C1B-NB	-5.26	1.30	1.35
24	c	509	CLA	C1D-C2D	-5.26	1.34	1.45
24	B	616	CLA	C1D-C2D	-5.25	1.35	1.45
24	c	503	CLA	C1D-C2D	-5.25	1.35	1.45
24	D	404	CLA	C1D-C2D	-5.24	1.35	1.45
24	c	506	CLA	C1D-C2D	-5.23	1.35	1.45
26	b	619	BCR	C23-C22	5.22	1.57	1.45
24	b	612	CLA	CHD-C1D	5.21	1.48	1.38
24	C	505	CLA	C1B-NB	-5.20	1.30	1.35
24	b	606	CLA	CHC-C1C	5.19	1.48	1.35
24	C	505	CLA	C1D-C2D	-5.19	1.35	1.45
24	C	501	CLA	CHC-C1C	5.19	1.48	1.35
24	C	501	CLA	C1D-C2D	-5.19	1.35	1.45
26	B	620	BCR	C17-C18	5.18	1.42	1.35
26	K	101	BCR	C24-C23	5.17	1.48	1.33
24	b	609	CLA	C1D-C2D	-5.17	1.35	1.45
24	b	615	CLA	C1D-C2D	-5.17	1.35	1.45
24	B	614	CLA	C4B-CHC	-5.16	1.26	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	CHC-C1C	5.15	1.48	1.35
24	b	610	CLA	C1D-C2D	-5.15	1.35	1.45
24	B	614	CLA	C1D-C2D	-5.15	1.35	1.45
24	c	510	CLA	C1D-C2D	-5.14	1.35	1.45
26	b	620	BCR	C11-C12	5.14	1.47	1.34
26	c	515	BCR	C24-C23	5.14	1.48	1.33
24	B	617	CLA	C4B-CHC	-5.14	1.26	1.41
24	c	512	CLA	C1D-C2D	-5.13	1.35	1.45
24	b	604	CLA	CHC-C1C	5.12	1.48	1.35
24	c	511	CLA	C1D-C2D	-5.11	1.35	1.45
24	C	513	CLA	CHD-C1D	5.11	1.48	1.38
24	c	513	CLA	CHD-C1D	5.10	1.48	1.38
26	b	619	BCR	C11-C12	5.10	1.47	1.34
24	c	513	CLA	C1D-C2D	-5.10	1.35	1.45
26	f	101	BCR	C11-C12	5.10	1.47	1.34
24	C	501	CLA	CHD-C1D	5.09	1.48	1.38
24	b	608[A]	CLA	CHD-C1D	5.08	1.48	1.38
24	B	604	CLA	C4B-CHC	-5.08	1.26	1.41
24	a	607	CLA	CHC-C1C	5.07	1.48	1.35
24	c	506	CLA	CHD-C1D	5.07	1.48	1.38
24	B	606	CLA	C1B-NB	-5.06	1.30	1.35
24	a	615	CLA	C4B-CHC	-5.06	1.26	1.41
24	c	505	CLA	CHD-C1D	5.06	1.48	1.38
30	l	102	LHG	O8-C23	5.05	1.48	1.33
24	c	501	CLA	CHD-C1D	5.05	1.48	1.38
24	b	611	CLA	C1B-NB	-5.04	1.30	1.35
24	C	510	CLA	C4B-CHC	-5.04	1.27	1.41
24	A	607	CLA	C1D-C2D	-5.04	1.35	1.45
24	b	618	CLA	C4B-CHC	-5.04	1.27	1.41
26	C	514	BCR	C24-C23	5.03	1.48	1.33
24	b	608[B]	CLA	CHD-C1D	5.03	1.48	1.38
24	B	609	CLA	C1D-C2D	-5.03	1.35	1.45
24	A	606	CLA	CHD-C4C	-5.03	1.27	1.39
24	C	504	CLA	CHD-C1D	5.03	1.48	1.38
24	c	502	CLA	C1D-C2D	-5.03	1.35	1.45
26	b	619	BCR	C24-C23	5.02	1.48	1.33
24	B	602	CLA	C1D-C2D	-5.02	1.35	1.45
24	D	402	CLA	CHD-C1D	5.02	1.48	1.38
24	C	512	CLA	C4B-CHC	-5.00	1.27	1.41
24	b	605	CLA	C4B-CHC	-5.00	1.27	1.41
24	c	511	CLA	C1B-NB	-5.00	1.30	1.35
29	c	520	LMG	O7-C10	5.00	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	CHC-C1C	4.99	1.47	1.35
26	B	620	BCR	C23-C22	4.99	1.56	1.45
24	C	513	CLA	CHC-C1C	4.99	1.47	1.35
24	b	616	CLA	CHC-C1C	4.99	1.47	1.35
24	b	609	CLA	CHC-C1C	4.99	1.47	1.35
24	B	602	CLA	C1B-NB	-4.99	1.30	1.35
24	b	612	CLA	C1D-C2D	-4.98	1.35	1.45
24	c	501	CLA	CHC-C1C	4.98	1.47	1.35
24	B	616	CLA	CHC-C1C	4.98	1.47	1.35
24	b	613	CLA	C4B-CHC	-4.98	1.27	1.41
29	C	518	LMG	O7-C10	4.97	1.48	1.34
24	B	609	CLA	C1B-NB	-4.97	1.30	1.35
24	c	502	CLA	CHD-C1D	4.97	1.48	1.38
24	d	403	CLA	C1D-C2D	-4.97	1.35	1.45
24	c	504	CLA	CHC-C1C	4.97	1.47	1.35
26	K	101	BCR	C11-C12	4.96	1.47	1.34
24	C	510	CLA	CHD-C1D	4.96	1.48	1.38
24	B	617	CLA	C1D-C2D	-4.95	1.35	1.45
24	a	606	CLA	CHD-C4C	-4.95	1.27	1.39
24	b	617	CLA	C4C-C3C	-4.95	1.36	1.45
24	c	511	CLA	CHC-C1C	4.95	1.47	1.35
26	A	610	BCR	C24-C25	4.95	1.62	1.45
24	a	607	CLA	C1D-C2D	-4.94	1.35	1.45
26	F	101	BCR	C24-C25	4.94	1.62	1.45
29	a	613	LMG	O7-C10	4.93	1.48	1.34
24	D	404	CLA	CHC-C1C	4.93	1.47	1.35
24	c	508	CLA	CHC-C1C	4.93	1.47	1.35
26	c	514	BCR	C24-C23	4.93	1.48	1.33
24	B	604	CLA	CHD-C1D	4.92	1.48	1.38
26	c	515	BCR	C23-C22	4.92	1.56	1.45
24	c	510	CLA	CHC-C1C	4.92	1.47	1.35
26	K	101	BCR	C23-C22	4.92	1.56	1.45
26	k	101	BCR	C24-C23	4.92	1.47	1.33
24	D	403	CLA	C4C-C3C	-4.92	1.36	1.45
24	B	617	CLA	CHD-C1D	4.91	1.47	1.38
24	a	607	CLA	CHD-C1D	4.91	1.47	1.38
24	b	611	CLA	CHC-C1C	4.91	1.47	1.35
24	A	607	CLA	CHD-C4C	-4.90	1.28	1.39
24	B	608	CLA	CHD-C4C	-4.89	1.28	1.39
24	B	613	CLA	C4B-CHC	-4.89	1.27	1.41
24	B	605	CLA	C4B-CHC	-4.89	1.27	1.41
24	C	510	CLA	C1D-C2D	-4.89	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	620	BCR	C24-C25	4.88	1.62	1.45
24	C	508	CLA	C4B-CHC	-4.88	1.27	1.41
24	b	603	CLA	C4C-C3C	-4.88	1.36	1.45
24	D	404	CLA	CHD-C1D	4.87	1.47	1.38
24	b	616	CLA	CHD-C4C	-4.87	1.28	1.39
24	c	507	CLA	CHD-C1D	4.87	1.47	1.38
26	t	101	BCR	C24-C23	4.87	1.47	1.33
24	d	403	CLA	C4C-C3C	-4.87	1.36	1.45
24	c	511	CLA	CHD-C1D	4.86	1.47	1.38
26	T	101	BCR	C24-C23	4.86	1.47	1.33
26	f	101	BCR	C24-C25	4.86	1.62	1.45
24	a	606	CLA	CHC-C1C	4.85	1.47	1.35
24	c	512	CLA	CHC-C1C	4.85	1.47	1.35
24	b	608[B]	CLA	CHC-C1C	4.85	1.47	1.35
24	b	604	CLA	CHD-C1D	4.85	1.47	1.38
24	A	607	CLA	CHC-C1C	4.84	1.47	1.35
24	C	503	CLA	CHD-C4C	-4.84	1.28	1.39
24	B	613	CLA	CHD-C1D	4.84	1.47	1.38
24	b	607	CLA	CHC-C1C	4.83	1.47	1.35
24	B	614	CLA	CHD-C1D	4.83	1.47	1.38
24	b	617	CLA	CHD-C4C	-4.83	1.28	1.39
24	c	509	CLA	CHC-C1C	4.83	1.47	1.35
24	a	609	CLA	CHC-C1C	4.83	1.47	1.35
24	b	615	CLA	CHD-C1D	4.83	1.47	1.38
26	k	101	BCR	C17-C18	4.83	1.42	1.35
24	a	606	CLA	C4B-CHC	-4.83	1.27	1.41
24	c	506	CLA	CHC-C1C	4.82	1.47	1.35
24	b	609	CLA	CHD-C4C	-4.82	1.28	1.39
30	d	407	LHG	O8-C23	4.82	1.47	1.33
24	b	614	CLA	CHC-C1C	4.81	1.47	1.35
24	B	606	CLA	CHC-C1C	4.81	1.47	1.35
24	c	513	CLA	CHC-C1C	4.81	1.47	1.35
24	B	602	CLA	CHD-C1D	4.81	1.47	1.38
24	b	608[A]	CLA	CHC-C1C	4.81	1.47	1.35
24	C	509	CLA	C4B-CHC	-4.80	1.27	1.41
24	b	610	CLA	CHD-C1D	4.79	1.47	1.38
24	C	507	CLA	CHD-C4C	-4.79	1.28	1.39
24	C	504	CLA	C1D-C2D	-4.79	1.35	1.45
24	c	512	CLA	CHD-C1D	4.79	1.47	1.38
24	C	511	CLA	CHC-C1C	4.79	1.47	1.35
24	C	510	CLA	C1C-NC	-4.79	1.30	1.37
24	d	403	CLA	CHC-C1C	4.79	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	C4B-CHC	-4.78	1.27	1.41
24	A	609	CLA	CHD-C4C	-4.78	1.28	1.39
24	A	609	CLA	CHD-C1D	4.78	1.47	1.38
29	c	519	LMG	O7-C10	4.78	1.47	1.34
24	B	607[B]	CLA	CHC-C1C	4.77	1.47	1.35
24	c	511	CLA	CHD-C4C	-4.77	1.28	1.39
24	B	611	CLA	CHC-C1C	4.77	1.47	1.35
24	c	502	CLA	CHC-C1C	4.77	1.47	1.35
24	d	403	CLA	CHD-C4C	-4.77	1.28	1.39
26	c	515	BCR	C17-C18	4.77	1.42	1.35
26	B	620	BCR	C24-C23	4.77	1.47	1.33
26	b	619	BCR	C17-C18	4.76	1.42	1.35
24	b	607	CLA	CHD-C4C	-4.76	1.28	1.39
30	D	406	LHG	O8-C23	4.76	1.47	1.33
24	a	609	CLA	CHD-C4C	-4.76	1.28	1.39
26	c	514	BCR	C17-C18	4.76	1.42	1.35
24	C	512	CLA	CHD-C4C	-4.75	1.28	1.39
26	b	620	BCR	C23-C22	4.75	1.56	1.45
24	B	608	CLA	CHC-C1C	4.74	1.47	1.35
24	D	404	CLA	C4B-CHC	-4.74	1.27	1.41
24	C	506	CLA	C4B-CHC	-4.74	1.27	1.41
26	h	101	BCR	C23-C22	4.74	1.56	1.45
24	b	607	CLA	C4C-C3C	-4.74	1.36	1.45
26	K	102	BCR	C23-C22	4.74	1.56	1.45
24	A	609	CLA	C4C-C3C	-4.73	1.36	1.45
24	C	507	CLA	CHC-C1C	4.73	1.47	1.35
24	d	402	CLA	CHC-C1C	4.73	1.47	1.35
24	B	612	CLA	CHD-C1D	4.73	1.47	1.38
24	B	614	CLA	C4C-C3C	-4.72	1.36	1.45
26	I	101	BCR	C23-C22	4.72	1.56	1.45
24	B	607[A]	CLA	CHD-C1D	4.72	1.47	1.38
24	C	508	CLA	CHC-C1C	4.72	1.47	1.35
24	a	615	CLA	CHD-C1D	4.72	1.47	1.38
24	c	508	CLA	CHD-C1D	4.71	1.47	1.38
24	B	605	CLA	CHD-C1D	4.71	1.47	1.38
24	b	615	CLA	CHC-C1C	4.71	1.47	1.35
24	A	607	CLA	CHD-C1D	4.71	1.47	1.38
24	c	504	CLA	C4B-CHC	-4.71	1.27	1.41
24	D	404	CLA	CHD-C4C	-4.71	1.28	1.39
24	B	610	CLA	CHC-C1C	4.70	1.47	1.35
24	A	606	CLA	CHC-C1C	4.70	1.47	1.35
24	A	607	CLA	C4B-CHC	-4.70	1.27	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	519	LMG	O7-C10	4.70	1.47	1.34
24	B	616	CLA	CHD-C4C	-4.70	1.28	1.39
24	b	614	CLA	C4B-CHC	-4.70	1.27	1.41
26	I	101	BCR	C24-C23	4.69	1.47	1.33
26	B	619	BCR	C17-C18	4.69	1.42	1.35
24	b	617	CLA	CHC-C1C	4.69	1.47	1.35
24	B	607[A]	CLA	CHC-C1C	4.68	1.47	1.35
24	A	606	CLA	C4B-CHC	-4.68	1.28	1.41
24	b	615	CLA	CHD-C4C	-4.68	1.28	1.39
24	b	611	CLA	CHD-C1D	4.68	1.47	1.38
24	B	602	CLA	CHC-C1C	4.68	1.47	1.35
24	b	606	CLA	C4B-CHC	-4.68	1.28	1.41
24	B	603	CLA	CHD-C1D	4.68	1.47	1.38
24	b	611	CLA	CHD-C4C	-4.67	1.28	1.39
24	b	613	CLA	CHD-C4C	-4.67	1.28	1.39
24	C	512	CLA	CHC-C1C	4.67	1.46	1.35
24	C	509	CLA	CHD-C4C	-4.67	1.28	1.39
24	C	506	CLA	CHC-C1C	4.67	1.46	1.35
24	B	615	CLA	CHC-C1C	4.67	1.46	1.35
24	B	610	CLA	CHD-C4C	-4.67	1.28	1.39
24	a	609	CLA	C1B-NB	-4.66	1.31	1.35
24	c	512	CLA	C4B-CHC	-4.66	1.28	1.41
24	a	607	CLA	CHD-C4C	-4.66	1.28	1.39
24	b	616	CLA	C4C-C3C	-4.66	1.37	1.45
24	c	505	CLA	C4B-CHC	-4.66	1.28	1.41
24	A	607	CLA	C1C-NC	-4.66	1.30	1.37
24	c	505	CLA	CHC-C1C	4.65	1.46	1.35
24	B	607[B]	CLA	CHD-C1D	4.65	1.47	1.38
24	B	615	CLA	CHD-C1D	4.65	1.47	1.38
24	a	615	CLA	C1C-NC	-4.65	1.30	1.37
24	A	609	CLA	CHC-C1C	4.65	1.46	1.35
24	b	614	CLA	CHD-C1D	4.65	1.47	1.38
24	C	502	CLA	CHC-C1C	4.65	1.46	1.35
26	K	102	BCR	C24-C23	4.65	1.47	1.33
24	C	504	CLA	C4B-CHC	-4.64	1.28	1.41
24	b	609	CLA	CHD-C1D	4.64	1.47	1.38
24	d	403	CLA	C4B-CHC	-4.64	1.28	1.41
24	d	402	CLA	CHD-C1D	4.64	1.47	1.38
24	b	615	CLA	C4C-C3C	-4.63	1.37	1.45
24	B	605	CLA	CHC-C1C	4.63	1.46	1.35
24	b	603	CLA	C4B-CHC	-4.63	1.28	1.41
32	E	101	DGD	O2G-C1B	4.63	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	615	CLA	CHD-C4C	-4.62	1.28	1.39
24	D	402	CLA	CHC-C1C	4.62	1.46	1.35
24	C	505	CLA	C4B-CHC	-4.62	1.28	1.41
27	a	611	PL9	C3-C4	-4.61	1.41	1.49
24	A	609	CLA	C1C-NC	-4.61	1.30	1.37
24	b	607	CLA	C4B-CHC	-4.61	1.28	1.41
24	b	616	CLA	CHD-C1D	4.61	1.47	1.38
27	d	404	PL9	C3-C4	-4.60	1.41	1.49
26	c	514	BCR	C23-C22	4.60	1.55	1.45
24	c	503	CLA	CHD-C1D	4.60	1.47	1.38
24	b	615	CLA	C4B-CHC	-4.60	1.28	1.41
29	z	101	LMG	O7-C10	4.60	1.47	1.34
24	D	403	CLA	CHD-C4C	-4.59	1.28	1.39
24	c	510	CLA	CHD-C4C	-4.59	1.28	1.39
26	K	101	BCR	C24-C25	4.59	1.61	1.45
24	B	612	CLA	CHD-C4C	-4.59	1.28	1.39
24	c	507	CLA	C4B-CHC	-4.58	1.28	1.41
24	b	610	CLA	C4B-CHC	-4.58	1.28	1.41
24	d	403	CLA	CHD-C1D	4.58	1.47	1.38
24	b	609	CLA	C4C-C3C	-4.58	1.37	1.45
24	C	502	CLA	C4B-CHC	-4.58	1.28	1.41
24	b	603	CLA	C1C-NC	-4.58	1.31	1.37
24	d	402	CLA	C4B-CHC	-4.57	1.28	1.41
24	b	617	CLA	C4B-CHC	-4.57	1.28	1.41
32	d	405	DGD	O2G-C1B	4.57	1.47	1.34
24	c	506	CLA	C4B-CHC	-4.57	1.28	1.41
24	B	606	CLA	CHD-C4C	-4.57	1.28	1.39
28	X	101	SQD	O48-C23	4.57	1.46	1.33
24	b	603	CLA	CHC-C1C	4.56	1.46	1.35
24	B	614	CLA	CHD-C4C	-4.56	1.28	1.39
24	b	610	CLA	CHC-C1C	4.56	1.46	1.35
24	b	606	CLA	CHD-C1D	4.56	1.47	1.38
24	D	402	CLA	CMA-C3A	-4.56	1.43	1.53
24	c	509	CLA	C4B-CHC	-4.55	1.28	1.41
29	A	613	LMG	O7-C10	4.55	1.47	1.34
24	B	613	CLA	CHC-C1C	4.55	1.46	1.35
24	B	611	CLA	CHD-C1D	4.55	1.47	1.38
24	b	612	CLA	C4B-CHC	-4.55	1.28	1.41
24	B	612	CLA	CHC-C1C	4.55	1.46	1.35
24	c	510	CLA	C4B-CHC	-4.55	1.28	1.41
24	B	602	CLA	CHD-C4C	-4.55	1.28	1.39
24	B	608	CLA	C4B-CHC	-4.55	1.28	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CHD-C4C	-4.55	1.28	1.39
24	b	606	CLA	CHD-C4C	-4.55	1.28	1.39
24	c	507	CLA	CHD-C4C	-4.54	1.28	1.39
24	c	502	CLA	C4B-CHC	-4.54	1.28	1.41
26	c	521	BCR	C24-C23	4.54	1.46	1.33
24	C	504	CLA	C4C-C3C	-4.54	1.37	1.45
24	B	607[B]	CLA	CHD-C4C	-4.53	1.28	1.39
24	c	511	CLA	C1C-NC	-4.53	1.31	1.37
24	B	610	CLA	C4B-CHC	-4.53	1.28	1.41
27	a	611	PL9	C7-C3	4.53	1.55	1.51
24	C	506	CLA	CHD-C1D	4.53	1.47	1.38
30	L	101	LHG	O8-C23	4.53	1.46	1.33
24	C	507	CLA	C4B-CHC	-4.53	1.28	1.41
24	C	512	CLA	C4C-C3C	-4.53	1.37	1.45
24	c	509	CLA	CHD-C4C	-4.53	1.28	1.39
24	B	607[B]	CLA	C4B-CHC	-4.53	1.28	1.41
24	b	605	CLA	CHD-C4C	-4.53	1.28	1.39
24	C	511	CLA	C4B-CHC	-4.52	1.28	1.41
24	C	505	CLA	CHC-C1C	4.52	1.46	1.35
28	x	101	SQD	O48-C23	4.52	1.46	1.33
24	C	511	CLA	CHD-C4C	-4.52	1.28	1.39
24	b	618	CLA	CHD-C1D	4.51	1.47	1.38
24	D	402	CLA	C4B-CHC	-4.51	1.28	1.41
26	K	102	BCR	C17-C18	4.50	1.41	1.35
26	H	101	BCR	C24-C25	4.50	1.61	1.45
24	c	509	CLA	CHD-C1D	4.50	1.47	1.38
24	C	508	CLA	CHD-C4C	-4.50	1.28	1.39
30	E	102	LHG	O7-C7	4.50	1.47	1.34
24	B	607[A]	CLA	CHD-C4C	-4.49	1.28	1.39
24	B	606	CLA	C4B-CHC	-4.49	1.28	1.41
24	d	403	CLA	C1C-NC	-4.49	1.31	1.37
26	T	101	BCR	C17-C18	4.49	1.41	1.35
24	C	503	CLA	C4C-C3C	-4.49	1.37	1.45
28	X	101	SQD	O47-C7	4.48	1.46	1.34
26	k	101	BCR	C24-C25	4.48	1.61	1.45
24	c	507	CLA	CHC-C1C	4.48	1.46	1.35
24	b	618	CLA	CHD-C4C	-4.48	1.29	1.39
28	a	614	SQD	O48-C23	4.48	1.46	1.33
28	A	614	SQD	O48-C23	4.47	1.46	1.33
26	k	101	BCR	C23-C22	4.47	1.55	1.45
30	D	407	LHG	O7-C7	4.47	1.46	1.34
24	b	614	CLA	CHD-C4C	-4.46	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	CHC-C1C	4.46	1.46	1.35
27	A	611	PL9	C3-C4	-4.46	1.42	1.49
24	D	403	CLA	CHD-C1D	4.46	1.47	1.38
24	b	609	CLA	C1C-NC	-4.46	1.31	1.37
24	c	511	CLA	C4C-C3C	-4.46	1.37	1.45
24	B	612	CLA	C4B-CHC	-4.45	1.28	1.41
24	b	608[B]	CLA	C4B-CHC	-4.45	1.28	1.41
24	b	605	CLA	CHD-C1D	4.45	1.47	1.38
28	x	101	SQD	O47-C7	4.45	1.46	1.34
24	b	616	CLA	C4B-CHC	-4.44	1.28	1.41
24	B	608	CLA	C4C-C3C	-4.44	1.37	1.45
24	C	510	CLA	CHD-C4C	-4.44	1.29	1.39
24	c	508	CLA	C4B-CHC	-4.44	1.28	1.41
24	b	609	CLA	C4B-CHC	-4.44	1.28	1.41
24	B	602	CLA	C4B-CHC	-4.43	1.28	1.41
29	Z	101	LMG	O7-C10	4.43	1.46	1.34
24	B	615	CLA	C4B-CHC	-4.43	1.28	1.41
24	c	513	CLA	C4B-CHC	-4.43	1.28	1.41
24	c	510	CLA	CHD-C1D	4.43	1.47	1.38
28	b	601	SQD	O47-C7	4.43	1.46	1.34
24	b	617	CLA	CHD-C1D	4.42	1.47	1.38
24	B	617	CLA	CHD-C4C	-4.42	1.29	1.39
24	C	504	CLA	C1C-NC	-4.42	1.31	1.37
24	B	615	CLA	CHD-C4C	-4.42	1.29	1.39
30	e	101	LHG	O7-C7	4.42	1.46	1.34
24	c	503	CLA	CHD-C4C	-4.41	1.29	1.39
24	B	607[A]	CLA	C4B-CHC	-4.41	1.28	1.41
28	b	601	SQD	O48-C23	4.41	1.46	1.33
24	A	606	CLA	C4C-C3C	-4.41	1.37	1.45
28	l	101	SQD	O47-C7	4.41	1.46	1.34
28	B	622	SQD	O48-C23	4.40	1.46	1.33
24	d	402	CLA	C1C-NC	-4.40	1.31	1.37
28	B	622	SQD	O47-C7	4.40	1.46	1.34
24	B	614	CLA	CHC-C1C	4.40	1.46	1.35
26	B	620	BCR	C40-C30	4.40	1.62	1.53
24	B	610	CLA	CHD-C1D	4.39	1.46	1.38
30	e	101	LHG	O8-C23	4.39	1.46	1.33
24	C	502	CLA	C1D-C2D	-4.39	1.36	1.45
26	K	102	BCR	C40-C30	4.39	1.62	1.53
24	B	616	CLA	CHD-C1D	4.39	1.46	1.38
24	a	607	CLA	C4B-CHC	-4.39	1.28	1.41
24	c	512	CLA	CHD-C4C	-4.39	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C4B-CHC	-4.39	1.28	1.41
24	B	609	CLA	CHC-C1C	4.38	1.46	1.35
28	L	102	SQD	O47-C7	4.38	1.46	1.34
24	B	616	CLA	C4C-C3C	-4.38	1.37	1.45
24	C	506	CLA	CHD-C4C	-4.37	1.29	1.39
24	d	402	CLA	CHD-C4C	-4.37	1.29	1.39
24	b	607	CLA	CHD-C1D	4.37	1.46	1.38
24	C	508	CLA	C1D-ND	-4.37	1.32	1.37
24	C	511	CLA	CHD-C1D	4.37	1.46	1.38
24	B	613	CLA	CHD-C4C	-4.36	1.29	1.39
24	b	613	CLA	C1D-ND	-4.36	1.32	1.37
24	C	509	CLA	CHC-C1C	4.36	1.46	1.35
24	B	604	CLA	CHC-C1C	4.36	1.46	1.35
33	V	201	HEM	C3C-CAC	4.36	1.56	1.47
24	B	608	CLA	CHD-C1D	4.36	1.46	1.38
24	b	618	CLA	CHC-C1C	4.36	1.46	1.35
24	c	509	CLA	C4C-C3C	-4.36	1.37	1.45
24	c	504	CLA	CHD-C1D	4.35	1.46	1.38
24	B	606	CLA	C4C-C3C	-4.35	1.37	1.45
24	c	511	CLA	C4B-CHC	-4.35	1.28	1.41
24	b	604	CLA	CHD-C4C	-4.35	1.29	1.39
24	b	604	CLA	C1C-NC	-4.35	1.31	1.37
30	E	102	LHG	O8-C23	4.35	1.46	1.33
32	C	515	DGD	O2G-C1B	4.35	1.46	1.34
24	B	603	CLA	CHD-C4C	-4.34	1.29	1.39
24	C	509	CLA	CHD-C1D	4.34	1.46	1.38
24	a	607	CLA	C1C-NC	-4.34	1.31	1.37
24	b	603	CLA	C1B-NB	-4.33	1.31	1.35
30	a	616	LHG	O8-C23	4.33	1.46	1.33
24	B	611	CLA	CHD-C4C	-4.33	1.29	1.39
29	b	622	LMG	O7-C10	4.33	1.46	1.34
24	b	618	CLA	C4C-C3C	-4.33	1.37	1.45
26	I	101	BCR	C24-C25	4.32	1.60	1.45
24	b	608[A]	CLA	C4B-CHC	-4.32	1.29	1.41
24	B	606	CLA	CHD-C1D	4.32	1.46	1.38
24	B	604	CLA	CHD-C4C	-4.32	1.29	1.39
29	B	621	LMG	O7-C10	4.31	1.46	1.34
24	D	403	CLA	CMA-C3A	-4.31	1.43	1.53
24	c	513	CLA	C4C-C3C	-4.31	1.37	1.45
24	C	504	CLA	CMA-C3A	-4.31	1.43	1.53
24	C	507	CLA	CHD-C1D	4.31	1.46	1.38
24	C	512	CLA	CHD-C1D	4.30	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	CHC-C1C	4.30	1.46	1.35
24	b	616	CLA	C1C-NC	-4.30	1.31	1.37
26	c	521	BCR	C40-C30	4.30	1.62	1.53
24	a	606	CLA	CHD-C1D	4.30	1.46	1.38
26	b	619	BCR	C24-C25	4.29	1.60	1.45
24	a	609	CLA	CHD-C1D	4.29	1.46	1.38
24	b	613	CLA	CHD-C1D	4.29	1.46	1.38
28	A	614	SQD	O47-C7	4.28	1.46	1.34
24	b	611	CLA	C4B-CHC	-4.28	1.29	1.41
24	B	611	CLA	C4B-CHC	-4.28	1.29	1.41
24	B	605	CLA	C1C-NC	-4.28	1.31	1.37
28	a	614	SQD	O47-C7	4.28	1.46	1.34
24	c	501	CLA	C4B-CHC	-4.28	1.29	1.41
24	D	403	CLA	CBD-CGD	-4.27	1.39	1.52
24	b	604	CLA	C4B-CHC	-4.27	1.29	1.41
24	b	605	CLA	CMA-C3A	-4.27	1.44	1.53
24	B	603	CLA	C4B-CHC	-4.27	1.29	1.41
24	B	608	CLA	CAA-C2A	-4.27	1.46	1.54
24	C	504	CLA	CHC-C1C	4.27	1.45	1.35
24	A	609	CLA	C4B-CHC	-4.26	1.29	1.41
24	b	608[B]	CLA	CHD-C4C	-4.26	1.29	1.39
24	a	615	CLA	CHC-C1C	4.26	1.45	1.35
24	b	605	CLA	CHC-C1C	4.26	1.45	1.35
24	C	513	CLA	C4B-CHC	-4.26	1.29	1.41
26	c	515	BCR	C24-C25	4.26	1.60	1.45
24	B	607[B]	CLA	CMA-C3A	-4.26	1.44	1.53
24	b	607	CLA	C1C-NC	-4.26	1.31	1.37
24	b	604	CLA	C3D-C4D	-4.25	1.34	1.44
24	c	504	CLA	CHD-C4C	-4.25	1.29	1.39
24	C	510	CLA	CHC-C1C	4.25	1.45	1.35
24	B	614	CLA	CMA-C3A	-4.24	1.44	1.53
32	h	102	DGD	O2G-C1B	4.24	1.46	1.34
24	B	612	CLA	C1C-NC	-4.24	1.31	1.37
24	b	616	CLA	C1A-CHA	-4.24	1.25	1.43
26	h	101	BCR	C24-C25	4.23	1.60	1.45
24	D	403	CLA	CHC-C1C	4.23	1.45	1.35
24	B	616	CLA	C4B-CHC	-4.23	1.29	1.41
24	C	509	CLA	C1C-NC	-4.23	1.31	1.37
24	C	504	CLA	CHD-C4C	-4.23	1.29	1.39
24	B	608	CLA	CMA-C3A	-4.23	1.44	1.53
24	C	513	CLA	C4C-C3C	-4.22	1.37	1.45
24	d	403	CLA	O2A-CGA	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	v	201	HEM	C3C-CAC	4.22	1.56	1.47
26	B	618	BCR	C24-C25	4.22	1.60	1.45
24	B	607[A]	CLA	CMA-C3A	-4.22	1.44	1.53
26	B	620	BCR	C24-C25	4.22	1.60	1.45
24	C	513	CLA	CHD-C4C	-4.22	1.29	1.39
30	d	407	LHG	O7-C7	4.22	1.46	1.34
24	B	607[B]	CLA	C4C-C3C	-4.22	1.37	1.45
24	c	503	CLA	C4B-CHC	-4.22	1.29	1.41
24	b	614	CLA	CMA-C3A	-4.22	1.44	1.53
24	D	404	CLA	CMA-C3A	-4.21	1.44	1.53
24	B	613	CLA	CMA-C3A	-4.21	1.44	1.53
26	a	610	BCR	C24-C25	4.21	1.60	1.45
24	c	501	CLA	CHD-C4C	-4.21	1.29	1.39
24	B	613	CLA	C1C-NC	-4.21	1.31	1.37
24	c	509	CLA	CMA-C3A	-4.21	1.44	1.53
24	a	609	CLA	C4B-CHC	-4.21	1.29	1.41
24	C	502	CLA	CHD-C4C	-4.20	1.29	1.39
24	A	606	CLA	CMA-C3A	-4.20	1.44	1.53
26	A	610	BCR	C17-C18	4.20	1.41	1.35
24	B	602	CLA	C4C-C3C	-4.19	1.37	1.45
24	B	613	CLA	C1A-CHA	-4.19	1.25	1.43
32	H	102	DGD	O1G-C1A	4.19	1.45	1.33
24	C	502	CLA	C4C-C3C	-4.19	1.37	1.45
24	b	616	CLA	C3D-C4D	-4.19	1.34	1.44
33	v	201	HEM	C3C-C2C	-4.18	1.34	1.40
30	d	406	LHG	O8-C23	4.18	1.45	1.33
24	B	614	CLA	C1C-NC	-4.18	1.31	1.37
24	C	501	CLA	C4B-CHC	-4.18	1.29	1.41
24	B	613	CLA	C1D-ND	-4.18	1.32	1.37
32	c	517	DGD	O2G-C2G	-4.18	1.36	1.46
24	a	615	CLA	C3D-C4D	-4.17	1.34	1.44
24	c	506	CLA	CHD-C4C	-4.17	1.29	1.39
24	c	508	CLA	CHD-C4C	-4.17	1.29	1.39
24	B	617	CLA	CHC-C1C	4.17	1.45	1.35
32	c	518	DGD	O2G-C2G	-4.17	1.36	1.46
24	B	617	CLA	C1C-NC	-4.17	1.31	1.37
24	C	507	CLA	C1C-NC	-4.17	1.31	1.37
24	b	617	CLA	C1C-NC	-4.17	1.31	1.37
24	B	605	CLA	CMA-C3A	-4.16	1.44	1.53
24	C	501	CLA	CMA-C3A	-4.16	1.44	1.53
24	b	606	CLA	O2A-CGA	4.16	1.45	1.33
24	D	403	CLA	C1C-NC	-4.16	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	C4C-C3C	-4.16	1.37	1.45
24	b	610	CLA	CHD-C4C	-4.16	1.29	1.39
24	c	502	CLA	CHD-C4C	-4.16	1.29	1.39
24	b	603	CLA	CHD-C1D	4.16	1.46	1.38
24	B	611	CLA	CMA-C3A	-4.16	1.44	1.53
24	D	402	CLA	C3D-C4D	-4.16	1.34	1.44
24	C	506	CLA	C1C-NC	-4.16	1.31	1.37
30	l	102	LHG	O7-C7	4.16	1.46	1.34
24	B	607[A]	CLA	C4C-C3C	-4.16	1.37	1.45
24	C	511	CLA	CMA-C3A	-4.15	1.44	1.53
24	B	608	CLA	C3D-C4D	-4.15	1.34	1.44
32	c	518	DGD	O2G-C1B	4.15	1.46	1.34
24	b	608[A]	CLA	CHD-C4C	-4.15	1.29	1.39
24	C	502	CLA	C1C-NC	-4.15	1.31	1.37
24	b	611	CLA	C4C-C3C	-4.15	1.37	1.45
24	A	609	CLA	C3D-C4D	-4.15	1.34	1.44
26	b	621	BCR	C40-C30	4.14	1.61	1.53
24	c	502	CLA	CMA-C3A	-4.14	1.44	1.53
26	c	521	BCR	C24-C25	4.14	1.59	1.45
24	b	605	CLA	O2A-CGA	4.14	1.45	1.33
24	C	501	CLA	CHD-C4C	-4.14	1.29	1.39
30	d	406	LHG	O7-C7	4.14	1.46	1.34
28	A	612	SQD	O47-C7	4.14	1.46	1.34
24	c	504	CLA	CMA-C3A	-4.14	1.44	1.53
24	d	402	CLA	CMA-C3A	-4.13	1.44	1.53
29	c	519	LMG	O8-C28	4.13	1.45	1.33
24	a	615	CLA	C4C-C3C	-4.13	1.37	1.45
24	C	510	CLA	CMA-C3A	-4.13	1.44	1.53
28	l	101	SQD	O48-C23	4.13	1.45	1.33
24	b	612	CLA	CHD-C4C	-4.13	1.29	1.39
33	E	103	HEM	C3C-CAC	4.13	1.56	1.47
28	a	612	SQD	O47-C7	4.13	1.45	1.34
30	A	615	LHG	O7-C7	4.13	1.45	1.34
24	b	613	CLA	C1C-NC	-4.13	1.31	1.37
32	C	516	DGD	O1G-C1A	4.13	1.45	1.33
24	b	608[A]	CLA	CMA-C3A	-4.13	1.44	1.53
26	F	101	BCR	C2-C3	4.12	1.62	1.52
24	c	511	CLA	CMA-C3A	-4.12	1.44	1.53
24	b	609	CLA	CMA-C3A	-4.12	1.44	1.53
26	C	514	BCR	C24-C25	4.12	1.59	1.45
29	C	518	LMG	O6-C1	4.12	1.52	1.41
26	k	101	BCR	C40-C30	4.12	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C3D-C2D	-4.12	1.27	1.39
24	b	608[B]	CLA	CMA-C3A	-4.12	1.44	1.53
24	c	512	CLA	C4C-C3C	-4.12	1.37	1.45
24	B	617	CLA	C4C-C3C	-4.12	1.37	1.45
28	L	102	SQD	O48-C23	4.11	1.45	1.33
24	A	609	CLA	CMA-C3A	-4.11	1.44	1.53
29	j	101	LMG	O7-C10	4.11	1.45	1.34
24	c	507	CLA	C1C-NC	-4.11	1.31	1.37
24	C	502	CLA	CMA-C3A	-4.11	1.44	1.53
24	a	615	CLA	CMA-C3A	-4.11	1.44	1.53
24	c	506	CLA	CMA-C3A	-4.11	1.44	1.53
32	c	516	DGD	O2G-C2G	-4.10	1.36	1.46
32	c	516	DGD	O2G-C1B	4.10	1.45	1.34
24	B	605	CLA	C4C-C3C	-4.10	1.38	1.45
32	C	516	DGD	O2G-C1B	4.10	1.45	1.34
24	B	610	CLA	C3D-C4D	-4.10	1.34	1.44
24	d	402	CLA	C4C-C3C	-4.10	1.38	1.45
27	A	611	PL9	C7-C3	4.10	1.55	1.51
24	C	508	CLA	C4C-C3C	-4.09	1.38	1.45
24	a	606	CLA	C4C-C3C	-4.09	1.38	1.45
24	a	609	CLA	C1C-NC	-4.09	1.31	1.37
30	A	615	LHG	O8-C23	4.08	1.45	1.33
24	B	612	CLA	C4C-C3C	-4.08	1.38	1.45
32	c	517	DGD	O1G-C1A	4.08	1.45	1.33
30	D	407	LHG	O8-C23	4.08	1.45	1.33
24	c	513	CLA	CHD-C4C	-4.08	1.29	1.39
24	C	508	CLA	C3D-C4D	-4.08	1.35	1.44
24	b	607	CLA	CMA-C3A	-4.08	1.44	1.53
26	b	621	BCR	C24-C25	4.08	1.59	1.45
32	C	517	DGD	O2G-C2G	-4.07	1.36	1.46
24	B	602	CLA	C1C-NC	-4.07	1.31	1.37
32	E	101	DGD	O1G-C1A	4.07	1.45	1.33
29	C	518	LMG	O8-C28	4.07	1.45	1.33
24	a	609	CLA	O2A-CGA	4.07	1.45	1.33
24	c	505	CLA	CHD-C4C	-4.06	1.29	1.39
24	B	604	CLA	C1C-NC	-4.06	1.31	1.37
24	B	610	CLA	C1D-ND	-4.06	1.32	1.37
24	D	404	CLA	O2A-CGA	4.06	1.45	1.33
24	B	615	CLA	C4C-C3C	-4.06	1.38	1.45
24	b	615	CLA	C1C-NC	-4.05	1.31	1.37
32	H	102	DGD	O2G-C2G	-4.05	1.36	1.46
24	C	503	CLA	CHD-C1D	4.05	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	102	BCR	C24-C25	4.05	1.59	1.45
24	b	610	CLA	CMA-C3A	-4.05	1.44	1.53
24	B	608	CLA	C1C-NC	-4.05	1.31	1.37
24	C	510	CLA	C4C-C3C	-4.05	1.38	1.45
24	B	611	CLA	C1C-NC	-4.05	1.31	1.37
24	c	504	CLA	C4C-C3C	-4.05	1.38	1.45
28	a	612	SQD	O48-C23	4.04	1.45	1.33
26	f	101	BCR	C27-C26	4.04	1.59	1.51
32	c	516	DGD	O1G-C1A	4.04	1.45	1.33
32	d	405	DGD	O1G-C1A	4.04	1.45	1.33
24	b	604	CLA	C4C-C3C	-4.03	1.38	1.45
26	a	610	BCR	C17-C18	4.03	1.41	1.35
24	a	609	CLA	CMA-C3A	-4.03	1.44	1.53
24	C	501	CLA	C1A-CHA	-4.03	1.26	1.43
24	B	609	CLA	CMA-C3A	-4.03	1.44	1.53
24	b	605	CLA	C4C-C3C	-4.03	1.38	1.45
24	C	508	CLA	CHD-C1D	4.03	1.46	1.38
24	C	511	CLA	C4C-C3C	-4.03	1.38	1.45
24	B	615	CLA	C1C-NC	-4.03	1.31	1.37
24	b	613	CLA	C4C-C3C	-4.03	1.38	1.45
26	H	101	BCR	C40-C30	4.02	1.61	1.53
24	B	614	CLA	C3D-C4D	-4.02	1.35	1.44
24	c	504	CLA	O2A-CGA	4.02	1.45	1.33
30	L	101	LHG	O7-C7	4.02	1.45	1.34
27	D	405	PL9	C6-C1	-4.02	1.41	1.48
29	c	520	LMG	O8-C28	4.02	1.45	1.33
32	C	517	DGD	O1G-C1A	4.02	1.45	1.33
24	c	512	CLA	C1C-NC	-4.02	1.31	1.37
24	b	604	CLA	CMA-C3A	-4.01	1.44	1.53
24	a	609	CLA	C4C-C3C	-4.01	1.38	1.45
24	B	606	CLA	C3D-C2D	-4.01	1.28	1.39
24	D	402	CLA	CHD-C4C	-4.01	1.30	1.39
24	B	612	CLA	CMA-C3A	-4.01	1.44	1.53
30	a	616	LHG	O7-C7	4.01	1.45	1.34
26	c	521	BCR	C12-C13	4.00	1.54	1.45
24	B	610	CLA	CMA-C3A	-4.00	1.44	1.53
29	D	408	LMG	O7-C10	4.00	1.45	1.34
32	C	517	DGD	O2G-C1B	4.00	1.45	1.34
33	E	103	HEM	C3C-C2C	-4.00	1.34	1.40
24	B	604	CLA	C3D-C4D	-4.00	1.35	1.44
24	a	606	CLA	CMA-C3A	-4.00	1.44	1.53
24	B	612	CLA	C1A-CHA	-4.00	1.26	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	C1C-NC	-3.99	1.31	1.37
24	C	509	CLA	C4C-C3C	-3.99	1.38	1.45
24	d	402	CLA	C3D-C4D	-3.99	1.35	1.44
24	c	508	CLA	C1C-NC	-3.98	1.31	1.37
28	A	612	SQD	O48-C23	3.97	1.44	1.33
24	D	402	CLA	C1C-NC	-3.97	1.31	1.37
24	C	507	CLA	O2A-CGA	3.97	1.44	1.33
24	b	606	CLA	CMA-C3A	-3.97	1.44	1.53
24	b	614	CLA	C3D-C2D	-3.97	1.28	1.39
24	b	611	CLA	C1C-NC	-3.97	1.31	1.37
24	b	613	CLA	CMA-C3A	-3.97	1.44	1.53
24	c	510	CLA	C4C-C3C	-3.97	1.38	1.45
24	c	502	CLA	C1C-NC	-3.97	1.31	1.37
24	B	615	CLA	CMA-C3A	-3.97	1.44	1.53
24	B	612	CLA	C3D-C4D	-3.97	1.35	1.44
24	C	513	CLA	C3D-C4D	-3.96	1.35	1.44
24	c	507	CLA	O2A-CGA	3.96	1.44	1.33
24	A	606	CLA	C1C-NC	-3.96	1.31	1.37
24	b	612	CLA	CMA-C3A	-3.96	1.44	1.53
24	b	611	CLA	CMA-C3A	-3.96	1.44	1.53
24	D	403	CLA	C3D-C4D	-3.95	1.35	1.44
24	C	505	CLA	CMA-C3A	-3.95	1.44	1.53
24	C	509	CLA	CMA-C3A	-3.95	1.44	1.53
24	B	615	CLA	C3D-C2D	-3.95	1.28	1.39
24	b	615	CLA	CMA-C3A	-3.95	1.44	1.53
24	B	614	CLA	C3D-C2D	-3.95	1.28	1.39
24	b	606	CLA	C3D-C4D	-3.95	1.35	1.44
24	C	512	CLA	C1C-NC	-3.95	1.31	1.37
24	A	607	CLA	C3D-C4D	-3.95	1.35	1.44
24	c	507	CLA	C4C-C3C	-3.95	1.38	1.45
26	c	514	BCR	C24-C25	3.94	1.59	1.45
26	B	618	BCR	C2-C3	3.94	1.62	1.52
24	b	609	CLA	C3D-C4D	-3.94	1.35	1.44
32	c	518	DGD	O6E-C5E	3.94	1.53	1.44
26	T	101	BCR	C2-C3	3.94	1.62	1.52
24	A	606	CLA	C1A-CHA	-3.94	1.26	1.43
24	c	512	CLA	CMA-C3A	-3.94	1.44	1.53
33	e	102	HEM	C3C-CAC	3.94	1.55	1.47
24	b	605	CLA	C1C-NC	-3.94	1.31	1.37
24	C	508	CLA	C1C-NC	-3.93	1.31	1.37
24	b	606	CLA	C1C-NC	-3.93	1.31	1.37
24	b	614	CLA	C1A-CHA	-3.93	1.26	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	609	CLA	C1A-CHA	-3.93	1.26	1.43
24	d	403	CLA	CMA-C3A	-3.93	1.44	1.53
24	C	502	CLA	O2A-CGA	3.93	1.44	1.33
24	b	616	CLA	CMA-C3A	-3.93	1.44	1.53
24	b	617	CLA	CMA-C3A	-3.93	1.44	1.53
32	c	518	DGD	O1G-C1A	3.93	1.44	1.33
32	C	516	DGD	O2G-C2G	-3.93	1.36	1.46
29	D	408	LMG	O6-C1	3.93	1.51	1.41
32	h	102	DGD	O1G-C1A	3.92	1.44	1.33
24	D	404	CLA	C1C-NC	-3.92	1.31	1.37
24	B	607[B]	CLA	C1C-NC	-3.92	1.32	1.37
24	b	610	CLA	C1C-NC	-3.92	1.32	1.37
24	C	511	CLA	C3D-C4D	-3.92	1.35	1.44
24	a	606	CLA	C3D-C4D	-3.91	1.35	1.44
24	B	602	CLA	O2A-CGA	3.91	1.44	1.33
24	B	610	CLA	C1C-NC	-3.91	1.32	1.37
24	c	508	CLA	C4C-C3C	-3.91	1.38	1.45
24	D	402	CLA	CBD-CGD	-3.91	1.40	1.52
24	C	508	CLA	CMA-C3A	-3.91	1.44	1.53
24	B	607[A]	CLA	C1C-NC	-3.91	1.32	1.37
24	b	612	CLA	C1C-NC	-3.91	1.32	1.37
24	c	510	CLA	CMA-C3A	-3.90	1.44	1.53
24	B	606	CLA	CMA-C3A	-3.90	1.44	1.53
32	E	101	DGD	O6E-C5E	3.90	1.53	1.44
30	D	406	LHG	O7-C7	3.90	1.45	1.34
32	C	515	DGD	O1G-C1A	3.90	1.44	1.33
24	C	503	CLA	C3D-C2D	-3.90	1.28	1.39
26	t	101	BCR	C24-C25	3.90	1.58	1.45
24	D	402	CLA	C1A-CHA	-3.90	1.26	1.43
24	A	607	CLA	O2A-CGA	3.90	1.44	1.33
24	B	617	CLA	O2A-CGA	3.90	1.44	1.33
24	B	610	CLA	C1A-CHA	-3.90	1.26	1.43
24	c	501	CLA	CMA-C3A	-3.89	1.44	1.53
24	c	510	CLA	CAA-C2A	-3.89	1.46	1.54
24	c	505	CLA	CMA-C3A	-3.89	1.44	1.53
24	B	604	CLA	C1D-ND	-3.89	1.33	1.37
24	a	615	CLA	C1A-CHA	-3.89	1.27	1.43
24	a	607	CLA	C3D-C4D	-3.89	1.35	1.44
24	b	604	CLA	CAA-C2A	-3.88	1.46	1.54
24	A	606	CLA	CHD-C1D	3.88	1.45	1.38
24	c	508	CLA	CMA-C3A	-3.88	1.44	1.53
24	C	503	CLA	C3D-C4D	-3.88	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	h	102	DGD	O2G-C2G	-3.88	1.36	1.46
24	B	607[B]	CLA	C3D-C4D	-3.88	1.35	1.44
27	d	404	PL9	C6-C1	-3.88	1.41	1.48
29	A	613	LMG	O8-C28	3.87	1.44	1.33
24	C	511	CLA	C3D-C2D	-3.87	1.28	1.39
24	a	606	CLA	C3D-C2D	-3.87	1.28	1.39
24	b	613	CLA	CBD-CGD	-3.87	1.40	1.52
29	j	101	LMG	O6-C1	3.86	1.51	1.41
24	c	502	CLA	C4C-C3C	-3.86	1.38	1.45
24	b	608[B]	CLA	C3D-C4D	-3.86	1.35	1.44
24	a	606	CLA	C1C-NC	-3.86	1.32	1.37
24	C	503	CLA	C1C-NC	-3.86	1.32	1.37
24	C	508	CLA	C1A-CHA	-3.86	1.27	1.43
24	c	506	CLA	C1C-NC	-3.86	1.32	1.37
24	c	503	CLA	CMA-C3A	-3.86	1.44	1.53
24	C	513	CLA	C1C-NC	-3.85	1.32	1.37
24	B	606	CLA	C1C-NC	-3.85	1.32	1.37
24	b	609	CLA	C1A-CHA	-3.85	1.27	1.43
29	a	613	LMG	O8-C28	3.85	1.44	1.33
24	A	609	CLA	CBD-CGD	-3.85	1.40	1.52
24	B	603	CLA	C3D-C4D	-3.85	1.35	1.44
26	c	515	BCR	C12-C13	3.85	1.54	1.45
29	b	622	LMG	O6-C1	3.85	1.51	1.41
32	h	102	DGD	O6E-C5E	3.84	1.53	1.44
26	b	619	BCR	C40-C30	3.84	1.61	1.53
24	b	618	CLA	C3D-C4D	-3.84	1.35	1.44
24	b	609	CLA	C3D-C2D	-3.84	1.28	1.39
24	b	614	CLA	CAA-C2A	-3.84	1.47	1.54
26	T	101	BCR	C24-C25	3.84	1.58	1.45
24	b	611	CLA	C1D-ND	-3.84	1.33	1.37
26	I	101	BCR	C12-C13	3.83	1.54	1.45
24	B	603	CLA	C4C-C3C	-3.83	1.38	1.45
26	f	101	BCR	C2-C3	3.83	1.62	1.52
24	C	506	CLA	C4C-C3C	-3.83	1.38	1.45
32	H	102	DGD	O2G-C1B	3.83	1.45	1.34
24	b	613	CLA	C3D-C2D	-3.83	1.28	1.39
24	b	605	CLA	C1D-ND	-3.83	1.33	1.37
32	C	516	DGD	O6E-C5E	3.83	1.53	1.44
24	b	606	CLA	C3D-C2D	-3.83	1.28	1.39
24	A	607	CLA	C4C-C3C	-3.82	1.38	1.45
24	b	606	CLA	C4C-C3C	-3.82	1.38	1.45
24	b	614	CLA	C3D-C4D	-3.82	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	615	CLA	C3D-C2D	-3.82	1.28	1.39
24	d	402	CLA	C1D-ND	-3.82	1.33	1.37
24	A	606	CLA	C1D-ND	-3.82	1.33	1.37
26	B	619	BCR	C2-C3	3.82	1.62	1.52
24	b	613	CLA	C3D-C4D	-3.81	1.35	1.44
26	c	521	BCR	C2-C3	3.81	1.62	1.52
24	b	608[B]	CLA	C4C-C3C	-3.81	1.38	1.45
24	b	611	CLA	O2D-CGD	3.81	1.42	1.33
24	B	608	CLA	C1A-CHA	-3.81	1.27	1.43
24	C	501	CLA	O2A-CGA	3.81	1.44	1.33
24	b	618	CLA	CAA-C2A	-3.80	1.47	1.54
24	B	603	CLA	CMA-C3A	-3.80	1.45	1.53
24	c	504	CLA	C1C-NC	-3.80	1.32	1.37
24	b	618	CLA	C1C-NC	-3.80	1.32	1.37
24	D	402	CLA	C3D-C2D	-3.80	1.28	1.39
24	A	606	CLA	C3D-C4D	-3.80	1.35	1.44
24	B	602	CLA	CMA-C3A	-3.80	1.45	1.53
24	C	507	CLA	C4C-C3C	-3.80	1.38	1.45
24	C	504	CLA	C1A-CHA	-3.80	1.27	1.43
24	B	604	CLA	O2A-CGA	3.80	1.44	1.33
24	B	605	CLA	C3D-C4D	-3.79	1.35	1.44
24	c	505	CLA	C1C-NC	-3.79	1.32	1.37
24	c	507	CLA	CMA-C3A	-3.79	1.45	1.53
26	c	514	BCR	C40-C30	3.79	1.61	1.53
32	C	515	DGD	O6E-C5E	3.79	1.53	1.44
24	C	501	CLA	C3D-C4D	-3.79	1.35	1.44
24	a	607	CLA	C4C-C3C	-3.78	1.38	1.45
24	C	506	CLA	O2D-CGD	3.78	1.42	1.33
24	a	607	CLA	CMA-C3A	-3.78	1.45	1.53
24	B	613	CLA	C3D-C4D	-3.78	1.35	1.44
24	c	513	CLA	CMA-C3A	-3.78	1.45	1.53
24	b	614	CLA	C1D-ND	-3.78	1.33	1.37
24	D	404	CLA	C4C-C3C	-3.77	1.38	1.45
26	t	101	BCR	C17-C18	3.77	1.40	1.35
29	c	519	LMG	O6-C1	3.77	1.51	1.41
24	b	614	CLA	C1C-NC	-3.77	1.32	1.37
24	b	618	CLA	CMA-C3A	-3.77	1.45	1.53
24	B	613	CLA	CAA-C2A	-3.76	1.47	1.54
32	c	517	DGD	O2G-C1B	3.76	1.44	1.34
24	C	505	CLA	CAA-C2A	-3.76	1.47	1.54
26	c	515	BCR	C40-C30	3.76	1.61	1.53
24	C	506	CLA	C3D-C4D	-3.76	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	O2A-CGA	3.76	1.44	1.33
32	C	515	DGD	O2G-C2G	-3.76	1.37	1.46
26	C	514	BCR	C40-C30	3.76	1.61	1.53
29	B	621	LMG	O8-C28	3.76	1.44	1.33
24	c	505	CLA	C3D-C4D	-3.76	1.35	1.44
24	b	608[A]	CLA	C3D-C4D	-3.76	1.35	1.44
24	b	610	CLA	C4C-C3C	-3.75	1.38	1.45
24	b	615	CLA	CAA-C2A	-3.75	1.47	1.54
24	C	508	CLA	C3D-C2D	-3.75	1.28	1.39
24	B	603	CLA	C1C-NC	-3.75	1.32	1.37
24	B	604	CLA	C4C-C3C	-3.75	1.38	1.45
24	c	512	CLA	O2A-CGA	3.75	1.44	1.33
26	F	101	BCR	C40-C30	3.75	1.61	1.53
24	c	506	CLA	O2A-CGA	3.75	1.44	1.33
29	b	622	LMG	O8-C28	3.75	1.44	1.33
24	B	607[A]	CLA	C3D-C4D	-3.75	1.35	1.44
24	c	509	CLA	O2A-CGA	3.74	1.44	1.33
24	c	513	CLA	C1C-NC	-3.74	1.32	1.37
24	c	504	CLA	C3D-C2D	-3.74	1.28	1.39
32	d	405	DGD	O6E-C5E	3.73	1.53	1.44
26	B	620	BCR	C2-C3	3.73	1.61	1.52
24	B	610	CLA	O2A-CGA	3.72	1.44	1.33
24	c	511	CLA	O2A-CGA	3.72	1.44	1.33
24	A	607	CLA	C1A-CHA	-3.72	1.27	1.43
24	b	604	CLA	C1A-CHA	-3.72	1.27	1.43
24	c	503	CLA	CBD-CGD	-3.72	1.40	1.52
24	C	511	CLA	O2A-CGA	3.72	1.44	1.33
29	D	408	LMG	O8-C28	3.72	1.44	1.33
24	B	609	CLA	C3D-C4D	-3.71	1.35	1.44
24	c	505	CLA	C1D-ND	-3.71	1.33	1.37
24	B	616	CLA	C1C-NC	-3.71	1.32	1.37
24	a	615	CLA	C1D-ND	-3.71	1.33	1.37
27	A	611	PL9	C6-C1	-3.71	1.42	1.48
24	b	605	CLA	C3D-C4D	-3.71	1.35	1.44
24	C	510	CLA	C1D-ND	-3.70	1.33	1.37
24	c	502	CLA	O2A-CGA	3.70	1.44	1.33
24	B	610	CLA	C4C-C3C	-3.70	1.38	1.45
29	C	519	LMG	O8-C28	3.70	1.44	1.33
32	H	102	DGD	O6E-C5E	3.70	1.53	1.44
24	C	507	CLA	CMA-C3A	-3.70	1.45	1.53
24	c	508	CLA	C3D-C4D	-3.70	1.35	1.44
24	b	608[A]	CLA	O2A-CGA	3.70	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	C3D-C2D	-3.69	1.29	1.39
24	c	503	CLA	O2A-CGA	3.69	1.44	1.33
26	K	102	BCR	C2-C3	3.69	1.61	1.52
24	c	511	CLA	C3D-C4D	-3.69	1.35	1.44
24	b	614	CLA	C4C-C3C	-3.69	1.38	1.45
24	B	609	CLA	C1C-NC	-3.69	1.32	1.37
24	A	609	CLA	C3D-C2D	-3.69	1.29	1.39
24	B	615	CLA	C3D-C4D	-3.69	1.35	1.44
24	b	608[A]	CLA	C4C-C3C	-3.68	1.38	1.45
24	B	606	CLA	C3D-C4D	-3.68	1.35	1.44
24	a	607	CLA	C3D-C2D	-3.68	1.29	1.39
26	B	618	BCR	C40-C30	3.68	1.61	1.53
24	b	609	CLA	CAA-C2A	-3.68	1.47	1.54
24	a	615	CLA	CBD-CGD	-3.68	1.40	1.52
32	C	517	DGD	O6E-C5E	3.68	1.53	1.44
24	A	606	CLA	CAA-C2A	-3.68	1.47	1.54
26	c	515	BCR	C2-C3	3.68	1.61	1.52
24	c	501	CLA	C1C-NC	-3.68	1.32	1.37
24	C	503	CLA	CMA-C3A	-3.68	1.45	1.53
24	b	612	CLA	C3D-C4D	-3.67	1.35	1.44
27	a	611	PL9	C36-C34	3.67	1.58	1.51
33	e	102	HEM	C3C-C2C	-3.67	1.35	1.40
24	B	614	CLA	C1A-CHA	-3.67	1.27	1.43
24	b	612	CLA	C1A-CHA	-3.67	1.27	1.43
24	a	609	CLA	C3D-C4D	-3.67	1.35	1.44
24	B	608	CLA	C3D-C2D	-3.67	1.29	1.39
24	C	510	CLA	C3D-C2D	-3.67	1.29	1.39
24	b	611	CLA	CAA-C2A	-3.67	1.47	1.54
24	B	614	CLA	CBD-CGD	-3.66	1.40	1.52
24	c	503	CLA	C3D-C4D	-3.66	1.35	1.44
24	D	404	CLA	CBD-CGD	-3.66	1.41	1.52
24	C	513	CLA	C1A-CHA	-3.66	1.27	1.43
26	K	102	BCR	C12-C13	3.66	1.53	1.45
24	B	613	CLA	MG-NA	-3.66	1.97	2.06
24	B	605	CLA	C1A-CHA	-3.66	1.27	1.43
24	C	513	CLA	CMA-C3A	-3.66	1.45	1.53
24	A	607	CLA	CMA-C3A	-3.66	1.45	1.53
26	I	101	BCR	C40-C30	3.66	1.61	1.53
24	C	511	CLA	C1C-NC	-3.66	1.32	1.37
24	b	608[A]	CLA	CBD-CGD	-3.66	1.41	1.52
24	d	403	CLA	CBD-CGD	-3.66	1.41	1.52
24	b	608[B]	CLA	C1A-CHA	-3.65	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	CBD-CGD	-3.65	1.41	1.52
26	B	619	BCR	C27-C26	3.65	1.58	1.51
24	d	402	CLA	C1A-CHA	-3.65	1.28	1.43
24	b	618	CLA	O2A-CGA	3.65	1.44	1.33
24	c	505	CLA	C4C-C3C	-3.65	1.38	1.45
24	b	603	CLA	C3D-C2D	-3.65	1.29	1.39
24	b	612	CLA	O2A-CGA	3.65	1.44	1.33
24	C	509	CLA	CBD-CGD	-3.65	1.41	1.52
29	Z	101	LMG	O6-C1	3.65	1.51	1.41
24	b	608[B]	CLA	O2A-CGA	3.64	1.44	1.33
24	C	511	CLA	C1B-CHB	3.64	1.51	1.41
24	a	615	CLA	MG-NA	-3.64	1.97	2.06
24	b	603	CLA	CMA-C3A	-3.64	1.45	1.53
24	B	617	CLA	C1B-CHB	3.64	1.51	1.41
26	A	610	BCR	C12-C13	3.64	1.53	1.45
24	B	614	CLA	CAA-C2A	-3.64	1.47	1.54
24	C	505	CLA	CHD-C4C	-3.64	1.30	1.39
24	a	606	CLA	C1A-CHA	-3.64	1.28	1.43
24	b	611	CLA	C3D-C4D	-3.64	1.36	1.44
24	a	615	CLA	CAA-C2A	-3.64	1.47	1.54
24	B	604	CLA	C1A-CHA	-3.63	1.28	1.43
24	B	612	CLA	C1D-ND	-3.63	1.33	1.37
24	C	506	CLA	CMA-C3A	-3.63	1.45	1.53
24	C	510	CLA	C1A-CHA	-3.63	1.28	1.43
24	c	510	CLA	C3D-C2D	-3.62	1.29	1.39
24	b	603	CLA	C3D-C4D	-3.62	1.36	1.44
24	C	512	CLA	CMA-C3A	-3.62	1.45	1.53
24	b	608[B]	CLA	CBD-CGD	-3.62	1.41	1.52
24	c	503	CLA	C3D-C2D	-3.62	1.29	1.39
27	a	611	PL9	C6-C1	-3.61	1.42	1.48
24	b	604	CLA	C3D-C2D	-3.61	1.29	1.39
24	b	608[B]	CLA	C1C-NC	-3.61	1.32	1.37
26	a	610	BCR	C2-C3	3.61	1.61	1.52
24	c	503	CLA	C1C-NC	-3.61	1.32	1.37
24	b	613	CLA	O2A-CGA	3.61	1.43	1.33
24	B	602	CLA	CBD-CGD	-3.61	1.41	1.52
24	B	607[A]	CLA	O2A-CGA	3.61	1.43	1.33
29	C	519	LMG	O6-C1	3.61	1.51	1.41
24	B	616	CLA	CMA-C3A	-3.61	1.45	1.53
24	A	607	CLA	MG-NA	-3.61	1.97	2.06
24	B	609	CLA	CHD-C4C	-3.61	1.31	1.39
29	z	101	LMG	O6-C1	3.61	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	501	CLA	C3D-C4D	-3.61	1.36	1.44
32	d	405	DGD	O2G-C2G	-3.60	1.37	1.46
24	b	610	CLA	CAA-C2A	-3.60	1.47	1.54
32	c	517	DGD	O6E-C5E	3.60	1.53	1.44
26	B	618	BCR	C1-C6	-3.60	1.48	1.53
26	b	620	BCR	C2-C3	3.60	1.61	1.52
26	b	621	BCR	C2-C3	3.60	1.61	1.52
24	A	607	CLA	CBD-CGD	-3.60	1.41	1.52
24	C	511	CLA	O2D-CGD	3.60	1.42	1.33
24	b	603	CLA	O2A-CGA	3.60	1.43	1.33
24	b	604	CLA	C1D-ND	-3.60	1.33	1.37
24	b	608[A]	CLA	C1A-CHA	-3.60	1.28	1.43
24	c	504	CLA	C3D-C4D	-3.60	1.36	1.44
24	b	608[B]	CLA	C3D-C2D	-3.60	1.29	1.39
24	c	512	CLA	C1A-CHA	-3.60	1.28	1.43
24	B	603	CLA	C1A-CHA	-3.60	1.28	1.43
27	A	611	PL9	C36-C34	3.60	1.58	1.51
26	b	621	BCR	C24-C23	3.59	1.43	1.33
24	B	611	CLA	C3D-C4D	-3.59	1.36	1.44
24	a	609	CLA	C3D-C2D	-3.59	1.29	1.39
24	c	501	CLA	O2A-CGA	3.59	1.43	1.33
26	h	101	BCR	C2-C3	3.59	1.61	1.52
24	d	402	CLA	C3D-C2D	-3.59	1.29	1.39
24	b	610	CLA	C3D-C4D	-3.59	1.36	1.44
24	b	604	CLA	O2D-CGD	3.59	1.42	1.33
24	D	404	CLA	C1A-CHA	-3.59	1.28	1.43
24	c	508	CLA	CAA-C2A	-3.59	1.47	1.54
24	c	505	CLA	C3D-C2D	-3.59	1.29	1.39
24	d	403	CLA	C1A-CHA	-3.58	1.28	1.43
26	c	514	BCR	C2-C3	3.58	1.61	1.52
24	b	608[A]	CLA	C3D-C2D	-3.58	1.29	1.39
24	b	607	CLA	C3D-C4D	-3.58	1.36	1.44
24	b	618	CLA	C1A-CHA	-3.58	1.28	1.43
29	c	520	LMG	O6-C1	3.58	1.51	1.41
24	b	618	CLA	C1D-ND	-3.58	1.33	1.37
24	b	615	CLA	C3D-C4D	-3.57	1.36	1.44
24	C	505	CLA	C1C-NC	-3.57	1.32	1.37
32	C	515	DGD	O6D-C5D	3.57	1.53	1.44
24	C	508	CLA	O2A-CGA	3.57	1.43	1.33
24	b	603	CLA	C1B-CHB	3.57	1.50	1.41
24	B	606	CLA	O2A-CGA	3.57	1.43	1.33
24	A	609	CLA	C3B-CAB	3.57	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C1A-CHA	-3.57	1.28	1.43
24	B	607[A]	CLA	C1A-CHA	-3.57	1.28	1.43
24	c	505	CLA	C1B-CHB	3.57	1.50	1.41
24	c	511	CLA	C3D-C2D	-3.57	1.29	1.39
24	C	509	CLA	C3D-C2D	-3.57	1.29	1.39
26	b	619	BCR	C2-C3	3.56	1.61	1.52
24	B	607[B]	CLA	C1A-CHA	-3.56	1.28	1.43
26	C	514	BCR	C4-C5	3.56	1.58	1.51
26	A	610	BCR	C2-C3	3.56	1.61	1.52
33	e	102	HEM	FE-ND	3.56	2.14	1.96
24	D	402	CLA	O2A-CGA	3.56	1.43	1.33
26	K	101	BCR	C40-C30	3.56	1.60	1.53
24	a	606	CLA	CAA-C2A	-3.56	1.47	1.54
24	D	402	CLA	C4C-C3C	-3.56	1.38	1.45
24	C	507	CLA	C3D-C4D	-3.56	1.36	1.44
24	A	607	CLA	C1D-ND	-3.56	1.33	1.37
24	d	402	CLA	MG-NA	-3.55	1.97	2.06
26	a	610	BCR	C40-C30	3.55	1.60	1.53
24	B	604	CLA	C3D-C2D	-3.55	1.29	1.39
24	b	607	CLA	C3D-C2D	-3.55	1.29	1.39
24	c	510	CLA	C1C-NC	-3.55	1.32	1.37
24	B	607[B]	CLA	CAA-C2A	-3.55	1.47	1.54
24	C	511	CLA	C1A-CHA	-3.55	1.28	1.43
24	A	606	CLA	O2A-CGA	3.54	1.43	1.33
26	F	101	BCR	C27-C26	3.54	1.58	1.51
26	t	101	BCR	C2-C3	3.54	1.61	1.52
24	c	504	CLA	C1A-CHA	-3.54	1.28	1.43
24	b	607	CLA	CAA-C2A	-3.54	1.47	1.54
24	B	606	CLA	O2D-CGD	3.54	1.41	1.33
24	D	404	CLA	C3D-C4D	-3.54	1.36	1.44
24	b	610	CLA	C1A-CHA	-3.54	1.28	1.43
24	B	610	CLA	CAA-C2A	-3.54	1.47	1.54
24	c	501	CLA	C4C-C3C	-3.53	1.38	1.45
24	b	618	CLA	C1B-CHB	3.53	1.50	1.41
24	C	506	CLA	C3D-C2D	-3.53	1.29	1.39
24	b	607	CLA	O2A-CGA	3.53	1.43	1.33
24	A	607	CLA	CAA-C2A	-3.53	1.47	1.54
24	B	607[B]	CLA	O2A-CGA	3.53	1.43	1.33
26	T	101	BCR	C40-C30	3.53	1.60	1.53
24	A	607	CLA	C3D-C2D	-3.53	1.29	1.39
24	D	403	CLA	C1A-CHA	-3.53	1.28	1.43
24	c	507	CLA	C3D-C4D	-3.53	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	607	CLA	C1A-CHA	-3.53	1.28	1.43
24	C	501	CLA	C1C-NC	-3.53	1.32	1.37
24	C	510	CLA	C3D-C4D	-3.52	1.36	1.44
33	v	201	HEM	CAB-C3B	3.52	1.57	1.47
24	a	607	CLA	CBD-CGD	-3.52	1.41	1.52
24	a	607	CLA	O2A-CGA	3.52	1.43	1.33
24	D	403	CLA	C1D-ND	-3.52	1.33	1.37
24	D	402	CLA	C1D-ND	-3.52	1.33	1.37
24	C	510	CLA	CAA-C2A	-3.52	1.47	1.54
32	E	101	DGD	O2G-C2G	-3.51	1.37	1.46
24	c	506	CLA	C4C-C3C	-3.51	1.39	1.45
33	V	201	HEM	C3C-C2C	-3.51	1.35	1.40
26	H	101	BCR	C2-C3	3.51	1.61	1.52
24	B	616	CLA	C1A-CHA	-3.51	1.28	1.43
24	b	608[A]	CLA	C1C-NC	-3.50	1.32	1.37
24	B	614	CLA	C1B-CHB	3.50	1.50	1.41
26	f	101	BCR	C40-C30	3.50	1.60	1.53
26	C	514	BCR	C2-C3	3.50	1.61	1.52
26	A	610	BCR	C27-C26	3.50	1.57	1.51
24	C	510	CLA	MG-NA	-3.49	1.98	2.06
24	D	402	CLA	MG-NA	-3.49	1.98	2.06
24	d	403	CLA	C1B-CHB	3.49	1.50	1.41
24	B	611	CLA	O2A-CGA	3.49	1.43	1.33
24	a	606	CLA	O2A-CGA	3.49	1.43	1.33
24	C	509	CLA	C3D-C4D	-3.49	1.36	1.44
24	c	501	CLA	O2D-CGD	3.49	1.41	1.33
24	B	609	CLA	C1B-CHB	3.49	1.50	1.41
26	h	101	BCR	C40-C30	3.49	1.60	1.53
24	B	617	CLA	CAA-C2A	-3.49	1.47	1.54
24	B	603	CLA	O2A-CGA	3.48	1.43	1.33
24	b	617	CLA	C3D-C2D	-3.48	1.29	1.39
24	B	607[B]	CLA	C3D-C2D	-3.48	1.29	1.39
24	B	617	CLA	CMA-C3A	-3.48	1.45	1.53
24	b	605	CLA	CBD-CGD	-3.48	1.41	1.52
24	A	609	CLA	O2A-CGA	3.48	1.43	1.33
24	b	606	CLA	C1A-CHA	-3.48	1.28	1.43
24	b	617	CLA	O2A-CGA	3.48	1.43	1.33
24	d	402	CLA	CAA-C2A	-3.47	1.47	1.54
26	b	620	BCR	C27-C26	3.47	1.57	1.51
24	B	616	CLA	CBD-CGD	-3.47	1.41	1.52
24	C	512	CLA	CAA-C2A	-3.47	1.47	1.54
24	B	616	CLA	O2A-CGA	3.47	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	101	BCR	C12-C13	3.46	1.53	1.45
24	b	609	CLA	CBD-CGD	-3.46	1.41	1.52
24	c	508	CLA	C1A-CHA	-3.46	1.28	1.43
24	b	616	CLA	C1D-ND	-3.46	1.33	1.37
24	a	609	CLA	C1B-CHB	3.46	1.50	1.41
24	C	513	CLA	O2D-CGD	3.45	1.41	1.33
24	C	502	CLA	C1A-CHA	-3.45	1.28	1.43
24	C	508	CLA	CAA-C2A	-3.45	1.47	1.54
24	c	512	CLA	C3D-C4D	-3.45	1.36	1.44
32	c	518	DGD	C3D-C2D	-3.45	1.43	1.52
24	D	404	CLA	C3D-C2D	-3.45	1.29	1.39
24	C	512	CLA	O2A-CGA	3.44	1.43	1.33
24	b	617	CLA	C3D-C4D	-3.44	1.36	1.44
29	B	621	LMG	O6-C1	3.44	1.50	1.41
24	c	509	CLA	CAA-C2A	-3.44	1.47	1.54
32	c	516	DGD	O6E-C5E	3.44	1.52	1.44
24	B	611	CLA	CBD-CGD	-3.44	1.41	1.52
33	v	201	HEM	FE-ND	3.44	2.13	1.96
24	B	607[A]	CLA	C3D-C2D	-3.44	1.29	1.39
32	c	516	DGD	C3D-C2D	-3.44	1.43	1.52
24	c	509	CLA	C1A-CHA	-3.43	1.28	1.43
26	I	101	BCR	C2-C3	3.43	1.61	1.52
24	B	609	CLA	C1A-CHA	-3.43	1.28	1.43
24	b	607	CLA	C1A-CHA	-3.43	1.28	1.43
24	B	617	CLA	CBD-CGD	-3.43	1.41	1.52
24	A	609	CLA	C1D-ND	-3.43	1.33	1.37
24	b	616	CLA	C3D-C2D	-3.43	1.29	1.39
24	b	606	CLA	O2D-CGD	3.42	1.41	1.33
24	B	607[A]	CLA	CAA-C2A	-3.42	1.47	1.54
32	C	515	DGD	C3D-C2D	-3.42	1.43	1.52
24	B	615	CLA	C1A-CHA	-3.42	1.28	1.43
26	f	101	BCR	C4-C5	3.41	1.57	1.51
26	t	101	BCR	C40-C30	3.41	1.60	1.53
24	B	616	CLA	C3D-C4D	-3.41	1.36	1.44
27	A	611	PL9	C21-C19	3.41	1.58	1.51
24	B	612	CLA	CBD-CGD	-3.41	1.41	1.52
24	c	507	CLA	C1A-CHA	-3.41	1.29	1.43
24	c	506	CLA	CAA-C2A	-3.41	1.47	1.54
24	b	611	CLA	O2A-CGA	3.41	1.43	1.33
24	C	505	CLA	C3D-C4D	-3.41	1.36	1.44
26	k	101	BCR	C4-C5	3.41	1.57	1.51
24	d	402	CLA	CBD-CGD	-3.40	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	502	CLA	C3D-C2D	-3.40	1.29	1.39
24	a	606	CLA	CBD-CGD	-3.40	1.41	1.52
24	c	511	CLA	C1B-CHB	3.40	1.50	1.41
32	H	102	DGD	C3D-C2D	-3.40	1.43	1.52
24	b	618	CLA	O2D-CGD	3.40	1.41	1.33
24	b	615	CLA	C1A-CHA	-3.40	1.29	1.43
24	B	602	CLA	C3D-C2D	-3.39	1.29	1.39
24	C	504	CLA	CAA-C2A	-3.39	1.47	1.54
24	b	616	CLA	CAA-C2A	-3.39	1.47	1.54
24	d	402	CLA	O2A-CGA	3.39	1.43	1.33
24	b	614	CLA	O2A-CGA	3.39	1.43	1.33
24	B	617	CLA	C1A-CHA	-3.39	1.29	1.43
24	B	610	CLA	C3D-C2D	-3.39	1.29	1.39
24	c	510	CLA	C1B-CHB	3.39	1.50	1.41
24	B	605	CLA	O2A-CGA	3.39	1.43	1.33
24	B	612	CLA	C3D-C2D	-3.39	1.29	1.39
24	B	603	CLA	C3D-C2D	-3.39	1.29	1.39
24	c	508	CLA	C1D-ND	-3.38	1.33	1.37
24	C	503	CLA	O2A-CGA	3.38	1.43	1.33
24	B	604	CLA	CMA-C3A	-3.38	1.45	1.53
24	b	616	CLA	CBD-CGD	-3.38	1.41	1.52
26	K	101	BCR	C2-C3	3.38	1.60	1.52
33	E	103	HEM	CAA-C2A	3.38	1.57	1.52
24	c	503	CLA	C1A-CHA	-3.38	1.29	1.43
32	C	517	DGD	O6D-C5D	3.38	1.52	1.44
29	A	613	LMG	O6-C1	3.37	1.50	1.41
24	B	609	CLA	CAA-C2A	-3.37	1.47	1.54
24	c	510	CLA	C3D-C4D	-3.37	1.36	1.44
24	c	509	CLA	O2D-CGD	3.37	1.41	1.33
24	C	503	CLA	C1A-CHA	-3.37	1.29	1.43
26	H	101	BCR	C27-C26	3.37	1.57	1.51
24	A	606	CLA	C3D-C2D	-3.37	1.29	1.39
24	D	403	CLA	O2A-CGA	3.37	1.43	1.33
24	c	511	CLA	C1A-CHA	-3.37	1.29	1.43
24	C	507	CLA	C3D-C2D	-3.37	1.29	1.39
24	C	512	CLA	C3D-C4D	-3.36	1.36	1.44
24	c	512	CLA	C1B-CHB	3.36	1.50	1.41
24	c	513	CLA	C3D-C4D	-3.36	1.36	1.44
24	c	502	CLA	C1A-CHA	-3.36	1.29	1.43
24	c	501	CLA	C1A-CHA	-3.36	1.29	1.43
24	B	615	CLA	CBD-CGD	-3.35	1.41	1.52
24	c	505	CLA	C1A-CHA	-3.35	1.29	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	CBD-CGD	-3.35	1.41	1.52
24	B	615	CLA	C1D-ND	-3.35	1.33	1.37
24	B	604	CLA	CBD-CGD	-3.35	1.41	1.52
24	c	505	CLA	CAA-C2A	-3.35	1.47	1.54
24	C	505	CLA	C1B-CHB	3.35	1.50	1.41
24	C	510	CLA	CBD-CGD	-3.35	1.41	1.52
24	B	608	CLA	O2A-CGA	3.34	1.43	1.33
24	c	508	CLA	O2D-CGD	3.34	1.41	1.33
26	B	620	BCR	C1-C6	-3.34	1.49	1.53
24	C	509	CLA	C1D-ND	-3.34	1.33	1.37
24	b	617	CLA	CAA-C2A	-3.34	1.47	1.54
27	d	404	PL9	C36-C34	3.34	1.58	1.51
24	C	511	CLA	C1D-ND	-3.33	1.33	1.37
24	B	605	CLA	CBD-CGD	-3.33	1.42	1.52
24	b	610	CLA	O2D-CGD	3.33	1.41	1.33
29	j	101	LMG	O8-C28	3.33	1.43	1.33
24	c	512	CLA	CBD-CGD	-3.33	1.42	1.52
26	b	621	BCR	C23-C22	3.33	1.53	1.45
24	b	604	CLA	O2A-CGA	3.33	1.43	1.33
24	b	605	CLA	C1B-CHB	3.33	1.50	1.41
24	c	513	CLA	C1A-CHA	-3.32	1.29	1.43
24	B	615	CLA	CAA-C2A	-3.32	1.47	1.54
24	c	509	CLA	C3D-C4D	-3.32	1.36	1.44
26	b	621	BCR	C4-C5	3.32	1.57	1.51
24	b	612	CLA	CAA-C2A	-3.32	1.47	1.54
24	C	508	CLA	CBD-CGD	-3.32	1.42	1.52
27	D	405	PL9	C21-C19	3.32	1.58	1.51
24	B	606	CLA	C1D-ND	-3.32	1.33	1.37
24	c	513	CLA	O2D-CGD	3.32	1.41	1.33
24	C	512	CLA	C1A-CHA	-3.32	1.29	1.43
32	d	405	DGD	O6D-C5D	3.32	1.52	1.44
24	D	402	CLA	CAA-C2A	-3.32	1.47	1.54
24	a	615	CLA	O2A-CGA	3.31	1.43	1.33
24	C	504	CLA	O2A-CGA	3.31	1.43	1.33
24	b	606	CLA	C1D-ND	-3.31	1.33	1.37
24	C	509	CLA	O2A-CGA	3.31	1.43	1.33
24	B	613	CLA	C4C-C3C	-3.31	1.39	1.45
24	b	615	CLA	CBD-CGD	-3.31	1.42	1.52
24	B	613	CLA	O2A-CGA	3.31	1.43	1.33
24	C	502	CLA	C1B-CHB	3.30	1.50	1.41
24	C	504	CLA	C3D-C4D	-3.30	1.36	1.44
24	b	603	CLA	O2D-CGD	3.30	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C1A-CHA	-3.30	1.29	1.43
24	D	403	CLA	CAA-C2A	-3.30	1.48	1.54
25	a	608	PHO	CAC-C3C	-3.30	1.46	1.52
24	B	607[A]	CLA	C1D-ND	-3.30	1.33	1.37
24	c	502	CLA	C3D-C4D	-3.29	1.36	1.44
24	c	504	CLA	CAA-C2A	-3.29	1.48	1.54
24	C	508	CLA	O2D-CGD	3.29	1.41	1.33
29	b	622	LMG	O7-C8	-3.29	1.38	1.46
24	c	513	CLA	O2A-CGA	3.29	1.42	1.33
24	c	506	CLA	C3D-C4D	-3.28	1.36	1.44
24	c	506	CLA	C3D-C2D	-3.28	1.30	1.39
24	c	509	CLA	CBD-CGD	-3.28	1.42	1.52
24	b	611	CLA	C1A-CHA	-3.28	1.29	1.43
24	B	609	CLA	O2D-CGD	3.28	1.41	1.33
24	b	605	CLA	C1A-CHA	-3.28	1.29	1.43
24	c	505	CLA	O2D-CGD	3.28	1.41	1.33
24	d	402	CLA	C3B-CAB	3.28	1.54	1.47
24	B	612	CLA	CAA-C2A	-3.28	1.48	1.54
26	K	101	BCR	C4-C5	3.28	1.57	1.51
24	B	613	CLA	C3D-C2D	-3.28	1.30	1.39
24	b	607	CLA	CBD-CGD	-3.28	1.42	1.52
26	b	621	BCR	C12-C13	3.27	1.53	1.45
24	b	613	CLA	C1B-CHB	3.27	1.50	1.41
24	b	614	CLA	MG-NA	-3.27	1.98	2.06
24	B	610	CLA	C1B-CHB	3.27	1.50	1.41
24	b	615	CLA	C3D-C2D	-3.27	1.30	1.39
32	h	102	DGD	C3D-C2D	-3.27	1.44	1.52
32	E	101	DGD	O6D-C5D	3.27	1.52	1.44
24	d	403	CLA	C3D-C4D	-3.26	1.36	1.44
24	a	606	CLA	C1D-ND	-3.26	1.33	1.37
26	A	610	BCR	C40-C30	3.26	1.60	1.53
24	c	508	CLA	C3D-C2D	-3.26	1.30	1.39
24	B	617	CLA	C3D-C4D	-3.26	1.36	1.44
24	b	612	CLA	C1B-CHB	3.26	1.50	1.41
24	B	607[A]	CLA	O2D-CGD	3.25	1.41	1.33
24	C	501	CLA	CAA-C2A	-3.25	1.48	1.54
24	c	502	CLA	CBD-CGD	-3.25	1.42	1.52
24	C	509	CLA	C1A-CHA	-3.25	1.29	1.43
24	B	603	CLA	C1D-ND	-3.25	1.33	1.37
26	H	101	BCR	C12-C13	3.25	1.52	1.45
24	C	512	CLA	CBD-CGD	-3.25	1.42	1.52
26	b	620	BCR	C17-C18	3.24	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C4C-C3C	-3.24	1.39	1.45
24	b	616	CLA	MG-NA	-3.24	1.98	2.06
33	V	201	HEM	CAB-C3B	3.24	1.56	1.47
24	c	503	CLA	C1B-CHB	3.24	1.50	1.41
24	b	612	CLA	CBD-CGD	-3.24	1.42	1.52
24	C	506	CLA	CAA-C2A	-3.24	1.48	1.54
24	B	615	CLA	O2A-CGA	3.24	1.42	1.33
24	C	510	CLA	O2A-CGA	3.23	1.42	1.33
24	c	510	CLA	C1D-ND	-3.23	1.33	1.37
24	B	613	CLA	CBD-CGD	-3.23	1.42	1.52
24	c	501	CLA	C1B-CHB	3.23	1.50	1.41
24	B	605	CLA	C3D-C2D	-3.23	1.30	1.39
24	C	513	CLA	C1D-ND	-3.23	1.33	1.37
24	c	512	CLA	C3D-C2D	-3.23	1.30	1.39
24	B	614	CLA	O2A-CGA	3.22	1.42	1.33
24	c	511	CLA	O2D-CGD	3.22	1.41	1.33
24	b	618	CLA	C3D-C2D	-3.22	1.30	1.39
24	C	507	CLA	C1A-CHA	-3.22	1.29	1.43
24	c	501	CLA	C3D-C2D	-3.22	1.30	1.39
26	k	101	BCR	C2-C3	3.22	1.60	1.52
24	B	607[B]	CLA	O2D-CGD	3.22	1.41	1.33
24	b	603	CLA	C1A-CHA	-3.22	1.29	1.43
24	c	502	CLA	O2D-CGD	3.22	1.41	1.33
24	b	607	CLA	C1D-ND	-3.22	1.33	1.37
24	B	610	CLA	O2D-CGD	3.21	1.41	1.33
24	C	511	CLA	MG-NA	-3.21	1.98	2.06
29	D	408	LMG	O7-C8	-3.21	1.38	1.46
24	B	605	CLA	O2D-CGD	3.21	1.41	1.33
24	c	510	CLA	O2A-CGA	3.21	1.42	1.33
32	c	518	DGD	O6D-C5D	3.21	1.52	1.44
24	b	608[B]	CLA	CAA-C2A	-3.21	1.48	1.54
24	C	501	CLA	O2D-CGD	3.20	1.41	1.33
24	a	607	CLA	C3B-CAB	3.20	1.54	1.47
26	c	515	BCR	C4-C5	3.20	1.57	1.51
27	a	611	PL9	C21-C19	3.20	1.57	1.51
26	h	101	BCR	C27-C26	3.20	1.57	1.51
24	B	612	CLA	O2D-CGD	3.19	1.41	1.33
24	B	612	CLA	O2A-CGA	3.19	1.42	1.33
24	a	609	CLA	C1A-CHA	-3.19	1.29	1.43
24	B	614	CLA	C1D-ND	-3.18	1.33	1.37
24	c	510	CLA	O2D-CGD	3.18	1.41	1.33
24	B	611	CLA	C3D-C2D	-3.18	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C1D-ND	-3.18	1.33	1.37
24	B	608	CLA	CBD-CGD	-3.18	1.42	1.52
24	C	512	CLA	C1B-CHB	3.18	1.49	1.41
24	b	605	CLA	CAA-C2A	-3.18	1.48	1.54
24	c	501	CLA	CAA-C2A	-3.17	1.48	1.54
26	c	514	BCR	C4-C5	3.17	1.57	1.51
24	b	613	CLA	C3B-CAB	3.17	1.54	1.47
26	h	101	BCR	C12-C13	3.17	1.52	1.45
24	b	605	CLA	O2D-CGD	3.17	1.40	1.33
24	B	611	CLA	C1A-CHA	-3.17	1.30	1.43
24	B	607[A]	CLA	CBD-CGD	-3.17	1.42	1.52
24	C	505	CLA	O2D-CGD	3.17	1.40	1.33
24	B	611	CLA	C4C-C3C	-3.17	1.39	1.45
24	b	615	CLA	C1B-CHB	3.16	1.49	1.41
33	E	103	HEM	CAB-C3B	3.16	1.56	1.47
24	c	507	CLA	C1B-CHB	3.16	1.49	1.41
24	c	505	CLA	O2A-CGA	3.16	1.42	1.33
24	b	604	CLA	MG-NA	-3.16	1.98	2.06
26	B	619	BCR	C12-C13	3.16	1.52	1.45
24	b	617	CLA	O2D-CGD	3.16	1.40	1.33
24	B	612	CLA	MG-NA	-3.16	1.98	2.06
24	b	610	CLA	C3D-C2D	-3.16	1.30	1.39
33	E	103	HEM	FE-ND	3.16	2.12	1.96
24	C	507	CLA	O2D-CGD	3.15	1.40	1.33
24	B	609	CLA	CBD-CGD	-3.15	1.42	1.52
24	b	603	CLA	C1D-ND	-3.15	1.33	1.37
24	c	511	CLA	CAA-C2A	-3.15	1.48	1.54
32	C	517	DGD	C3D-C2D	-3.15	1.44	1.52
24	b	611	CLA	C1B-CHB	3.15	1.49	1.41
24	B	609	CLA	C3D-C2D	-3.15	1.30	1.39
24	C	503	CLA	C1D-ND	-3.15	1.33	1.37
32	h	102	DGD	O6D-C5D	3.15	1.52	1.44
27	D	405	PL9	C36-C34	3.14	1.57	1.51
24	C	502	CLA	C3D-C4D	-3.14	1.37	1.44
24	C	513	CLA	C1B-CHB	3.14	1.49	1.41
24	C	505	CLA	O2A-CGA	3.14	1.42	1.33
24	C	505	CLA	C1D-ND	-3.14	1.33	1.37
24	b	612	CLA	O2D-CGD	3.14	1.40	1.33
26	k	101	BCR	C12-C13	3.14	1.52	1.45
24	C	513	CLA	MG-NA	-3.13	1.98	2.06
26	B	620	BCR	C4-C5	3.13	1.57	1.51
24	d	403	CLA	C3D-C2D	-3.13	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	C3D-C2D	-3.13	1.30	1.39
24	a	607	CLA	O2D-CGD	3.13	1.40	1.33
24	c	501	CLA	C3B-CAB	3.13	1.54	1.47
26	T	101	BCR	C4-C5	3.13	1.57	1.51
26	b	619	BCR	C1-C6	-3.13	1.49	1.53
24	c	510	CLA	C1A-CHA	-3.13	1.30	1.43
24	C	507	CLA	CAA-C2A	-3.13	1.48	1.54
24	B	605	CLA	CAA-C2A	-3.12	1.48	1.54
24	B	606	CLA	CAA-C2A	-3.12	1.48	1.54
24	A	606	CLA	MG-NA	-3.12	1.98	2.06
24	B	613	CLA	C2A-C1A	-3.12	1.45	1.52
24	B	607[B]	CLA	CBD-CGD	-3.12	1.42	1.52
24	C	506	CLA	O2A-CGA	3.12	1.42	1.33
24	C	505	CLA	C3D-C2D	-3.12	1.30	1.39
24	B	602	CLA	C3D-C4D	-3.12	1.37	1.44
24	B	609	CLA	O2A-CGA	3.11	1.42	1.33
24	C	501	CLA	C4C-C3C	-3.11	1.39	1.45
33	e	102	HEM	CAB-C3B	3.11	1.55	1.47
24	B	603	CLA	O2D-CGD	3.11	1.40	1.33
24	a	607	CLA	MG-NA	-3.11	1.98	2.06
26	b	620	BCR	C1-C6	-3.11	1.49	1.53
26	k	101	BCR	C27-C26	3.11	1.57	1.51
24	c	509	CLA	C3D-C2D	-3.11	1.30	1.39
24	b	612	CLA	C4C-C3C	-3.10	1.39	1.45
26	h	101	BCR	C4-C5	3.10	1.57	1.51
24	b	617	CLA	C1A-CHA	-3.10	1.30	1.43
24	b	609	CLA	O2D-CGD	3.10	1.40	1.33
24	c	513	CLA	CAA-C2A	-3.09	1.48	1.54
24	b	615	CLA	O2A-CGA	3.09	1.42	1.33
32	E	101	DGD	C3D-C2D	-3.09	1.44	1.52
24	B	608	CLA	C1B-CHB	3.09	1.49	1.41
24	C	504	CLA	C3B-CAB	3.09	1.54	1.47
24	A	606	CLA	O2D-CGD	3.09	1.40	1.33
24	c	509	CLA	C1B-CHB	3.08	1.49	1.41
24	C	513	CLA	C3D-C2D	-3.08	1.30	1.39
24	B	606	CLA	C1B-CHB	3.08	1.49	1.41
24	a	606	CLA	C1B-CHB	3.08	1.49	1.41
29	a	613	LMG	O6-C1	3.08	1.49	1.41
24	B	610	CLA	MG-NA	-3.08	1.99	2.06
24	C	502	CLA	C3D-C2D	-3.08	1.30	1.39
24	b	614	CLA	C1B-CHB	3.08	1.49	1.41
24	B	615	CLA	O2D-CGD	3.07	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	CBD-CGD	-3.07	1.42	1.52
24	A	609	CLA	C1B-CHB	3.07	1.49	1.41
24	B	617	CLA	O2D-CGD	3.06	1.40	1.33
24	B	607[B]	CLA	C1D-ND	-3.06	1.34	1.37
24	B	611	CLA	C1D-ND	-3.06	1.34	1.37
32	E	101	DGD	O5D-C1E	3.06	1.45	1.40
24	b	608[A]	CLA	CAA-C2A	-3.06	1.48	1.54
24	A	606	CLA	C1B-CHB	3.05	1.49	1.41
24	b	612	CLA	C3D-C2D	-3.05	1.30	1.39
24	c	502	CLA	C1D-ND	-3.05	1.34	1.37
24	a	609	CLA	C1D-ND	-3.05	1.34	1.37
24	b	614	CLA	C2A-C1A	-3.05	1.45	1.52
24	C	508	CLA	MG-NA	-3.04	1.99	2.06
24	D	403	CLA	C3B-CAB	3.04	1.54	1.47
32	H	102	DGD	C6E-C5E	-3.04	1.41	1.51
26	C	514	BCR	C27-C26	3.04	1.57	1.51
24	b	605	CLA	C3B-CAB	3.03	1.54	1.47
32	E	101	DGD	O6E-C1E	3.03	1.49	1.41
24	B	606	CLA	C1A-CHA	-3.03	1.30	1.43
24	c	513	CLA	C3D-CAD	3.03	1.55	1.45
24	c	504	CLA	C3B-CAB	3.03	1.54	1.47
24	C	501	CLA	CBD-CGD	-3.03	1.42	1.52
24	C	510	CLA	C2A-C1A	-3.03	1.45	1.52
32	c	517	DGD	C3D-C2D	-3.02	1.44	1.52
24	B	604	CLA	O2D-CGD	3.02	1.40	1.33
24	b	612	CLA	C1D-ND	-3.02	1.34	1.37
24	c	512	CLA	C3B-CAB	3.02	1.54	1.47
26	a	610	BCR	C35-C13	-3.02	1.44	1.50
24	c	510	CLA	CBD-CGD	-3.02	1.43	1.52
24	B	602	CLA	C1A-CHA	-3.02	1.30	1.43
24	B	607[B]	CLA	C1B-CHB	3.02	1.49	1.41
24	b	608[B]	CLA	C1B-CHB	3.01	1.49	1.41
24	B	616	CLA	C3D-C2D	-3.01	1.30	1.39
24	c	504	CLA	MG-NA	-3.01	1.99	2.06
24	a	609	CLA	O2D-CGD	3.01	1.40	1.33
26	c	521	BCR	C4-C5	3.01	1.56	1.51
24	b	616	CLA	C1B-CHB	3.00	1.49	1.41
24	b	610	CLA	C1B-CHB	3.00	1.49	1.41
24	c	504	CLA	C1D-ND	-3.00	1.34	1.37
24	C	504	CLA	C3D-C2D	-3.00	1.30	1.39
24	b	609	CLA	MG-NA	-3.00	1.99	2.06
24	b	608[A]	CLA	C1B-CHB	3.00	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	V	201	HEM	FE-ND	3.00	2.11	1.96
24	c	507	CLA	C3D-C2D	-3.00	1.30	1.39
24	c	501	CLA	C1D-ND	-2.99	1.34	1.37
24	B	616	CLA	O2D-CGD	2.99	1.40	1.33
26	b	619	BCR	C12-C13	2.99	1.52	1.45
24	C	503	CLA	C1B-CHB	2.99	1.49	1.41
24	c	503	CLA	C3B-CAB	2.99	1.54	1.47
24	C	501	CLA	C1D-ND	-2.99	1.34	1.37
24	C	501	CLA	C3D-CAD	2.99	1.55	1.45
29	Z	101	LMG	O7-C8	-2.99	1.39	1.46
24	c	504	CLA	CBD-CGD	-2.99	1.43	1.52
24	B	608	CLA	C1D-ND	-2.99	1.34	1.37
24	b	607	CLA	MG-NA	-2.98	1.99	2.06
26	t	101	BCR	C4-C5	2.98	1.56	1.51
32	H	102	DGD	O6D-C5D	2.98	1.51	1.44
24	A	607	CLA	C1B-CHB	2.98	1.49	1.41
27	d	404	PL9	C41-C39	2.98	1.57	1.51
24	A	606	CLA	C3D-CAD	2.98	1.55	1.45
26	B	618	BCR	C12-C13	2.98	1.52	1.45
24	B	617	CLA	C3D-CAD	2.98	1.55	1.45
24	C	502	CLA	C3D-CAD	2.98	1.55	1.45
24	b	607	CLA	O2D-CGD	2.98	1.40	1.33
24	b	603	CLA	CBD-CGD	-2.97	1.43	1.52
24	b	611	CLA	MG-NA	-2.97	1.99	2.06
24	c	502	CLA	C1B-CHB	2.97	1.49	1.41
24	B	604	CLA	C1B-CHB	2.97	1.49	1.41
24	C	502	CLA	CBD-CGD	-2.97	1.43	1.52
24	C	501	CLA	C1B-CHB	2.97	1.49	1.41
29	j	101	LMG	O7-C8	-2.97	1.39	1.46
24	b	608[A]	CLA	C1D-ND	-2.97	1.34	1.37
24	a	607	CLA	C1D-ND	-2.96	1.34	1.37
24	c	506	CLA	C1B-CHB	2.96	1.49	1.41
24	B	603	CLA	MG-NA	-2.96	1.99	2.06
24	C	509	CLA	O2D-CGD	2.96	1.40	1.33
33	e	102	HEM	CAA-C2A	2.96	1.56	1.52
24	D	404	CLA	C1B-CHB	2.95	1.49	1.41
24	c	508	CLA	O2A-CGA	2.95	1.42	1.33
24	B	602	CLA	C1B-CHB	2.95	1.49	1.41
24	C	501	CLA	C3D-C2D	-2.95	1.31	1.39
24	B	615	CLA	MG-NA	-2.95	1.99	2.06
24	B	607[A]	CLA	C1B-CHB	2.95	1.49	1.41
24	A	609	CLA	CAA-C2A	-2.94	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C3B-CAB	2.94	1.53	1.47
24	C	509	CLA	CAA-C2A	-2.94	1.48	1.54
32	d	405	DGD	C3D-C2D	-2.94	1.44	1.52
24	b	610	CLA	C1D-ND	-2.94	1.34	1.37
24	d	402	CLA	C2A-C1A	-2.94	1.45	1.52
26	K	101	BCR	C12-C13	2.94	1.52	1.45
24	b	610	CLA	C3D-CAD	2.94	1.55	1.45
24	b	606	CLA	C1B-CHB	2.93	1.49	1.41
24	c	513	CLA	C3D-C2D	-2.93	1.31	1.39
24	C	508	CLA	MG-NC	-2.93	1.99	2.06
24	C	508	CLA	C1B-CHB	2.93	1.49	1.41
24	b	617	CLA	C1B-CHB	2.93	1.49	1.41
24	b	614	CLA	O2D-CGD	2.93	1.40	1.33
24	B	603	CLA	CAA-C2A	-2.93	1.48	1.54
24	b	610	CLA	O2A-CGA	2.93	1.41	1.33
24	B	602	CLA	C3B-CAB	2.93	1.53	1.47
24	C	507	CLA	C1D-ND	-2.93	1.34	1.37
24	B	604	CLA	MG-NA	-2.92	1.99	2.06
24	B	604	CLA	CAA-C2A	-2.92	1.48	1.54
32	C	516	DGD	O6E-C1E	2.92	1.49	1.41
24	b	609	CLA	O2A-CGA	2.92	1.41	1.33
24	a	606	CLA	O2D-CGD	2.92	1.40	1.33
24	B	616	CLA	C1B-CHB	2.92	1.49	1.41
26	B	619	BCR	C40-C30	2.92	1.59	1.53
32	C	517	DGD	C3E-C2E	-2.92	1.44	1.52
24	b	604	CLA	C2A-C1A	-2.91	1.45	1.52
24	b	609	CLA	C2A-C1A	-2.91	1.45	1.52
24	B	613	CLA	O2D-CGD	2.91	1.40	1.33
26	H	101	BCR	C4-C5	2.91	1.56	1.51
24	C	512	CLA	C3D-C2D	-2.91	1.31	1.39
24	C	506	CLA	C1A-CHA	-2.91	1.31	1.43
24	a	607	CLA	C1B-CHB	2.91	1.49	1.41
24	C	511	CLA	CBD-CGD	-2.91	1.43	1.52
24	C	507	CLA	MG-NA	-2.91	1.99	2.06
26	K	101	BCR	C27-C26	2.91	1.56	1.51
24	C	503	CLA	C3B-CAB	2.90	1.53	1.47
24	c	508	CLA	C3D-CAD	2.90	1.55	1.45
24	c	506	CLA	C1A-CHA	-2.90	1.31	1.43
24	a	615	CLA	O2D-CGD	2.90	1.40	1.33
24	c	508	CLA	MG-NA	-2.90	1.99	2.06
26	T	101	BCR	C35-C13	-2.90	1.44	1.50
26	c	514	BCR	C27-C26	2.90	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	MG-NA	-2.90	1.99	2.06
26	C	514	BCR	C31-C1	-2.89	1.48	1.53
26	c	514	BCR	C35-C13	-2.89	1.44	1.50
24	B	605	CLA	C1B-CHB	2.89	1.49	1.41
24	c	506	CLA	O2D-CGD	2.89	1.40	1.33
24	a	609	CLA	CBD-CGD	-2.89	1.43	1.52
24	b	611	CLA	C3D-CAD	2.89	1.54	1.45
24	b	604	CLA	CBD-CGD	-2.89	1.43	1.52
24	C	503	CLA	CAA-C2A	-2.88	1.48	1.54
26	B	620	BCR	C27-C26	2.88	1.56	1.51
24	B	610	CLA	C3B-CAB	2.88	1.53	1.47
24	C	509	CLA	MG-NA	-2.88	1.99	2.06
24	b	606	CLA	CBD-CGD	-2.88	1.43	1.52
24	b	615	CLA	O2D-CGD	2.88	1.40	1.33
24	C	504	CLA	C3D-CAD	2.88	1.54	1.45
24	B	609	CLA	C4C-C3C	-2.88	1.40	1.45
24	D	404	CLA	O2D-CED	-2.87	1.38	1.45
24	C	512	CLA	O2D-CGD	2.87	1.40	1.33
24	C	512	CLA	C1D-ND	-2.87	1.34	1.37
24	C	507	CLA	C1B-CHB	2.87	1.49	1.41
32	C	516	DGD	O2D-C2D	2.87	1.49	1.43
24	C	510	CLA	O2D-CGD	2.87	1.40	1.33
24	C	506	CLA	C1B-CHB	2.86	1.49	1.41
24	c	504	CLA	O2D-CGD	2.86	1.40	1.33
27	d	404	PL9	C21-C19	2.86	1.57	1.51
26	b	621	BCR	C31-C1	-2.86	1.48	1.53
26	f	101	BCR	C12-C13	2.86	1.52	1.45
24	a	606	CLA	O2D-CED	-2.86	1.38	1.45
26	K	102	BCR	C27-C26	2.86	1.56	1.51
24	c	501	CLA	C3D-CAD	2.86	1.54	1.45
26	c	514	BCR	C31-C1	-2.85	1.48	1.53
24	c	502	CLA	CAA-C2A	-2.85	1.48	1.54
24	c	503	CLA	CAA-C2A	-2.85	1.48	1.54
24	c	512	CLA	CAA-C2A	-2.85	1.48	1.54
29	C	518	LMG	O7-C8	-2.85	1.39	1.46
24	b	615	CLA	C1D-ND	-2.85	1.34	1.37
24	D	403	CLA	C1B-CHB	2.85	1.48	1.41
24	b	614	CLA	C3B-CAB	2.85	1.53	1.47
24	a	606	CLA	MG-NA	-2.85	1.99	2.06
24	c	507	CLA	O2D-CGD	2.84	1.40	1.33
24	C	501	CLA	C3B-CAB	2.84	1.53	1.47
24	B	602	CLA	O2D-CGD	2.84	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	620	BCR	C40-C30	2.84	1.59	1.53
26	K	102	BCR	C4-C5	2.84	1.56	1.51
24	B	615	CLA	C1B-CHB	2.84	1.48	1.41
24	C	509	CLA	C1B-CHB	2.84	1.48	1.41
24	c	510	CLA	MG-NA	-2.83	1.99	2.06
24	C	512	CLA	C3B-CAB	2.83	1.53	1.47
24	c	507	CLA	C3D-CAD	2.83	1.54	1.45
24	B	611	CLA	MG-NA	-2.83	1.99	2.06
24	c	503	CLA	O2D-CED	-2.83	1.38	1.45
24	B	605	CLA	MG-NA	-2.83	1.99	2.06
24	B	608	CLA	O2D-CGD	2.83	1.40	1.33
24	A	606	CLA	MG-NC	-2.83	1.99	2.06
24	B	611	CLA	O2D-CGD	2.83	1.40	1.33
24	b	615	CLA	C3D-CAD	2.83	1.54	1.45
24	C	505	CLA	C3D-CAD	2.83	1.54	1.45
26	B	620	BCR	C31-C1	-2.83	1.48	1.53
24	c	504	CLA	C1B-CHB	2.82	1.48	1.41
24	B	608	CLA	C2A-C1A	-2.82	1.45	1.52
24	c	513	CLA	C1B-CHB	2.82	1.48	1.41
24	c	513	CLA	C3B-CAB	2.82	1.53	1.47
24	c	509	CLA	C3D-CAD	2.82	1.54	1.45
24	C	513	CLA	CAA-C2A	-2.82	1.48	1.54
26	h	101	BCR	C31-C1	-2.81	1.48	1.53
24	a	615	CLA	C1B-CHB	2.81	1.48	1.41
29	c	519	LMG	O7-C8	-2.81	1.39	1.46
24	b	618	CLA	C3D-CAD	2.81	1.54	1.45
26	f	101	BCR	C17-C18	2.81	1.39	1.35
24	C	504	CLA	O2D-CGD	2.81	1.40	1.33
24	C	513	CLA	C3D-CAD	2.81	1.54	1.45
24	D	404	CLA	C3B-CAB	2.81	1.53	1.47
32	c	516	DGD	O6D-C5D	2.80	1.51	1.44
26	c	514	BCR	C12-C13	2.80	1.52	1.45
24	B	613	CLA	C3D-CAD	2.80	1.54	1.45
24	b	616	CLA	C2A-C1A	-2.80	1.45	1.52
24	b	611	CLA	C3B-CAB	2.80	1.53	1.47
24	C	512	CLA	C3D-CAD	2.80	1.54	1.45
24	B	613	CLA	C1B-CHB	2.80	1.48	1.41
26	t	101	BCR	C12-C13	2.80	1.51	1.45
26	H	101	BCR	C1-C6	-2.79	1.49	1.53
24	c	508	CLA	C1B-CHB	2.79	1.48	1.41
28	A	612	SQD	C6-S	-2.79	1.67	1.77
24	B	610	CLA	CBD-CGD	-2.79	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C3B-CAB	2.79	1.53	1.47
32	c	516	DGD	C6E-C5E	-2.79	1.42	1.51
24	B	611	CLA	O2D-CED	-2.79	1.38	1.45
32	H	102	DGD	O5D-C1E	2.78	1.44	1.40
24	c	506	CLA	CBD-CGD	-2.78	1.43	1.52
32	c	518	DGD	O5D-C1E	2.78	1.44	1.40
24	C	510	CLA	C3B-CAB	2.78	1.53	1.47
29	A	613	LMG	O7-C8	-2.78	1.39	1.46
29	B	621	LMG	O7-C8	-2.78	1.39	1.46
32	c	516	DGD	O6E-C1E	2.77	1.48	1.41
28	a	612	SQD	C6-S	-2.77	1.67	1.77
24	B	617	CLA	C3D-C2D	-2.77	1.31	1.39
26	a	610	BCR	C4-C5	2.77	1.56	1.51
26	k	101	BCR	C31-C1	-2.77	1.48	1.53
24	c	510	CLA	C3B-CAB	2.77	1.53	1.47
27	D	405	PL9	C41-C39	2.77	1.57	1.51
24	d	403	CLA	C3D-CAD	2.77	1.54	1.45
26	F	101	BCR	C4-C5	2.77	1.56	1.51
24	b	608[A]	CLA	O2D-CGD	2.77	1.40	1.33
24	A	607	CLA	C3B-CAB	2.76	1.53	1.47
24	C	505	CLA	CBD-CGD	-2.76	1.43	1.52
24	c	502	CLA	MG-NA	-2.76	1.99	2.06
26	b	620	BCR	C4-C5	2.76	1.56	1.51
24	B	606	CLA	CBD-CGD	-2.76	1.43	1.52
24	C	504	CLA	C1B-CHB	2.76	1.48	1.41
32	d	405	DGD	O3G-C1D	2.76	1.44	1.40
24	b	606	CLA	C3B-CAB	2.76	1.53	1.47
24	B	610	CLA	C2A-C1A	-2.75	1.46	1.52
24	b	613	CLA	O2D-CGD	2.75	1.39	1.33
24	B	606	CLA	C3B-CAB	2.75	1.53	1.47
32	d	405	DGD	O6E-C1E	2.75	1.48	1.41
24	A	607	CLA	MG-NC	-2.75	1.99	2.06
24	b	613	CLA	CAA-C2A	-2.75	1.49	1.54
26	B	619	BCR	C4-C5	2.75	1.56	1.51
24	C	504	CLA	MG-NA	-2.75	1.99	2.06
24	A	607	CLA	C3D-CAD	2.75	1.54	1.45
26	A	610	BCR	C4-C5	2.75	1.56	1.51
32	h	102	DGD	C6E-C5E	-2.74	1.42	1.51
24	B	602	CLA	C3D-CAD	2.74	1.54	1.45
26	k	101	BCR	C7-C6	2.74	1.54	1.45
24	b	609	CLA	C1B-CHB	2.74	1.48	1.41
24	c	511	CLA	CBD-CGD	-2.74	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	C3D-CAD	2.74	1.54	1.45
24	B	608	CLA	MG-NA	-2.74	1.99	2.06
32	c	516	DGD	C3E-C2E	-2.74	1.45	1.52
24	C	507	CLA	C3D-CAD	2.74	1.54	1.45
24	c	511	CLA	C3B-CAB	2.74	1.53	1.47
24	B	610	CLA	C3D-CAD	2.74	1.54	1.45
24	A	606	CLA	O2D-CED	-2.73	1.38	1.45
26	C	514	BCR	C12-C13	2.73	1.51	1.45
24	b	607	CLA	C1B-CHB	2.73	1.48	1.41
24	c	512	CLA	C1D-ND	-2.73	1.34	1.37
24	A	606	CLA	C2A-C1A	-2.73	1.46	1.52
24	D	402	CLA	C3B-CAB	2.73	1.53	1.47
26	K	102	BCR	C31-C1	-2.73	1.48	1.53
24	C	502	CLA	CAA-C2A	-2.73	1.49	1.54
24	c	505	CLA	CBD-CGD	-2.73	1.43	1.52
24	C	502	CLA	O2D-CGD	2.73	1.39	1.33
24	D	404	CLA	O2D-CGD	2.73	1.39	1.33
24	c	506	CLA	C1D-ND	-2.73	1.34	1.37
26	I	101	BCR	C27-C26	2.73	1.56	1.51
24	D	402	CLA	O2D-CED	-2.73	1.38	1.45
32	H	102	DGD	O6E-C1E	2.73	1.48	1.41
26	B	619	BCR	C35-C13	-2.72	1.45	1.50
32	C	516	DGD	O5D-C1E	2.72	1.44	1.40
24	B	616	CLA	C3D-CAD	2.71	1.54	1.45
24	c	502	CLA	C3D-CAD	2.71	1.54	1.45
24	C	511	CLA	CAA-C2A	-2.71	1.49	1.54
24	B	603	CLA	C3D-CAD	2.71	1.54	1.45
26	b	619	BCR	C27-C26	2.71	1.56	1.51
24	D	403	CLA	MG-NA	-2.71	1.99	2.06
24	B	603	CLA	C1B-CHB	2.71	1.48	1.41
24	B	612	CLA	C3D-CAD	2.70	1.54	1.45
24	B	609	CLA	C1D-ND	-2.70	1.34	1.37
32	C	515	DGD	C1D-C2D	-2.70	1.44	1.52
24	b	608[B]	CLA	O2D-CGD	2.70	1.39	1.33
24	B	617	CLA	C1D-ND	-2.70	1.34	1.37
24	c	505	CLA	C3B-CAB	2.70	1.53	1.47
24	B	605	CLA	C1D-ND	-2.70	1.34	1.37
24	B	611	CLA	C3D-CAD	2.69	1.54	1.45
24	C	501	CLA	C2A-C1A	-2.69	1.46	1.52
24	C	504	CLA	C2A-C1A	-2.69	1.46	1.52
26	B	620	BCR	C12-C13	2.69	1.51	1.45
24	b	608[B]	CLA	C1D-ND	-2.69	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C3B-CAB	2.69	1.53	1.47
24	c	508	CLA	C3B-CAB	2.69	1.53	1.47
24	d	403	CLA	O2D-CED	-2.69	1.39	1.45
24	B	616	CLA	CAA-C2A	-2.69	1.49	1.54
24	c	509	CLA	MG-NA	-2.69	1.99	2.06
32	c	517	DGD	O6D-C5D	2.69	1.50	1.44
28	A	614	SQD	C6-S	-2.68	1.67	1.77
28	a	614	SQD	C6-S	-2.68	1.67	1.77
24	D	403	CLA	O2D-CED	-2.68	1.39	1.45
26	t	101	BCR	C27-C26	2.68	1.56	1.51
26	c	521	BCR	C7-C6	2.68	1.54	1.45
24	c	507	CLA	CAA-C2A	-2.67	1.49	1.54
24	d	403	CLA	C3B-CAB	2.67	1.53	1.47
24	B	603	CLA	CBD-CGD	-2.67	1.44	1.52
32	h	102	DGD	C3E-C2E	-2.67	1.45	1.52
24	b	612	CLA	C3D-CAD	2.67	1.54	1.45
24	b	614	CLA	CBD-CGD	-2.67	1.44	1.52
24	C	505	CLA	MG-NA	-2.67	1.99	2.06
26	K	101	BCR	C31-C1	-2.67	1.48	1.53
26	b	619	BCR	C4-C5	2.66	1.56	1.51
32	C	516	DGD	C3D-C2D	-2.66	1.45	1.52
24	C	509	CLA	C3D-CAD	2.66	1.54	1.45
32	c	517	DGD	C6E-C5E	-2.66	1.42	1.51
24	b	617	CLA	CBD-CGD	-2.66	1.44	1.52
24	b	603	CLA	C3B-CAB	2.65	1.53	1.47
24	c	506	CLA	C3B-CAB	2.65	1.53	1.47
32	C	515	DGD	C6E-C5E	-2.65	1.43	1.51
24	B	612	CLA	C2A-C1A	-2.65	1.46	1.52
24	a	607	CLA	CAA-C2A	-2.65	1.49	1.54
24	D	402	CLA	C1B-CHB	2.65	1.48	1.41
32	C	517	DGD	O2D-C2D	2.65	1.49	1.43
29	z	101	LMG	O7-C8	-2.65	1.40	1.46
24	A	607	CLA	O2D-CGD	2.65	1.39	1.33
24	C	503	CLA	O2D-CED	-2.65	1.39	1.45
26	b	620	BCR	C31-C1	-2.64	1.48	1.53
24	A	609	CLA	O2D-CGD	2.64	1.39	1.33
32	c	518	DGD	C6E-C5E	-2.64	1.43	1.51
24	d	403	CLA	O2D-CGD	2.64	1.39	1.33
26	b	621	BCR	C27-C26	2.64	1.56	1.51
24	B	614	CLA	O2D-CED	-2.64	1.39	1.45
24	B	607[A]	CLA	C3D-CAD	2.64	1.54	1.45
24	a	615	CLA	C2A-C1A	-2.63	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	C3D-CAD	2.63	1.54	1.45
32	c	518	DGD	O2D-C2D	2.63	1.49	1.43
24	B	614	CLA	MG-NC	-2.63	2.00	2.06
24	c	512	CLA	O2D-CGD	2.63	1.39	1.33
24	B	607[A]	CLA	MG-NA	-2.63	2.00	2.06
28	X	101	SQD	C6-S	-2.63	1.67	1.77
24	a	609	CLA	CAA-C2A	-2.63	1.49	1.54
24	C	503	CLA	MG-NA	-2.63	2.00	2.06
24	a	609	CLA	O2D-CED	-2.63	1.39	1.45
24	b	610	CLA	C2A-C1A	-2.63	1.46	1.52
24	a	615	CLA	MG-NC	-2.63	2.00	2.06
24	a	609	CLA	C3B-CAB	2.62	1.53	1.47
24	B	612	CLA	C1B-CHB	2.62	1.48	1.41
28	x	101	SQD	C6-S	-2.62	1.67	1.77
24	B	607[B]	CLA	C2A-C1A	-2.62	1.46	1.52
32	C	517	DGD	C6E-C5E	-2.62	1.43	1.51
24	C	508	CLA	C2A-C1A	-2.62	1.46	1.52
24	b	604	CLA	C3B-CAB	2.61	1.53	1.47
24	b	615	CLA	MG-NA	-2.61	2.00	2.06
24	B	604	CLA	C3B-CAB	2.61	1.53	1.47
24	b	609	CLA	C1D-ND	-2.61	1.34	1.37
24	C	502	CLA	O2D-CED	-2.61	1.39	1.45
24	b	616	CLA	O2A-CGA	2.61	1.41	1.33
26	c	515	BCR	C27-C26	2.61	1.56	1.51
24	B	615	CLA	C3B-CAB	2.61	1.53	1.47
26	c	521	BCR	C27-C26	2.60	1.56	1.51
24	a	607	CLA	C3D-CAD	2.60	1.54	1.45
24	c	512	CLA	C3D-CAD	2.60	1.54	1.45
24	C	501	CLA	CMC-C2C	2.60	1.56	1.50
24	B	611	CLA	C3B-CAB	2.60	1.53	1.47
26	T	101	BCR	C27-C26	2.60	1.56	1.51
26	h	101	BCR	C35-C13	-2.60	1.45	1.50
32	d	405	DGD	C6E-C5E	-2.60	1.43	1.51
24	a	615	CLA	C3B-CAB	2.59	1.53	1.47
26	b	620	BCR	C12-C13	2.59	1.51	1.45
24	D	402	CLA	O2D-CGD	2.59	1.39	1.33
24	A	606	CLA	CBD-CGD	-2.59	1.44	1.52
24	B	607[B]	CLA	C3D-CAD	2.59	1.53	1.45
24	D	403	CLA	MG-NC	-2.59	2.00	2.06
24	C	506	CLA	C3D-CAD	2.59	1.53	1.45
24	b	603	CLA	CAA-C2A	-2.59	1.49	1.54
24	C	505	CLA	C2A-C1A	-2.59	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k	101	BCR	C1-C6	-2.59	1.50	1.53
24	A	609	CLA	OBD-CAD	-2.59	1.18	1.22
24	C	513	CLA	CBD-CGD	-2.59	1.44	1.52
24	B	614	CLA	MG-NA	-2.58	2.00	2.06
24	b	616	CLA	O2D-CGD	2.58	1.39	1.33
24	c	505	CLA	C2A-C1A	-2.58	1.46	1.52
24	B	603	CLA	C3B-CAB	2.57	1.53	1.47
24	C	502	CLA	C3B-CAB	2.57	1.53	1.47
24	d	402	CLA	O2D-CGD	2.57	1.39	1.33
24	C	506	CLA	MG-NA	-2.57	2.00	2.06
24	D	402	CLA	OBD-CAD	-2.57	1.18	1.22
24	D	402	CLA	C2A-C1A	-2.57	1.46	1.52
24	C	508	CLA	C3B-CAB	2.57	1.53	1.47
24	B	607[A]	CLA	C2A-C1A	-2.57	1.46	1.52
24	b	608[B]	CLA	O2D-CED	-2.56	1.39	1.45
24	d	402	CLA	C3D-CAD	2.56	1.53	1.45
24	b	618	CLA	MG-NA	-2.56	2.00	2.06
27	D	405	PL9	C26-C24	2.56	1.56	1.51
32	c	516	DGD	O2D-C2D	2.56	1.49	1.43
24	b	607	CLA	C2A-C1A	-2.56	1.46	1.52
24	b	606	CLA	MG-NA	-2.55	2.00	2.06
24	B	614	CLA	OBD-CAD	-2.55	1.18	1.22
24	B	611	CLA	C1B-CHB	2.55	1.48	1.41
24	c	510	CLA	C3D-CAD	2.55	1.53	1.45
32	h	102	DGD	C1D-C2D	-2.55	1.45	1.52
28	b	601	SQD	C6-S	-2.55	1.68	1.77
24	D	404	CLA	C3D-CAD	2.55	1.53	1.45
24	B	611	CLA	CAA-C2A	-2.55	1.49	1.54
24	A	609	CLA	MG-NA	-2.55	2.00	2.06
24	C	503	CLA	CMC-C2C	2.55	1.56	1.50
24	b	609	CLA	C3B-CAB	2.54	1.53	1.47
24	b	615	CLA	C3B-CAB	2.54	1.53	1.47
24	C	506	CLA	C3B-CAB	2.54	1.53	1.47
24	B	606	CLA	MG-NA	-2.54	2.00	2.06
32	C	516	DGD	C6D-C5D	-2.54	1.43	1.51
24	c	513	CLA	MG-NA	-2.54	2.00	2.06
24	d	403	CLA	CAA-C2A	-2.53	1.49	1.54
24	C	509	CLA	C3B-CAB	2.53	1.53	1.47
32	C	515	DGD	C3E-C2E	-2.53	1.45	1.52
24	B	612	CLA	C3B-CAB	2.53	1.53	1.47
24	c	501	CLA	CBD-CGD	-2.53	1.44	1.52
26	f	101	BCR	C35-C13	-2.53	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	519	LMG	O7-C8	-2.53	1.40	1.46
24	c	503	CLA	O2D-CGD	2.53	1.39	1.33
32	E	101	DGD	O3G-C1D	2.52	1.44	1.40
24	b	606	CLA	CAA-C2A	-2.52	1.49	1.54
26	B	618	BCR	C27-C26	2.52	1.56	1.51
32	h	102	DGD	O6E-C1E	2.52	1.48	1.41
26	t	101	BCR	C35-C13	-2.52	1.45	1.50
24	c	507	CLA	C1D-ND	-2.52	1.34	1.37
32	d	405	DGD	O6D-C1D	2.52	1.48	1.41
24	b	613	CLA	MG-NC	-2.52	2.00	2.06
24	A	609	CLA	O2D-CED	-2.52	1.39	1.45
24	c	507	CLA	MG-NA	-2.52	2.00	2.06
24	b	603	CLA	C3D-CAD	2.52	1.53	1.45
24	c	511	CLA	C3D-CAD	2.52	1.53	1.45
24	B	605	CLA	C3B-CAB	2.51	1.53	1.47
26	H	101	BCR	C31-C1	-2.51	1.48	1.53
32	d	405	DGD	O5D-C1E	2.51	1.44	1.40
24	C	504	CLA	C1D-ND	-2.51	1.34	1.37
24	c	501	CLA	MG-NA	-2.51	2.00	2.06
24	c	504	CLA	CMC-C2C	2.51	1.56	1.50
28	B	622	SQD	C6-S	-2.51	1.68	1.77
24	c	504	CLA	MG-NC	-2.51	2.00	2.06
24	a	609	CLA	C3D-CAD	2.51	1.53	1.45
24	c	504	CLA	C3D-CAD	2.51	1.53	1.45
32	H	102	DGD	O2D-C2D	2.50	1.48	1.43
24	A	607	CLA	O2D-CED	-2.50	1.39	1.45
24	c	506	CLA	O2D-CED	-2.50	1.39	1.45
24	D	404	CLA	CAA-C2A	-2.50	1.49	1.54
24	c	511	CLA	O2D-CED	-2.50	1.39	1.45
24	c	511	CLA	MG-NA	-2.50	2.00	2.06
26	a	610	BCR	C12-C13	2.50	1.51	1.45
24	C	503	CLA	OBD-CAD	-2.50	1.18	1.22
26	b	621	BCR	C35-C13	-2.50	1.45	1.50
24	C	507	CLA	CBD-CGD	-2.50	1.44	1.52
24	d	402	CLA	O2D-CED	-2.49	1.39	1.45
24	b	612	CLA	MG-NA	-2.49	2.00	2.06
26	C	514	BCR	C33-C5	2.49	1.55	1.50
24	B	616	CLA	C1D-ND	-2.49	1.34	1.37
24	c	508	CLA	C2A-C1A	-2.49	1.46	1.52
24	b	608[A]	CLA	O2D-CED	-2.49	1.39	1.45
24	C	508	CLA	C3D-CAD	2.49	1.53	1.45
24	b	618	CLA	CBD-CGD	-2.49	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C3D-CAD	2.48	1.53	1.45
32	d	405	DGD	O2D-C2D	2.48	1.48	1.43
24	C	510	CLA	C1B-CHB	2.48	1.47	1.41
24	B	603	CLA	C2A-C1A	-2.48	1.46	1.52
24	b	610	CLA	CBD-CGD	-2.48	1.44	1.52
32	c	517	DGD	O6E-C1E	2.48	1.48	1.41
24	b	610	CLA	MG-NA	-2.48	2.00	2.06
24	B	608	CLA	O2D-CED	-2.48	1.39	1.45
24	c	503	CLA	CMC-C2C	2.47	1.56	1.50
24	B	607[B]	CLA	MG-NA	-2.47	2.00	2.06
24	D	403	CLA	O2D-CGD	2.47	1.39	1.33
26	B	618	BCR	C31-C1	-2.47	1.48	1.53
32	c	516	DGD	O5D-C1E	2.47	1.44	1.40
24	b	611	CLA	C2A-C1A	-2.47	1.46	1.52
24	c	512	CLA	O2D-CED	-2.47	1.39	1.45
24	b	604	CLA	OBD-CAD	-2.47	1.18	1.22
26	K	101	BCR	C7-C6	2.47	1.53	1.45
24	B	614	CLA	C2A-C1A	-2.47	1.46	1.52
24	B	605	CLA	C3D-CAD	2.47	1.53	1.45
28	l	101	SQD	C6-S	-2.47	1.68	1.77
26	K	101	BCR	C1-C6	-2.47	1.50	1.53
24	c	507	CLA	C3B-CAB	2.46	1.53	1.47
24	B	616	CLA	O2D-CED	-2.46	1.39	1.45
24	c	502	CLA	C3B-CAB	2.46	1.53	1.47
24	B	602	CLA	C1D-ND	-2.46	1.34	1.37
24	D	403	CLA	OBD-CAD	-2.46	1.18	1.22
24	B	602	CLA	O2D-CED	-2.46	1.39	1.45
24	c	509	CLA	C3B-CAB	2.46	1.52	1.47
24	B	617	CLA	C3B-CAB	2.46	1.52	1.47
24	c	501	CLA	CMC-C2C	2.46	1.56	1.50
24	C	501	CLA	MG-NA	-2.46	2.00	2.06
24	C	511	CLA	C3B-CAB	2.46	1.52	1.47
32	C	515	DGD	O6E-C1E	2.46	1.48	1.41
32	E	101	DGD	O3D-C3D	2.45	1.48	1.43
24	A	607	CLA	C2A-C1A	-2.45	1.46	1.52
24	C	509	CLA	MG-NC	-2.45	2.00	2.06
32	C	516	DGD	O6D-C5D	2.45	1.50	1.44
26	C	514	BCR	C35-C13	-2.45	1.45	1.50
24	b	604	CLA	C1B-CHB	2.45	1.47	1.41
24	B	617	CLA	O2D-CED	-2.45	1.39	1.45
24	c	505	CLA	MG-NA	-2.45	2.00	2.06
26	a	610	BCR	C31-C1	-2.45	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	O2D-CED	-2.45	1.39	1.45
28	L	102	SQD	C6-S	-2.44	1.68	1.77
24	B	605	CLA	C2A-C1A	-2.44	1.46	1.52
26	A	610	BCR	C7-C6	2.44	1.53	1.45
32	c	518	DGD	O6E-C1E	2.44	1.48	1.41
24	c	509	CLA	C2A-C1A	-2.44	1.46	1.52
24	b	615	CLA	O2D-CED	-2.44	1.39	1.45
24	b	607	CLA	C3B-CAB	2.44	1.52	1.47
24	c	513	CLA	CBD-CGD	-2.44	1.44	1.52
26	k	101	BCR	C35-C13	-2.44	1.45	1.50
24	C	513	CLA	C2A-C1A	-2.44	1.46	1.52
24	c	511	CLA	C1D-ND	-2.44	1.34	1.37
24	D	403	CLA	C2A-C1A	-2.44	1.46	1.52
24	d	403	CLA	MG-NA	-2.43	2.00	2.06
29	a	613	LMG	O7-C8	-2.43	1.40	1.46
24	C	505	CLA	C3B-CAB	2.43	1.52	1.47
24	b	616	CLA	C3D-CAD	2.43	1.53	1.45
24	b	608[A]	CLA	C3D-CAD	2.43	1.53	1.45
26	B	619	BCR	C1-C6	-2.43	1.50	1.53
29	c	520	LMG	O7-C8	-2.42	1.40	1.46
26	I	101	BCR	C35-C13	-2.42	1.45	1.50
26	K	101	BCR	C35-C13	-2.42	1.45	1.50
26	c	521	BCR	C31-C1	-2.42	1.49	1.53
26	B	619	BCR	C30-C25	2.42	1.57	1.53
24	c	503	CLA	C3D-CAD	2.42	1.53	1.45
24	C	504	CLA	O2D-CED	-2.42	1.39	1.45
24	C	508	CLA	OBD-CAD	-2.42	1.18	1.22
24	b	614	CLA	C3D-CAD	2.42	1.53	1.45
32	C	517	DGD	O3D-C3D	2.42	1.48	1.43
26	a	610	BCR	C7-C6	2.41	1.53	1.45
24	b	609	CLA	MG-NC	-2.41	2.00	2.06
24	C	503	CLA	O2D-CGD	2.41	1.39	1.33
32	h	102	DGD	O2D-C2D	2.41	1.48	1.43
24	b	608[B]	CLA	C3D-CAD	2.41	1.53	1.45
26	K	102	BCR	C7-C6	2.41	1.53	1.45
24	b	607	CLA	C3D-CAD	2.41	1.53	1.45
24	c	504	CLA	O2D-CED	-2.41	1.39	1.45
27	d	404	PL9	C7-C3	2.41	1.53	1.51
24	d	403	CLA	MG-NC	-2.40	2.00	2.06
32	E	101	DGD	O6D-C1D	2.40	1.48	1.41
32	h	102	DGD	O5D-C1E	2.40	1.44	1.40
24	b	605	CLA	MG-NA	-2.40	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	615	CLA	O2D-CED	-2.40	1.39	1.45
26	t	101	BCR	C7-C6	2.40	1.53	1.45
24	c	507	CLA	O2D-CED	-2.40	1.39	1.45
26	B	618	BCR	C4-C5	2.39	1.55	1.51
24	a	606	CLA	C3D-CAD	2.39	1.53	1.45
24	b	605	CLA	C3D-CAD	2.39	1.53	1.45
24	b	608[A]	CLA	MG-NA	-2.39	2.00	2.06
32	c	516	DGD	C6D-C5D	-2.39	1.44	1.51
24	C	510	CLA	O2D-CED	-2.39	1.39	1.45
24	c	513	CLA	C2A-C1A	-2.39	1.46	1.52
24	b	612	CLA	OBD-CAD	-2.39	1.18	1.22
32	c	518	DGD	O3D-C3D	2.39	1.48	1.43
26	b	621	BCR	C1-C6	-2.38	1.50	1.53
32	E	101	DGD	C6E-C5E	-2.38	1.43	1.51
24	b	610	CLA	O2D-CED	-2.38	1.39	1.45
24	c	505	CLA	C3D-CAD	2.38	1.53	1.45
24	C	503	CLA	MG-NC	-2.38	2.00	2.06
29	C	518	LMG	O6-C5	2.38	1.50	1.44
26	I	101	BCR	C4-C5	2.38	1.55	1.51
24	B	609	CLA	O2D-CED	-2.37	1.39	1.45
26	H	101	BCR	C7-C6	2.37	1.53	1.45
24	B	608	CLA	CMC-C2C	2.37	1.55	1.50
24	C	512	CLA	CMC-C2C	2.37	1.55	1.50
24	A	606	CLA	C3B-CAB	2.37	1.52	1.47
32	C	515	DGD	O2D-C2D	2.37	1.48	1.43
32	C	517	DGD	C1E-C2E	-2.37	1.45	1.52
26	f	101	BCR	C7-C6	2.37	1.53	1.45
26	c	515	BCR	C7-C6	2.37	1.53	1.45
26	T	101	BCR	C12-C13	2.37	1.51	1.45
32	C	515	DGD	O6D-C1D	2.37	1.47	1.41
32	c	516	DGD	O6D-C1D	2.37	1.47	1.41
26	T	101	BCR	C7-C6	2.36	1.53	1.45
24	B	608	CLA	C3B-CAB	2.36	1.52	1.47
32	c	517	DGD	O2D-C2D	2.36	1.48	1.43
24	B	610	CLA	O2D-CED	-2.36	1.39	1.45
24	B	605	CLA	OBD-CAD	-2.36	1.18	1.22
32	H	102	DGD	O3D-C3D	2.36	1.48	1.43
24	d	402	CLA	C3A-C4A	-2.35	1.44	1.51
26	c	515	BCR	C35-C13	-2.35	1.46	1.50
24	C	502	CLA	C1D-ND	-2.35	1.34	1.37
24	D	404	CLA	MG-NA	-2.35	2.00	2.06
24	B	603	CLA	O2D-CED	-2.35	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	O2D-CED	-2.35	1.39	1.45
24	b	617	CLA	O2D-CED	-2.35	1.39	1.45
32	C	516	DGD	C6E-C5E	-2.35	1.44	1.51
29	z	101	LMG	O8-C28	2.34	1.45	1.33
24	B	617	CLA	C4D-CHA	2.34	1.46	1.38
24	c	504	CLA	C2A-C1A	-2.34	1.46	1.52
26	t	101	BCR	C31-C1	-2.34	1.49	1.53
24	C	512	CLA	MG-NC	-2.34	2.00	2.06
24	C	507	CLA	CMC-C2C	2.34	1.55	1.50
24	b	618	CLA	C2A-C1A	-2.34	1.47	1.52
24	b	613	CLA	C3D-CAD	2.34	1.53	1.45
26	c	514	BCR	C7-C6	2.34	1.53	1.45
24	b	617	CLA	C3D-CAD	2.34	1.53	1.45
24	c	511	CLA	MG-NC	-2.34	2.00	2.06
29	Z	101	LMG	O8-C28	2.33	1.44	1.33
24	B	607[B]	CLA	O2D-CED	-2.33	1.39	1.45
32	d	405	DGD	O3D-C3D	2.33	1.48	1.43
24	C	504	CLA	MG-NC	-2.33	2.00	2.06
24	B	602	CLA	CMC-C2C	2.33	1.55	1.50
26	a	610	BCR	C27-C26	2.33	1.55	1.51
24	b	608[B]	CLA	MG-NA	-2.33	2.00	2.06
24	B	607[A]	CLA	O2D-CED	-2.33	1.39	1.45
24	c	509	CLA	MG-NC	-2.33	2.00	2.06
24	a	607	CLA	CMC-C2C	2.33	1.55	1.50
24	C	511	CLA	O2D-CED	-2.33	1.39	1.45
24	B	603	CLA	MG-NC	-2.32	2.00	2.06
26	b	619	BCR	C31-C1	-2.32	1.49	1.53
24	b	616	CLA	O2D-CED	-2.32	1.39	1.45
24	c	510	CLA	O2D-CED	-2.32	1.39	1.45
24	d	402	CLA	C1B-CHB	2.32	1.47	1.41
24	b	603	CLA	MG-NC	-2.32	2.00	2.06
24	b	614	CLA	O2D-CED	-2.32	1.39	1.45
30	e	101	LHG	C8-C7	2.32	1.57	1.50
26	b	621	BCR	C7-C6	2.32	1.53	1.45
24	B	615	CLA	C3D-CAD	2.32	1.53	1.45
24	C	503	CLA	C3D-CAD	2.31	1.53	1.45
24	B	617	CLA	MG-NC	-2.31	2.00	2.06
26	b	620	BCR	C35-C13	-2.31	1.46	1.50
24	B	617	CLA	C2A-C1A	-2.31	1.47	1.52
32	E	101	DGD	O2D-C2D	2.31	1.48	1.43
24	a	607	CLA	O2D-CED	-2.31	1.39	1.45
24	c	506	CLA	C4D-CHA	2.31	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	101	BCR	C7-C6	2.31	1.53	1.45
26	B	620	BCR	C33-C5	2.31	1.54	1.50
24	B	615	CLA	CMC-C2C	2.31	1.55	1.50
24	C	505	CLA	O2D-CED	-2.31	1.39	1.45
24	B	602	CLA	CAA-C2A	-2.31	1.49	1.54
24	d	402	CLA	MG-NC	-2.30	2.00	2.06
24	b	617	CLA	C2A-C1A	-2.30	1.47	1.52
24	D	404	CLA	CMC-C2C	2.30	1.55	1.50
24	B	613	CLA	O2D-CED	-2.30	1.39	1.45
24	B	608	CLA	C3D-CAD	2.30	1.52	1.45
26	A	610	BCR	C31-C1	-2.29	1.49	1.53
24	b	615	CLA	C2A-C1A	-2.29	1.47	1.52
24	D	402	CLA	C3A-C4A	-2.29	1.44	1.51
24	b	607	CLA	O2D-CED	-2.29	1.39	1.45
26	K	101	BCR	C33-C5	2.29	1.54	1.50
24	b	605	CLA	O2D-CED	-2.29	1.39	1.45
24	b	608[B]	CLA	C2A-C1A	-2.29	1.47	1.52
27	a	611	PL9	C41-C39	2.29	1.56	1.51
24	B	606	CLA	C3D-CAD	2.29	1.52	1.45
24	b	603	CLA	O2D-CED	-2.28	1.39	1.45
24	A	609	CLA	MG-NC	-2.28	2.00	2.06
32	c	517	DGD	O5D-C1E	2.28	1.44	1.40
32	C	517	DGD	O6E-C1E	2.28	1.47	1.41
24	d	403	CLA	C2A-C1A	-2.28	1.47	1.52
24	a	615	CLA	C3D-CAD	2.28	1.52	1.45
32	C	515	DGD	O5D-C1E	2.28	1.44	1.40
32	C	515	DGD	C1E-C2E	-2.28	1.45	1.52
24	d	402	CLA	OBD-CAD	-2.28	1.18	1.22
33	E	103	HEM	CMB-C2B	2.28	1.55	1.50
24	a	609	CLA	C4D-CHA	2.28	1.46	1.38
26	c	514	BCR	C33-C5	2.28	1.54	1.50
24	b	605	CLA	MG-NC	-2.28	2.00	2.06
24	b	613	CLA	O2D-CED	-2.28	1.40	1.45
26	f	101	BCR	C1-C6	-2.27	1.50	1.53
24	D	404	CLA	C1D-ND	-2.27	1.35	1.37
24	A	609	CLA	C3D-CAD	2.27	1.52	1.45
24	c	512	CLA	CMC-C2C	2.27	1.55	1.50
24	C	511	CLA	CBA-CGA	2.27	1.57	1.50
24	B	604	CLA	C3D-CAD	2.27	1.52	1.45
32	C	516	DGD	O3D-C3D	2.26	1.48	1.43
24	B	604	CLA	O2D-CED	-2.26	1.40	1.45
24	B	606	CLA	O2D-CED	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	OBD-CAD	-2.26	1.18	1.22
24	b	611	CLA	C4D-CHA	2.26	1.46	1.38
29	C	518	LMG	C11-C10	2.26	1.57	1.50
24	c	501	CLA	C4D-CHA	2.26	1.46	1.38
24	b	610	CLA	C3B-CAB	2.26	1.52	1.47
32	c	516	DGD	O3D-C3D	2.26	1.48	1.43
26	c	515	BCR	C31-C1	-2.26	1.49	1.53
24	b	604	CLA	C3D-CAD	2.26	1.52	1.45
24	A	607	CLA	CMC-C2C	2.25	1.55	1.50
24	c	510	CLA	C2A-C1A	-2.25	1.47	1.52
24	b	612	CLA	C2A-C1A	-2.25	1.47	1.52
24	c	508	CLA	CBD-CGD	-2.25	1.45	1.52
24	c	510	CLA	CMC-C2C	2.25	1.55	1.50
24	C	510	CLA	MG-NC	-2.25	2.00	2.06
24	a	609	CLA	CBA-CGA	2.25	1.57	1.50
32	d	405	DGD	C6D-C5D	-2.25	1.44	1.51
24	c	512	CLA	C2A-C1A	-2.25	1.47	1.52
24	b	618	CLA	O2D-CED	-2.25	1.40	1.45
24	B	616	CLA	MG-NA	-2.25	2.00	2.06
24	b	603	CLA	MG-NA	-2.25	2.00	2.06
24	B	611	CLA	OBD-CAD	-2.24	1.18	1.22
32	C	516	DGD	C3E-C2E	-2.24	1.46	1.52
26	A	610	BCR	C1-C6	-2.24	1.50	1.53
24	c	503	CLA	OBD-CAD	-2.24	1.18	1.22
24	C	506	CLA	C4D-CHA	2.24	1.46	1.38
32	C	517	DGD	C1D-C2D	-2.24	1.46	1.52
24	b	606	CLA	C3D-CAD	2.24	1.52	1.45
24	D	402	CLA	C3D-CAD	2.24	1.52	1.45
24	C	512	CLA	MG-NA	-2.24	2.00	2.06
29	c	520	LMG	C7-C8	2.24	1.57	1.50
26	c	521	BCR	C35-C13	-2.24	1.46	1.50
24	C	512	CLA	C4D-CHA	2.24	1.46	1.38
24	C	506	CLA	MG-NC	-2.24	2.01	2.06
25	a	608	PHO	CMD-C2D	-2.24	1.46	1.51
33	V	201	HEM	CMD-C2D	2.24	1.55	1.50
24	c	513	CLA	C4D-CHA	2.23	1.46	1.38
24	C	510	CLA	CMC-C2C	2.23	1.55	1.50
24	a	606	CLA	C2A-C1A	-2.23	1.47	1.52
24	C	512	CLA	O2D-CED	-2.23	1.40	1.45
24	c	512	CLA	MG-NA	-2.23	2.01	2.06
24	B	602	CLA	MG-NA	-2.23	2.01	2.06
24	b	615	CLA	C4D-CHA	2.23	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	619	BCR	C7-C6	2.23	1.53	1.45
32	H	102	DGD	C3E-C2E	-2.23	1.46	1.52
24	d	403	CLA	C4D-CHA	2.23	1.46	1.38
24	c	502	CLA	C2A-C1A	-2.23	1.47	1.52
25	A	608	PHO	C3B-C2B	-2.22	1.37	1.40
33	e	102	HEM	CMB-C2B	2.22	1.55	1.50
24	c	503	CLA	C1D-ND	-2.22	1.35	1.37
24	B	609	CLA	C3B-CAB	2.22	1.52	1.47
26	b	621	BCR	C33-C5	2.22	1.54	1.50
24	c	508	CLA	O2D-CED	-2.22	1.40	1.45
30	E	102	LHG	C8-C7	2.22	1.57	1.50
24	c	509	CLA	O2D-CED	-2.22	1.40	1.45
26	I	101	BCR	C1-C6	-2.21	1.50	1.53
32	H	102	DGD	C6D-C5D	-2.21	1.44	1.51
25	D	401	PHO	CAC-C3C	-2.21	1.48	1.52
27	D	405	PL9	C22-C23	2.21	1.57	1.50
24	A	609	CLA	C2A-C1A	-2.21	1.47	1.52
29	c	519	LMG	C11-C10	2.21	1.57	1.50
24	b	605	CLA	CMC-C2C	2.21	1.55	1.50
24	B	615	CLA	O2D-CED	-2.21	1.40	1.45
26	I	101	BCR	C7-C6	2.20	1.52	1.45
26	T	101	BCR	C32-C1	2.20	1.58	1.53
24	B	604	CLA	CMC-C2C	2.20	1.55	1.50
24	c	506	CLA	MG-NA	-2.20	2.01	2.06
24	C	509	CLA	CMC-C2C	2.20	1.55	1.50
24	D	404	CLA	C4D-CHA	2.20	1.46	1.38
24	b	608[B]	CLA	CMC-C2C	2.20	1.55	1.50
24	c	513	CLA	CMC-C2C	2.19	1.55	1.50
24	C	502	CLA	C4D-CHA	2.19	1.46	1.38
24	C	508	CLA	O2D-CED	-2.19	1.40	1.45
24	c	505	CLA	O2D-CED	-2.19	1.40	1.45
32	c	518	DGD	C1D-C2D	-2.19	1.46	1.52
27	A	611	PL9	C41-C39	2.19	1.55	1.51
24	B	606	CLA	CMC-C2C	2.19	1.55	1.50
24	c	502	CLA	O2D-CED	-2.19	1.40	1.45
33	v	201	HEM	CMD-C2D	2.19	1.55	1.50
24	b	609	CLA	C3D-CAD	2.19	1.52	1.45
24	D	404	CLA	CBA-CGA	2.19	1.57	1.50
24	B	612	CLA	MG-NC	-2.18	2.01	2.06
24	B	611	CLA	C3A-C4A	-2.18	1.44	1.51
24	b	618	CLA	MG-NC	-2.18	2.01	2.06
24	B	614	CLA	C3B-CAB	2.18	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	OBD-CAD	-2.18	1.18	1.22
26	H	101	BCR	C35-C13	-2.18	1.46	1.50
24	C	507	CLA	O2D-CED	-2.18	1.40	1.45
29	C	519	LMG	C7-C8	2.18	1.57	1.50
26	a	610	BCR	C1-C6	-2.18	1.50	1.53
24	c	509	CLA	C1D-ND	-2.18	1.35	1.37
24	C	506	CLA	CBD-CGD	-2.18	1.45	1.52
27	a	611	PL9	C2-C3	2.18	1.40	1.34
24	C	511	CLA	C3D-CAD	2.17	1.52	1.45
32	E	101	DGD	C3G-C2G	2.17	1.57	1.50
24	b	615	CLA	OBD-CAD	-2.17	1.18	1.22
24	b	606	CLA	OBD-CAD	-2.17	1.18	1.22
24	B	604	CLA	C2A-C1A	-2.17	1.47	1.52
24	C	507	CLA	C4D-CHA	2.17	1.46	1.38
24	B	612	CLA	O2D-CED	-2.17	1.40	1.45
32	c	517	DGD	C1E-C2E	-2.17	1.46	1.52
24	B	606	CLA	MG-NC	-2.17	2.01	2.06
24	c	511	CLA	C4D-CHA	2.17	1.46	1.38
32	c	518	DGD	C3E-C2E	-2.17	1.46	1.52
24	b	613	CLA	OBD-CAD	-2.17	1.18	1.22
24	b	609	CLA	O2D-CED	-2.17	1.40	1.45
24	b	617	CLA	MG-NA	-2.16	2.01	2.06
26	C	514	BCR	C7-C6	2.16	1.52	1.45
24	b	608[B]	CLA	C3B-CAB	2.16	1.52	1.47
24	b	608[A]	CLA	C2A-C1A	-2.16	1.47	1.52
26	c	515	BCR	C1-C6	-2.16	1.50	1.53
24	C	509	CLA	C4D-CHA	2.16	1.46	1.38
24	c	513	CLA	O2D-CED	-2.16	1.40	1.45
24	c	503	CLA	MG-NC	-2.16	2.01	2.06
26	K	102	BCR	C1-C6	-2.16	1.50	1.53
24	C	502	CLA	MG-NA	-2.16	2.01	2.06
24	c	507	CLA	C4D-CHA	2.16	1.46	1.38
24	b	608[A]	CLA	C3B-CAB	2.16	1.52	1.47
24	B	602	CLA	C4D-CHA	2.15	1.46	1.38
24	B	604	CLA	OBD-CAD	-2.15	1.18	1.22
27	A	611	PL9	C22-C23	2.15	1.57	1.50
32	c	516	DGD	C1D-C2D	-2.15	1.46	1.52
28	B	622	SQD	O6-C1	2.15	1.43	1.40
24	B	614	CLA	C3D-CAD	2.15	1.52	1.45
24	c	512	CLA	CBA-CGA	2.15	1.57	1.50
24	b	603	CLA	C4D-CHA	2.15	1.46	1.38
24	c	504	CLA	OBD-CAD	-2.15	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	102	SQD	O6-C1	2.15	1.43	1.40
24	B	614	CLA	O2D-CGD	2.14	1.38	1.33
27	D	405	PL9	C37-C38	2.14	1.57	1.50
24	C	502	CLA	C2A-C1A	-2.14	1.47	1.52
24	C	511	CLA	C2A-C1A	-2.14	1.47	1.52
26	c	515	BCR	C33-C5	2.14	1.54	1.50
24	b	618	CLA	C4D-CHA	2.14	1.46	1.38
24	C	511	CLA	OBD-CAD	-2.14	1.18	1.22
24	c	510	CLA	C4D-CHA	2.14	1.46	1.38
24	D	402	CLA	MG-NC	-2.13	2.01	2.06
24	C	513	CLA	O2D-CED	-2.13	1.40	1.45
24	B	607[B]	CLA	C3B-CAB	2.13	1.52	1.47
24	B	604	CLA	MG-NC	-2.13	2.01	2.06
24	c	509	CLA	C4D-CHA	2.13	1.46	1.38
24	b	616	CLA	MG-NC	-2.13	2.01	2.06
32	C	516	DGD	O6D-C1D	2.13	1.47	1.41
32	H	102	DGD	O6D-C1D	2.13	1.47	1.41
26	B	618	BCR	C17-C18	2.13	1.38	1.35
24	b	617	CLA	C4D-CHA	2.13	1.46	1.38
26	B	618	BCR	C35-C13	-2.13	1.46	1.50
27	d	404	PL9	C37-C38	2.13	1.57	1.50
24	b	608[A]	CLA	OBD-CAD	-2.12	1.18	1.22
28	b	601	SQD	O6-C1	2.12	1.43	1.40
29	D	408	LMG	O6-C5	2.12	1.49	1.44
24	B	607[B]	CLA	MG-NC	-2.12	2.01	2.06
24	b	607	CLA	MG-NC	-2.12	2.01	2.06
24	b	617	CLA	MG-NC	-2.12	2.01	2.06
24	d	403	CLA	CBA-CGA	2.12	1.56	1.50
32	E	101	DGD	C6D-C5D	-2.12	1.45	1.51
24	b	612	CLA	CMC-C2C	2.12	1.55	1.50
32	c	518	DGD	O6D-C1D	2.12	1.47	1.41
24	B	609	CLA	C2A-C1A	-2.12	1.47	1.52
24	b	614	CLA	CMC-C2C	2.11	1.55	1.50
32	C	517	DGD	O6D-C1D	2.11	1.47	1.41
32	c	517	DGD	C6D-C5D	-2.11	1.45	1.51
24	c	503	CLA	MG-NA	-2.11	2.01	2.06
24	B	603	CLA	OBD-CAD	-2.11	1.18	1.22
24	c	508	CLA	MG-NC	-2.11	2.01	2.06
24	a	606	CLA	CMC-C2C	2.11	1.55	1.50
32	d	405	DGD	C3G-C2G	2.11	1.57	1.50
24	B	602	CLA	CBA-CGA	2.10	1.56	1.50
27	A	611	PL9	C2-C3	2.10	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	404	PL9	C26-C24	2.10	1.55	1.51
24	B	611	CLA	CMC-C2C	2.10	1.55	1.50
24	b	617	CLA	OBD-CAD	-2.10	1.18	1.22
32	h	102	DGD	O3D-C3D	2.10	1.47	1.43
24	c	513	CLA	C1D-ND	-2.10	1.35	1.37
24	a	609	CLA	CMC-C2C	2.10	1.55	1.50
24	c	501	CLA	C2A-C1A	-2.10	1.47	1.52
32	c	517	DGD	C3E-C2E	-2.10	1.47	1.52
32	h	102	DGD	C6D-C5D	-2.10	1.45	1.51
24	a	615	CLA	C3A-C4A	-2.09	1.45	1.51
24	b	607	CLA	OBD-CAD	-2.09	1.18	1.22
24	b	608[A]	CLA	CMC-C2C	2.09	1.55	1.50
28	l	101	SQD	O6-C1	2.09	1.43	1.40
24	C	513	CLA	OBD-CAD	-2.09	1.18	1.22
32	h	102	DGD	O6D-C1D	2.09	1.47	1.41
26	T	101	BCR	C31-C1	-2.09	1.49	1.53
24	C	501	CLA	O2D-CED	-2.09	1.40	1.45
24	b	610	CLA	CMC-C2C	2.09	1.55	1.50
24	C	512	CLA	C2A-C1A	-2.09	1.47	1.52
32	C	515	DGD	O3D-C3D	2.09	1.47	1.43
26	A	610	BCR	C35-C13	-2.08	1.46	1.50
24	a	606	CLA	C3B-CAB	2.08	1.52	1.47
24	c	502	CLA	CBA-CGA	2.08	1.56	1.50
24	B	615	CLA	OBD-CAD	-2.08	1.18	1.22
24	b	616	CLA	CBD-CHA	-2.08	1.42	1.52
32	c	517	DGD	C1D-C2D	-2.08	1.46	1.52
26	F	101	BCR	C7-C6	2.08	1.52	1.45
24	B	603	CLA	CMC-C2C	2.08	1.55	1.50
30	A	615	LHG	C8-C7	2.08	1.56	1.50
24	B	613	CLA	CMC-C2C	2.07	1.55	1.50
24	C	504	CLA	CMC-C2C	2.07	1.55	1.50
24	B	611	CLA	C4D-CHA	2.07	1.45	1.38
24	C	506	CLA	O2D-CED	-2.07	1.40	1.45
24	C	507	CLA	MG-NC	-2.07	2.01	2.06
27	a	611	PL9	C37-C38	2.07	1.57	1.50
24	c	509	CLA	CMC-C2C	2.07	1.55	1.50
24	A	606	CLA	CMC-C2C	2.06	1.55	1.50
24	D	402	CLA	CMC-C2C	2.06	1.55	1.50
27	D	405	PL9	C17-C18	2.06	1.57	1.50
24	b	605	CLA	C4D-CHA	2.06	1.45	1.38
24	B	615	CLA	MG-NC	-2.06	2.01	2.06
26	k	101	BCR	C33-C5	2.06	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	501	CLA	O2D-CED	-2.06	1.40	1.45
33	e	102	HEM	FE-NB	2.06	2.07	1.96
24	c	501	CLA	MG-NC	-2.06	2.01	2.06
32	c	517	DGD	O3G-C1D	2.06	1.43	1.40
27	d	404	PL9	C22-C23	2.05	1.57	1.50
24	b	604	CLA	C3A-C4A	-2.05	1.45	1.51
24	B	609	CLA	CMC-C2C	2.05	1.55	1.50
24	A	606	CLA	C4D-CHA	2.05	1.45	1.38
24	b	617	CLA	C1D-ND	-2.05	1.35	1.37
27	a	611	PL9	C17-C18	2.05	1.57	1.50
29	a	613	LMG	C7-C8	2.04	1.57	1.50
24	B	607[A]	CLA	C3B-CAB	2.04	1.52	1.47
27	a	611	PL9	C22-C23	2.04	1.57	1.50
24	D	404	CLA	MG-NC	-2.04	2.01	2.06
30	D	407	LHG	C8-C7	2.04	1.56	1.50
24	c	513	CLA	MG-NC	-2.04	2.01	2.06
24	b	613	CLA	C2A-C1A	-2.04	1.47	1.52
24	C	510	CLA	OBD-CAD	-2.04	1.19	1.22
24	D	402	CLA	CBD-CHA	-2.04	1.42	1.52
24	c	503	CLA	C4D-CHA	2.04	1.45	1.38
24	c	504	CLA	C4D-CHA	2.04	1.45	1.38
24	c	507	CLA	CMC-C2C	2.04	1.55	1.50
28	X	101	SQD	O6-C1	2.04	1.43	1.40
29	j	101	LMG	O8-C9	-2.03	1.40	1.45
33	V	201	HEM	CMC-C2C	2.03	1.56	1.51
24	A	609	CLA	CBD-CHA	-2.03	1.42	1.52
24	B	616	CLA	MG-NC	-2.03	2.01	2.06
25	D	401	PHO	CHA-CBD	-2.03	1.49	1.52
26	B	619	BCR	C31-C1	-2.03	1.49	1.53
26	I	101	BCR	C32-C1	2.03	1.57	1.53
24	B	612	CLA	OBD-CAD	-2.03	1.19	1.22
30	d	407	LHG	C8-C7	2.03	1.56	1.50
24	B	611	CLA	CBA-CGA	2.03	1.56	1.50
25	A	608	PHO	CMB-C2B	-2.02	1.46	1.51
26	h	101	BCR	C1-C6	-2.02	1.51	1.53
26	t	101	BCR	C39-C30	-2.02	1.49	1.53
32	C	517	DGD	O3G-C3G	-2.02	1.40	1.43
33	V	201	HEM	C1B-NB	-2.02	1.36	1.40
32	d	405	DGD	C3E-C2E	-2.02	1.47	1.52
24	B	616	CLA	C2A-C1A	-2.01	1.47	1.52
24	C	503	CLA	C4D-CHA	2.01	1.45	1.38
26	I	101	BCR	C31-C1	-2.01	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	x	101	SQD	O6-C1	2.01	1.43	1.40
24	C	508	CLA	CMC-C2C	2.01	1.55	1.50
24	C	507	CLA	C3B-CAB	2.01	1.52	1.47
27	A	611	PL9	C17-C18	2.01	1.57	1.50
32	c	518	DGD	O3G-C3G	-2.01	1.40	1.43
25	a	608	PHO	CMC-C2C	-2.01	1.46	1.51
24	b	610	CLA	C4D-CHA	2.01	1.45	1.38
24	B	603	CLA	C4D-CHA	2.01	1.45	1.38
32	c	517	DGD	O6D-C1D	2.01	1.47	1.41
24	b	606	CLA	O2D-CED	-2.00	1.40	1.45
25	D	401	PHO	O2D-CGD	2.00	1.38	1.33
24	B	616	CLA	C4D-CHA	2.00	1.45	1.38
32	C	516	DGD	C1D-C2D	-2.00	1.46	1.52

All (2340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	621	BCR	C15-C16-C17	25.00	174.68	123.47
26	k	101	BCR	C15-C16-C17	24.97	174.62	123.47
26	T	101	BCR	C15-C16-C17	24.91	174.50	123.47
26	t	101	BCR	C15-C16-C17	24.76	174.19	123.47
26	A	610	BCR	C15-C16-C17	23.82	172.26	123.47
26	B	620	BCR	C15-C16-C17	23.09	170.76	123.47
26	I	101	BCR	C15-C16-C17	23.08	170.75	123.47
26	F	101	BCR	C15-C16-C17	23.06	170.72	123.47
26	C	514	BCR	C15-C16-C17	22.99	170.57	123.47
26	B	618	BCR	C15-C16-C17	22.79	170.16	123.47
26	c	521	BCR	C15-C16-C17	22.79	170.15	123.47
26	H	101	BCR	C15-C16-C17	22.69	169.95	123.47
26	c	515	BCR	C15-C16-C17	22.57	169.72	123.47
26	K	102	BCR	C15-C16-C17	22.45	169.46	123.47
26	b	620	BCR	C15-C16-C17	22.32	169.19	123.47
26	B	619	BCR	C15-C16-C17	22.09	168.72	123.47
26	f	101	BCR	C15-C16-C17	21.73	167.99	123.47
26	h	101	BCR	C15-C16-C17	21.61	167.74	123.47
26	c	514	BCR	C15-C16-C17	21.60	167.72	123.47
26	b	619	BCR	C15-C16-C17	21.27	167.04	123.47
26	K	101	BCR	C15-C16-C17	21.21	166.92	123.47
26	a	610	BCR	C15-C16-C17	20.30	165.06	123.47
26	b	619	BCR	C21-C20-C19	18.01	179.43	123.22
26	T	101	BCR	C21-C20-C19	17.74	178.57	123.22
26	a	610	BCR	C21-C20-C19	17.43	177.61	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	514	BCR	C21-C20-C19	17.42	177.57	123.22
26	I	101	BCR	C21-C20-C19	17.33	177.31	123.22
26	c	515	BCR	C21-C20-C19	17.25	177.04	123.22
26	K	102	BCR	C21-C20-C19	17.18	176.83	123.22
26	h	101	BCR	C21-C20-C19	17.14	176.72	123.22
26	t	101	BCR	C21-C20-C19	17.11	176.60	123.22
26	A	610	BCR	C21-C20-C19	17.08	176.52	123.22
26	b	621	BCR	C21-C20-C19	16.91	175.99	123.22
26	b	620	BCR	C21-C20-C19	16.82	175.72	123.22
26	F	101	BCR	C21-C20-C19	16.80	175.63	123.22
26	B	618	BCR	C21-C20-C19	16.78	175.59	123.22
26	C	514	BCR	C21-C20-C19	16.69	175.30	123.22
26	c	521	BCR	C21-C20-C19	16.52	174.78	123.22
26	B	619	BCR	C21-C20-C19	16.31	174.13	123.22
26	k	101	BCR	C21-C20-C19	16.06	173.33	123.22
26	f	101	BCR	C21-C20-C19	15.91	172.85	123.22
26	K	101	BCR	C21-C20-C19	15.82	172.58	123.22
26	B	620	BCR	C21-C20-C19	15.49	171.57	123.22
26	F	101	BCR	C33-C5-C6	-15.38	107.26	124.53
26	B	618	BCR	C33-C5-C6	-15.09	107.59	124.53
26	T	101	BCR	C38-C26-C25	-14.94	107.75	124.53
26	B	618	BCR	C38-C26-C25	-14.58	108.15	124.53
26	b	619	BCR	C33-C5-C6	-14.40	108.36	124.53
26	f	101	BCR	C33-C5-C6	-14.22	108.56	124.53
26	H	101	BCR	C21-C20-C19	14.16	167.40	123.22
26	b	621	BCR	C38-C26-C25	-14.09	108.71	124.53
26	H	101	BCR	C33-C5-C6	-13.87	108.95	124.53
26	b	620	BCR	C33-C5-C6	-13.84	108.98	124.53
26	B	620	BCR	C38-C26-C25	-13.71	109.14	124.53
26	C	514	BCR	C38-C26-C25	-13.66	109.18	124.53
26	K	101	BCR	C38-C26-C25	-13.55	109.31	124.53
26	k	101	BCR	C33-C5-C6	-13.45	109.42	124.53
26	B	619	BCR	C33-C5-C6	-13.32	109.57	124.53
26	t	101	BCR	C38-C26-C25	-13.30	109.59	124.53
26	c	515	BCR	C38-C26-C25	-13.23	109.68	124.53
26	b	621	BCR	C15-C14-C13	-13.22	108.44	127.31
26	K	101	BCR	C33-C5-C6	-13.09	109.83	124.53
26	a	610	BCR	C33-C5-C6	-13.06	109.86	124.53
26	A	610	BCR	C33-C5-C6	-13.03	109.90	124.53
26	I	101	BCR	C38-C26-C25	-13.02	109.91	124.53
26	c	514	BCR	C38-C26-C25	-12.94	110.00	124.53
26	k	101	BCR	C38-C26-C25	-12.82	110.13	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	610	BCR	C38-C26-C25	-12.66	110.31	124.53
26	b	619	BCR	C38-C26-C25	-12.64	110.33	124.53
26	K	102	BCR	C33-C5-C6	-12.54	110.45	124.53
26	A	610	BCR	C38-C26-C25	-12.37	110.63	124.53
26	T	101	BCR	C33-C5-C6	-12.35	110.66	124.53
26	t	101	BCR	C33-C5-C6	-12.25	110.78	124.53
26	h	101	BCR	C33-C5-C6	-11.94	111.12	124.53
26	b	620	BCR	C24-C23-C22	-11.64	108.64	126.23
26	F	101	BCR	C16-C17-C18	-11.63	110.72	127.31
26	b	621	BCR	C16-C17-C18	-11.59	110.77	127.31
26	H	101	BCR	C38-C26-C25	-11.50	111.62	124.53
27	D	405	PL9	C7-C8-C9	-11.45	107.74	126.79
26	c	521	BCR	C33-C5-C6	-11.44	111.69	124.53
26	C	514	BCR	C33-C5-C6	-11.44	111.69	124.53
26	K	102	BCR	C16-C17-C18	-11.36	111.09	127.31
26	h	101	BCR	C38-C26-C25	-11.36	111.78	124.53
26	b	619	BCR	C16-C17-C18	-11.34	111.13	127.31
27	d	404	PL9	C7-C8-C9	-11.29	108.00	126.79
26	b	621	BCR	C33-C5-C6	-11.27	111.88	124.53
26	c	514	BCR	C16-C17-C18	-11.24	111.27	127.31
26	c	521	BCR	C38-C26-C25	-11.20	111.95	124.53
26	c	521	BCR	C20-C21-C22	-11.09	111.48	127.31
26	f	101	BCR	C16-C17-C18	-11.08	111.49	127.31
26	B	620	BCR	C33-C5-C6	-11.07	112.10	124.53
26	b	621	BCR	C24-C23-C22	-10.99	109.62	126.23
26	c	514	BCR	C33-C5-C6	-10.81	112.39	124.53
26	b	621	BCR	C20-C21-C22	-10.77	111.94	127.31
26	c	521	BCR	C24-C23-C22	-10.57	110.26	126.23
26	B	620	BCR	C16-C17-C18	-10.55	112.26	127.31
26	h	101	BCR	C15-C14-C13	-10.25	112.69	127.31
26	c	514	BCR	C24-C23-C22	-10.24	110.77	126.23
26	F	101	BCR	C7-C8-C9	-10.18	110.85	126.23
26	I	101	BCR	C4-C5-C6	-10.16	107.98	122.73
26	F	101	BCR	C11-C10-C9	-10.16	112.81	127.31
26	t	101	BCR	C24-C23-C22	-10.15	110.89	126.23
26	c	521	BCR	C16-C17-C18	-10.13	112.85	127.31
26	c	515	BCR	C33-C5-C6	-10.00	113.30	124.53
26	a	610	BCR	C16-C17-C18	-9.95	113.11	127.31
26	B	619	BCR	C11-C10-C9	-9.82	113.30	127.31
26	h	101	BCR	C16-C17-C18	-9.81	113.31	127.31
26	B	619	BCR	C16-C17-C18	-9.75	113.40	127.31
26	K	102	BCR	C38-C26-C25	-9.72	113.61	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	BCR	C24-C23-C22	-9.72	111.55	126.23
26	F	101	BCR	C36-C18-C17	-9.54	109.56	122.92
26	I	101	BCR	C33-C5-C6	-9.46	113.91	124.53
26	I	101	BCR	C24-C23-C22	-9.45	111.95	126.23
26	f	101	BCR	C30-C25-C26	-9.34	109.45	122.61
26	C	514	BCR	C11-C10-C9	-9.29	114.05	127.31
26	I	101	BCR	C11-C10-C9	-9.22	114.15	127.31
26	B	620	BCR	C8-C7-C6	-9.20	101.36	127.20
26	H	101	BCR	C37-C22-C21	-9.18	110.06	122.92
26	B	618	BCR	C16-C17-C18	-9.12	114.30	127.31
26	H	101	BCR	C15-C14-C13	-9.09	114.33	127.31
26	K	102	BCR	C24-C23-C22	-9.04	112.57	126.23
26	A	610	BCR	C16-C17-C18	-8.98	114.50	127.31
26	t	101	BCR	C30-C25-C26	-8.97	109.97	122.61
26	b	620	BCR	C38-C26-C25	-8.89	114.55	124.53
26	f	101	BCR	C4-C5-C6	-8.84	109.90	122.73
26	c	515	BCR	C11-C10-C9	-8.83	114.71	127.31
26	I	101	BCR	C16-C17-C18	-8.81	114.74	127.31
26	F	101	BCR	C24-C23-C22	-8.80	112.94	126.23
26	T	101	BCR	C16-C17-C18	-8.74	114.84	127.31
26	T	101	BCR	C30-C25-C26	-8.64	110.44	122.61
26	b	619	BCR	C11-C10-C9	-8.62	115.01	127.31
26	I	101	BCR	C7-C8-C9	-8.58	113.27	126.23
26	b	619	BCR	C4-C5-C6	-8.58	110.28	122.73
26	b	620	BCR	C8-C7-C6	-8.57	103.13	127.20
26	B	619	BCR	C38-C26-C25	-8.52	114.97	124.53
26	F	101	BCR	C38-C26-C25	-8.51	114.97	124.53
26	k	101	BCR	C16-C17-C18	-8.50	115.18	127.31
26	b	620	BCR	C11-C10-C9	-8.44	115.27	127.31
26	F	101	BCR	C4-C5-C6	-8.43	110.50	122.73
24	A	606	CLA	C4A-NA-C1A	-8.34	102.96	106.71
26	K	101	BCR	C30-C25-C26	-8.32	110.90	122.61
26	B	619	BCR	C7-C8-C9	-8.28	113.73	126.23
26	F	101	BCR	C30-C25-C26	-8.27	110.96	122.61
24	C	510	CLA	C4A-NA-C1A	-8.27	102.99	106.71
26	b	619	BCR	C7-C8-C9	-8.22	113.82	126.23
26	K	102	BCR	C20-C21-C22	-8.17	115.66	127.31
26	C	514	BCR	C7-C8-C9	-8.16	113.90	126.23
26	t	101	BCR	C27-C26-C25	-8.16	110.88	122.73
26	b	620	BCR	C15-C14-C13	-8.15	115.68	127.31
26	a	610	BCR	C27-C26-C25	-8.14	110.91	122.73
26	T	101	BCR	C27-C26-C25	-8.11	110.96	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C7-C8-C9	-8.06	114.06	126.23
26	T	101	BCR	C15-C14-C13	-8.05	115.83	127.31
26	H	101	BCR	C16-C17-C18	-8.05	115.83	127.31
27	A	611	PL9	C37-C38-C39	-8.03	108.31	127.66
26	C	514	BCR	C16-C17-C18	-8.01	115.88	127.31
26	c	515	BCR	C24-C23-C22	-7.98	114.18	126.23
26	c	515	BCR	C4-C5-C6	-7.96	111.17	122.73
26	c	514	BCR	C11-C10-C9	-7.95	115.97	127.31
26	a	610	BCR	C4-C5-C6	-7.95	111.19	122.73
27	A	611	PL9	C42-C43-C44	-7.91	108.62	127.66
26	H	101	BCR	C24-C23-C22	-7.84	114.38	126.23
26	C	514	BCR	C20-C21-C22	-7.81	116.17	127.31
26	f	101	BCR	C38-C26-C25	-7.79	115.78	124.53
26	C	514	BCR	C24-C23-C22	-7.76	114.50	126.23
26	B	619	BCR	C8-C7-C6	-7.76	105.41	127.20
27	a	611	PL9	C7-C8-C9	-7.73	113.93	126.79
27	a	611	PL9	C37-C38-C39	-7.70	109.11	127.66
27	A	611	PL9	C7-C8-C9	-7.70	113.98	126.79
26	K	101	BCR	C11-C10-C9	-7.70	116.33	127.31
26	B	620	BCR	C27-C26-C25	-7.69	111.56	122.73
26	I	101	BCR	C27-C26-C25	-7.66	111.61	122.73
26	C	514	BCR	C15-C14-C13	-7.63	116.41	127.31
26	c	514	BCR	C15-C14-C13	-7.62	116.44	127.31
26	B	618	BCR	C11-C10-C9	-7.58	116.49	127.31
26	f	101	BCR	C11-C10-C9	-7.57	116.51	127.31
27	d	404	PL9	C12-C13-C14	-7.57	109.44	127.66
27	a	611	PL9	C16-C14-C13	-7.55	105.84	121.12
27	D	405	PL9	C32-C33-C34	-7.54	109.51	127.66
26	t	101	BCR	C7-C6-C5	-7.54	103.20	121.46
26	T	101	BCR	C7-C8-C9	-7.53	114.86	126.23
26	H	101	BCR	C8-C7-C6	-7.50	106.14	127.20
26	b	621	BCR	C36-C18-C19	-7.49	106.28	118.08
26	f	101	BCR	C24-C23-C22	-7.48	114.93	126.23
27	D	405	PL9	C22-C23-C24	-7.47	109.67	127.66
26	B	618	BCR	C4-C5-C6	-7.45	111.92	122.73
26	A	610	BCR	C4-C5-C6	-7.41	111.97	122.73
27	A	611	PL9	C16-C14-C13	-7.37	106.19	121.12
26	b	620	BCR	C4-C5-C6	-7.37	112.03	122.73
26	I	101	BCR	C1-C6-C5	-7.35	112.26	122.61
26	b	621	BCR	C8-C7-C6	-7.30	106.71	127.20
26	k	101	BCR	C24-C23-C22	-7.30	115.21	126.23
26	a	610	BCR	C30-C25-C26	-7.29	112.35	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C4-C5-C6	-7.29	112.15	122.73
26	c	514	BCR	C30-C25-C26	-7.29	112.35	122.61
27	a	611	PL9	C27-C28-C29	-7.24	110.22	127.66
24	C	505	CLA	C3A-C2A-C1A	7.23	112.17	101.34
27	a	611	PL9	C42-C43-C44	-7.22	110.26	127.66
27	a	611	PL9	C22-C23-C24	-7.22	110.29	127.66
26	t	101	BCR	C11-C10-C9	-7.21	117.02	127.31
26	f	101	BCR	C7-C8-C9	-7.19	115.37	126.23
27	D	405	PL9	C27-C28-C29	-7.17	110.39	127.66
27	A	611	PL9	C27-C28-C29	-7.17	110.39	127.66
26	f	101	BCR	C1-C6-C5	-7.17	112.51	122.61
26	K	102	BCR	C30-C25-C26	-7.16	112.52	122.61
26	c	515	BCR	C7-C8-C9	-7.15	115.42	126.23
27	d	404	PL9	C32-C33-C34	-7.14	110.47	127.66
26	c	515	BCR	C27-C26-C25	-7.09	112.44	122.73
27	d	404	PL9	C22-C23-C24	-7.02	110.75	127.66
26	B	620	BCR	C30-C25-C26	-7.02	112.72	122.61
26	k	101	BCR	C30-C25-C26	-6.99	112.77	122.61
26	b	620	BCR	C16-C17-C18	-6.96	117.37	127.31
26	b	619	BCR	C1-C6-C5	-6.96	112.82	122.61
24	D	404	CLA	C4A-NA-C1A	-6.95	103.58	106.71
26	b	621	BCR	C11-C10-C9	-6.93	117.42	127.31
27	A	611	PL9	C41-C39-C38	-6.93	107.10	121.12
26	T	101	BCR	C7-C6-C5	-6.91	104.73	121.46
27	D	405	PL9	C16-C14-C13	-6.90	107.15	121.12
26	B	618	BCR	C1-C6-C5	-6.90	112.89	122.61
26	c	514	BCR	C20-C21-C22	-6.86	117.52	127.31
26	c	514	BCR	C27-C26-C25	-6.85	112.79	122.73
26	c	515	BCR	C1-C6-C5	-6.83	112.99	122.61
24	C	507	CLA	O2D-CGD-CBD	6.83	123.40	111.27
26	a	610	BCR	C1-C6-C5	-6.79	113.05	122.61
26	c	514	BCR	C34-C9-C10	-6.76	113.46	122.92
27	d	404	PL9	C46-C44-C43	-6.75	107.47	121.12
26	c	515	BCR	C15-C14-C13	-6.72	117.72	127.31
26	K	102	BCR	C27-C26-C25	-6.72	112.97	122.73
26	B	619	BCR	C7-C6-C5	-6.71	105.20	121.46
27	A	611	PL9	C17-C18-C19	-6.71	111.51	127.66
26	h	101	BCR	C36-C18-C17	-6.68	113.56	122.92
27	a	611	PL9	C17-C18-C19	-6.63	111.70	127.66
24	c	505	CLA	C3A-C2A-C1A	6.63	111.27	101.34
26	c	521	BCR	C30-C25-C26	-6.62	113.29	122.61
26	t	101	BCR	C15-C14-C13	-6.61	117.88	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	515	BCR	C16-C17-C18	-6.60	117.89	127.31
26	B	619	BCR	C19-C18-C17	6.59	129.06	118.94
24	C	512	CLA	C3A-C2A-C1A	6.58	111.20	101.34
24	b	604	CLA	O2D-CGD-CBD	6.58	122.97	111.27
26	B	620	BCR	C4-C5-C6	-6.57	113.19	122.73
24	b	614	CLA	O2D-CGD-CBD	6.56	122.92	111.27
24	a	606	CLA	C4A-NA-C1A	-6.53	103.77	106.71
27	a	611	PL9	C32-C33-C34	-6.53	111.94	127.66
27	d	404	PL9	C16-C14-C13	-6.52	107.93	121.12
26	f	101	BCR	C27-C26-C25	-6.50	113.30	122.73
26	f	101	BCR	C36-C18-C17	-6.49	113.83	122.92
26	A	610	BCR	C15-C14-C13	-6.45	118.11	127.31
24	C	506	CLA	C3A-C2A-C1A	6.43	110.97	101.34
26	a	610	BCR	C24-C23-C22	-6.42	116.53	126.23
26	B	618	BCR	C20-C21-C22	-6.42	118.15	127.31
24	C	505	CLA	O2D-CGD-CBD	6.41	122.66	111.27
27	d	404	PL9	C21-C19-C18	-6.41	108.14	121.12
26	K	101	BCR	C8-C7-C6	-6.41	109.21	127.20
26	K	101	BCR	C27-C26-C25	-6.40	113.44	122.73
24	c	507	CLA	C4A-NA-C1A	-6.39	103.83	106.71
24	B	603	CLA	O2D-CGD-CBD	6.39	122.62	111.27
27	A	611	PL9	C22-C23-C24	-6.38	112.31	127.66
27	A	611	PL9	C26-C24-C23	-6.37	108.22	121.12
26	b	621	BCR	C27-C26-C25	-6.36	113.50	122.73
26	b	619	BCR	C36-C18-C17	-6.36	114.01	122.92
26	k	101	BCR	C27-C26-C25	-6.36	113.50	122.73
26	h	101	BCR	C24-C23-C22	-6.36	116.63	126.23
26	c	514	BCR	C8-C7-C6	-6.35	109.38	127.20
26	f	101	BCR	C15-C14-C13	-6.34	118.27	127.31
26	F	101	BCR	C27-C26-C25	-6.30	113.59	122.73
27	d	404	PL9	C11-C9-C8	-6.29	108.39	121.12
26	k	101	BCR	C8-C7-C6	-6.29	109.55	127.20
24	c	511	CLA	C3A-C2A-C1A	6.28	110.74	101.34
26	t	101	BCR	C16-C17-C18	-6.27	118.37	127.31
26	b	620	BCR	C12-C13-C14	-6.24	109.37	118.94
26	A	610	BCR	C11-C10-C9	-6.23	118.41	127.31
27	a	611	PL9	C40-C39-C38	-6.22	107.73	123.68
27	d	404	PL9	C17-C18-C19	-6.21	112.70	127.66
26	B	619	BCR	C15-C14-C13	-6.20	118.46	127.31
26	F	101	BCR	C23-C22-C21	6.20	128.45	118.94
27	a	611	PL9	C12-C13-C14	-6.19	112.76	127.66
26	H	101	BCR	C1-C6-C5	-6.17	113.92	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	C3A-C2A-C1A	6.17	110.58	101.34
27	A	611	PL9	C12-C13-C14	-6.16	112.83	127.66
26	I	101	BCR	C37-C22-C21	-6.14	114.32	122.92
27	d	404	PL9	C27-C28-C29	-6.14	112.87	127.66
27	A	611	PL9	C40-C39-C38	-6.13	107.95	123.68
27	A	611	PL9	C32-C33-C34	-6.13	112.90	127.66
26	C	514	BCR	C23-C24-C25	-6.12	110.00	127.20
26	B	620	BCR	C24-C23-C22	-6.12	116.98	126.23
26	C	514	BCR	C8-C7-C6	-6.09	110.08	127.20
26	A	610	BCR	C1-C6-C5	-6.08	114.04	122.61
27	a	611	PL9	C45-C44-C43	-6.07	108.11	123.68
26	B	620	BCR	C15-C14-C13	-6.05	118.67	127.31
24	b	617	CLA	C3A-C2A-C1A	6.05	110.41	101.34
26	B	619	BCR	C24-C23-C22	-6.05	117.09	126.23
24	c	506	CLA	C3A-C2A-C1A	6.05	110.40	101.34
26	B	620	BCR	C36-C18-C17	-6.04	114.46	122.92
24	c	507	CLA	O2D-CGD-CBD	6.04	122.00	111.27
24	B	609	CLA	C3A-C2A-C1A	6.03	110.38	101.34
26	h	101	BCR	C1-C6-C5	-6.02	114.14	122.61
27	d	404	PL9	C37-C38-C39	-6.01	113.19	127.66
24	b	610	CLA	C3A-C2A-C1A	6.00	110.33	101.34
26	b	620	BCR	C1-C6-C5	-6.00	114.16	122.61
26	C	514	BCR	C30-C25-C26	-5.99	114.17	122.61
24	c	501	CLA	C3A-C2A-C1A	5.99	110.31	101.34
27	A	611	PL9	C10-C9-C8	-5.98	108.33	123.68
24	c	508	CLA	C3A-C2A-C1A	5.98	110.30	101.34
27	d	404	PL9	C42-C43-C44	-5.98	113.26	127.66
26	k	101	BCR	C34-C9-C10	-5.98	114.55	122.92
27	A	611	PL9	C45-C44-C43	-5.96	108.40	123.68
26	B	620	BCR	C11-C10-C9	-5.95	118.81	127.31
24	b	616	CLA	C3A-C2A-C1A	5.95	110.25	101.34
27	a	611	PL9	C11-C9-C8	-5.95	109.08	121.12
24	C	509	CLA	C4A-NA-C1A	-5.93	104.04	106.71
24	b	612	CLA	C4A-NA-C1A	-5.93	104.04	106.71
26	H	101	BCR	C36-C18-C17	-5.93	114.62	122.92
26	H	101	BCR	C31-C1-C6	-5.90	100.72	110.30
24	B	610	CLA	C3A-C2A-C1A	5.90	110.18	101.34
24	b	615	CLA	C3A-C2A-C1A	5.90	110.18	101.34
26	c	521	BCR	C11-C10-C9	-5.90	118.89	127.31
24	b	618	CLA	C3A-C2A-C1A	5.89	110.17	101.34
24	C	511	CLA	C3A-C2A-C1A	5.89	110.16	101.34
27	A	611	PL9	C11-C9-C8	-5.89	109.21	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C3A-C2A-C1A	5.88	110.15	101.34
24	C	502	CLA	C4A-NA-C1A	-5.88	104.06	106.71
26	h	101	BCR	C20-C21-C22	-5.88	118.92	127.31
26	b	620	BCR	C7-C6-C5	-5.88	107.23	121.46
26	K	101	BCR	C34-C9-C10	-5.86	114.71	122.92
24	b	613	CLA	O2D-CGD-CBD	5.86	121.68	111.27
24	b	606	CLA	C4A-NA-C1A	-5.86	104.07	106.71
26	b	621	BCR	C4-C5-C6	-5.86	114.23	122.73
26	c	514	BCR	C24-C25-C26	-5.85	107.28	121.46
26	k	101	BCR	C1-C6-C5	-5.85	114.38	122.61
24	b	611	CLA	C3A-C2A-C1A	5.84	110.09	101.34
26	A	610	BCR	C30-C25-C26	-5.82	114.42	122.61
24	b	608[B]	CLA	C2A-C3A-C4A	5.81	111.25	101.87
26	c	515	BCR	C30-C25-C26	-5.81	114.44	122.61
24	B	606	CLA	C3A-C2A-C1A	5.80	110.02	101.34
26	K	101	BCR	C7-C8-C9	-5.79	117.49	126.23
24	B	615	CLA	C3A-C2A-C1A	5.79	110.01	101.34
24	b	618	CLA	O2D-CGD-CBD	5.79	121.55	111.27
26	c	521	BCR	C27-C26-C25	-5.79	114.33	122.73
27	A	611	PL9	C46-C44-C43	-5.78	109.43	121.12
24	b	604	CLA	C3A-C2A-C1A	5.77	109.99	101.34
24	B	613	CLA	C2A-C3A-C4A	5.77	111.19	101.87
27	D	405	PL9	C17-C18-C19	-5.77	113.77	127.66
26	a	610	BCR	C20-C21-C22	-5.76	119.09	127.31
27	a	611	PL9	C10-C9-C8	-5.76	108.91	123.68
27	d	404	PL9	C35-C34-C33	-5.75	108.93	123.68
27	D	405	PL9	C11-C9-C8	-5.74	109.50	121.12
26	B	618	BCR	C27-C26-C25	-5.74	114.40	122.73
26	b	620	BCR	C20-C21-C22	-5.73	119.13	127.31
26	b	619	BCR	C38-C26-C27	-5.72	102.62	113.62
27	D	405	PL9	C21-C19-C18	-5.72	109.54	121.12
27	a	611	PL9	C40-C39-C41	-5.72	105.65	115.27
24	C	503	CLA	C3A-C2A-C1A	5.72	109.90	101.34
24	B	613	CLA	C4A-NA-C1A	-5.71	104.14	106.71
26	k	101	BCR	C15-C14-C13	-5.71	119.16	127.31
26	a	610	BCR	C7-C8-C9	-5.70	117.62	126.23
26	F	101	BCR	C7-C6-C5	-5.70	107.66	121.46
27	a	611	PL9	C26-C24-C23	-5.70	109.59	121.12
24	C	501	CLA	C2A-C3A-C4A	5.69	111.07	101.87
26	K	102	BCR	C15-C14-C13	-5.69	119.19	127.31
24	b	608[A]	CLA	C2A-C3A-C4A	5.69	111.06	101.87
24	C	501	CLA	O2D-CGD-CBD	5.68	121.36	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C7-C6-C5	-5.67	107.72	121.46
26	a	610	BCR	C15-C14-C13	-5.67	119.22	127.31
24	B	616	CLA	C2A-C3A-C4A	5.65	111.00	101.87
24	b	617	CLA	C2A-C3A-C4A	5.65	110.99	101.87
26	B	618	BCR	C8-C7-C6	-5.64	111.35	127.20
24	c	512	CLA	O2D-CGD-CBD	5.64	121.30	111.27
26	b	619	BCR	C20-C21-C22	-5.64	119.26	127.31
24	c	509	CLA	C2A-C3A-C4A	5.63	110.96	101.87
24	c	502	CLA	C3A-C2A-C1A	5.62	109.76	101.34
24	c	513	CLA	C3A-C2A-C1A	5.62	109.76	101.34
26	t	101	BCR	C7-C8-C9	-5.62	117.74	126.23
24	b	611	CLA	C2A-C3A-C4A	5.62	110.94	101.87
26	a	610	BCR	C11-C10-C9	-5.61	119.30	127.31
24	b	605	CLA	C2A-C3A-C4A	5.61	110.93	101.87
26	I	101	BCR	C20-C21-C22	-5.61	119.31	127.31
24	B	617	CLA	C3A-C2A-C1A	5.60	109.73	101.34
26	c	521	BCR	C4-C5-C6	-5.60	114.60	122.73
26	B	619	BCR	C4-C5-C6	-5.59	114.62	122.73
24	B	607[B]	CLA	C2A-C3A-C4A	5.59	110.89	101.87
24	A	607	CLA	O2D-CGD-CBD	5.59	121.19	111.27
27	a	611	PL9	C35-C34-C33	-5.58	109.36	123.68
26	K	102	BCR	C7-C6-C5	-5.58	107.95	121.46
26	K	102	BCR	C11-C10-C9	-5.57	119.36	127.31
24	C	508	CLA	C3A-C2A-C1A	5.57	109.69	101.34
24	C	512	CLA	O2D-CGD-CBD	5.57	121.17	111.27
26	B	618	BCR	C15-C14-C13	-5.57	119.36	127.31
27	a	611	PL9	C15-C14-C13	-5.57	109.39	123.68
30	A	615	LHG	O7-C7-C8	5.57	123.50	111.50
24	B	608	CLA	C2A-C3A-C4A	5.57	110.86	101.87
26	B	618	BCR	C37-C22-C21	-5.55	115.15	122.92
24	b	603	CLA	C3A-C2A-C1A	5.54	109.64	101.34
24	B	608	CLA	C3A-C2A-C1A	5.54	109.64	101.34
26	h	101	BCR	C2-C1-C6	5.54	119.00	110.48
24	B	612	CLA	O2D-CGD-CBD	5.53	121.09	111.27
24	c	509	CLA	C3A-C2A-C1A	5.53	109.61	101.34
26	c	514	BCR	C7-C6-C5	-5.52	108.09	121.46
24	b	613	CLA	C3A-C2A-C1A	5.52	109.60	101.34
24	c	505	CLA	O2D-CGD-CBD	5.52	121.07	111.27
26	B	618	BCR	C24-C23-C22	-5.51	117.90	126.23
24	B	602	CLA	C3A-C2A-C1A	5.50	109.58	101.34
26	C	514	BCR	C7-C6-C5	-5.50	108.14	121.46
24	C	507	CLA	C3A-C2A-C1A	5.50	109.58	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	BCR	C24-C23-C22	-5.49	117.93	126.23
27	D	405	PL9	C42-C43-C44	-5.49	114.45	127.66
24	B	614	CLA	C3A-C2A-C1A	5.48	109.55	101.34
24	b	614	CLA	C2A-C3A-C4A	5.47	110.71	101.87
26	H	101	BCR	C29-C30-C25	5.47	118.90	110.48
24	B	607[B]	CLA	C3A-C2A-C1A	5.47	109.53	101.34
24	B	617	CLA	C4A-NA-C1A	-5.45	104.25	106.71
24	B	607[A]	CLA	C2A-C3A-C4A	5.45	110.67	101.87
24	b	605	CLA	C2A-C1A-CHA	5.44	133.37	123.86
27	D	405	PL9	C46-C44-C43	-5.44	110.11	121.12
24	C	504	CLA	C2A-C3A-C4A	5.43	110.65	101.87
24	c	503	CLA	C3A-C2A-C1A	5.43	109.47	101.34
26	T	101	BCR	C11-C10-C9	-5.42	119.57	127.31
33	V	201	HEM	CBA-CAA-C2A	-5.41	103.38	112.62
24	C	509	CLA	C2A-C3A-C4A	5.41	110.61	101.87
24	c	507	CLA	C2A-C3A-C4A	5.41	110.61	101.87
24	B	610	CLA	C2A-C3A-C4A	5.41	110.60	101.87
24	b	606	CLA	C3A-C2A-C1A	5.40	109.43	101.34
24	C	507	CLA	C2A-C3A-C4A	5.40	110.59	101.87
26	C	514	BCR	C16-C15-C14	-5.40	112.42	123.47
26	C	514	BCR	C2-C1-C6	5.40	118.79	110.48
26	h	101	BCR	C4-C5-C6	-5.39	114.90	122.73
24	b	605	CLA	C3A-C2A-C1A	5.39	109.42	101.34
26	K	102	BCR	C8-C7-C6	-5.38	112.10	127.20
24	B	607[A]	CLA	C3A-C2A-C1A	5.38	109.39	101.34
27	D	405	PL9	C30-C29-C28	-5.37	109.90	123.68
24	C	506	CLA	C2A-C1A-CHA	5.37	133.24	123.86
24	b	609	CLA	C2A-C3A-C4A	5.36	110.53	101.87
24	c	508	CLA	O2D-CGD-CBD	5.36	120.80	111.27
26	K	101	BCR	C7-C6-C5	-5.36	108.47	121.46
27	D	405	PL9	C37-C38-C39	-5.36	114.76	127.66
26	c	521	BCR	C8-C7-C6	-5.36	112.16	127.20
24	C	504	CLA	C4A-NA-C1A	-5.35	104.30	106.71
24	c	501	CLA	O2D-CGD-CBD	5.35	120.78	111.27
26	F	101	BCR	C1-C6-C5	-5.35	115.08	122.61
27	A	611	PL9	C15-C14-C13	-5.34	109.97	123.68
24	b	612	CLA	O2D-CGD-CBD	5.33	120.73	111.27
24	B	614	CLA	C2A-C3A-C4A	5.33	110.47	101.87
26	c	521	BCR	C7-C6-C5	-5.32	108.57	121.46
26	B	619	BCR	C34-C9-C10	-5.32	115.47	122.92
24	C	511	CLA	O2D-CGD-CBD	5.30	120.69	111.27
24	c	506	CLA	C2A-C1A-CHA	5.30	133.13	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	C2A-C3A-C4A	5.30	110.43	101.87
24	a	609	CLA	C3A-C2A-C1A	5.29	109.27	101.34
24	b	607	CLA	C2A-C3A-C4A	5.29	110.41	101.87
24	b	609	CLA	C3A-C2A-C1A	5.29	109.25	101.34
24	C	502	CLA	C2A-C3A-C4A	5.28	110.40	101.87
26	B	620	BCR	C7-C6-C5	-5.27	108.69	121.46
24	B	612	CLA	C3A-C2A-C1A	5.26	109.22	101.34
24	b	609	CLA	C4A-NA-C1A	-5.26	104.34	106.71
24	B	605	CLA	C2A-C3A-C4A	5.26	110.36	101.87
26	b	621	BCR	C30-C25-C26	-5.26	115.21	122.61
24	B	610	CLA	O2D-CGD-CBD	5.26	120.61	111.27
24	B	612	CLA	C2A-C3A-C4A	5.25	110.36	101.87
24	B	606	CLA	C2A-C1A-CHA	5.25	133.04	123.86
24	c	512	CLA	C3A-C2A-C1A	5.25	109.21	101.34
27	D	405	PL9	C25-C24-C23	-5.25	110.22	123.68
24	A	607	CLA	C3A-C2A-C1A	5.24	109.19	101.34
26	K	102	BCR	C36-C18-C17	-5.24	115.58	122.92
26	B	619	BCR	C38-C26-C27	-5.24	103.55	113.62
27	D	405	PL9	C10-C9-C8	-5.24	110.23	123.68
26	I	101	BCR	C16-C15-C14	-5.24	112.75	123.47
26	C	514	BCR	C27-C26-C25	-5.23	115.13	122.73
24	b	608[B]	CLA	C3A-C2A-C1A	5.23	109.18	101.34
24	a	615	CLA	O2D-CGD-CBD	5.23	120.56	111.27
27	A	611	PL9	C21-C19-C18	-5.23	110.53	121.12
27	d	404	PL9	C25-C24-C23	-5.23	110.26	123.68
26	b	621	BCR	C35-C13-C14	-5.23	115.60	122.92
26	C	514	BCR	C24-C25-C26	-5.23	108.80	121.46
24	A	609	CLA	C3A-C2A-C1A	5.22	109.16	101.34
27	D	405	PL9	C45-C44-C43	-5.22	110.30	123.68
26	K	101	BCR	C16-C17-C18	-5.22	119.87	127.31
24	B	602	CLA	C2A-C3A-C4A	5.22	110.29	101.87
27	a	611	PL9	C46-C44-C43	-5.20	110.59	121.12
24	C	511	CLA	C2A-C1A-CHA	5.20	132.95	123.86
24	d	403	CLA	C2A-C3A-C4A	5.20	110.27	101.87
26	h	101	BCR	C27-C26-C25	-5.20	115.19	122.73
26	H	101	BCR	C27-C26-C25	-5.20	115.19	122.73
24	B	605	CLA	C3A-C2A-C1A	5.19	109.11	101.34
27	D	405	PL9	C15-C14-C13	-5.17	110.41	123.68
24	b	603	CLA	C2A-C1A-CHA	5.17	132.90	123.86
24	a	607	CLA	C2A-C1A-CHA	5.17	132.90	123.86
26	I	101	BCR	C34-C9-C10	-5.16	115.69	122.92
24	c	504	CLA	C2A-C3A-C4A	5.16	110.20	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	O2D-CGD-CBD	5.16	120.43	111.27
24	b	608[A]	CLA	C3A-C2A-C1A	5.15	109.05	101.34
27	a	611	PL9	C25-C24-C23	-5.14	110.49	123.68
33	v	201	HEM	C4D-ND-C1D	5.14	110.38	105.07
27	d	404	PL9	C15-C14-C13	-5.14	110.50	123.68
26	B	620	BCR	C7-C8-C9	-5.13	118.48	126.23
26	B	618	BCR	C30-C25-C26	-5.13	115.38	122.61
26	T	101	BCR	C23-C24-C25	-5.13	112.80	127.20
24	b	614	CLA	C3A-C2A-C1A	5.12	109.01	101.34
26	t	101	BCR	C35-C13-C12	-5.11	110.02	118.08
24	c	502	CLA	C2A-C3A-C4A	5.11	110.12	101.87
26	b	621	BCR	C37-C22-C23	5.11	126.13	118.08
24	b	617	CLA	O2D-CGD-CBD	5.11	120.34	111.27
24	d	402	CLA	C1B-CHB-C4A	-5.10	120.01	130.12
24	B	604	CLA	C3A-C2A-C1A	5.10	108.98	101.34
24	d	402	CLA	C3A-C2A-C1A	5.10	108.97	101.34
26	h	101	BCR	C7-C8-C9	-5.09	118.54	126.23
24	D	404	CLA	C2A-C1A-CHA	5.09	132.76	123.86
24	B	616	CLA	C3A-C2A-C1A	5.08	108.95	101.34
24	C	509	CLA	C3A-C2A-C1A	5.08	108.94	101.34
27	A	611	PL9	C35-C34-C33	-5.07	110.67	123.68
27	D	405	PL9	C20-C19-C18	-5.07	110.67	123.68
24	B	615	CLA	C2A-C1A-CHA	5.07	132.72	123.86
24	C	513	CLA	C3A-C2A-C1A	5.07	108.93	101.34
24	c	503	CLA	C2A-C3A-C4A	5.06	110.05	101.87
24	a	615	CLA	C3A-C2A-C1A	5.06	108.92	101.34
27	d	404	PL9	C26-C24-C23	-5.06	110.88	121.12
26	B	620	BCR	C20-C19-C18	-5.05	112.22	126.42
26	B	619	BCR	C1-C6-C5	-5.05	115.50	122.61
24	B	609	CLA	O2D-CGD-CBD	5.05	120.23	111.27
24	B	605	CLA	O1D-CGD-CBD	-5.04	114.17	124.48
27	d	404	PL9	C10-C9-C8	-5.04	110.75	123.68
24	D	403	CLA	C2A-C3A-C4A	5.04	110.00	101.87
24	C	502	CLA	C3A-C2A-C1A	5.03	108.87	101.34
24	d	402	CLA	O2D-CGD-CBD	5.03	120.20	111.27
27	D	405	PL9	C40-C39-C38	-5.03	110.78	123.68
26	c	514	BCR	C7-C8-C9	-5.03	118.64	126.23
24	B	609	CLA	C2A-C1A-CHA	5.02	132.65	123.86
24	b	603	CLA	C2A-C3A-C4A	5.02	109.98	101.87
26	K	101	BCR	C38-C26-C27	-5.02	103.97	113.62
24	C	501	CLA	C3A-C2A-C1A	5.01	108.85	101.34
27	a	611	PL9	C41-C39-C38	-5.01	110.98	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	607	CLA	C3A-C2A-C1A	5.00	108.83	101.34
24	B	611	CLA	C2A-C3A-C4A	5.00	109.94	101.87
27	d	404	PL9	C45-C44-C43	-4.99	110.88	123.68
26	t	101	BCR	C4-C5-C6	-4.99	115.49	122.73
26	c	514	BCR	C4-C5-C6	-4.98	115.50	122.73
26	T	101	BCR	C8-C7-C6	-4.98	113.23	127.20
27	D	405	PL9	C47-C48-C49	-4.97	110.76	127.75
26	c	514	BCR	C23-C24-C25	-4.97	113.24	127.20
27	a	611	PL9	C30-C29-C28	-4.97	110.93	123.68
24	c	506	CLA	C2A-C3A-C4A	4.97	109.89	101.87
24	b	612	CLA	C3A-C2A-C1A	4.96	108.77	101.34
24	c	510	CLA	C2A-C1A-CHA	4.95	132.52	123.86
33	e	102	HEM	C4D-ND-C1D	4.95	110.19	105.07
24	B	607[A]	CLA	O2D-CGD-CBD	4.95	120.07	111.27
24	c	510	CLA	O2D-CGD-CBD	4.95	120.07	111.27
24	C	503	CLA	C2A-C3A-C4A	4.95	109.86	101.87
24	c	511	CLA	C2A-C1A-CHA	4.94	132.50	123.86
24	b	608[A]	CLA	C2A-C1A-CHA	4.94	132.50	123.86
26	b	619	BCR	C23-C24-C25	-4.94	113.33	127.20
24	A	609	CLA	C2A-C3A-C4A	4.94	109.85	101.87
24	B	611	CLA	C3A-C2A-C1A	4.94	108.73	101.34
24	D	404	CLA	C2A-C3A-C4A	4.92	109.82	101.87
24	B	604	CLA	C2A-C3A-C4A	4.92	109.82	101.87
24	B	613	CLA	O2D-CGD-CBD	4.92	120.01	111.27
26	h	101	BCR	C29-C30-C25	4.92	118.05	110.48
26	t	101	BCR	C8-C7-C6	-4.91	113.40	127.20
24	b	610	CLA	O2D-CGD-CBD	4.91	119.99	111.27
24	c	512	CLA	C4A-NA-C1A	-4.90	104.50	106.71
24	B	607[B]	CLA	O2D-CGD-CBD	4.90	119.98	111.27
26	H	101	BCR	C2-C1-C6	4.90	118.02	110.48
26	b	619	BCR	C34-C9-C10	-4.90	116.07	122.92
26	h	101	BCR	C8-C7-C6	-4.89	113.46	127.20
24	c	506	CLA	O2D-CGD-CBD	4.89	119.96	111.27
26	A	610	BCR	C24-C23-C22	-4.89	118.84	126.23
30	a	616	LHG	O7-C7-C8	4.89	122.04	111.50
24	C	513	CLA	C2A-C3A-C4A	4.89	109.77	101.87
24	A	607	CLA	C2A-C3A-C4A	4.89	109.77	101.87
24	c	501	CLA	C2A-C3A-C4A	4.89	109.76	101.87
24	b	606	CLA	C2A-C1A-CHA	4.89	132.40	123.86
30	d	407	LHG	O7-C7-C8	4.88	122.03	111.50
26	I	101	BCR	C36-C18-C17	-4.88	116.09	122.92
24	b	615	CLA	C2A-C3A-C4A	4.88	109.75	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C24-C25-C26	-4.87	109.65	121.46
24	c	511	CLA	O2D-CGD-CBD	4.87	119.92	111.27
24	b	606	CLA	C2A-C3A-C4A	4.87	109.73	101.87
26	K	101	BCR	C1-C6-C5	-4.87	115.76	122.61
26	T	101	BCR	C35-C13-C12	-4.87	110.41	118.08
26	h	101	BCR	C35-C13-C14	-4.86	116.12	122.92
24	B	602	CLA	C4A-NA-C1A	-4.86	104.52	106.71
24	b	613	CLA	C2A-C3A-C4A	4.85	109.71	101.87
26	b	621	BCR	C24-C25-C26	-4.85	109.72	121.46
27	D	405	PL9	C35-C34-C33	-4.84	111.25	123.68
26	B	618	BCR	C7-C6-C5	-4.84	109.74	121.46
24	B	611	CLA	C2A-C1A-CHA	4.83	132.30	123.86
24	d	403	CLA	C2A-C1A-CHA	4.82	132.29	123.86
26	C	514	BCR	C4-C5-C6	-4.82	115.73	122.73
26	B	618	BCR	C24-C25-C26	-4.82	109.78	121.46
24	a	609	CLA	C2A-C1A-CHA	4.82	132.29	123.86
24	c	513	CLA	O2D-CGD-CBD	4.82	119.83	111.27
27	D	405	PL9	C12-C13-C14	-4.82	116.06	127.66
26	k	101	BCR	C11-C10-C9	-4.81	120.45	127.31
24	a	606	CLA	C2A-C1A-CHA	4.81	132.27	123.86
27	d	404	PL9	C30-C29-C28	-4.80	111.35	123.68
24	C	502	CLA	O2D-CGD-CBD	4.80	119.79	111.27
24	B	615	CLA	C4A-NA-C1A	-4.79	104.55	106.71
24	c	513	CLA	C2A-C3A-C4A	4.78	109.60	101.87
24	D	402	CLA	C3A-C2A-C1A	4.77	108.49	101.34
26	B	620	BCR	C20-C21-C22	-4.77	120.50	127.31
26	b	620	BCR	C7-C8-C9	-4.77	119.03	126.23
26	K	101	BCR	C15-C14-C13	-4.76	120.51	127.31
24	c	504	CLA	C3A-C2A-C1A	4.75	108.46	101.34
24	c	504	CLA	C4A-NA-C1A	-4.75	104.57	106.71
26	C	514	BCR	C31-C1-C6	-4.75	102.59	110.30
24	c	507	CLA	C3A-C2A-C1A	4.75	108.45	101.34
24	B	603	CLA	C2A-C1A-CHA	4.75	132.16	123.86
26	k	101	BCR	C7-C6-C5	-4.74	109.98	121.46
24	b	608[B]	CLA	C2A-C1A-CHA	4.74	132.15	123.86
30	e	101	LHG	O7-C7-C8	4.74	121.71	111.50
26	K	102	BCR	C7-C8-C9	-4.74	119.08	126.23
27	A	611	PL9	C30-C29-C28	-4.74	111.53	123.68
24	B	608	CLA	C2A-C1A-CHA	4.73	132.14	123.86
24	b	604	CLA	C1B-CHB-C4A	-4.73	120.75	130.12
24	b	606	CLA	O2D-CGD-CBD	4.73	119.67	111.27
26	b	621	BCR	C31-C1-C6	-4.73	102.64	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C2A-C1A-CHA	4.72	132.12	123.86
24	C	508	CLA	C2A-C3A-C4A	4.72	109.49	101.87
24	d	403	CLA	C3A-C2A-C1A	4.72	108.41	101.34
27	d	404	PL9	C47-C48-C49	-4.72	111.63	127.75
27	d	404	PL9	C40-C39-C38	-4.72	111.58	123.68
24	C	507	CLA	C2A-C1A-CHA	4.71	132.10	123.86
26	c	515	BCR	C38-C26-C27	-4.71	104.56	113.62
24	b	615	CLA	C2A-C1A-CHA	4.71	132.10	123.86
24	c	503	CLA	C4A-NA-C1A	-4.71	104.59	106.71
24	b	607	CLA	O2D-CGD-CBD	4.70	119.62	111.27
24	A	607	CLA	C2A-C1A-CHA	4.70	132.07	123.86
32	c	518	DGD	O2G-C1B-C2B	4.69	121.62	111.50
24	B	602	CLA	C2A-C1A-CHA	4.69	132.05	123.86
26	K	102	BCR	C1-C6-C5	-4.69	116.01	122.61
28	A	612	SQD	O6-C1-C2	4.68	115.62	108.30
26	b	621	BCR	C7-C6-C5	-4.68	110.12	121.46
26	I	101	BCR	C33-C5-C4	-4.68	104.62	113.62
26	h	101	BCR	C23-C24-C25	-4.68	114.06	127.20
24	C	513	CLA	O2D-CGD-CBD	4.68	119.58	111.27
24	D	404	CLA	C3A-C2A-C1A	4.68	108.35	101.34
24	a	606	CLA	C3A-C2A-C1A	4.68	108.34	101.34
28	a	612	SQD	O6-C1-C2	4.67	115.59	108.30
24	B	611	CLA	C1B-CHB-C4A	-4.66	120.88	130.12
27	A	611	PL9	C20-C19-C18	-4.66	111.72	123.68
24	C	507	CLA	C4A-NA-C1A	-4.66	104.61	106.71
26	H	101	BCR	C7-C6-C5	-4.65	110.20	121.46
24	b	604	CLA	C2A-C3A-C4A	4.65	109.38	101.87
26	t	101	BCR	C24-C25-C26	-4.64	110.21	121.46
24	B	605	CLA	O2D-CGD-O1D	-4.64	114.76	123.84
26	H	101	BCR	C38-C26-C27	-4.64	104.70	113.62
24	b	612	CLA	C2A-C3A-C4A	4.64	109.36	101.87
24	B	609	CLA	C2A-C3A-C4A	4.64	109.36	101.87
26	T	101	BCR	C11-C12-C13	-4.63	113.42	126.42
26	K	101	BCR	C24-C23-C22	-4.63	119.25	126.23
26	c	514	BCR	C36-C18-C17	-4.62	116.45	122.92
26	t	101	BCR	C11-C12-C13	-4.62	113.44	126.42
24	C	510	CLA	C3A-C2A-C1A	4.62	108.25	101.34
27	A	611	PL9	C40-C39-C41	-4.62	107.51	115.27
26	c	521	BCR	C38-C26-C27	-4.61	104.75	113.62
24	a	609	CLA	C2A-C3A-C4A	4.61	109.32	101.87
24	C	510	CLA	C2A-C3A-C4A	4.61	109.32	101.87
24	B	606	CLA	O2D-CGD-CBD	4.61	119.46	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	l	101	SQD	O6-C1-C2	4.60	115.49	108.30
28	L	102	SQD	O6-C1-C2	4.60	115.49	108.30
24	c	508	CLA	C2A-C3A-C4A	4.60	109.30	101.87
24	c	512	CLA	C2A-C3A-C4A	4.59	109.28	101.87
26	K	101	BCR	C4-C5-C6	-4.59	116.07	122.73
24	a	615	CLA	C1B-CHB-C4A	-4.59	121.04	130.12
24	a	609	CLA	O2D-CGD-CBD	4.58	119.42	111.27
32	h	102	DGD	O2G-C1B-C2B	4.58	121.38	111.50
26	a	610	BCR	C7-C6-C5	-4.58	110.37	121.46
26	F	101	BCR	C15-C14-C13	-4.57	120.78	127.31
24	C	508	CLA	C2A-C1A-CHA	4.57	131.86	123.86
26	B	618	BCR	C34-C9-C10	-4.57	116.52	122.92
26	F	101	BCR	C8-C7-C6	-4.57	114.36	127.20
27	D	405	PL9	C45-C44-C46	-4.57	107.58	115.27
26	B	620	BCR	C31-C1-C6	-4.57	102.89	110.30
26	h	101	BCR	C38-C26-C27	-4.57	104.84	113.62
24	b	610	CLA	C2A-C3A-C4A	4.56	109.24	101.87
24	c	502	CLA	O2D-CGD-CBD	4.56	119.37	111.27
24	c	504	CLA	C2A-C1A-CHA	4.56	131.83	123.86
24	c	504	CLA	O2D-CGD-CBD	4.56	119.37	111.27
24	B	607[A]	CLA	C4A-NA-C1A	-4.56	104.66	106.71
24	C	512	CLA	C4A-NA-C1A	-4.55	104.66	106.71
24	C	506	CLA	O2D-CGD-CBD	4.55	119.35	111.27
24	d	402	CLA	C2A-C3A-C4A	4.54	109.21	101.87
24	b	616	CLA	C2A-C3A-C4A	4.54	109.20	101.87
24	C	511	CLA	C2A-C3A-C4A	4.53	109.19	101.87
26	K	102	BCR	C4-C5-C6	-4.52	116.17	122.73
24	D	403	CLA	C3A-C2A-C1A	4.52	108.11	101.34
26	c	515	BCR	C8-C7-C6	-4.52	114.51	127.20
24	b	611	CLA	O2D-CGD-CBD	4.51	119.29	111.27
24	b	603	CLA	C4A-NA-C1A	-4.51	104.68	106.71
26	A	610	BCR	C7-C8-C9	-4.51	119.42	126.23
24	C	511	CLA	C4A-NA-C1A	-4.51	104.68	106.71
27	a	611	PL9	C21-C19-C18	-4.50	112.01	121.12
24	b	613	CLA	C2A-C1A-CHA	4.49	131.71	123.86
24	c	509	CLA	C2A-C1A-CHA	4.49	131.71	123.86
27	A	611	PL9	C25-C24-C23	-4.49	112.17	123.68
26	B	619	BCR	C30-C25-C26	-4.48	116.30	122.61
24	B	617	CLA	CHC-C1C-NC	4.48	131.00	124.20
24	B	613	CLA	C3A-C2A-C1A	4.47	108.04	101.34
24	C	512	CLA	C2A-C3A-C4A	4.46	109.08	101.87
26	a	610	BCR	C38-C26-C27	-4.46	105.05	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	514	BCR	C2-C1-C6	4.46	117.34	110.48
24	A	609	CLA	O2D-CGD-CBD	4.46	119.19	111.27
24	B	615	CLA	C2A-C3A-C4A	4.46	109.07	101.87
24	C	504	CLA	O2D-CGD-CBD	4.45	119.18	111.27
24	b	612	CLA	C2A-C1A-CHA	4.45	131.65	123.86
24	c	511	CLA	C4A-NA-C1A	-4.45	104.70	106.71
24	c	505	CLA	C2A-C1A-CHA	4.45	131.63	123.86
24	B	603	CLA	C1B-CHB-C4A	-4.45	121.31	130.12
24	c	502	CLA	C2A-C1A-CHA	4.44	131.63	123.86
26	b	619	BCR	C7-C6-C5	-4.44	110.70	121.46
24	A	606	CLA	C2A-C1A-CHA	4.44	131.63	123.86
29	c	520	LMG	O7-C10-C11	4.44	121.07	111.50
24	D	402	CLA	C2A-C3A-C4A	4.44	109.04	101.87
26	c	521	BCR	C1-C6-C5	-4.44	116.36	122.61
26	K	102	BCR	C38-C26-C27	-4.43	105.10	113.62
24	A	607	CLA	C4D-CHA-C1A	-4.43	115.86	121.25
24	C	504	CLA	C3A-C2A-C1A	4.42	107.96	101.34
24	c	511	CLA	C2A-C3A-C4A	4.42	109.00	101.87
24	C	506	CLA	C1B-CHB-C4A	-4.41	121.38	130.12
26	T	101	BCR	C4-C5-C6	-4.41	116.33	122.73
27	a	611	PL9	C20-C19-C18	-4.41	112.37	123.68
26	T	101	BCR	C35-C13-C14	-4.41	116.75	122.92
27	A	611	PL9	C36-C34-C33	-4.40	112.20	121.12
24	B	614	CLA	C2A-C1A-CHA	4.39	131.53	123.86
24	B	605	CLA	O2D-CGD-CBD	4.38	119.04	111.27
24	b	610	CLA	C2A-C1A-CHA	4.37	131.51	123.86
24	b	607	CLA	C2A-C1A-CHA	4.37	131.51	123.86
24	c	510	CLA	C2A-C3A-C4A	4.37	108.93	101.87
26	c	521	BCR	C15-C14-C13	-4.37	121.07	127.31
26	H	101	BCR	C30-C25-C26	-4.37	116.46	122.61
26	k	101	BCR	C38-C26-C27	-4.37	105.22	113.62
24	a	606	CLA	C2A-C3A-C4A	4.37	108.92	101.87
24	b	618	CLA	C2A-C3A-C4A	4.37	108.92	101.87
24	A	606	CLA	O2D-CGD-CBD	4.36	119.02	111.27
24	D	402	CLA	C1B-CHB-C4A	-4.36	121.48	130.12
24	B	607[A]	CLA	C2A-C1A-CHA	4.36	131.48	123.86
28	a	612	SQD	O9-S-C6	4.35	112.11	106.94
24	c	505	CLA	C2A-C3A-C4A	4.34	108.88	101.87
24	c	508	CLA	C2A-C1A-CHA	4.33	131.44	123.86
24	C	501	CLA	C4A-NA-C1A	-4.33	104.76	106.71
24	b	615	CLA	O2D-CGD-CBD	4.33	118.96	111.27
24	a	607	CLA	C2A-C3A-C4A	4.33	108.86	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C24-C25-C26	-4.33	110.98	121.46
28	a	612	SQD	O47-C7-C8	4.32	120.82	111.50
26	I	101	BCR	C30-C25-C26	-4.32	116.52	122.61
24	D	402	CLA	CHA-C1A-NA	-4.32	116.50	126.40
26	T	101	BCR	C24-C25-C26	-4.32	111.00	121.46
28	A	612	SQD	O47-C7-C8	4.31	120.80	111.50
28	A	612	SQD	O9-S-C6	4.31	112.06	106.94
24	c	507	CLA	C2A-C1A-CHA	4.31	131.39	123.86
26	b	620	BCR	C38-C26-C27	-4.30	105.35	113.62
30	d	406	LHG	O7-C7-C8	4.30	120.77	111.50
24	C	502	CLA	C2A-C1A-CHA	4.30	131.38	123.86
24	B	617	CLA	C2A-C3A-C4A	4.30	108.81	101.87
26	b	619	BCR	C37-C22-C21	-4.30	116.90	122.92
26	B	619	BCR	C36-C18-C19	-4.29	111.32	118.08
26	T	101	BCR	C20-C21-C22	-4.28	121.20	127.31
24	C	504	CLA	C1B-CHB-C4A	-4.27	121.66	130.12
26	f	101	BCR	C8-C7-C6	-4.27	115.20	127.20
24	b	616	CLA	O2D-CGD-CBD	4.27	118.86	111.27
24	C	505	CLA	C2A-C1A-CHA	4.27	131.32	123.86
26	b	621	BCR	C37-C22-C21	-4.26	116.95	122.92
24	C	506	CLA	C2A-C3A-C4A	4.26	108.75	101.87
24	c	509	CLA	O2D-CGD-CBD	4.26	118.83	111.27
24	b	608[A]	CLA	O2D-CGD-CBD	4.25	118.83	111.27
26	H	101	BCR	C23-C24-C25	-4.25	115.26	127.20
24	B	604	CLA	O2D-CGD-CBD	4.25	118.82	111.27
24	d	403	CLA	C1-O2A-CGA	4.25	127.59	116.44
26	B	620	BCR	C23-C22-C21	-4.24	112.43	118.94
26	C	514	BCR	C20-C19-C18	-4.24	114.50	126.42
24	b	608[A]	CLA	C4A-NA-C1A	-4.24	104.80	106.71
26	A	610	BCR	C7-C6-C5	-4.23	111.21	121.46
24	C	513	CLA	C4A-NA-C1A	-4.23	104.80	106.71
24	C	508	CLA	O2D-CGD-CBD	4.23	118.78	111.27
28	B	622	SQD	O6-C1-C2	4.22	114.90	108.30
28	b	601	SQD	O6-C1-C2	4.22	114.89	108.30
32	c	516	DGD	O2G-C1B-C2B	4.22	120.60	111.50
24	B	616	CLA	C2A-C1A-CHA	4.22	131.24	123.86
26	t	101	BCR	C23-C24-C25	-4.22	115.36	127.20
25	d	401	PHO	CMB-C2B-C3B	4.21	132.56	124.68
24	b	608[B]	CLA	O2D-CGD-CBD	4.21	118.75	111.27
24	C	504	CLA	C2A-C1A-CHA	4.21	131.22	123.86
24	c	513	CLA	C2A-C1A-CHA	4.20	131.21	123.86
26	f	101	BCR	C7-C6-C5	-4.20	111.28	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	607	CLA	C1B-CHB-C4A	-4.20	121.80	130.12
24	b	616	CLA	C4A-NA-C1A	-4.20	104.82	106.71
27	d	404	PL9	C20-C19-C18	-4.19	112.92	123.68
24	B	608	CLA	C4A-NA-C1A	-4.19	104.82	106.71
24	b	610	CLA	C1B-CHB-C4A	-4.18	121.83	130.12
26	C	514	BCR	C36-C18-C17	-4.18	117.07	122.92
24	B	615	CLA	O2D-CGD-CBD	4.18	118.70	111.27
30	E	102	LHG	O7-C7-C8	4.18	120.50	111.50
27	d	404	PL9	C31-C29-C28	-4.17	112.67	121.12
24	C	505	CLA	C2A-C3A-C4A	4.17	108.61	101.87
24	c	503	CLA	C2A-C1A-CHA	4.17	131.15	123.86
26	B	619	BCR	C20-C19-C18	-4.17	114.70	126.42
24	b	616	CLA	C2A-C1A-CHA	4.17	131.15	123.86
24	B	607[B]	CLA	C2A-C1A-CHA	4.16	131.14	123.86
24	c	501	CLA	C2A-C1A-CHA	4.16	131.13	123.86
26	c	521	BCR	C35-C13-C14	-4.16	117.10	122.92
26	b	621	BCR	C38-C26-C27	-4.15	105.64	113.62
24	c	513	CLA	C1B-CHB-C4A	-4.15	121.91	130.12
24	a	607	CLA	C4A-NA-C1A	-4.14	104.84	106.71
26	A	610	BCR	C39-C30-C25	4.14	117.01	110.30
24	d	403	CLA	C4A-NA-C1A	-4.13	104.85	106.71
27	d	404	PL9	C36-C34-C33	-4.13	112.76	121.12
24	C	513	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
32	d	405	DGD	O2G-C1B-C2B	4.12	120.39	111.50
24	D	402	CLA	O1D-CGD-CBD	-4.12	116.05	124.48
24	b	609	CLA	O2D-CGD-CBD	4.12	118.58	111.27
24	B	603	CLA	C2A-C3A-C4A	4.12	108.52	101.87
28	X	101	SQD	O6-C1-C2	4.12	114.73	108.30
27	A	611	PL9	C47-C48-C49	-4.11	113.70	127.75
26	a	610	BCR	C24-C25-C26	-4.11	111.51	121.46
24	C	510	CLA	O2D-CGD-CBD	4.11	118.57	111.27
26	C	514	BCR	C38-C26-C27	-4.11	105.72	113.62
26	B	618	BCR	C36-C18-C17	-4.11	117.17	122.92
28	x	101	SQD	O6-C1-C2	4.10	114.71	108.30
26	a	610	BCR	C36-C18-C17	-4.10	117.19	122.92
24	B	614	CLA	CHC-C1C-NC	4.09	130.41	124.20
26	k	101	BCR	C23-C24-C25	-4.09	115.71	127.20
26	c	514	BCR	C16-C15-C14	-4.09	115.10	123.47
24	C	513	CLA	C1B-CHB-C4A	-4.08	122.03	130.12
24	b	611	CLA	C1B-CHB-C4A	-4.08	122.03	130.12
26	B	618	BCR	C23-C24-C25	-4.08	115.73	127.20
29	C	518	LMG	O7-C10-C11	4.08	120.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C23-C22-C21	-4.08	112.68	118.94
26	B	619	BCR	C11-C12-C13	-4.07	114.99	126.42
27	D	405	PL9	C7-C3-C4	4.07	120.18	116.88
24	C	512	CLA	CHC-C1C-NC	4.06	130.36	124.20
26	F	101	BCR	C37-C22-C21	-4.06	117.24	122.92
27	a	611	PL9	C47-C48-C49	-4.06	113.88	127.75
24	B	613	CLA	C1B-CHB-C4A	-4.05	122.09	130.12
26	A	610	BCR	C34-C9-C10	-4.05	117.25	122.92
26	K	102	BCR	C23-C24-C25	-4.04	115.85	127.20
24	B	603	CLA	CHC-C1C-NC	4.04	130.34	124.20
26	k	101	BCR	C4-C5-C6	-4.04	116.87	122.73
27	a	611	PL9	C31-C29-C28	-4.03	112.95	121.12
27	A	611	PL9	C31-C29-C28	-4.03	112.96	121.12
24	a	615	CLA	C2A-C3A-C4A	4.03	108.38	101.87
32	C	515	DGD	O2G-C1B-C2B	4.03	120.18	111.50
26	a	610	BCR	C8-C7-C6	-4.03	115.89	127.20
26	F	101	BCR	C36-C18-C19	4.02	124.41	118.08
24	b	613	CLA	C4A-NA-C1A	-4.02	104.90	106.71
24	D	402	CLA	C2A-C1A-CHA	4.01	130.87	123.86
24	B	609	CLA	CAC-C3C-C4C	4.00	130.00	124.81
24	A	609	CLA	C2A-C1A-CHA	4.00	130.85	123.86
26	B	619	BCR	C35-C13-C14	-3.99	117.33	122.92
23	a	605	BCT	O2-C-O1	-3.99	109.19	119.55
26	I	101	BCR	C38-C26-C27	-3.99	105.96	113.62
24	D	404	CLA	C1-O2A-CGA	3.99	126.91	116.44
24	a	607	CLA	O1D-CGD-CBD	-3.98	116.33	124.48
24	a	609	CLA	CHA-C1A-NA	-3.98	117.29	126.40
26	c	515	BCR	C20-C21-C22	-3.97	121.64	127.31
27	D	405	PL9	C51-C49-C48	-3.97	111.17	122.65
24	c	508	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
28	b	601	SQD	O47-C7-C8	3.97	120.06	111.50
28	B	622	SQD	O47-C7-C8	3.97	120.05	111.50
32	E	101	DGD	O2G-C1B-C2B	3.97	120.05	111.50
24	a	607	CLA	C1B-CHB-C4A	-3.96	122.27	130.12
26	B	618	BCR	C33-C5-C4	-3.96	106.00	113.62
26	b	620	BCR	C37-C22-C21	-3.96	117.38	122.92
24	c	503	CLA	O2D-CGD-CBD	3.96	118.30	111.27
32	C	517	DGD	O2G-C1B-C2B	3.95	120.02	111.50
24	c	508	CLA	C4D-C3D-CAD	-3.95	103.44	108.10
24	b	618	CLA	CHC-C1C-NC	3.94	130.19	124.20
24	B	612	CLA	C1B-CHB-C4A	-3.94	122.31	130.12
24	c	510	CLA	CHC-C1C-NC	3.94	130.18	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	C1B-CHB-C4A	-3.93	122.33	130.12
24	b	611	CLA	C2A-C1A-CHA	3.93	130.73	123.86
24	B	606	CLA	C4-C3-C5	3.93	121.88	115.27
24	C	507	CLA	C1D-ND-C4D	-3.92	103.55	106.33
24	d	403	CLA	C1D-ND-C4D	-3.92	103.55	106.33
24	C	508	CLA	CHC-C1C-NC	3.92	130.15	124.20
28	b	601	SQD	O7-S-C6	3.92	111.60	106.94
24	a	615	CLA	CHC-C1C-NC	3.91	130.13	124.20
24	B	617	CLA	O2D-CGD-CBD	3.90	118.21	111.27
24	c	505	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
24	b	607	CLA	C4-C3-C5	3.90	121.83	115.27
24	c	504	CLA	C1B-CHB-C4A	-3.90	122.39	130.12
24	D	404	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
28	B	622	SQD	O7-S-C6	3.89	111.56	106.94
25	D	401	PHO	O2D-CGD-O1D	-3.89	116.23	123.84
26	b	619	BCR	C30-C25-C26	-3.88	117.15	122.61
30	l	102	LHG	O7-C7-C8	3.88	119.86	111.50
24	b	603	CLA	O2D-CGD-CBD	3.88	118.16	111.27
26	b	621	BCR	C19-C18-C17	3.87	124.88	118.94
27	D	405	PL9	C41-C39-C38	-3.87	113.29	121.12
26	b	620	BCR	C30-C25-C26	-3.87	117.17	122.61
24	A	607	CLA	CHC-C1C-NC	3.86	130.06	124.20
26	h	101	BCR	C31-C1-C6	-3.86	104.04	110.30
24	c	502	CLA	C4A-NA-C1A	-3.86	104.97	106.71
29	C	519	LMG	O7-C10-C11	3.86	119.82	111.50
26	f	101	BCR	C37-C22-C23	-3.86	112.00	118.08
24	A	606	CLA	CHC-C1C-NC	3.85	130.05	124.20
27	d	404	PL9	C50-C49-C48	-3.85	111.52	122.65
24	b	613	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
24	b	614	CLA	O2D-CGD-O1D	-3.85	116.32	123.84
24	B	612	CLA	C4A-NA-C1A	-3.84	104.98	106.71
26	K	101	BCR	C35-C13-C14	-3.84	117.54	122.92
24	b	613	CLA	CHC-C1C-NC	3.84	130.03	124.20
27	A	611	PL9	C50-C49-C48	-3.84	111.55	122.65
26	A	610	BCR	C23-C22-C21	-3.84	113.05	118.94
24	B	607[B]	CLA	CHC-C1C-NC	3.84	130.02	124.20
24	D	404	CLA	C1B-CHB-C4A	-3.83	122.52	130.12
24	C	503	CLA	C2A-C1A-CHA	3.83	130.56	123.86
28	B	622	SQD	C3-C4-C5	3.83	117.07	110.24
24	B	615	CLA	C1B-CHB-C4A	-3.82	122.55	130.12
28	b	601	SQD	C3-C4-C5	3.82	117.05	110.24
27	d	404	PL9	C41-C39-C38	-3.82	113.39	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C40-C30-C25	-3.82	104.11	110.30
24	C	506	CLA	CED-O2D-CGD	3.81	124.56	115.94
26	A	610	BCR	C8-C7-C6	-3.81	116.52	127.20
33	e	102	HEM	CBD-CAD-C3D	-3.80	102.08	112.63
24	b	612	CLA	C1B-CHB-C4A	-3.80	122.60	130.12
27	A	611	PL9	C7-C3-C4	3.79	119.96	116.88
24	b	610	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
24	b	603	CLA	CHC-C1C-NC	3.79	129.95	124.20
26	b	621	BCR	C2-C1-C6	3.78	116.30	110.48
26	B	618	BCR	C38-C26-C27	-3.78	106.36	113.62
26	c	521	BCR	C24-C25-C26	-3.78	112.31	121.46
24	b	605	CLA	CHB-C4A-NA	-3.78	119.29	124.51
26	b	619	BCR	C8-C7-C6	-3.77	116.60	127.20
28	X	101	SQD	O47-C7-C8	3.77	119.63	111.50
29	Z	101	LMG	O1-C1-C2	3.77	114.19	108.30
24	C	503	CLA	C4A-NA-C1A	-3.77	105.01	106.71
32	c	518	DGD	O3G-C3G-C2G	-3.77	101.80	110.90
28	x	101	SQD	O47-C7-C8	3.77	119.62	111.50
27	D	405	PL9	C10-C9-C11	-3.77	108.93	115.27
26	A	610	BCR	C36-C18-C17	-3.77	117.64	122.92
24	b	604	CLA	O1D-CGD-CBD	-3.77	116.78	124.48
24	a	615	CLA	O2A-CGA-CBA	3.76	123.72	111.91
33	v	201	HEM	C3B-C2B-C1B	3.76	109.28	106.49
24	B	607[A]	CLA	CHC-C1C-NC	3.76	129.91	124.20
24	C	505	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
24	b	605	CLA	O1D-CGD-CBD	-3.76	116.80	124.48
25	D	401	PHO	CMB-C2B-C3B	3.76	131.70	124.68
26	C	514	BCR	C34-C9-C10	-3.75	117.66	122.92
29	a	613	LMG	O7-C10-C11	3.75	119.59	111.50
24	C	511	CLA	CHC-C1C-NC	3.74	129.87	124.20
24	b	607	CLA	C1-O2A-CGA	3.73	126.24	116.44
27	a	611	PL9	C7-C3-C4	3.73	119.91	116.88
33	E	103	HEM	C4D-ND-C1D	3.73	108.93	105.07
24	c	504	CLA	C1D-ND-C4D	-3.73	103.68	106.33
24	d	403	CLA	CHC-C1C-NC	3.73	129.86	124.20
26	B	620	BCR	C38-C26-C27	-3.73	106.45	113.62
24	C	501	CLA	C2A-C1A-CHA	3.73	130.37	123.86
28	L	102	SQD	O47-C7-C8	3.72	119.52	111.50
26	B	620	BCR	C24-C25-C26	-3.71	112.47	121.46
26	h	101	BCR	C33-C5-C4	-3.71	106.49	113.62
24	A	606	CLA	C1B-CHB-C4A	-3.71	122.78	130.12
26	c	514	BCR	C20-C19-C18	-3.71	116.00	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	C2A-C1A-CHA	3.70	130.34	123.86
32	C	517	DGD	O3G-C3G-C2G	-3.70	101.96	110.90
24	b	609	CLA	C1B-CHB-C4A	-3.70	122.79	130.12
24	D	404	CLA	O2D-CGD-CBD	3.70	117.84	111.27
24	c	502	CLA	C1B-CHB-C4A	-3.70	122.79	130.12
26	B	619	BCR	C37-C22-C21	-3.69	117.75	122.92
24	B	612	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
24	c	503	CLA	C1B-CHB-C4A	-3.69	122.82	130.12
24	b	616	CLA	C1B-CHB-C4A	-3.68	122.83	130.12
28	L	102	SQD	O7-S-C6	3.68	111.31	106.94
26	B	620	BCR	C16-C15-C14	-3.67	115.95	123.47
24	c	507	CLA	CHC-C1C-NC	3.67	129.78	124.20
28	l	101	SQD	O7-S-C6	3.67	111.31	106.94
28	l	101	SQD	O47-C7-C8	3.67	119.42	111.50
33	E	103	HEM	CBD-CAD-C3D	-3.66	102.45	112.63
27	a	611	PL9	C45-C44-C46	-3.66	109.11	115.27
24	c	501	CLA	C1B-CHB-C4A	-3.66	122.87	130.12
24	A	609	CLA	C1B-CHB-C4A	-3.65	122.88	130.12
24	A	607	CLA	C4A-NA-C1A	-3.65	105.06	106.71
24	a	615	CLA	C2A-C1A-CHA	3.65	130.24	123.86
24	C	508	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
24	a	606	CLA	CHC-C1C-NC	3.65	129.74	124.20
26	I	101	BCR	C8-C7-C6	-3.65	116.96	127.20
24	C	506	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
24	c	506	CLA	C1B-CHB-C4A	-3.64	122.90	130.12
24	B	610	CLA	C1B-CHB-C4A	-3.64	122.91	130.12
24	B	605	CLA	C4D-C3D-CAD	-3.63	103.81	108.10
24	c	505	CLA	C1B-CHB-C4A	-3.63	122.93	130.12
24	B	607[B]	CLA	C4A-NA-C1A	-3.63	105.08	106.71
24	c	503	CLA	C1D-ND-C4D	-3.62	103.76	106.33
27	d	404	PL9	C51-C49-C48	-3.62	112.17	122.65
24	B	604	CLA	CHB-C4A-NA	-3.62	119.50	124.51
24	B	616	CLA	O2D-CGD-CBD	3.61	117.69	111.27
26	c	515	BCR	C23-C24-C25	-3.61	117.06	127.20
26	c	515	BCR	C34-C9-C10	-3.61	117.86	122.92
24	b	615	CLA	CHC-C1C-NC	3.61	129.68	124.20
24	b	616	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
26	I	101	BCR	C20-C19-C18	-3.61	116.28	126.42
26	h	101	BCR	C30-C25-C26	-3.61	117.53	122.61
24	B	603	CLA	C4A-NA-C1A	-3.61	105.08	106.71
29	z	101	LMG	O7-C10-C11	3.60	119.25	111.50
24	b	609	CLA	C1D-ND-C4D	-3.60	103.78	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	405	PL9	C50-C49-C48	-3.59	112.26	122.65
27	a	611	PL9	C50-C49-C48	-3.59	112.26	122.65
24	b	609	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
24	a	609	CLA	C4-C3-C5	3.59	121.30	115.27
26	I	101	BCR	C7-C6-C5	-3.59	112.78	121.46
26	c	515	BCR	C7-C6-C5	-3.58	112.79	121.46
24	c	508	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
24	A	609	CLA	C4-C3-C5	3.58	121.29	115.27
29	Z	101	LMG	O7-C10-C11	3.57	119.20	111.50
26	t	101	BCR	C34-C9-C10	-3.57	117.93	122.92
33	V	201	HEM	C4D-ND-C1D	3.56	108.75	105.07
24	C	502	CLA	C1-O2A-CGA	3.56	125.79	116.44
24	a	607	CLA	CHA-C1A-NA	-3.56	118.24	126.40
24	d	402	CLA	C2A-C1A-CHA	3.56	130.09	123.86
24	a	615	CLA	CHA-C1A-NA	-3.56	118.25	126.40
26	K	102	BCR	C33-C5-C4	-3.56	106.78	113.62
24	a	615	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
24	D	403	CLA	C4A-NA-C1A	-3.55	105.11	106.71
24	B	602	CLA	C1B-CHB-C4A	-3.55	123.09	130.12
24	C	503	CLA	O2D-CGD-CBD	3.54	117.56	111.27
24	C	507	CLA	C1B-CHB-C4A	-3.54	123.11	130.12
26	k	101	BCR	C24-C25-C26	-3.54	112.89	121.46
24	C	510	CLA	C1B-CHB-C4A	-3.54	123.11	130.12
30	D	407	LHG	O7-C7-C8	3.53	119.12	111.50
29	c	519	LMG	O7-C10-C11	3.53	119.11	111.50
26	c	515	BCR	C33-C5-C4	-3.53	106.83	113.62
26	a	610	BCR	C34-C9-C10	-3.53	117.98	122.92
24	b	617	CLA	CHC-C1C-NC	3.52	129.55	124.20
26	A	610	BCR	C33-C5-C4	-3.52	106.85	113.62
24	D	403	CLA	C1B-CHB-C4A	-3.52	123.15	130.12
24	c	510	CLA	C4A-NA-C1A	-3.52	105.12	106.71
24	B	613	CLA	CHB-C4A-NA	-3.52	119.65	124.51
33	V	201	HEM	C3B-C2B-C1B	3.52	109.09	106.49
29	D	408	LMG	O6-C5-C4	3.52	116.08	109.69
24	c	509	CLA	CHC-C1C-NC	3.51	129.53	124.20
24	b	605	CLA	CHC-C1C-NC	3.51	129.53	124.20
26	k	101	BCR	C20-C21-C22	-3.51	122.31	127.31
27	A	611	PL9	C15-C14-C16	-3.50	109.38	115.27
24	b	613	CLA	O1D-CGD-CBD	-3.50	117.32	124.48
24	B	605	CLA	CHC-C1C-NC	3.50	129.51	124.20
24	B	617	CLA	C4D-C3D-CAD	-3.50	103.98	108.10
24	B	610	CLA	CHC-C1C-NC	3.50	129.51	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608[B]	CLA	C4A-NA-C1A	-3.49	105.14	106.71
26	K	102	BCR	C24-C25-C26	-3.49	113.00	121.46
27	A	611	PL9	C45-C44-C46	-3.49	109.40	115.27
24	A	607	CLA	O2A-CGA-CBA	3.49	122.86	111.91
24	B	616	CLA	CHC-C1C-NC	3.49	129.50	124.20
24	c	511	CLA	C1B-CHB-C4A	-3.49	123.21	130.12
24	b	611	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
24	c	509	CLA	C1D-ND-C4D	-3.49	103.86	106.33
27	a	611	PL9	C36-C34-C33	-3.48	114.08	121.12
26	A	610	BCR	C16-C15-C14	-3.48	116.35	123.47
24	c	501	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
24	B	606	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
24	d	403	CLA	O2D-CGD-CBD	3.47	117.44	111.27
23	a	605	BCT	O3-C-O1	-3.47	110.55	119.55
24	B	604	CLA	O1D-CGD-CBD	-3.47	117.39	124.48
24	D	404	CLA	CHA-C1A-NA	-3.46	118.47	126.40
24	B	610	CLA	C2A-C1A-CHA	3.46	129.91	123.86
24	c	508	CLA	CHC-C1C-NC	3.46	129.45	124.20
26	I	101	BCR	C30-C25-C24	-3.46	106.00	115.78
28	A	614	SQD	O9-S-C6	3.46	111.05	106.94
24	a	606	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
24	C	503	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
24	b	616	CLA	C4-C3-C5	3.45	121.08	115.27
24	c	508	CLA	C4A-NA-C1A	-3.45	105.16	106.71
26	K	102	BCR	C40-C30-C25	3.45	115.89	110.30
24	C	508	CLA	C1B-CHB-C4A	-3.44	123.30	130.12
24	B	615	CLA	C4-C3-C5	3.44	121.06	115.27
24	b	616	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
26	b	619	BCR	C24-C25-C26	-3.44	113.13	121.46
24	C	507	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
24	C	509	CLA	C2A-C1A-CHA	3.44	129.87	123.86
24	c	505	CLA	C4A-NA-C1A	-3.44	105.16	106.71
26	b	620	BCR	C16-C15-C14	-3.44	116.44	123.47
24	B	609	CLA	CHC-C1C-NC	3.44	129.41	124.20
24	a	615	CLA	C4D-CHA-C1A	-3.43	117.07	121.25
24	c	506	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
26	b	620	BCR	C27-C26-C25	-3.43	117.75	122.73
24	A	606	CLA	C3A-C2A-C1A	3.42	106.47	101.34
24	A	606	CLA	C2A-C3A-C4A	3.42	107.40	101.87
24	c	506	CLA	CHB-C4A-NA	-3.42	119.78	124.51
30	L	101	LHG	O7-C7-C8	3.42	118.87	111.50
24	B	602	CLA	O2D-CGD-CBD	3.41	117.34	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C1D-ND-C4D	-3.41	103.91	106.33
24	B	603	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
28	a	614	SQD	O9-S-C6	3.41	110.99	106.94
26	t	101	BCR	C1-C6-C5	-3.40	117.82	122.61
24	B	607[B]	CLA	C1B-CHB-C4A	-3.40	123.39	130.12
24	b	610	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
24	C	511	CLA	C1B-CHB-C4A	-3.40	123.39	130.12
27	a	611	PL9	C15-C14-C16	-3.39	109.56	115.27
24	c	507	CLA	C1-O2A-CGA	3.39	125.35	116.44
24	b	606	CLA	C1-O2A-CGA	3.39	125.34	116.44
24	a	607	CLA	C1-O2A-CGA	3.39	125.33	116.44
28	A	614	SQD	O47-C7-C8	3.37	118.77	111.50
28	a	614	SQD	O47-C7-C8	3.37	118.77	111.50
24	b	605	CLA	O2A-C1-C2	3.37	117.50	108.64
24	A	609	CLA	CHA-C1A-NA	-3.36	118.70	126.40
24	B	605	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
29	C	518	LMG	O8-C28-C29	3.36	122.44	111.91
24	b	604	CLA	C2A-C1A-CHA	3.36	129.73	123.86
26	b	621	BCR	C1-C6-C5	-3.35	117.89	122.61
29	D	408	LMG	O7-C10-C11	3.35	118.73	111.50
24	C	512	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
28	A	612	SQD	O8-S-C6	3.35	111.08	105.74
25	A	608	PHO	CMB-C2B-C3B	3.34	130.93	124.68
24	b	605	CLA	O2D-CGD-CBD	3.34	117.20	111.27
27	A	611	PL9	C51-C49-C48	-3.34	113.00	122.65
24	b	617	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
24	C	508	CLA	C4D-C3D-CAD	-3.34	104.16	108.10
24	B	602	CLA	C1D-ND-C4D	-3.34	103.97	106.33
24	a	607	CLA	CHC-C1C-NC	3.33	129.26	124.20
24	B	616	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
28	a	612	SQD	C1-C2-C3	-3.33	103.06	110.00
32	c	517	DGD	O2G-C1B-C2B	3.33	118.67	111.50
24	b	606	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
24	d	402	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
24	C	501	CLA	C4D-C3D-CAD	-3.32	104.19	108.10
24	C	509	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
24	A	607	CLA	O1D-CGD-CBD	-3.32	117.70	124.48
28	a	612	SQD	O8-S-C6	3.31	111.02	105.74
28	A	612	SQD	C1-C2-C3	-3.31	103.10	110.00
32	E	101	DGD	C4E-C3E-C2E	3.31	116.60	110.82
24	c	507	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
24	b	609	CLA	C2A-C1A-CHA	3.31	129.64	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	608	PHO	CMB-C2B-C3B	3.31	130.86	124.68
26	t	101	BCR	C35-C13-C14	-3.30	118.30	122.92
24	C	512	CLA	C4-C3-C5	3.30	120.82	115.27
27	D	405	PL9	C15-C14-C16	-3.30	109.72	115.27
24	c	512	CLA	CHC-C1C-NC	3.29	129.20	124.20
24	c	504	CLA	CHC-C1C-NC	3.29	129.20	124.20
26	B	620	BCR	C37-C22-C21	-3.29	118.31	122.92
24	c	505	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
24	a	607	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
26	c	521	BCR	C34-C9-C10	-3.28	118.32	122.92
24	C	507	CLA	CHC-C1C-NC	3.28	129.19	124.20
24	c	512	CLA	C4-C3-C5	3.28	120.80	115.27
24	C	509	CLA	CHC-C1C-NC	3.28	129.18	124.20
24	b	608[B]	CLA	CHC-C1C-NC	3.28	129.18	124.20
32	C	516	DGD	O1G-C1A-C2A	3.28	122.20	111.91
24	B	604	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
24	c	512	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
24	D	402	CLA	CHC-C1C-NC	3.28	129.18	124.20
24	C	501	CLA	C1B-CHB-C4A	-3.28	123.63	130.12
24	C	505	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
26	B	620	BCR	C12-C13-C14	-3.27	113.92	118.94
26	T	101	BCR	C37-C22-C21	-3.27	118.34	122.92
26	F	101	BCR	C20-C21-C22	-3.27	122.64	127.31
24	c	501	CLA	CHC-C1C-NC	3.27	129.16	124.20
24	c	511	CLA	CHC-C1C-NC	3.27	129.16	124.20
26	k	101	BCR	C23-C22-C21	-3.26	113.94	118.94
26	K	101	BCR	C11-C12-C13	-3.26	117.27	126.42
24	a	607	CLA	C1D-ND-C4D	-3.25	104.02	106.33
24	C	502	CLA	CHC-C1C-NC	3.25	129.14	124.20
24	c	509	CLA	O1D-CGD-CBD	-3.25	117.83	124.48
24	b	614	CLA	C4-C3-C5	3.25	120.74	115.27
24	a	606	CLA	O2D-CGD-CBD	3.25	117.04	111.27
24	b	604	CLA	CHC-C1C-NC	3.25	129.13	124.20
26	h	101	BCR	C20-C19-C18	-3.25	117.30	126.42
24	b	614	CLA	CHC-C1C-NC	3.25	129.13	124.20
24	B	611	CLA	C4A-NA-C1A	-3.25	105.25	106.71
26	h	101	BCR	C37-C22-C21	-3.24	118.38	122.92
24	B	614	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	b	604	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
26	K	101	BCR	C23-C24-C25	-3.24	118.10	127.20
24	a	609	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
24	c	509	CLA	C1B-CHB-C4A	-3.24	123.71	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	O2A-CGA-CBA	3.24	122.06	111.91
26	t	101	BCR	C16-C15-C14	-3.24	116.85	123.47
24	B	604	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
26	T	101	BCR	C16-C15-C14	-3.23	116.85	123.47
24	B	603	CLA	C3A-C2A-C1A	3.23	106.18	101.34
26	t	101	BCR	C38-C26-C27	-3.23	107.42	113.62
24	B	615	CLA	C1D-ND-C4D	-3.22	104.05	106.33
26	K	101	BCR	C37-C22-C21	-3.22	118.41	122.92
26	T	101	BCR	C33-C5-C4	-3.22	107.43	113.62
24	c	502	CLA	CHC-C1C-NC	3.22	129.09	124.20
26	K	101	BCR	C33-C5-C4	-3.22	107.44	113.62
24	B	607[A]	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
28	x	101	SQD	O7-S-C6	3.22	110.76	106.94
24	b	606	CLA	O1D-CGD-CBD	-3.21	117.91	124.48
24	B	613	CLA	C4-C3-C5	3.21	120.68	115.27
27	D	405	PL9	C7-C3-C2	-3.21	119.08	123.30
27	D	405	PL9	C31-C29-C28	-3.21	114.62	121.12
24	B	608	CLA	CHB-C4A-NA	-3.21	120.08	124.51
25	D	401	PHO	CBA-CAA-C2A	-3.21	104.44	113.81
24	b	617	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
24	B	613	CLA	CBA-CAA-C2A	-3.21	104.40	113.86
24	C	509	CLA	O2D-CGD-CBD	3.20	116.96	111.27
24	b	615	CLA	C4A-NA-C1A	-3.20	105.27	106.71
24	C	502	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
24	c	512	CLA	C1-O2A-CGA	3.20	124.83	116.44
26	b	621	BCR	C20-C19-C18	-3.20	117.44	126.42
26	b	619	BCR	C27-C26-C25	-3.20	118.09	122.73
24	B	603	CLA	C4-C3-C5	3.19	120.64	115.27
26	k	101	BCR	C33-C5-C4	-3.19	107.48	113.62
26	b	621	BCR	C7-C8-C9	-3.19	121.41	126.23
26	k	101	BCR	C37-C22-C21	-3.19	118.46	122.92
24	B	613	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
24	B	613	CLA	C4D-C3D-CAD	-3.18	104.34	108.10
24	B	609	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
26	b	619	BCR	C30-C25-C24	-3.18	106.78	115.78
24	C	510	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
24	b	617	CLA	C1D-ND-C4D	-3.18	104.08	106.33
24	b	614	CLA	C4A-NA-C1A	-3.17	105.28	106.71
24	B	602	CLA	O2A-CGA-CBA	3.17	121.86	111.91
28	X	101	SQD	O7-S-C6	3.17	110.71	106.94
24	b	606	CLA	CHC-C1C-NC	3.17	129.01	124.20
24	d	402	CLA	CHC-C1C-NC	3.17	129.01	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	403	CLA	CHC-C1C-NC	3.17	129.01	124.20
24	C	513	CLA	C4D-C3D-CAD	-3.16	104.37	108.10
24	C	510	CLA	CHC-C1C-NC	3.16	129.00	124.20
24	c	504	CLA	C1-O2A-CGA	3.16	124.74	116.44
26	T	101	BCR	C38-C26-C27	-3.16	107.54	113.62
32	C	516	DGD	O6D-C5D-C4D	-3.16	103.96	109.69
24	B	609	CLA	CHD-C4C-C3C	3.16	129.48	124.84
24	b	604	CLA	C4-C3-C5	3.16	120.58	115.27
32	d	405	DGD	C4E-C3E-C2E	3.16	116.33	110.82
24	d	403	CLA	C4D-C3D-CAD	-3.15	104.38	108.10
23	A	605	BCT	O2-C-O1	-3.15	111.37	119.55
26	a	610	BCR	C11-C12-C13	-3.15	117.57	126.42
24	a	607	CLA	C4-C3-C5	3.15	120.57	115.27
32	C	516	DGD	C3E-C4E-C5E	3.15	115.86	110.24
27	d	404	PL9	C7-C3-C2	-3.15	119.16	123.30
24	a	609	CLA	C4A-NA-C1A	-3.15	105.29	106.71
26	b	620	BCR	C20-C19-C18	-3.15	117.58	126.42
24	C	510	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
24	B	607[A]	CLA	C1-O2A-CGA	3.14	124.69	116.44
24	b	604	CLA	CHB-C4A-NA	-3.14	120.17	124.51
26	A	610	BCR	C38-C26-C27	-3.14	107.58	113.62
33	v	201	HEM	C1B-NB-C4B	3.14	108.31	105.07
24	c	513	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
24	D	404	CLA	O1D-CGD-CBD	-3.13	118.07	124.48
24	A	607	CLA	C4-C3-C5	3.13	120.54	115.27
24	B	606	CLA	CHC-C1C-NC	3.13	128.95	124.20
26	B	619	BCR	C27-C26-C25	-3.13	118.19	122.73
24	C	513	CLA	C2A-C1A-CHA	3.13	129.33	123.86
33	v	201	HEM	CBA-CAA-C2A	-3.13	107.28	112.62
30	d	406	LHG	C5-O7-C7	-3.13	110.10	117.79
28	a	614	SQD	O6-C1-C2	3.13	113.18	108.30
29	A	613	LMG	O7-C10-C11	3.12	118.23	111.50
24	C	513	CLA	C4D-CHA-C1A	-3.12	117.45	121.25
24	B	608	CLA	CHC-C1C-NC	3.12	128.94	124.20
24	c	507	CLA	C4-C3-C5	3.12	120.52	115.27
27	D	405	PL9	C26-C24-C23	-3.12	114.80	121.12
24	C	505	CLA	C4D-C3D-CAD	-3.12	104.42	108.10
25	d	401	PHO	CMA-C3A-C4A	-3.12	107.54	114.38
24	D	404	CLA	CHC-C1C-NC	3.12	128.94	124.20
32	C	516	DGD	O2G-C1B-C2B	3.12	118.22	111.50
24	C	506	CLA	C4-C3-C5	3.12	120.52	115.27
24	D	403	CLA	CMC-C2C-C1C	3.12	129.79	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
24	B	606	CLA	C1D-ND-C4D	-3.12	104.12	106.33
24	b	612	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
29	B	621	LMG	C6-C5-C4	-3.11	105.72	113.00
28	X	101	SQD	O9-S-C6	3.10	110.63	106.94
24	b	608[A]	CLA	CHC-C1C-NC	3.10	128.91	124.20
24	B	609	CLA	O1D-CGD-CBD	-3.10	118.14	124.48
24	b	607	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
24	c	501	CLA	C4A-NA-C1A	-3.10	105.31	106.71
26	H	101	BCR	C8-C9-C10	-3.10	114.19	118.94
33	e	102	HEM	C4B-CHC-C1C	3.09	126.64	122.56
24	B	613	CLA	C2A-C1A-CHA	3.09	129.27	123.86
29	b	622	LMG	O7-C10-C11	3.09	118.17	111.50
24	c	506	CLA	C4-C3-C5	3.09	120.47	115.27
24	C	504	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
24	d	403	CLA	CHA-C1A-NA	-3.09	119.33	126.40
24	b	607	CLA	CHC-C1C-NC	3.08	128.88	124.20
24	B	611	CLA	C4D-C3D-CAD	-3.08	104.46	108.10
26	f	101	BCR	C36-C18-C19	3.08	122.93	118.08
28	x	101	SQD	O9-S-C6	3.08	110.60	106.94
26	H	101	BCR	C35-C13-C14	-3.08	118.61	122.92
24	B	612	CLA	C2A-C1A-CHA	3.08	129.24	123.86
24	A	606	CLA	O2A-CGA-CBA	3.08	121.56	111.91
26	f	101	BCR	C34-C9-C10	-3.08	118.61	122.92
24	C	507	CLA	O2A-CGA-CBA	3.08	121.56	111.91
27	a	611	PL9	C53-C6-C1	3.08	121.28	114.99
24	B	608	CLA	O2D-CGD-CBD	3.07	116.73	111.27
27	d	404	PL9	C7-C3-C4	3.07	119.37	116.88
26	I	101	BCR	C15-C14-C13	-3.07	122.93	127.31
24	b	617	CLA	C2A-C1A-CHA	3.07	129.22	123.86
24	b	614	CLA	CHA-C1A-NA	-3.07	119.37	126.40
24	C	507	CLA	C2D-C1D-ND	3.07	112.36	110.10
24	c	510	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
24	B	604	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
28	A	614	SQD	O6-C1-C2	3.06	113.09	108.30
29	b	622	LMG	C6-C5-C4	-3.06	105.83	113.00
24	b	610	CLA	C4A-NA-C1A	-3.06	105.33	106.71
33	v	201	HEM	C4C-CHD-C1D	3.06	126.60	122.56
24	a	615	CLA	O1D-CGD-CBD	-3.06	118.22	124.48
24	B	612	CLA	CHA-C1A-NA	-3.06	119.39	126.40
26	H	101	BCR	C10-C11-C12	-3.06	113.67	123.22
32	E	101	DGD	C3E-C4E-C5E	3.06	115.69	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	606	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
24	B	610	CLA	C4D-C3D-CAD	-3.05	104.50	108.10
24	C	513	CLA	CMB-C2B-C3B	3.05	130.39	124.68
27	D	405	PL9	C36-C34-C33	-3.05	114.94	121.12
24	b	613	CLA	C1-O2A-CGA	3.05	124.45	116.44
24	B	617	CLA	O2A-CGA-CBA	3.05	121.48	111.91
24	c	507	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	B	604	CLA	CHC-C1C-NC	3.05	128.83	124.20
24	b	606	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
26	b	620	BCR	C34-C9-C10	-3.05	118.65	122.92
26	B	620	BCR	C23-C24-C25	-3.05	118.65	127.20
24	B	611	CLA	CHC-C1C-NC	3.05	128.82	124.20
24	C	507	CLA	C4-C3-C5	3.04	120.39	115.27
24	B	612	CLA	O1D-CGD-CBD	-3.04	118.26	124.48
24	C	504	CLA	C4-C3-C5	3.04	120.38	115.27
26	A	610	BCR	C27-C26-C25	-3.04	118.32	122.73
26	F	101	BCR	C12-C13-C14	-3.03	114.29	118.94
32	c	517	DGD	O6D-C5D-C4D	-3.03	104.19	109.69
24	a	606	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
24	B	609	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
27	a	611	PL9	C51-C49-C48	-3.03	113.90	122.65
24	b	603	CLA	CHA-C1A-NA	-3.03	119.47	126.40
24	B	604	CLA	C4-C3-C5	3.03	120.36	115.27
24	A	609	CLA	C4A-NA-C1A	-3.03	105.35	106.71
24	b	605	CLA	C4-C3-C5	3.02	120.36	115.27
26	c	515	BCR	C36-C18-C17	-3.02	118.69	122.92
26	c	521	BCR	C33-C5-C4	-3.02	107.81	113.62
26	c	514	BCR	C3-C4-C5	-3.02	108.69	114.08
24	B	611	CLA	O2A-CGA-CBA	3.02	121.38	111.91
24	b	618	CLA	C2A-C1A-CHA	3.02	129.13	123.86
24	B	609	CLA	CAC-C3C-C2C	-3.01	122.37	127.53
24	a	609	CLA	C1-O2A-CGA	3.01	124.35	116.44
24	C	504	CLA	C4D-C3D-CAD	-3.01	104.55	108.10
24	b	612	CLA	O2A-CGA-CBA	3.01	121.36	111.91
25	a	608	PHO	O1D-CGD-CBD	3.01	129.75	124.74
32	c	517	DGD	O1G-C1A-C2A	3.01	121.34	111.91
24	c	504	CLA	C4-C3-C5	3.00	120.33	115.27
30	A	615	LHG	O8-C23-O10	-3.00	116.01	123.59
24	C	503	CLA	CHC-C1C-NC	3.00	128.76	124.20
24	c	506	CLA	C4A-NA-C1A	-2.99	105.36	106.71
24	c	513	CLA	C4D-C3D-CAD	-2.99	104.57	108.10
24	B	611	CLA	O2D-CGD-CBD	2.99	116.58	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
29	Z	101	LMG	O2-C2-C3	-2.99	103.44	110.35
24	b	606	CLA	C4D-C3D-CAD	-2.99	104.57	108.10
24	C	510	CLA	CHA-C1A-NA	-2.99	119.56	126.40
26	t	101	BCR	C20-C21-C22	-2.99	123.05	127.31
24	C	505	CLA	CHC-C1C-NC	2.99	128.73	124.20
26	c	515	BCR	C24-C25-C26	-2.99	114.23	121.46
24	C	511	CLA	C1-O2A-CGA	2.98	124.27	116.44
30	A	615	LHG	C5-O7-C7	-2.98	110.45	117.79
24	C	509	CLA	C4D-C3D-CAD	-2.98	104.58	108.10
24	B	612	CLA	C4D-C3D-CAD	-2.98	104.58	108.10
24	c	502	CLA	O1D-CGD-CBD	-2.98	118.39	124.48
24	B	612	CLA	CHC-C1C-NC	2.98	128.72	124.20
24	b	608[A]	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	b	604	CLA	C4D-C3D-CAD	-2.98	104.59	108.10
26	a	610	BCR	C33-C5-C4	-2.98	107.90	113.62
26	c	514	BCR	C31-C1-C6	-2.97	105.48	110.30
24	c	505	CLA	O2A-C1-C2	2.97	116.44	108.64
24	c	511	CLA	C1D-ND-C4D	-2.96	104.23	106.33
24	C	506	CLA	CHC-C1C-NC	2.96	128.70	124.20
24	C	504	CLA	CHC-C1C-NC	2.96	128.70	124.20
24	d	402	CLA	C3C-C4C-NC	-2.96	107.25	110.57
26	t	101	BCR	C2-C1-C6	2.96	115.04	110.48
24	D	403	CLA	O2A-CGA-CBA	2.96	121.19	111.91
24	b	613	CLA	CHA-C1A-NA	-2.96	119.63	126.40
24	b	608[B]	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
26	b	620	BCR	C35-C13-C14	-2.96	118.78	122.92
24	C	509	CLA	C1D-ND-C4D	-2.96	104.23	106.33
24	d	403	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
24	B	607[B]	CLA	C1-O2A-CGA	2.96	124.20	116.44
24	a	615	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
30	D	406	LHG	O7-C7-C8	2.95	117.86	111.50
26	t	101	BCR	C36-C18-C17	-2.95	118.79	122.92
24	A	607	CLA	CHA-C1A-NA	-2.95	119.64	126.40
24	a	606	CLA	CHA-C1A-NA	-2.95	119.65	126.40
26	B	620	BCR	C1-C6-C7	-2.95	107.44	115.78
24	b	605	CLA	CHA-C1A-NA	-2.95	119.65	126.40
33	E	103	HEM	C4B-CHC-C1C	2.95	126.45	122.56
24	B	608	CLA	C1-C2-C3	-2.94	120.95	126.04
24	A	609	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
24	b	618	CLA	C4D-C3D-CAD	-2.94	104.63	108.10
28	a	614	SQD	O48-C23-C24	2.94	121.13	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607[B]	CLA	C4-C3-C5	2.94	120.21	115.27
28	X	101	SQD	O48-C23-C24	2.94	121.12	111.91
24	b	610	CLA	CHC-C1C-NC	2.94	128.66	124.20
26	H	101	BCR	C33-C5-C4	-2.94	107.98	113.62
28	x	101	SQD	O48-C23-C24	2.93	121.11	111.91
24	b	608[B]	CLA	C4-C3-C5	2.93	120.20	115.27
29	C	518	LMG	C4-C3-C2	2.93	115.94	110.82
24	a	607	CLA	CMD-C2D-C1D	2.93	129.88	124.71
24	b	610	CLA	C4D-C3D-CAD	-2.93	104.65	108.10
32	C	516	DGD	C1D-O6D-C5D	-2.92	107.95	113.69
24	B	613	CLA	CHC-C1C-NC	2.92	128.64	124.20
27	a	611	PL9	C25-C24-C26	-2.92	110.36	115.27
25	D	401	PHO	C1-C2-C3	-2.92	120.99	126.04
28	A	614	SQD	O48-C23-C24	2.92	121.08	111.91
24	B	607[A]	CLA	C4-C3-C5	2.92	120.18	115.27
32	C	516	DGD	C4E-C3E-C2E	2.92	115.92	110.82
24	A	609	CLA	O1D-CGD-CBD	-2.92	118.51	124.48
26	a	610	BCR	C23-C24-C25	-2.92	119.01	127.20
26	F	101	BCR	C37-C22-C23	-2.91	113.49	118.08
24	B	608	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
24	c	502	CLA	CED-O2D-CGD	2.91	122.52	115.94
32	C	516	DGD	O6E-C5E-C6E	2.91	113.67	106.44
32	c	516	DGD	O6D-C5D-C4D	-2.91	104.41	109.69
24	C	505	CLA	O1D-CGD-CBD	-2.91	118.53	124.48
24	b	609	CLA	CHC-C1C-NC	2.91	128.62	124.20
26	H	101	BCR	C34-C9-C8	2.91	122.66	118.08
24	b	616	CLA	CHC-C1C-NC	2.91	128.61	124.20
26	A	610	BCR	C20-C19-C18	-2.91	118.25	126.42
27	d	404	PL9	C45-C44-C46	-2.91	110.38	115.27
24	a	609	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
24	b	609	CLA	C1-C2-C3	-2.90	121.02	126.04
24	c	507	CLA	O2A-CGA-CBA	2.90	121.02	111.91
24	B	611	CLA	C1D-ND-C4D	-2.90	104.27	106.33
24	B	616	CLA	O2A-CGA-CBA	2.90	121.02	111.91
24	b	608[A]	CLA	C1-O2A-CGA	2.90	124.05	116.44
25	d	401	PHO	C1-C2-C3	-2.90	121.03	126.04
26	c	514	BCR	C19-C18-C17	2.89	123.38	118.94
29	C	518	LMG	O6-C5-C4	2.89	114.93	109.69
24	b	608[A]	CLA	O1D-CGD-CBD	-2.88	118.58	124.48
26	K	101	BCR	C24-C25-C26	-2.88	114.48	121.46
24	B	611	CLA	CED-O2D-CGD	2.88	122.45	115.94
24	b	608[A]	CLA	C4-C3-C5	2.88	120.11	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	CHC-C1C-NC	2.88	128.57	124.20
24	a	615	CLA	C4-C3-C5	2.87	120.11	115.27
24	D	403	CLA	O2D-CGD-CBD	2.87	116.37	111.27
24	B	612	CLA	C1-C2-C3	-2.87	121.08	126.04
24	D	402	CLA	C4A-NA-C1A	-2.87	105.42	106.71
24	B	617	CLA	C2A-C1A-CHA	2.87	128.88	123.86
24	c	502	CLA	C4D-C3D-CAD	-2.87	104.72	108.10
24	b	614	CLA	O2A-CGA-CBA	2.87	120.90	111.91
24	c	512	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
24	b	606	CLA	CHA-C1A-NA	-2.86	119.84	126.40
24	A	607	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
28	A	612	SQD	C45-O47-C7	-2.86	110.75	117.79
24	A	606	CLA	CHA-C1A-NA	-2.86	119.84	126.40
24	C	502	CLA	C4D-C3D-CAD	-2.86	104.72	108.10
24	C	505	CLA	C1-O2A-CGA	2.86	123.95	116.44
28	a	612	SQD	C45-O47-C7	-2.86	110.76	117.79
24	b	616	CLA	C1D-ND-C4D	-2.85	104.31	106.33
24	c	509	CLA	C4D-C3D-CAD	-2.85	104.73	108.10
29	c	519	LMG	O8-C28-C29	2.85	120.86	111.91
24	c	507	CLA	C1D-ND-C4D	-2.85	104.31	106.33
26	B	618	BCR	C29-C30-C25	2.85	114.86	110.48
24	B	608	CLA	C4-C3-C5	2.85	120.06	115.27
24	b	613	CLA	C1-C2-C3	-2.85	121.12	126.04
29	c	520	LMG	O8-C28-C29	2.84	120.83	111.91
24	b	605	CLA	C1B-CHB-C4A	-2.84	124.48	130.12
24	a	606	CLA	CHB-C4A-NA	-2.84	120.58	124.51
24	D	402	CLA	C4-C3-C5	2.84	120.05	115.27
26	c	514	BCR	C10-C11-C12	-2.84	114.35	123.22
24	b	612	CLA	CHC-C1C-NC	2.84	128.51	124.20
26	B	620	BCR	C1-C6-C5	-2.84	118.62	122.61
24	b	612	CLA	O1D-CGD-CBD	-2.83	118.69	124.48
24	B	609	CLA	C4A-NA-C1A	-2.83	105.43	106.71
26	H	101	BCR	C20-C19-C18	-2.83	118.46	126.42
24	c	501	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	b	619	BCR	C2-C3-C4	2.83	117.70	111.38
24	D	403	CLA	CHB-C4A-NA	-2.83	120.60	124.51
24	b	615	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	b	618	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
24	c	513	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	c	512	CLA	O2A-CGA-CBA	2.83	120.77	111.91
24	a	609	CLA	CHC-C1C-NC	2.82	128.49	124.20
24	B	614	CLA	CHC-C1C-C2C	-2.82	118.91	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
32	h	102	DGD	C4D-C3D-C2D	2.82	115.75	110.82
24	b	609	CLA	C4-C3-C5	2.82	120.02	115.27
32	C	517	DGD	C3G-C2G-C1G	-2.82	105.12	111.79
24	B	611	CLA	CMA-C3A-C4A	-2.81	104.22	111.77
24	B	616	CLA	C1D-ND-C4D	-2.81	104.34	106.33
32	E	101	DGD	C1E-C2E-C3E	2.81	115.84	110.00
24	c	505	CLA	CHC-C1C-NC	2.81	128.46	124.20
24	d	403	CLA	O2A-CGA-CBA	2.81	120.72	111.91
24	b	611	CLA	CHC-C1C-NC	2.81	128.46	124.20
24	c	504	CLA	C4D-C3D-CAD	-2.81	104.79	108.10
24	b	613	CLA	CHC-C1C-C2C	-2.80	118.96	126.72
24	b	611	CLA	O2A-CGA-CBA	2.80	120.70	111.91
24	b	605	CLA	C4D-C3D-CAD	-2.80	104.79	108.10
26	k	101	BCR	C35-C13-C14	-2.80	119.00	122.92
24	c	501	CLA	O2A-CGA-CBA	2.80	120.70	111.91
28	a	612	SQD	C44-O6-C1	-2.80	108.27	113.74
26	C	514	BCR	C37-C22-C21	-2.80	119.00	122.92
24	D	402	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
24	b	615	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
26	B	618	BCR	C30-C25-C24	-2.79	107.88	115.78
28	l	101	SQD	C1-O5-C5	-2.79	108.21	113.69
24	b	606	CLA	CED-O2D-CGD	2.79	122.24	115.94
26	f	101	BCR	C19-C18-C17	2.78	123.21	118.94
28	L	102	SQD	C1-O5-C5	-2.78	108.22	113.69
26	b	621	BCR	C23-C24-C25	-2.78	119.39	127.20
28	A	612	SQD	C44-O6-C1	-2.78	108.31	113.74
27	d	404	PL9	C30-C29-C31	-2.78	110.60	115.27
24	b	605	CLA	C1-O2A-CGA	2.78	123.73	116.44
24	d	402	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
24	c	502	CLA	C1D-ND-C4D	-2.78	104.36	106.33
24	c	513	CLA	C1D-ND-C4D	-2.78	104.36	106.33
26	I	101	BCR	C1-C6-C7	-2.78	107.93	115.78
24	B	604	CLA	C4D-C3D-CAD	-2.77	104.83	108.10
33	V	201	HEM	C1D-C2D-C3D	-2.77	104.04	106.96
24	b	605	CLA	CED-O2D-CGD	2.77	122.20	115.94
30	D	406	LHG	O8-C23-C24	2.77	120.58	111.91
24	b	606	CLA	C4-C3-C5	2.76	119.92	115.27
24	C	508	CLA	C4-C3-C5	2.76	119.92	115.27
24	c	507	CLA	C4D-C3D-CAD	-2.76	104.84	108.10
24	c	507	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
24	c	508	CLA	C4-C3-C5	2.76	119.91	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608[B]	CLA	C1-O2A-CGA	2.76	123.68	116.44
25	d	401	PHO	O1D-CGD-CBD	2.76	129.33	124.74
24	C	512	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
25	D	401	PHO	O1D-CGD-CBD	2.76	129.33	124.74
24	C	511	CLA	CMB-C2B-C1B	-2.75	124.23	128.46
24	B	609	CLA	C4D-C3D-CAD	-2.75	104.85	108.10
25	a	608	PHO	C1-C2-C3	-2.75	121.29	126.04
24	b	609	CLA	CMD-C2D-C1D	2.75	129.56	124.71
24	C	513	CLA	O2A-CGA-CBA	2.75	120.53	111.91
24	D	402	CLA	C4D-C3D-CAD	-2.75	104.86	108.10
24	b	611	CLA	CED-O2D-CGD	2.75	122.15	115.94
24	b	613	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
24	C	506	CLA	CHB-C4A-NA	-2.75	120.72	124.51
24	b	610	CLA	C1D-ND-C4D	-2.74	104.39	106.33
24	B	614	CLA	C4A-NA-C1A	-2.74	105.47	106.71
24	B	608	CLA	C1D-ND-C4D	-2.74	104.39	106.33
24	B	605	CLA	C4-C3-C5	2.74	119.89	115.27
24	c	513	CLA	CHC-C1C-NC	2.74	128.36	124.20
27	A	611	PL9	C53-C6-C1	2.74	120.59	114.99
24	B	608	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	c	509	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
28	B	622	SQD	O48-C23-C24	2.74	120.50	111.91
24	A	609	CLA	C4D-C3D-CAD	-2.74	104.87	108.10
24	C	502	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
27	D	405	PL9	C40-C39-C41	-2.73	110.68	115.27
26	b	620	BCR	C10-C11-C12	-2.73	114.71	123.22
24	c	513	CLA	C4A-NA-C1A	-2.72	105.48	106.71
24	B	603	CLA	C4D-C3D-CAD	-2.72	104.89	108.10
24	b	616	CLA	C4D-C3D-CAD	-2.72	104.89	108.10
28	b	601	SQD	O48-C23-C24	2.72	120.44	111.91
30	E	102	LHG	O8-C23-C24	2.72	120.44	111.91
24	b	615	CLA	C4D-C3D-CAD	-2.72	104.89	108.10
30	l	102	LHG	O8-C23-C24	2.72	120.44	111.91
24	C	511	CLA	O1D-CGD-CBD	-2.72	118.93	124.48
24	b	610	CLA	CMB-C2B-C3B	2.72	129.76	124.68
30	D	406	LHG	C5-O7-C7	-2.71	111.11	117.79
28	L	102	SQD	O48-C23-C24	2.71	120.42	111.91
26	H	101	BCR	C19-C18-C17	2.71	123.10	118.94
26	T	101	BCR	C1-C6-C5	-2.71	118.80	122.61
25	D	401	PHO	O2D-CGD-CBD	2.71	114.43	111.00
24	c	506	CLA	C4D-C3D-CAD	-2.71	104.90	108.10
28	l	101	SQD	O48-C23-C24	2.71	120.41	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	CED-O2D-CGD	2.71	122.06	115.94
24	B	614	CLA	C1D-ND-C4D	-2.71	104.41	106.33
29	b	622	LMG	O8-C28-C29	2.71	120.40	111.91
24	C	504	CLA	CED-O2D-CGD	2.71	122.06	115.94
24	D	403	CLA	CMB-C2B-C1B	-2.71	124.31	128.46
26	A	610	BCR	C24-C25-C26	-2.70	114.91	121.46
26	h	101	BCR	C11-C12-C13	-2.70	118.82	126.42
24	c	504	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
24	b	612	CLA	CHB-C4A-NA	-2.70	120.78	124.51
24	b	618	CLA	CHA-C1A-NA	-2.70	120.21	126.40
24	D	403	CLA	CHA-C1A-NA	-2.70	120.21	126.40
26	b	621	BCR	C34-C9-C10	-2.70	119.14	122.92
24	C	512	CLA	O2A-CGA-CBA	2.70	120.37	111.91
24	D	403	CLA	C4-C3-C5	2.69	119.80	115.27
24	c	503	CLA	C4-C3-C5	2.69	119.80	115.27
26	I	101	BCR	C24-C25-C26	-2.69	114.94	121.46
26	B	618	BCR	C36-C18-C19	2.69	122.32	118.08
28	L	102	SQD	O8-S-C6	2.69	110.03	105.74
28	b	601	SQD	O9-S-C6	2.69	110.14	106.94
24	D	402	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	e	101	LHG	O8-C23-C24	2.69	120.35	111.91
26	K	101	BCR	C35-C13-C12	2.69	122.31	118.08
24	c	503	CLA	CHC-C1C-NC	2.69	128.28	124.20
24	c	512	CLA	CHA-C1A-NA	-2.69	120.24	126.40
25	d	401	PHO	O2D-CGD-O1D	-2.69	118.58	123.84
24	a	607	CLA	O2D-CGD-CBD	2.69	116.04	111.27
24	a	606	CLA	O2A-CGA-CBA	2.69	120.34	111.91
24	b	616	CLA	CMB-C2B-C3B	2.69	129.70	124.68
28	b	601	SQD	C4-C3-C2	2.68	115.50	110.82
26	K	102	BCR	C16-C15-C14	-2.68	117.98	123.47
24	b	603	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
30	d	406	LHG	O8-C23-C24	2.68	120.32	111.91
24	c	511	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	C	504	CLA	C1D-ND-C4D	-2.68	104.43	106.33
24	b	612	CLA	C4D-C3D-CAD	-2.68	104.94	108.10
28	B	622	SQD	O9-S-C6	2.68	110.12	106.94
32	c	518	DGD	C3G-O3G-C1D	-2.68	108.51	113.74
29	c	520	LMG	C3-C4-C5	2.67	115.01	110.24
28	B	622	SQD	C4-C3-C2	2.67	115.49	110.82
24	A	606	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
24	d	402	CLA	C4-C3-C5	2.67	119.76	115.27
24	b	607	CLA	O2D-CGD-O1D	-2.67	118.62	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	CED-O2D-CGD	2.67	121.97	115.94
24	b	617	CLA	C4D-C3D-CAD	-2.67	104.95	108.10
24	B	607[A]	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
24	b	618	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	c	511	CLA	O2A-CGA-CBA	2.67	120.28	111.91
24	B	608	CLA	CMB-C2B-C1B	-2.67	124.37	128.46
24	b	603	CLA	O2A-CGA-CBA	2.66	120.27	111.91
28	l	101	SQD	O8-S-C6	2.66	109.98	105.74
24	C	503	CLA	C4-C3-C5	2.66	119.75	115.27
26	c	515	BCR	C1-C6-C7	-2.66	108.24	115.78
26	I	101	BCR	C8-C9-C10	2.66	123.03	118.94
32	c	518	DGD	C2G-O2G-C1B	-2.66	111.24	117.79
24	b	608[B]	CLA	C1-C2-C3	-2.66	121.45	126.04
24	A	606	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
26	b	619	BCR	C36-C18-C19	2.66	122.26	118.08
24	c	510	CLA	CMB-C2B-C1B	-2.66	124.38	128.46
24	D	404	CLA	C4D-C3D-CAD	-2.65	104.97	108.10
24	C	513	CLA	CHA-C1A-NA	-2.65	120.32	126.40
32	E	101	DGD	O1G-C1A-C2A	2.65	120.23	111.91
24	b	608[B]	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
25	A	608	PHO	O2D-CGD-O1D	-2.65	118.66	123.84
24	d	402	CLA	O2A-CGA-CBA	2.65	120.21	111.91
24	B	607[B]	CLA	C1-C2-C3	-2.65	121.47	126.04
26	b	619	BCR	C33-C5-C4	-2.65	108.53	113.62
26	C	514	BCR	C12-C13-C14	-2.65	114.88	118.94
30	D	407	LHG	O8-C23-C24	2.64	120.20	111.91
24	C	509	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
27	d	404	PL9	C15-C14-C16	-2.64	110.83	115.27
24	B	611	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
24	c	512	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
24	a	615	CLA	CMB-C2B-C3B	2.64	129.62	124.68
30	d	407	LHG	C5-O7-C7	-2.64	111.30	117.79
26	c	521	BCR	C7-C8-C9	-2.64	122.25	126.23
24	b	607	CLA	C1D-ND-C4D	-2.64	104.46	106.33
24	C	513	CLA	CED-O2D-CGD	2.63	121.89	115.94
24	b	608[A]	CLA	CHA-C1A-NA	-2.63	120.37	126.40
24	c	509	CLA	O2A-CGA-CBA	2.63	120.16	111.91
24	A	607	CLA	C1D-ND-C4D	-2.63	104.47	106.33
24	B	606	CLA	CED-O2D-CGD	2.63	121.88	115.94
26	c	514	BCR	C29-C30-C25	2.63	114.53	110.48
24	c	504	CLA	C2D-C1D-ND	2.62	112.04	110.10
24	C	513	CLA	CHC-C1C-NC	2.62	128.18	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	CED-O2D-CGD	2.62	121.87	115.94
26	t	101	BCR	C30-C25-C24	-2.62	108.36	115.78
24	c	502	CLA	C4-C3-C5	2.62	119.68	115.27
24	C	508	CLA	C4A-NA-C1A	-2.62	105.53	106.71
26	T	101	BCR	C20-C19-C18	-2.62	119.06	126.42
24	A	607	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
32	d	405	DGD	O1G-C1A-C2A	2.62	120.13	111.91
26	t	101	BCR	C29-C30-C25	2.62	114.51	110.48
26	h	101	BCR	C30-C25-C24	-2.62	108.37	115.78
24	C	509	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
24	c	506	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	C	501	CLA	CHD-C4C-C3C	2.61	128.68	124.84
24	b	615	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
24	C	511	CLA	C4-C3-C5	2.61	119.66	115.27
26	K	101	BCR	C16-C15-C14	-2.61	118.13	123.47
32	C	517	DGD	O2E-C2E-C3E	-2.61	104.31	110.35
24	b	605	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
24	b	609	CLA	O1D-CGD-CBD	-2.61	119.15	124.48
27	D	405	PL9	C53-C6-C1	2.61	120.32	114.99
24	b	617	CLA	C4-C3-C5	2.61	119.65	115.27
24	a	609	CLA	O2A-CGA-CBA	2.60	120.08	111.91
24	C	509	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
30	D	406	LHG	O7-C7-O9	-2.59	117.43	123.70
26	B	619	BCR	C29-C30-C25	2.59	114.47	110.48
24	B	613	CLA	O2A-CGA-CBA	2.59	120.03	111.91
26	t	101	BCR	C8-C9-C10	-2.58	114.97	118.94
24	B	604	CLA	O2A-CGA-CBA	2.58	120.02	111.91
24	c	505	CLA	O1D-CGD-CBD	-2.58	119.20	124.48
33	v	201	HEM	CMB-C2B-C1B	-2.58	121.11	125.04
24	B	611	CLA	O2A-C1-C2	2.58	115.42	108.64
26	k	101	BCR	C36-C18-C17	-2.58	119.31	122.92
24	c	511	CLA	C4-C3-C5	2.58	119.61	115.27
24	b	618	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
24	C	502	CLA	C4-C3-C5	2.58	119.61	115.27
24	C	509	CLA	C1-O2A-CGA	2.58	123.21	116.44
24	c	501	CLA	C4D-C3D-CAD	-2.58	105.06	108.10
24	B	616	CLA	C4-C3-C5	2.58	119.61	115.27
26	c	514	BCR	C38-C26-C27	-2.58	108.67	113.62
24	C	512	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
24	c	512	CLA	C1-C2-C3	-2.58	121.59	126.04
32	h	102	DGD	O1G-C1A-C2A	2.57	119.99	111.91
26	B	620	BCR	C33-C5-C4	-2.57	108.67	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C4-C3-C5	2.57	119.60	115.27
24	B	603	CLA	C1-O2A-CGA	2.57	123.19	116.44
24	b	615	CLA	C4-C3-C5	2.57	119.60	115.27
26	c	521	BCR	C19-C18-C17	2.57	122.88	118.94
24	a	615	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
26	F	101	BCR	C34-C9-C10	-2.56	119.33	122.92
26	B	619	BCR	C36-C18-C17	-2.56	119.33	122.92
26	c	521	BCR	C29-C28-C27	2.56	117.10	111.38
24	D	402	CLA	C4D-CHA-C1A	-2.56	118.13	121.25
24	b	611	CLA	CHB-C4A-NA	-2.56	120.97	124.51
24	B	610	CLA	C1-O2A-CGA	2.56	123.16	116.44
24	B	614	CLA	C4-C3-C5	2.56	119.58	115.27
24	c	512	CLA	C2A-C1A-CHA	2.56	128.33	123.86
24	B	602	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
30	a	616	LHG	O8-C23-C24	2.56	119.93	111.91
24	b	613	CLA	CHB-C4A-NA	-2.56	120.98	124.51
24	C	502	CLA	CHA-C1A-NA	-2.55	120.55	126.40
24	b	603	CLA	CED-O2D-CGD	2.55	121.71	115.94
24	D	403	CLA	C2A-C1A-CHA	2.55	128.32	123.86
32	C	515	DGD	O6D-C5D-C6D	2.55	111.81	106.67
26	c	515	BCR	C30-C25-C24	-2.55	108.57	115.78
28	a	614	SQD	O8-S-C6	2.55	109.80	105.74
26	c	514	BCR	C30-C25-C24	-2.55	108.57	115.78
29	c	520	LMG	O6-C5-C4	2.55	114.32	109.69
28	A	612	SQD	C1-O5-C5	-2.55	108.69	113.69
24	c	501	CLA	CHA-C1A-NA	-2.54	120.57	126.40
24	A	609	CLA	CED-O2D-CGD	2.54	121.69	115.94
26	C	514	BCR	C1-C6-C5	-2.54	119.03	122.61
24	D	402	CLA	O2A-CGA-CBA	2.54	119.88	111.91
24	C	512	CLA	C1-C2-C3	-2.54	121.65	126.04
24	b	608[B]	CLA	CHA-C1A-NA	-2.54	120.58	126.40
24	b	618	CLA	CHB-C4A-NA	-2.54	121.00	124.51
24	b	615	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
26	a	610	BCR	C20-C19-C18	-2.54	119.29	126.42
28	A	614	SQD	O8-S-C6	2.53	109.78	105.74
32	c	517	DGD	O3G-C1D-C2D	2.53	112.26	108.30
24	B	602	CLA	CHC-C1C-NC	2.53	128.04	124.20
26	B	620	BCR	C2-C1-C6	2.53	114.38	110.48
32	c	516	DGD	C2G-O2G-C1B	-2.53	111.56	117.79
24	C	512	CLA	C4D-C3D-CAD	-2.53	105.11	108.10
24	C	513	CLA	C3C-C4C-NC	-2.53	107.73	110.57
32	c	517	DGD	O6E-C5E-C6E	2.53	112.72	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	z	101	LMG	O2-C2-C3	-2.53	104.51	110.35
24	B	609	CLA	CHB-C4A-NA	-2.53	121.02	124.51
24	C	512	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
24	d	403	CLA	C4-C3-C5	2.53	119.52	115.27
24	D	404	CLA	C4-C3-C5	2.52	119.52	115.27
24	B	615	CLA	CHA-C1A-NA	-2.52	120.62	126.40
32	c	516	DGD	O3G-C3G-C2G	-2.52	104.81	110.90
26	T	101	BCR	C36-C18-C17	-2.52	119.39	122.92
26	t	101	BCR	C3-C4-C5	-2.52	109.57	114.08
24	b	606	CLA	O2A-CGA-CBA	2.52	119.82	111.91
24	B	605	CLA	C4A-NA-C1A	-2.52	105.57	106.71
25	A	608	PHO	CMA-C3A-C4A	-2.52	108.86	114.38
24	c	510	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
24	c	502	CLA	C1-O2A-CGA	2.51	123.04	116.44
24	C	501	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
24	B	607[B]	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
32	E	101	DGD	C6D-C5D-C4D	-2.51	106.85	112.09
24	b	603	CLA	C1D-ND-C4D	-2.51	104.55	106.33
26	I	101	BCR	C23-C22-C21	-2.51	115.09	118.94
24	c	510	CLA	C1D-ND-C4D	-2.51	104.55	106.33
24	c	507	CLA	CHA-C1A-NA	-2.51	120.66	126.40
24	a	606	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
24	b	612	CLA	C4-C3-C5	2.50	119.48	115.27
24	c	505	CLA	C4D-C3D-CAD	-2.50	105.15	108.10
32	d	405	DGD	O2G-C1B-O1B	-2.50	117.66	123.70
28	a	612	SQD	C1-O5-C5	-2.50	108.78	113.69
24	B	616	CLA	CHA-C1A-NA	-2.50	120.68	126.40
24	b	604	CLA	CED-O2D-CGD	2.50	121.58	115.94
24	B	607[B]	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
24	D	402	CLA	CHC-C1C-C2C	-2.49	119.82	126.72
24	C	511	CLA	CHC-C1C-C2C	-2.49	119.82	126.72
24	C	504	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
24	b	612	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
24	C	501	CLA	C1-O2A-CGA	2.49	122.98	116.44
27	A	611	PL9	C7-C3-C2	-2.49	120.02	123.30
24	b	615	CLA	C1D-ND-C4D	-2.49	104.57	106.33
30	a	616	LHG	C5-O7-C7	-2.49	111.67	117.79
24	b	613	CLA	C4D-C3D-CAD	-2.49	105.17	108.10
26	B	618	BCR	C2-C1-C6	-2.49	106.66	110.48
24	b	611	CLA	C4D-C3D-CAD	-2.48	105.17	108.10
26	A	610	BCR	C40-C30-C25	-2.48	106.27	110.30
26	c	515	BCR	C8-C9-C10	2.48	122.74	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C4D-C3D-CAD	-2.48	105.18	108.10
24	b	605	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
24	c	501	CLA	C4D-CHA-C1A	-2.47	118.24	121.25
25	a	608	PHO	O2A-CGA-O1A	-2.47	117.35	123.59
24	B	613	CLA	CAC-C3C-C4C	2.47	128.02	124.81
24	b	611	CLA	C1-C2-C3	-2.47	121.77	126.04
24	D	404	CLA	C1D-ND-C4D	-2.47	104.58	106.33
24	B	617	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
24	B	604	CLA	C4A-NA-C1A	-2.47	105.60	106.71
24	B	615	CLA	CHC-C1C-NC	2.47	127.94	124.20
24	B	612	CLA	CED-O2D-CGD	2.47	121.52	115.94
24	C	510	CLA	C2A-C1A-CHA	2.46	128.17	123.86
26	C	514	BCR	C30-C25-C24	-2.46	108.81	115.78
32	h	102	DGD	O2G-C1B-O1B	-2.46	117.75	123.70
24	B	609	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
24	b	618	CLA	CBA-CAA-C2A	-2.46	106.59	113.86
32	E	101	DGD	O6D-C5D-C6D	2.46	111.64	106.67
26	b	621	BCR	C11-C12-C13	-2.46	119.50	126.42
24	b	608[A]	CLA	C1-C2-C3	-2.46	121.79	126.04
24	c	512	CLA	C4D-C3D-CAD	-2.46	105.20	108.10
24	D	403	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
24	C	512	CLA	O1D-CGD-CBD	-2.46	119.46	124.48
24	B	607[A]	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
26	c	515	BCR	C16-C15-C14	-2.46	118.44	123.47
24	b	612	CLA	CHA-C1A-NA	-2.46	120.78	126.40
33	E	103	HEM	C1D-C2D-C3D	-2.45	104.38	106.96
24	B	609	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
24	B	609	CLA	O2A-CGA-CBA	2.45	119.60	111.91
24	d	403	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
24	B	615	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
32	d	405	DGD	O6D-C5D-C6D	2.45	111.60	106.67
24	C	508	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
32	c	518	DGD	C3G-C2G-C1G	-2.45	106.00	111.79
24	c	504	CLA	CHA-C1A-NA	-2.45	120.80	126.40
24	b	606	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
24	C	507	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
24	b	603	CLA	CHC-C1C-C2C	-2.44	119.96	126.72
24	d	402	CLA	C4D-C3D-CAD	-2.44	105.22	108.10
24	b	614	CLA	CAC-C3C-C4C	2.44	127.98	124.81
24	B	604	CLA	CHA-C1A-NA	-2.44	120.81	126.40
29	D	408	LMG	O7-C10-O9	-2.44	117.80	123.70
24	b	604	CLA	CHA-C1A-NA	-2.44	120.81	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C4-C3-C5	2.44	119.37	115.27
24	c	513	CLA	C4-C3-C5	2.44	119.37	115.27
24	C	501	CLA	C1D-ND-C4D	-2.44	104.60	106.33
24	C	507	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
26	A	610	BCR	C34-C9-C8	2.43	121.91	118.08
26	c	514	BCR	C33-C5-C4	-2.43	108.94	113.62
24	B	605	CLA	CED-O2D-CGD	2.43	121.44	115.94
24	b	617	CLA	C1D-CHD-C4C	-2.43	120.81	126.06
26	B	619	BCR	C24-C25-C26	-2.43	115.57	121.46
26	b	619	BCR	C19-C18-C17	2.43	122.67	118.94
24	B	605	CLA	O2A-CGA-CBA	2.43	119.53	111.91
24	D	403	CLA	C1D-CHD-C4C	-2.43	120.81	126.06
24	c	513	CLA	O2A-CGA-CBA	2.43	119.53	111.91
24	B	607[A]	CLA	C1-C2-C3	-2.43	121.84	126.04
24	c	504	CLA	CHB-C4A-NA	-2.43	121.16	124.51
24	B	605	CLA	C1D-ND-C4D	-2.43	104.61	106.33
26	B	619	BCR	C12-C13-C14	2.42	122.66	118.94
26	T	101	BCR	C2-C1-C6	2.42	114.21	110.48
29	D	408	LMG	O8-C28-O10	-2.42	117.48	123.59
24	C	511	CLA	CHA-C1A-NA	-2.42	120.85	126.40
24	a	615	CLA	C4A-NA-C1A	-2.42	105.62	106.71
32	C	517	DGD	O6E-C5E-C6E	2.42	112.45	106.44
24	b	614	CLA	C1D-ND-C4D	-2.42	104.62	106.33
24	C	512	CLA	C1-O2A-CGA	2.42	122.78	116.44
26	b	621	BCR	C33-C5-C4	-2.41	108.98	113.62
24	B	610	CLA	C1-C2-C3	-2.41	121.87	126.04
29	a	613	LMG	O8-C28-C29	2.41	119.47	111.91
26	K	101	BCR	C34-C9-C8	2.41	121.88	118.08
24	C	510	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
26	b	620	BCR	C34-C9-C8	2.41	121.87	118.08
24	B	608	CLA	CHC-C1C-C2C	-2.41	120.07	126.72
24	C	501	CLA	CAC-C3C-C4C	2.40	127.93	124.81
32	C	515	DGD	O3G-C3G-C2G	-2.40	105.10	110.90
24	b	607	CLA	C4D-C3D-CAD	-2.40	105.26	108.10
24	c	511	CLA	CHA-C1A-NA	-2.40	120.90	126.40
24	a	609	CLA	C1D-ND-C4D	-2.40	104.63	106.33
24	C	503	CLA	CHA-C1A-NA	-2.40	120.90	126.40
24	B	612	CLA	C1D-ND-C4D	-2.40	104.63	106.33
24	D	402	CLA	C1D-ND-C4D	-2.40	104.63	106.33
24	C	512	CLA	CHA-C1A-NA	-2.40	120.90	126.40
24	B	603	CLA	CMB-C2B-C1B	-2.40	124.78	128.46
24	b	611	CLA	CBA-CAA-C2A	-2.40	106.79	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	C1D-ND-C4D	-2.40	104.63	106.33
26	f	101	BCR	C30-C25-C24	-2.39	109.00	115.78
24	c	508	CLA	C1D-ND-C4D	-2.39	104.63	106.33
32	H	102	DGD	C1D-C2D-C3D	2.39	114.98	110.00
26	K	101	BCR	C1-C6-C7	-2.39	109.01	115.78
24	b	618	CLA	O2A-CGA-CBA	2.39	119.42	111.91
24	d	403	CLA	C2D-C1D-ND	2.39	111.86	110.10
26	h	101	BCR	C10-C11-C12	-2.39	115.76	123.22
24	C	504	CLA	O2A-CGA-CBA	2.39	119.40	111.91
26	B	619	BCR	C40-C30-C25	2.39	114.17	110.30
24	B	612	CLA	C1-O2A-CGA	2.39	122.70	116.44
24	B	613	CLA	CHA-C1A-NA	-2.39	120.93	126.40
29	C	518	LMG	C1-C2-C3	2.38	114.96	110.00
24	b	609	CLA	CMB-C2B-C3B	2.38	129.14	124.68
24	C	501	CLA	CHC-C1C-NC	2.38	127.82	124.20
24	c	504	CLA	C4D-CHA-C1A	-2.38	118.35	121.25
24	B	617	CLA	CED-O2D-CGD	2.38	121.32	115.94
26	h	101	BCR	C11-C10-C9	-2.38	123.91	127.31
24	b	611	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
24	B	603	CLA	C1-C2-C3	-2.38	121.93	126.04
27	d	404	PL9	C53-C6-C1	2.38	119.85	114.99
24	B	613	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	C	510	CLA	C4D-C3D-CAD	-2.38	105.30	108.10
26	B	618	BCR	C1-C6-C7	-2.38	109.06	115.78
24	c	507	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
24	b	614	CLA	CHC-C1C-C2C	-2.37	120.15	126.72
24	b	607	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
24	c	503	CLA	C4D-C3D-CAD	-2.37	105.30	108.10
24	B	616	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
24	D	402	CLA	CHD-C4C-C3C	2.37	128.33	124.84
24	C	501	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
24	b	608[A]	CLA	C4D-C3D-CAD	-2.37	105.30	108.10
24	C	509	CLA	CHA-C1A-NA	-2.37	120.98	126.40
24	b	614	CLA	CBA-CAA-C2A	-2.37	106.88	113.86
24	B	616	CLA	C4D-C3D-CAD	-2.36	105.31	108.10
26	B	618	BCR	C2-C3-C4	2.36	116.66	111.38
26	k	101	BCR	C12-C13-C14	-2.36	115.31	118.94
24	A	606	CLA	C1D-CHD-C4C	-2.36	120.96	126.06
24	c	513	CLA	C3C-C4C-NC	-2.36	107.92	110.57
24	C	506	CLA	CMB-C2B-C3B	2.36	129.10	124.68
24	B	602	CLA	CMC-C2C-C1C	2.36	128.63	125.04
24	B	604	CLA	CHC-C1C-C2C	-2.36	120.19	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	608	PHO	C1-C2-C3	-2.36	121.97	126.04
24	b	612	CLA	CED-O2D-CGD	2.36	121.27	115.94
26	c	514	BCR	C12-C13-C14	-2.36	115.33	118.94
29	B	621	LMG	C3-C4-C5	2.35	114.44	110.24
24	B	605	CLA	CHC-C1C-C2C	-2.35	120.21	126.72
24	B	610	CLA	O2A-CGA-CBA	2.35	119.29	111.91
24	C	513	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	B	610	CLA	CHC-C1C-C2C	-2.35	120.22	126.72
30	A	615	LHG	O7-C7-O9	-2.35	118.02	123.70
24	C	508	CLA	CHC-C1C-C2C	-2.35	120.22	126.72
26	h	101	BCR	C1-C6-C7	-2.35	109.13	115.78
24	c	504	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	C	501	CLA	CHA-C1A-NA	-2.35	121.02	126.40
24	b	615	CLA	C1-O2A-CGA	2.35	122.61	116.44
24	B	603	CLA	O1D-CGD-CBD	-2.35	119.69	124.48
32	c	516	DGD	O1G-C1A-O1A	-2.35	117.67	123.59
33	V	201	HEM	C4C-CHD-C1D	2.34	125.65	122.56
24	a	615	CLA	CAA-CBA-CGA	-2.34	106.41	113.25
24	c	504	CLA	CED-O2D-CGD	2.34	121.23	115.94
26	c	521	BCR	C16-C15-C14	-2.34	118.68	123.47
24	b	605	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
24	b	604	CLA	O2A-CGA-CBA	2.34	119.25	111.91
29	A	613	LMG	O1-C1-C2	2.34	111.95	108.30
24	c	503	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
24	B	602	CLA	CHA-C1A-NA	-2.34	121.04	126.40
24	c	501	CLA	C1-O2A-CGA	2.34	122.57	116.44
24	b	609	CLA	CED-O2D-CGD	2.34	121.22	115.94
24	A	606	CLA	C1-O2A-CGA	2.33	122.57	116.44
24	b	604	CLA	C1-C2-C3	-2.33	122.01	126.04
26	T	101	BCR	C1-C6-C7	-2.33	109.18	115.78
24	c	501	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
24	b	618	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
24	B	612	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
24	A	609	CLA	C1-O2A-CGA	2.33	122.55	116.44
29	c	519	LMG	O7-C10-O9	-2.33	118.08	123.70
32	C	517	DGD	C2G-O2G-C1B	-2.33	112.06	117.79
26	f	101	BCR	C16-C15-C14	-2.32	118.71	123.47
25	A	608	PHO	O1D-CGD-CBD	2.32	128.61	124.74
24	d	403	CLA	CHB-C4A-NA	-2.32	121.30	124.51
24	a	607	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
26	F	101	BCR	C8-C9-C10	2.32	122.50	118.94
24	B	607[A]	CLA	O2A-CGA-CBA	2.32	119.19	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	h	102	DGD	O6D-C5D-C6D	2.32	111.35	106.67
24	B	607[B]	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
24	B	608	CLA	C4D-C3D-CAD	-2.32	105.36	108.10
24	b	617	CLA	O2A-CGA-CBA	2.32	119.19	111.91
24	c	506	CLA	CHA-C1A-NA	-2.32	121.09	126.40
24	B	607[A]	CLA	C4D-C3D-CAD	-2.32	105.36	108.10
32	H	102	DGD	O5E-C6E-C5E	-2.32	103.34	111.29
24	C	511	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
24	B	606	CLA	CMD-C2D-C1D	2.31	128.79	124.71
24	B	616	CLA	C4A-NA-C1A	-2.31	105.67	106.71
24	D	403	CLA	CBC-CAC-C3C	-2.31	106.05	112.43
24	B	610	CLA	CED-O2D-CGD	2.31	121.16	115.94
24	B	616	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
24	c	510	CLA	CHA-C1A-NA	-2.31	121.11	126.40
24	C	507	CLA	C4D-C3D-CAD	-2.31	105.38	108.10
24	C	504	CLA	C3C-C4C-NC	-2.31	107.98	110.57
28	a	614	SQD	C3-C4-C5	2.31	114.36	110.24
24	b	616	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
24	b	618	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
24	C	511	CLA	CHB-C4A-NA	-2.31	121.32	124.51
26	B	620	BCR	C11-C12-C13	-2.30	119.95	126.42
24	B	610	CLA	CHA-C1A-NA	-2.30	121.13	126.40
24	D	402	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
26	C	514	BCR	C11-C12-C13	-2.30	119.95	126.42
29	Z	101	LMG	O6-C5-C4	2.30	113.87	109.69
24	B	608	CLA	CHA-C1A-NA	-2.30	121.13	126.40
24	b	608[B]	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
24	C	503	CLA	O2A-C1-C2	2.30	114.67	108.64
24	c	511	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
24	B	610	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
24	C	506	CLA	C1D-ND-C4D	-2.30	104.70	106.33
26	c	515	BCR	C35-C13-C14	-2.30	119.71	122.92
29	D	408	LMG	O8-C28-C29	2.29	119.11	111.91
26	t	101	BCR	C33-C5-C4	-2.29	109.21	113.62
24	b	613	CLA	C1D-ND-C4D	-2.29	104.71	106.33
24	C	507	CLA	C1-O2A-CGA	2.29	122.46	116.44
24	b	610	CLA	C4-C3-C5	2.29	119.12	115.27
24	D	404	CLA	O2A-CGA-CBA	2.29	119.09	111.91
32	d	405	DGD	C1E-C2E-C3E	2.29	114.77	110.00
24	B	607[A]	CLA	CHA-C1A-NA	-2.29	121.15	126.40
32	c	516	DGD	O6D-C5D-C6D	2.29	111.29	106.67
24	b	608[B]	CLA	CMB-C2B-C1B	-2.29	124.94	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C1-O2A-CGA	2.29	122.45	116.44
24	c	508	CLA	CMB-C2B-C3B	2.29	128.96	124.68
24	d	402	CLA	CMA-C3A-C4A	-2.29	105.63	111.77
24	C	507	CLA	CHA-C1A-NA	-2.29	121.16	126.40
29	c	519	LMG	O6-C5-C4	2.29	113.84	109.69
24	C	505	CLA	CHD-C4C-C3C	2.28	128.20	124.84
32	E	101	DGD	O2G-C1B-O1B	-2.28	118.18	123.70
33	e	102	HEM	C1B-NB-C4B	2.28	107.43	105.07
24	B	609	CLA	C4-C3-C5	2.28	119.11	115.27
32	C	516	DGD	O1G-C1A-O1A	-2.28	117.83	123.59
30	d	407	LHG	O8-C23-C24	2.28	119.07	111.91
24	B	606	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
24	b	610	CLA	C11-C12-C13	-2.28	108.55	115.92
24	A	606	CLA	C4-C3-C5	2.28	119.11	115.27
24	A	606	CLA	C3C-C4C-NC	-2.28	108.01	110.57
25	D	401	PHO	C4A-C3A-C2A	-2.28	100.67	102.84
26	K	102	BCR	C39-C30-C25	-2.28	106.61	110.30
24	a	609	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
26	k	101	BCR	C11-C12-C13	-2.27	120.04	126.42
27	a	611	PL9	C3-C4-C5	2.27	121.55	118.60
24	d	402	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
24	C	504	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
28	A	614	SQD	C3-C4-C5	2.26	114.28	110.24
30	A	615	LHG	O8-C23-C24	2.26	119.01	111.91
24	A	607	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
32	d	405	DGD	C3E-C4E-C5E	2.26	114.28	110.24
24	a	607	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
24	B	610	CLA	CAC-C3C-C4C	2.26	127.74	124.81
24	d	403	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
24	b	614	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
24	B	611	CLA	CHA-C1A-NA	-2.26	121.22	126.40
32	c	518	DGD	O4D-C4D-C3D	-2.26	105.13	110.35
24	a	609	CLA	CED-O2D-CGD	2.26	121.05	115.94
24	B	605	CLA	CHA-C1A-NA	-2.26	121.23	126.40
26	F	101	BCR	C30-C25-C24	-2.26	109.39	115.78
24	C	508	CLA	CMB-C2B-C3B	2.26	128.90	124.68
29	C	518	LMG	O1-C7-C8	-2.25	105.46	110.90
24	B	616	CLA	CHC-C1C-C2C	-2.25	120.48	126.72
24	A	609	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
24	c	502	CLA	CMB-C2B-C1B	-2.25	125.00	128.46
25	a	608	PHO	O2D-CGD-O1D	-2.25	119.43	123.84
24	B	607[B]	CLA	C3C-C4C-NC	-2.25	108.05	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	CMB-C2B-C3B	2.25	128.89	124.68
24	B	604	CLA	CHD-C4C-C3C	2.25	128.15	124.84
24	c	504	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
24	A	609	CLA	CHC-C1C-NC	2.25	127.61	124.20
24	c	513	CLA	CMB-C2B-C3B	2.25	128.88	124.68
24	b	608[B]	CLA	C1D-ND-C4D	-2.25	104.74	106.33
24	B	609	CLA	C11-C12-C13	-2.25	108.65	115.92
24	c	504	CLA	C3C-C4C-NC	-2.25	108.05	110.57
29	A	613	LMG	O8-C28-O10	-2.25	117.92	123.59
24	c	513	CLA	CHA-C1A-NA	-2.24	121.26	126.40
24	B	613	CLA	CHD-C4C-C3C	2.24	128.14	124.84
24	B	611	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
24	C	511	CLA	O2A-CGA-CBA	2.24	118.95	111.91
26	k	101	BCR	C20-C19-C18	-2.24	120.11	126.42
29	j	101	LMG	O8-C28-O10	-2.24	117.93	123.59
24	a	606	CLA	C4-C3-C5	2.24	119.04	115.27
29	D	408	LMG	C1-O6-C5	2.24	118.09	113.69
24	D	402	CLA	C3C-C4C-NC	-2.24	108.06	110.57
24	b	614	CLA	C2A-C1A-CHA	2.24	127.78	123.86
24	A	609	CLA	CHD-C4C-C3C	2.24	128.13	124.84
24	c	510	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
32	C	515	DGD	C3G-C2G-C1G	-2.24	106.49	111.79
26	F	101	BCR	C38-C26-C27	-2.24	109.32	113.62
24	c	503	CLA	CHA-C1A-NA	-2.24	121.27	126.40
24	b	607	CLA	CED-O2D-CGD	2.24	121.00	115.94
24	B	608	CLA	O2A-CGA-CBA	2.24	118.92	111.91
24	B	610	CLA	CHD-C4C-C3C	2.24	128.13	124.84
32	C	516	DGD	C1E-C2E-C3E	2.23	114.65	110.00
33	V	201	HEM	C4B-C3B-C2B	-2.23	105.34	107.11
24	c	502	CLA	CHA-C1A-NA	-2.23	121.28	126.40
24	a	606	CLA	C4D-C3D-CAD	-2.23	105.47	108.10
24	b	605	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
24	B	614	CLA	CMD-C2D-C1D	2.23	128.65	124.71
24	A	609	CLA	O2A-CGA-CBA	2.23	118.91	111.91
24	C	512	CLA	C2A-C1A-CHA	2.23	127.76	123.86
24	B	610	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
29	C	518	LMG	O4-C4-C5	2.23	114.83	109.30
24	C	503	CLA	C1D-CHD-C4C	-2.23	121.25	126.06
24	B	615	CLA	CMD-C2D-C1D	2.23	128.63	124.71
24	C	505	CLA	C4D-CHA-C1A	-2.23	118.54	121.25
24	C	502	CLA	CHC-C1C-C2C	-2.22	120.57	126.72
24	B	616	CLA	CED-O2D-CGD	2.22	120.96	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	101	BCR	C28-C27-C26	-2.22	110.11	114.08
29	a	613	LMG	O8-C28-O10	-2.22	118.00	123.59
29	B	621	LMG	O7-C10-C11	2.22	116.28	111.50
24	b	615	CLA	C1-C2-C3	-2.21	122.21	126.04
28	A	612	SQD	O48-C23-C24	2.21	118.86	111.91
28	x	101	SQD	O48-C23-O10	-2.21	118.01	123.59
24	B	609	CLA	C1D-ND-C4D	-2.21	104.76	106.33
24	D	404	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
26	B	618	BCR	C16-C15-C14	-2.21	118.94	123.47
26	A	610	BCR	C1-C6-C7	-2.21	109.52	115.78
26	C	514	BCR	C8-C9-C10	2.21	122.33	118.94
24	b	615	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	j	101	LMG	O7-C10-C11	2.21	116.26	111.50
26	c	514	BCR	C37-C22-C21	-2.21	119.83	122.92
32	c	517	DGD	O2G-C1B-O1B	-2.21	118.37	123.70
28	X	101	SQD	O48-C23-O10	-2.21	118.03	123.59
24	B	607[B]	CLA	O2A-CGA-CBA	2.20	118.83	111.91
24	c	509	CLA	CHC-C1C-C2C	-2.20	120.62	126.72
32	E	101	DGD	O6E-C5E-C6E	2.20	111.91	106.44
24	A	607	CLA	CHD-C4C-C3C	2.20	128.08	124.84
24	b	608[A]	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
24	B	603	CLA	O2A-CGA-CBA	2.20	118.81	111.91
24	D	403	CLA	CED-O2D-CGD	2.20	120.91	115.94
24	B	614	CLA	C1-O2A-CGA	2.20	122.22	116.44
24	C	501	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
28	a	612	SQD	O48-C23-C24	2.20	118.81	111.91
26	I	101	BCR	C23-C24-C25	-2.20	121.03	127.20
26	T	101	BCR	C30-C25-C24	-2.20	109.56	115.78
24	C	503	CLA	CMD-C2D-C1D	2.20	128.59	124.71
29	Z	101	LMG	O7-C10-O9	-2.20	118.39	123.70
24	B	614	CLA	C1-C2-C3	-2.20	122.25	126.04
24	d	403	CLA	CHC-C1C-C2C	-2.20	120.65	126.72
24	B	607[A]	CLA	C3C-C4C-NC	-2.20	108.11	110.57
26	B	620	BCR	C3-C4-C5	-2.19	110.16	114.08
24	B	602	CLA	C1-O2A-CGA	2.19	122.20	116.44
24	c	501	CLA	CHD-C4C-C3C	2.19	128.06	124.84
24	c	510	CLA	CED-O2D-CGD	2.19	120.89	115.94
26	H	101	BCR	C11-C12-C13	-2.19	120.26	126.42
33	V	201	HEM	CAD-C3D-C4D	2.19	128.49	124.66
24	C	511	CLA	C1D-ND-C4D	-2.19	104.78	106.33
29	A	613	LMG	O8-C28-C29	2.19	118.78	111.91
24	c	503	CLA	O2A-CGA-CBA	2.19	118.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	518	LMG	O8-C28-O10	-2.19	118.07	123.59
24	b	609	CLA	CHA-C1A-NA	-2.19	121.39	126.40
24	C	501	CLA	C4-C3-C5	2.19	118.95	115.27
24	c	501	CLA	CED-O2D-CGD	2.18	120.88	115.94
33	E	103	HEM	CMD-C2D-C1D	2.18	128.37	125.04
24	A	607	CLA	CMD-C2D-C1D	2.18	128.56	124.71
24	C	502	CLA	C1D-ND-C4D	-2.18	104.78	106.33
24	a	606	CLA	C1D-CHD-C4C	-2.18	121.35	126.06
24	a	609	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
26	h	101	BCR	C2-C3-C4	2.18	116.25	111.38
26	b	620	BCR	C29-C30-C25	2.18	113.84	110.48
28	a	612	SQD	O48-C23-O10	-2.18	118.09	123.59
32	d	405	DGD	C6D-C5D-C4D	-2.18	107.54	112.09
24	c	506	CLA	O2A-CGA-CBA	2.18	118.75	111.91
26	t	101	BCR	C39-C30-C25	-2.18	106.76	110.30
24	c	501	CLA	C4-C3-C5	2.18	118.94	115.27
24	b	617	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
24	C	511	CLA	C3C-C4C-NC	-2.17	108.13	110.57
24	b	609	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	I	101	BCR	C19-C18-C17	2.17	122.27	118.94
26	B	619	BCR	C28-C27-C26	2.17	117.95	114.08
24	c	505	CLA	CMB-C2B-C3B	2.17	128.74	124.68
24	C	508	CLA	CHA-C1A-NA	-2.17	121.42	126.40
26	b	620	BCR	C28-C27-C26	2.17	117.95	114.08
28	A	612	SQD	O48-C23-O10	-2.17	118.12	123.59
24	c	512	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
26	T	101	BCR	C3-C4-C5	-2.17	110.21	114.08
26	f	101	BCR	C20-C19-C18	-2.17	120.33	126.42
26	c	514	BCR	C35-C13-C12	2.17	121.49	118.08
24	b	608[B]	CLA	CHD-C4C-C3C	2.17	128.02	124.84
24	c	508	CLA	C3C-C4C-NC	-2.16	108.14	110.57
24	c	509	CLA	C2D-C1D-ND	2.16	111.70	110.10
26	t	101	BCR	C1-C6-C7	-2.16	109.66	115.78
24	c	510	CLA	CMD-C2D-C1D	2.16	128.52	124.71
24	A	606	CLA	C4D-C3D-CAD	-2.16	105.55	108.10
24	B	612	CLA	CHD-C4C-C3C	2.16	128.01	124.84
30	D	407	LHG	O8-C23-O10	-2.16	118.15	123.59
29	D	408	LMG	C3-C4-C5	2.15	114.08	110.24
24	B	609	CLA	CMB-C2B-C3B	2.15	128.71	124.68
24	b	614	CLA	CMB-C2B-C1B	-2.15	125.15	128.46
29	C	519	LMG	O8-C28-C29	2.15	118.66	111.91
24	B	607[B]	CLA	C1D-ND-C4D	-2.15	104.81	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CHA-C1A-NA	-2.15	121.47	126.40
24	b	618	CLA	C4A-NA-C1A	-2.15	105.74	106.71
32	d	405	DGD	O1G-C1A-O1A	-2.15	118.17	123.59
24	c	508	CLA	O2A-CGA-CBA	2.15	118.65	111.91
24	c	511	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
24	B	614	CLA	CHA-C1A-NA	-2.15	121.48	126.40
24	B	611	CLA	C2D-C1D-ND	2.15	111.69	110.10
24	b	612	CLA	CHD-C4C-C3C	2.14	127.99	124.84
24	a	607	CLA	CED-O2D-CGD	2.14	120.78	115.94
24	b	614	CLA	CAC-C3C-C2C	-2.14	123.87	127.53
28	b	601	SQD	O47-C7-O49	-2.14	118.53	123.70
24	B	610	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
26	c	521	BCR	C23-C24-C25	-2.14	121.19	127.20
24	B	617	CLA	CAC-C3C-C4C	2.14	127.59	124.81
24	b	608[A]	CLA	O2A-CGA-CBA	2.14	118.62	111.91
24	C	506	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
26	C	514	BCR	C1-C6-C7	-2.14	109.73	115.78
29	C	519	LMG	C3-C4-C5	2.14	114.05	110.24
24	B	612	CLA	CMB-C2B-C3B	2.14	128.68	124.68
24	B	613	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
24	B	607[B]	CLA	CHA-C1A-NA	-2.14	121.51	126.40
26	C	514	BCR	C35-C13-C14	-2.14	119.93	122.92
26	T	101	BCR	C23-C22-C21	2.13	122.22	118.94
24	B	617	CLA	CHA-C1A-NA	-2.13	121.51	126.40
24	C	505	CLA	CHA-C1A-NA	-2.13	121.51	126.40
24	B	614	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
24	B	617	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
24	b	608[A]	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
28	B	622	SQD	O47-C7-O49	-2.13	118.55	123.70
24	c	504	CLA	C7-C6-C5	-2.13	107.58	113.36
24	B	608	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
24	A	607	CLA	CMB-C2B-C3B	2.12	128.65	124.68
32	c	516	DGD	O2G-C1B-O1B	-2.12	118.58	123.70
24	B	608	CLA	C4D-CHA-C1A	-2.12	118.67	121.25
24	b	616	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	c	509	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	B	607[B]	CLA	C4D-C3D-CAD	-2.12	105.60	108.10
24	C	504	CLA	C7-C6-C5	-2.12	107.61	113.36
24	B	603	CLA	CHC-C1C-C2C	-2.12	120.87	126.72
24	C	509	CLA	O2A-CGA-CBA	2.12	118.55	111.91
26	K	101	BCR	C20-C21-C22	-2.12	124.29	127.31
32	C	515	DGD	O1G-C1A-O1A	-2.11	118.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	101	LHG	O8-C23-C24	2.11	118.54	111.91
25	d	401	PHO	CMD-C2D-C3D	2.11	128.63	124.68
24	b	608[A]	CLA	C1D-ND-C4D	-2.11	104.83	106.33
24	C	512	CLA	CED-O2D-CGD	2.11	120.72	115.94
24	a	607	CLA	C4D-C3D-CAD	-2.11	105.61	108.10
24	C	508	CLA	C1D-ND-C4D	-2.11	104.83	106.33
28	b	601	SQD	O5-C1-C2	-2.11	105.88	110.35
24	c	505	CLA	CHD-C4C-C3C	2.11	127.94	124.84
24	d	402	CLA	CHD-C4C-C3C	2.11	127.94	124.84
26	c	514	BCR	C37-C22-C23	-2.11	114.76	118.08
24	C	504	CLA	CHA-C1A-NA	-2.11	121.57	126.40
24	C	510	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
24	b	618	CLA	C4-C3-C5	2.10	118.81	115.27
24	b	603	CLA	CHB-C4A-NA	-2.10	121.60	124.51
24	a	615	CLA	C4D-C3D-CAD	-2.10	105.62	108.10
24	c	509	CLA	C4-C3-C5	2.10	118.81	115.27
24	c	502	CLA	CHC-C1C-C2C	-2.10	120.91	126.72
24	B	617	CLA	C4-C3-C5	2.10	118.81	115.27
25	D	401	PHO	CMA-C3A-C4A	-2.10	109.78	114.38
29	z	101	LMG	O1-C1-C2	2.10	111.58	108.30
24	A	606	CLA	C1D-ND-C4D	-2.10	104.84	106.33
28	B	622	SQD	O5-C1-C2	-2.10	105.91	110.35
30	L	101	LHG	O8-C23-O10	-2.10	118.30	123.59
24	b	612	CLA	C1D-ND-C4D	-2.10	104.85	106.33
23	A	605	BCT	O3-C-O1	-2.10	114.11	119.55
24	b	614	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
24	C	501	CLA	C1-C2-C3	-2.09	122.42	126.04
24	C	510	CLA	CMD-C2D-C1D	2.09	128.40	124.71
24	C	511	CLA	C4D-C3D-CAD	-2.09	105.63	108.10
26	C	514	BCR	C3-C4-C5	-2.09	110.34	114.08
26	t	101	BCR	C19-C18-C17	2.09	122.15	118.94
24	C	512	CLA	C1D-CHD-C4C	-2.09	121.55	126.06
32	c	517	DGD	C4E-C3E-C2E	2.09	114.47	110.82
24	B	609	CLA	C11-C10-C8	-2.09	109.17	115.92
24	b	610	CLA	C11-C10-C8	-2.09	109.17	115.92
24	c	512	CLA	CHC-C1C-C2C	-2.09	120.95	126.72
24	D	404	CLA	CMB-C2B-C3B	2.09	128.58	124.68
24	a	606	CLA	CBA-CAA-C2A	-2.09	107.71	113.86
24	b	618	CLA	CED-O2D-CGD	2.09	120.65	115.94
24	c	501	CLA	C1-C2-C3	-2.08	122.44	126.04
24	B	611	CLA	CHD-C4C-C3C	2.08	127.90	124.84
24	b	617	CLA	C11-C10-C8	-2.08	109.18	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	403	CLA	CHC-C1C-C2C	-2.08	120.96	126.72
24	C	509	CLA	C4-C3-C5	2.08	118.77	115.27
24	B	603	CLA	CHB-C4A-NA	-2.08	121.64	124.51
33	E	103	HEM	CMA-C3A-C4A	-2.08	125.27	128.46
28	X	101	SQD	C3-C4-C5	2.08	113.95	110.24
26	b	620	BCR	C36-C18-C17	-2.08	120.01	122.92
24	B	605	CLA	C1-O2A-CGA	2.08	121.90	116.44
24	B	615	CLA	CED-O2D-CGD	2.08	120.64	115.94
26	b	619	BCR	C35-C13-C14	2.08	125.83	122.92
26	B	618	BCR	C39-C30-C25	-2.08	106.93	110.30
30	a	616	LHG	C9-C8-C7	-2.07	106.08	113.62
24	b	605	CLA	O2A-CGA-CBA	2.07	118.41	111.91
24	B	616	CLA	C11-C10-C8	-2.07	109.23	115.92
32	h	102	DGD	O3G-C3G-C2G	-2.07	105.90	110.90
29	C	519	LMG	O6-C5-C4	2.07	113.45	109.69
26	b	620	BCR	C32-C1-C6	-2.07	106.94	110.30
24	C	501	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
26	b	620	BCR	C11-C12-C13	-2.07	120.60	126.42
24	b	608[B]	CLA	O2A-CGA-CBA	2.07	118.40	111.91
24	b	608[B]	CLA	C3C-C4C-NC	-2.07	108.25	110.57
27	D	405	PL9	C20-C19-C21	-2.07	111.79	115.27
27	d	404	PL9	C10-C9-C11	-2.07	111.79	115.27
24	d	402	CLA	C1D-ND-C4D	-2.07	104.87	106.33
24	C	503	CLA	O2A-CGA-CBA	2.07	118.39	111.91
24	B	615	CLA	CHC-C1C-C2C	-2.07	121.01	126.72
24	B	607[A]	CLA	CMB-C2B-C1B	-2.07	125.29	128.46
29	b	622	LMG	O1-C7-C8	-2.06	105.92	110.90
24	b	610	CLA	CHB-C4A-NA	-2.06	121.66	124.51
24	B	606	CLA	CBA-CAA-C2A	-2.06	107.77	113.86
26	F	101	BCR	C28-C27-C26	-2.06	110.39	114.08
25	A	608	PHO	O2A-CGA-O1A	-2.06	118.39	123.59
26	b	620	BCR	C35-C13-C12	2.06	121.32	118.08
24	c	503	CLA	CMD-C2D-C1D	2.06	128.34	124.71
32	c	518	DGD	C3D-C4D-C5D	2.06	113.91	110.24
24	C	510	CLA	C4-C3-C5	2.06	118.73	115.27
24	b	611	CLA	CHA-C1A-NA	-2.06	121.69	126.40
24	C	506	CLA	C4A-NA-C1A	-2.06	105.78	106.71
29	j	101	LMG	O7-C10-O9	-2.05	118.74	123.70
24	B	603	CLA	C3C-C4C-NC	-2.05	108.27	110.57
24	a	606	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
28	A	612	SQD	O5-C1-C2	-2.05	106.00	110.35
26	b	621	BCR	C1-C6-C7	-2.05	109.97	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j	101	LMG	O6-C5-C4	2.05	113.42	109.69
24	b	610	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
24	b	617	CLA	CHA-C1A-NA	-2.05	121.70	126.40
24	B	616	CLA	C3C-C4C-NC	-2.05	108.27	110.57
26	f	101	BCR	C12-C13-C14	-2.05	115.80	118.94
30	a	616	LHG	O7-C7-O9	-2.05	118.75	123.70
24	C	502	CLA	O2A-CGA-CBA	2.05	118.34	111.91
26	k	101	BCR	C8-C9-C10	-2.05	115.80	118.94
28	x	101	SQD	C3-C4-C5	2.05	113.89	110.24
24	a	615	CLA	CMA-C3A-C4A	-2.05	106.27	111.77
24	d	402	CLA	CHB-C4A-NA	-2.05	121.68	124.51
24	d	403	CLA	C6-C7-C8	-2.04	109.31	115.92
26	c	521	BCR	C36-C18-C19	-2.04	114.86	118.08
24	D	402	CLA	O2D-CGD-CBD	2.04	114.90	111.27
24	a	609	CLA	C4D-C3D-CAD	-2.04	105.69	108.10
24	b	616	CLA	C1-O2A-CGA	2.04	121.80	116.44
26	H	101	BCR	C35-C13-C12	2.04	121.29	118.08
29	C	518	LMG	O6-C5-C6	2.04	111.51	106.44
32	c	518	DGD	O2G-C1B-O1B	-2.04	118.77	123.70
24	a	615	CLA	CHD-C4C-C3C	2.04	127.84	124.84
28	l	101	SQD	C4-C3-C2	2.04	114.38	110.82
24	b	608[B]	CLA	C4D-C3D-CAD	-2.04	105.69	108.10
32	c	517	DGD	C1E-O6E-C5E	-2.04	109.69	113.69
24	B	603	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	b	612	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
27	A	611	PL9	C25-C24-C26	-2.03	111.85	115.27
32	c	517	DGD	O1G-C1A-O1A	-2.03	118.46	123.59
29	b	622	LMG	C8-O7-C10	-2.03	112.78	117.79
24	b	603	CLA	CMD-C2D-C1D	2.03	128.30	124.71
24	c	508	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
28	L	102	SQD	C4-C3-C2	2.03	114.37	110.82
24	a	606	CLA	C1D-ND-C4D	-2.03	104.89	106.33
27	D	405	PL9	C3-C2-C1	-2.03	118.70	122.52
24	B	613	CLA	CHD-C1D-ND	2.03	126.32	124.45
33	v	201	HEM	CAA-CBA-CGA	-2.03	108.07	113.76
24	B	610	CLA	CHB-C4A-NA	-2.03	121.70	124.51
24	b	613	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
28	a	612	SQD	O5-C1-C2	-2.03	106.05	110.35
24	c	510	CLA	C1-O2A-CGA	2.03	121.76	116.44
24	c	510	CLA	C4-C3-C5	2.03	118.68	115.27
33	e	102	HEM	CMC-C2C-C3C	2.03	128.47	124.68
24	B	609	CLA	C3C-C4C-NC	-2.03	108.30	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	518	LMG	O7-C10-O9	-2.03	118.80	123.70
24	B	606	CLA	CHC-C1C-C2C	-2.03	121.12	126.72
24	C	505	CLA	CHC-C1C-C2C	-2.03	121.12	126.72
24	C	513	CLA	CMC-C2C-C1C	2.03	128.12	125.04
24	D	404	CLA	C6-C7-C8	-2.03	109.37	115.92
32	E	101	DGD	O1B-C1B-C2B	-2.03	115.83	123.73
24	b	611	CLA	CHC-C1C-C2C	-2.02	121.12	126.72
24	c	504	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
28	L	102	SQD	O9-S-C6	2.02	109.34	106.94
32	C	516	DGD	O2G-C1B-O1B	-2.02	118.82	123.70
32	H	102	DGD	O6D-C1D-C2D	2.02	114.63	110.35
26	b	619	BCR	C39-C30-C25	-2.02	107.02	110.30
26	f	101	BCR	C28-C29-C30	-2.02	107.38	114.60
26	B	620	BCR	C10-C11-C12	-2.02	116.91	123.22
28	l	101	SQD	O9-S-C6	2.02	109.34	106.94
24	B	607[A]	CLA	C1D-ND-C4D	-2.02	104.90	106.33
24	C	505	CLA	C1D-ND-C4D	-2.02	104.90	106.33
24	c	501	CLA	CMB-C2B-C3B	2.02	128.46	124.68
24	b	603	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
24	A	609	CLA	CHC-C1C-C2C	-2.02	121.14	126.72
24	a	606	CLA	CMB-C2B-C3B	2.02	128.45	124.68
29	c	519	LMG	O1-C7-C8	-2.02	106.03	110.90
24	b	613	CLA	CHD-C4C-C3C	2.02	127.80	124.84
30	E	102	LHG	O7-C7-O9	-2.02	118.83	123.70
26	K	102	BCR	C1-C6-C7	-2.02	110.07	115.78
24	b	608[A]	CLA	CHD-C4C-C3C	2.01	127.80	124.84
24	c	508	CLA	CED-O2D-CGD	2.01	120.49	115.94
24	C	506	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
24	d	402	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
24	C	510	CLA	CMB-C2B-C3B	2.01	128.44	124.68
29	Z	101	LMG	C6-C5-C4	-2.01	108.30	113.00
24	b	604	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
32	h	102	DGD	C2G-O2G-C1B	-2.01	112.84	117.79
24	b	613	CLA	O2A-CGA-CBA	2.01	118.21	111.91
26	B	620	BCR	C34-C9-C8	2.01	121.24	118.08
32	H	102	DGD	O3D-C3D-C2D	-2.01	105.71	110.35
24	B	607[A]	CLA	CED-O2D-CGD	2.01	120.48	115.94
24	c	511	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
29	z	101	LMG	C4-C3-C2	2.01	114.33	110.82
24	b	607	CLA	C4A-NA-C1A	-2.01	105.80	106.71
28	L	102	SQD	O47-C7-O49	-2.01	118.86	123.70
32	h	102	DGD	O5D-C1E-C2E	2.00	111.43	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C1-O2A-CGA	2.00	121.70	116.44
30	a	616	LHG	O8-C23-O10	-2.00	118.54	123.59
24	c	511	CLA	CHB-C4A-NA	-2.00	121.74	124.51
24	B	617	CLA	CHB-C4A-NA	-2.00	121.75	124.51
33	v	201	HEM	C2B-C1B-NB	-2.00	107.47	109.84

All (72) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
24	D	402	CLA	ND
24	D	403	CLA	ND
24	D	404	CLA	ND
24	a	606	CLA	ND
24	a	607	CLA	ND
24	a	609	CLA	ND
24	a	615	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608[A]	CLA	ND
24	b	608[B]	CLA	ND
24	b	609	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	618	CLA	ND
24	c	501	CLA	ND
24	c	502	CLA	ND
24	c	503	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	d	402	CLA	ND
24	d	403	CLA	ND

All (2162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	607	CLA	CHA-CBD-CGD-O2D
24	A	609	CLA	C1A-C2A-CAA-CBA
24	B	602	CLA	C1A-C2A-CAA-CBA
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	607[A]	CLA	CHA-CBD-CGD-O2D
24	B	607[B]	CLA	CHA-CBD-CGD-O2D
24	B	608	CLA	C1A-C2A-CAA-CBA
24	B	608	CLA	C3A-C2A-CAA-CBA
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	504	CLA	CHA-CBD-CGD-O1D
24	C	505	CLA	C1A-C2A-CAA-CBA
24	C	512	CLA	C1A-C2A-CAA-CBA
24	a	615	CLA	CHA-CBD-CGD-O1D
24	a	615	CLA	CHA-CBD-CGD-O2D
24	b	603	CLA	C1A-C2A-CAA-CBA
24	b	603	CLA	CHA-CBD-CGD-O1D
24	b	603	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	C2-C3-C5-C6
24	b	607	CLA	C4-C3-C5-C6
24	b	608[A]	CLA	CHA-CBD-CGD-O2D
24	b	608[B]	CLA	CHA-CBD-CGD-O2D
24	b	609	CLA	C1A-C2A-CAA-CBA
24	b	609	CLA	C3A-C2A-CAA-CBA
24	b	611	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CHA-CBD-CGD-O1D
24	b	616	CLA	CAD-CBD-CGD-O1D
24	b	616	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O1D
26	A	610	BCR	C11-C12-C13-C14
26	A	610	BCR	C12-C13-C14-C15
26	A	610	BCR	C35-C13-C14-C15
26	A	610	BCR	C13-C14-C15-C16
26	A	610	BCR	C14-C15-C16-C17
26	A	610	BCR	C16-C17-C18-C19
26	A	610	BCR	C16-C17-C18-C36
26	A	610	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
26	A	610	BCR	C18-C19-C20-C21
26	A	610	BCR	C20-C21-C22-C37
26	A	610	BCR	C23-C24-C25-C30
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C9-C10-C11-C12
26	B	618	BCR	C10-C11-C12-C13
26	B	618	BCR	C11-C12-C13-C14
26	B	618	BCR	C11-C12-C13-C35
26	B	618	BCR	C14-C15-C16-C17
26	B	618	BCR	C15-C16-C17-C18
26	B	618	BCR	C16-C17-C18-C19
26	B	618	BCR	C16-C17-C18-C36
26	B	618	BCR	C36-C18-C19-C20
26	B	618	BCR	C20-C21-C22-C23
26	B	618	BCR	C20-C21-C22-C37
26	B	618	BCR	C21-C22-C23-C24
26	B	618	BCR	C22-C23-C24-C25
26	B	618	BCR	C23-C24-C25-C26
26	B	619	BCR	C5-C6-C7-C8
26	B	619	BCR	C7-C8-C9-C34
26	B	619	BCR	C11-C10-C9-C8
26	B	619	BCR	C11-C10-C9-C34
26	B	619	BCR	C10-C11-C12-C13
26	B	619	BCR	C14-C15-C16-C17
26	B	619	BCR	C16-C17-C18-C19
26	B	619	BCR	C16-C17-C18-C36
26	B	619	BCR	C18-C19-C20-C21
26	B	619	BCR	C20-C21-C22-C23
26	B	619	BCR	C20-C21-C22-C37
26	B	619	BCR	C21-C22-C23-C24
26	B	620	BCR	C5-C6-C7-C8
26	B	620	BCR	C11-C10-C9-C8
26	B	620	BCR	C10-C11-C12-C13
26	B	620	BCR	C11-C12-C13-C14
26	B	620	BCR	C14-C15-C16-C17
26	B	620	BCR	C16-C17-C18-C19
26	B	620	BCR	C16-C17-C18-C36
26	B	620	BCR	C17-C18-C19-C20
26	B	620	BCR	C36-C18-C19-C20
26	B	620	BCR	C18-C19-C20-C21
26	B	620	BCR	C19-C20-C21-C22
26	B	620	BCR	C20-C21-C22-C23

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

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Mol	Chain	Res	Type	Atoms
26	H	101	BCR	C22-C23-C24-C25
26	I	101	BCR	C6-C7-C8-C9
26	I	101	BCR	C7-C8-C9-C34
26	I	101	BCR	C11-C10-C9-C8
26	I	101	BCR	C12-C13-C14-C15
26	I	101	BCR	C35-C13-C14-C15
26	I	101	BCR	C14-C15-C16-C17
26	I	101	BCR	C36-C18-C19-C20
26	I	101	BCR	C18-C19-C20-C21
26	I	101	BCR	C20-C21-C22-C23
26	K	101	BCR	C7-C8-C9-C10
26	K	101	BCR	C7-C8-C9-C34
26	K	101	BCR	C10-C11-C12-C13
26	K	101	BCR	C11-C12-C13-C35
26	K	101	BCR	C12-C13-C14-C15
26	K	101	BCR	C14-C15-C16-C17
26	K	101	BCR	C16-C17-C18-C19
26	K	101	BCR	C16-C17-C18-C36
26	K	101	BCR	C17-C18-C19-C20
26	K	101	BCR	C36-C18-C19-C20
26	K	101	BCR	C20-C21-C22-C37
26	K	102	BCR	C6-C7-C8-C9
26	K	102	BCR	C7-C8-C9-C10
26	K	102	BCR	C7-C8-C9-C34
26	K	102	BCR	C10-C11-C12-C13
26	K	102	BCR	C11-C12-C13-C14
26	K	102	BCR	C13-C14-C15-C16
26	K	102	BCR	C14-C15-C16-C17
26	K	102	BCR	C17-C18-C19-C20
26	K	102	BCR	C18-C19-C20-C21
26	K	102	BCR	C20-C21-C22-C37
26	K	102	BCR	C21-C22-C23-C24
26	K	102	BCR	C37-C22-C23-C24
26	K	102	BCR	C22-C23-C24-C25
26	T	101	BCR	C6-C7-C8-C9
26	T	101	BCR	C11-C10-C9-C8
26	T	101	BCR	C11-C10-C9-C34
26	T	101	BCR	C10-C11-C12-C13
26	T	101	BCR	C11-C12-C13-C14
26	T	101	BCR	C12-C13-C14-C15
26	T	101	BCR	C14-C15-C16-C17
26	T	101	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	T	101	BCR	C16-C17-C18-C36
26	T	101	BCR	C18-C19-C20-C21
26	T	101	BCR	C37-C22-C23-C24
26	T	101	BCR	C22-C23-C24-C25
26	a	610	BCR	C7-C8-C9-C10
26	a	610	BCR	C11-C10-C9-C34
26	a	610	BCR	C11-C12-C13-C14
26	a	610	BCR	C12-C13-C14-C15
26	a	610	BCR	C35-C13-C14-C15
26	a	610	BCR	C14-C15-C16-C17
26	a	610	BCR	C15-C16-C17-C18
26	a	610	BCR	C17-C18-C19-C20
26	a	610	BCR	C18-C19-C20-C21
26	a	610	BCR	C20-C21-C22-C23
26	a	610	BCR	C20-C21-C22-C37
26	a	610	BCR	C21-C22-C23-C24
26	b	619	BCR	C9-C10-C11-C12
26	b	619	BCR	C10-C11-C12-C13
26	b	619	BCR	C11-C12-C13-C14
26	b	619	BCR	C11-C12-C13-C35
26	b	619	BCR	C12-C13-C14-C15
26	b	619	BCR	C35-C13-C14-C15
26	b	619	BCR	C14-C15-C16-C17
26	b	619	BCR	C15-C16-C17-C18
26	b	619	BCR	C16-C17-C18-C19
26	b	619	BCR	C16-C17-C18-C36
26	b	619	BCR	C18-C19-C20-C21
26	b	619	BCR	C19-C20-C21-C22
26	b	619	BCR	C21-C22-C23-C24
26	b	619	BCR	C22-C23-C24-C25
26	b	620	BCR	C5-C6-C7-C8
26	b	620	BCR	C11-C12-C13-C35
26	b	620	BCR	C12-C13-C14-C15
26	b	620	BCR	C14-C15-C16-C17
26	b	620	BCR	C16-C17-C18-C19
26	b	620	BCR	C16-C17-C18-C36
26	b	620	BCR	C17-C18-C19-C20
26	b	620	BCR	C36-C18-C19-C20
26	b	620	BCR	C18-C19-C20-C21
26	b	620	BCR	C20-C21-C22-C23
26	b	620	BCR	C20-C21-C22-C37
26	b	620	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	b	621	BCR	C5-C6-C7-C8
26	b	621	BCR	C7-C8-C9-C34
26	b	621	BCR	C11-C10-C9-C8
26	b	621	BCR	C11-C10-C9-C34
26	b	621	BCR	C12-C13-C14-C15
26	b	621	BCR	C35-C13-C14-C15
26	b	621	BCR	C14-C15-C16-C17
26	b	621	BCR	C16-C17-C18-C19
26	b	621	BCR	C16-C17-C18-C36
26	b	621	BCR	C36-C18-C19-C20
26	b	621	BCR	C18-C19-C20-C21
26	b	621	BCR	C19-C20-C21-C22
26	b	621	BCR	C20-C21-C22-C23
26	b	621	BCR	C20-C21-C22-C37
26	c	514	BCR	C5-C6-C7-C8
26	c	514	BCR	C6-C7-C8-C9
26	c	514	BCR	C7-C8-C9-C10
26	c	514	BCR	C11-C10-C9-C8
26	c	514	BCR	C11-C10-C9-C34
26	c	514	BCR	C10-C11-C12-C13
26	c	514	BCR	C12-C13-C14-C15
26	c	514	BCR	C35-C13-C14-C15
26	c	514	BCR	C14-C15-C16-C17
26	c	514	BCR	C15-C16-C17-C18
26	c	514	BCR	C16-C17-C18-C19
26	c	514	BCR	C16-C17-C18-C36
26	c	514	BCR	C17-C18-C19-C20
26	c	514	BCR	C36-C18-C19-C20
26	c	514	BCR	C18-C19-C20-C21
26	c	514	BCR	C20-C21-C22-C23
26	c	514	BCR	C20-C21-C22-C37
26	c	514	BCR	C21-C22-C23-C24
26	c	514	BCR	C22-C23-C24-C25
26	c	514	BCR	C23-C24-C25-C26
26	c	515	BCR	C6-C7-C8-C9
26	c	515	BCR	C12-C13-C14-C15
26	c	515	BCR	C35-C13-C14-C15
26	c	515	BCR	C14-C15-C16-C17
26	c	515	BCR	C16-C17-C18-C36
26	c	515	BCR	C36-C18-C19-C20
26	c	515	BCR	C18-C19-C20-C21
26	c	515	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
26	c	515	BCR	C37-C22-C23-C24
26	c	521	BCR	C6-C7-C8-C9
26	c	521	BCR	C7-C8-C9-C34
26	c	521	BCR	C11-C10-C9-C8
26	c	521	BCR	C10-C11-C12-C13
26	c	521	BCR	C12-C13-C14-C15
26	c	521	BCR	C13-C14-C15-C16
26	c	521	BCR	C14-C15-C16-C17
26	c	521	BCR	C18-C19-C20-C21
26	c	521	BCR	C20-C21-C22-C37
26	c	521	BCR	C22-C23-C24-C25
26	c	521	BCR	C23-C24-C25-C30
26	f	101	BCR	C10-C11-C12-C13
26	f	101	BCR	C11-C12-C13-C35
26	f	101	BCR	C12-C13-C14-C15
26	f	101	BCR	C35-C13-C14-C15
26	f	101	BCR	C14-C15-C16-C17
26	f	101	BCR	C16-C17-C18-C19
26	f	101	BCR	C16-C17-C18-C36
26	f	101	BCR	C18-C19-C20-C21
26	f	101	BCR	C20-C21-C22-C37
26	f	101	BCR	C22-C23-C24-C25
26	f	101	BCR	C23-C24-C25-C26
26	h	101	BCR	C6-C7-C8-C9
26	h	101	BCR	C7-C8-C9-C34
26	h	101	BCR	C11-C10-C9-C8
26	h	101	BCR	C11-C10-C9-C34
26	h	101	BCR	C10-C11-C12-C13
26	h	101	BCR	C11-C12-C13-C14
26	h	101	BCR	C12-C13-C14-C15
26	h	101	BCR	C13-C14-C15-C16
26	h	101	BCR	C14-C15-C16-C17
26	h	101	BCR	C16-C17-C18-C19
26	h	101	BCR	C16-C17-C18-C36
26	h	101	BCR	C36-C18-C19-C20
26	h	101	BCR	C18-C19-C20-C21
26	h	101	BCR	C20-C21-C22-C23
26	h	101	BCR	C20-C21-C22-C37
26	h	101	BCR	C21-C22-C23-C24
26	k	101	BCR	C7-C8-C9-C34
26	k	101	BCR	C11-C10-C9-C8
26	k	101	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	k	101	BCR	C11-C12-C13-C35
26	k	101	BCR	C12-C13-C14-C15
26	k	101	BCR	C16-C17-C18-C19
26	k	101	BCR	C16-C17-C18-C36
26	k	101	BCR	C36-C18-C19-C20
26	k	101	BCR	C20-C21-C22-C23
26	k	101	BCR	C20-C21-C22-C37
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C10-C9-C8
26	t	101	BCR	C11-C12-C13-C14
26	t	101	BCR	C12-C13-C14-C15
26	t	101	BCR	C35-C13-C14-C15
26	t	101	BCR	C14-C15-C16-C17
26	t	101	BCR	C16-C17-C18-C19
26	t	101	BCR	C16-C17-C18-C36
26	t	101	BCR	C18-C19-C20-C21
26	t	101	BCR	C21-C22-C23-C24
26	t	101	BCR	C37-C22-C23-C24
26	t	101	BCR	C22-C23-C24-C25
26	t	101	BCR	C23-C24-C25-C30
27	A	611	PL9	C7-C8-C9-C10
27	A	611	PL9	C12-C11-C9-C10
27	A	611	PL9	C12-C13-C14-C15
27	A	611	PL9	C14-C16-C17-C18
27	A	611	PL9	C19-C21-C22-C23
27	A	611	PL9	C22-C23-C24-C25
27	A	611	PL9	C32-C33-C34-C35
27	A	611	PL9	C35-C34-C36-C37
27	D	405	PL9	C7-C8-C9-C10
27	D	405	PL9	C12-C13-C14-C15
27	D	405	PL9	C17-C18-C19-C20
27	D	405	PL9	C22-C23-C24-C25
27	D	405	PL9	C42-C43-C44-C46
27	D	405	PL9	C44-C46-C47-C48
27	a	611	PL9	C12-C11-C9-C10
27	a	611	PL9	C12-C13-C14-C15
27	a	611	PL9	C14-C16-C17-C18
27	a	611	PL9	C18-C19-C21-C22
27	a	611	PL9	C19-C21-C22-C23
27	a	611	PL9	C22-C23-C24-C25
27	a	611	PL9	C25-C24-C26-C27
27	a	611	PL9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
27	d	404	PL9	C17-C18-C19-C20
27	d	404	PL9	C25-C24-C26-C27
27	d	404	PL9	C27-C28-C29-C30
27	d	404	PL9	C42-C43-C44-C46
28	A	614	SQD	O6-C44-C45-O47
28	B	622	SQD	O5-C1-O6-C44
28	B	622	SQD	C8-C7-O47-C45
28	B	622	SQD	O5-C5-C6-S
28	L	102	SQD	C8-C7-O47-C45
28	L	102	SQD	O5-C5-C6-S
28	X	101	SQD	C2-C1-O6-C44
28	X	101	SQD	O5-C1-O6-C44
28	a	614	SQD	O6-C44-C45-O47
28	b	601	SQD	O5-C1-O6-C44
28	b	601	SQD	C8-C7-O47-C45
28	b	601	SQD	O5-C5-C6-S
28	l	101	SQD	C8-C7-O47-C45
28	l	101	SQD	O5-C5-C6-S
28	x	101	SQD	C2-C1-O6-C44
28	x	101	SQD	O5-C1-O6-C44
29	Z	101	LMG	O6-C1-O1-C7
29	Z	101	LMG	O1-C7-C8-O7
29	Z	101	LMG	O9-C10-O7-C8
29	Z	101	LMG	C11-C10-O7-C8
29	z	101	LMG	O6-C1-O1-C7
29	z	101	LMG	O1-C7-C8-O7
29	z	101	LMG	O9-C10-O7-C8
29	z	101	LMG	C11-C10-O7-C8
30	D	407	LHG	O1-C1-C2-C3
30	D	407	LHG	O2-C2-C3-O3
30	D	407	LHG	C3-O3-P-O5
30	D	407	LHG	C4-O6-P-O4
30	D	407	LHG	C4-O6-P-O5
30	L	101	LHG	C4-O6-P-O4
30	d	407	LHG	O1-C1-C2-C3
30	d	407	LHG	C3-O3-P-O4
30	d	407	LHG	C3-O3-P-O5
30	e	101	LHG	C8-C7-O7-C5
30	e	101	LHG	C24-C23-O8-C6
30	l	102	LHG	C4-O6-P-O4
32	C	515	DGD	O6D-C1D-O3G-C3G
32	E	101	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
32	d	405	DGD	C2B-C1B-O2G-C2G
32	d	405	DGD	O1B-C1B-O2G-C2G
32	d	405	DGD	C2E-C1E-O5D-C6D
29	z	101	LMG	C29-C28-O8-C9
24	b	611	CLA	CBD-CGD-O2D-CED
28	X	101	SQD	O10-C23-O48-C46
28	x	101	SQD	O10-C23-O48-C46
30	E	102	LHG	O10-C23-O8-C6
30	e	101	LHG	O10-C23-O8-C6
24	b	611	CLA	O1D-CGD-O2D-CED
28	X	101	SQD	C24-C23-O48-C46
28	x	101	SQD	C24-C23-O48-C46
30	E	102	LHG	C24-C23-O8-C6
29	Z	101	LMG	C29-C28-O8-C9
24	C	503	CLA	CBD-CGD-O2D-CED
24	b	606	CLA	CBD-CGD-O2D-CED
24	B	617	CLA	O1A-CGA-O2A-C1
24	b	618	CLA	O1A-CGA-O2A-C1
29	Z	101	LMG	O10-C28-O8-C9
29	z	101	LMG	O10-C28-O8-C9
24	b	612	CLA	O1D-CGD-O2D-CED
28	B	622	SQD	O49-C7-O47-C45
28	b	601	SQD	O49-C7-O47-C45
29	A	613	LMG	O9-C10-O7-C8
32	E	101	DGD	O1B-C1B-O2G-C2G
24	B	615	CLA	C3-C5-C6-C7
24	b	616	CLA	C3-C5-C6-C7
24	B	609	CLA	C2C-C3C-CAC-CBC
30	E	102	LHG	C8-C7-O7-C5
24	c	510	CLA	CBD-CGD-O2D-CED
29	C	519	LMG	O6-C5-C6-O5
27	A	611	PL9	C25-C24-C26-C27
27	A	611	PL9	C18-C19-C21-C22
24	b	612	CLA	CBD-CGD-O2D-CED
24	B	607[A]	CLA	C2A-CAA-CBA-CGA
24	B	607[B]	CLA	C2A-CAA-CBA-CGA
24	b	608[A]	CLA	C2A-CAA-CBA-CGA
24	b	608[B]	CLA	C2A-CAA-CBA-CGA
24	B	602	CLA	C3-C5-C6-C7
24	b	603	CLA	C3-C5-C6-C7
24	b	618	CLA	CBA-CGA-O2A-C1
27	A	611	PL9	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	A	611	PL9	C37-C38-C39-C40
27	A	611	PL9	C42-C43-C44-C45
27	D	405	PL9	C32-C33-C34-C35
27	D	405	PL9	C37-C38-C39-C40
27	a	611	PL9	C7-C8-C9-C10
27	a	611	PL9	C27-C28-C29-C30
27	a	611	PL9	C32-C33-C34-C35
27	a	611	PL9	C37-C38-C39-C40
27	a	611	PL9	C42-C43-C44-C45
27	d	404	PL9	C7-C8-C9-C10
27	d	404	PL9	C12-C13-C14-C15
27	d	404	PL9	C22-C23-C24-C25
27	d	404	PL9	C32-C33-C34-C35
27	d	404	PL9	C37-C38-C39-C40
24	B	602	CLA	O1D-CGD-O2D-CED
24	b	607	CLA	O1D-CGD-O2D-CED
28	L	102	SQD	O49-C7-O47-C45
28	l	101	SQD	O49-C7-O47-C45
30	E	102	LHG	O9-C7-O7-C5
26	A	610	BCR	C9-C10-C11-C12
26	B	619	BCR	C15-C16-C17-C18
26	B	620	BCR	C13-C14-C15-C16
26	C	514	BCR	C15-C16-C17-C18
26	F	101	BCR	C15-C16-C17-C18
26	H	101	BCR	C19-C20-C21-C22
26	I	101	BCR	C13-C14-C15-C16
26	I	101	BCR	C19-C20-C21-C22
26	T	101	BCR	C15-C16-C17-C18
26	c	514	BCR	C19-C20-C21-C22
26	f	101	BCR	C13-C14-C15-C16
26	h	101	BCR	C15-C16-C17-C18
26	k	101	BCR	C15-C16-C17-C18
32	H	102	DGD	O6E-C5E-C6E-O5E
24	A	609	CLA	CBD-CGD-O2D-CED
24	B	605	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	CBD-CGD-O2D-CED
24	b	607	CLA	CBD-CGD-O2D-CED
24	b	609	CLA	CBD-CGD-O2D-CED
24	c	503	CLA	CBD-CGD-O2D-CED
30	d	407	LHG	O2-C2-C3-O3
24	B	617	CLA	CBA-CGA-O2A-C1
29	j	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
24	a	606	CLA	O1D-CGD-O2D-CED
24	B	602	CLA	CBD-CGD-O2D-CED
24	b	616	CLA	CBD-CGD-O2D-CED
29	D	408	LMG	O6-C5-C6-O5
32	c	516	DGD	C4D-C5D-C6D-O5D
29	c	520	LMG	O6-C5-C6-O5
27	A	611	PL9	C47-C48-C49-C51
27	D	405	PL9	C47-C48-C49-C50
27	A	611	PL9	C38-C39-C41-C42
27	a	611	PL9	C38-C39-C41-C42
30	D	407	LHG	C14-C15-C16-C17
24	c	505	CLA	O1A-CGA-O2A-C1
32	H	102	DGD	O6E-C1E-O5D-C6D
27	A	611	PL9	C24-C26-C27-C28
27	d	404	PL9	C29-C31-C32-C33
27	d	404	PL9	C44-C46-C47-C48
32	H	102	DGD	C6B-C7B-C8B-C9B
27	A	611	PL9	C17-C18-C19-C20
24	B	616	CLA	O1D-CGD-O2D-CED
30	D	407	LHG	C1-C2-C3-O3
30	d	407	LHG	C1-C2-C3-O3
32	c	516	DGD	O6E-C5E-C6E-O5E
29	C	519	LMG	C4-C5-C6-O5
29	c	520	LMG	C4-C5-C6-O5
24	C	509	CLA	O1D-CGD-O2D-CED
28	L	102	SQD	C24-C23-O48-C46
28	l	101	SQD	C24-C23-O48-C46
32	c	518	DGD	C2A-C1A-O1G-C1G
32	h	102	DGD	O6E-C5E-C6E-O5E
24	B	612	CLA	CBD-CGD-O2D-CED
24	a	606	CLA	CBD-CGD-O2D-CED
32	h	102	DGD	C6B-C7B-C8B-C9B
26	B	620	BCR	C15-C16-C17-C18
26	a	610	BCR	C13-C14-C15-C16
26	h	101	BCR	C19-C20-C21-C22
32	H	102	DGD	C4E-C5E-C6E-O5E
29	Z	101	LMG	C2-C1-O1-C7
29	z	101	LMG	C2-C1-O1-C7
32	c	518	DGD	O1A-C1A-O1G-C1G
24	B	602	CLA	C11-C10-C8-C9
24	C	501	CLA	C11-C12-C13-C14
24	C	502	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	C11-C12-C13-C14
24	C	509	CLA	C6-C7-C8-C9
24	b	603	CLA	C11-C10-C8-C9
24	c	501	CLA	C11-C12-C13-C14
24	c	502	CLA	C14-C13-C15-C16
24	c	504	CLA	C11-C12-C13-C14
24	c	509	CLA	C6-C7-C8-C9
26	A	610	BCR	C11-C12-C13-C35
26	A	610	BCR	C36-C18-C19-C20
26	A	610	BCR	C37-C22-C23-C24
26	B	618	BCR	C37-C22-C23-C24
26	B	619	BCR	C36-C18-C19-C20
26	C	514	BCR	C37-C22-C23-C24
26	F	101	BCR	C11-C12-C13-C35
26	I	101	BCR	C37-C22-C23-C24
26	T	101	BCR	C7-C8-C9-C34
26	b	620	BCR	C7-C8-C9-C34
26	c	514	BCR	C7-C8-C9-C34
26	c	515	BCR	C7-C8-C9-C34
26	f	101	BCR	C36-C18-C19-C20
26	h	101	BCR	C11-C12-C13-C35
26	C	514	BCR	C7-C8-C9-C10
26	C	514	BCR	C17-C18-C19-C20
26	C	514	BCR	C21-C22-C23-C24
26	H	101	BCR	C17-C18-C19-C20
26	b	620	BCR	C7-C8-C9-C10
26	b	621	BCR	C7-C8-C9-C10
26	t	101	BCR	C7-C8-C9-C10
29	A	613	LMG	O6-C5-C6-O5
29	B	621	LMG	O9-C10-O7-C8
29	a	613	LMG	O9-C10-O7-C8
24	B	609	CLA	C4C-C3C-CAC-CBC
32	C	516	DGD	C4E-C5E-C6E-O5E
29	a	613	LMG	C28-C29-C30-C31
27	a	611	PL9	C47-C48-C49-C51
27	d	404	PL9	C47-C48-C49-C51
28	L	102	SQD	O10-C23-O48-C46
28	l	101	SQD	O10-C23-O48-C46
29	a	613	LMG	O10-C28-O8-C9
24	A	609	CLA	C10-C11-C12-C13
24	B	616	CLA	C5-C6-C7-C8
24	a	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	b	617	CLA	C5-C6-C7-C8
24	B	616	CLA	CBD-CGD-O2D-CED
32	C	516	DGD	O6E-C5E-C6E-O5E
29	D	408	LMG	C4-C5-C6-O5
24	A	609	CLA	C13-C15-C16-C17
24	B	602	CLA	C10-C11-C12-C13
24	a	609	CLA	C13-C15-C16-C17
24	b	603	CLA	C10-C11-C12-C13
32	c	516	DGD	C2A-C3A-C4A-C5A
32	C	516	DGD	C1B-C2B-C3B-C4B
32	d	405	DGD	C1A-C2A-C3A-C4A
24	B	608	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED
32	c	516	DGD	O6D-C5D-C6D-O5D
24	B	615	CLA	C5-C6-C7-C8
24	B	615	CLA	C10-C11-C12-C13
24	C	509	CLA	C8-C10-C11-C12
24	b	616	CLA	C5-C6-C7-C8
24	b	616	CLA	C10-C11-C12-C13
24	c	509	CLA	C8-C10-C11-C12
32	h	102	DGD	C4E-C5E-C6E-O5E
24	c	510	CLA	O1D-CGD-O2D-CED
30	D	407	LHG	O1-C1-C2-O2
30	d	407	LHG	O1-C1-C2-O2
27	a	611	PL9	C17-C18-C19-C20
28	B	622	SQD	C7-C8-C9-C10
28	b	601	SQD	C7-C8-C9-C10
29	B	621	LMG	C10-C11-C12-C13
29	C	518	LMG	C28-C29-C30-C31
29	Z	101	LMG	C10-C11-C12-C13
29	c	520	LMG	C28-C29-C30-C31
32	E	101	DGD	C1B-C2B-C3B-C4B
32	c	517	DGD	C1A-C2A-C3A-C4A
32	c	517	DGD	C1B-C2B-C3B-C4B
32	d	405	DGD	C1B-C2B-C3B-C4B
24	B	613	CLA	CBD-CGD-O2D-CED
24	B	607[A]	CLA	C13-C15-C16-C17
24	b	608[A]	CLA	C13-C15-C16-C17
30	e	101	LHG	O9-C7-O7-C5
24	C	506	CLA	C5-C6-C7-C8
24	D	404	CLA	C8-C10-C11-C12
24	d	403	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	A	614	SQD	C23-C24-C25-C26
28	a	614	SQD	C23-C24-C25-C26
29	A	613	LMG	C28-C29-C30-C31
29	C	519	LMG	C28-C29-C30-C31
32	C	516	DGD	C1A-C2A-C3A-C4A
32	E	101	DGD	C1A-C2A-C3A-C4A
24	c	506	CLA	C5-C6-C7-C8
24	C	513	CLA	O1D-CGD-O2D-CED
26	a	610	BCR	C9-C10-C11-C12
26	a	610	BCR	C19-C20-C21-C22
26	b	620	BCR	C13-C14-C15-C16
26	b	621	BCR	C9-C10-C11-C12
26	c	514	BCR	C13-C14-C15-C16
26	c	521	BCR	C15-C16-C17-C18
26	c	521	BCR	C19-C20-C21-C22
29	z	101	LMG	C10-C11-C12-C13
24	b	604	CLA	O1D-CGD-O2D-CED
24	B	607[A]	CLA	C15-C16-C17-C18
24	D	404	CLA	C10-C11-C12-C13
24	b	608[A]	CLA	C15-C16-C17-C18
24	d	403	CLA	C10-C11-C12-C13
24	C	504	CLA	O1A-CGA-O2A-C1
24	C	511	CLA	O1A-CGA-O2A-C1
32	d	405	DGD	O6E-C1E-O5D-C6D
24	A	607	CLA	C13-C15-C16-C17
24	a	607	CLA	C13-C15-C16-C17
27	A	611	PL9	C9-C11-C12-C13
27	D	405	PL9	C9-C11-C12-C13
27	D	405	PL9	C14-C16-C17-C18
27	D	405	PL9	C29-C31-C32-C33
27	d	404	PL9	C9-C11-C12-C13
27	d	404	PL9	C39-C41-C42-C43
29	C	518	LMG	C10-C11-C12-C13
29	c	519	LMG	C28-C29-C30-C31
26	I	101	BCR	C10-C11-C12-C13
26	c	515	BCR	C10-C11-C12-C13
27	d	404	PL9	C47-C48-C49-C50
30	l	102	LHG	O2-C2-C3-O3
29	j	101	LMG	C4-C5-C6-O5
24	C	509	CLA	C13-C15-C16-C17
24	c	509	CLA	C13-C15-C16-C17
29	z	101	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
24	A	609	CLA	C15-C16-C17-C18
24	B	612	CLA	C15-C16-C17-C18
24	a	609	CLA	C15-C16-C17-C18
24	b	613	CLA	C15-C16-C17-C18
29	A	613	LMG	C11-C10-O7-C8
24	B	607[B]	CLA	C10-C11-C12-C13
24	B	617	CLA	C10-C11-C12-C13
24	C	501	CLA	C15-C16-C17-C18
24	C	506	CLA	C10-C11-C12-C13
24	b	608[B]	CLA	C10-C11-C12-C13
24	b	618	CLA	C10-C11-C12-C13
24	c	501	CLA	C15-C16-C17-C18
24	c	506	CLA	C10-C11-C12-C13
30	D	407	LHG	C4-O6-P-O3
30	L	101	LHG	C4-O6-P-O3
30	d	407	LHG	C3-O3-P-O6
30	l	102	LHG	C4-O6-P-O3
24	c	505	CLA	CBA-CGA-O2A-C1
24	A	607	CLA	C16-C17-C18-C20
24	a	607	CLA	C16-C17-C18-C20
29	a	613	LMG	C29-C28-O8-C9
30	A	615	LHG	C24-C23-O8-C6
26	k	101	BCR	C14-C15-C16-C17
26	B	618	BCR	C13-C14-C15-C16
26	B	618	BCR	C19-C20-C21-C22
26	C	514	BCR	C19-C20-C21-C22
26	T	101	BCR	C19-C20-C21-C22
26	b	619	BCR	C13-C14-C15-C16
26	f	101	BCR	C19-C20-C21-C22
28	X	101	SQD	C29-C30-C31-C32
29	D	408	LMG	C16-C17-C18-C19
32	H	102	DGD	CBA-CCA-CDA-CEA
24	b	603	CLA	O1D-CGD-O2D-CED
24	c	513	CLA	CBD-CGD-O2D-CED
29	a	613	LMG	C11-C10-O7-C8
26	A	610	BCR	C11-C10-C9-C34
26	B	618	BCR	C35-C13-C14-C15
26	B	620	BCR	C11-C10-C9-C34
26	I	101	BCR	C16-C17-C18-C36
26	a	610	BCR	C16-C17-C18-C36
26	c	515	BCR	C20-C21-C22-C37
26	t	101	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
28	A	612	SQD	C11-C12-C13-C14
28	A	614	SQD	C15-C16-C17-C18
28	L	102	SQD	C15-C16-C17-C18
28	X	101	SQD	C26-C27-C28-C29
28	X	101	SQD	C34-C35-C36-C37
28	a	612	SQD	C11-C12-C13-C14
28	a	614	SQD	C15-C16-C17-C18
28	l	101	SQD	C11-C10-C9-C8
28	l	101	SQD	C10-C11-C12-C13
28	l	101	SQD	C15-C16-C17-C18
28	x	101	SQD	C26-C27-C28-C29
28	x	101	SQD	C29-C30-C31-C32
28	x	101	SQD	C34-C35-C36-C37
29	b	622	LMG	C32-C33-C34-C35
29	b	622	LMG	C34-C35-C36-C37
29	c	519	LMG	C15-C16-C17-C18
29	c	520	LMG	C29-C30-C31-C32
30	D	406	LHG	C29-C30-C31-C32
30	E	102	LHG	C15-C16-C17-C18
32	E	101	DGD	C7B-C8B-C9B-CAB
32	H	102	DGD	C7A-C8A-C9A-CAA
32	c	516	DGD	C5B-C6B-C7B-C8B
32	d	405	DGD	CCA-CDA-CEA-CFA
24	C	506	CLA	C16-C17-C18-C19
27	D	405	PL9	C47-C48-C49-C51
33	V	201	HEM	C2D-C3D-CAD-CBD
28	A	612	SQD	C28-C29-C30-C31
28	L	102	SQD	C11-C10-C9-C8
28	L	102	SQD	C10-C11-C12-C13
28	a	612	SQD	C28-C29-C30-C31
29	A	613	LMG	C18-C19-C20-C21
29	D	408	LMG	C38-C39-C40-C41
29	b	622	LMG	C17-C18-C19-C20
29	j	101	LMG	C14-C15-C16-C17
30	E	102	LHG	C24-C25-C26-C27
30	d	406	LHG	C32-C33-C34-C35
30	l	102	LHG	C11-C12-C13-C14
30	l	102	LHG	C31-C32-C33-C34
32	d	405	DGD	C9B-CAB-CBB-CCB
28	L	102	SQD	C46-C45-O47-C7
28	l	101	SQD	C46-C45-O47-C7
32	c	517	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
32	c	517	DGD	C9A-CAA-CBA-CCA
32	c	517	DGD	C6B-C7B-C8B-C9B
24	c	511	CLA	O1A-CGA-O2A-C1
29	z	101	LMG	O6-C5-C6-O5
28	A	612	SQD	C12-C13-C14-C15
28	A	612	SQD	C15-C16-C17-C18
28	a	612	SQD	C12-C13-C14-C15
28	a	612	SQD	C15-C16-C17-C18
29	B	621	LMG	C12-C13-C14-C15
29	C	519	LMG	C30-C31-C32-C33
30	E	102	LHG	C14-C15-C16-C17
30	L	101	LHG	C33-C34-C35-C36
30	e	101	LHG	C18-C19-C20-C21
32	C	516	DGD	C6B-C7B-C8B-C9B
32	C	516	DGD	CAB-CBB-CCB-CDB
32	E	101	DGD	C9A-CAA-CBA-CCA
32	E	101	DGD	C9B-CAB-CBB-CCB
32	c	518	DGD	C6A-C7A-C8A-C9A
28	L	102	SQD	C12-C13-C14-C15
28	l	101	SQD	C12-C13-C14-C15
29	a	613	LMG	C13-C14-C15-C16
29	j	101	LMG	C16-C17-C18-C19
30	e	101	LHG	C7-C8-C9-C10
24	C	508	CLA	O1D-CGD-O2D-CED
26	B	618	BCR	C11-C10-C9-C8
26	B	618	BCR	C12-C13-C14-C15
26	B	619	BCR	C12-C13-C14-C15
26	C	514	BCR	C12-C13-C14-C15
26	F	101	BCR	C20-C21-C22-C23
26	H	101	BCR	C12-C13-C14-C15
26	K	101	BCR	C11-C10-C9-C8
26	K	102	BCR	C12-C13-C14-C15
26	K	102	BCR	C20-C21-C22-C23
26	T	101	BCR	C20-C21-C22-C23
26	a	610	BCR	C11-C10-C9-C8
26	a	610	BCR	C16-C17-C18-C19
26	b	619	BCR	C20-C21-C22-C23
26	c	515	BCR	C16-C17-C18-C19
26	c	521	BCR	C16-C17-C18-C19
26	c	521	BCR	C20-C21-C22-C23
26	t	101	BCR	C20-C21-C22-C23
32	C	516	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
32	E	101	DGD	C2D-C1D-O3G-C3G
32	E	101	DGD	C2E-C1E-O5D-C6D
32	d	405	DGD	C2D-C1D-O3G-C3G
28	L	102	SQD	C17-C18-C19-C20
28	L	102	SQD	C24-C25-C26-C27
28	l	101	SQD	C17-C18-C19-C20
28	l	101	SQD	C18-C19-C20-C21
29	C	518	LMG	C15-C16-C17-C18
29	j	101	LMG	C12-C13-C14-C15
30	D	406	LHG	C32-C33-C34-C35
30	L	101	LHG	C34-C35-C36-C37
30	e	101	LHG	C24-C25-C26-C27
30	l	102	LHG	C33-C34-C35-C36
32	E	101	DGD	CCA-CDA-CEA-CFA
32	c	517	DGD	CAA-CBA-CCA-CDA
24	B	614	CLA	C15-C16-C17-C18
24	b	615	CLA	C15-C16-C17-C18
24	D	404	CLA	C16-C17-C18-C19
24	c	506	CLA	C16-C17-C18-C19
24	d	403	CLA	C16-C17-C18-C19
27	D	405	PL9	C27-C28-C29-C30
28	L	102	SQD	C18-C19-C20-C21
28	X	101	SQD	C24-C25-C26-C27
28	l	101	SQD	C24-C25-C26-C27
29	A	613	LMG	C14-C15-C16-C17
29	B	621	LMG	C37-C38-C39-C40
29	C	519	LMG	C31-C32-C33-C34
32	c	516	DGD	C4B-C5B-C6B-C7B
32	c	518	DGD	C9B-CAB-CBB-CCB
24	B	604	CLA	C6-C7-C8-C9
24	b	605	CLA	C6-C7-C8-C9
28	B	622	SQD	C34-C35-C36-C37
28	L	102	SQD	C29-C30-C31-C32
28	b	601	SQD	C34-C35-C36-C37
28	l	101	SQD	C29-C30-C31-C32
28	x	101	SQD	C24-C25-C26-C27
29	A	613	LMG	C12-C13-C14-C15
29	D	408	LMG	C12-C13-C14-C15
29	D	408	LMG	C15-C16-C17-C18
29	b	622	LMG	C37-C38-C39-C40
29	c	520	LMG	C31-C32-C33-C34
30	E	102	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	d	406	LHG	C29-C30-C31-C32
32	H	102	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	C2A-C3A-C4A-C5A
32	d	405	DGD	CBA-CCA-CDA-CEA
24	B	617	CLA	C8-C10-C11-C12
24	b	618	CLA	C8-C10-C11-C12
32	c	516	DGD	C4E-C5E-C6E-O5E
26	C	514	BCR	C7-C8-C9-C34
26	H	101	BCR	C37-C22-C23-C24
26	b	619	BCR	C37-C22-C23-C24
26	c	514	BCR	C37-C22-C23-C24
28	A	612	SQD	C16-C17-C18-C19
28	B	622	SQD	C31-C32-C33-C34
28	a	612	SQD	C16-C17-C18-C19
29	C	519	LMG	C29-C30-C31-C32
29	j	101	LMG	C30-C31-C32-C33
29	j	101	LMG	C39-C40-C41-C42
30	E	102	LHG	C13-C14-C15-C16
30	L	101	LHG	C11-C12-C13-C14
32	d	405	DGD	CCB-CDB-CEB-CFB
30	D	406	LHG	O1-C1-C2-C3
30	a	616	LHG	O1-C1-C2-C3
26	B	619	BCR	C7-C8-C9-C10
26	B	619	BCR	C17-C18-C19-C20
26	I	101	BCR	C21-C22-C23-C24
26	T	101	BCR	C7-C8-C9-C10
26	T	101	BCR	C21-C22-C23-C24
26	c	515	BCR	C17-C18-C19-C20
26	f	101	BCR	C11-C12-C13-C14
26	f	101	BCR	C17-C18-C19-C20
26	h	101	BCR	C17-C18-C19-C20
26	k	101	BCR	C7-C8-C9-C10
26	k	101	BCR	C17-C18-C19-C20
24	c	503	CLA	O1D-CGD-O2D-CED
24	b	610	CLA	C2C-C3C-CAC-CBC
28	B	622	SQD	C11-C12-C13-C14
28	L	102	SQD	C27-C28-C29-C30
28	b	601	SQD	C31-C32-C33-C34
28	l	101	SQD	C27-C28-C29-C30
29	B	621	LMG	C38-C39-C40-C41
29	Z	101	LMG	C16-C17-C18-C19
29	a	613	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	b	622	LMG	C14-C15-C16-C17
29	j	101	LMG	C15-C16-C17-C18
30	L	101	LHG	C13-C14-C15-C16
30	d	406	LHG	C25-C26-C27-C28
30	e	101	LHG	C25-C26-C27-C28
32	C	515	DGD	C6B-C7B-C8B-C9B
29	c	519	LMG	C10-C11-C12-C13
30	E	102	LHG	C7-C8-C9-C10
28	A	614	SQD	C16-C17-C18-C19
28	B	622	SQD	C11-C10-C9-C8
28	L	102	SQD	C32-C33-C34-C35
28	a	614	SQD	C16-C17-C18-C19
28	b	601	SQD	C11-C10-C9-C8
28	b	601	SQD	C11-C12-C13-C14
28	l	101	SQD	C14-C15-C16-C17
29	B	621	LMG	C16-C17-C18-C19
29	D	408	LMG	C14-C15-C16-C17
29	c	520	LMG	C17-C18-C19-C20
29	c	520	LMG	C30-C31-C32-C33
29	j	101	LMG	C13-C14-C15-C16
29	z	101	LMG	C12-C13-C14-C15
30	e	101	LHG	C14-C15-C16-C17
32	C	515	DGD	C6A-C7A-C8A-C9A
32	C	516	DGD	C3A-C4A-C5A-C6A
32	C	517	DGD	C6A-C7A-C8A-C9A
32	E	101	DGD	C2A-C3A-C4A-C5A
32	E	101	DGD	C5B-C6B-C7B-C8B
32	c	517	DGD	C4A-C5A-C6A-C7A
32	c	517	DGD	CAB-CBB-CCB-CDB
32	c	517	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	C9A-CAA-CBA-CCA
32	h	102	DGD	CBA-CCA-CDA-CEA
32	E	101	DGD	O6D-C1D-O3G-C3G
32	E	101	DGD	O6E-C1E-O5D-C6D
32	d	405	DGD	O6D-C1D-O3G-C3G
28	A	612	SQD	C9-C10-C11-C12
28	A	614	SQD	C26-C27-C28-C29
28	B	622	SQD	C24-C25-C26-C27
28	L	102	SQD	C14-C15-C16-C17
28	a	612	SQD	C9-C10-C11-C12
28	a	614	SQD	C26-C27-C28-C29
28	b	601	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
28	l	101	SQD	C32-C33-C34-C35
29	B	621	LMG	C14-C15-C16-C17
29	C	518	LMG	C16-C17-C18-C19
29	a	613	LMG	C38-C39-C40-C41
29	j	101	LMG	C36-C37-C38-C39
29	z	101	LMG	C19-C20-C21-C22
32	C	515	DGD	CAB-CBB-CCB-CDB
32	C	516	DGD	C9A-CAA-CBA-CCA
32	C	517	DGD	C2A-C3A-C4A-C5A
32	c	517	DGD	C9B-CAB-CBB-CCB
32	d	405	DGD	C7B-C8B-C9B-CAB
24	C	505	CLA	CBD-CGD-O2D-CED
28	A	614	SQD	C28-C29-C30-C31
29	A	613	LMG	C36-C37-C38-C39
29	B	621	LMG	C32-C33-C34-C35
29	c	519	LMG	C16-C17-C18-C19
29	z	101	LMG	C16-C17-C18-C19
30	L	101	LHG	C25-C26-C27-C28
30	e	101	LHG	C13-C14-C15-C16
32	C	515	DGD	C4B-C5B-C6B-C7B
32	C	516	DGD	CAA-CBA-CCA-CDA
32	C	516	DGD	C5B-C6B-C7B-C8B
32	c	516	DGD	C6A-C7A-C8A-C9A
32	c	516	DGD	C6B-C7B-C8B-C9B
28	a	614	SQD	C28-C29-C30-C31
29	D	408	LMG	C20-C21-C22-C23
30	E	102	LHG	C27-C28-C29-C30
30	a	616	LHG	C15-C16-C17-C18
30	l	102	LHG	C13-C14-C15-C16
32	c	518	DGD	C2A-C3A-C4A-C5A
29	c	520	LMG	C18-C19-C20-C21
30	L	101	LHG	C12-C13-C14-C15
30	a	616	LHG	C27-C28-C29-C30
24	c	504	CLA	O1D-CGD-O2D-CED
28	L	102	SQD	C16-C17-C18-C19
28	X	101	SQD	C31-C32-C33-C34
28	l	101	SQD	C16-C17-C18-C19
28	l	101	SQD	C28-C29-C30-C31
28	x	101	SQD	C31-C32-C33-C34
29	B	621	LMG	C17-C18-C19-C20
29	b	622	LMG	C31-C32-C33-C34
29	c	519	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	A	615	LHG	C15-C16-C17-C18
30	a	616	LHG	C30-C31-C32-C33
30	d	406	LHG	C13-C14-C15-C16
32	C	515	DGD	C5B-C6B-C7B-C8B
32	E	101	DGD	CCB-CDB-CEB-CFB
24	C	510	CLA	O1A-CGA-O2A-C1
29	A	613	LMG	O10-C28-O8-C9
30	d	407	LHG	O10-C23-O8-C6
24	a	615	CLA	C2C-C3C-CAC-CBC
28	B	622	SQD	C10-C11-C12-C13
28	L	102	SQD	C28-C29-C30-C31
28	b	601	SQD	C10-C11-C12-C13
29	A	613	LMG	C31-C32-C33-C34
29	a	613	LMG	C14-C15-C16-C17
29	a	613	LMG	C32-C33-C34-C35
30	L	101	LHG	C31-C32-C33-C34
32	H	102	DGD	CCA-CDA-CEA-CFA
32	c	518	DGD	C8B-C9B-CAB-CBB
32	h	102	DGD	C7B-C8B-C9B-CAB
24	D	402	CLA	O1D-CGD-O2D-CED
32	h	102	DGD	O1G-C1G-C2G-C3G
29	a	613	LMG	C12-C13-C14-C15
29	c	519	LMG	C19-C20-C21-C22
29	c	519	LMG	C38-C39-C40-C41
32	C	515	DGD	O6D-C5D-C6D-O5D
32	E	101	DGD	O6D-C5D-C6D-O5D
29	b	622	LMG	C16-C17-C18-C19
29	c	520	LMG	C33-C34-C35-C36
27	D	405	PL9	C45-C44-C46-C47
27	d	404	PL9	C30-C29-C31-C32
24	c	511	CLA	CBA-CGA-O2A-C1
27	D	405	PL9	C28-C29-C31-C32
27	D	405	PL9	C43-C44-C46-C47
27	d	404	PL9	C28-C29-C31-C32
28	X	101	SQD	C30-C31-C32-C33
28	x	101	SQD	C30-C31-C32-C33
30	A	615	LHG	C12-C13-C14-C15
32	c	518	DGD	C9A-CAA-CBA-CCA
29	A	613	LMG	C30-C31-C32-C33
29	a	613	LMG	C31-C32-C33-C34
29	b	622	LMG	C12-C13-C14-C15
30	E	102	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
32	C	516	DGD	C3B-C4B-C5B-C6B
32	c	516	DGD	CAB-CBB-CCB-CDB
32	c	517	DGD	C8B-C9B-CAB-CBB
24	C	507	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C19
29	b	622	LMG	C36-C37-C38-C39
24	B	605	CLA	C13-C15-C16-C17
29	C	518	LMG	C13-C14-C15-C16
29	Z	101	LMG	C19-C20-C21-C22
30	l	102	LHG	C16-C17-C18-C19
28	A	612	SQD	C32-C33-C34-C35
32	C	516	DGD	CBB-CCB-CDB-CEB
24	b	606	CLA	C13-C15-C16-C17
30	l	102	LHG	C1-C2-C3-O3
28	a	612	SQD	C32-C33-C34-C35
29	b	622	LMG	C38-C39-C40-C41
30	A	615	LHG	C10-C11-C12-C13
32	H	102	DGD	CCB-CDB-CEB-CFB
29	C	519	LMG	C38-C39-C40-C41
29	c	519	LMG	C32-C33-C34-C35
29	j	101	LMG	C20-C21-C22-C23
30	e	101	LHG	C12-C13-C14-C15
32	C	515	DGD	C7B-C8B-C9B-CAB
32	c	516	DGD	C4A-C5A-C6A-C7A
32	c	516	DGD	CAA-CBA-CCA-CDA
29	D	408	LMG	C39-C40-C41-C42
30	d	406	LHG	C33-C34-C35-C36
30	l	102	LHG	C12-C13-C14-C15
26	A	610	BCR	C5-C6-C7-C8
26	A	610	BCR	C23-C24-C25-C26
26	B	619	BCR	C23-C24-C25-C30
26	B	620	BCR	C23-C24-C25-C30
26	F	101	BCR	C5-C6-C7-C8
26	F	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C26
26	I	101	BCR	C5-C6-C7-C8
26	I	101	BCR	C23-C24-C25-C26
26	K	101	BCR	C5-C6-C7-C8
26	K	101	BCR	C23-C24-C25-C26
26	K	102	BCR	C5-C6-C7-C8
26	K	102	BCR	C23-C24-C25-C30
26	T	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	T	101	BCR	C23-C24-C25-C26
26	a	610	BCR	C1-C6-C7-C8
26	a	610	BCR	C23-C24-C25-C26
26	b	619	BCR	C1-C6-C7-C8
26	b	620	BCR	C23-C24-C25-C30
26	b	621	BCR	C23-C24-C25-C26
26	c	515	BCR	C5-C6-C7-C8
26	c	515	BCR	C23-C24-C25-C26
26	c	521	BCR	C5-C6-C7-C8
26	f	101	BCR	C1-C6-C7-C8
26	h	101	BCR	C5-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C26
26	k	101	BCR	C1-C6-C7-C8
26	k	101	BCR	C5-C6-C7-C8
26	t	101	BCR	C1-C6-C7-C8
26	t	101	BCR	C5-C6-C7-C8
29	A	613	LMG	C13-C14-C15-C16
29	a	613	LMG	C30-C31-C32-C33
30	D	406	LHG	C33-C34-C35-C36
28	A	614	SQD	C24-C23-O48-C46
28	a	614	SQD	C24-C23-O48-C46
30	a	616	LHG	C24-C23-O8-C6
24	C	506	CLA	C13-C15-C16-C17
24	c	506	CLA	C13-C15-C16-C17
28	X	101	SQD	C8-C7-O47-C45
28	x	101	SQD	C8-C7-O47-C45
32	C	517	DGD	C9B-CAB-CBB-CCB
32	d	405	DGD	O6E-C5E-C6E-O5E
30	D	406	LHG	C23-C24-C25-C26
28	B	622	SQD	C32-C33-C34-C35
28	b	601	SQD	C32-C33-C34-C35
32	C	515	DGD	CAA-CBA-CCA-CDA
32	c	516	DGD	C8B-C9B-CAB-CBB
27	a	611	PL9	C47-C48-C49-C50
29	D	408	LMG	C13-C14-C15-C16
30	d	406	LHG	C11-C10-C9-C8
30	d	406	LHG	C31-C32-C33-C34
30	e	101	LHG	C27-C28-C29-C30
24	B	606	CLA	O1D-CGD-O2D-CED
24	A	607	CLA	C6-C7-C8-C10
24	B	604	CLA	C6-C7-C8-C10
24	B	611	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	617	CLA	C6-C7-C8-C10
24	C	504	CLA	C11-C12-C13-C15
24	C	510	CLA	C2-C3-C5-C6
24	a	607	CLA	C6-C7-C8-C10
24	b	605	CLA	C6-C7-C8-C10
24	b	612	CLA	C12-C13-C15-C16
24	b	618	CLA	C6-C7-C8-C10
24	c	504	CLA	C11-C12-C13-C15
24	c	510	CLA	C2-C3-C5-C6
24	A	609	CLA	O1A-CGA-O2A-C1
28	B	622	SQD	C29-C30-C31-C32
28	b	601	SQD	C29-C30-C31-C32
30	e	101	LHG	C17-C18-C19-C20
32	d	405	DGD	C5B-C6B-C7B-C8B
24	C	504	CLA	C13-C15-C16-C17
24	c	504	CLA	C13-C15-C16-C17
26	A	610	BCR	C19-C20-C21-C22
29	c	520	LMG	O9-C10-O7-C8
28	L	102	SQD	C7-C8-C9-C10
28	l	101	SQD	C7-C8-C9-C10
24	C	504	CLA	CBA-CGA-O2A-C1
29	D	408	LMG	C29-C28-O8-C9
30	L	101	LHG	C27-C28-C29-C30
32	C	516	DGD	C4A-C5A-C6A-C7A
24	C	503	CLA	C2A-CAA-CBA-CGA
24	C	503	CLA	O1D-CGD-O2D-CED
28	b	601	SQD	C18-C19-C20-C21
32	c	517	DGD	C3B-C4B-C5B-C6B
28	B	622	SQD	C18-C19-C20-C21
30	d	406	LHG	C23-C24-C25-C26
29	C	519	LMG	C15-C16-C17-C18
30	A	615	LHG	C29-C30-C31-C32
30	E	102	LHG	C11-C10-C9-C8
32	E	101	DGD	C8B-C9B-CAB-CBB
27	D	405	PL9	C42-C43-C44-C45
28	a	612	SQD	C30-C31-C32-C33
29	C	518	LMG	C32-C33-C34-C35
32	C	517	DGD	C6B-C7B-C8B-C9B
32	c	518	DGD	C2B-C3B-C4B-C5B
26	B	619	BCR	C6-C7-C8-C9
26	C	514	BCR	C6-C7-C8-C9
26	h	101	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
32	C	515	DGD	O6E-C1E-O5D-C6D
32	C	516	DGD	O6E-C1E-O5D-C6D
32	c	517	DGD	O6E-C1E-O5D-C6D
24	C	501	CLA	C13-C15-C16-C17
24	c	501	CLA	C13-C15-C16-C17
27	a	611	PL9	C9-C11-C12-C13
28	A	612	SQD	C30-C31-C32-C33
29	A	613	LMG	C29-C30-C31-C32
29	j	101	LMG	C38-C39-C40-C41
30	l	102	LHG	C34-C35-C36-C37
32	c	517	DGD	C7B-C8B-C9B-CAB
32	d	405	DGD	C5A-C6A-C7A-C8A
29	B	621	LMG	C11-C10-O7-C8
30	D	406	LHG	C8-C7-O7-C5
26	t	101	BCR	C10-C11-C12-C13
29	C	519	LMG	C17-C18-C19-C20
30	a	616	LHG	C29-C30-C31-C32
24	B	607[A]	CLA	CBD-CGD-O2D-CED
32	d	405	DGD	C8B-C9B-CAB-CBB
28	X	101	SQD	O49-C7-O47-C45
28	x	101	SQD	O49-C7-O47-C45
29	j	101	LMG	C19-C20-C21-C22
32	h	102	DGD	C7A-C8A-C9A-CAA
32	d	405	DGD	O1A-C1A-O1G-C1G
32	C	517	DGD	C9A-CAA-CBA-CCA
32	d	405	DGD	C3A-C4A-C5A-C6A
24	C	510	CLA	C4-C3-C5-C6
24	c	510	CLA	C4-C3-C5-C6
27	D	405	PL9	C30-C29-C31-C32
29	b	622	LMG	C10-C11-C12-C13
29	b	622	LMG	C28-C29-C30-C31
27	A	611	PL9	C4-C3-C7-C8
27	a	611	PL9	C4-C3-C7-C8
29	A	613	LMG	C34-C35-C36-C37
24	A	607	CLA	C6-C7-C8-C9
24	B	611	CLA	C14-C13-C15-C16
24	B	616	CLA	C14-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C9
24	D	404	CLA	C11-C10-C8-C9
24	a	607	CLA	C6-C7-C8-C9
24	b	612	CLA	C14-C13-C15-C16
24	b	617	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	b	618	CLA	C6-C7-C8-C9
24	d	403	CLA	C11-C10-C8-C9
29	C	518	LMG	C38-C39-C40-C41
30	l	102	LHG	C32-C33-C34-C35
24	b	616	CLA	C2A-CAA-CBA-CGA
28	A	614	SQD	C18-C19-C20-C21
28	a	614	SQD	C18-C19-C20-C21
29	a	613	LMG	C18-C19-C20-C21
33	V	201	HEM	C4D-C3D-CAD-CBD
26	a	610	BCR	C36-C18-C19-C20
26	b	619	BCR	C36-C18-C19-C20
26	c	521	BCR	C37-C22-C23-C24
28	X	101	SQD	C23-C24-C25-C26
28	A	612	SQD	C34-C35-C36-C37
32	C	517	DGD	C3B-C4B-C5B-C6B
26	T	101	BCR	C17-C18-C19-C20
26	c	521	BCR	C11-C12-C13-C14
26	c	521	BCR	C17-C18-C19-C20
28	A	614	SQD	O10-C23-O48-C46
28	a	614	SQD	O10-C23-O48-C46
24	C	506	CLA	C1A-C2A-CAA-CBA
24	D	402	CLA	C1A-C2A-CAA-CBA
24	a	615	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
24	B	605	CLA	C16-C17-C18-C20
24	C	506	CLA	C16-C17-C18-C20
24	D	404	CLA	C16-C17-C18-C20
24	b	606	CLA	C16-C17-C18-C20
24	d	403	CLA	C16-C17-C18-C20
29	b	622	LMG	O9-C10-O7-C8
28	a	612	SQD	C34-C35-C36-C37
32	c	518	DGD	C4A-C5A-C6A-C7A
26	B	619	BCR	C13-C14-C15-C16
26	I	101	BCR	C9-C10-C11-C12
26	b	621	BCR	C15-C16-C17-C18
26	f	101	BCR	C15-C16-C17-C18
24	B	607[B]	CLA	C15-C16-C17-C18
24	C	507	CLA	C5-C6-C7-C8
24	b	608[B]	CLA	C15-C16-C17-C18
24	c	507	CLA	C5-C6-C7-C8
30	D	407	LHG	C3-O3-P-O6
30	e	101	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
29	c	519	LMG	C11-C12-C13-C14
30	D	406	LHG	C25-C26-C27-C28
32	C	516	DGD	C6A-C7A-C8A-C9A
28	x	101	SQD	C23-C24-C25-C26
29	C	518	LMG	C17-C18-C19-C20
24	D	404	CLA	C13-C15-C16-C17
24	d	403	CLA	C13-C15-C16-C17
29	C	519	LMG	C29-C28-O8-C9
29	b	622	LMG	C33-C34-C35-C36
29	c	520	LMG	C38-C39-C40-C41
32	C	515	DGD	O6E-C5E-C6E-O5E
24	A	609	CLA	C16-C17-C18-C19
24	C	507	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C20
24	c	507	CLA	C16-C17-C18-C20
28	B	622	SQD	C27-C28-C29-C30
28	b	601	SQD	C27-C28-C29-C30
30	l	102	LHG	C27-C28-C29-C30
32	C	515	DGD	C4A-C5A-C6A-C7A
29	C	518	LMG	C11-C12-C13-C14
29	D	408	LMG	C35-C36-C37-C38
29	Z	101	LMG	C12-C13-C14-C15
29	a	613	LMG	C15-C16-C17-C18
30	a	616	LHG	C12-C13-C14-C15
28	B	622	SQD	C28-C29-C30-C31
29	C	519	LMG	C18-C19-C20-C21
30	a	616	LHG	C16-C17-C18-C19
30	e	101	LHG	C11-C10-C9-C8
32	C	515	DGD	C4D-C5D-C6D-O5D
29	A	613	LMG	C4-C5-C6-O5
28	b	601	SQD	C28-C29-C30-C31
29	b	622	LMG	C15-C16-C17-C18
29	c	520	LMG	C15-C16-C17-C18
32	C	516	DGD	C7B-C8B-C9B-CAB
28	a	612	SQD	C27-C28-C29-C30
29	B	621	LMG	C36-C37-C38-C39
30	d	406	LHG	C24-C25-C26-C27
32	C	517	DGD	C4A-C5A-C6A-C7A
32	E	101	DGD	CBA-CCA-CDA-CEA
28	A	612	SQD	C27-C28-C29-C30
29	c	519	LMG	C13-C14-C15-C16
33	v	201	HEM	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
24	A	607	CLA	C16-C17-C18-C19
24	a	607	CLA	C16-C17-C18-C19
24	a	609	CLA	C16-C17-C18-C19
28	A	614	SQD	O6-C44-C45-C46
28	X	101	SQD	C35-C36-C37-C38
28	a	614	SQD	O6-C44-C45-C46
29	Z	101	LMG	O1-C7-C8-C9
29	a	613	LMG	C7-C8-C9-O8
29	b	622	LMG	C18-C19-C20-C21
29	z	101	LMG	O1-C7-C8-C9
24	C	509	CLA	C10-C11-C12-C13
24	c	509	CLA	C10-C11-C12-C13
28	x	101	SQD	C35-C36-C37-C38
32	E	101	DGD	CAB-CBB-CCB-CDB
33	v	201	HEM	C4D-C3D-CAD-CBD
29	c	520	LMG	C8-C7-O1-C1
32	c	517	DGD	C5D-C6D-O5D-C1E
24	C	502	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	O1D-CGD-O2D-CED
30	d	407	LHG	C34-C35-C36-C37
32	h	102	DGD	C9A-CAA-CBA-CCA
32	h	102	DGD	CCB-CDB-CEB-CFB
28	B	622	SQD	C13-C14-C15-C16
28	B	622	SQD	C35-C36-C37-C38
28	b	601	SQD	C13-C14-C15-C16
28	b	601	SQD	C35-C36-C37-C38
32	C	517	DGD	C8B-C9B-CAB-CBB
29	D	408	LMG	O6-C1-O1-C7
24	C	511	CLA	O1D-CGD-O2D-CED
28	A	614	SQD	C19-C20-C21-C22
32	c	517	DGD	C5B-C6B-C7B-C8B
26	A	610	BCR	C15-C16-C17-C18
28	a	614	SQD	C19-C20-C21-C22
32	h	102	DGD	CCA-CDA-CEA-CFA
30	a	616	LHG	O10-C23-O8-C6
29	B	621	LMG	C28-C29-C30-C31
29	C	518	LMG	C29-C30-C31-C32
30	D	406	LHG	C24-C25-C26-C27
32	h	102	DGD	CBB-CCB-CDB-CEB
28	A	612	SQD	C35-C36-C37-C38
28	a	612	SQD	C35-C36-C37-C38
30	e	101	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	E	101	DGD	C3A-C4A-C5A-C6A
24	b	614	CLA	C13-C15-C16-C17
26	h	101	BCR	C35-C13-C14-C15
25	A	608	PHO	C4-C3-C5-C6
29	B	621	LMG	C15-C16-C17-C18
24	C	511	CLA	CBA-CGA-O2A-C1
24	A	609	CLA	C5-C6-C7-C8
32	h	102	DGD	CDB-CEB-CFB-CGB
24	a	609	CLA	C5-C6-C7-C8
24	c	509	CLA	C2-C1-O2A-CGA
32	d	405	DGD	CAA-CBA-CCA-CDA
29	B	621	LMG	C30-C31-C32-C33
30	D	407	LHG	C9-C10-C11-C12
30	a	616	LHG	C10-C11-C12-C13
32	H	102	DGD	CAA-CBA-CCA-CDA
24	B	608	CLA	O1A-CGA-O2A-C1
28	L	102	SQD	C19-C20-C21-C22
28	l	101	SQD	C19-C20-C21-C22
30	e	101	LHG	C26-C27-C28-C29
32	C	516	DGD	C8B-C9B-CAB-CBB
24	B	613	CLA	C13-C15-C16-C17
30	A	615	LHG	C25-C26-C27-C28
32	c	518	DGD	CBA-CCA-CDA-CEA
26	A	610	BCR	C11-C10-C9-C8
32	C	515	DGD	C2E-C1E-O5D-C6D
32	c	517	DGD	C2E-C1E-O5D-C6D
29	c	519	LMG	C34-C35-C36-C37
30	A	615	LHG	C33-C34-C35-C36
24	b	614	CLA	O1A-CGA-O2A-C1
24	a	609	CLA	C16-C17-C18-C20
32	C	516	DGD	CDA-CEA-CFA-CGA
32	E	101	DGD	C6A-C7A-C8A-C9A
29	c	519	LMG	C39-C40-C41-C42
29	z	101	LMG	C15-C16-C17-C18
24	A	609	CLA	C11-C10-C8-C7
24	B	602	CLA	C6-C7-C8-C10
24	B	602	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	B	617	CLA	C11-C12-C13-C15
24	C	501	CLA	C11-C12-C13-C15
24	C	506	CLA	C11-C12-C13-C15
24	C	508	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	C	512	CLA	C11-C10-C8-C7
24	C	513	CLA	C6-C7-C8-C10
24	D	404	CLA	C11-C10-C8-C7
24	a	609	CLA	C11-C10-C8-C7
24	b	603	CLA	C6-C7-C8-C10
24	b	603	CLA	C11-C10-C8-C7
24	b	617	CLA	C12-C13-C15-C16
24	b	618	CLA	C11-C12-C13-C15
24	c	501	CLA	C11-C12-C13-C15
24	c	506	CLA	C11-C12-C13-C15
24	c	508	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C10-C8-C7
24	c	513	CLA	C6-C7-C8-C10
24	d	403	CLA	C11-C10-C8-C7
27	d	404	PL9	C13-C14-C16-C17
24	c	504	CLA	O1A-CGA-O2A-C1
24	B	617	CLA	C11-C12-C13-C14
24	C	501	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C14
24	C	508	CLA	C11-C10-C8-C9
24	C	513	CLA	C11-C12-C13-C14
24	b	618	CLA	C11-C12-C13-C14
24	c	501	CLA	C14-C13-C15-C16
24	c	506	CLA	C11-C12-C13-C14
24	c	508	CLA	C11-C10-C8-C9
24	c	513	CLA	C11-C12-C13-C14
26	K	101	BCR	C15-C16-C17-C18
26	K	102	BCR	C15-C16-C17-C18
26	t	101	BCR	C15-C16-C17-C18
28	A	612	SQD	C14-C15-C16-C17
28	a	612	SQD	C14-C15-C16-C17
29	Z	101	LMG	C13-C14-C15-C16
30	E	102	LHG	C26-C27-C28-C29
26	t	101	BCR	C36-C18-C19-C20
24	A	609	CLA	C16-C17-C18-C20
24	B	605	CLA	C16-C17-C18-C19
24	B	617	CLA	C16-C17-C18-C20
24	b	606	CLA	C16-C17-C18-C19
24	b	618	CLA	C16-C17-C18-C20
28	A	614	SQD	C25-C26-C27-C28
29	A	613	LMG	C22-C23-C24-C25
26	F	101	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
26	c	521	BCR	C21-C22-C23-C24
28	a	614	SQD	C25-C26-C27-C28
29	A	613	LMG	C21-C22-C23-C24
32	E	101	DGD	C4B-C5B-C6B-C7B
32	E	101	DGD	O1A-C1A-O1G-C1G
28	B	622	SQD	C24-C23-O48-C46
28	b	601	SQD	C24-C23-O48-C46
28	A	612	SQD	C19-C20-C21-C22
28	a	612	SQD	C19-C20-C21-C22
29	B	621	LMG	C31-C32-C33-C34
30	E	102	LHG	C9-C10-C11-C12
32	c	517	DGD	CDA-CEA-CFA-CGA
29	Z	101	LMG	C4-C5-C6-O5
29	D	408	LMG	C30-C31-C32-C33
30	A	615	LHG	C17-C18-C19-C20
32	C	517	DGD	C5B-C6B-C7B-C8B
26	B	618	BCR	C6-C7-C8-C9
26	c	515	BCR	C22-C23-C24-C25
24	a	607	CLA	CBD-CGD-O2D-CED
28	a	614	SQD	C31-C32-C33-C34
28	A	614	SQD	O5-C1-O6-C44
28	a	614	SQD	O5-C1-O6-C44
30	L	101	LHG	O6-C4-C5-C6
30	l	102	LHG	O6-C4-C5-C6
28	A	614	SQD	C31-C32-C33-C34
30	d	407	LHG	C13-C14-C15-C16
29	c	519	LMG	C20-C21-C22-C23
27	A	611	PL9	C28-C29-C31-C32
27	d	404	PL9	C43-C44-C46-C47
24	D	403	CLA	O1D-CGD-O2D-CED
24	B	609	CLA	C13-C15-C16-C17
24	b	610	CLA	C13-C15-C16-C17
24	B	604	CLA	C16-C17-C18-C20
24	b	605	CLA	C16-C17-C18-C20
29	z	101	LMG	C13-C14-C15-C16
32	E	101	DGD	CAA-CBA-CCA-CDA
29	C	518	LMG	C14-C15-C16-C17
24	B	602	CLA	C3A-C2A-CAA-CBA
24	B	605	CLA	C4C-C3C-CAC-CBC
29	C	519	LMG	C33-C34-C35-C36
28	l	101	SQD	C35-C36-C37-C38
24	C	508	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	b	617	CLA	C13-C15-C16-C17
24	c	508	CLA	C5-C6-C7-C8
28	L	102	SQD	C35-C36-C37-C38
29	C	518	LMG	C34-C35-C36-C37
30	D	406	LHG	C27-C28-C29-C30
30	l	102	LHG	C14-C15-C16-C17
28	A	614	SQD	C32-C33-C34-C35
28	a	614	SQD	C32-C33-C34-C35
30	D	406	LHG	C31-C32-C33-C34
28	B	622	SQD	C44-C45-C46-O48
28	L	102	SQD	C44-C45-C46-O48
28	b	601	SQD	C44-C45-C46-O48
28	l	101	SQD	C44-C45-C46-O48
29	D	408	LMG	C7-C8-C9-O8
29	C	519	LMG	O9-C10-O7-C8
32	C	516	DGD	C5A-C6A-C7A-C8A
29	a	613	LMG	C39-C40-C41-C42
30	A	615	LHG	C24-C25-C26-C27
24	B	616	CLA	C13-C15-C16-C17
30	E	102	LHG	C19-C20-C21-C22
32	C	515	DGD	CBA-CCA-CDA-CEA
30	A	615	LHG	C27-C28-C29-C30
24	B	605	CLA	C2C-C3C-CAC-CBC
24	b	606	CLA	C2C-C3C-CAC-CBC
30	A	615	LHG	C18-C19-C20-C21
32	C	516	DGD	C9B-CAB-CBB-CCB
30	E	102	LHG	C3-O3-P-O6
30	D	407	LHG	O10-C23-O8-C6
24	B	613	CLA	O1D-CGD-O2D-CED
28	A	614	SQD	C35-C36-C37-C38
28	a	614	SQD	C35-C36-C37-C38
32	C	516	DGD	CDB-CEB-CFB-CGB
32	E	101	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	C6A-C7A-C8A-C9A
24	B	616	CLA	C10-C11-C12-C13
24	b	617	CLA	C10-C11-C12-C13
24	B	602	CLA	O1A-CGA-O2A-C1
30	D	406	LHG	C15-C16-C17-C18
28	B	622	SQD	O47-C45-C46-O48
28	L	102	SQD	O47-C45-C46-O48
28	b	601	SQD	O47-C45-C46-O48
28	l	101	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
32	E	101	DGD	O1G-C1G-C2G-O2G
32	d	405	DGD	O1G-C1G-C2G-O2G
24	b	615	CLA	O1D-CGD-O2D-CED
28	L	102	SQD	C30-C31-C32-C33
26	I	101	BCR	C15-C16-C17-C18
26	c	515	BCR	C15-C16-C17-C18
29	c	520	LMG	C11-C10-O7-C8
24	B	602	CLA	C16-C17-C18-C20
24	b	603	CLA	C16-C17-C18-C20
28	l	101	SQD	C30-C31-C32-C33
27	D	405	PL9	C39-C41-C42-C43
24	b	603	CLA	C2-C1-O2A-CGA
27	D	405	PL9	C13-C14-C16-C17
30	d	407	LHG	C32-C33-C34-C35
24	B	615	CLA	C11-C12-C13-C14
24	B	615	CLA	C14-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C9
24	b	616	CLA	C11-C12-C13-C14
24	b	616	CLA	C14-C13-C15-C16
24	c	507	CLA	C11-C10-C8-C9
29	B	621	LMG	C33-C34-C35-C36
29	B	621	LMG	C34-C35-C36-C37
29	c	520	LMG	C11-C12-C13-C14
24	B	602	CLA	C15-C16-C17-C18
24	B	607[A]	CLA	C8-C10-C11-C12
24	b	603	CLA	C15-C16-C17-C18
24	b	608[A]	CLA	C8-C10-C11-C12
30	A	615	LHG	C2-C3-O3-P
29	C	518	LMG	C20-C21-C22-C23
30	L	101	LHG	C32-C33-C34-C35
32	H	102	DGD	C5A-C6A-C7A-C8A
24	B	606	CLA	CBD-CGD-O2D-CED
26	K	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	b	619	BCR	C23-C24-C25-C26
26	k	101	BCR	C23-C24-C25-C30
29	a	613	LMG	C22-C23-C24-C25
32	H	102	DGD	O2G-C1B-C2B-C3B
26	K	102	BCR	C36-C18-C19-C20
27	A	611	PL9	C47-C48-C49-C50
28	B	622	SQD	C16-C17-C18-C19
24	B	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	H	101	BCR	C21-C22-C23-C24
26	k	101	BCR	C21-C22-C23-C24
24	C	502	CLA	C15-C16-C17-C18
24	c	502	CLA	C15-C16-C17-C18
28	b	601	SQD	C16-C17-C18-C19
30	l	102	LHG	C25-C26-C27-C28
24	a	615	CLA	C4C-C3C-CAC-CBC
29	c	520	LMG	C40-C41-C42-C43
30	D	406	LHG	C13-C14-C15-C16
24	B	607[B]	CLA	C16-C17-C18-C19
24	C	501	CLA	C16-C17-C18-C19
24	C	502	CLA	C16-C17-C18-C20
24	b	608[B]	CLA	C16-C17-C18-C19
24	c	501	CLA	C16-C17-C18-C19
24	c	502	CLA	C16-C17-C18-C20
30	D	407	LHG	O6-C4-C5-C6
24	B	612	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C15
24	B	616	CLA	C11-C10-C8-C7
24	B	617	CLA	C12-C13-C15-C16
24	C	501	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	C	513	CLA	C11-C12-C13-C15
24	D	404	CLA	C6-C7-C8-C10
24	b	613	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C12-C13-C15
24	b	617	CLA	C11-C10-C8-C7
24	b	618	CLA	C12-C13-C15-C16
24	c	501	CLA	C12-C13-C15-C16
24	c	507	CLA	C11-C10-C8-C7
24	c	513	CLA	C11-C12-C13-C15
24	d	403	CLA	C6-C7-C8-C10
28	b	601	SQD	O10-C23-O48-C46
32	c	516	DGD	O1A-C1A-O1G-C1G
29	A	613	LMG	C15-C16-C17-C18
26	F	101	BCR	C19-C20-C21-C22
26	H	101	BCR	C13-C14-C15-C16
26	b	620	BCR	C15-C16-C17-C18
26	t	101	BCR	C9-C10-C11-C12
24	B	617	CLA	C16-C17-C18-C19
28	B	622	SQD	O10-C23-O48-C46
26	I	101	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
26	c	521	BCR	C16-C17-C18-C36
30	L	101	LHG	C24-C25-C26-C27
32	d	405	DGD	O6D-C5D-C6D-O5D
32	H	102	DGD	CDB-CEB-CFB-CGB
24	b	618	CLA	C16-C17-C18-C19
24	A	609	CLA	CBA-CGA-O2A-C1
30	D	407	LHG	C24-C23-O8-C6
32	E	101	DGD	C4D-C5D-C6D-O5D
28	x	101	SQD	C11-C10-C9-C8
29	c	519	LMG	C30-C31-C32-C33
30	d	406	LHG	C34-C35-C36-C37
32	c	518	DGD	C3A-C4A-C5A-C6A
32	d	405	DGD	CAB-CBB-CCB-CDB
24	C	503	CLA	C8-C10-C11-C12
24	c	503	CLA	C8-C10-C11-C12
24	A	606	CLA	CAD-CBD-CGD-O2D
24	A	609	CLA	CAD-CBD-CGD-O2D
24	C	501	CLA	CAD-CBD-CGD-O2D
24	C	509	CLA	CAD-CBD-CGD-O2D
24	b	603	CLA	CAD-CBD-CGD-O2D
24	c	513	CLA	CAD-CBD-CGD-O2D
25	A	608	PHO	CAD-CBD-CGD-O2D
29	c	519	LMG	O9-C10-O7-C8
28	X	101	SQD	C11-C10-C9-C8
32	C	517	DGD	C7A-C8A-C9A-CAA
30	D	406	LHG	C11-C10-C9-C8
26	B	620	BCR	C6-C7-C8-C9
29	A	613	LMG	C7-C8-C9-O8
32	E	101	DGD	O1G-C1G-C2G-C3G
32	H	102	DGD	O1G-C1G-C2G-C3G
24	B	606	CLA	O1A-CGA-O2A-C1
30	L	101	LHG	O6-C4-C5-O7
28	A	614	SQD	C24-C25-C26-C27
28	a	614	SQD	C24-C25-C26-C27
24	C	510	CLA	CBA-CGA-O2A-C1
24	B	615	CLA	C2A-CAA-CBA-CGA
24	B	604	CLA	C16-C17-C18-C19
24	b	605	CLA	C16-C17-C18-C19
29	C	518	LMG	C22-C23-C24-C25
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	604	CLA	CHA-CBD-CGD-O2D
24	B	607[A]	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	607[B]	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	B	610	CLA	CHA-CBD-CGD-O1D
24	B	610	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	504	CLA	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	b	604	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	b	608[A]	CLA	CHA-CBD-CGD-O1D
24	b	608[B]	CLA	CHA-CBD-CGD-O1D
24	b	614	CLA	CHA-CBD-CGD-O1D
24	b	614	CLA	CHA-CBD-CGD-O2D
24	c	504	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
32	C	515	DGD	CBB-CCB-CDB-CEB
28	A	614	SQD	C2-C1-O6-C44
28	a	614	SQD	C2-C1-O6-C44
29	C	519	LMG	C11-C12-C13-C14
32	C	515	DGD	CDA-CEA-CFA-CGA
32	C	517	DGD	CAB-CBB-CCB-CDB
29	a	613	LMG	O7-C8-C9-O8
30	d	407	LHG	C10-C11-C12-C13
24	b	609	CLA	O1A-CGA-O2A-C1
32	C	517	DGD	O1A-C1A-O1G-C1G
28	A	614	SQD	C29-C30-C31-C32
28	a	614	SQD	C29-C30-C31-C32
29	B	621	LMG	C18-C19-C20-C21
24	B	602	CLA	C16-C17-C18-C19
24	C	501	CLA	C16-C17-C18-C20
24	b	603	CLA	C16-C17-C18-C19
24	c	501	CLA	C16-C17-C18-C20
30	E	102	LHG	C12-C13-C14-C15
32	c	517	DGD	CDB-CEB-CFB-CGB
27	a	611	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
32	C	516	DGD	CCA-CDA-CEA-CFA
32	C	515	DGD	O1A-C1A-O1G-C1G
25	A	608	PHO	C2-C3-C5-C6
27	a	611	PL9	C28-C29-C31-C32
28	A	614	SQD	C27-C28-C29-C30
28	a	614	SQD	C27-C28-C29-C30
24	A	609	CLA	C11-C12-C13-C14
24	B	612	CLA	C14-C13-C15-C16
24	D	404	CLA	C6-C7-C8-C9
24	a	609	CLA	C11-C12-C13-C14
24	b	613	CLA	C14-C13-C15-C16
24	d	403	CLA	C6-C7-C8-C9
24	C	512	CLA	O1D-CGD-O2D-CED
29	c	519	LMG	C14-C15-C16-C17
29	a	613	LMG	O6-C5-C6-O5
32	C	516	DGD	C8A-C9A-CAA-CBA
32	C	516	DGD	CBA-CCA-CDA-CEA
26	T	101	BCR	C36-C18-C19-C20
26	c	521	BCR	C36-C18-C19-C20
30	E	102	LHG	O1-C1-C2-C3
26	I	101	BCR	C17-C18-C19-C20
26	b	619	BCR	C17-C18-C19-C20
26	b	621	BCR	C17-C18-C19-C20
26	t	101	BCR	C17-C18-C19-C20
24	b	612	CLA	C8-C10-C11-C12
29	j	101	LMG	C17-C18-C19-C20
24	B	602	CLA	C2-C1-O2A-CGA
24	a	606	CLA	C2-C1-O2A-CGA
24	b	618	CLA	C2-C1-O2A-CGA
29	A	613	LMG	C11-C12-C13-C14
29	C	518	LMG	C19-C20-C21-C22
26	T	101	BCR	C9-C10-C11-C12
30	E	102	LHG	C4-O6-P-O3
30	a	616	LHG	C11-C10-C9-C8
24	b	606	CLA	C4C-C3C-CAC-CBC
24	B	614	CLA	C13-C15-C16-C17
30	a	616	LHG	C2-C3-O3-P
29	C	518	LMG	C31-C32-C33-C34
30	L	101	LHG	C14-C15-C16-C17
32	C	516	DGD	C7A-C8A-C9A-CAA
30	D	407	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
30	e	101	LHG	C3-O3-P-O4
30	l	102	LHG	C4-O6-P-O5
24	B	611	CLA	C16-C17-C18-C19
24	b	612	CLA	C16-C17-C18-C19
30	d	406	LHG	C15-C16-C17-C18
32	c	516	DGD	C9A-CAA-CBA-CCA
32	c	516	DGD	O6D-C1D-O3G-C3G
24	B	611	CLA	C8-C10-C11-C12
24	b	615	CLA	C13-C15-C16-C17
29	A	613	LMG	C29-C28-O8-C9
24	B	615	CLA	CBD-CGD-O2D-CED
29	c	519	LMG	O10-C28-O8-C9
28	a	614	SQD	C9-C10-C11-C12
28	A	614	SQD	C9-C10-C11-C12
29	j	101	LMG	C11-C12-C13-C14
32	C	515	DGD	C5A-C6A-C7A-C8A
29	Z	101	LMG	C18-C19-C20-C21
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	510	CLA	CAD-CBD-CGD-O1D
24	b	603	CLA	CAD-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
28	A	612	SQD	C23-C24-C25-C26
28	a	612	SQD	C23-C24-C25-C26
29	a	613	LMG	C29-C30-C31-C32
32	H	102	DGD	C8A-C9A-CAA-CBA
32	c	517	DGD	C5A-C6A-C7A-C8A
24	B	605	CLA	C3-C5-C6-C7
24	b	606	CLA	C3-C5-C6-C7
24	D	402	CLA	C2C-C3C-CAC-CBC
28	B	622	SQD	C19-C20-C21-C22
28	b	601	SQD	C19-C20-C21-C22
28	X	101	SQD	C28-C29-C30-C31
32	c	517	DGD	C6A-C7A-C8A-C9A
24	B	602	CLA	CBA-CGA-O2A-C1
24	b	603	CLA	CBA-CGA-O2A-C1
28	x	101	SQD	C28-C29-C30-C31
32	c	518	DGD	CAB-CBB-CCB-CDB
24	b	617	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	c	502	CLA	CBD-CGD-O2D-CED
24	A	607	CLA	C11-C10-C8-C7
24	B	615	CLA	C12-C13-C15-C16
24	C	504	CLA	C12-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C10
24	C	509	CLA	C6-C7-C8-C10
24	D	404	CLA	C11-C12-C13-C15
24	D	404	CLA	C12-C13-C15-C16
24	a	607	CLA	C11-C10-C8-C7
24	b	616	CLA	C12-C13-C15-C16
24	c	504	CLA	C12-C13-C15-C16
24	c	506	CLA	C6-C7-C8-C10
24	c	509	CLA	C6-C7-C8-C10
24	d	403	CLA	C12-C13-C15-C16
29	a	613	LMG	C10-C11-C12-C13
30	l	102	LHG	O6-C4-C5-O7
32	C	515	DGD	C9A-CAA-CBA-CCA
32	c	516	DGD	C5A-C6A-C7A-C8A
32	c	518	DGD	CDB-CEB-CFB-CGB
27	A	611	PL9	C2-C3-C7-C8
29	A	613	LMG	C10-C11-C12-C13
29	A	613	LMG	C17-C18-C19-C20
29	j	101	LMG	C34-C35-C36-C37
30	a	616	LHG	C17-C18-C19-C20
32	h	102	DGD	C5A-C6A-C7A-C8A
24	B	616	CLA	C16-C17-C18-C20
29	C	519	LMG	C40-C41-C42-C43
29	C	519	LMG	C16-C17-C18-C19
29	a	613	LMG	O1-C7-C8-C9
30	A	615	LHG	C30-C31-C32-C33
32	c	518	DGD	C3B-C4B-C5B-C6B
32	c	518	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	O1G-C1G-C2G-C3G
29	A	613	LMG	O1-C7-C8-O7
29	A	613	LMG	O7-C8-C9-O8
29	D	408	LMG	O7-C8-C9-O8
29	a	613	LMG	O1-C7-C8-O7
30	E	102	LHG	O7-C5-C6-O8
32	h	102	DGD	O1G-C1G-C2G-O2G
30	e	101	LHG	C9-C10-C11-C12
29	C	519	LMG	C8-C7-O1-C1
32	C	516	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
32	C	516	DGD	C5D-C6D-O5D-C1E
32	c	517	DGD	C2G-C3G-O3G-C1D
24	c	513	CLA	C3-C5-C6-C7
27	A	611	PL9	C15-C14-C16-C17
29	a	613	LMG	C33-C34-C35-C36
29	A	613	LMG	C39-C40-C41-C42
32	d	405	DGD	CBB-CCB-CDB-CEB
24	A	607	CLA	C11-C10-C8-C9
24	A	609	CLA	C11-C10-C8-C9
24	B	617	CLA	C14-C13-C15-C16
24	C	504	CLA	C14-C13-C15-C16
24	a	607	CLA	C11-C10-C8-C9
24	b	618	CLA	C14-C13-C15-C16
24	c	504	CLA	C14-C13-C15-C16
24	c	512	CLA	C11-C10-C8-C9
26	t	101	BCR	C6-C7-C8-C9
24	C	513	CLA	C3-C5-C6-C7
28	l	101	SQD	C13-C14-C15-C16
30	E	102	LHG	O1-C1-C2-O2
29	b	622	LMG	C35-C36-C37-C38
30	E	102	LHG	C17-C18-C19-C20
30	d	407	LHG	C11-C10-C9-C8
26	c	515	BCR	C13-C14-C15-C16
28	L	102	SQD	C13-C14-C15-C16
29	a	613	LMG	C17-C18-C19-C20
29	D	408	LMG	C11-C12-C13-C14
28	B	622	SQD	C14-C15-C16-C17
28	b	601	SQD	C14-C15-C16-C17
29	B	621	LMG	C39-C40-C41-C42
29	C	519	LMG	C36-C37-C38-C39
29	Z	101	LMG	C15-C16-C17-C18
32	c	518	DGD	C7A-C8A-C9A-CAA
28	B	622	SQD	C46-C45-O47-C7
28	b	601	SQD	C46-C45-O47-C7
29	c	520	LMG	C16-C17-C18-C19
29	C	518	LMG	O9-C10-O7-C8
24	B	617	CLA	C2-C1-O2A-CGA
24	C	506	CLA	C2-C1-O2A-CGA
29	C	518	LMG	C30-C31-C32-C33
29	c	519	LMG	C29-C28-O8-C9
26	K	102	BCR	C19-C20-C21-C22
30	L	101	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
30	D	407	LHG	O6-C4-C5-O7
24	B	603	CLA	O1D-CGD-O2D-CED
27	a	611	PL9	C35-C34-C36-C37
29	c	520	LMG	C36-C37-C38-C39
32	c	517	DGD	C7A-C8A-C9A-CAA
26	A	610	BCR	C1-C6-C7-C8
26	F	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C23-C24-C25-C30
26	t	101	BCR	C23-C24-C25-C26
24	b	603	CLA	CAA-CBA-CGA-O2A
29	B	621	LMG	O8-C28-C29-C30
30	l	102	LHG	C28-C29-C30-C31
24	C	512	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C19
24	b	612	CLA	C2A-CAA-CBA-CGA
26	K	101	BCR	C20-C21-C22-C23
29	A	613	LMG	C2-C1-O1-C7
30	D	406	LHG	C3-O3-P-O6
30	e	101	LHG	C4-O6-P-O3
29	A	613	LMG	O1-C7-C8-C9
29	b	622	LMG	C30-C31-C32-C33
24	C	506	CLA	C12-C13-C15-C16
24	c	506	CLA	C12-C13-C15-C16
24	d	403	CLA	C11-C12-C13-C15
32	c	516	DGD	CBA-CCA-CDA-CEA
24	B	602	CLA	C6-C7-C8-C9
24	B	616	CLA	C11-C10-C8-C9
24	C	506	CLA	C6-C7-C8-C9
24	C	512	CLA	C11-C10-C8-C9
24	C	513	CLA	C6-C7-C8-C9
24	a	609	CLA	C11-C10-C8-C9
24	b	603	CLA	C6-C7-C8-C9
24	b	617	CLA	C11-C10-C8-C9
24	c	506	CLA	C6-C7-C8-C9
24	c	513	CLA	C6-C7-C8-C9
26	B	619	BCR	C19-C20-C21-C22
24	B	611	CLA	C16-C17-C18-C20
24	b	612	CLA	C16-C17-C18-C20
29	A	613	LMG	C19-C20-C21-C22
30	l	102	LHG	C9-C10-C11-C12
24	C	502	CLA	C16-C17-C18-C19
24	c	502	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	C	519	LMG	C39-C40-C41-C42
32	E	101	DGD	C5A-C6A-C7A-C8A
27	D	405	PL9	C36-C37-C38-C39
30	D	406	LHG	O1-C1-C2-O2
24	B	616	CLA	C16-C17-C18-C19
24	b	617	CLA	C16-C17-C18-C19
24	c	504	CLA	CBA-CGA-O2A-C1
32	d	405	DGD	C2A-C1A-O1G-C1G
30	d	406	LHG	C17-C18-C19-C20
24	a	609	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	CBD-CGD-O2D-CED
32	C	515	DGD	CCA-CDA-CEA-CFA
32	E	101	DGD	CDB-CEB-CFB-CGB
24	C	501	CLA	O1A-CGA-O2A-C1
24	b	615	CLA	O1A-CGA-O2A-C1
29	A	613	LMG	O6-C1-O1-C7
26	b	620	BCR	C9-C10-C11-C12
24	b	613	CLA	O1A-CGA-O2A-C1
24	A	607	CLA	C2C-C3C-CAC-CBC
24	A	607	CLA	C4C-C3C-CAC-CBC
29	B	621	LMG	C13-C14-C15-C16
32	h	102	DGD	C8B-C9B-CAB-CBB
26	k	101	BCR	C18-C19-C20-C21
24	d	403	CLA	O1A-CGA-O2A-C1
32	H	102	DGD	C7B-C8B-C9B-CAB
27	d	404	PL9	C15-C14-C16-C17
24	B	611	CLA	C13-C15-C16-C17
24	b	612	CLA	C13-C15-C16-C17
29	c	519	LMG	C21-C22-C23-C24
30	L	101	LHG	C16-C17-C18-C19
32	c	518	DGD	O6D-C5D-C6D-O5D
28	a	614	SQD	C10-C11-C12-C13
28	A	614	SQD	C10-C11-C12-C13
27	d	404	PL9	C42-C43-C44-C45
24	B	611	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
24	c	509	CLA	C2A-CAA-CBA-CGA
32	C	516	DGD	C2B-C3B-C4B-C5B
24	B	616	CLA	C3A-C2A-CAA-CBA
24	b	603	CLA	C3A-C2A-CAA-CBA
29	z	101	LMG	C14-C15-C16-C17
30	e	101	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
33	e	102	HEM	CAD-CBD-CGD-O1D
29	c	519	LMG	C22-C23-C24-C25
24	B	617	CLA	C13-C15-C16-C17
26	B	619	BCR	C35-C13-C14-C15
30	A	615	LHG	C13-C14-C15-C16
24	C	512	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C20
24	C	506	CLA	CBA-CGA-O2A-C1
24	C	510	CLA	C8-C10-C11-C12
24	b	618	CLA	C13-C15-C16-C17
24	c	510	CLA	C8-C10-C11-C12
24	c	505	CLA	CBD-CGD-O2D-CED
29	C	519	LMG	C12-C13-C14-C15
27	d	404	PL9	C35-C34-C36-C37
24	B	603	CLA	C1A-C2A-CAA-CBA
24	B	611	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C1A-C2A-CAA-CBA
24	D	403	CLA	C1A-C2A-CAA-CBA
29	b	622	LMG	C39-C40-C41-C42
24	A	609	CLA	C12-C13-C15-C16
24	B	607[B]	CLA	C11-C10-C8-C7
24	C	502	CLA	C12-C13-C15-C16
24	C	504	CLA	C11-C10-C8-C7
24	a	609	CLA	C12-C13-C15-C16
24	b	608[B]	CLA	C11-C10-C8-C7
24	c	502	CLA	C12-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C7
24	C	505	CLA	C2A-CAA-CBA-CGA
29	a	613	LMG	C21-C22-C23-C24
30	D	407	LHG	C35-C36-C37-C38
29	Z	101	LMG	O6-C5-C6-O5
24	B	608	CLA	CBA-CGA-O2A-C1
33	e	102	HEM	CAD-CBD-CGD-O2D
27	a	611	PL9	C45-C44-C46-C47
27	d	404	PL9	C12-C11-C9-C10
32	C	515	DGD	C1B-C2B-C3B-C4B
24	C	513	CLA	C16-C17-C18-C19
24	c	513	CLA	C16-C17-C18-C19
29	c	520	LMG	C39-C40-C41-C42
30	d	406	LHG	C11-C12-C13-C14
29	C	518	LMG	C33-C34-C35-C36
28	A	612	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
28	a	612	SQD	O6-C44-C45-O47
32	E	101	DGD	O2G-C2G-C3G-O3G
32	H	102	DGD	O1G-C1G-C2G-O2G
30	d	407	LHG	C26-C27-C28-C29
32	C	517	DGD	CBA-CCA-CDA-CEA
24	c	502	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	C6-C7-C8-C9
29	c	520	LMG	C32-C33-C34-C35
24	c	501	CLA	C2A-CAA-CBA-CGA
24	c	505	CLA	C2A-CAA-CBA-CGA
26	B	619	BCR	C1-C6-C7-C8
26	C	514	BCR	C1-C6-C7-C8
26	K	101	BCR	C23-C24-C25-C30
26	a	610	BCR	C23-C24-C25-C30
26	c	515	BCR	C1-C6-C7-C8
24	b	610	CLA	C4C-C3C-CAC-CBC
32	d	405	DGD	CDB-CEB-CFB-CGB
29	c	520	LMG	C37-C38-C39-C40
24	C	513	CLA	C4-C3-C5-C6
24	c	513	CLA	C4-C3-C5-C6
25	a	608	PHO	C4-C3-C5-C6
27	A	611	PL9	C45-C44-C46-C47
32	E	101	DGD	O6E-C5E-C6E-O5E
26	K	101	BCR	C21-C22-C23-C24
30	d	407	LHG	C16-C17-C18-C19
24	B	610	CLA	C2-C3-C5-C6
24	b	611	CLA	C2-C3-C5-C6
25	a	608	PHO	C2-C3-C5-C6
24	B	602	CLA	CAA-CBA-CGA-O2A
29	A	613	LMG	C20-C21-C22-C23
30	e	101	LHG	O6-C4-C5-O7
32	c	516	DGD	CCA-CDA-CEA-CFA
32	h	102	DGD	CDA-CEA-CFA-CGA
24	C	506	CLA	CBD-CGD-O2D-CED
24	B	613	CLA	CBA-CGA-O2A-C1
24	B	615	CLA	CBA-CGA-O2A-C1
32	d	405	DGD	C4E-C5E-C6E-O5E
25	D	401	PHO	C8-C10-C11-C12
24	c	507	CLA	C4-C3-C5-C6
27	D	405	PL9	C19-C21-C22-C23
26	b	620	BCR	C19-C20-C21-C22
33	E	103	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
32	H	102	DGD	CDA-CEA-CFA-CGA
30	a	616	LHG	O7-C5-C6-O8
32	C	515	DGD	C8B-C9B-CAB-CBB
24	a	615	CLA	C2A-CAA-CBA-CGA
25	D	401	PHO	C5-C6-C7-C8
30	D	407	LHG	C25-C26-C27-C28
30	l	102	LHG	C17-C18-C19-C20
26	k	101	BCR	C35-C13-C14-C15
30	D	407	LHG	C13-C14-C15-C16
32	C	517	DGD	C2B-C3B-C4B-C5B
24	C	507	CLA	C4-C3-C5-C6
24	a	609	CLA	C4-C3-C5-C6
27	D	405	PL9	C12-C11-C9-C10
29	C	518	LMG	C29-C28-O8-C9
30	l	102	LHG	O7-C7-C8-C9
28	b	601	SQD	C33-C34-C35-C36
32	c	518	DGD	C6B-C7B-C8B-C9B
24	B	607[A]	CLA	C11-C12-C13-C14
24	B	607[B]	CLA	C11-C10-C8-C9
24	D	404	CLA	C11-C12-C13-C14
24	b	608[A]	CLA	C11-C12-C13-C14
24	b	608[B]	CLA	C11-C10-C8-C9
24	c	510	CLA	C6-C7-C8-C9
24	d	403	CLA	C11-C12-C13-C14
28	B	622	SQD	C33-C34-C35-C36
32	c	516	DGD	C3B-C4B-C5B-C6B
24	b	605	CLA	C13-C15-C16-C17
24	A	609	CLA	C3A-C2A-CAA-CBA
24	C	512	CLA	C3A-C2A-CAA-CBA
24	b	617	CLA	C3A-C2A-CAA-CBA
24	B	604	CLA	C13-C15-C16-C17
24	C	510	CLA	CAA-CBA-CGA-O2A
24	D	403	CLA	CAA-CBA-CGA-O2A
30	E	102	LHG	O7-C7-C8-C9
32	d	405	DGD	C4B-C5B-C6B-C7B
24	B	606	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	C	508	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	606	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	b	615	CLA	CAD-CBD-CGD-O2D
24	c	501	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CAD-CBD-CGD-O2D
24	D	402	CLA	C4C-C3C-CAC-CBC
30	D	406	LHG	C17-C18-C19-C20
28	B	622	SQD	C17-C18-C19-C20
28	L	102	SQD	O48-C23-C24-C25
24	A	609	CLA	C4-C3-C5-C6
28	l	101	SQD	O48-C23-C24-C25
29	j	101	LMG	O7-C10-C11-C12
30	L	101	LHG	O7-C7-C8-C9
28	b	601	SQD	C17-C18-C19-C20
26	A	610	BCR	C21-C22-C23-C24
26	C	514	BCR	C11-C12-C13-C14
26	h	101	BCR	C7-C8-C9-C10
29	c	520	LMG	C14-C15-C16-C17
30	d	406	LHG	C27-C28-C29-C30
25	D	401	PHO	C2C-C3C-CAC-CBC
25	d	401	PHO	C2C-C3C-CAC-CBC
30	E	102	LHG	C4-C5-C6-O8
27	A	611	PL9	C21-C22-C23-C24
24	c	510	CLA	CAA-CBA-CGA-O2A
32	c	518	DGD	O1G-C1A-C2A-C3A
24	B	605	CLA	O2A-C1-C2-C3
24	C	512	CLA	O2A-C1-C2-C3
24	D	403	CLA	O2A-C1-C2-C3
24	b	604	CLA	O2A-C1-C2-C3
24	b	606	CLA	O2A-C1-C2-C3
24	c	509	CLA	O2A-C1-C2-C3
24	c	512	CLA	O2A-C1-C2-C3
24	d	402	CLA	O2A-C1-C2-C3
25	A	608	PHO	O2A-C1-C2-C3
25	a	608	PHO	O2A-C1-C2-C3
32	c	518	DGD	C5B-C6B-C7B-C8B
24	A	607	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	D	402	CLA	CHA-CBD-CGD-O2D
24	a	607	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	c	505	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O1D
29	a	613	LMG	C19-C20-C21-C22
24	B	607[A]	CLA	C16-C17-C18-C20
24	b	608[A]	CLA	C16-C17-C18-C20
27	a	611	PL9	C2-C3-C7-C8
32	C	517	DGD	O1G-C1A-C2A-C3A
30	D	406	LHG	O7-C5-C6-O8
24	a	607	CLA	C4C-C3C-CAC-CBC
24	b	614	CLA	CAA-CBA-CGA-O2A
29	D	408	LMG	O7-C10-C11-C12
29	a	613	LMG	C16-C17-C18-C19
30	d	406	LHG	C10-C11-C12-C13
24	C	501	CLA	C2A-CAA-CBA-CGA
24	b	605	CLA	C2A-CAA-CBA-CGA
25	D	401	PHO	CHA-CBD-CGD-O1D
25	d	401	PHO	CHA-CBD-CGD-O1D
30	a	616	LHG	O1-C1-C2-O2
32	C	517	DGD	CDB-CEB-CFB-CGB
32	h	102	DGD	O2G-C1B-C2B-C3B
27	d	404	PL9	C36-C37-C38-C39
24	B	610	CLA	C4-C3-C5-C6
24	A	609	CLA	C11-C12-C13-C15
24	a	609	CLA	C11-C12-C13-C15
32	H	102	DGD	C9B-CAB-CBB-CCB
24	B	614	CLA	CAA-CBA-CGA-O2A
30	e	101	LHG	O7-C7-C8-C9
24	B	605	CLA	C6-C7-C8-C9
24	C	504	CLA	C11-C10-C8-C9
24	C	505	CLA	C14-C13-C15-C16
24	C	506	CLA	C14-C13-C15-C16
24	D	404	CLA	C14-C13-C15-C16
24	b	606	CLA	C6-C7-C8-C9
24	c	504	CLA	C11-C10-C8-C9
24	c	505	CLA	C14-C13-C15-C16
24	c	506	CLA	C14-C13-C15-C16
24	d	403	CLA	C14-C13-C15-C16
30	A	615	LHG	O10-C23-C24-C25
26	t	101	BCR	C19-C20-C21-C22
32	E	101	DGD	C3B-C4B-C5B-C6B
28	A	612	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
28	a	612	SQD	C18-C19-C20-C21
29	D	408	LMG	C32-C33-C34-C35
32	d	405	DGD	C3B-C4B-C5B-C6B
32	c	517	DGD	O1B-C1B-C2B-C3B
30	D	406	LHG	C34-C35-C36-C37
33	E	103	HEM	CAD-CBD-CGD-O2D
24	C	513	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C20
24	b	611	CLA	C4-C3-C5-C6
29	C	518	LMG	C21-C22-C23-C24
24	a	607	CLA	C2C-C3C-CAC-CBC
30	e	101	LHG	O9-C7-C8-C9
24	B	609	CLA	C1A-C2A-CAA-CBA
24	b	604	CLA	C1A-C2A-CAA-CBA
24	b	610	CLA	C1A-C2A-CAA-CBA
24	b	612	CLA	C1A-C2A-CAA-CBA
24	c	505	CLA	C1A-C2A-CAA-CBA
32	c	516	DGD	C7B-C8B-C9B-CAB
32	C	516	DGD	O1B-C1B-C2B-C3B
24	c	509	CLA	O1D-CGD-O2D-CED
24	B	608	CLA	C2-C1-O2A-CGA
24	d	402	CLA	C2-C1-O2A-CGA
28	A	614	SQD	C11-C12-C13-C14
29	c	519	LMG	C17-C18-C19-C20
32	E	101	DGD	C2A-C1A-O1G-C1G
32	E	101	DGD	C1G-C2G-C3G-O3G
28	a	614	SQD	C11-C12-C13-C14
24	D	403	CLA	CAA-CBA-CGA-O1A
24	B	606	CLA	C13-C15-C16-C17
24	b	607	CLA	C13-C15-C16-C17
32	c	517	DGD	C8A-C9A-CAA-CBA
27	D	405	PL9	C18-C19-C21-C22
33	E	103	HEM	CAA-CBA-CGA-O2A
32	c	516	DGD	C2E-C1E-O5D-C6D
30	A	615	LHG	C4-O6-P-O5
30	d	407	LHG	C4-O6-P-O5
28	L	102	SQD	O10-C23-C24-C25
30	a	616	LHG	O8-C23-C24-C25
24	B	610	CLA	O1A-CGA-O2A-C1
28	l	101	SQD	O10-C23-C24-C25
29	z	101	LMG	O7-C10-C11-C12
24	c	512	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	A	613	LMG	O10-C28-C29-C30
27	d	404	PL9	C45-C44-C46-C47
30	D	406	LHG	C28-C29-C30-C31
27	d	404	PL9	C38-C39-C41-C42
24	B	610	CLA	CAD-CBD-CGD-O1D
24	B	613	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CAD-CBD-CGD-O1D
24	A	609	CLA	C14-C13-C15-C16
24	B	607[B]	CLA	C14-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C9
24	D	402	CLA	C11-C12-C13-C14
24	a	609	CLA	C14-C13-C15-C16
24	a	615	CLA	C11-C12-C13-C14
24	b	608[B]	CLA	C14-C13-C15-C16
24	c	511	CLA	C6-C7-C8-C9
29	a	613	LMG	C36-C37-C38-C39
24	c	501	CLA	CAA-CBA-CGA-O2A
29	D	408	LMG	C19-C20-C21-C22
24	B	616	CLA	C15-C16-C17-C18
33	e	102	HEM	CAA-CBA-CGA-O1A
32	H	102	DGD	C5B-C6B-C7B-C8B
28	B	622	SQD	C45-C46-O48-C23
28	b	601	SQD	C45-C46-O48-C23
24	b	604	CLA	C2A-CAA-CBA-CGA
24	C	505	CLA	CAA-CBA-CGA-O2A
32	C	516	DGD	O2G-C1B-C2B-C3B
27	D	405	PL9	C25-C24-C26-C27
24	b	617	CLA	C15-C16-C17-C18
24	B	607[B]	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C10-C8-C7
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C15
24	C	510	CLA	C6-C7-C8-C10
24	C	511	CLA	C6-C7-C8-C10
24	D	403	CLA	C12-C13-C15-C16
24	b	608[B]	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C7
24	c	505	CLA	C12-C13-C15-C16
24	c	507	CLA	C11-C12-C13-C15
24	c	510	CLA	C6-C7-C8-C10
24	c	511	CLA	C6-C7-C8-C10

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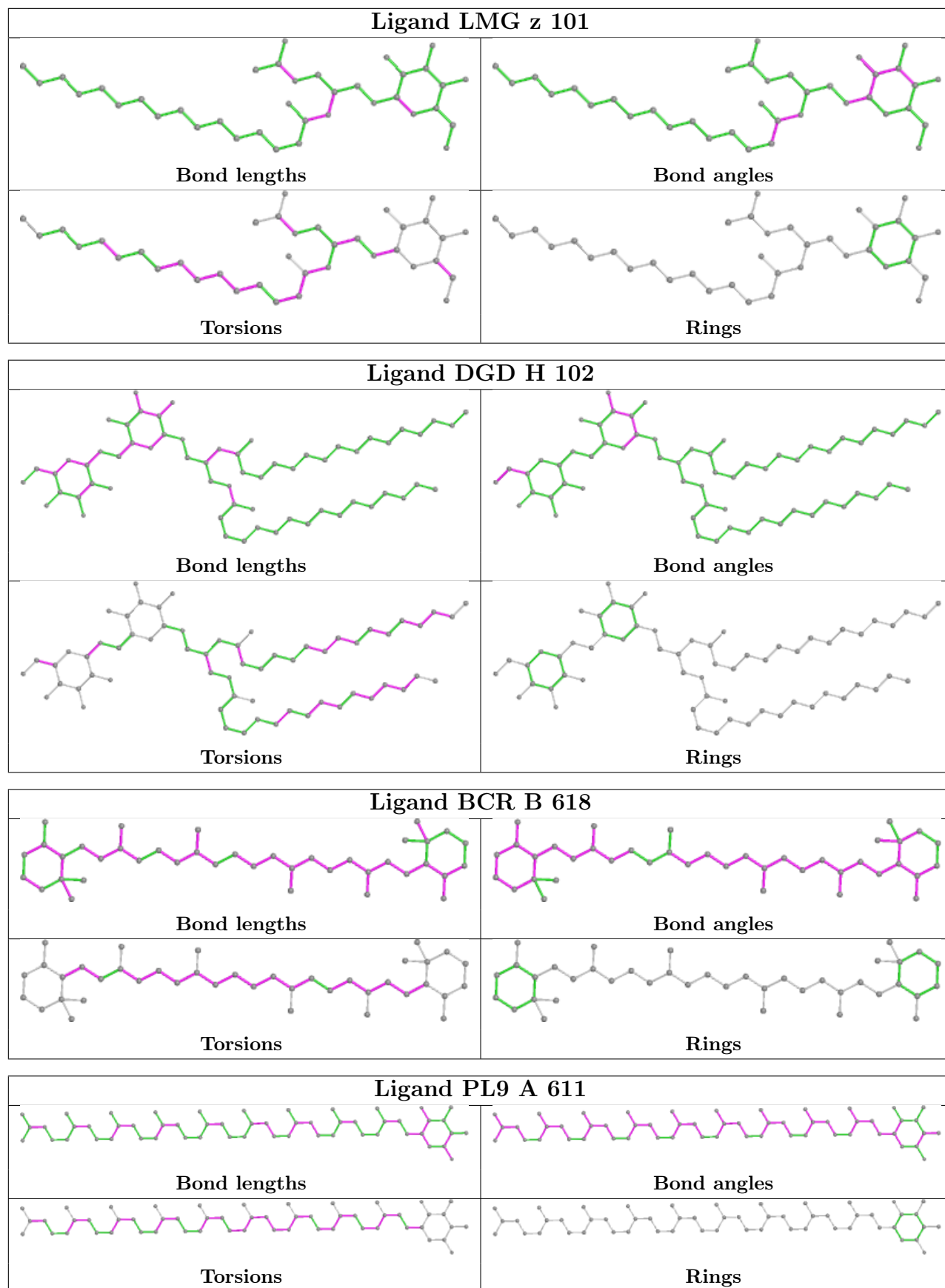
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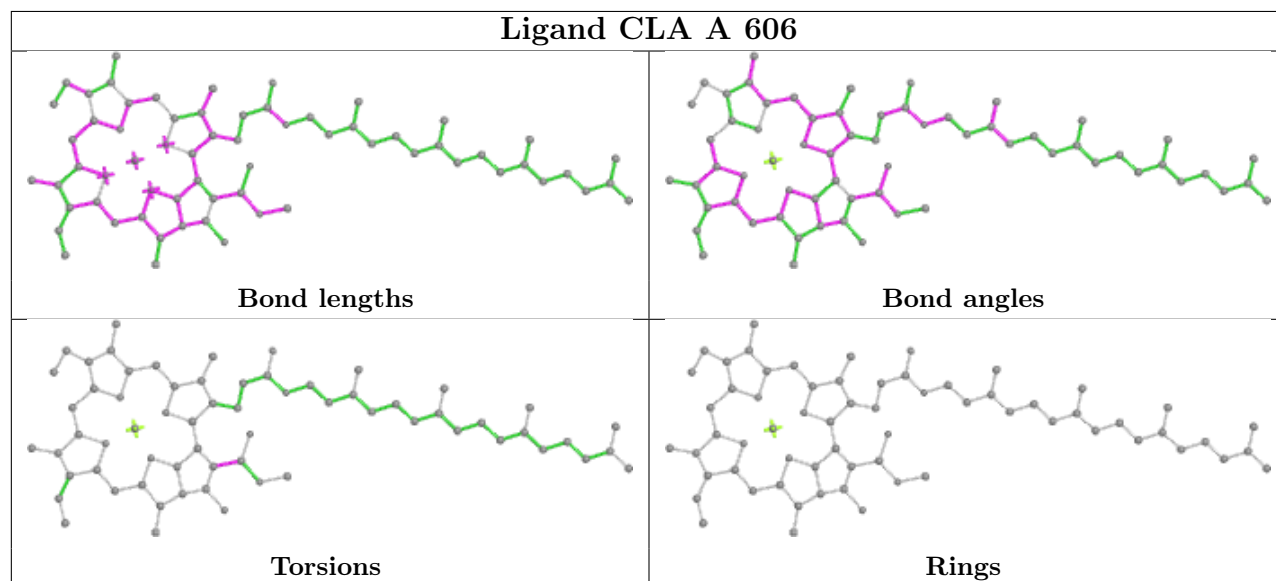
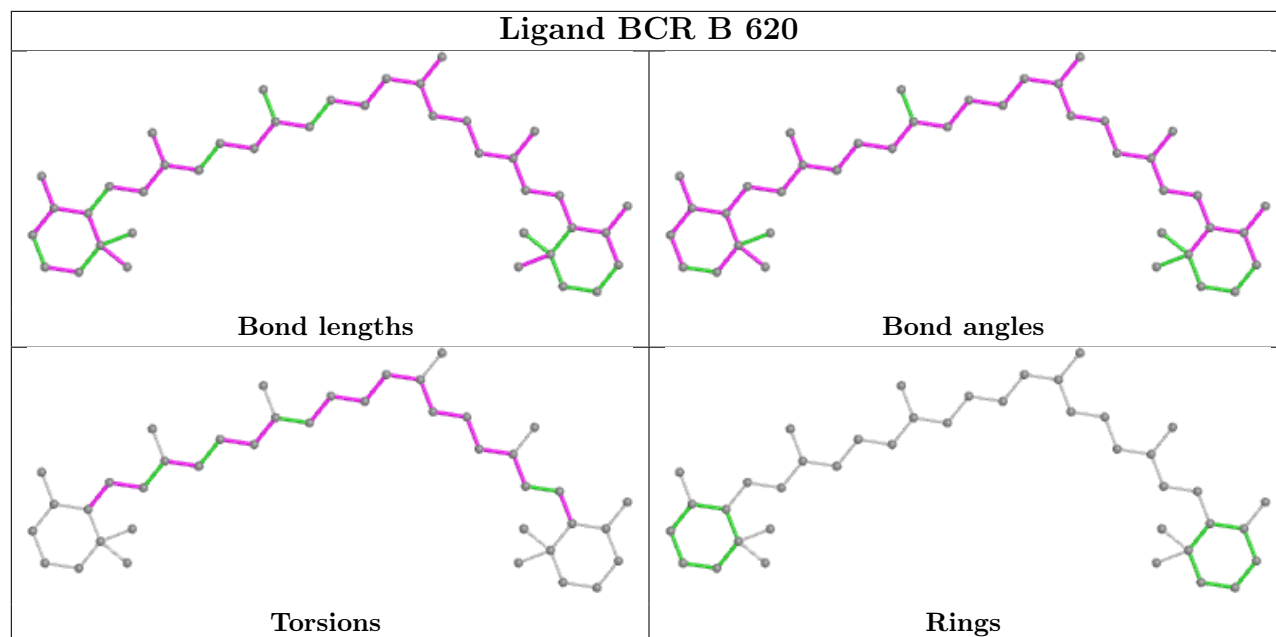
Mol	Chain	Res	Type	Atoms
24	d	402	CLA	C12-C13-C15-C16
24	C	501	CLA	CAA-CBA-CGA-O1A
32	c	517	DGD	O2G-C1B-C2B-C3B
32	C	517	DGD	CCA-CDA-CEA-CFA
30	d	407	LHG	C12-C13-C14-C15
26	B	618	BCR	C17-C18-C19-C20
26	b	621	BCR	C21-C22-C23-C24
24	B	613	CLA	CAA-CBA-CGA-O1A
24	B	613	CLA	C8-C10-C11-C12
24	b	614	CLA	C8-C10-C11-C12
32	c	518	DGD	O6E-C5E-C6E-O5E
29	C	518	LMG	O8-C28-C29-C30
24	C	506	CLA	C15-C16-C17-C18
24	c	506	CLA	C15-C16-C17-C18
30	E	102	LHG	O9-C7-C8-C9
30	a	616	LHG	O10-C23-C24-C25
30	l	102	LHG	O9-C7-C8-C9
32	d	405	DGD	O1A-C1A-C2A-C3A
30	d	407	LHG	O8-C23-C24-C25

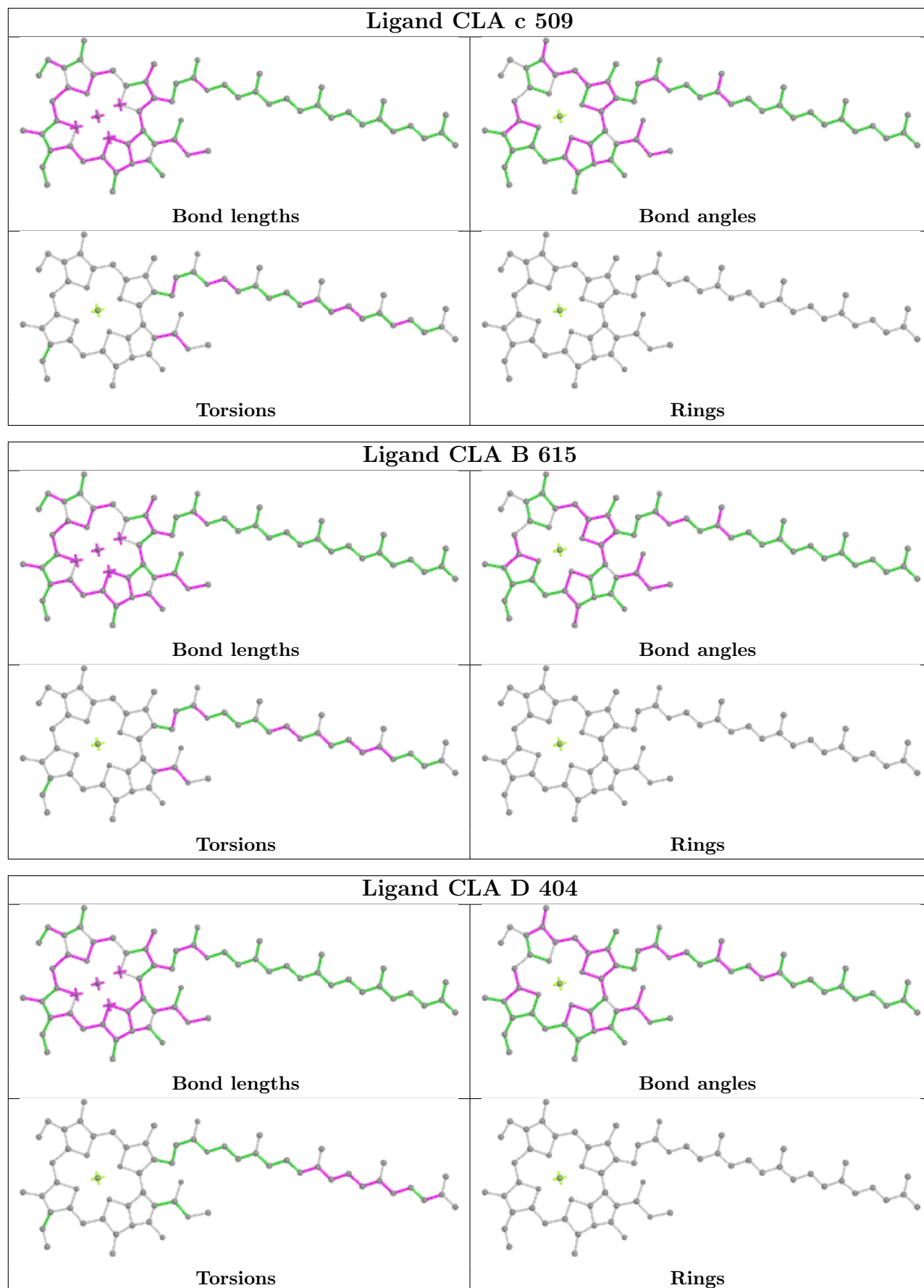
There are no ring outliers.

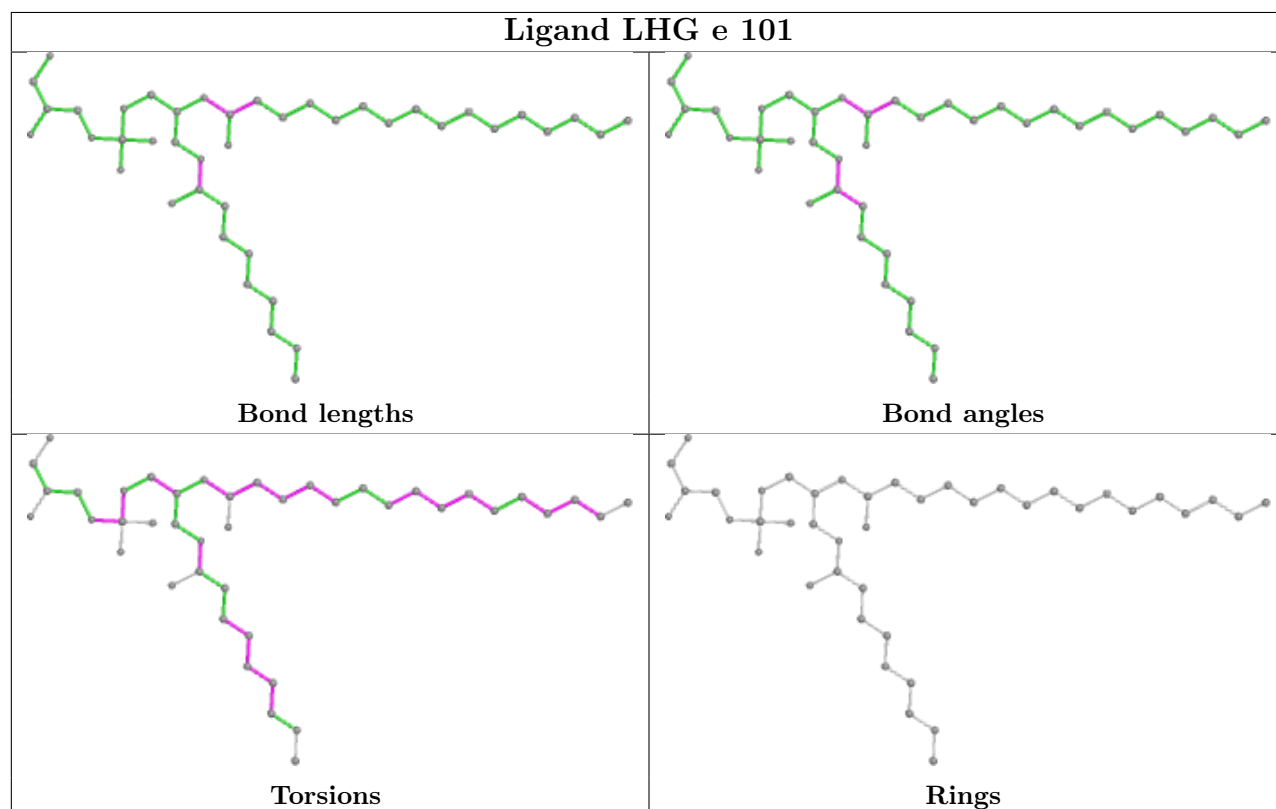
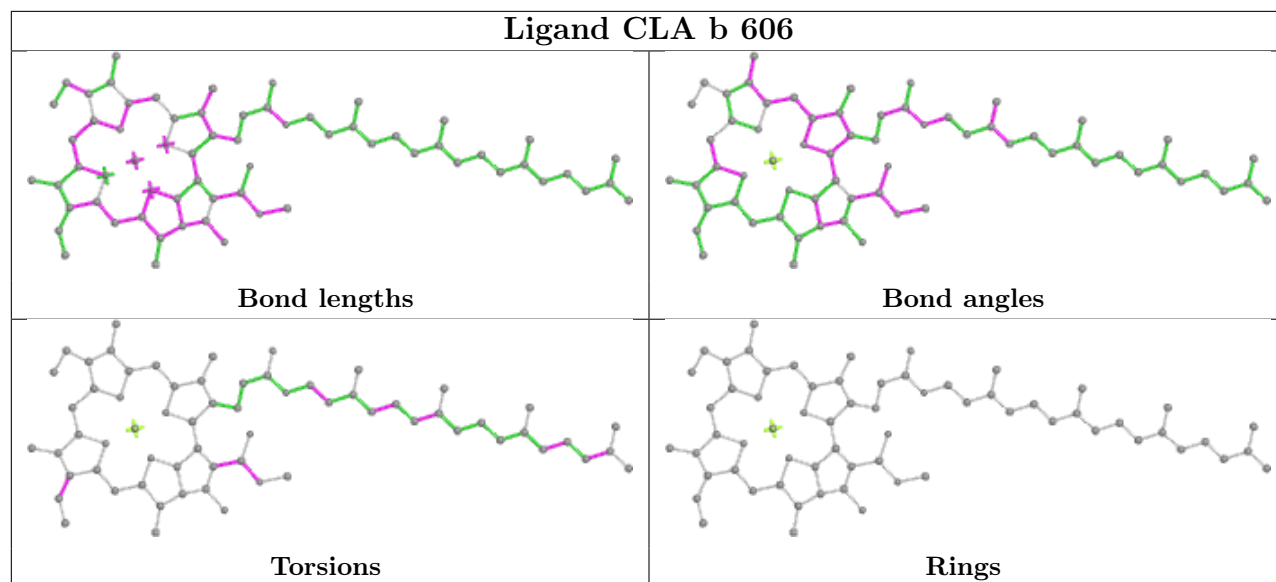
No monomer is involved in short contacts.

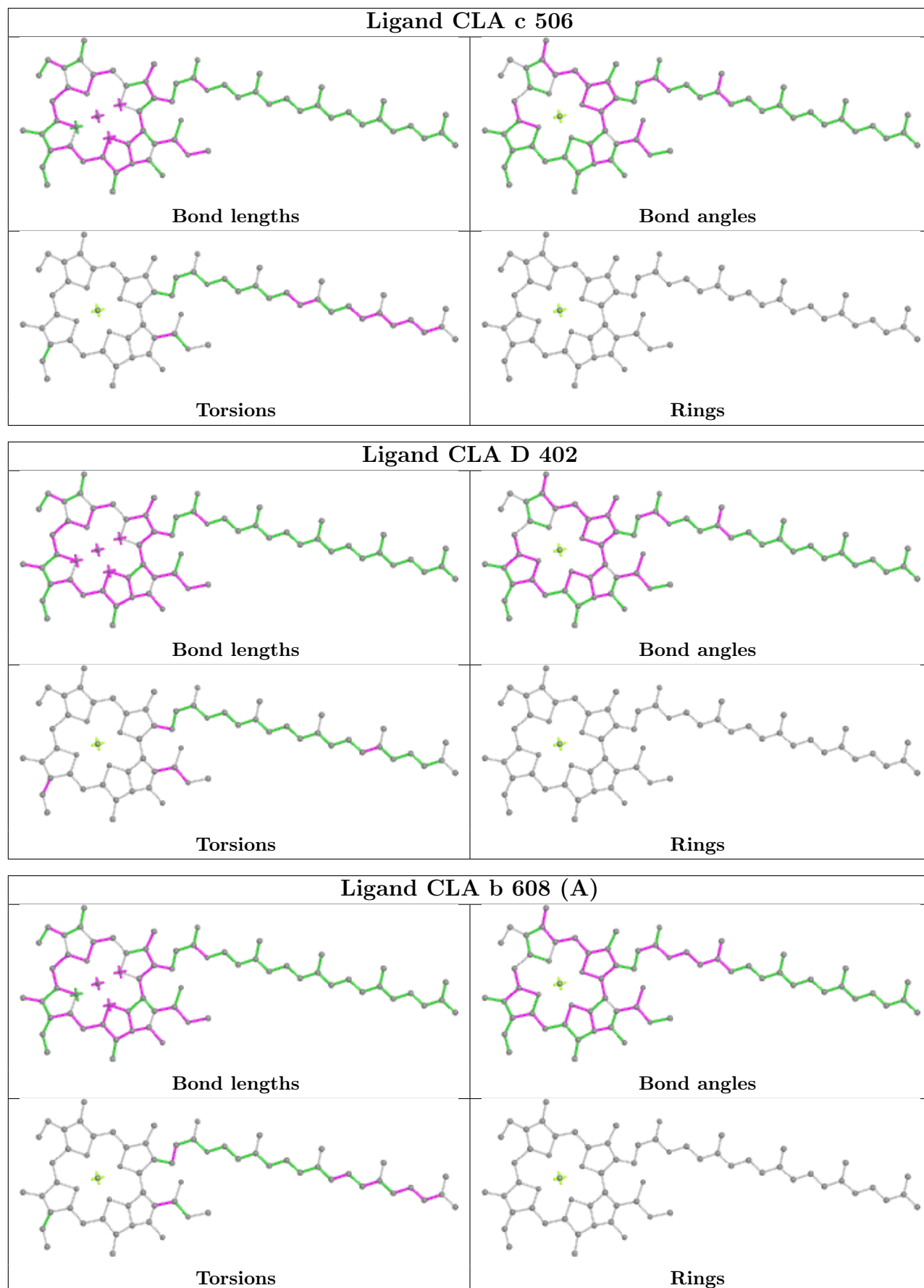
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

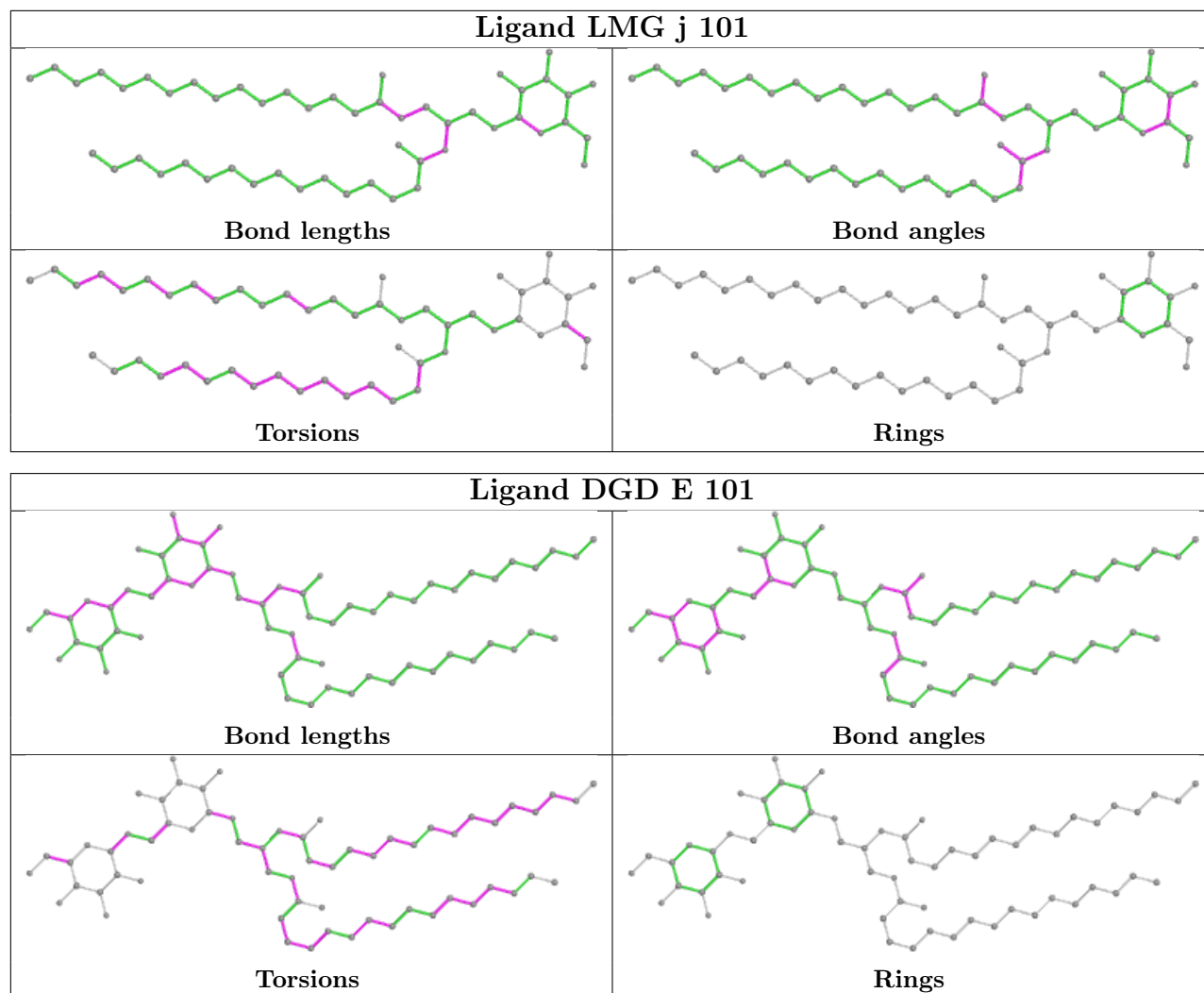


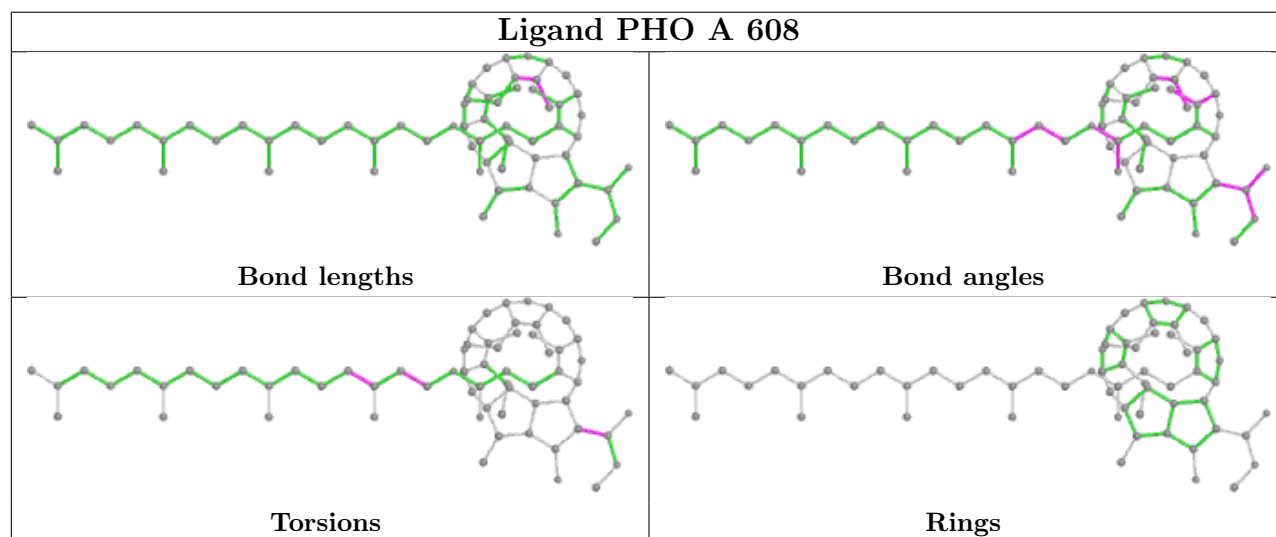
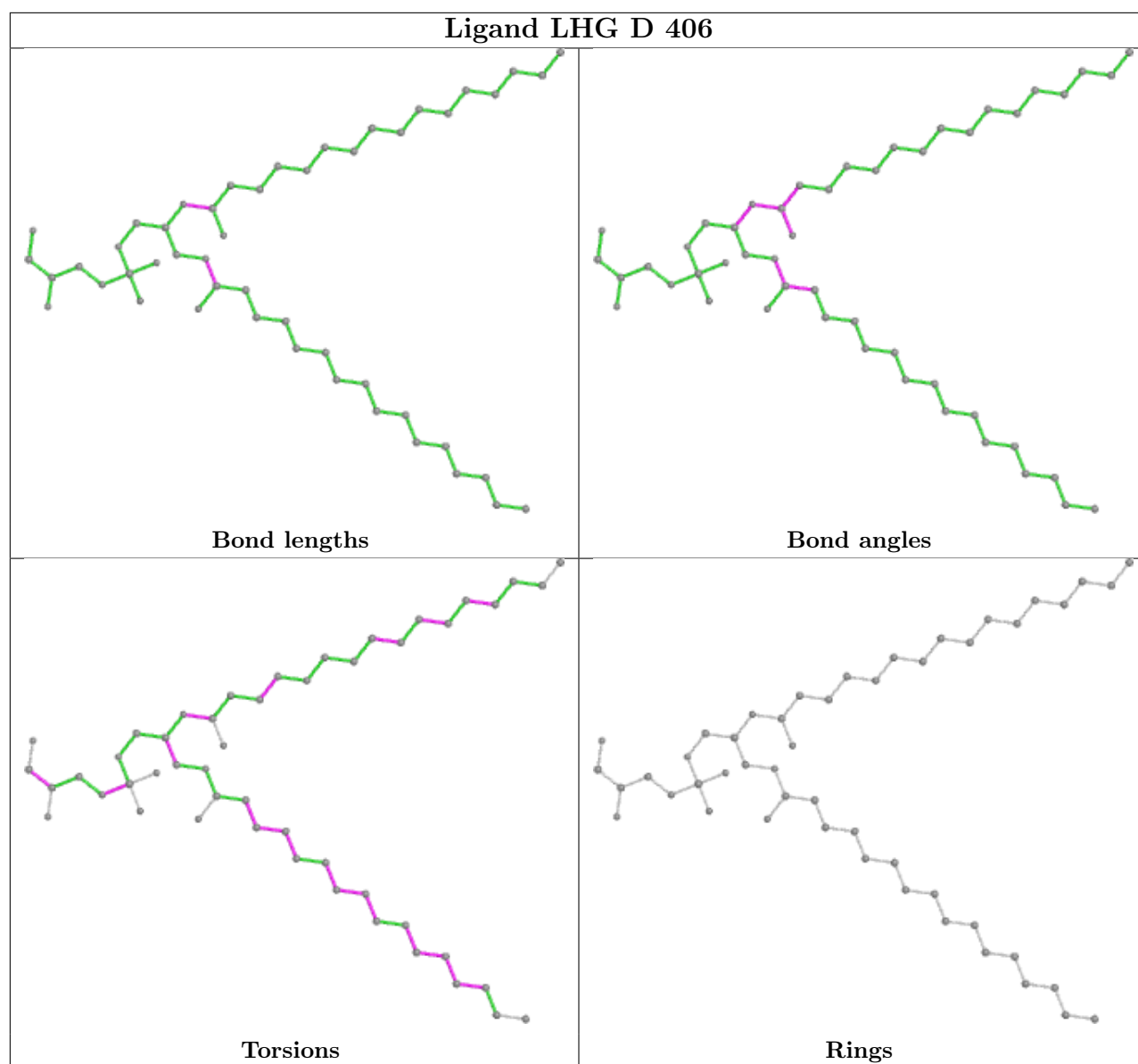


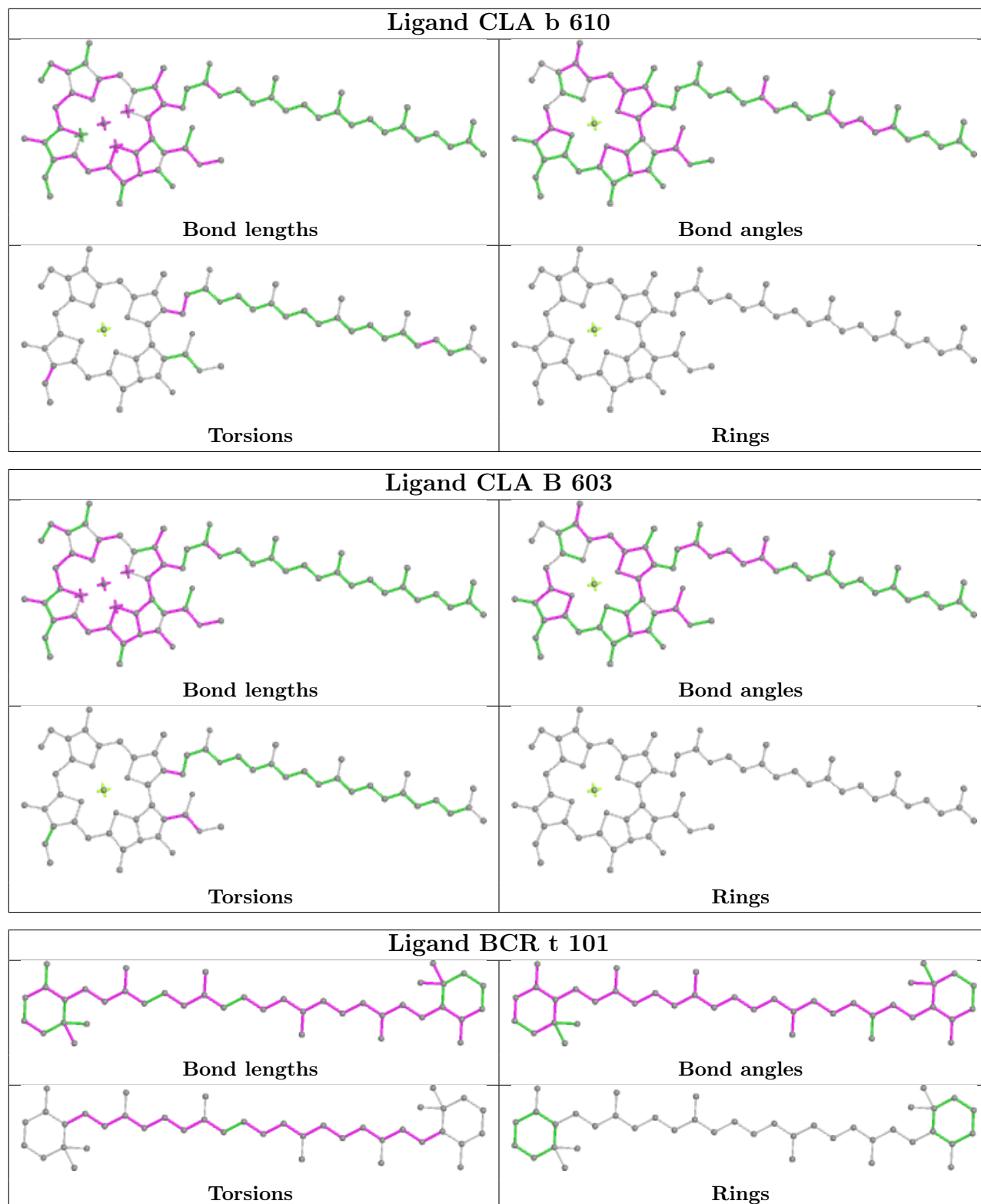


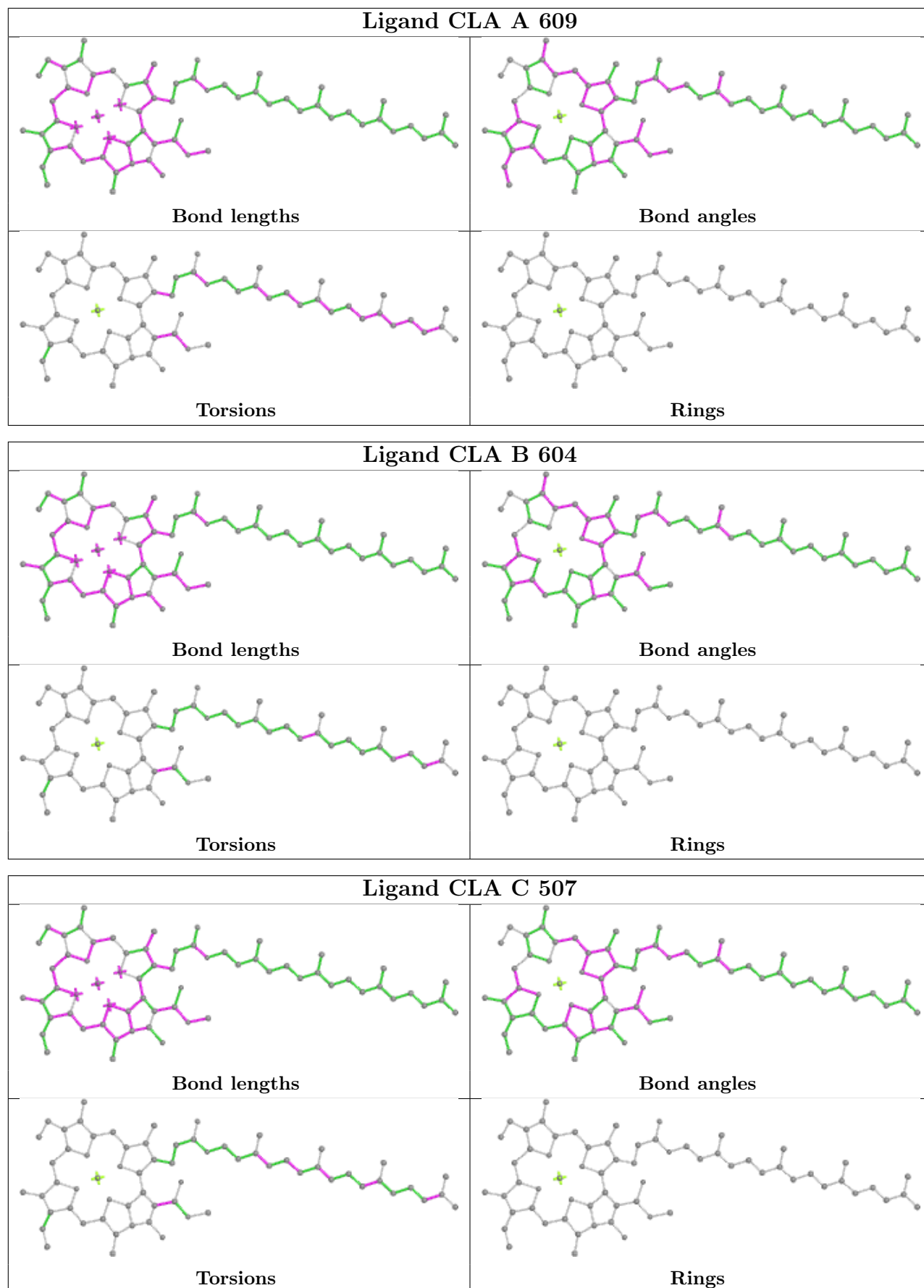


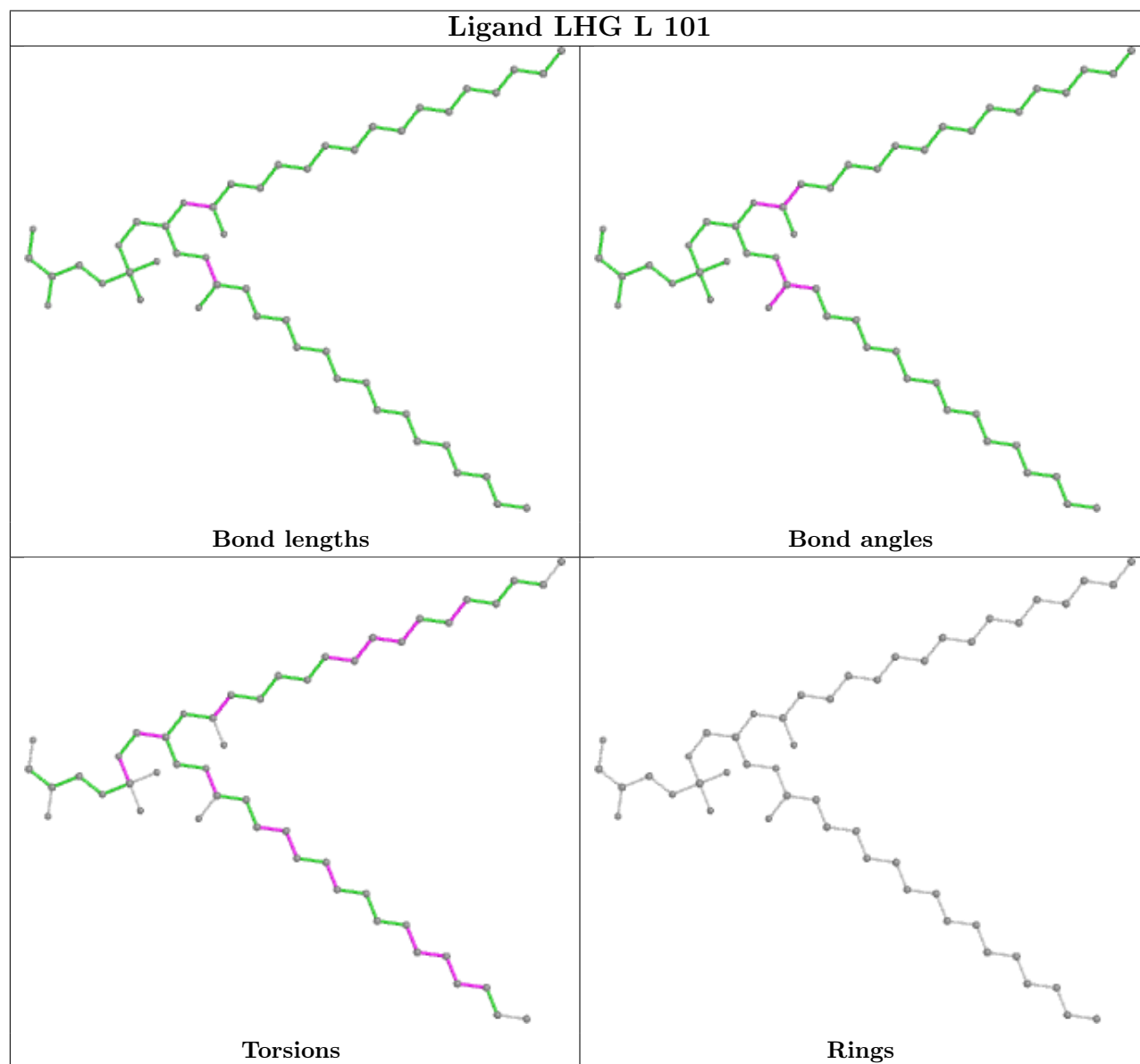
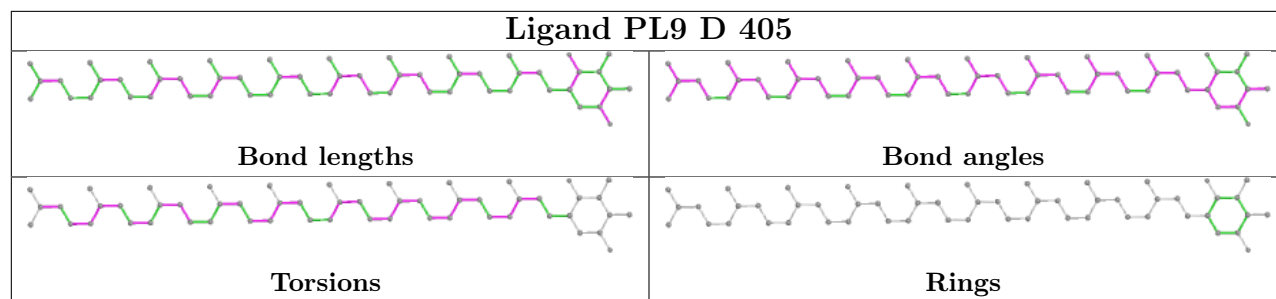


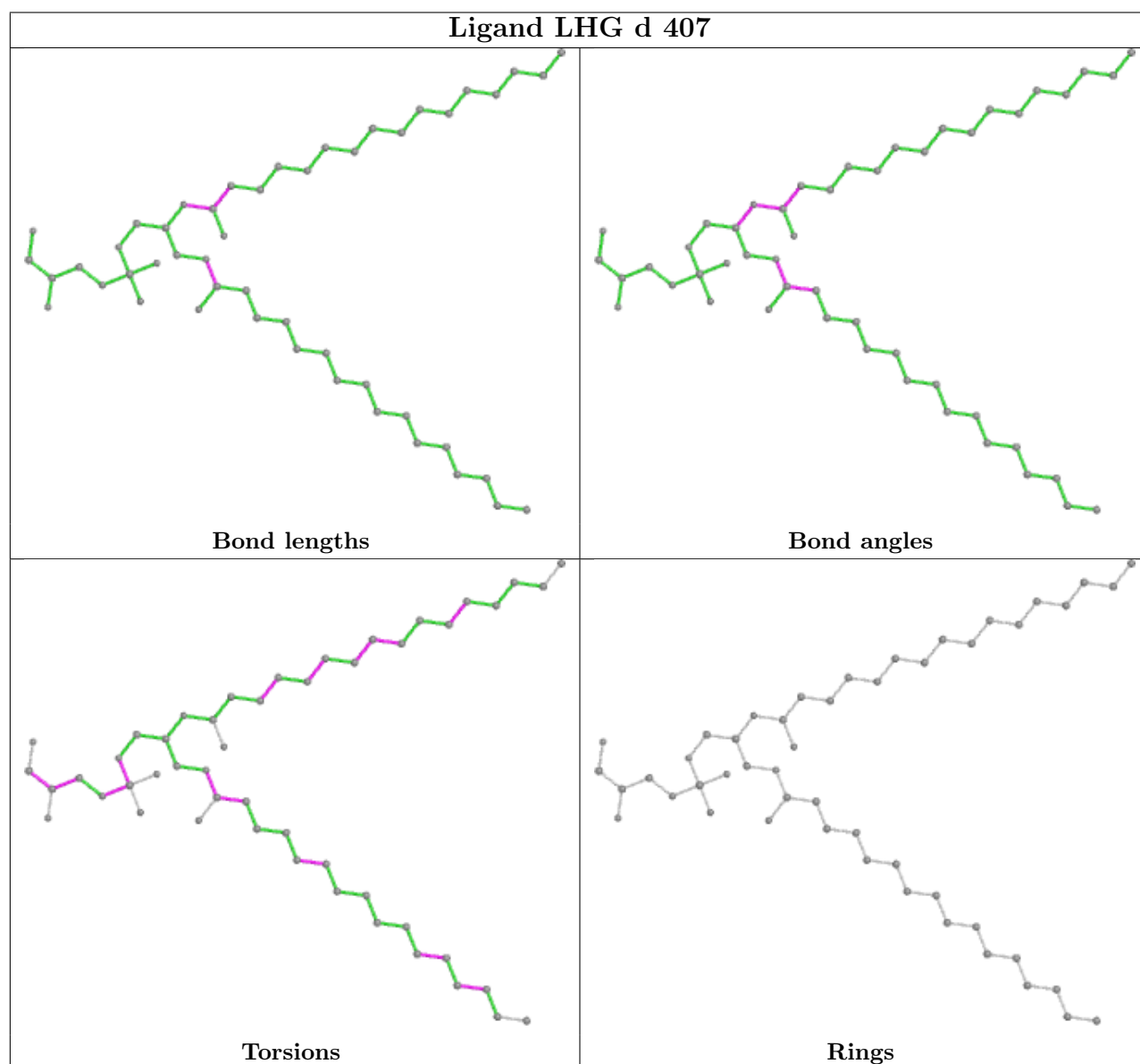
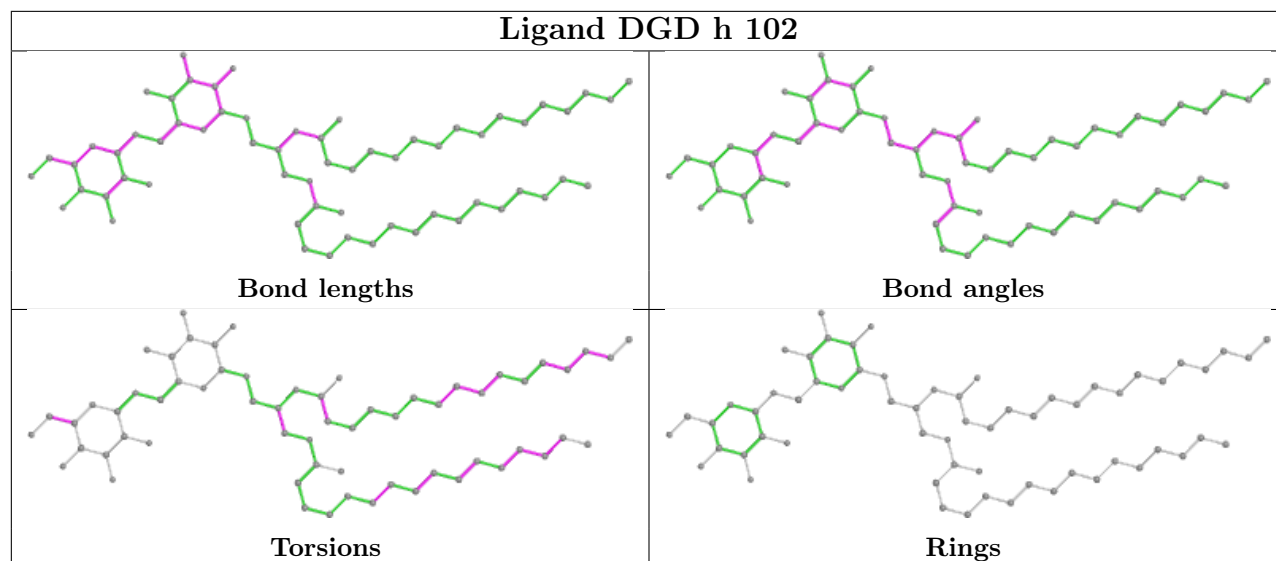


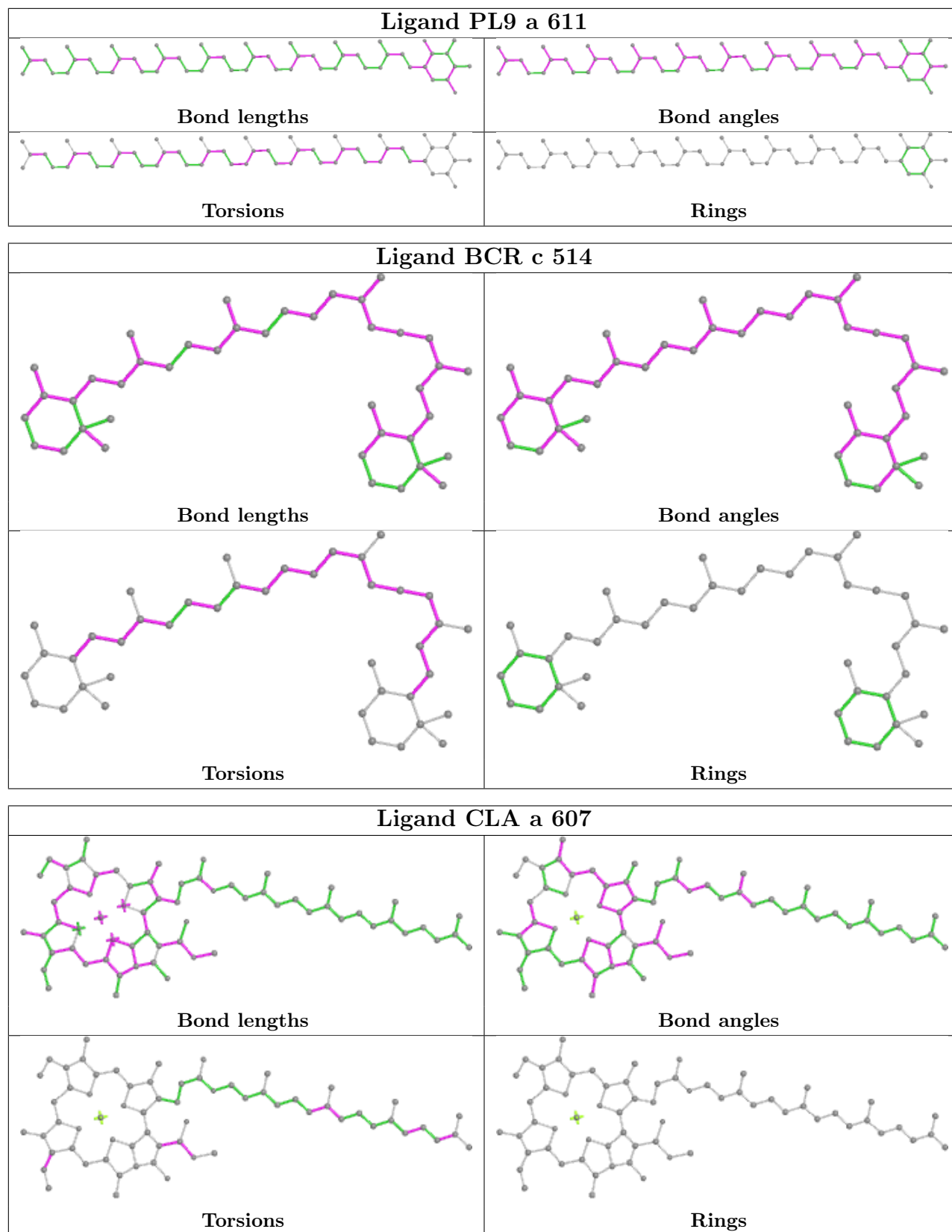


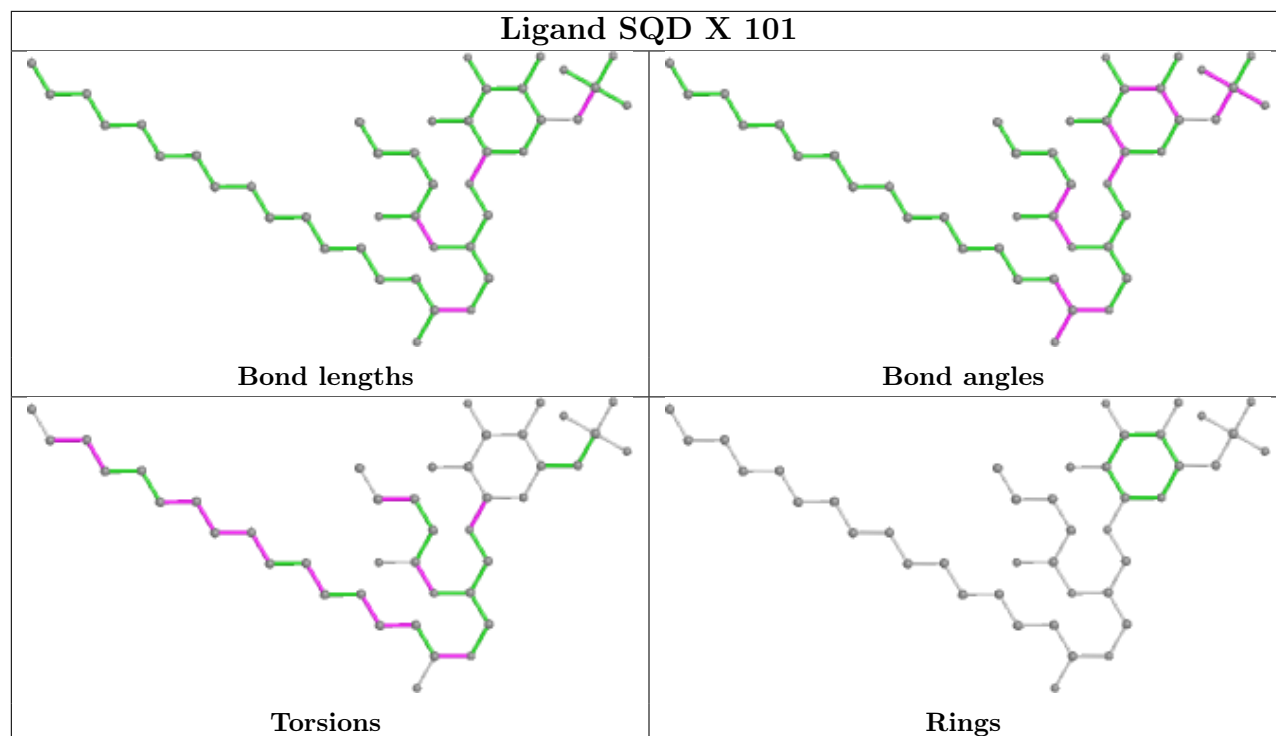


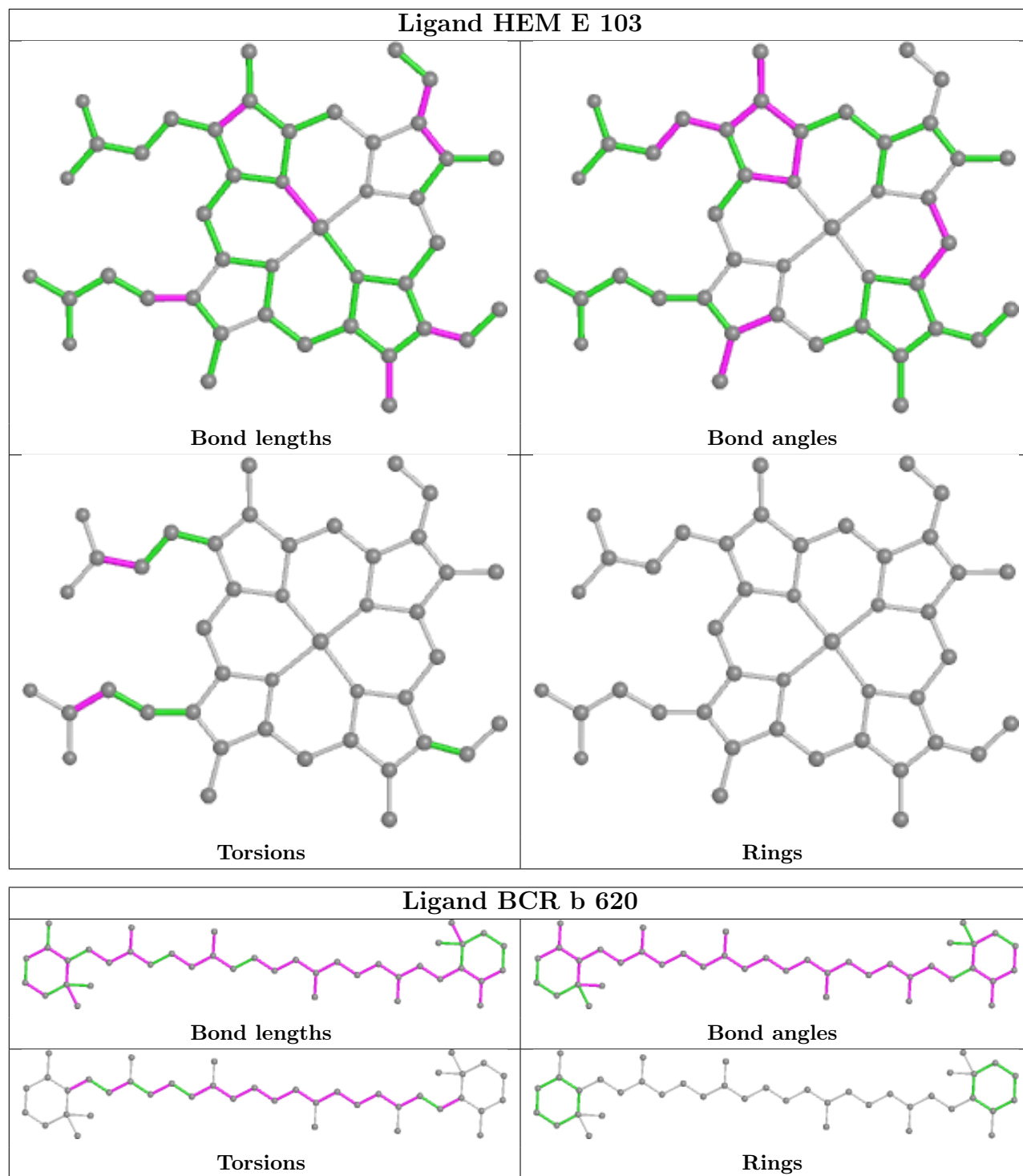


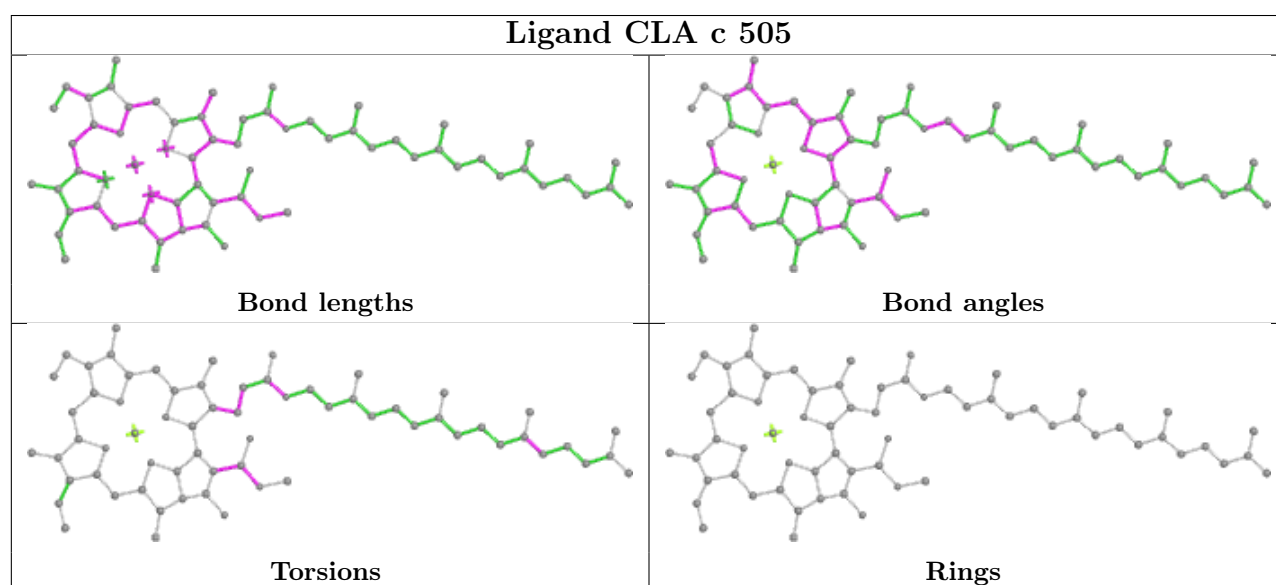
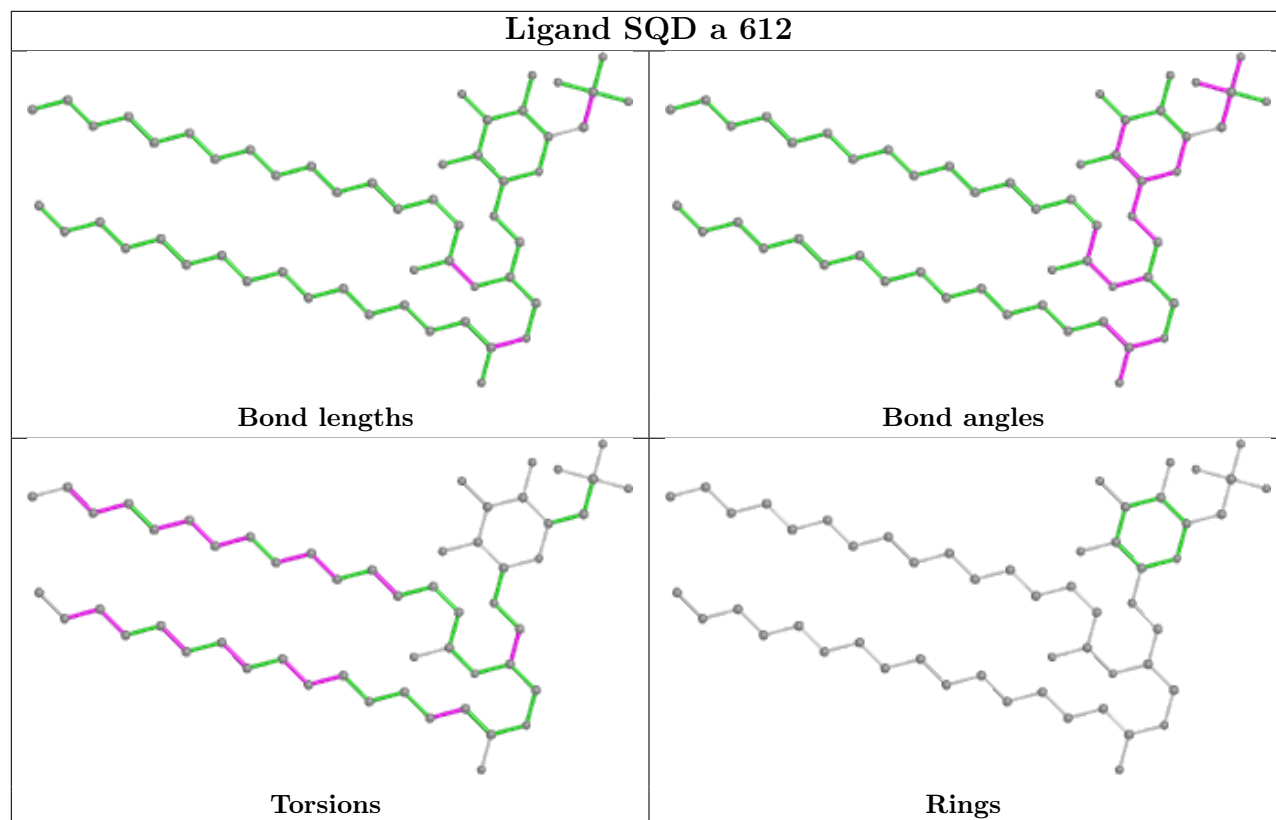
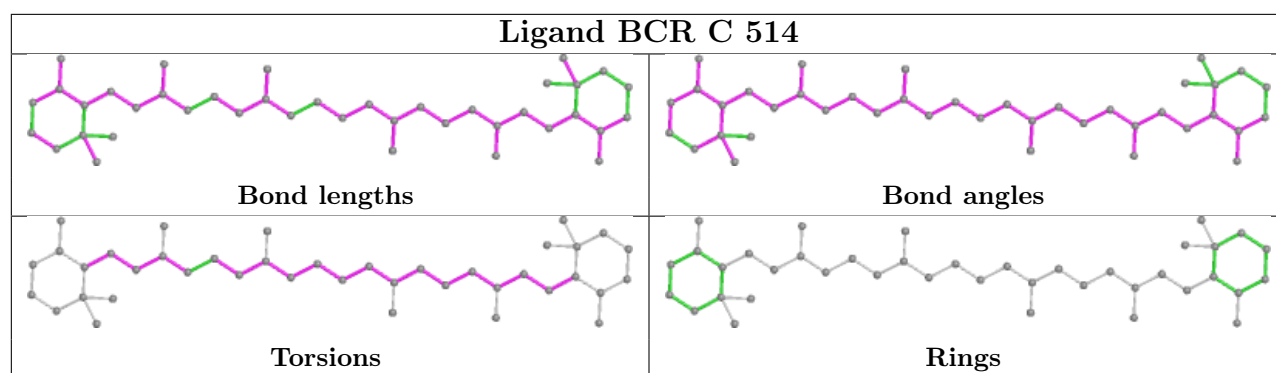


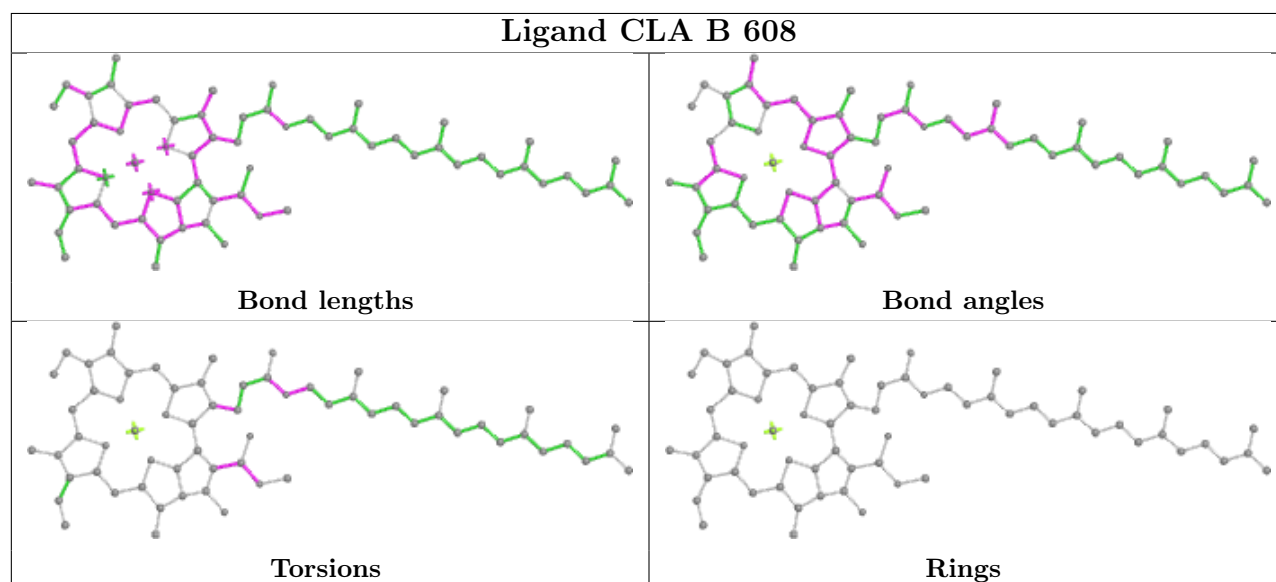
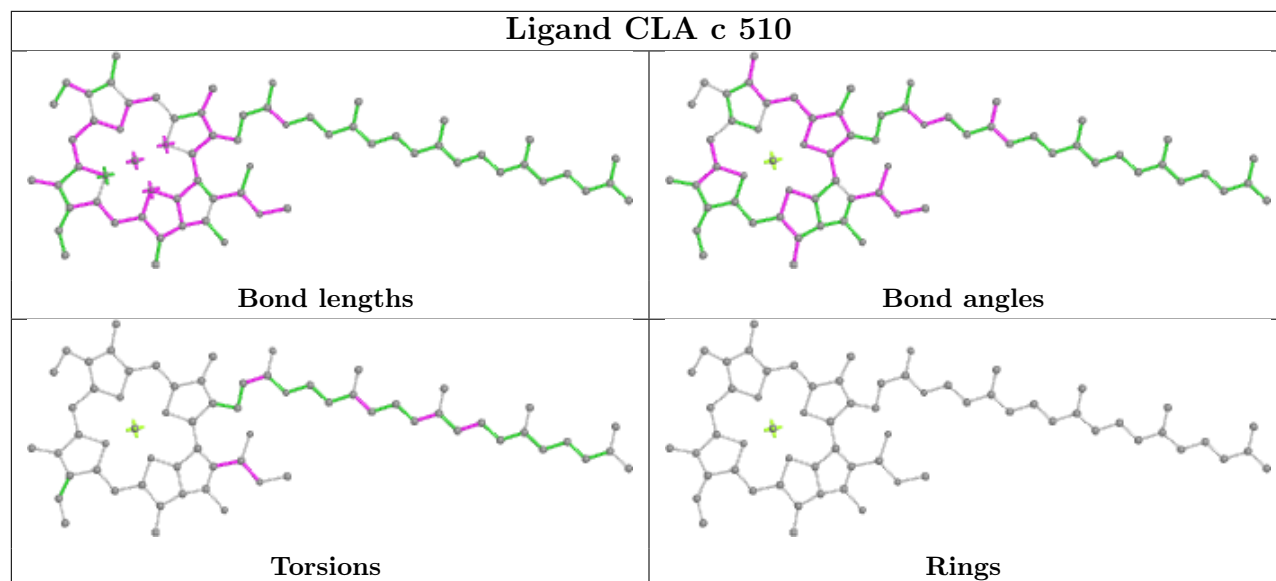
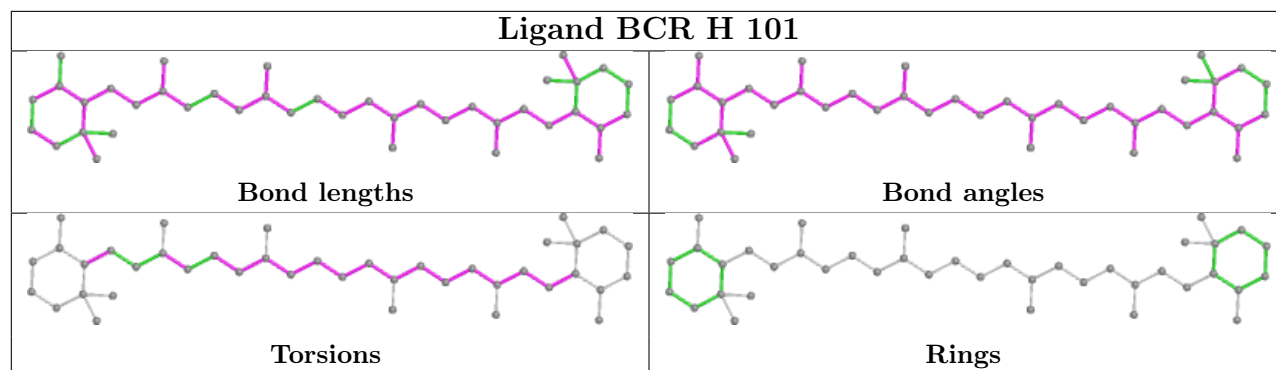


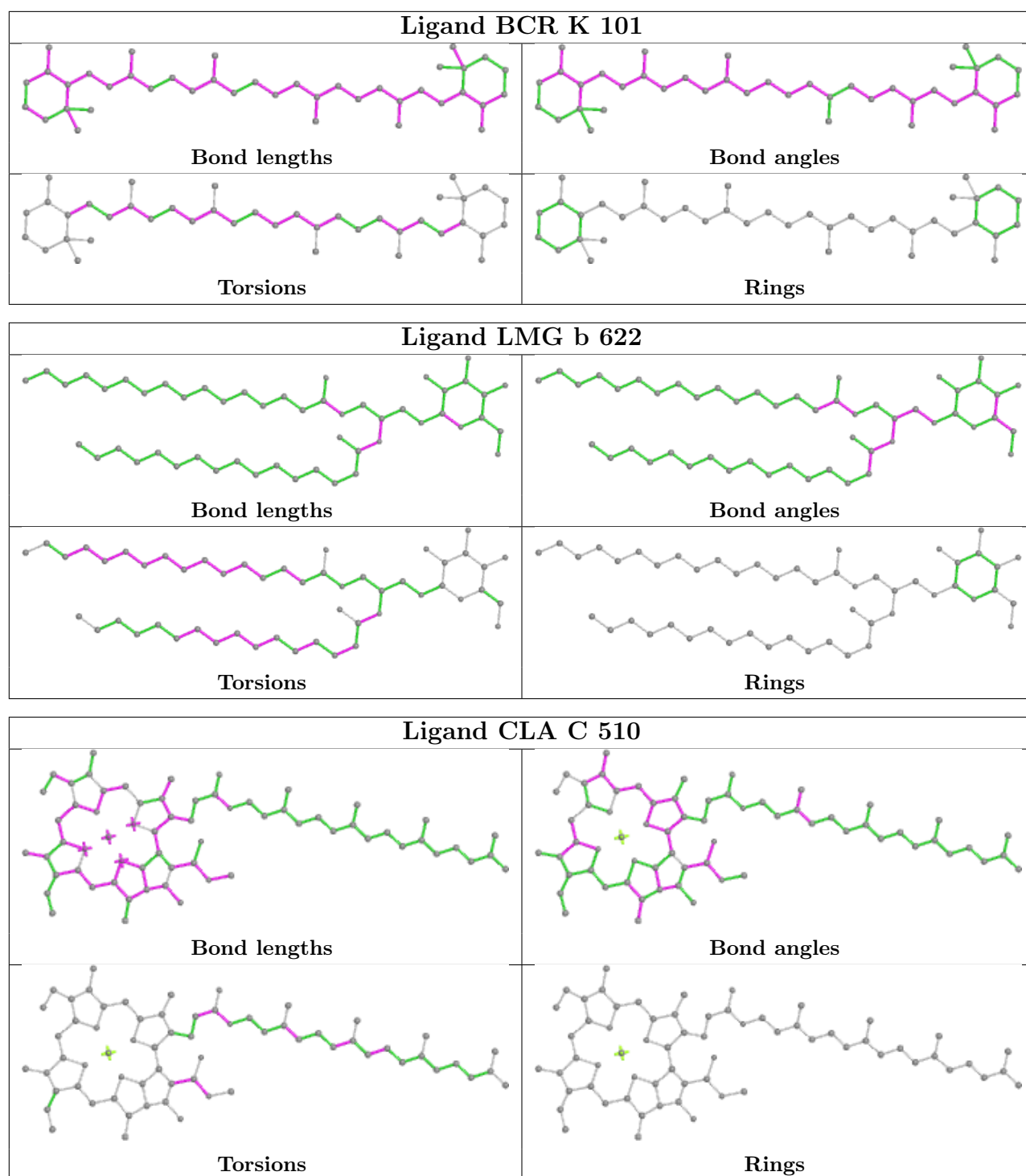


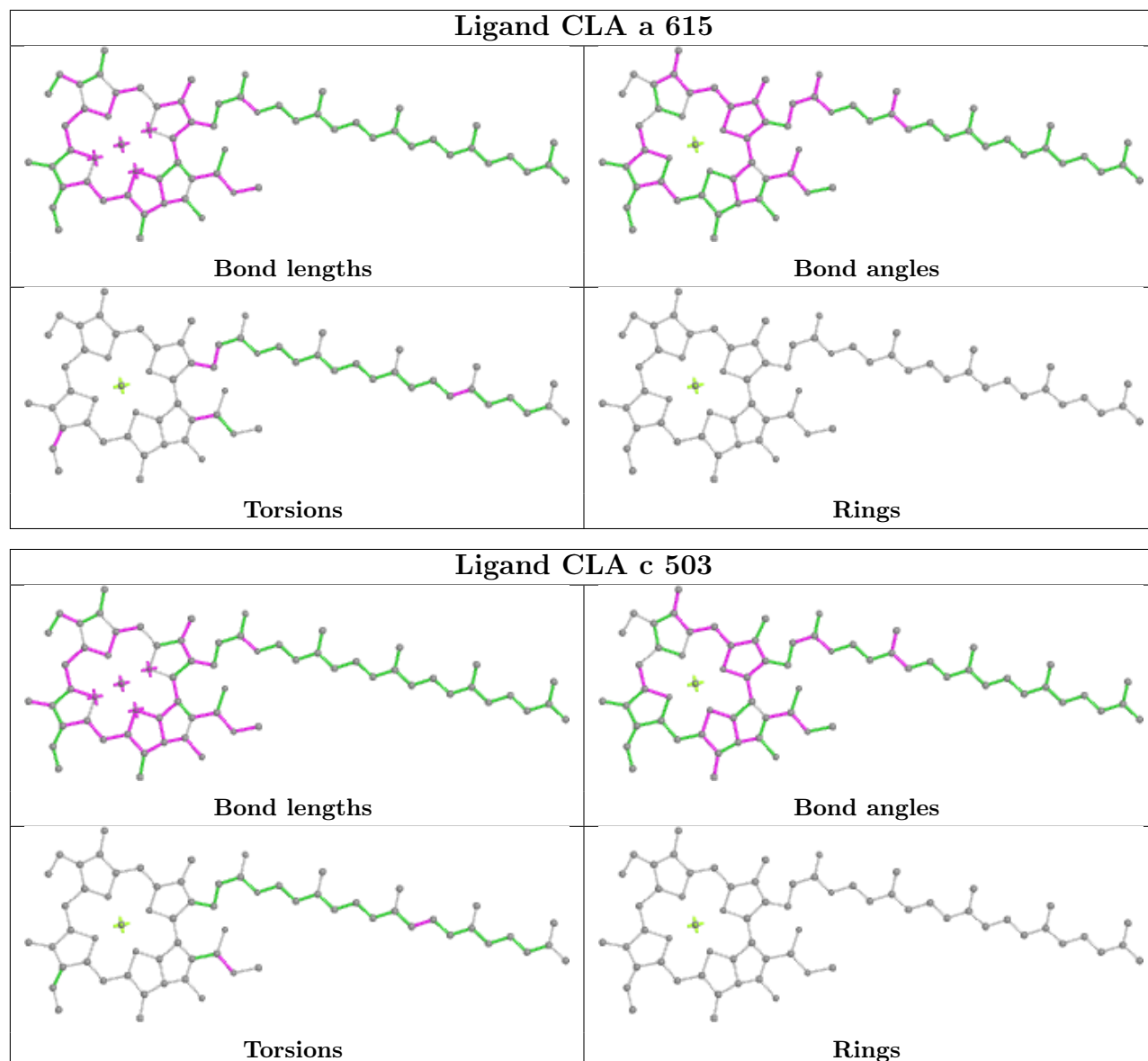


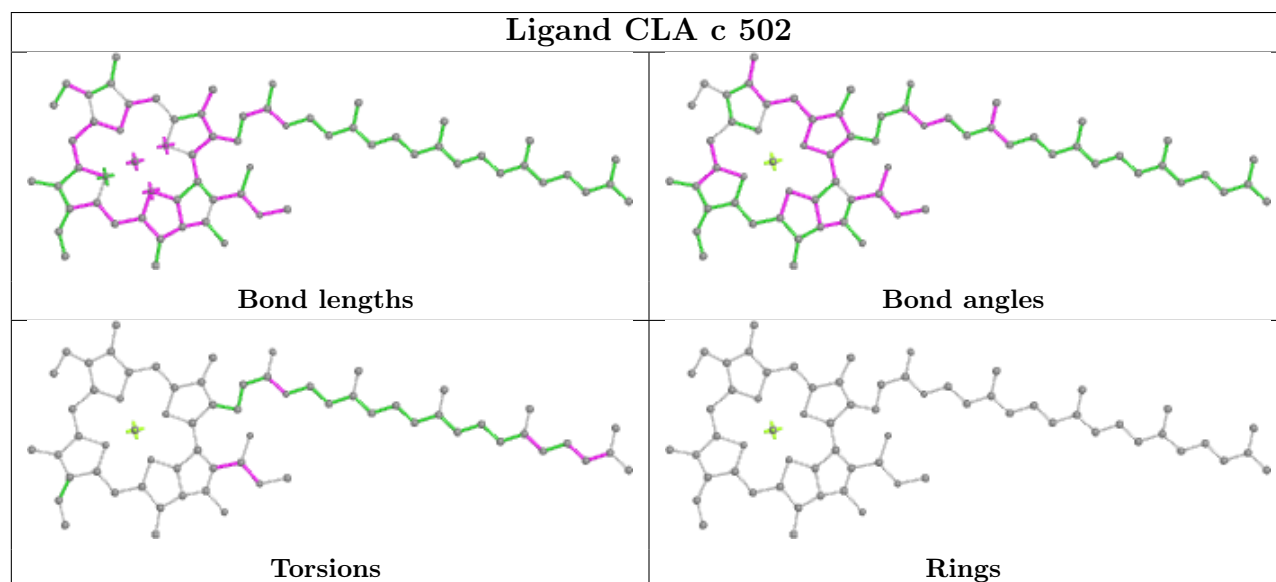
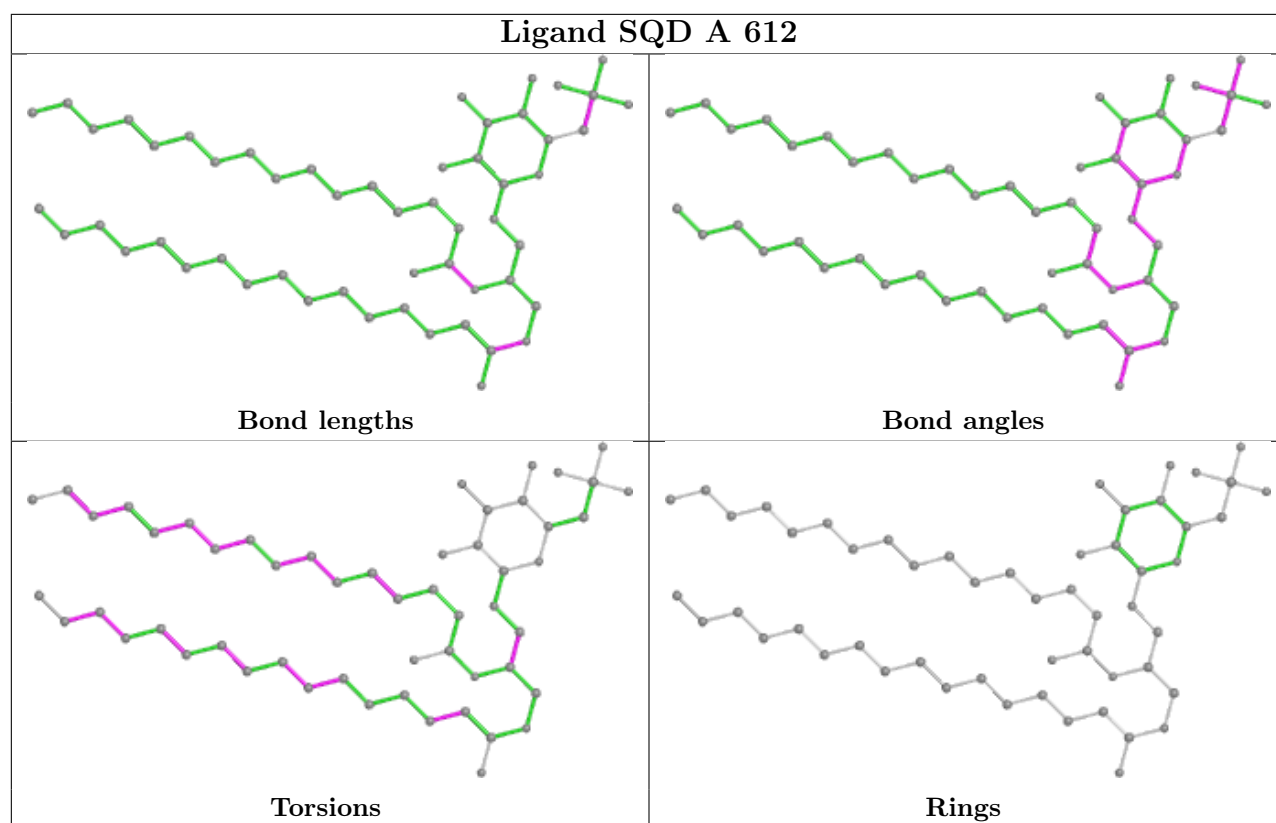


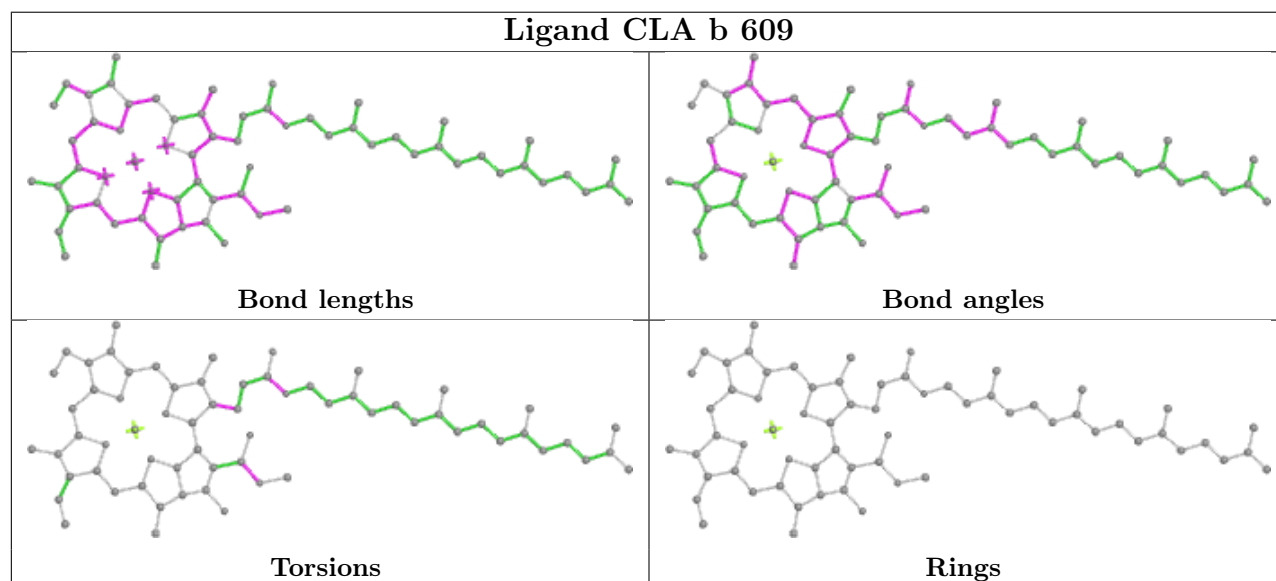
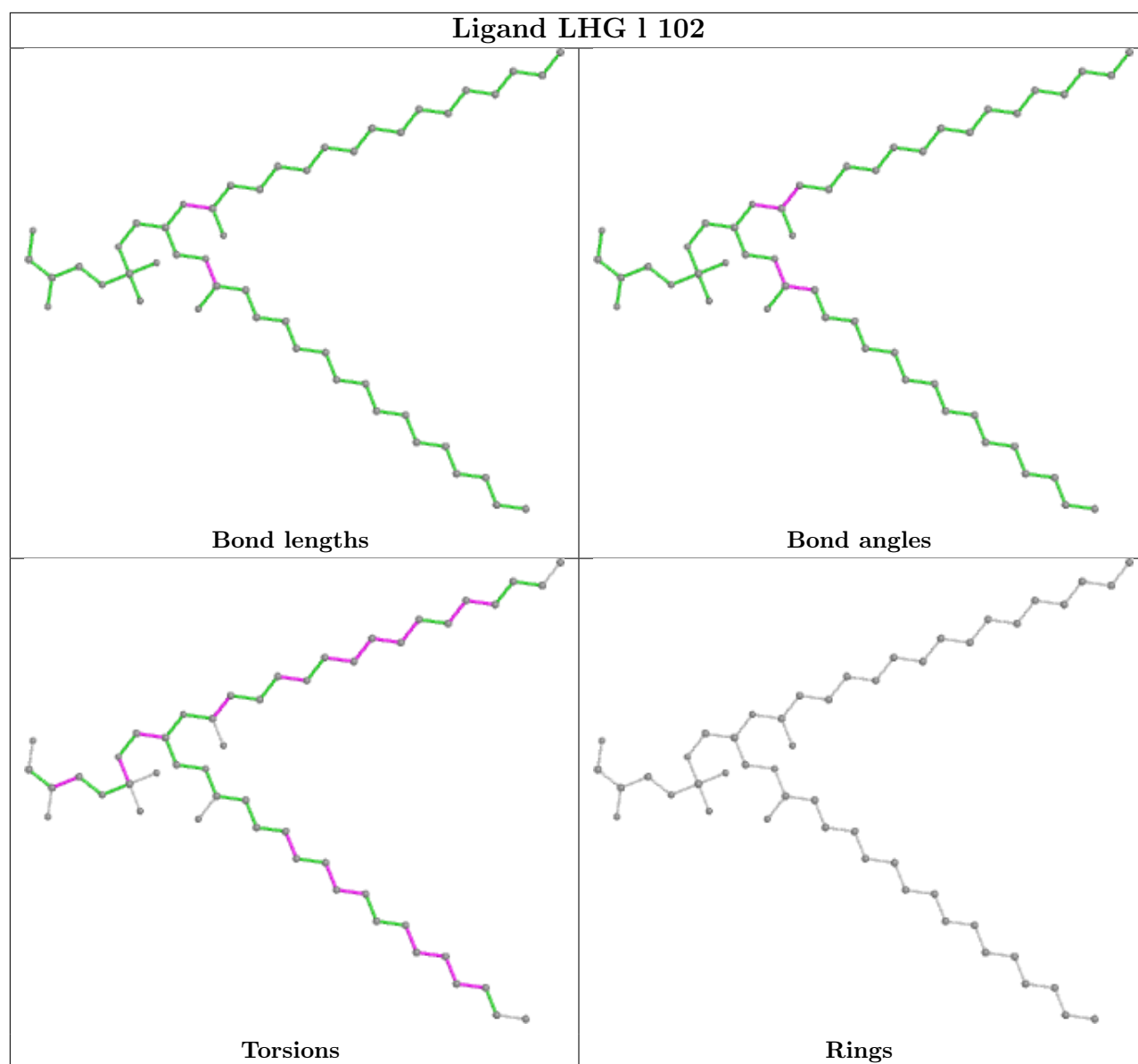


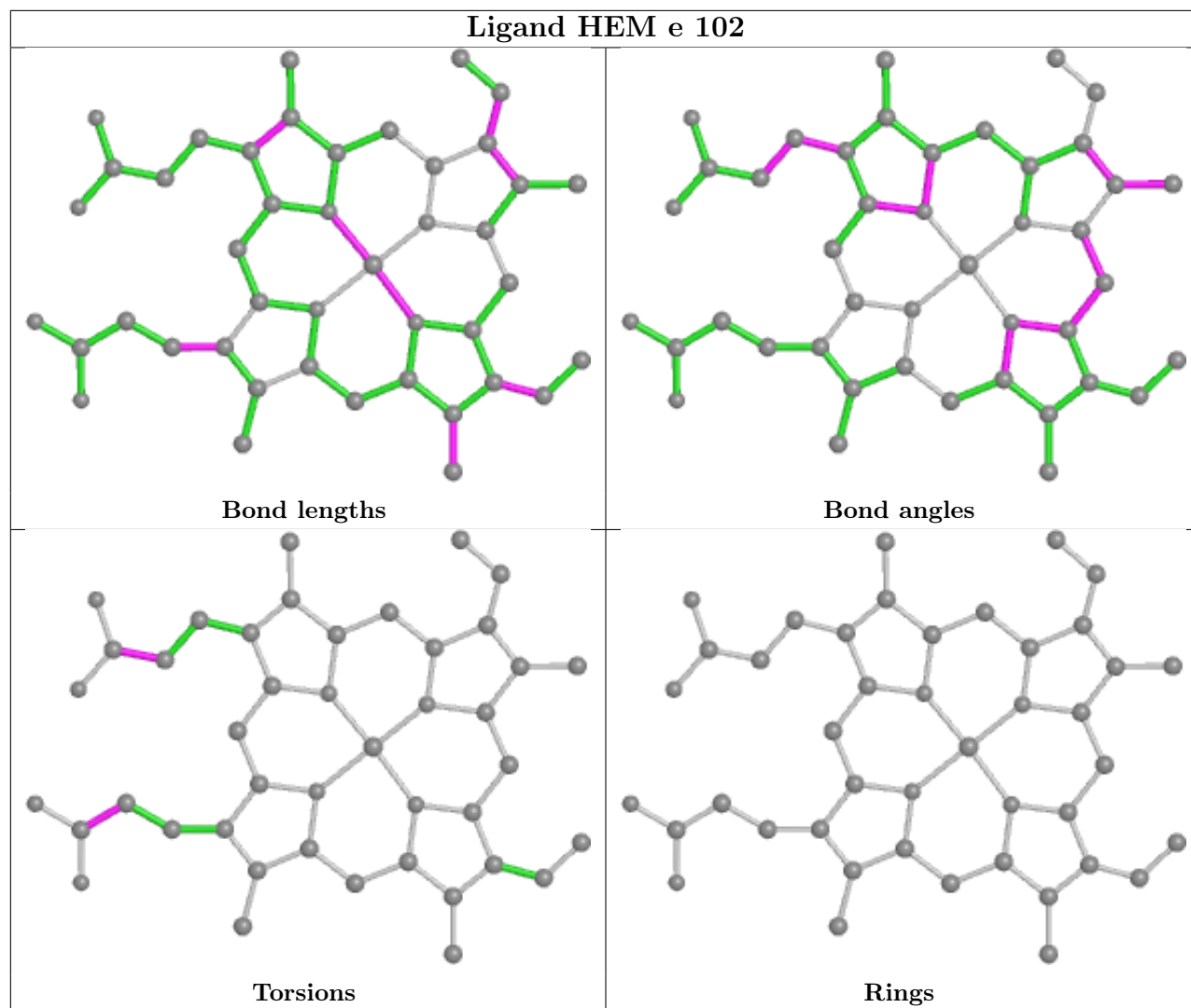


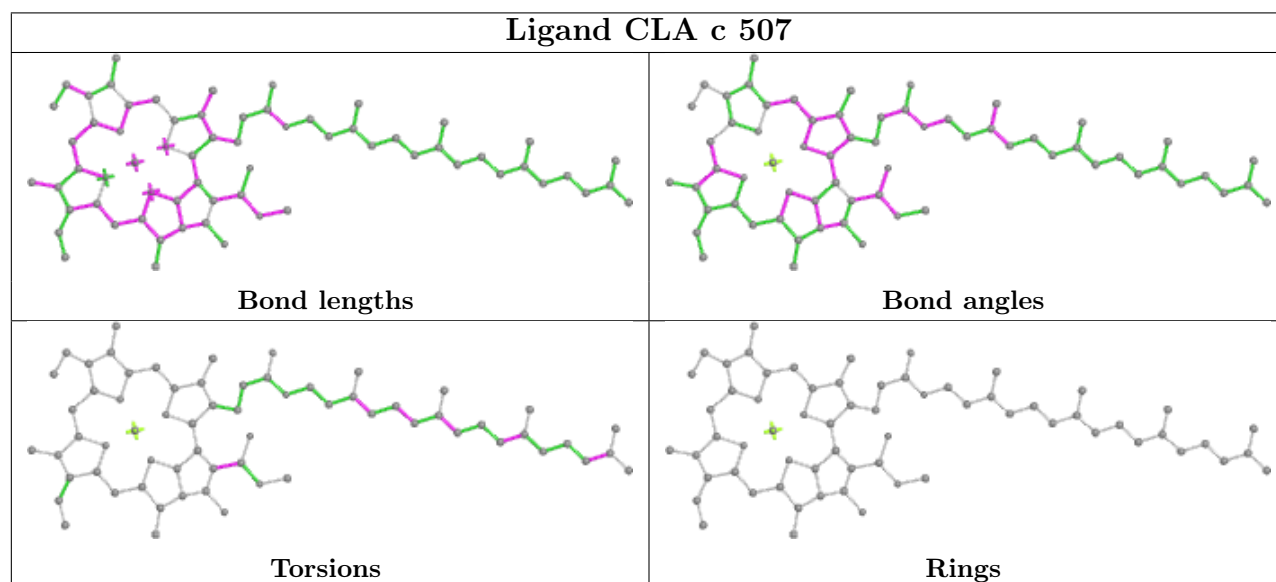
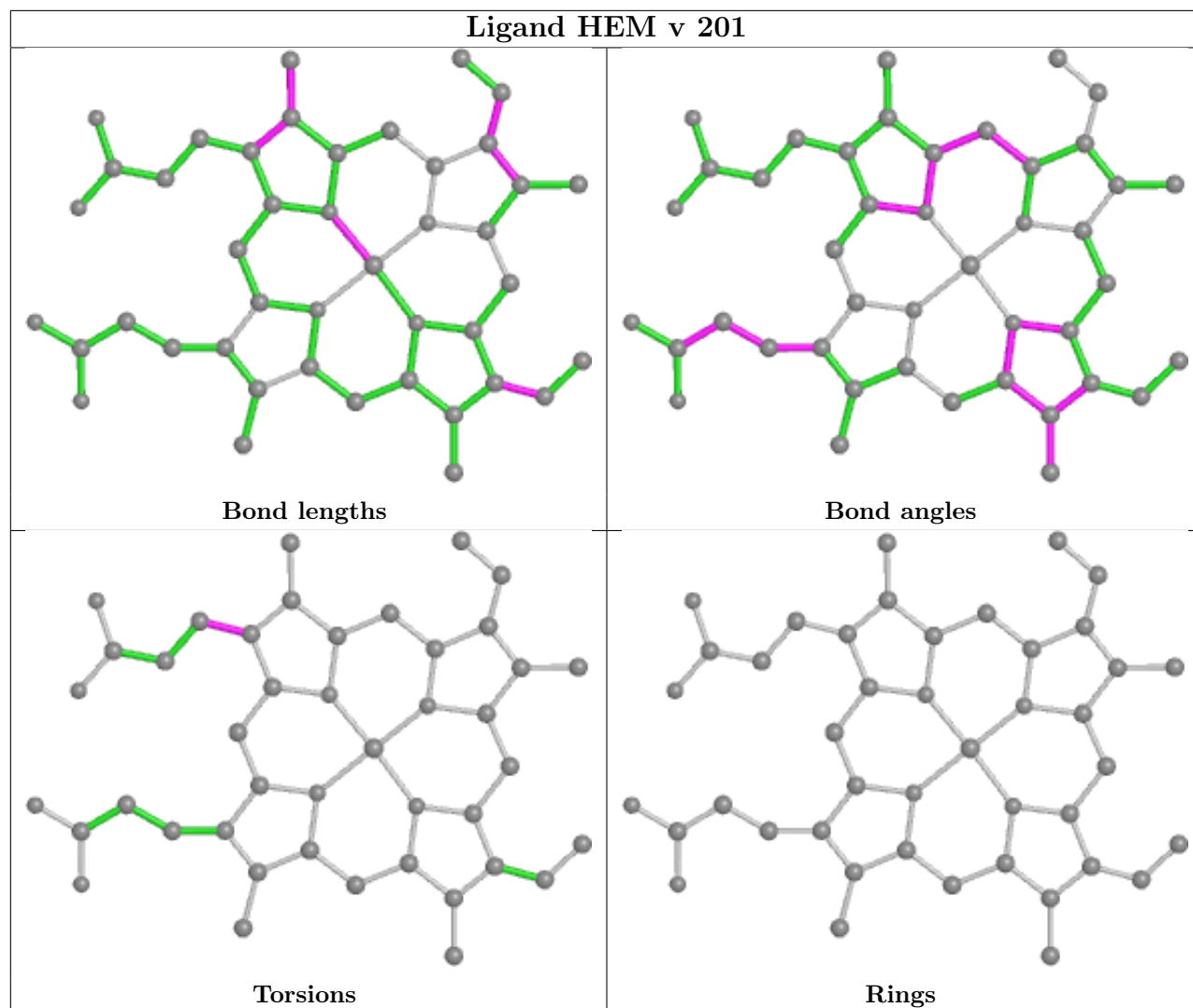


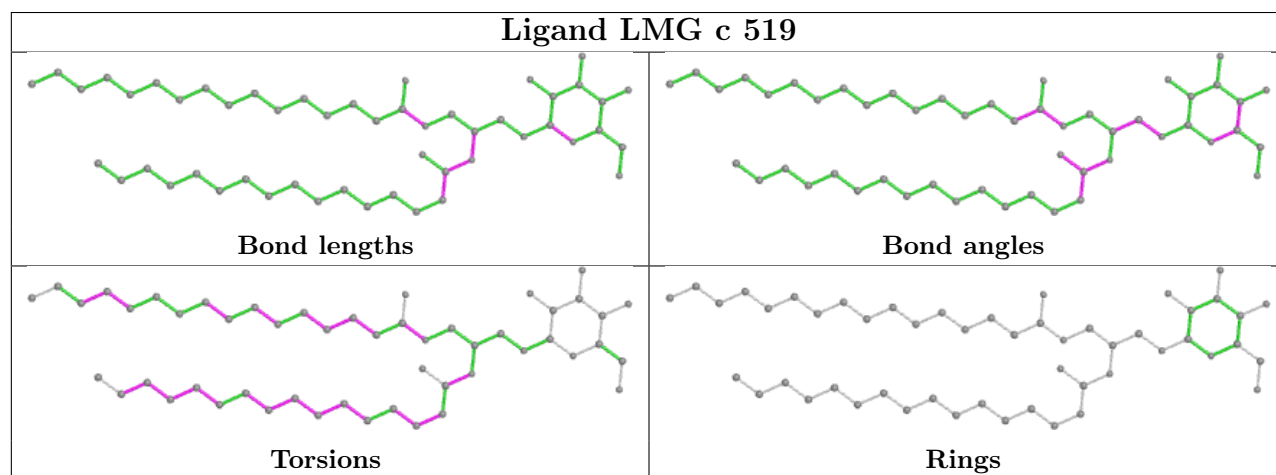
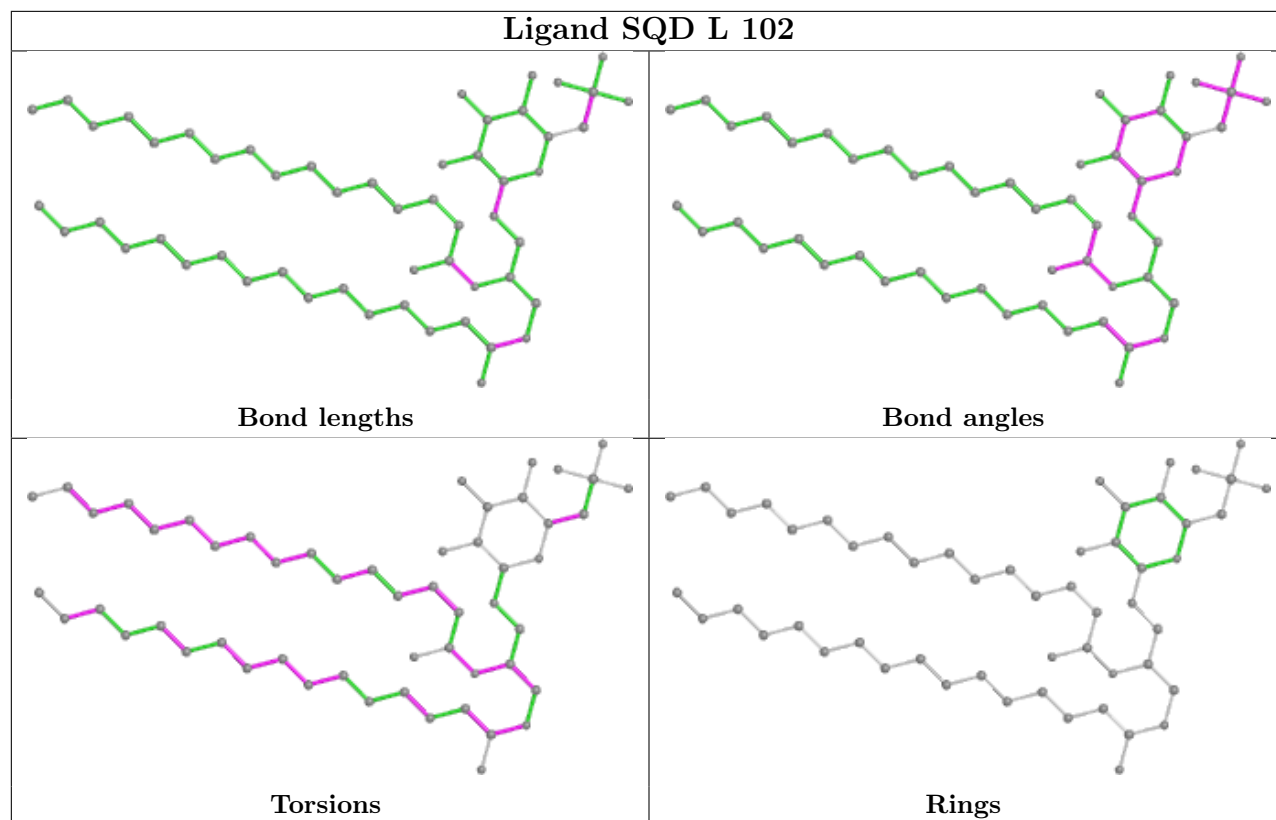


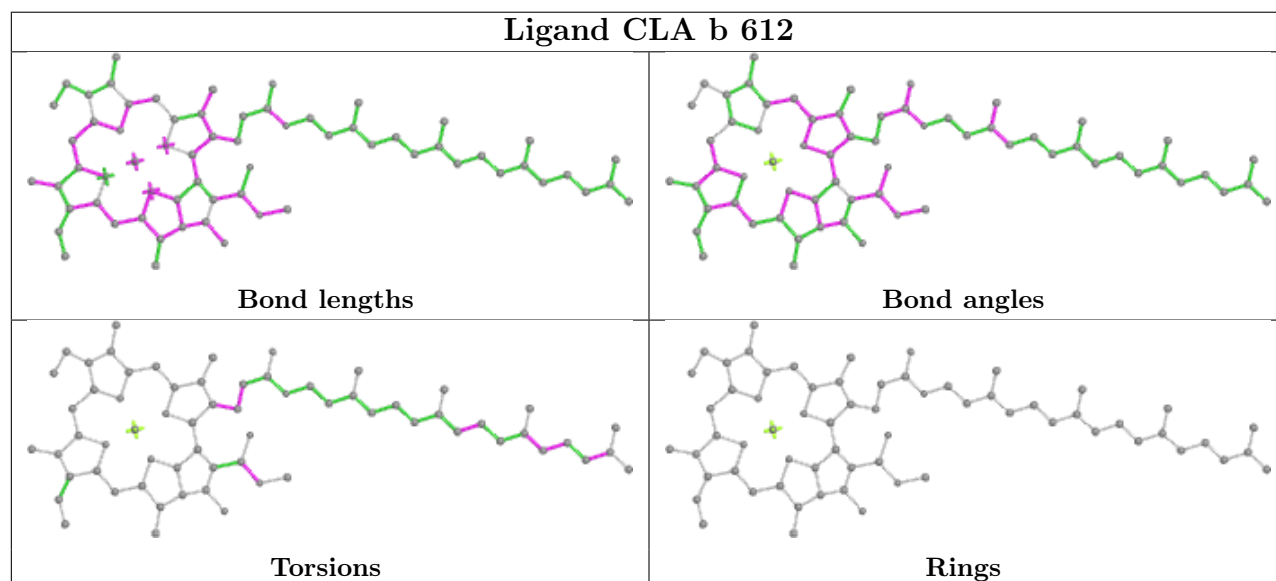
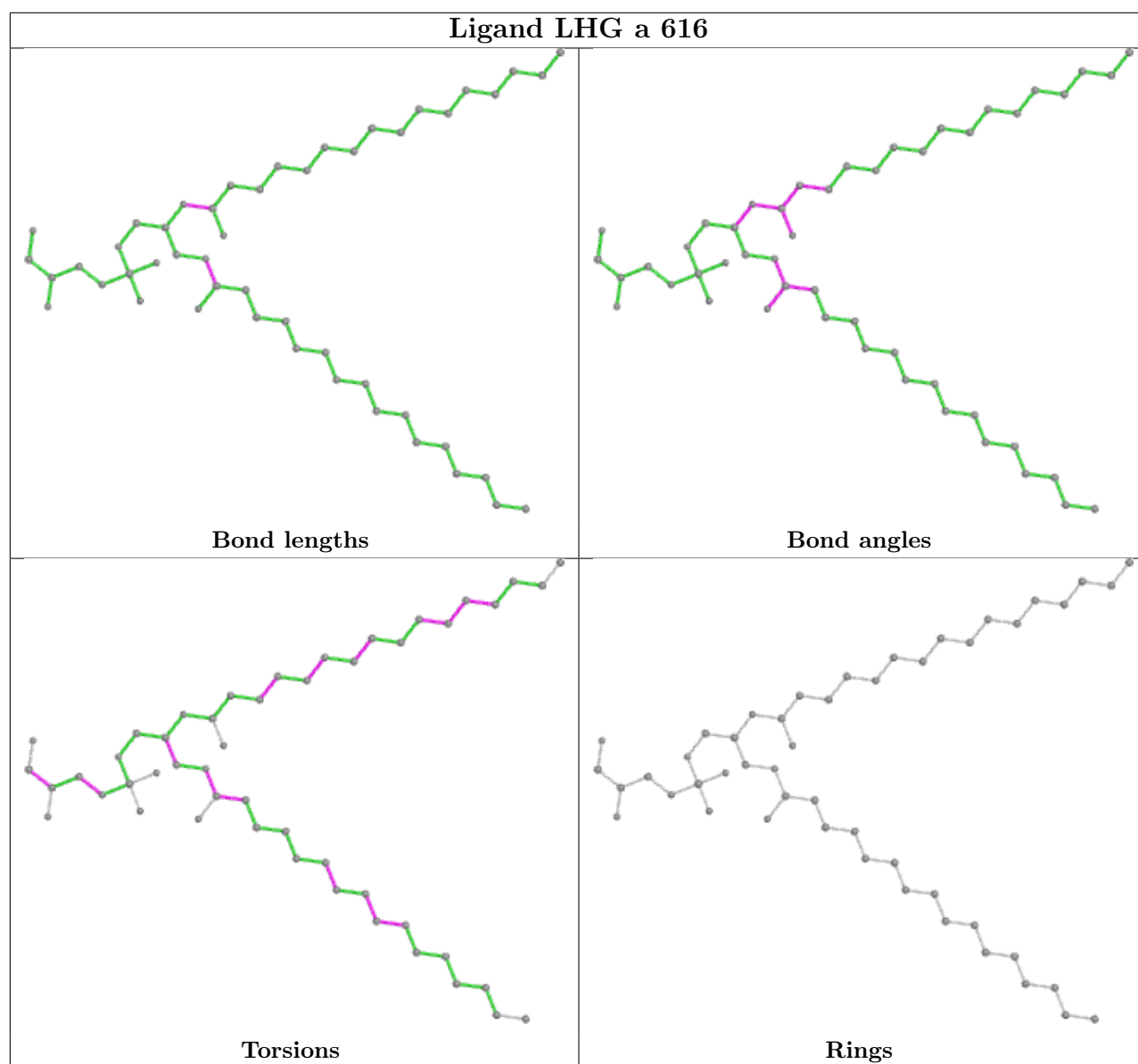


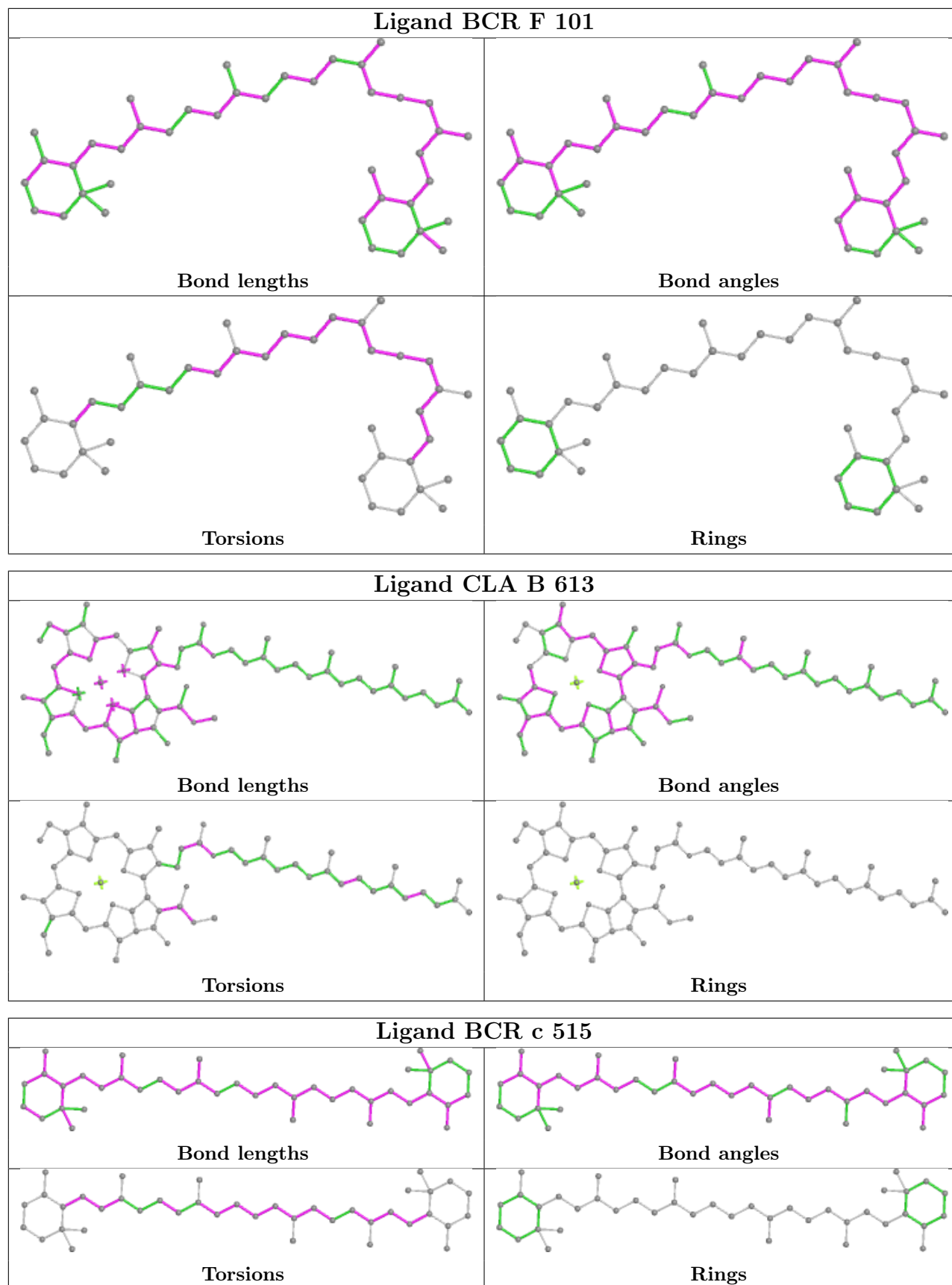


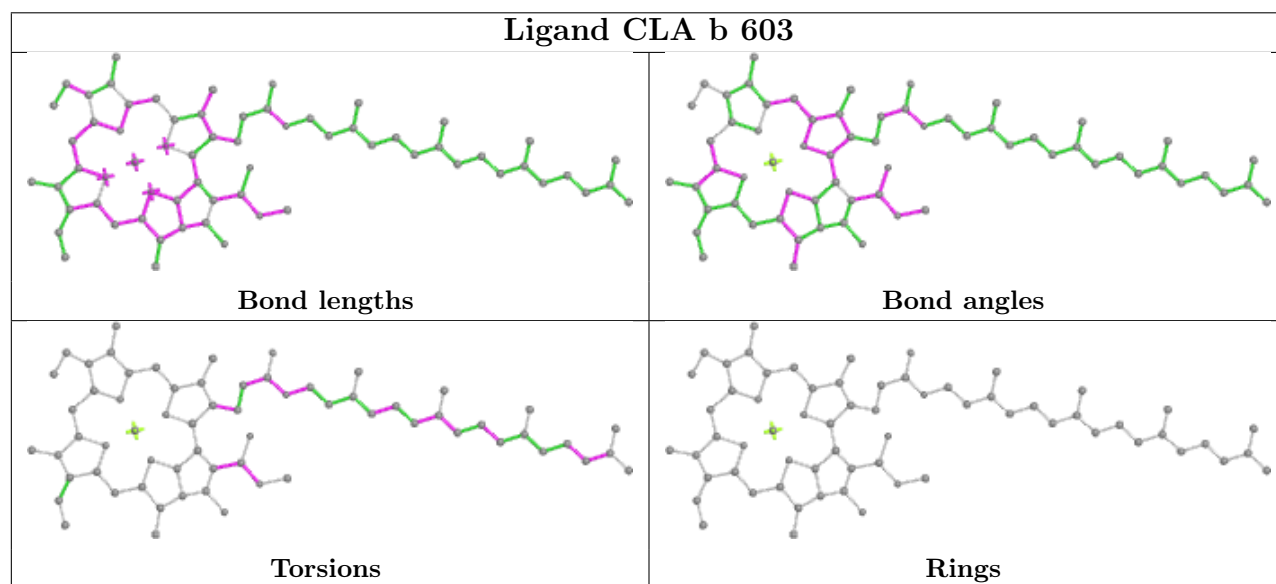
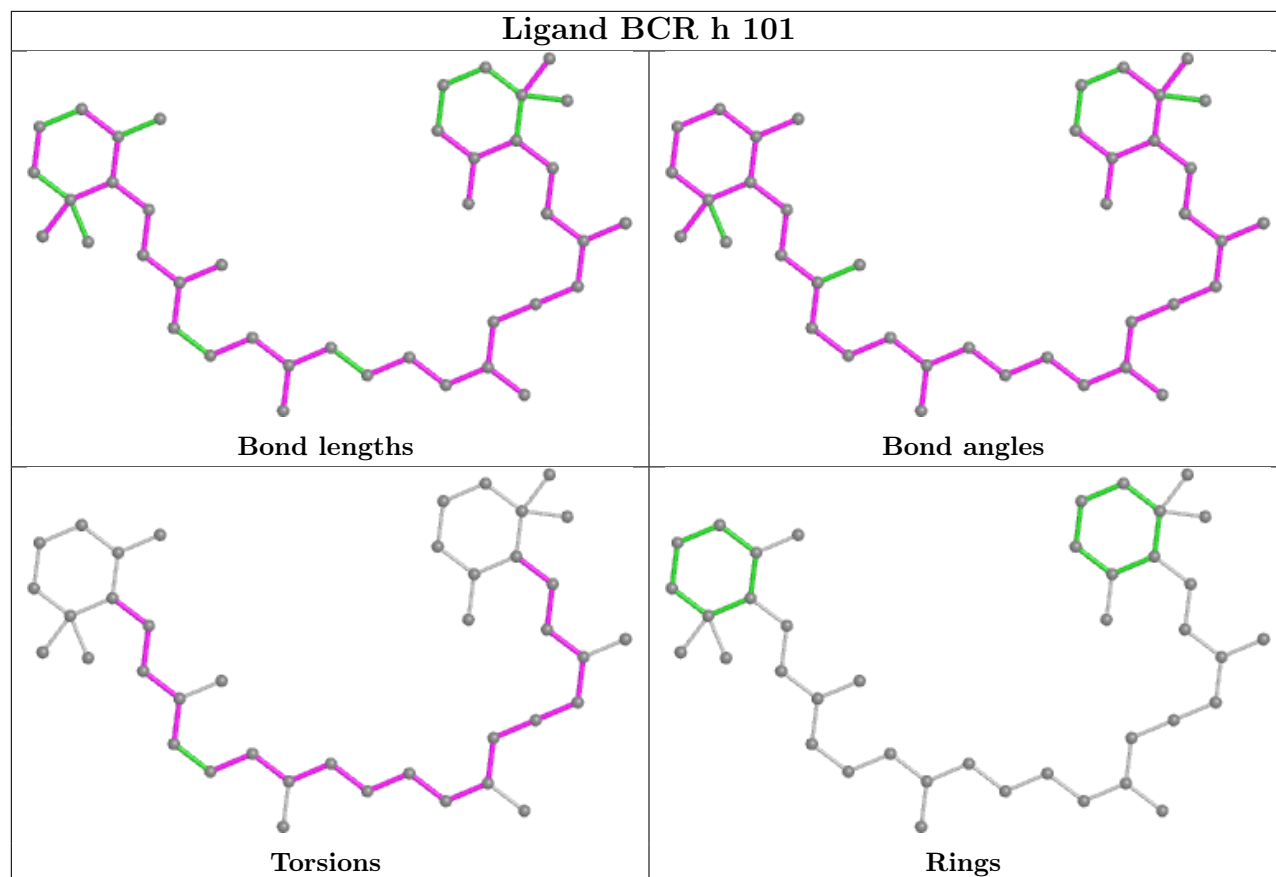


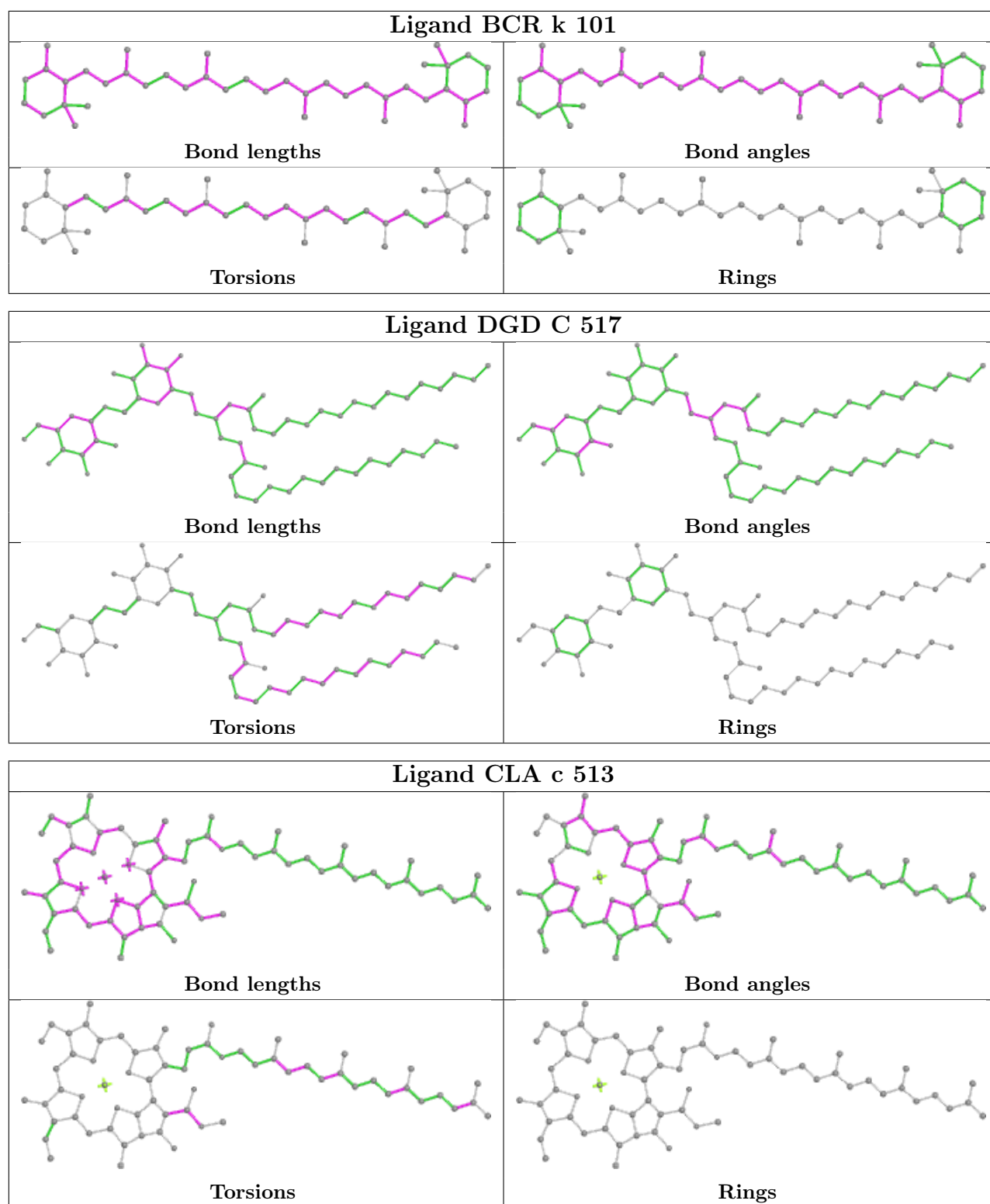


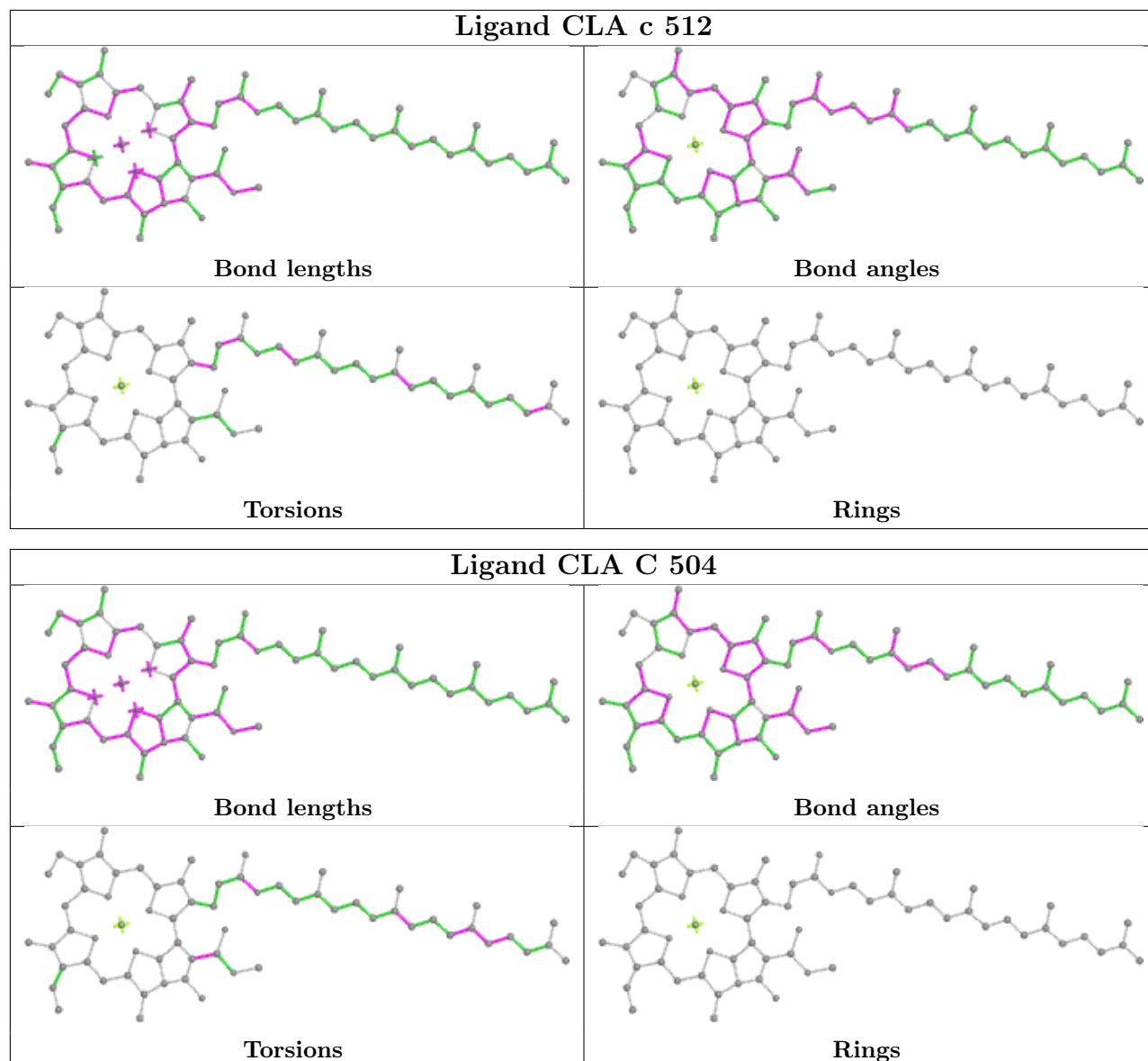


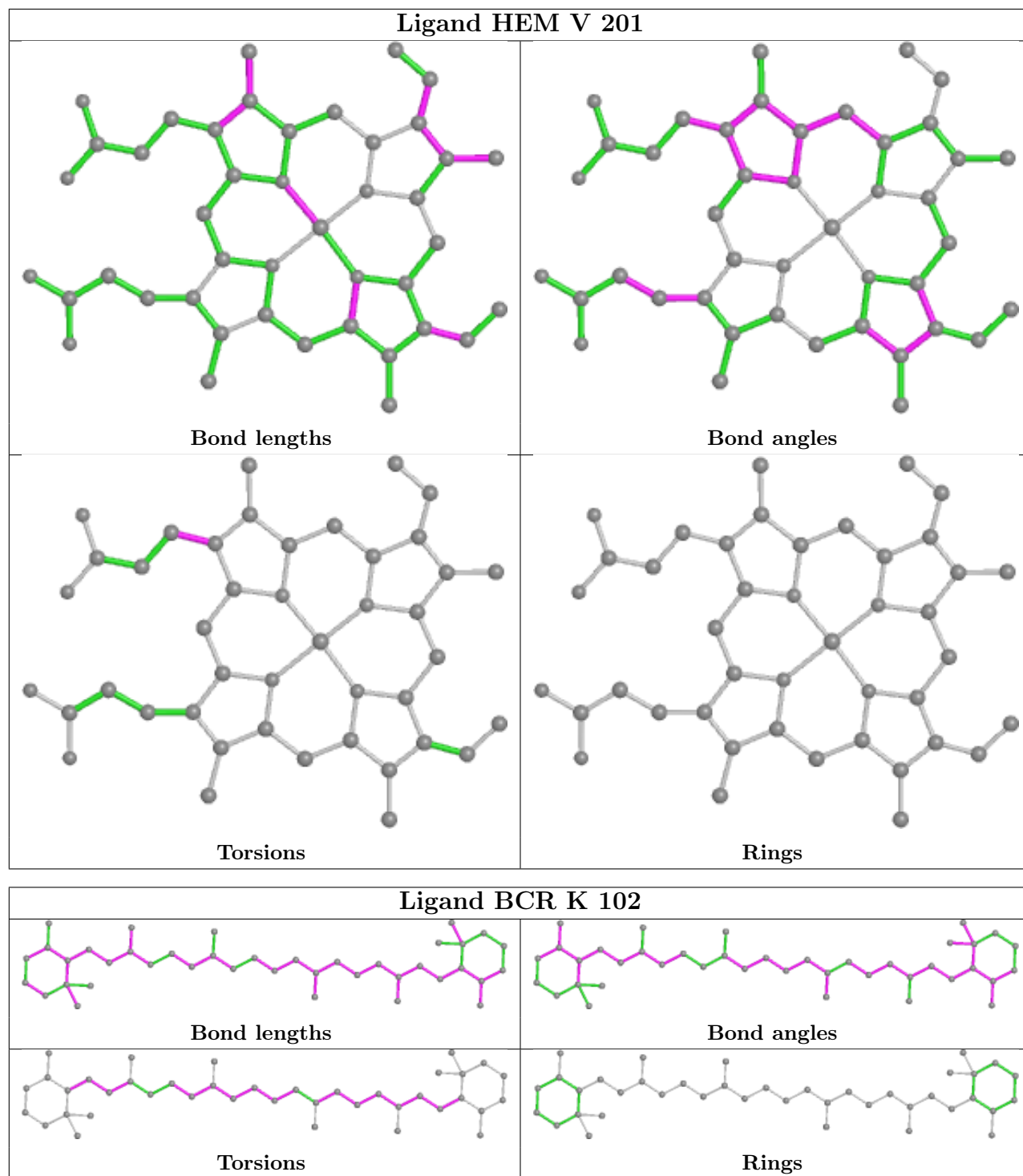


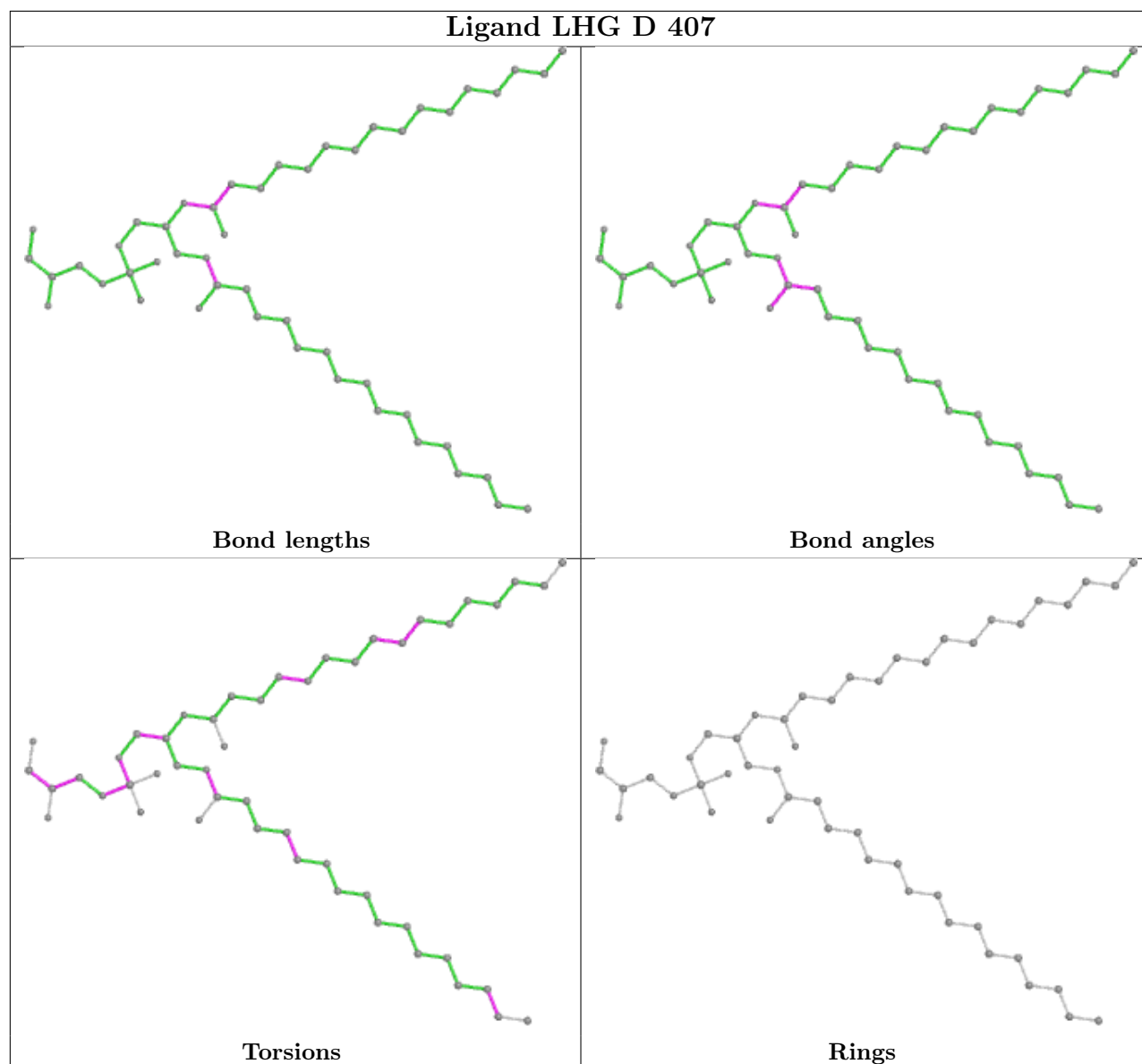
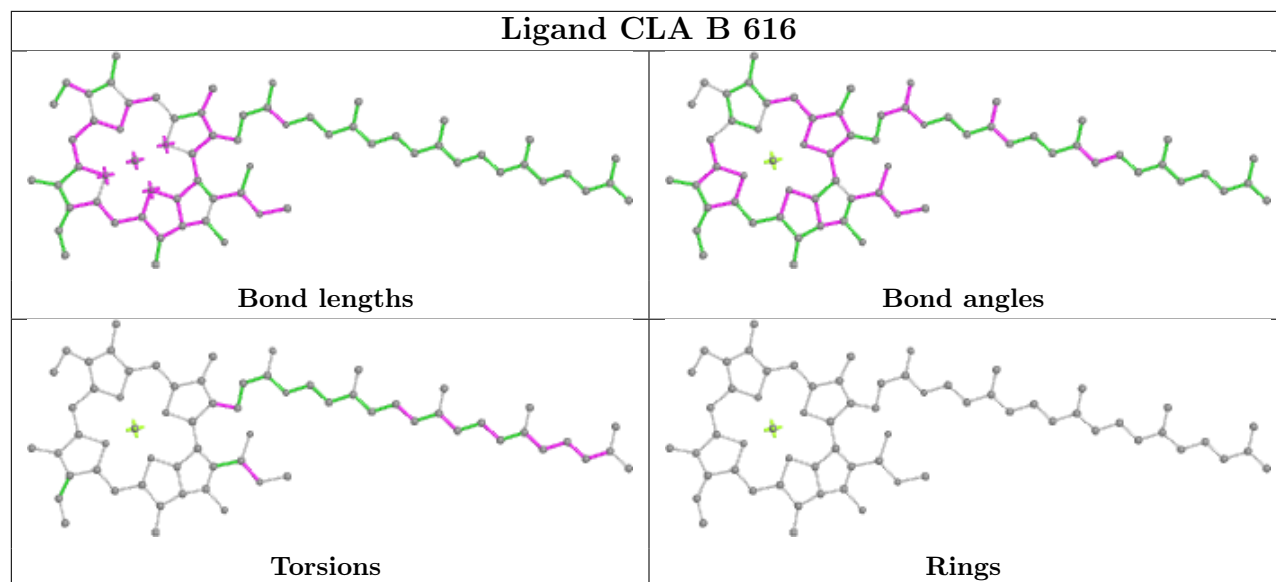


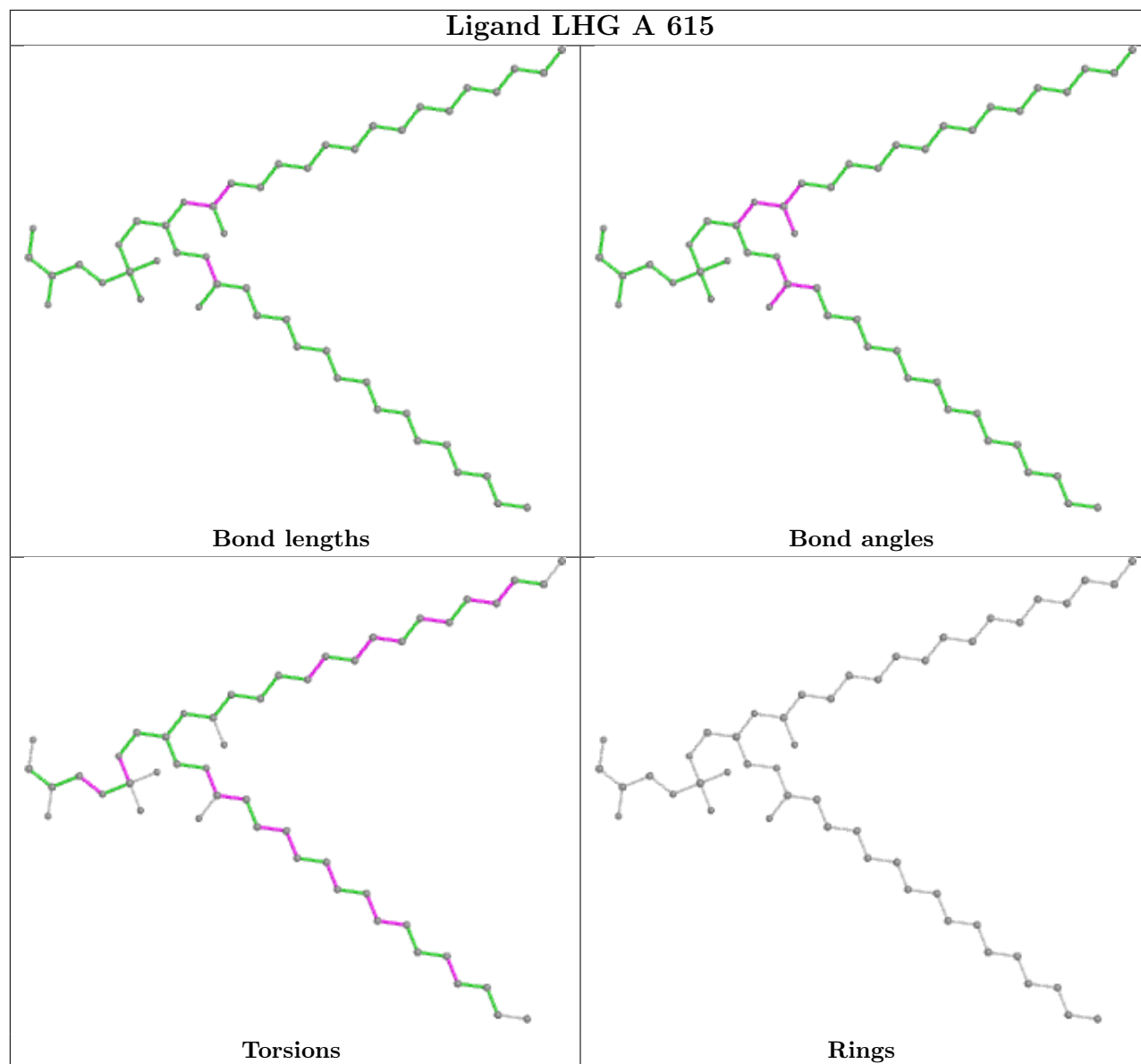


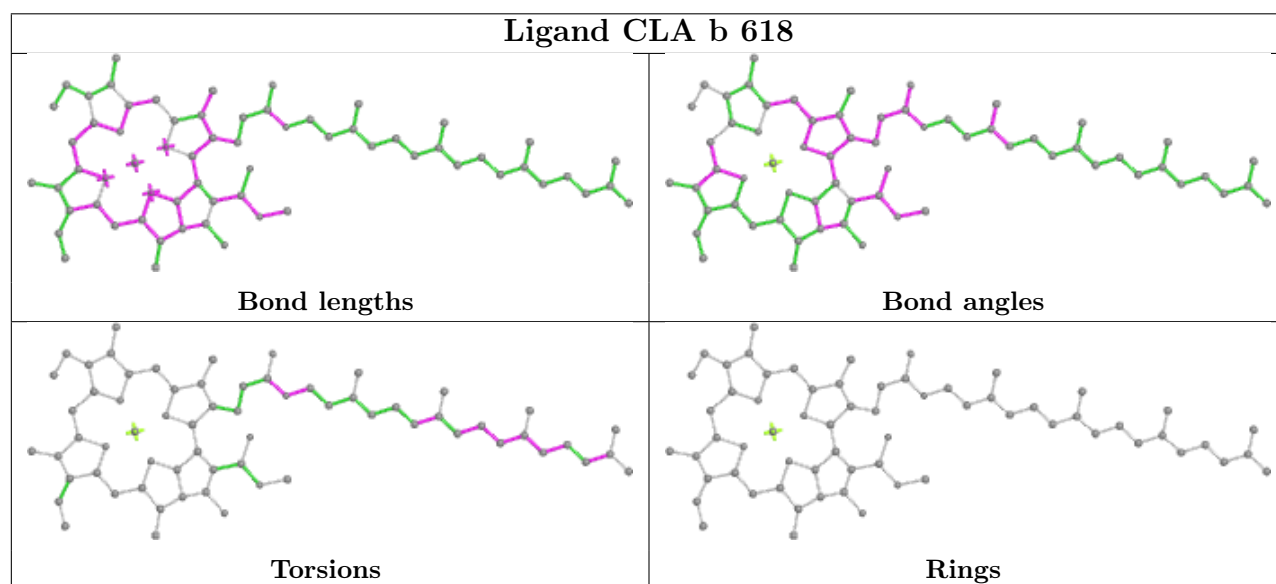
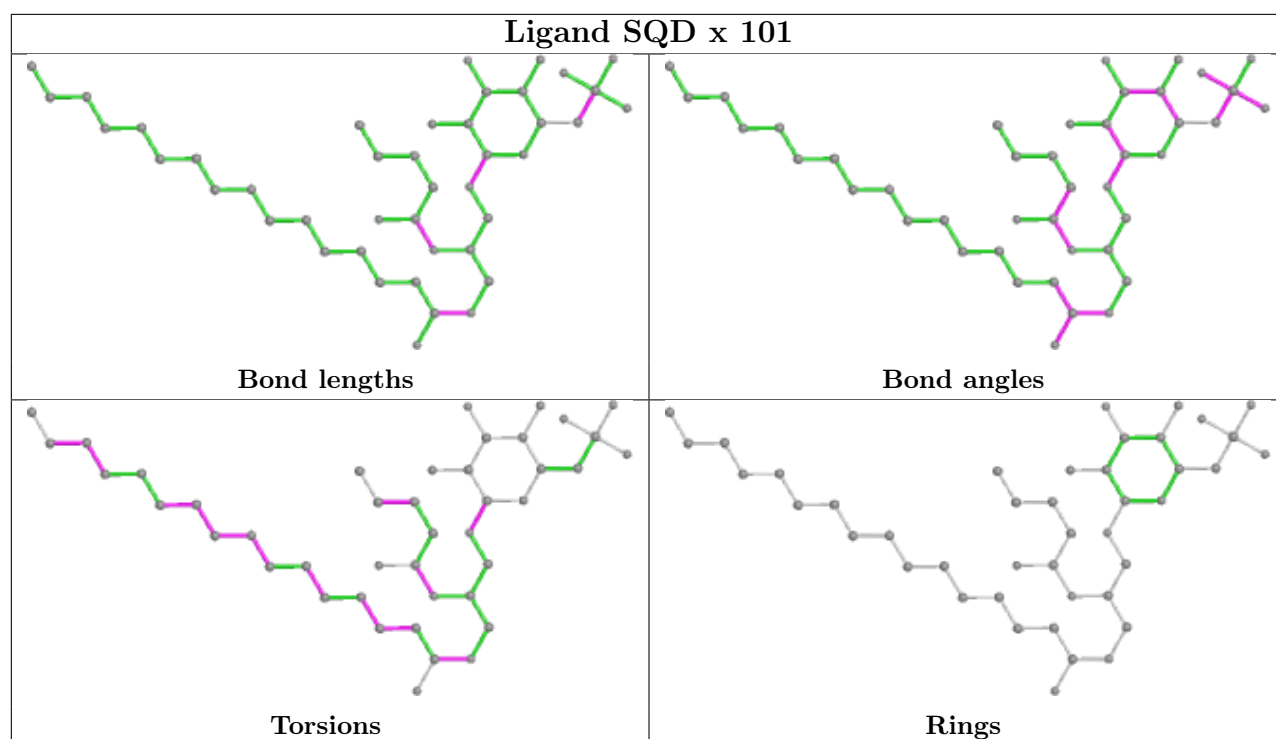


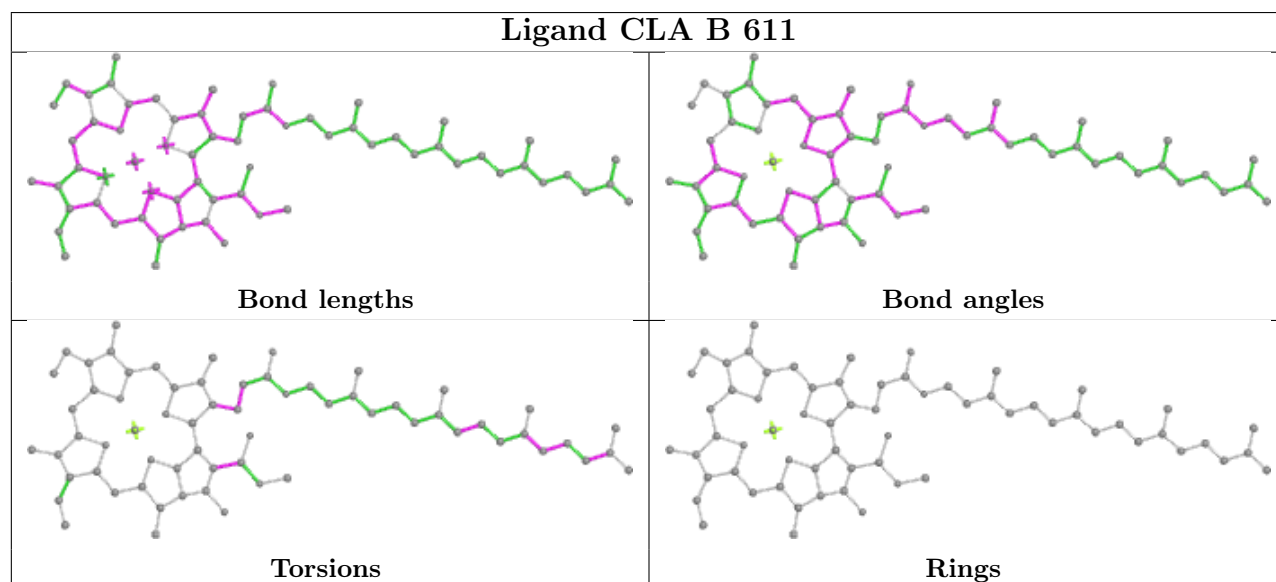
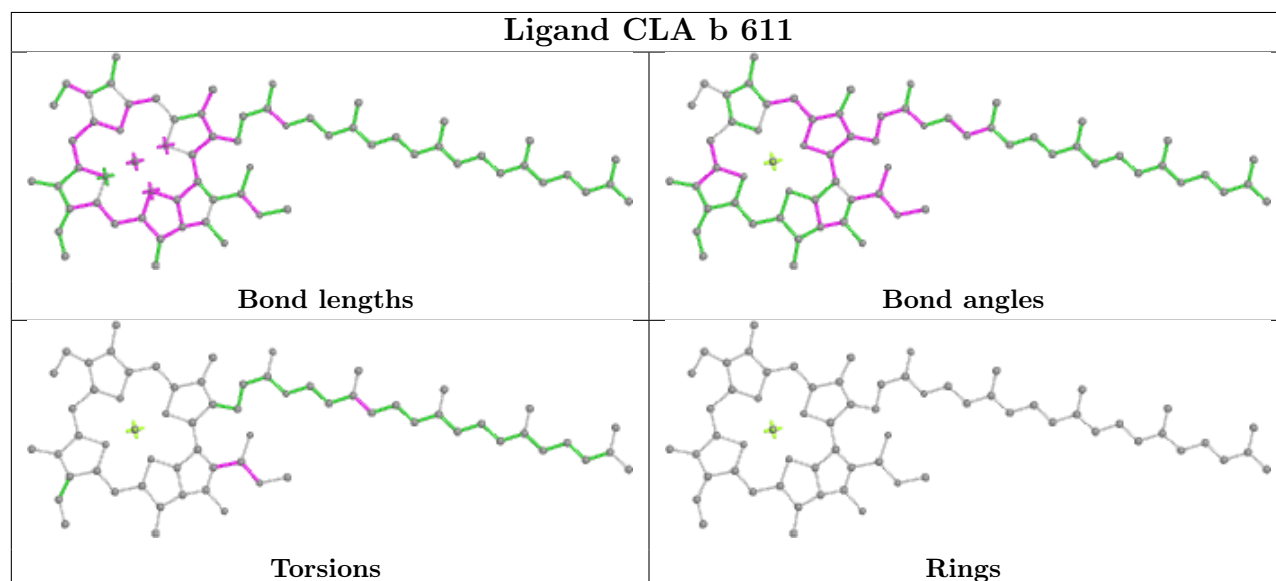
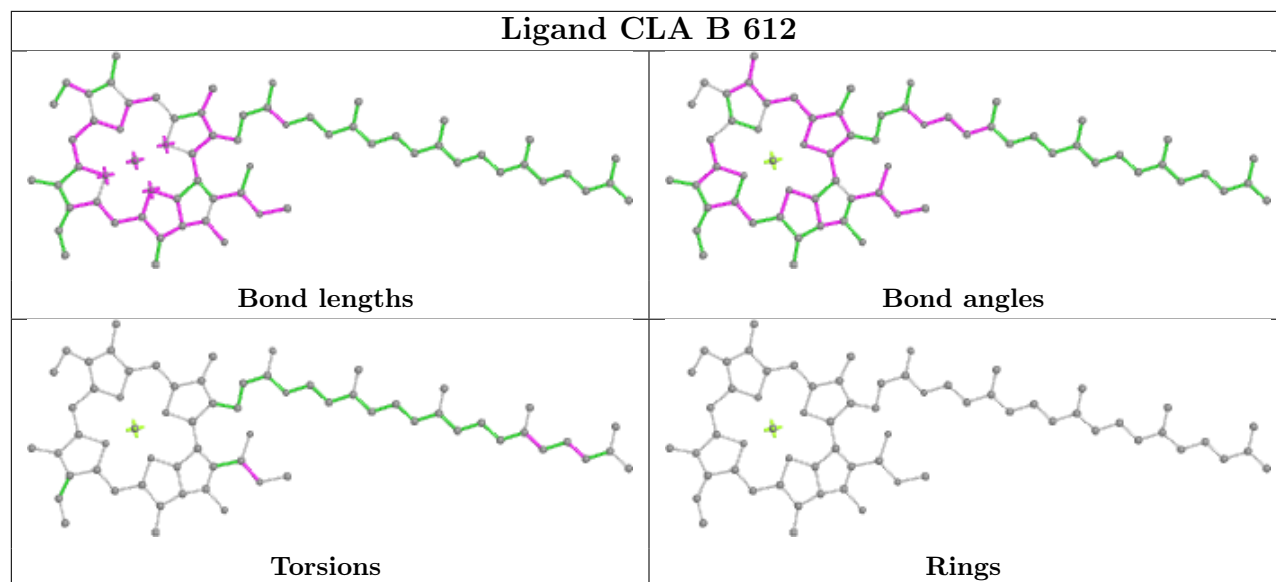


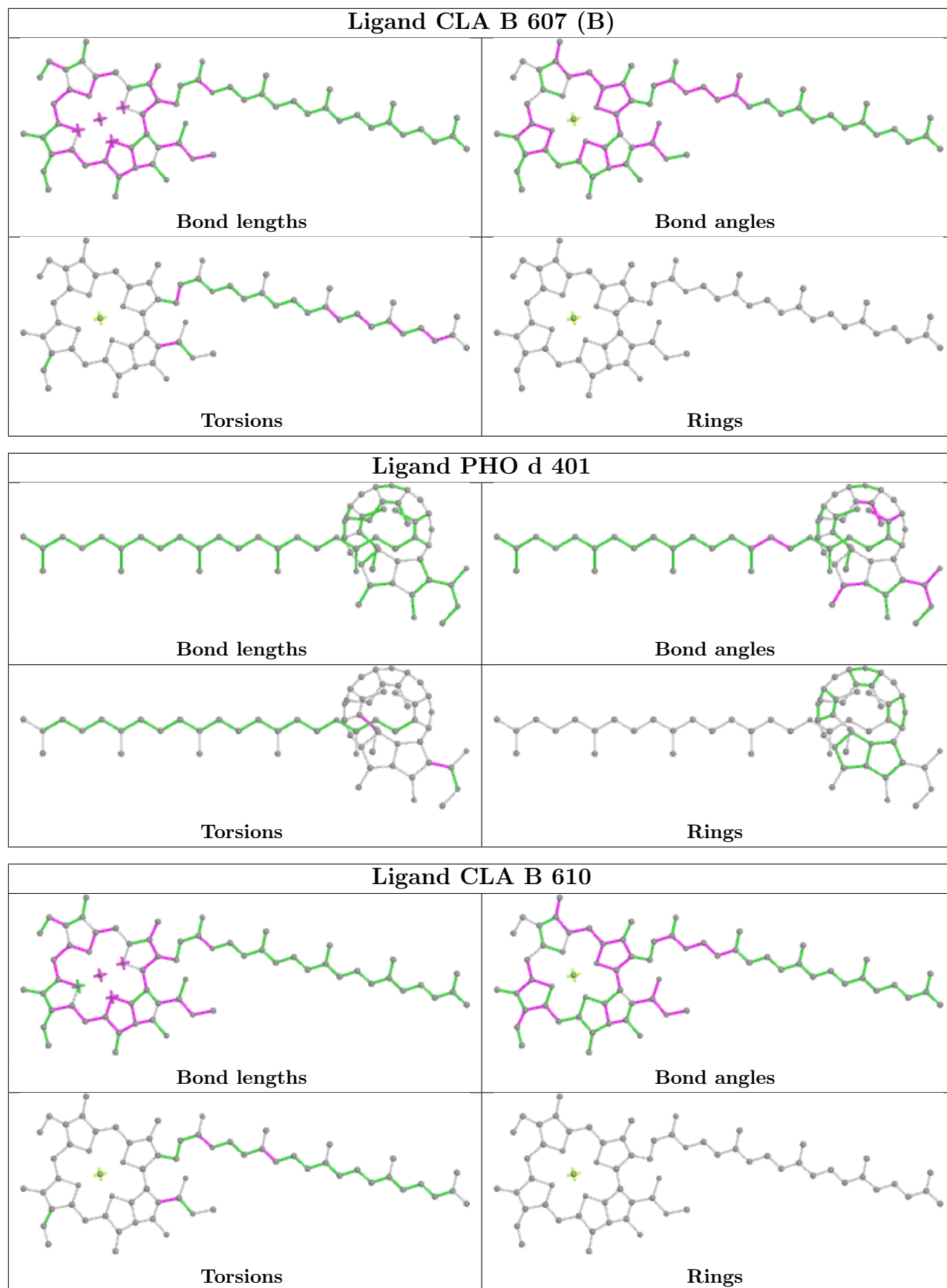


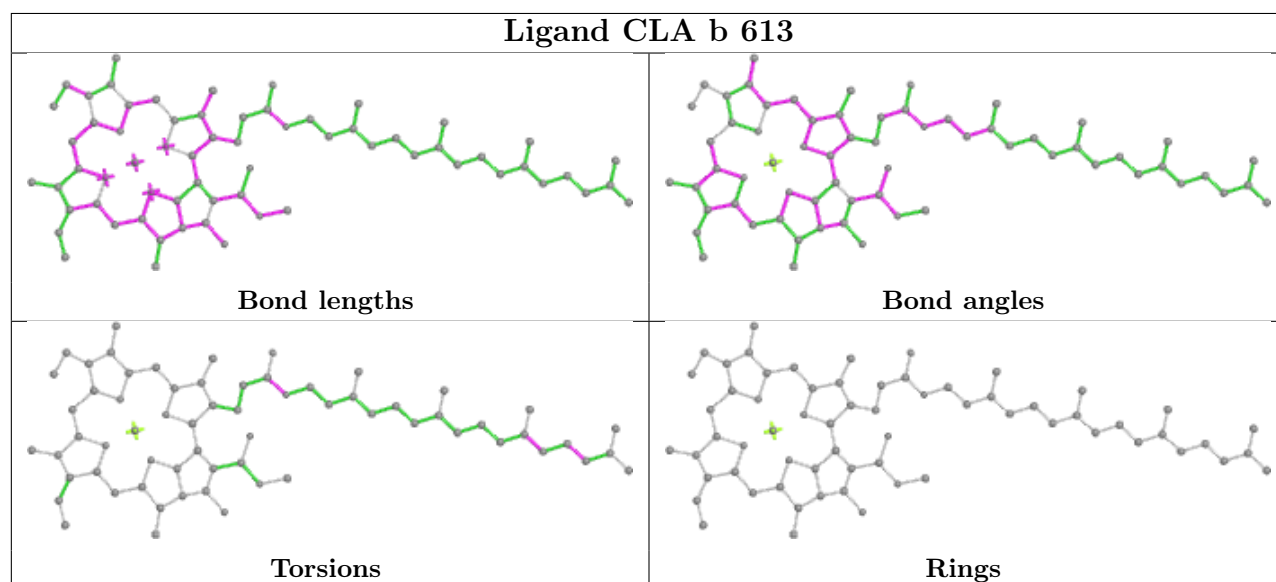
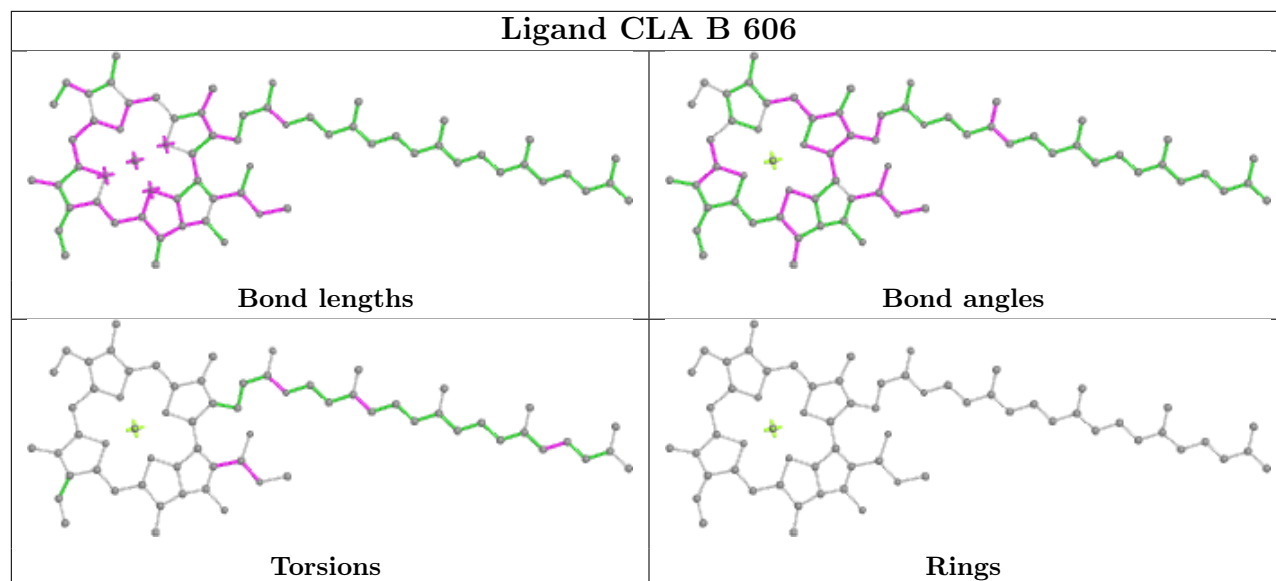
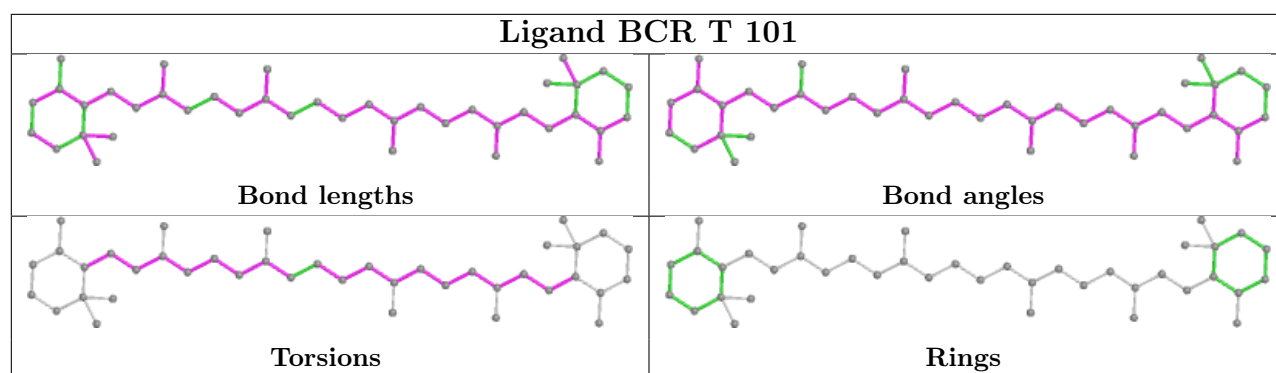


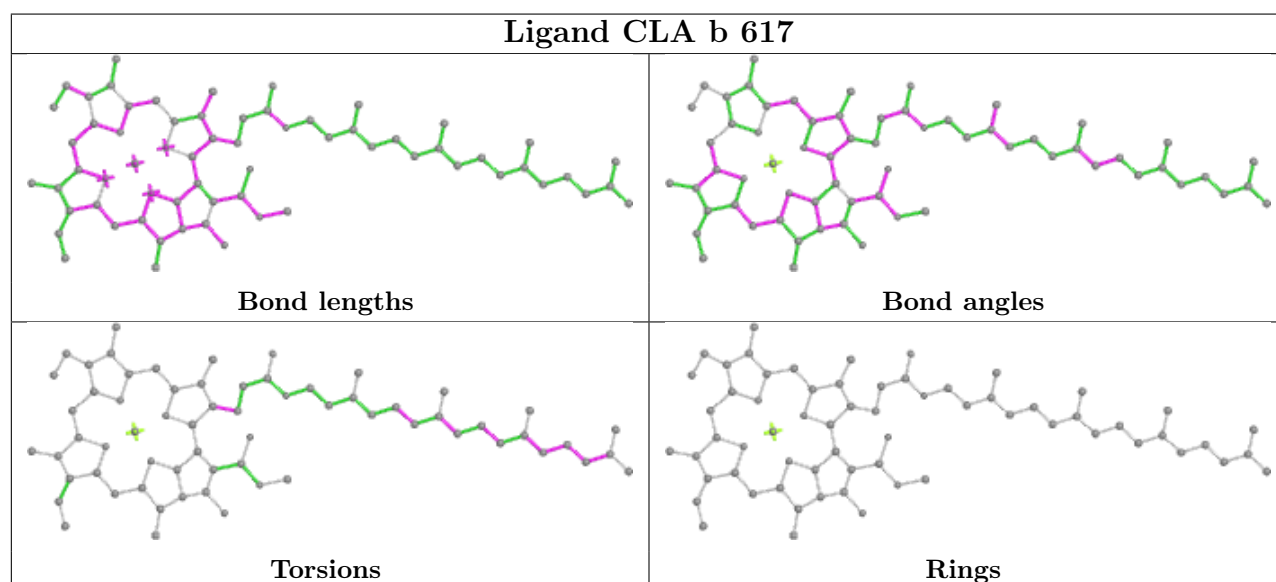
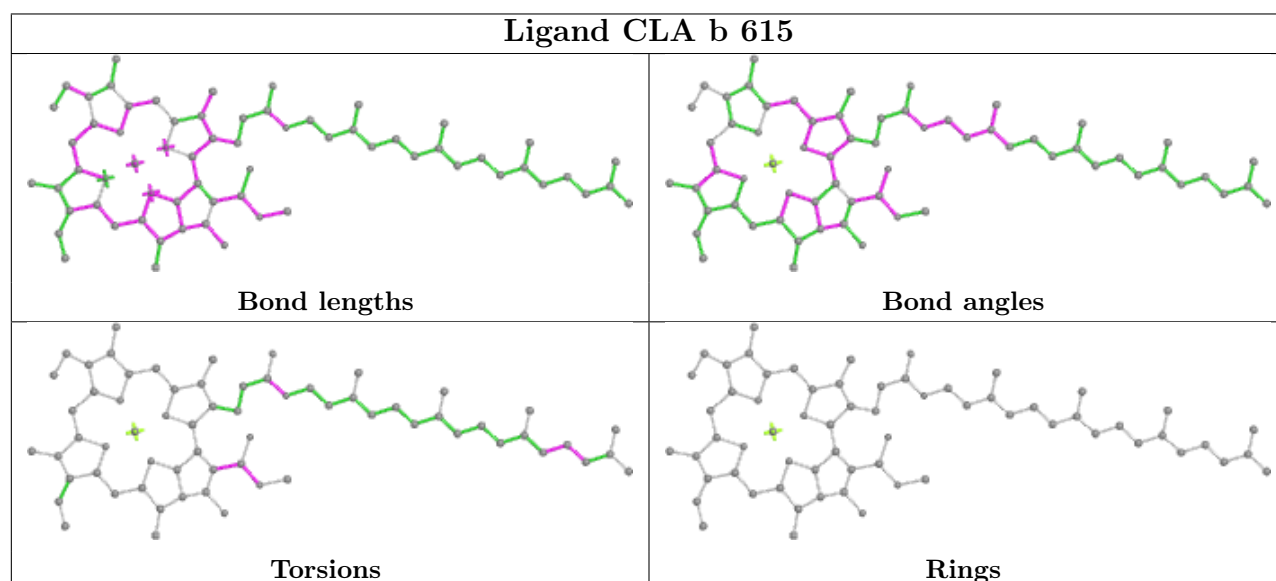
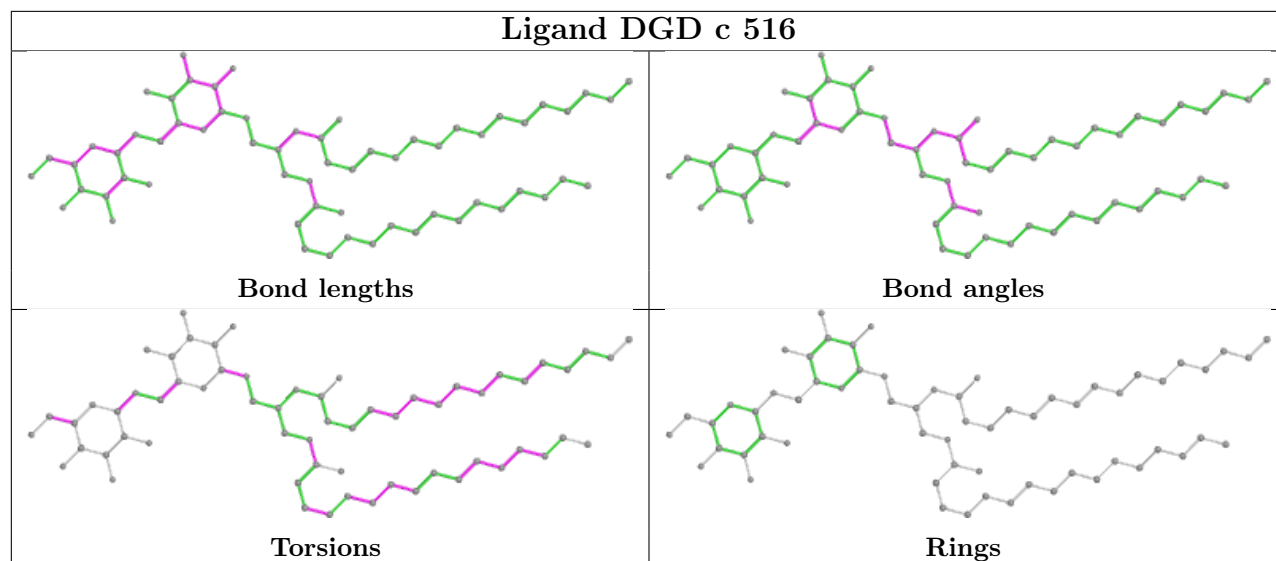


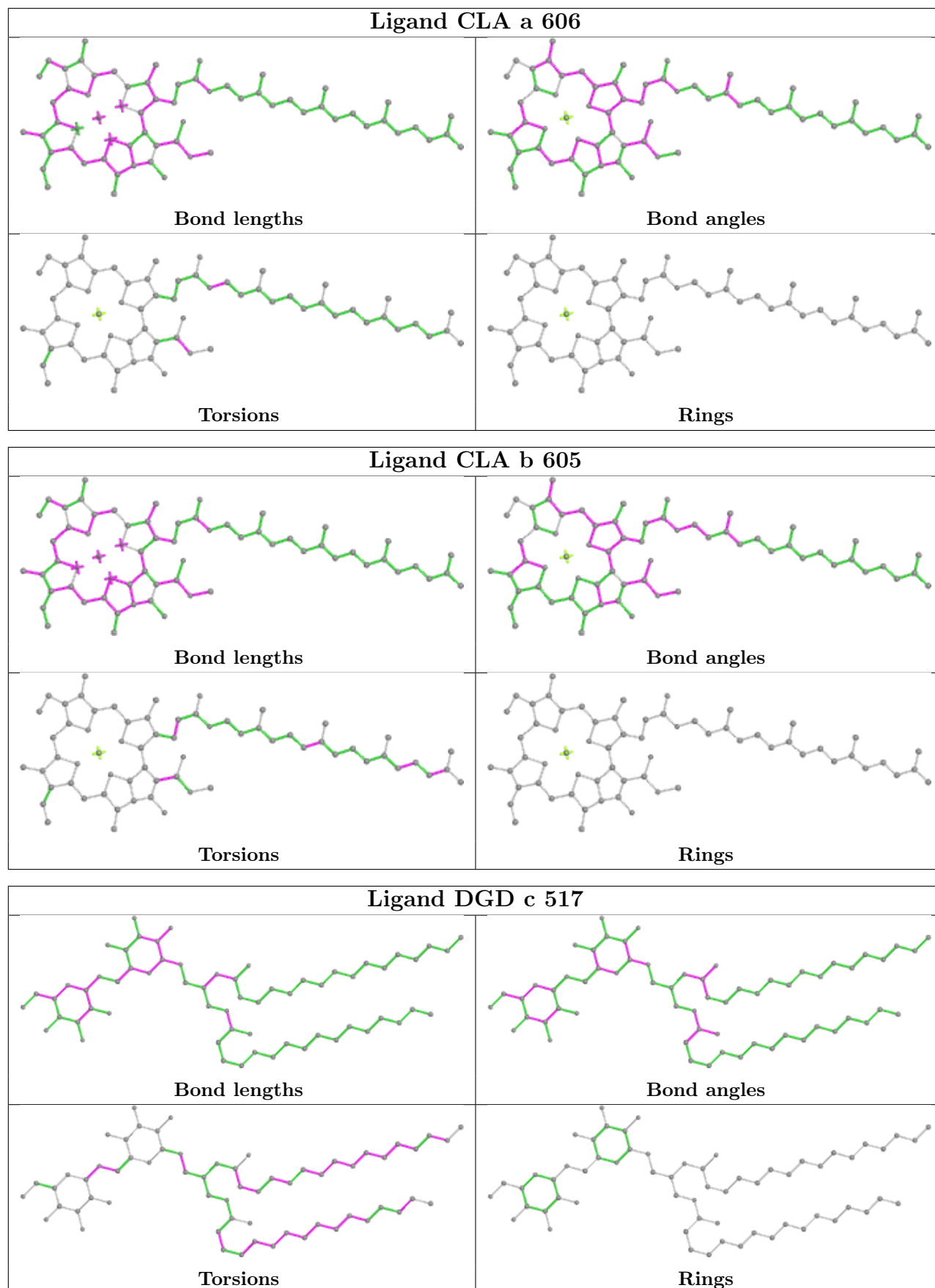


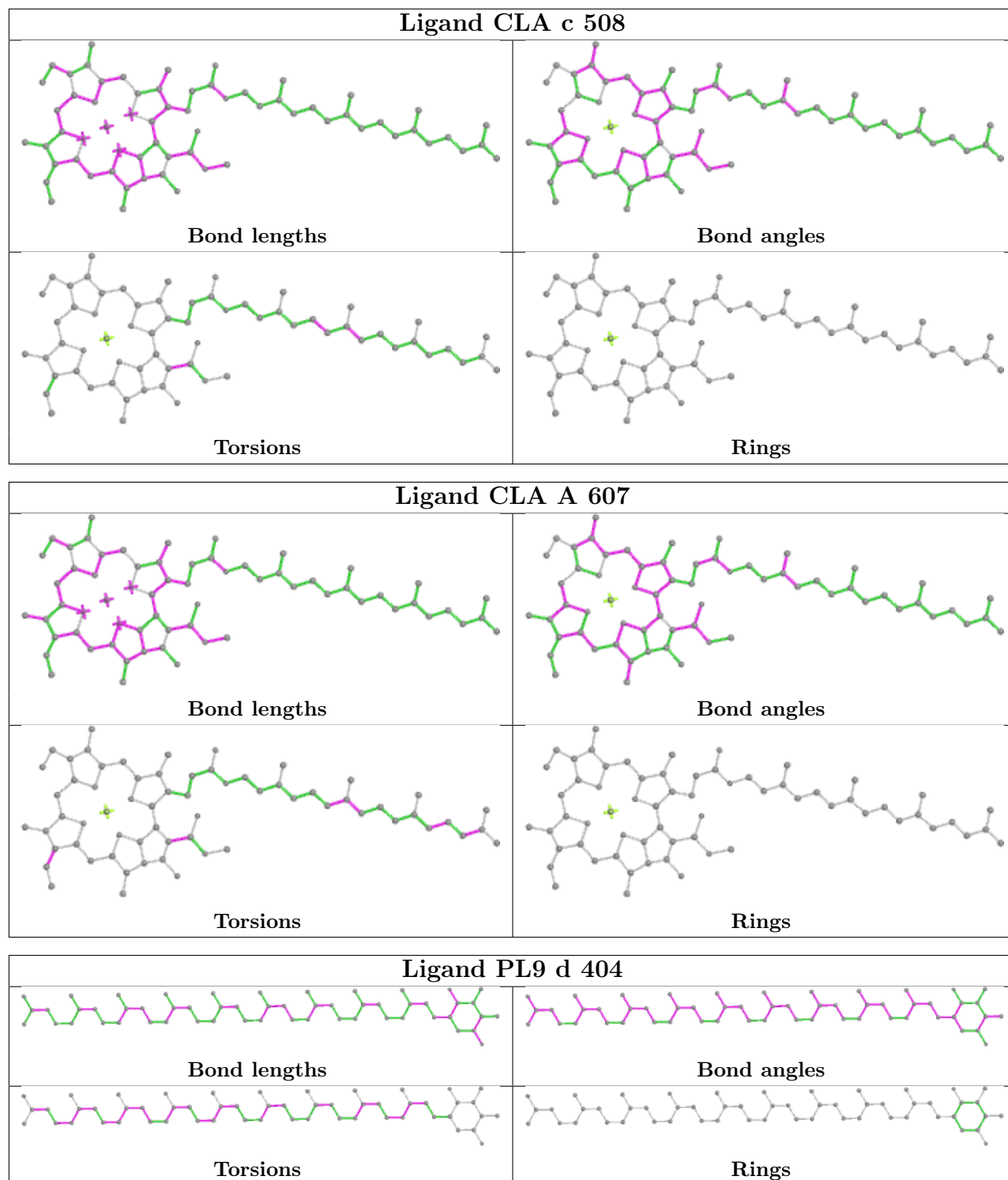


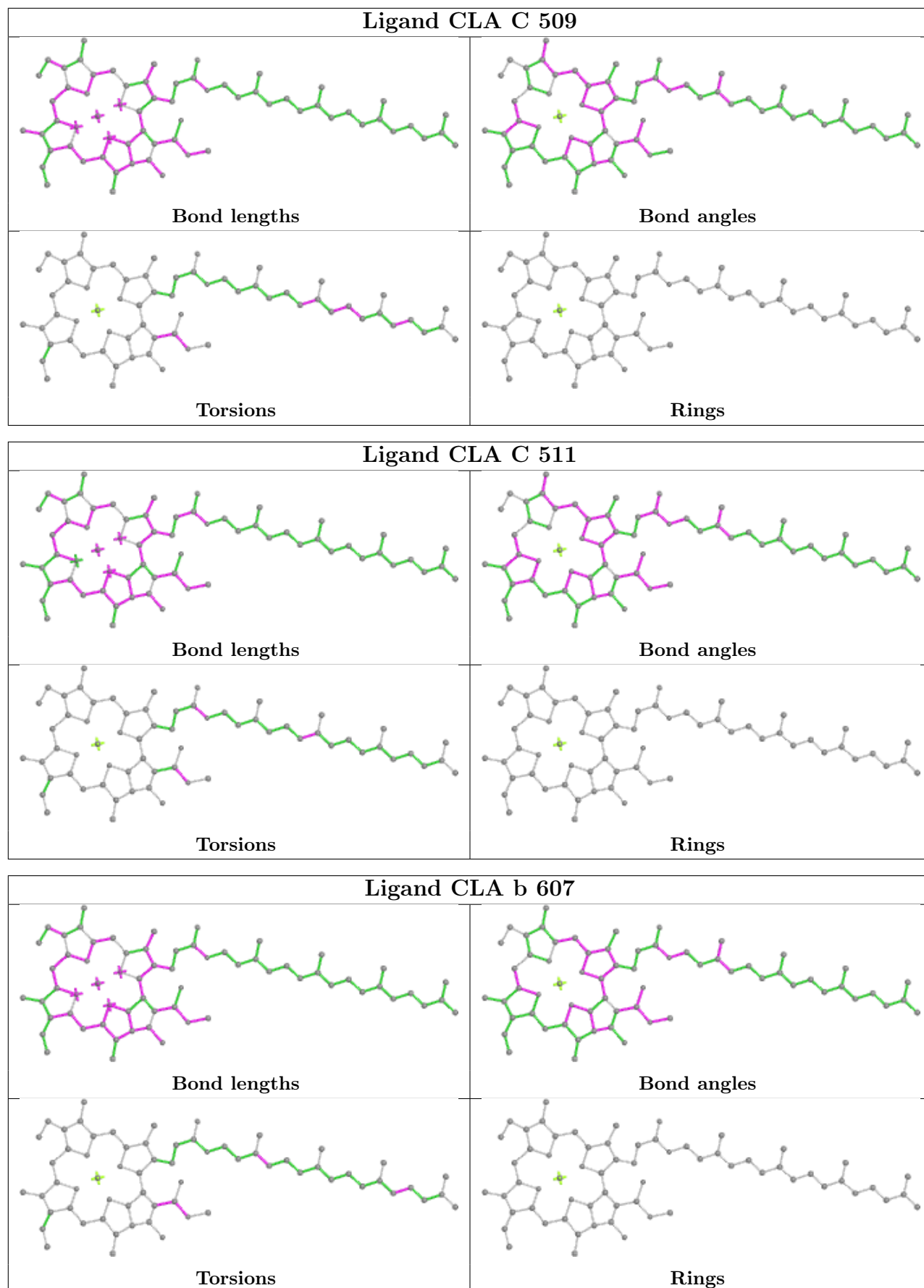


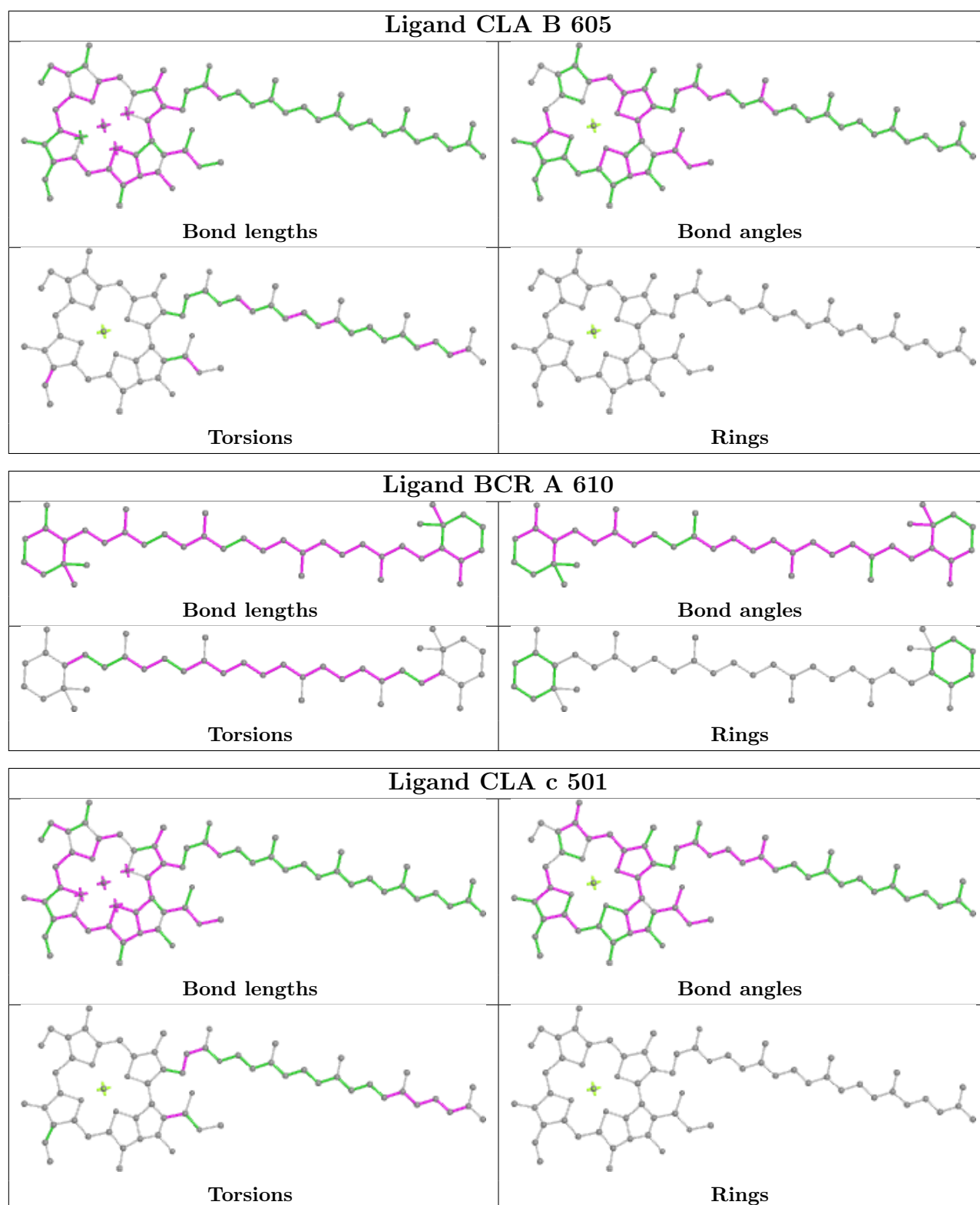


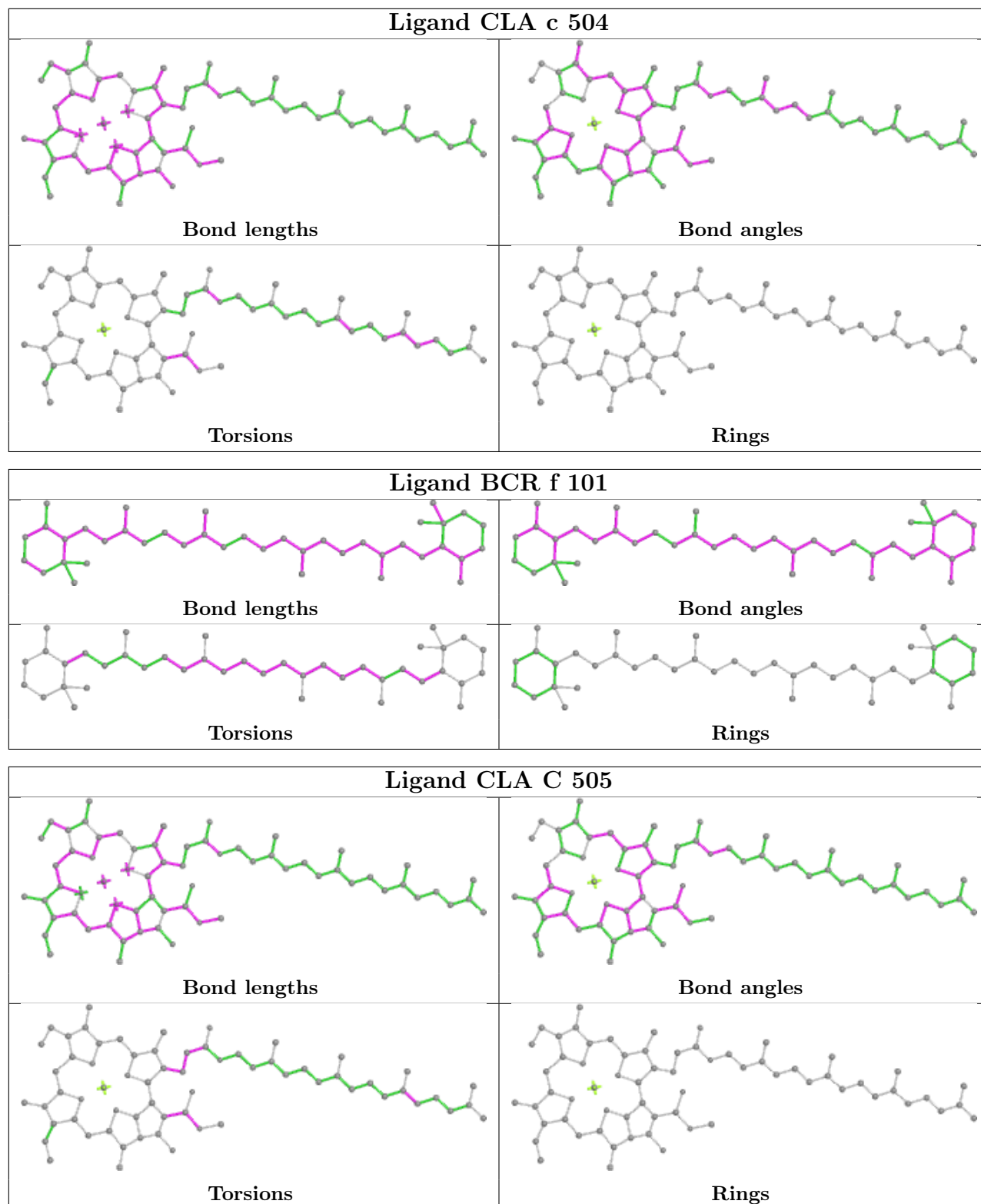


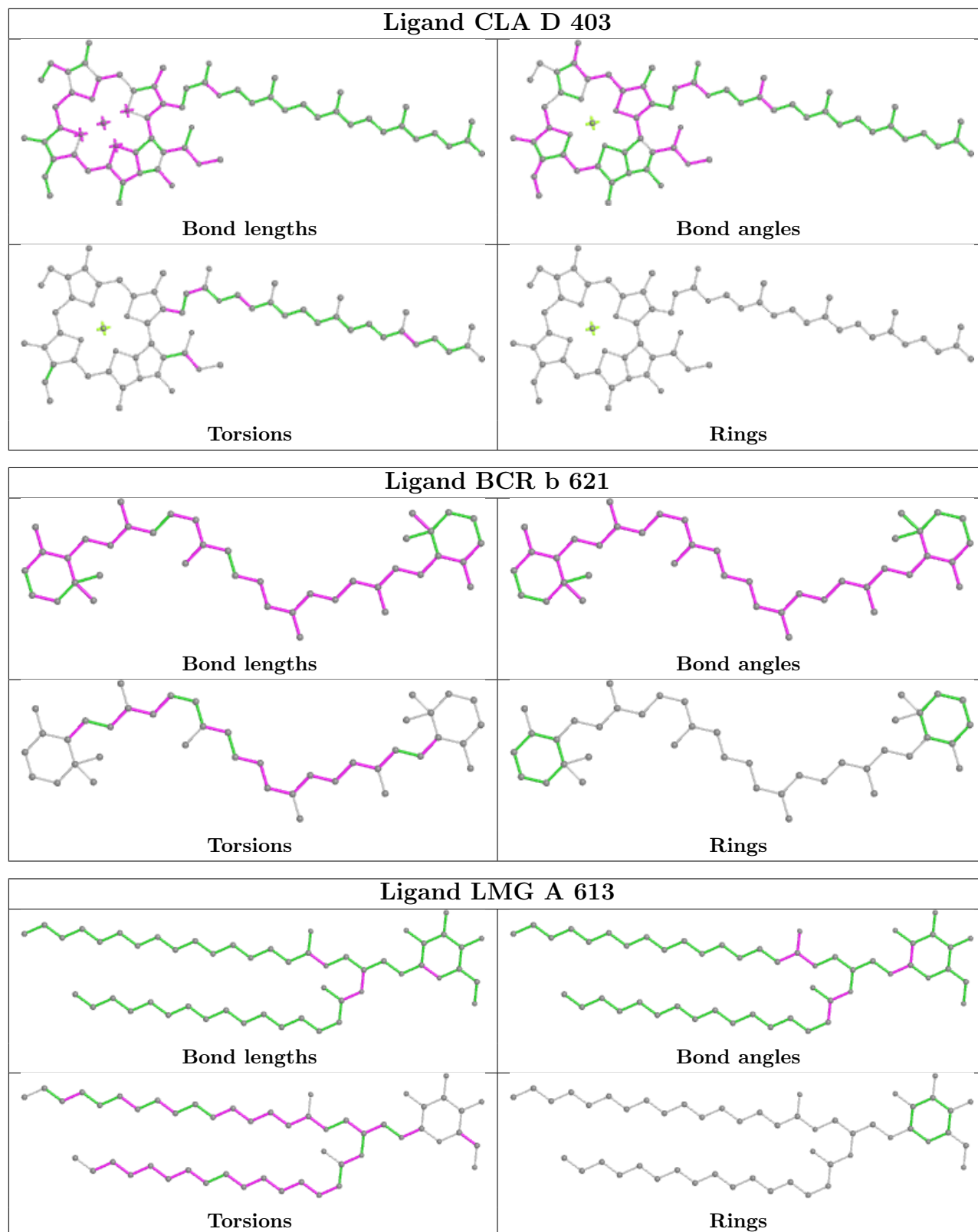


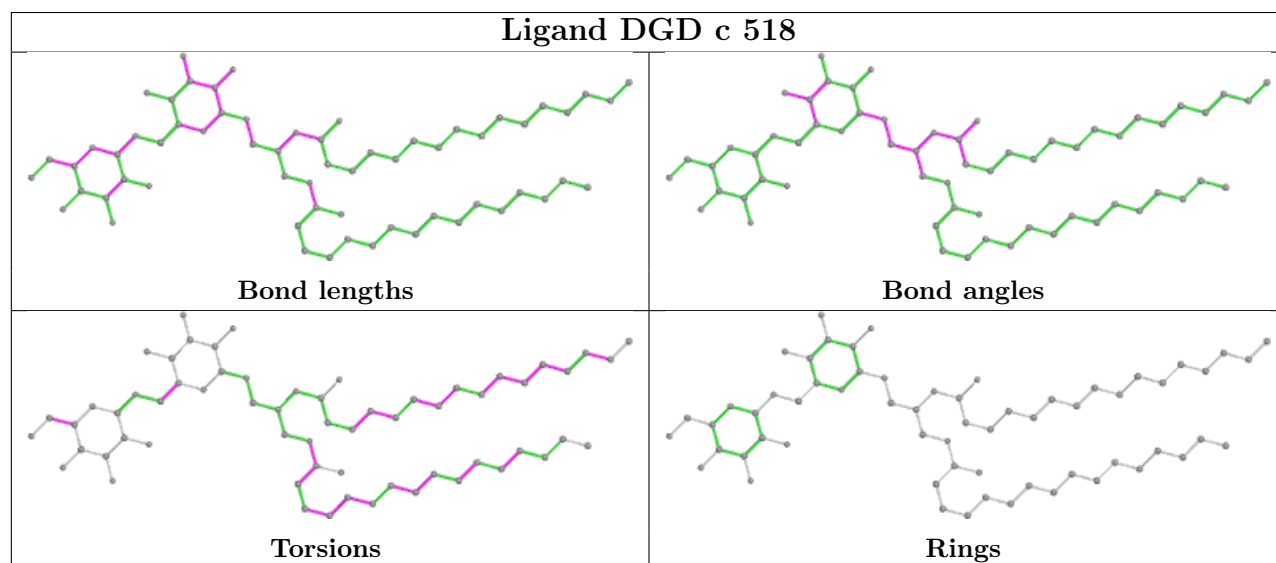
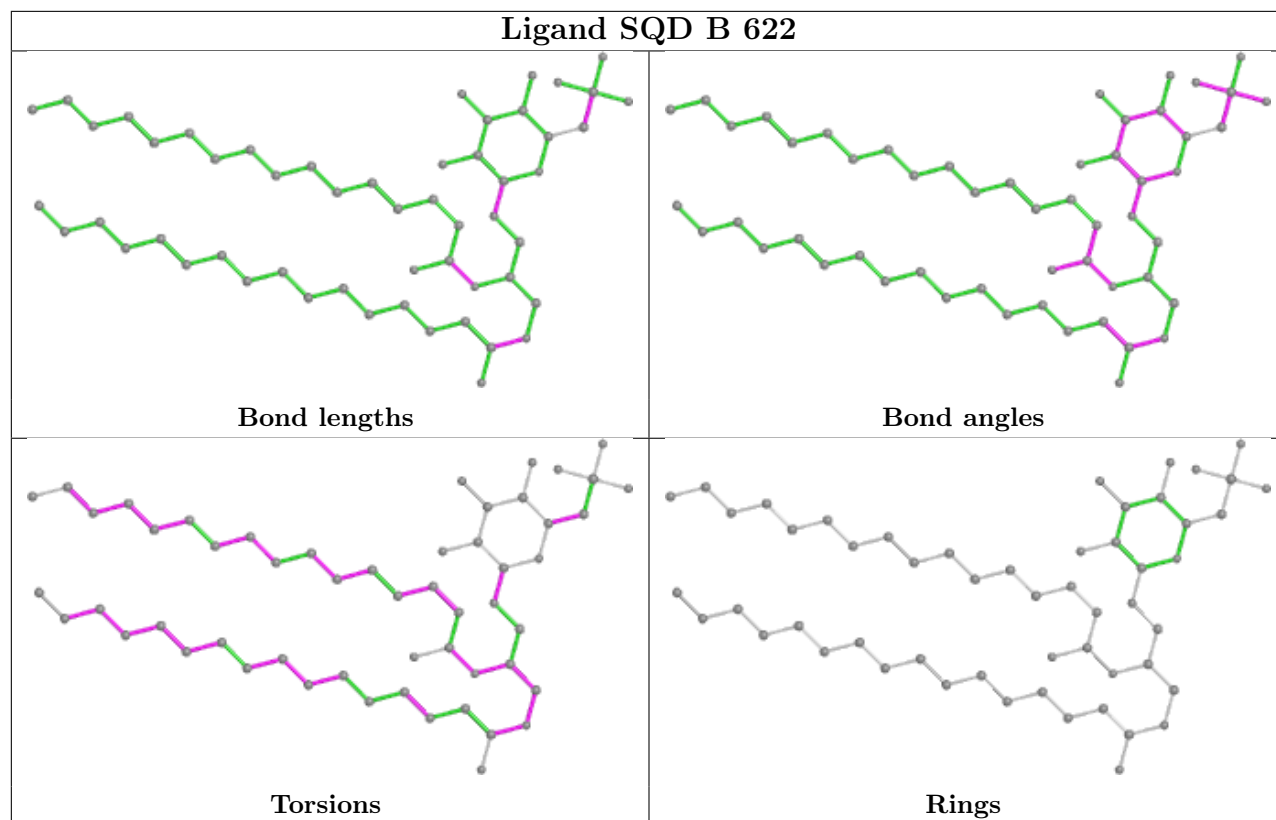


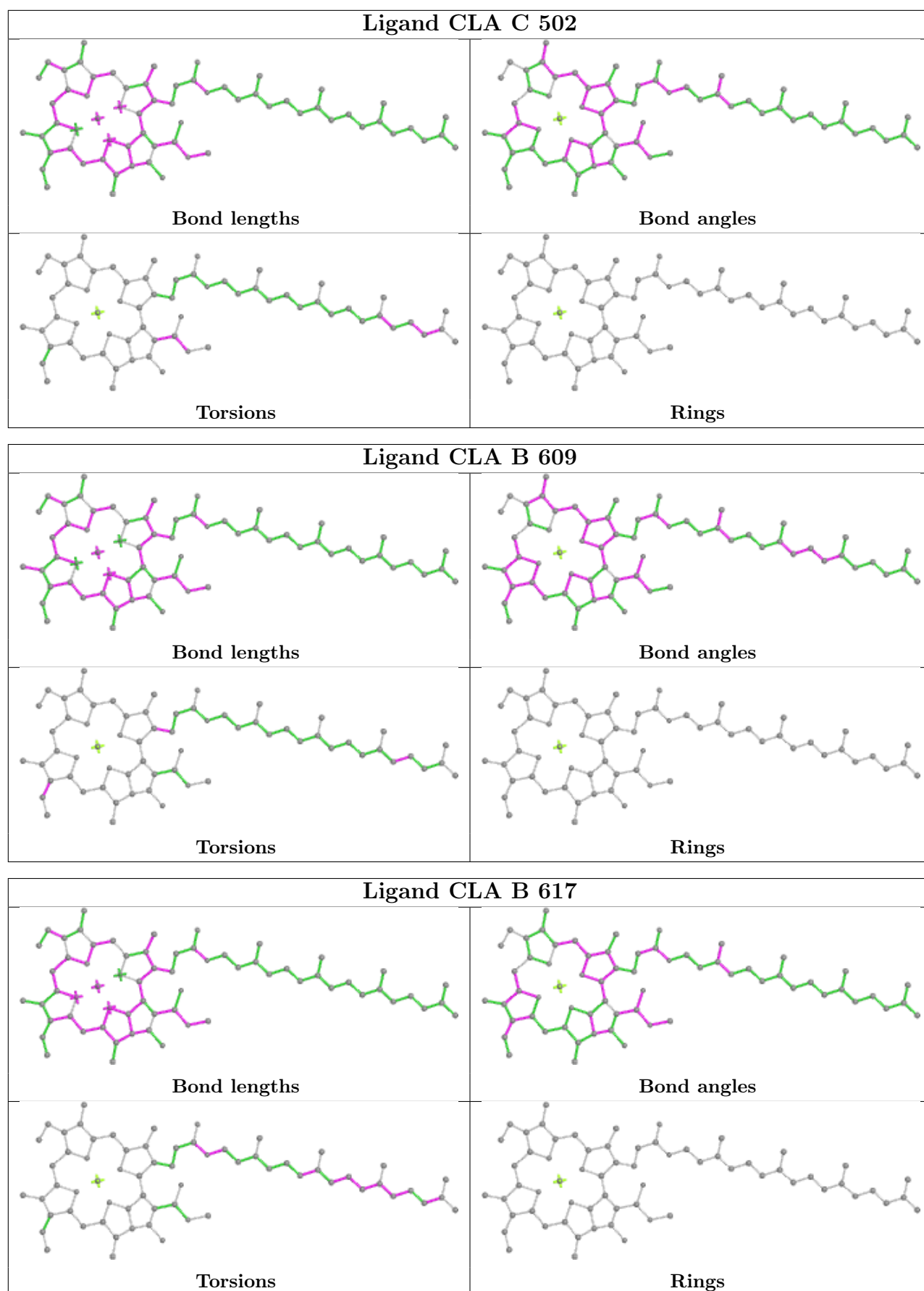


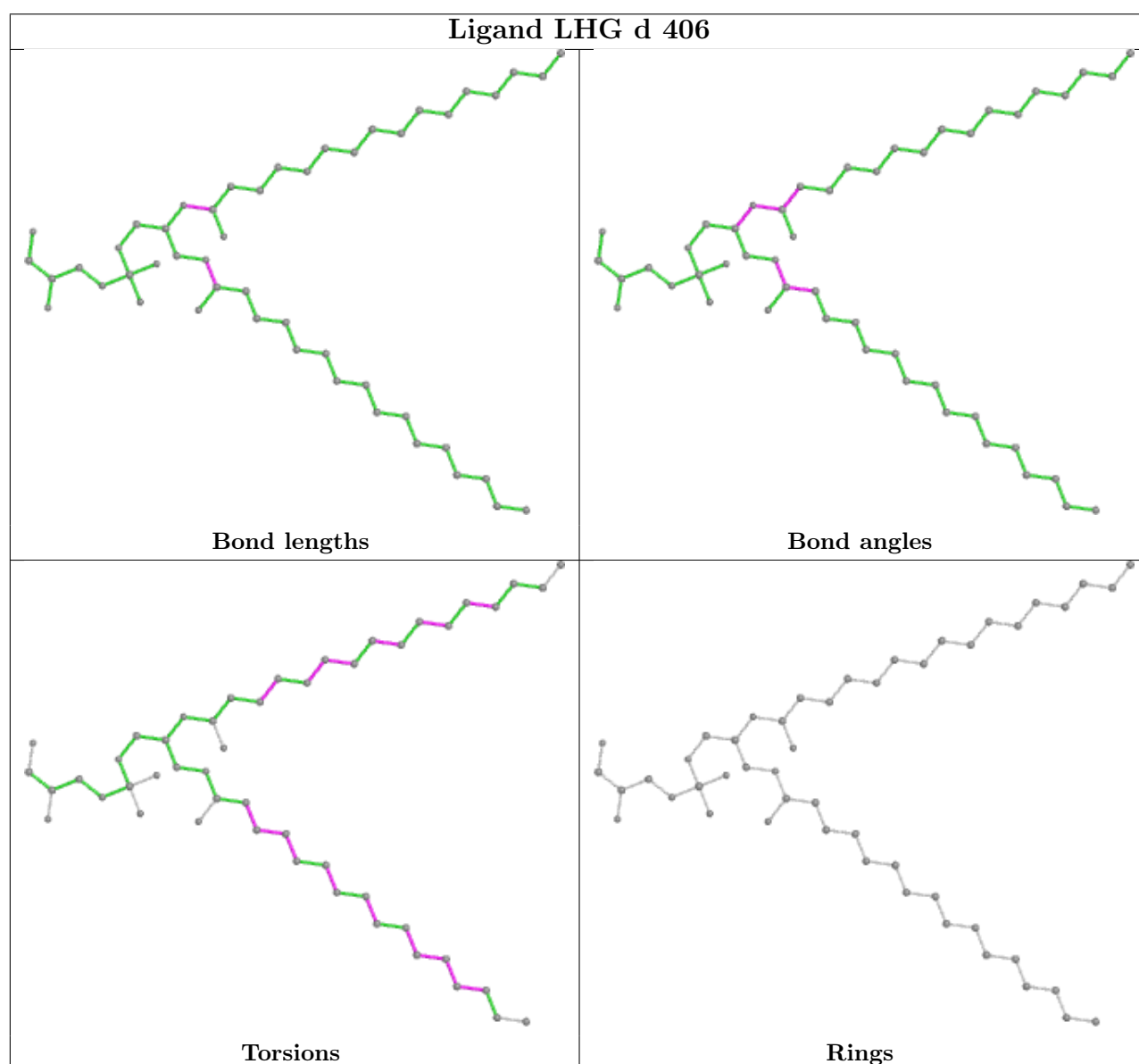
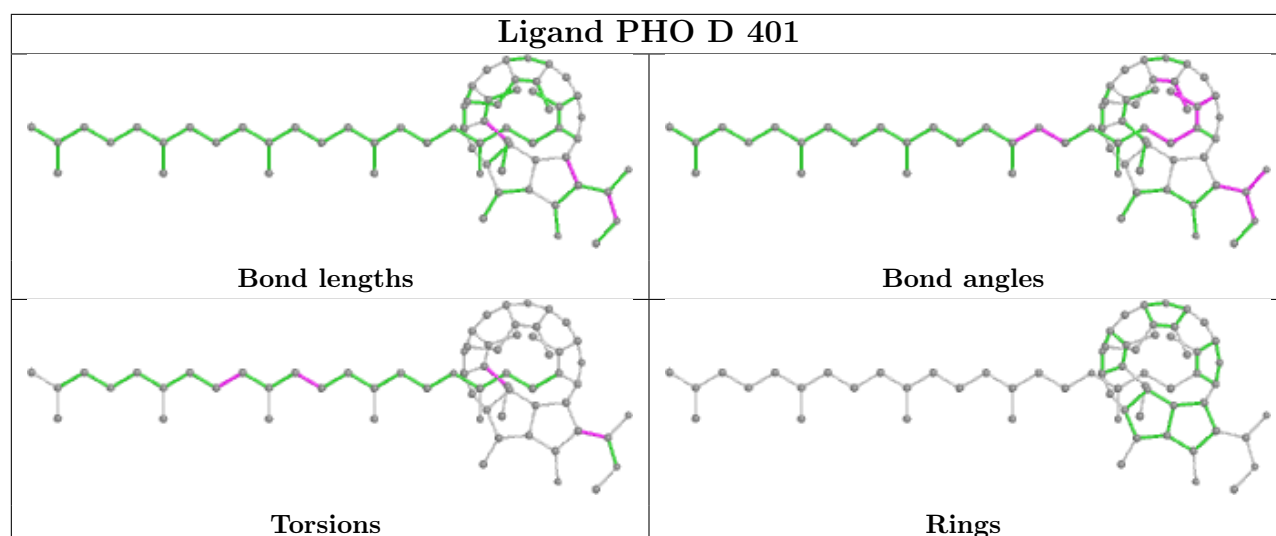


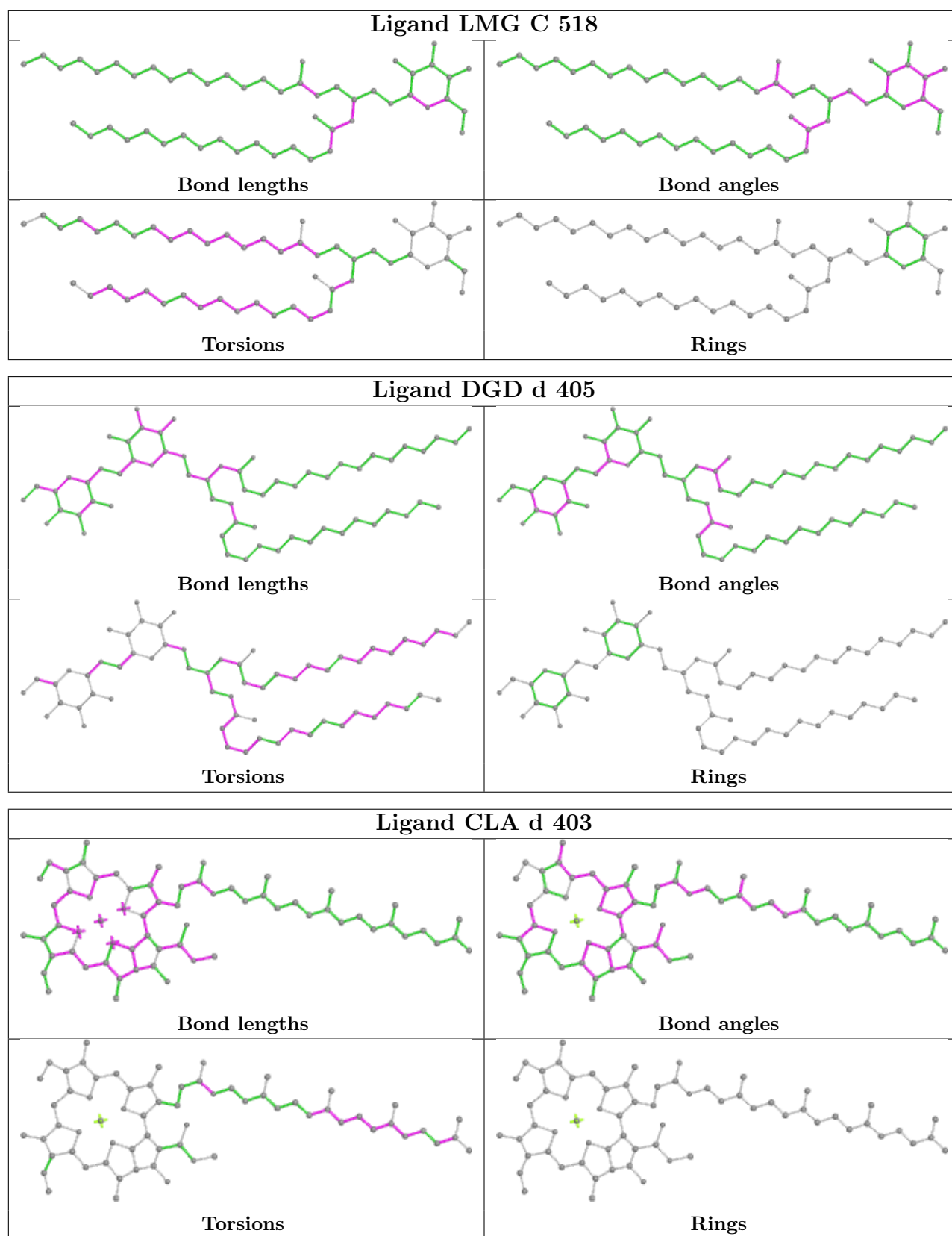


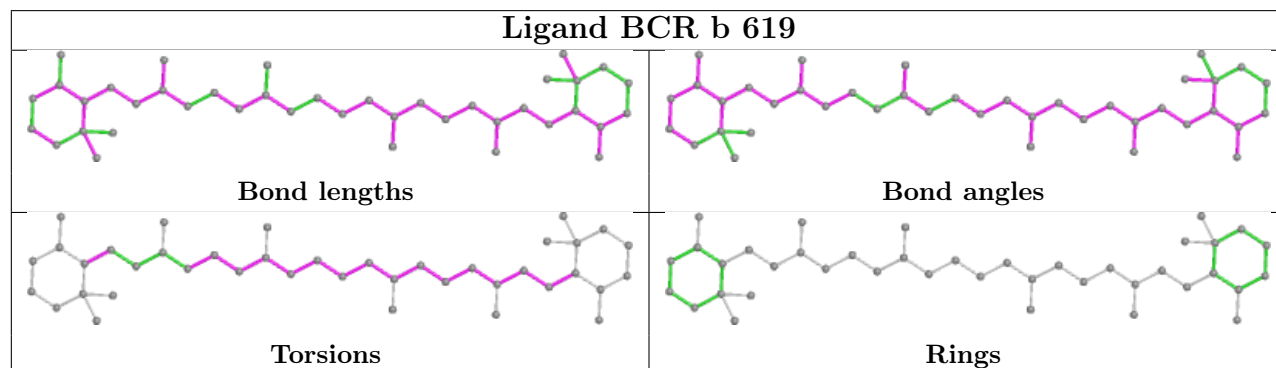
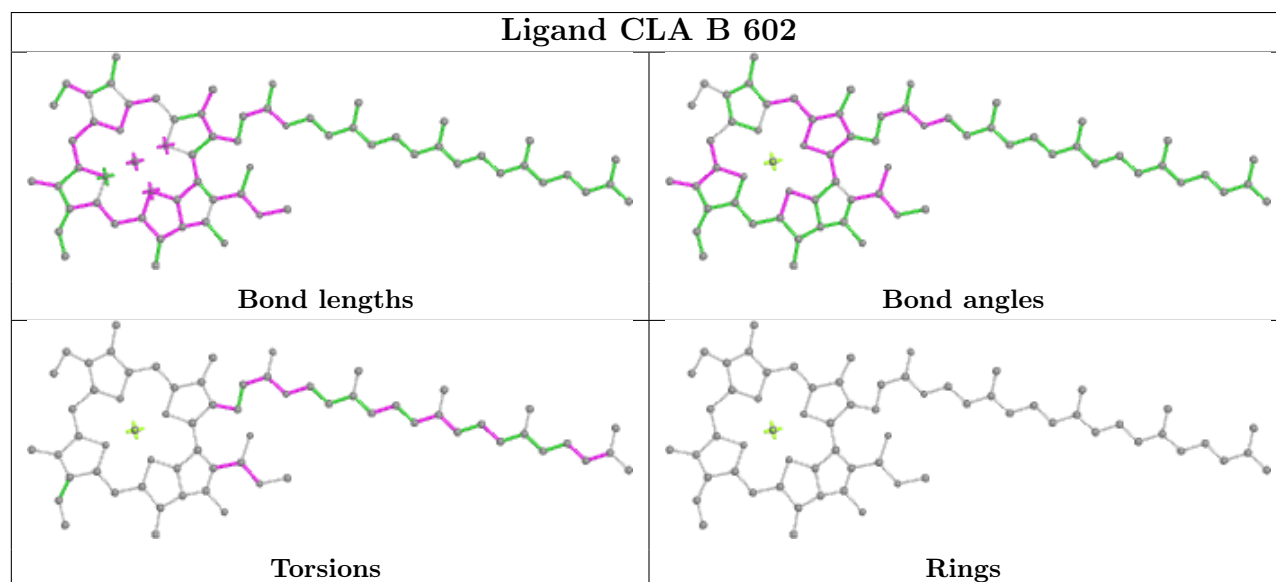
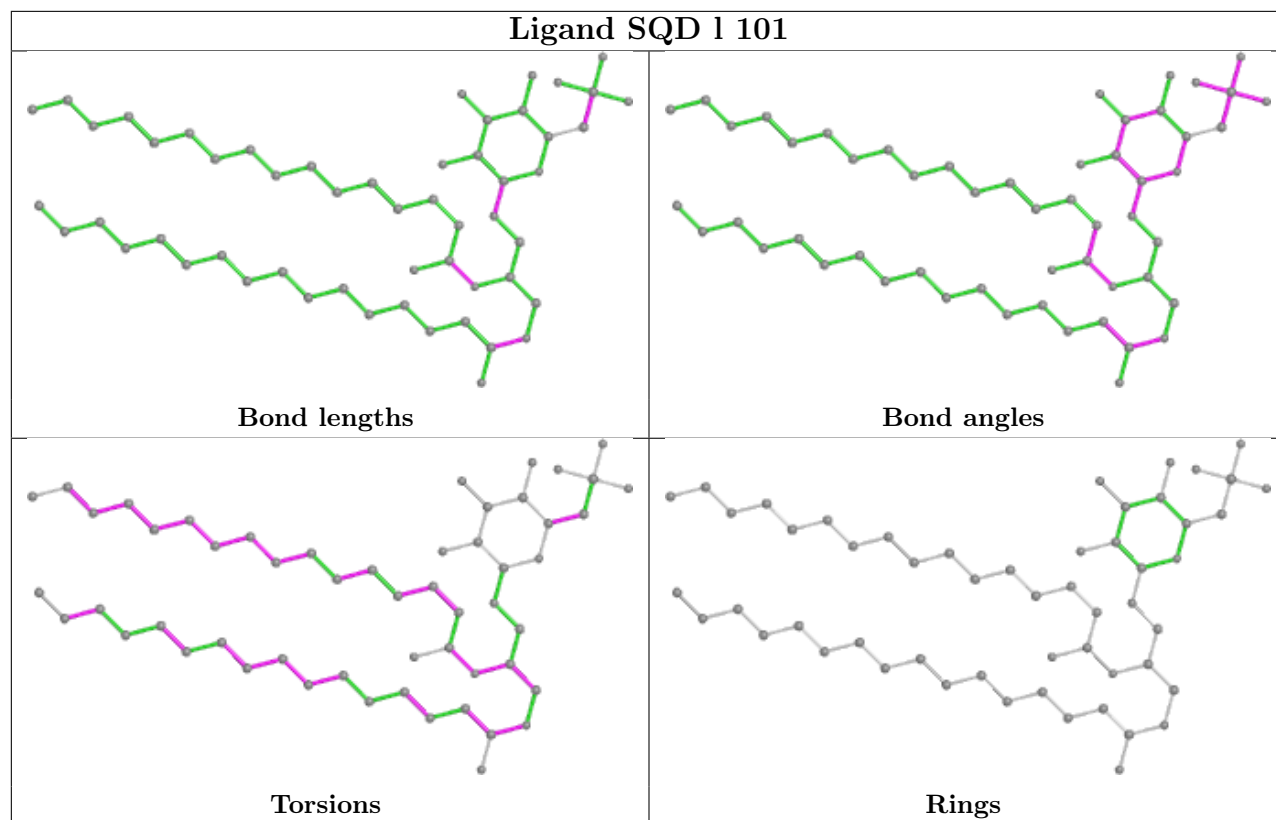


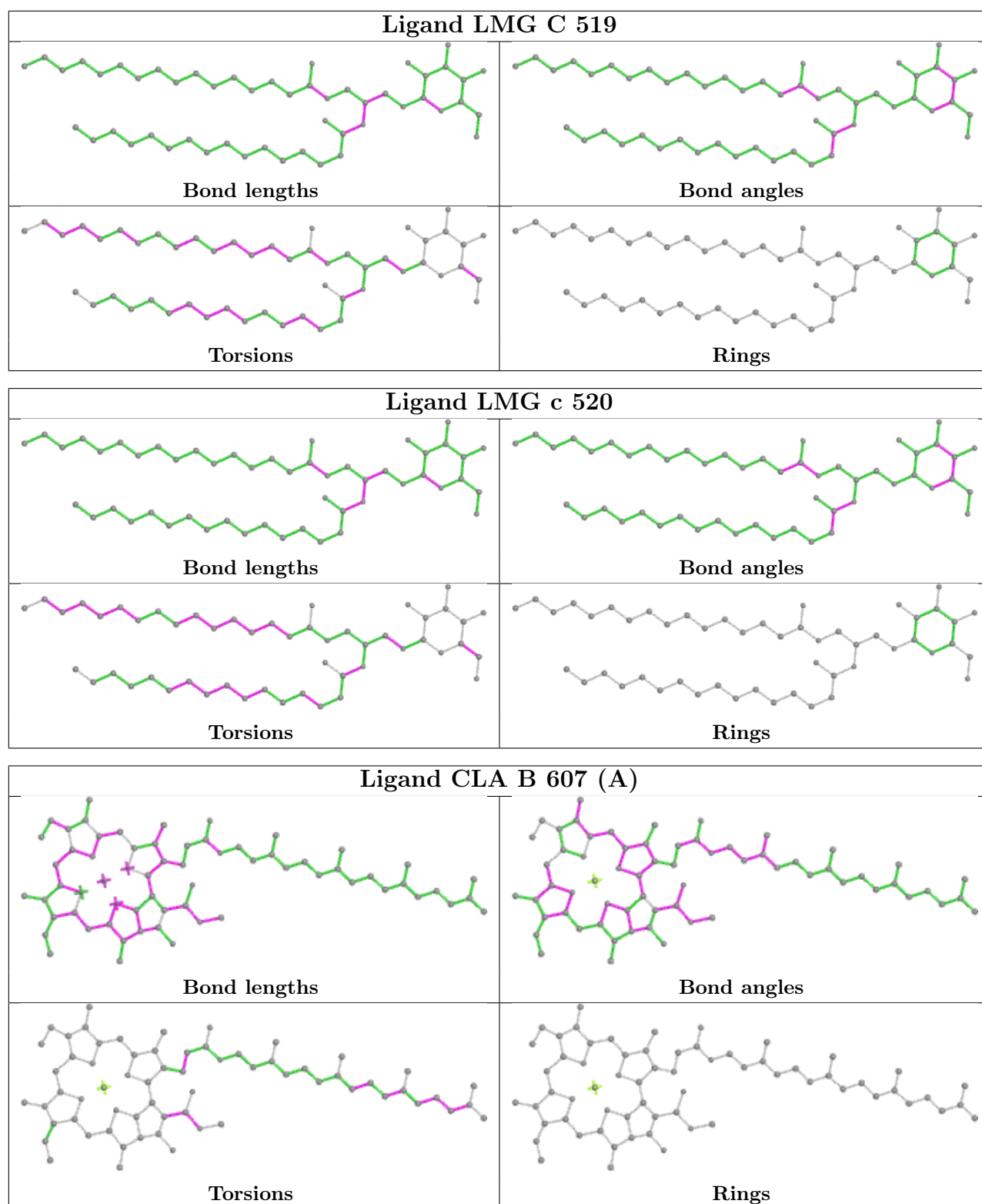


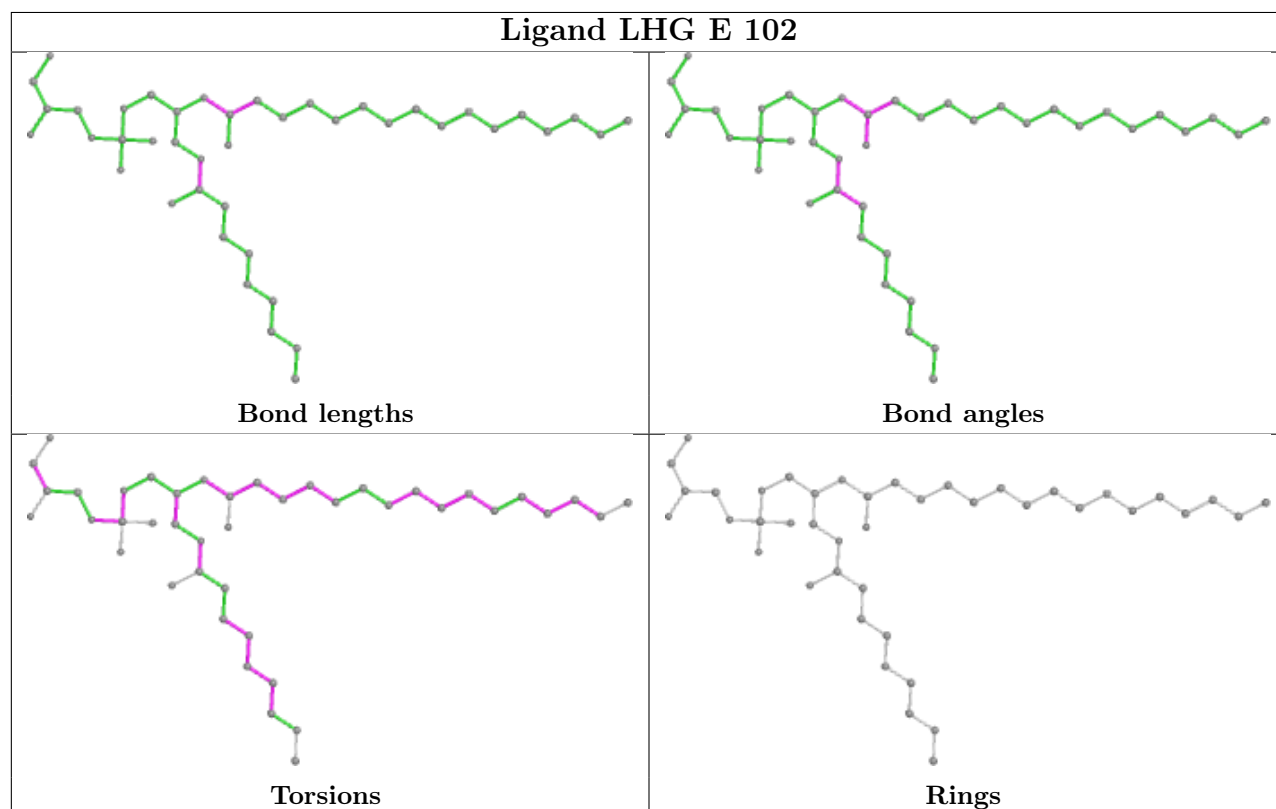
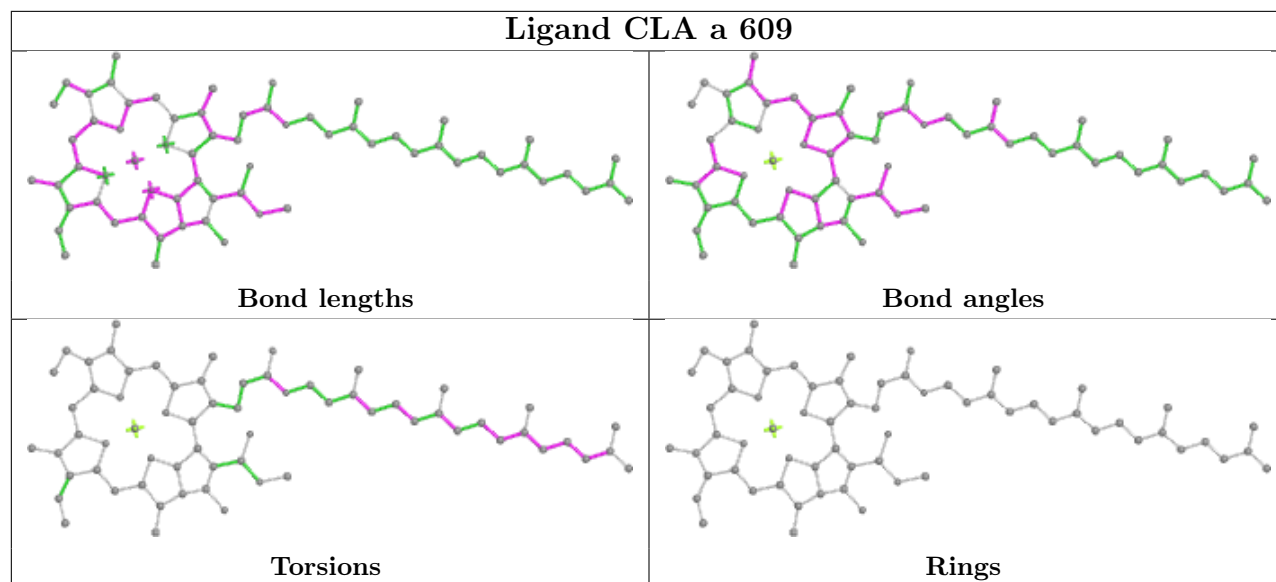


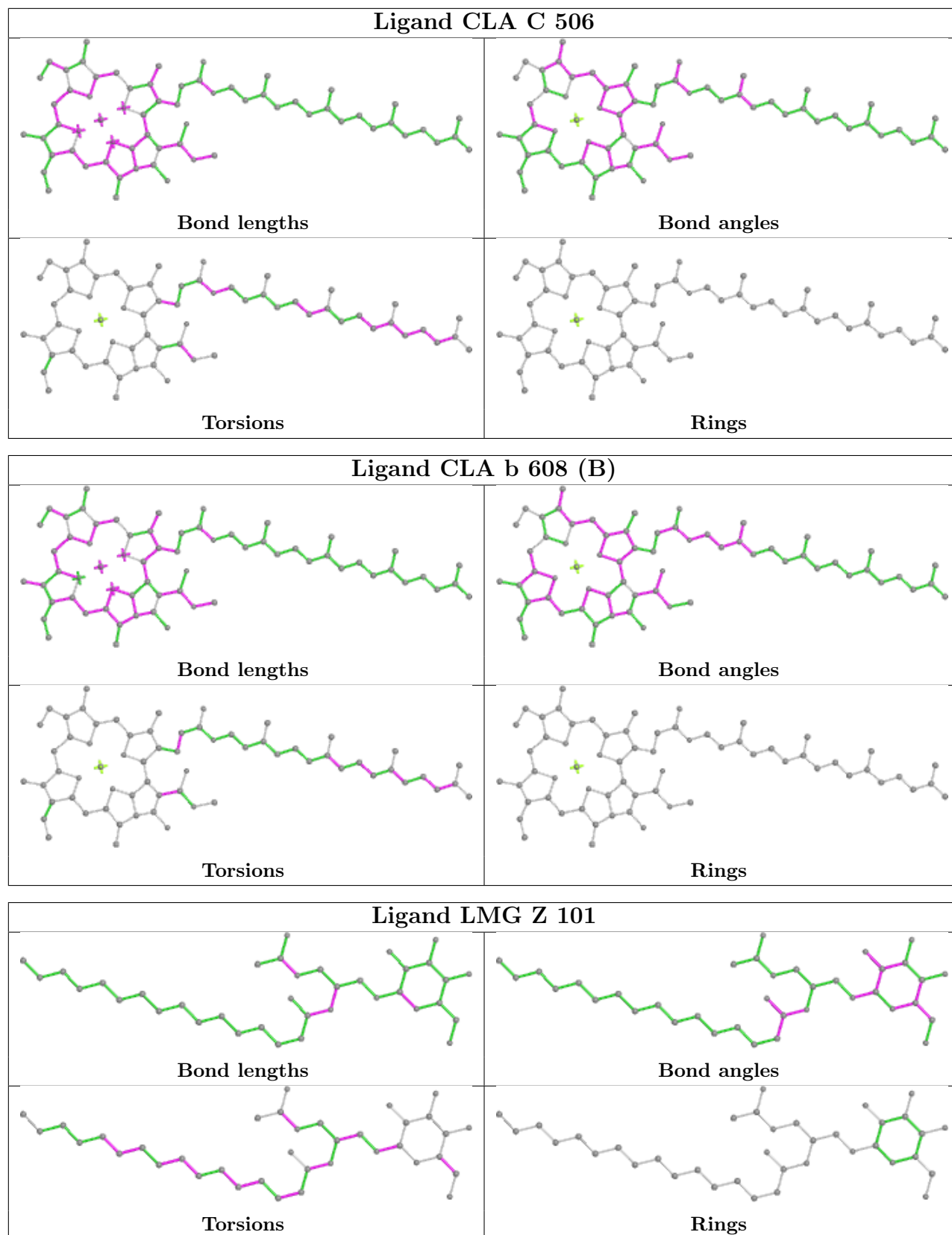


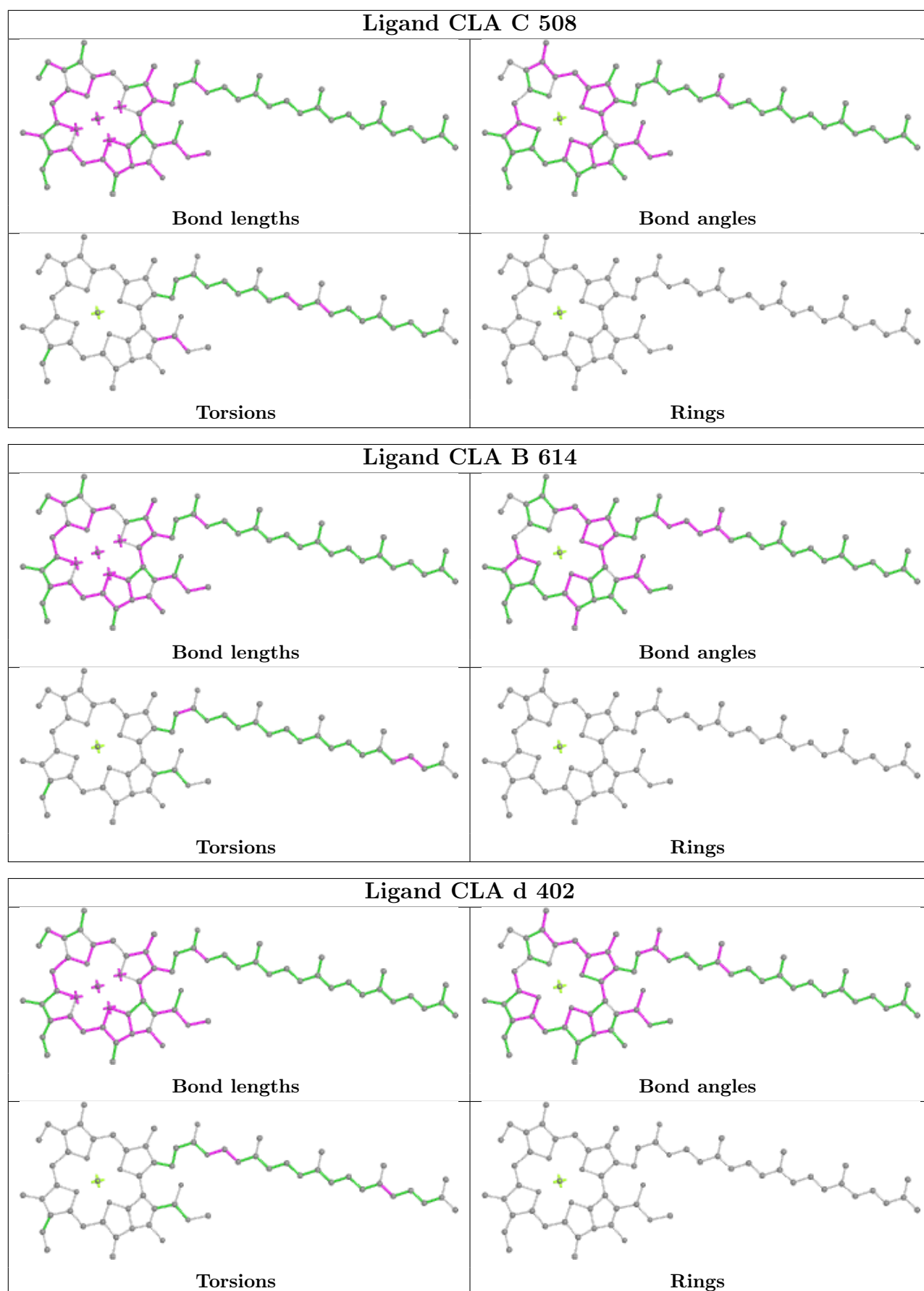


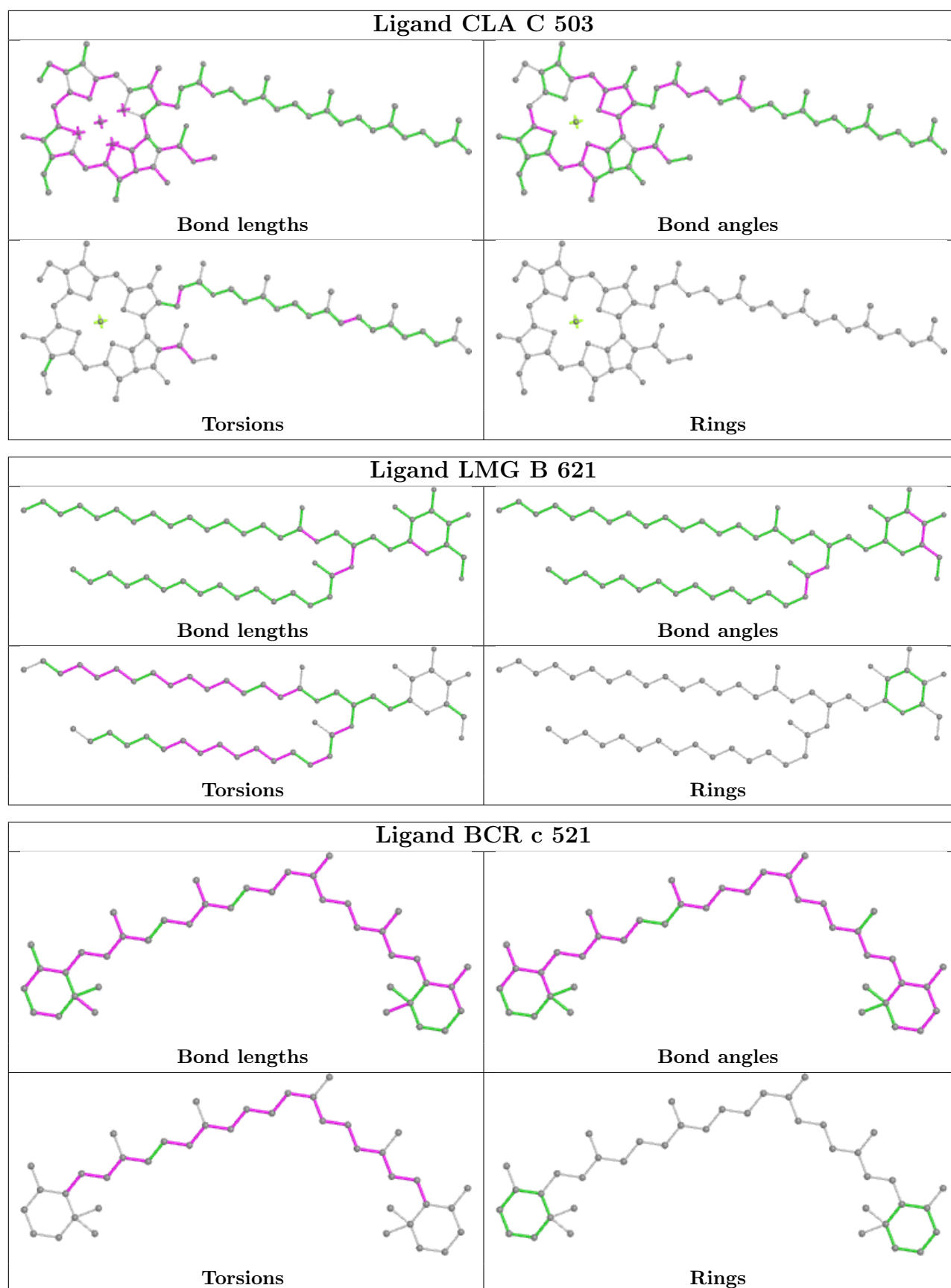


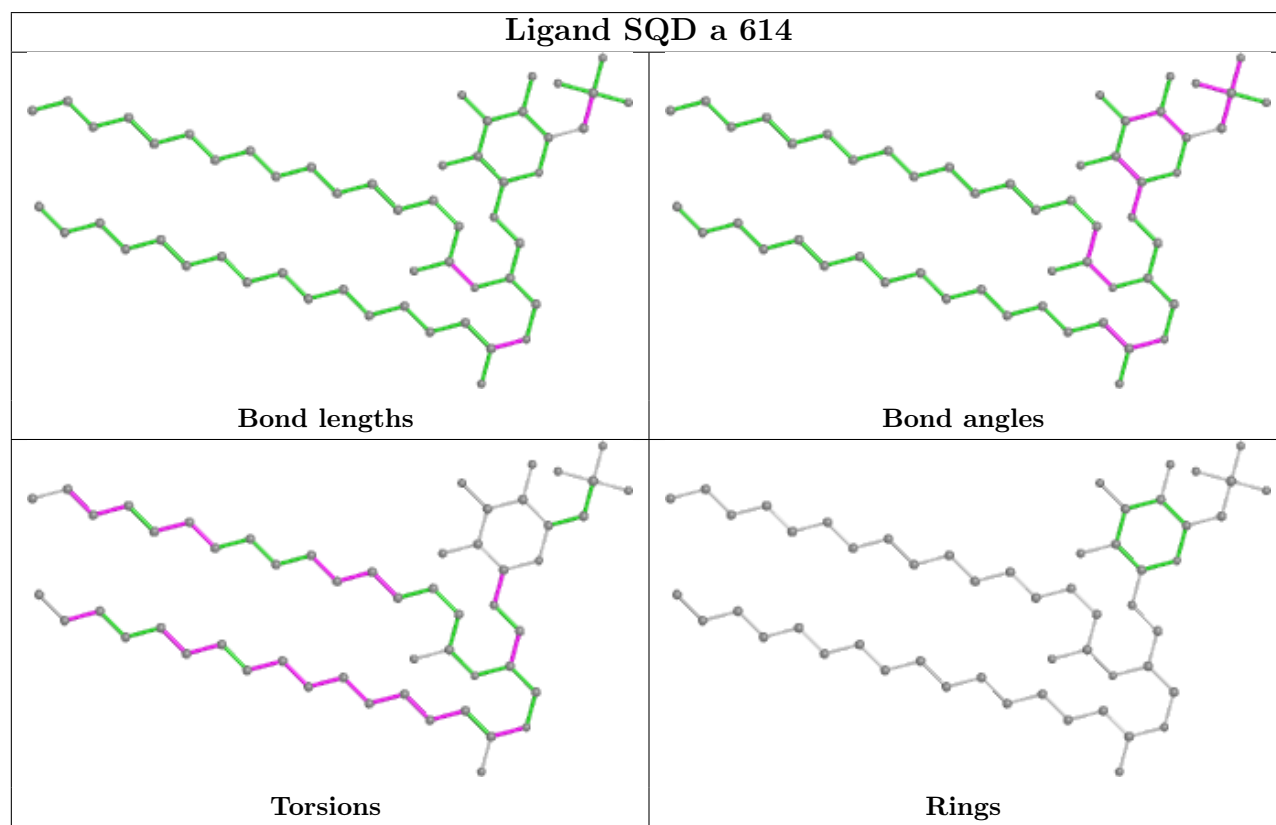
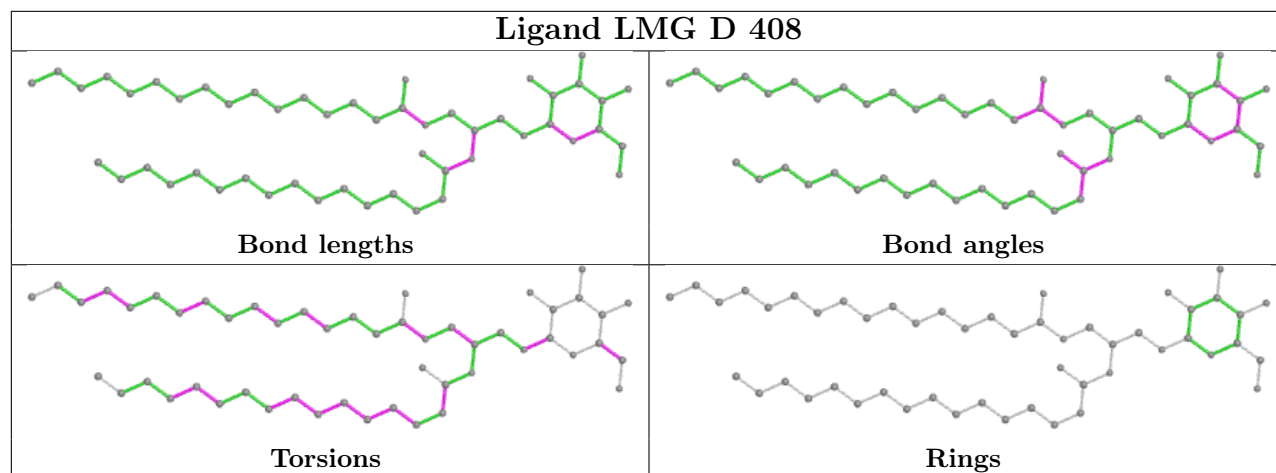
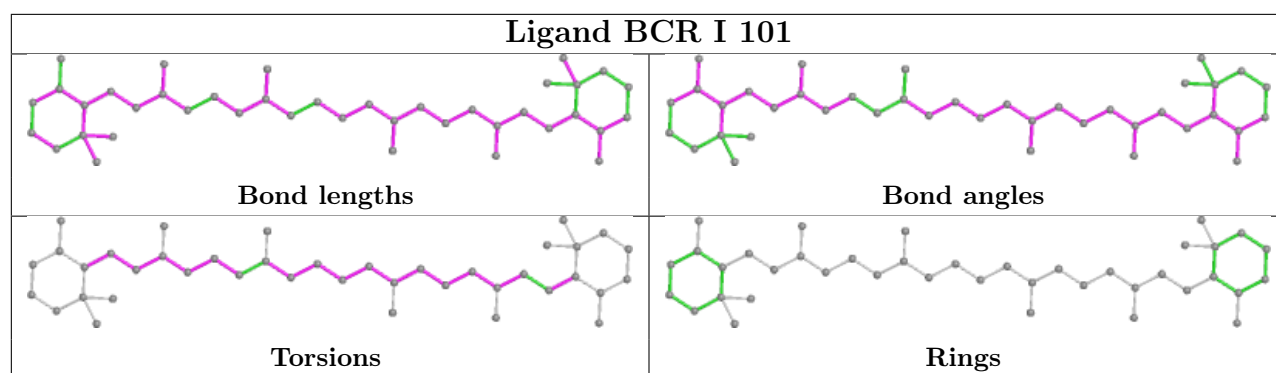


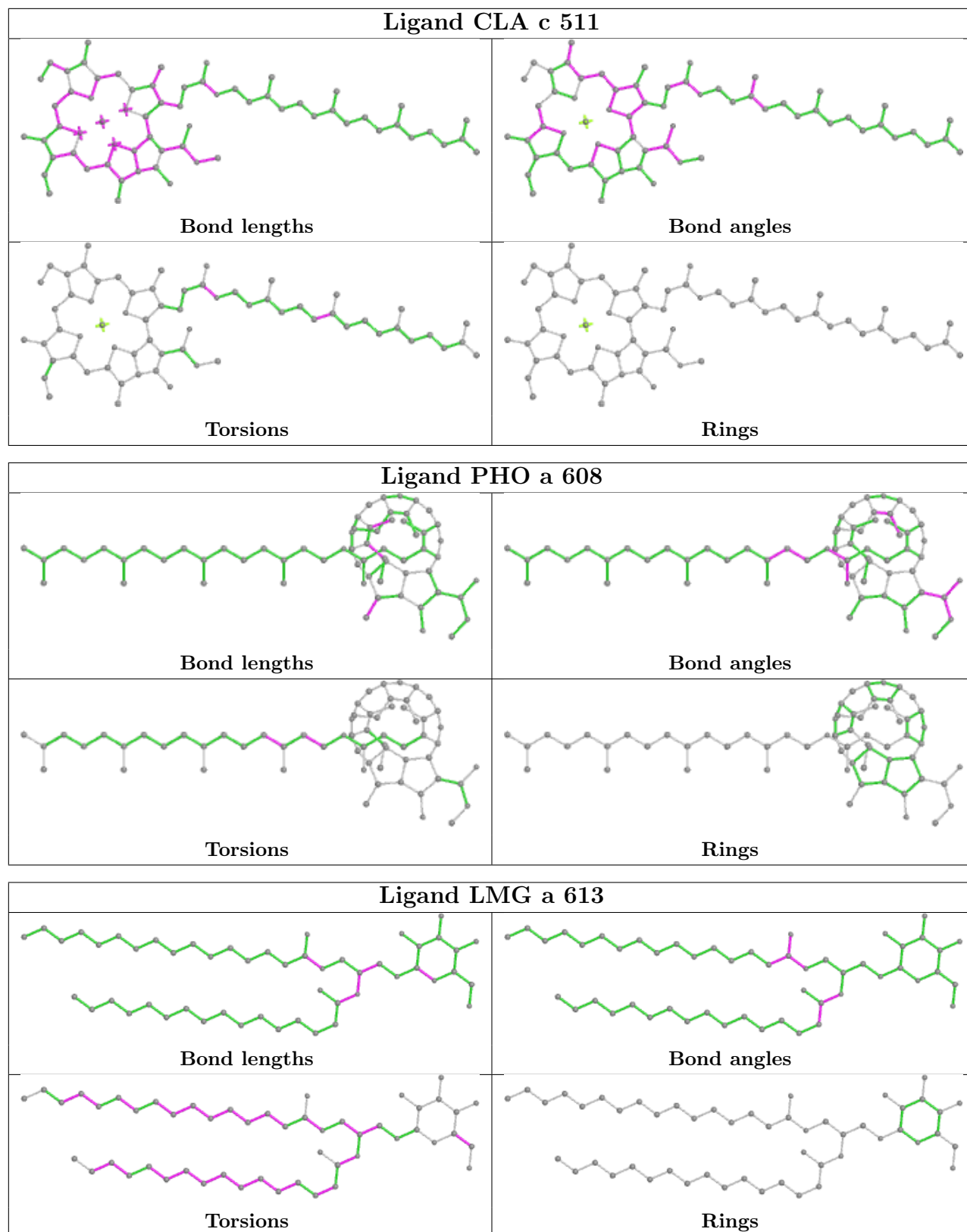


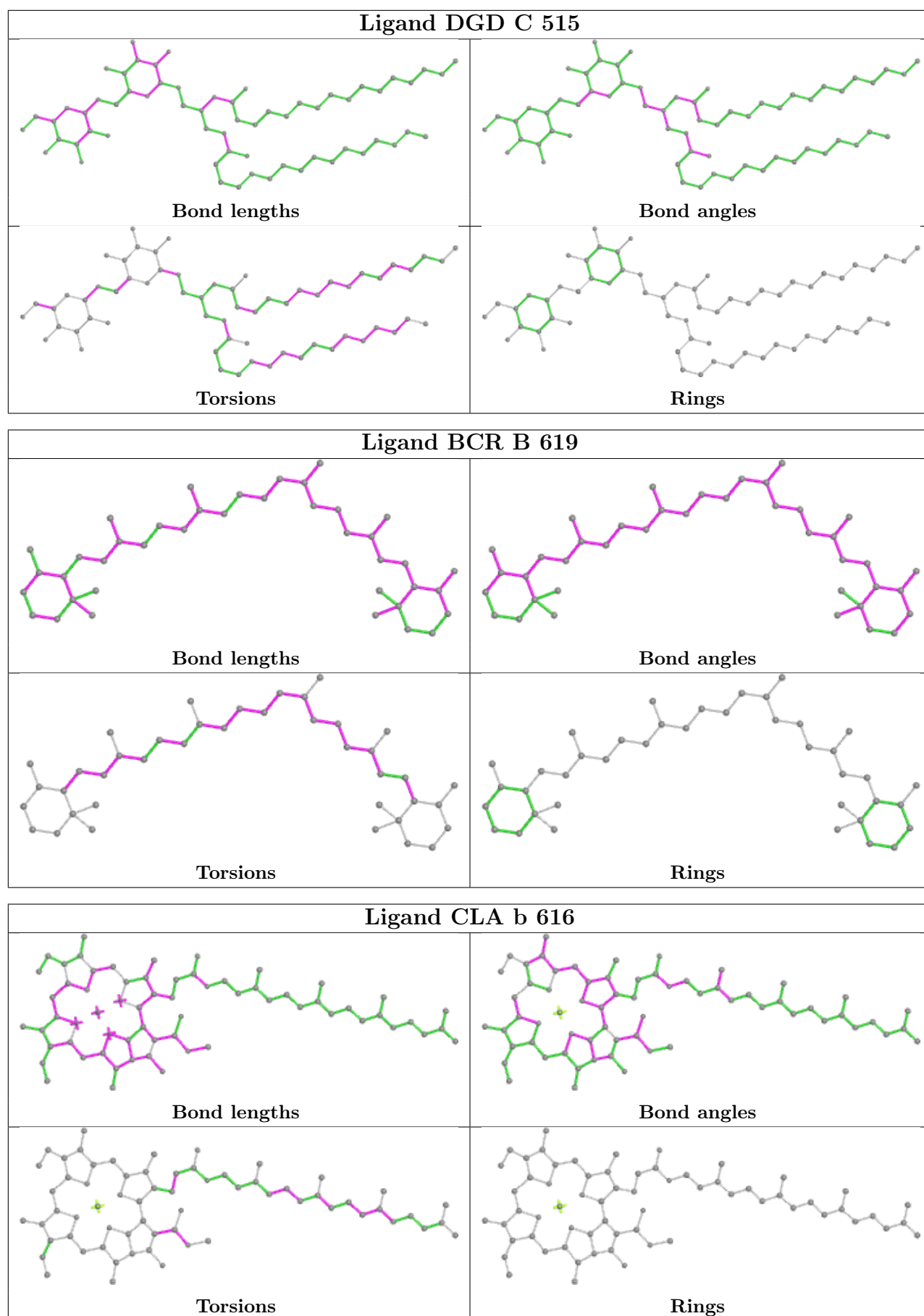


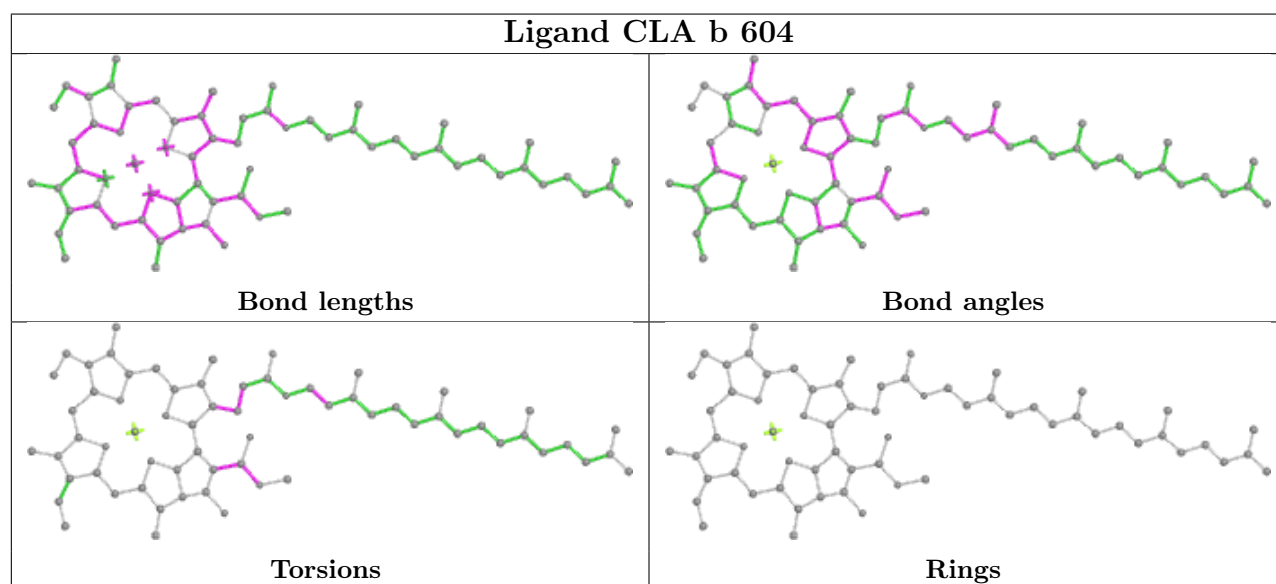
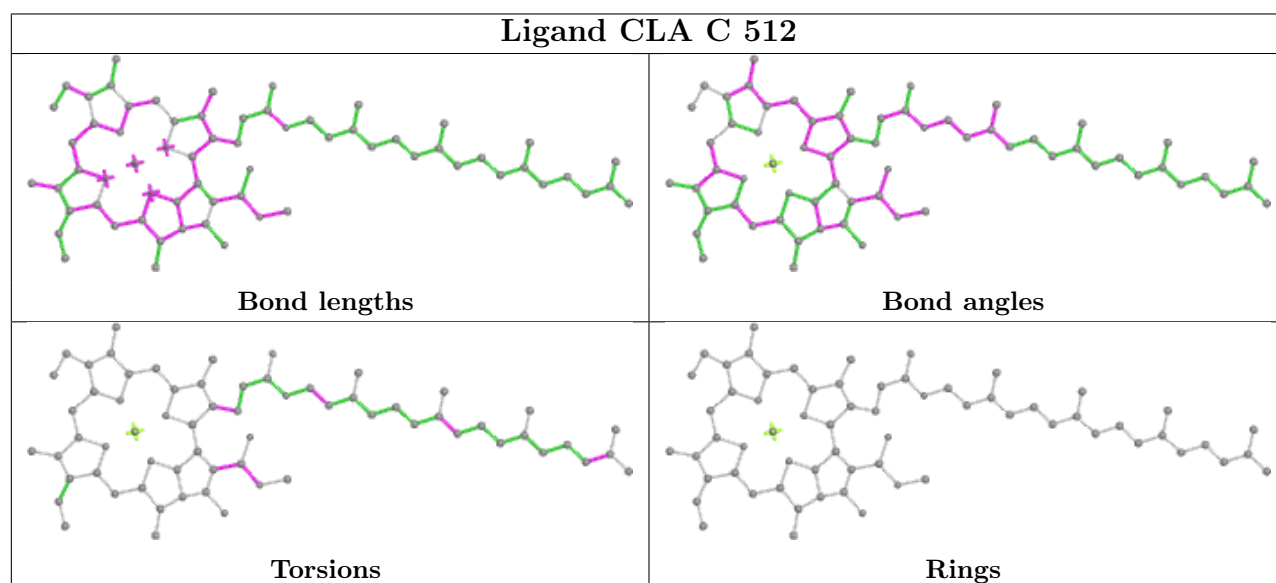
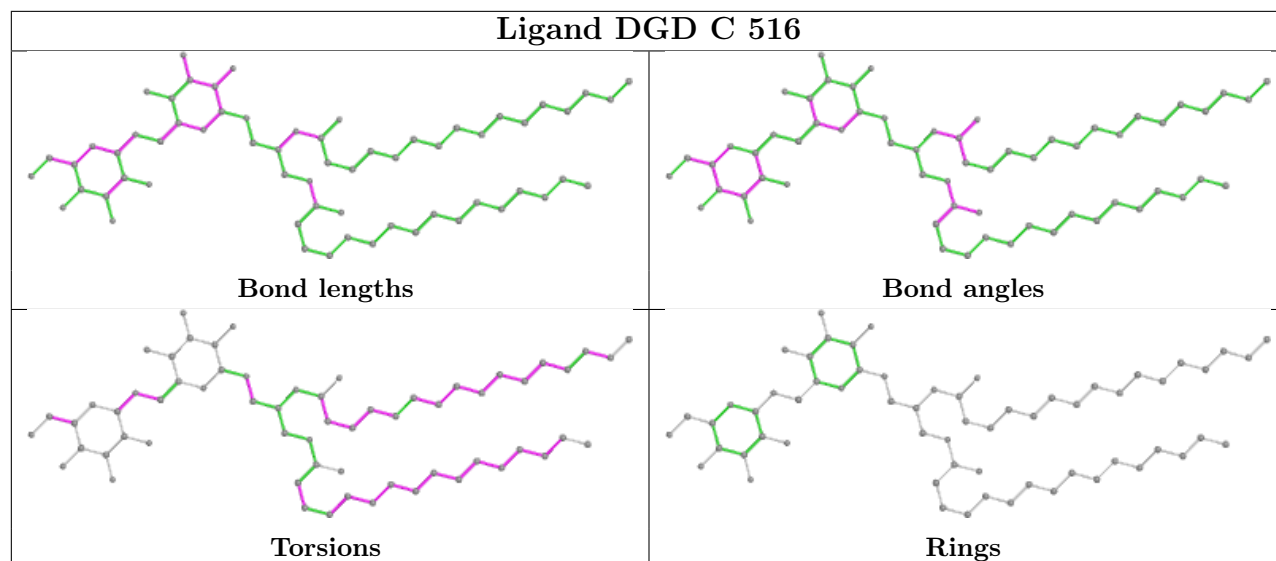


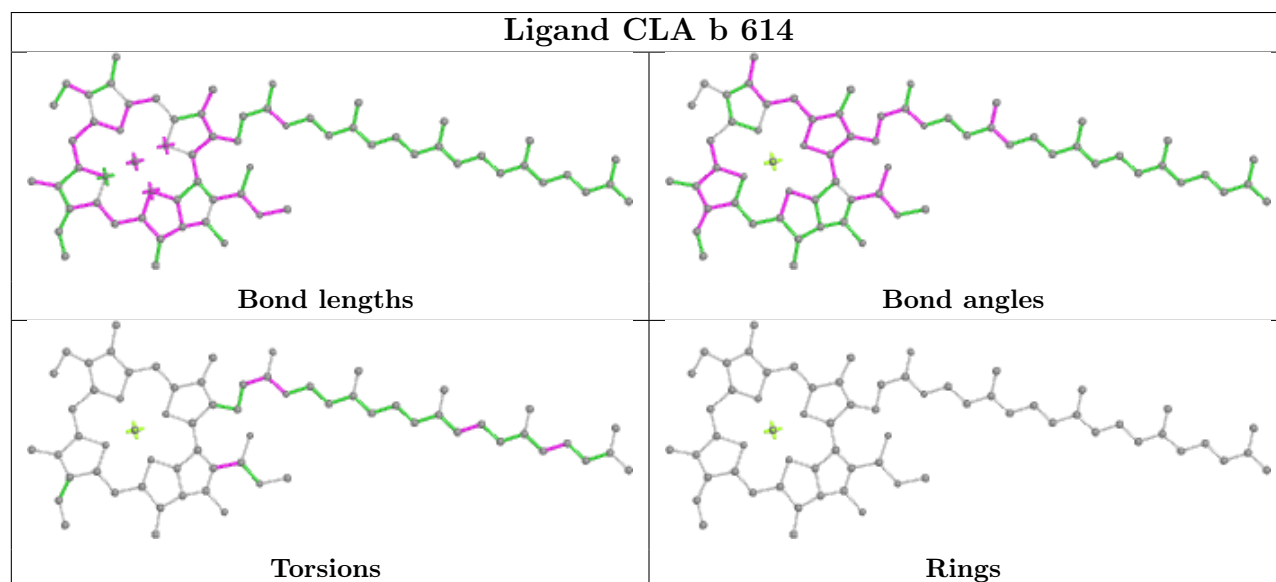
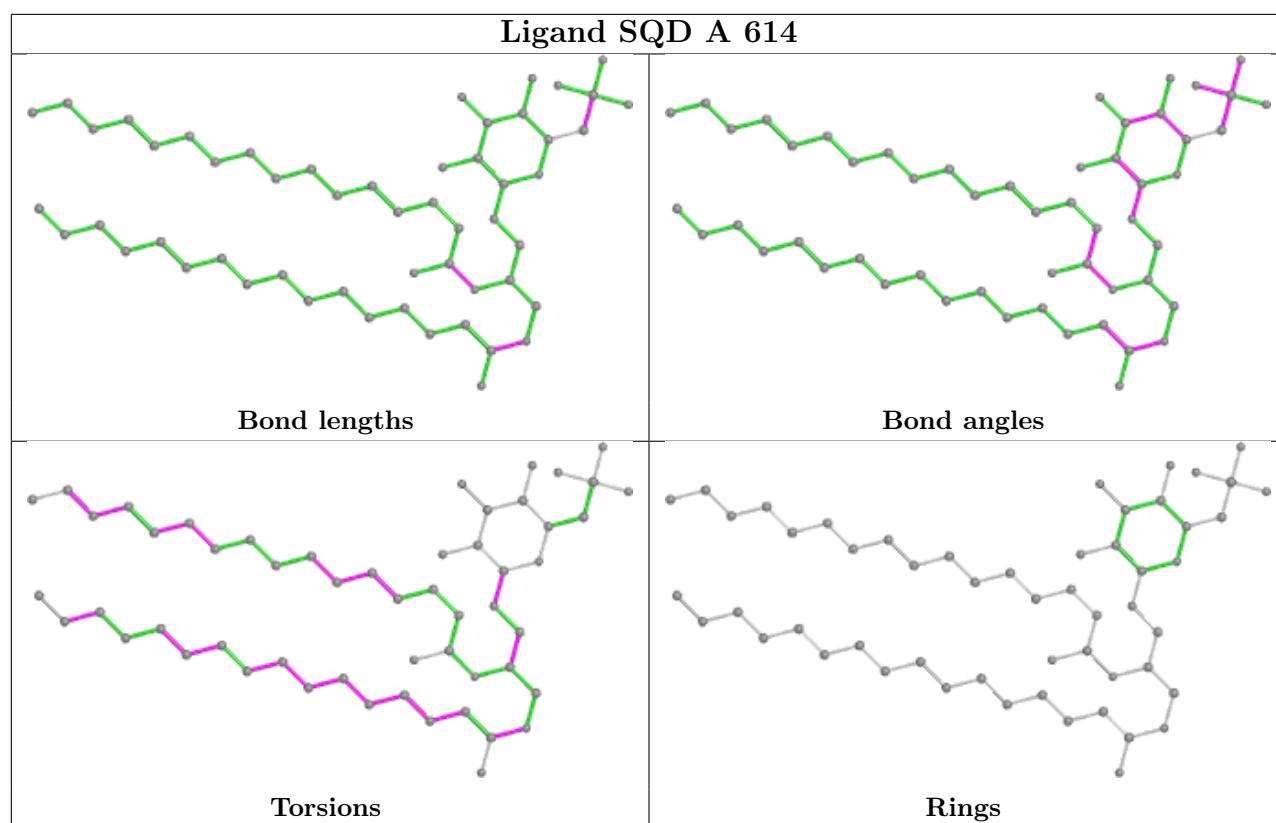


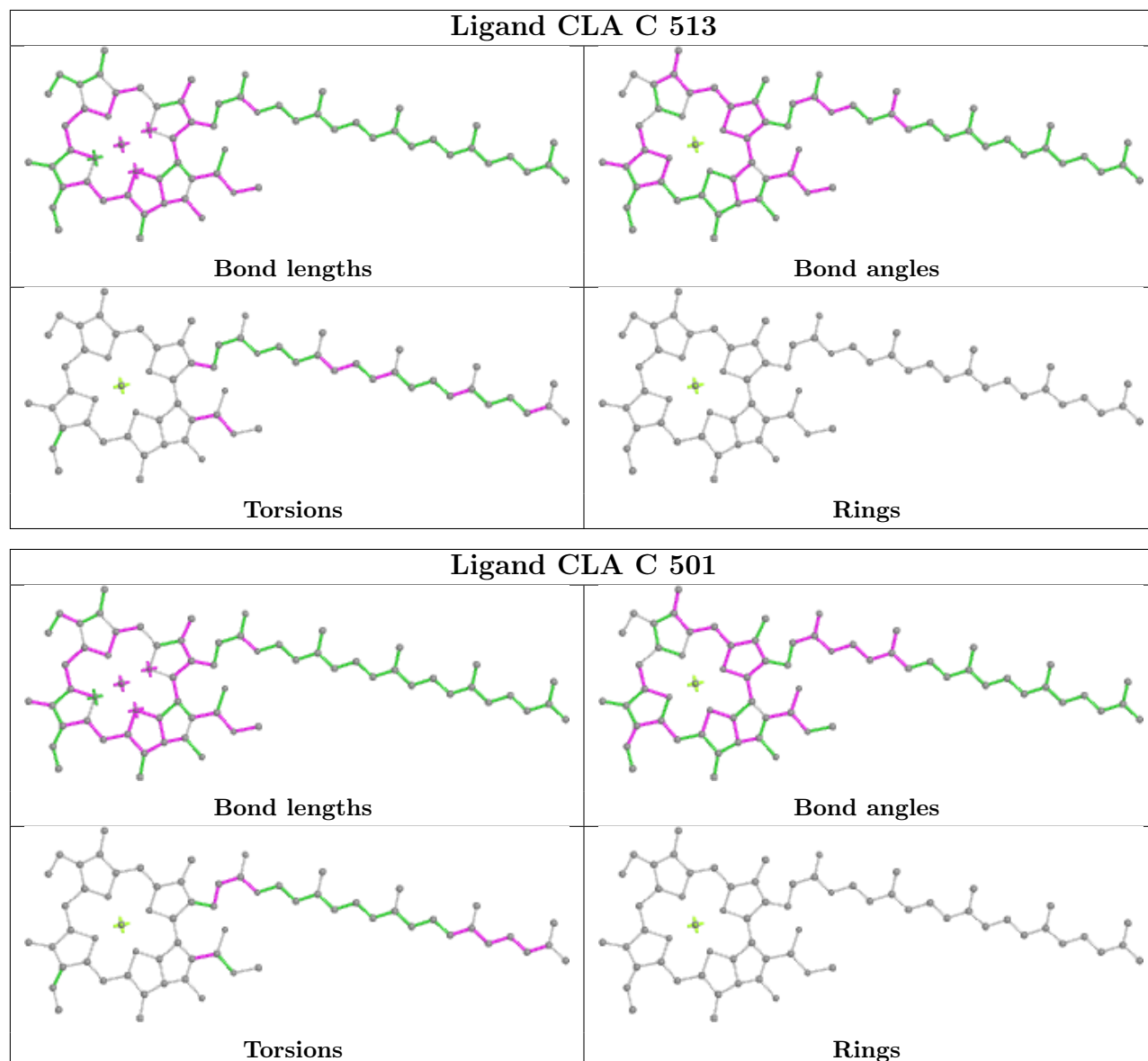


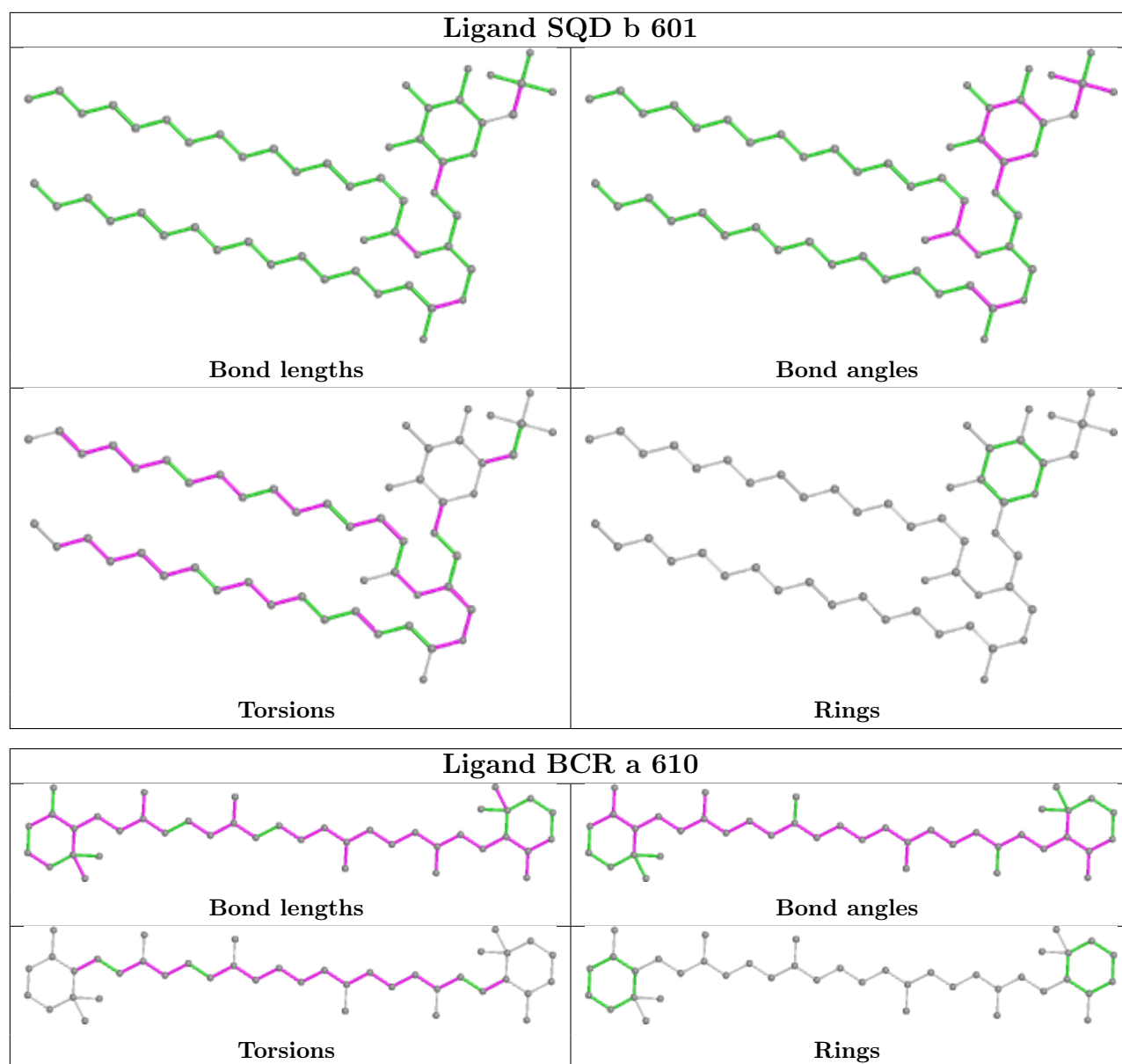












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

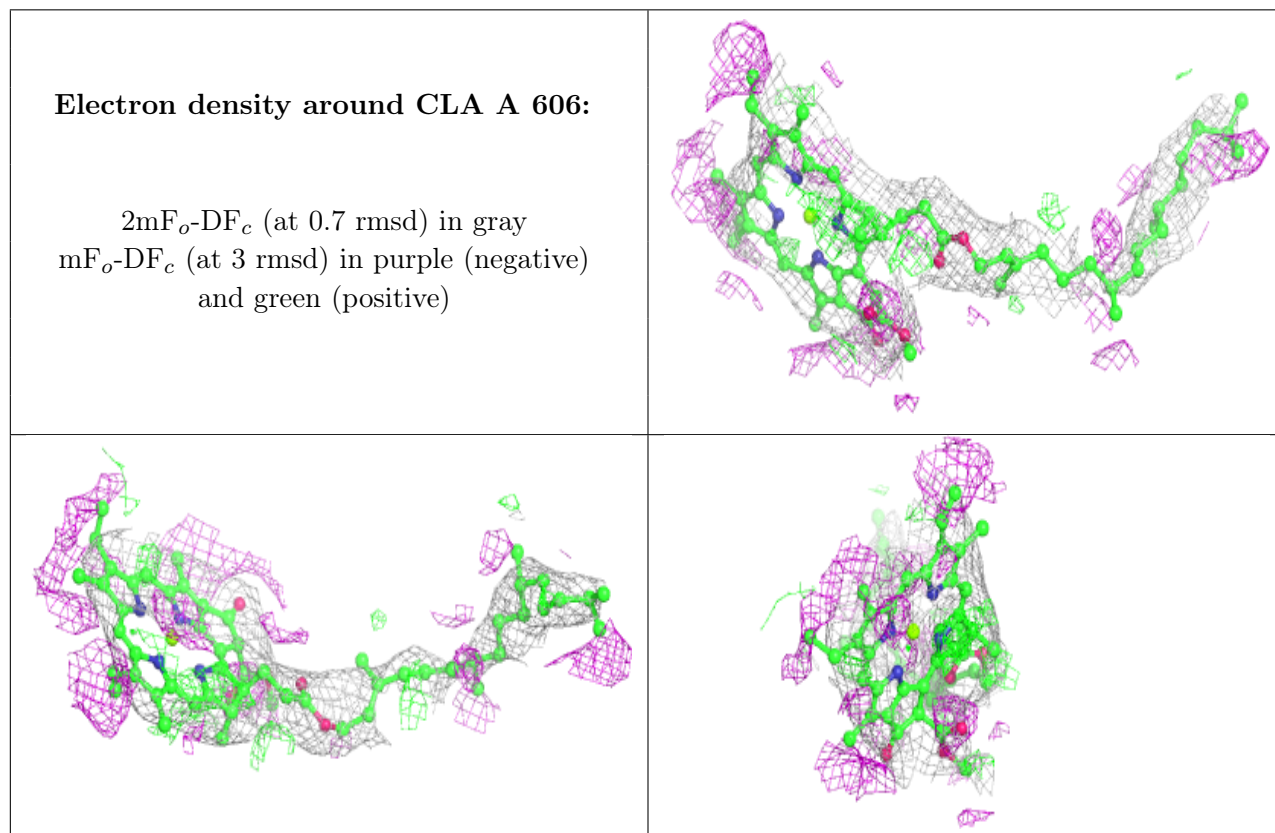
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

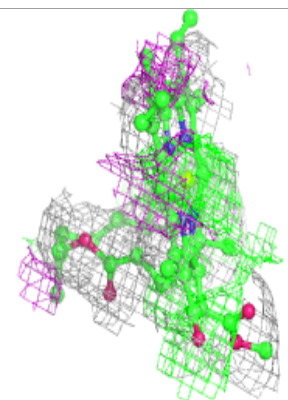
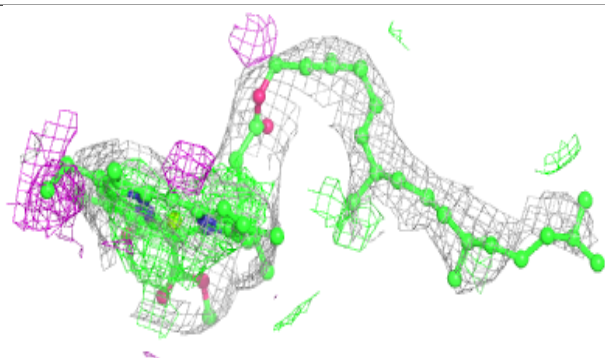
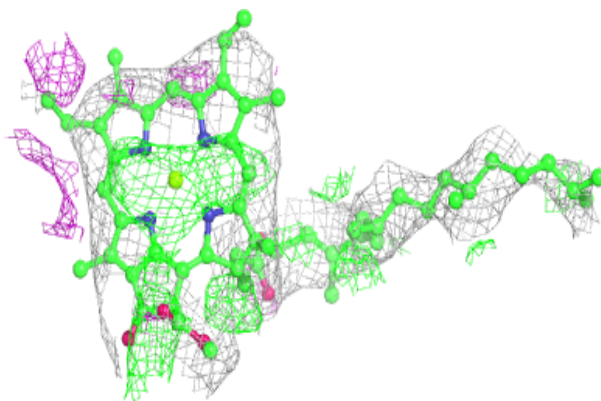
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

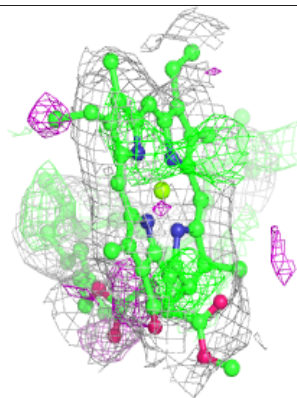
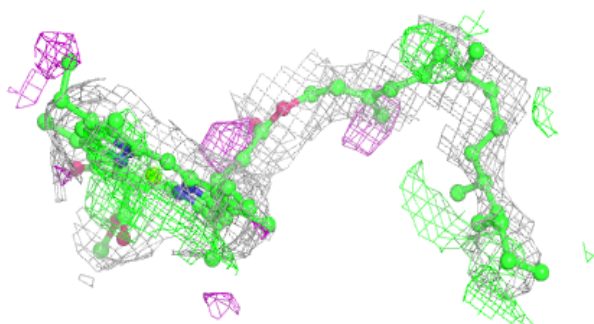
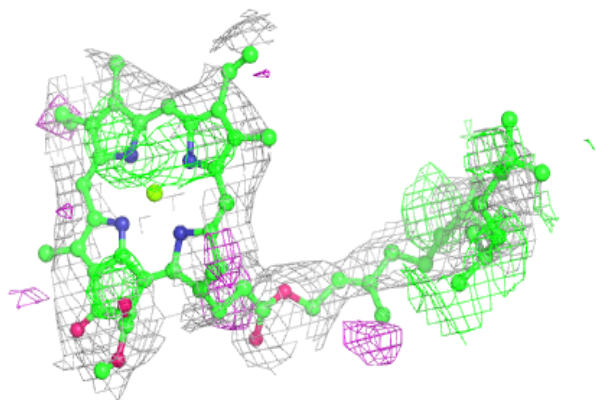


Electron density around CLA A 607:

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

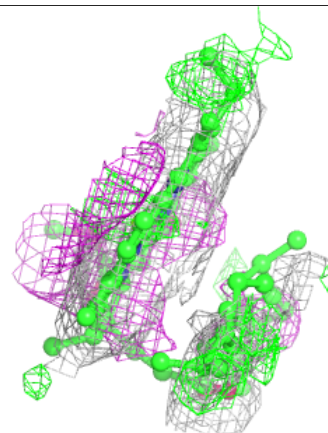
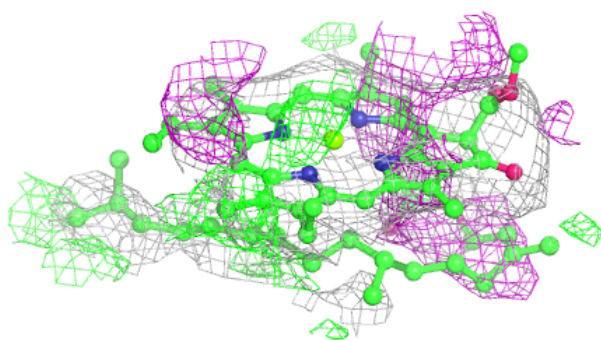
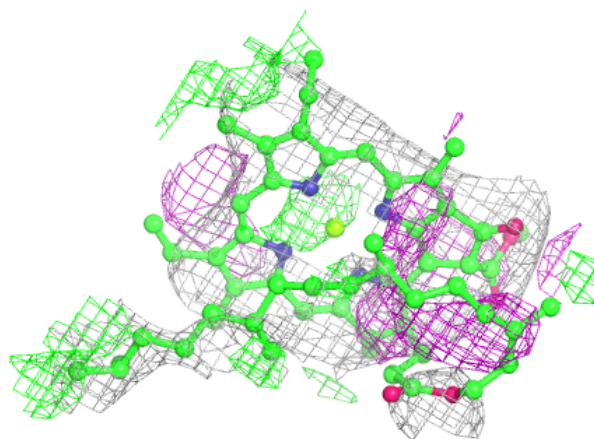
**Electron density around CLA A 609:**

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

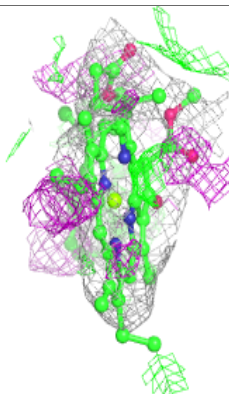
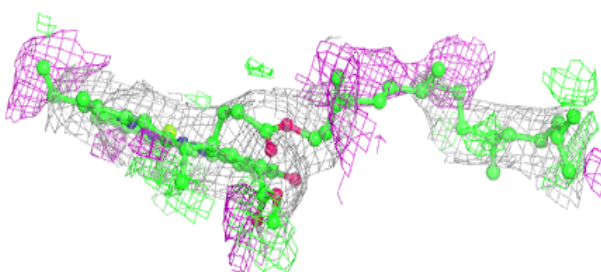
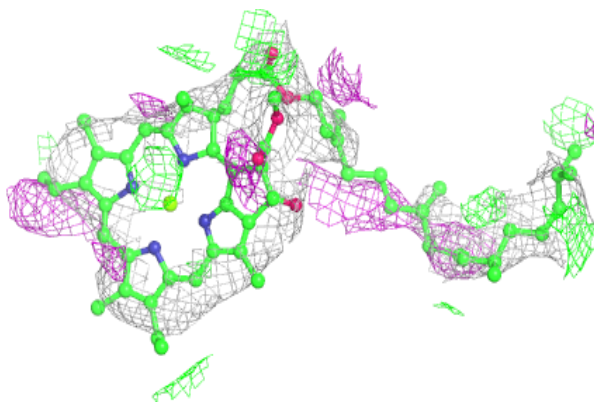


Electron density around CLA B 602:

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

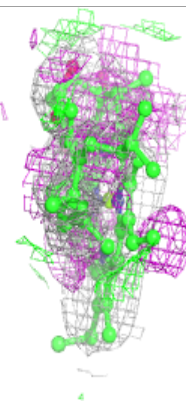
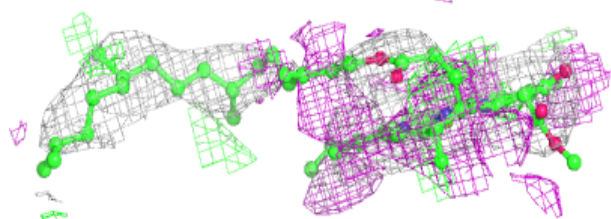
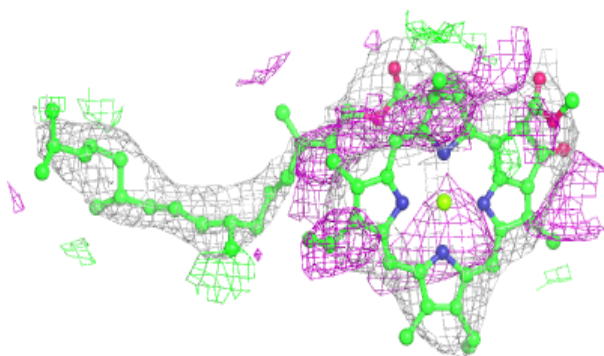
**Electron density around CLA B 603:**

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

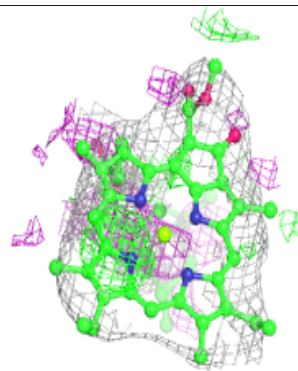
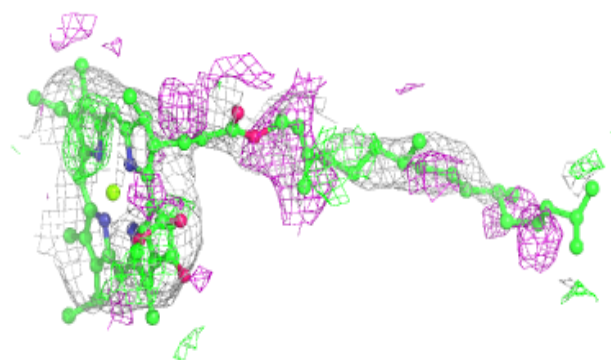
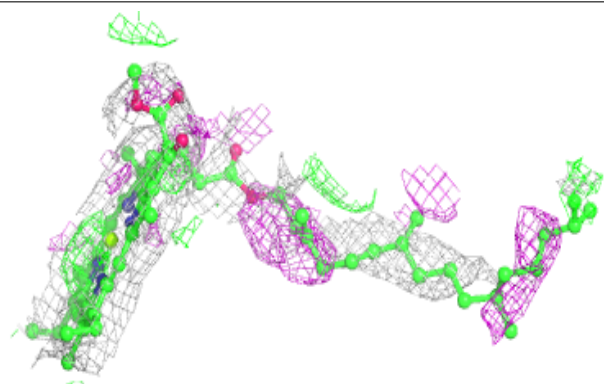


Electron density around CLA B 604:

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

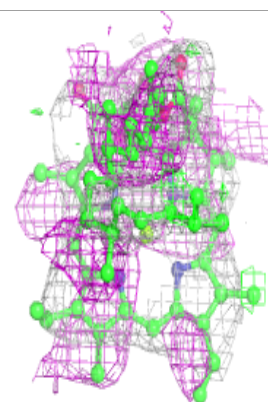
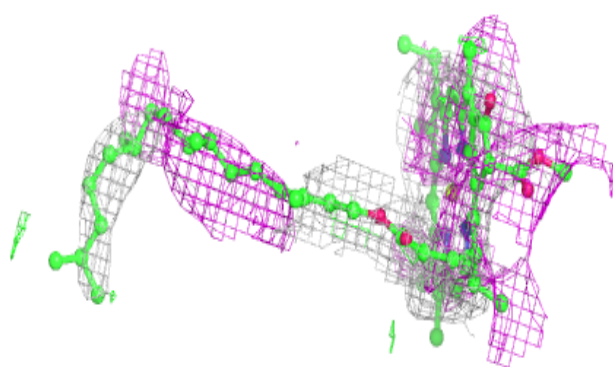
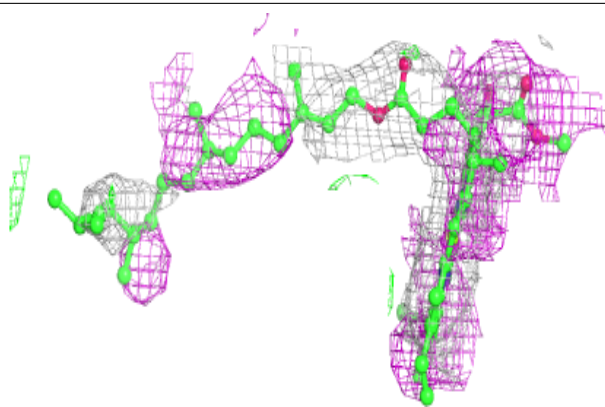
**Electron density around CLA B 605:**

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

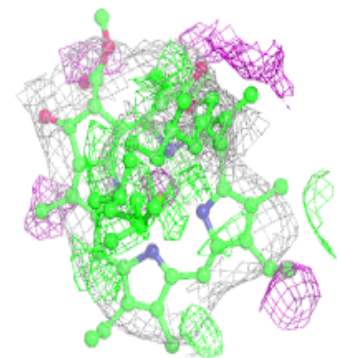
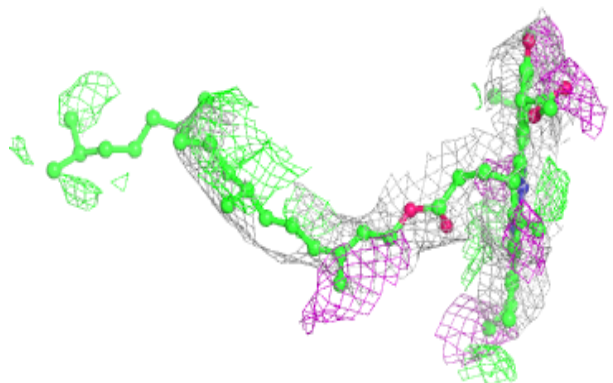
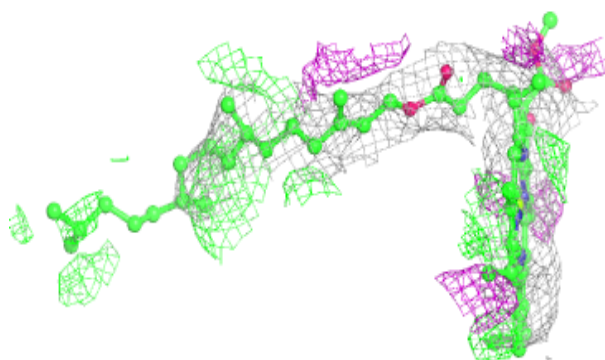


Electron density around CLA B 606:

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

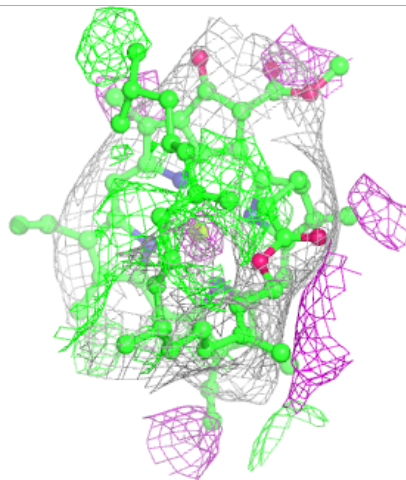
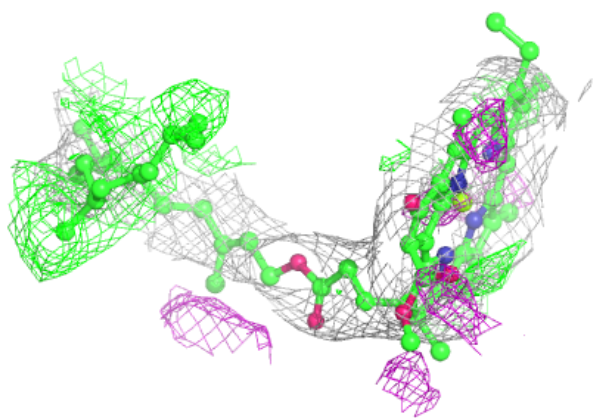
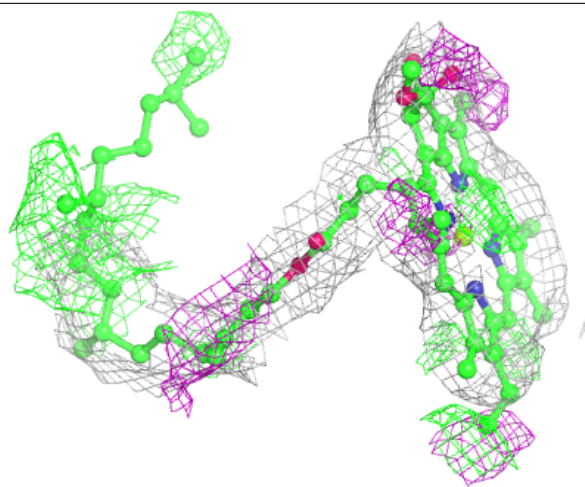
**Electron density around CLA B 607 (A):**

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



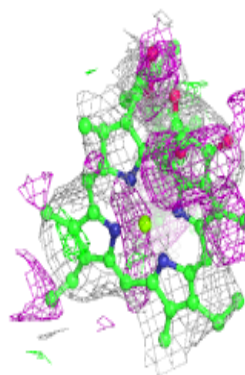
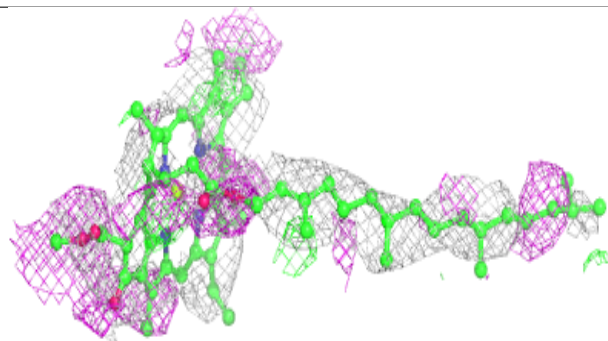
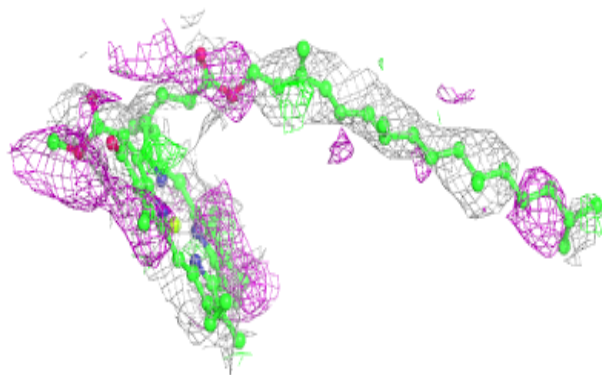
Electron density around CLA B 607 (B):

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

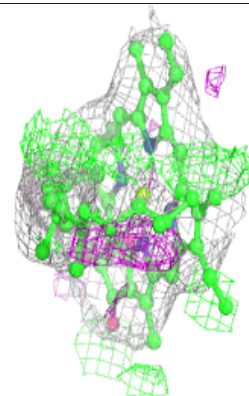
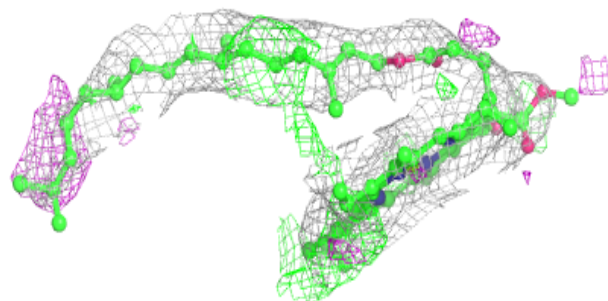
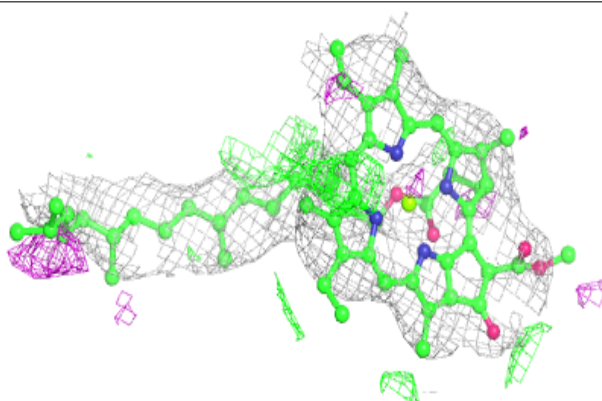


Electron density around CLA B 608:

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

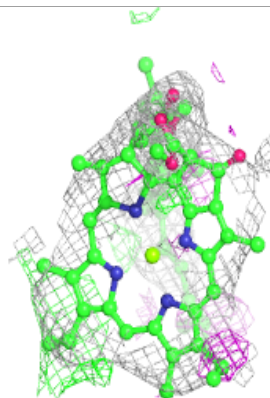
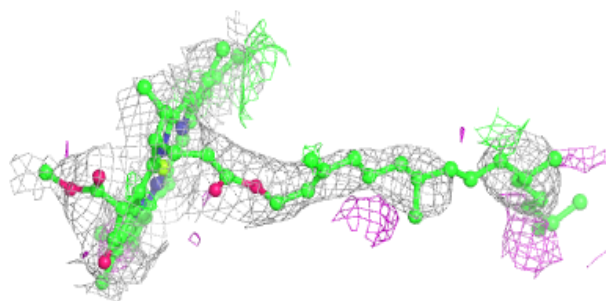
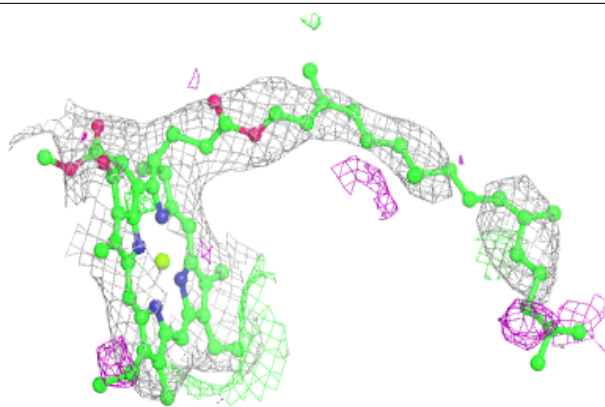
**Electron density around CLA B 609:**

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

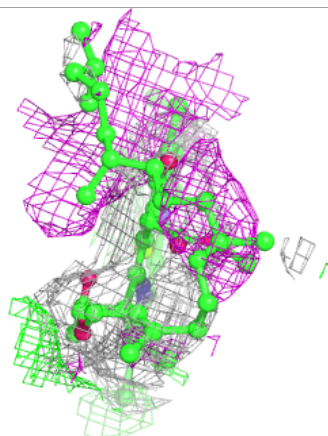
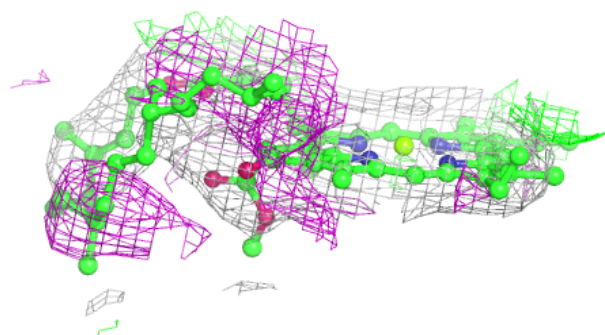
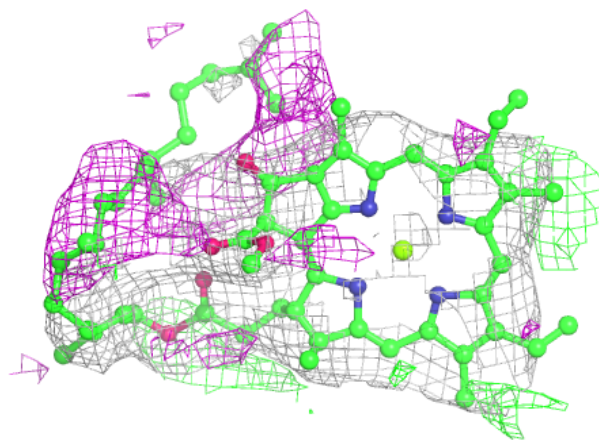


Electron density around CLA B 610:

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

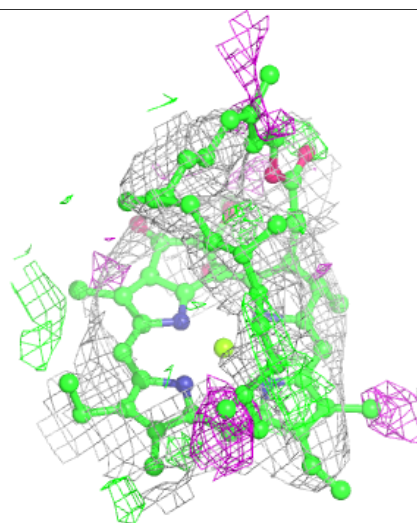
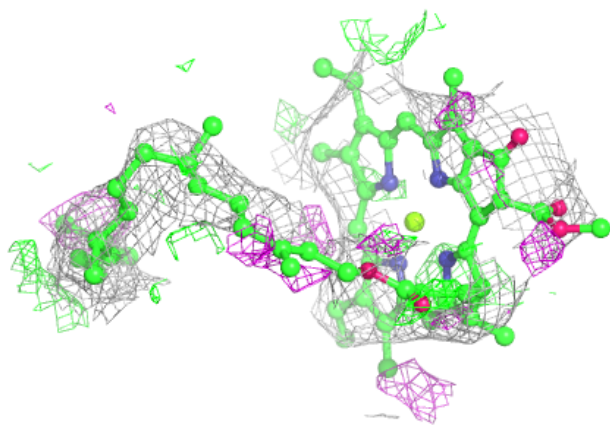
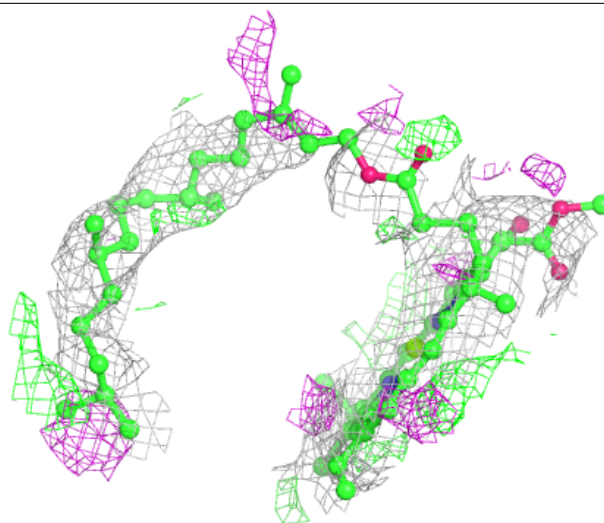
**Electron density around CLA B 611:**

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



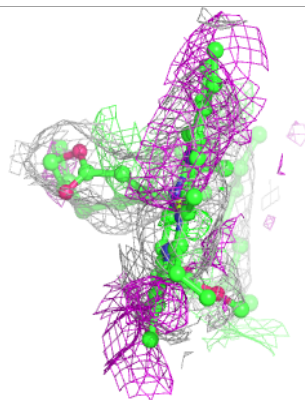
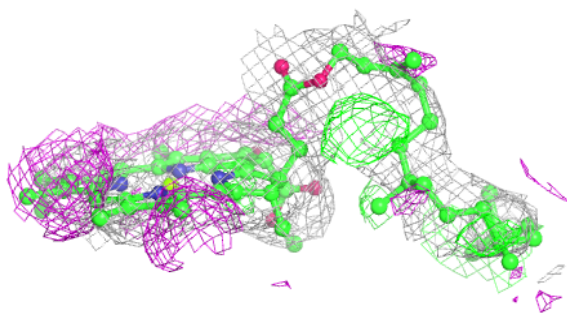
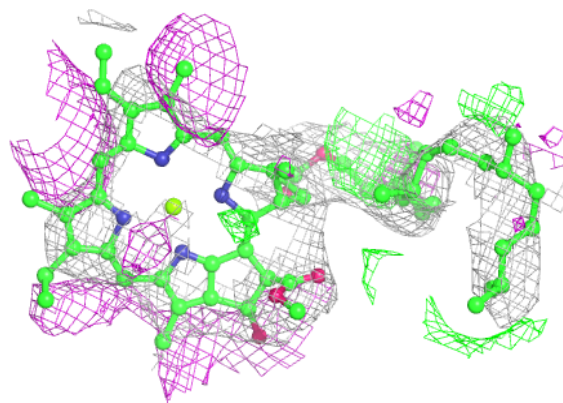
Electron density around CLA B 612:

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



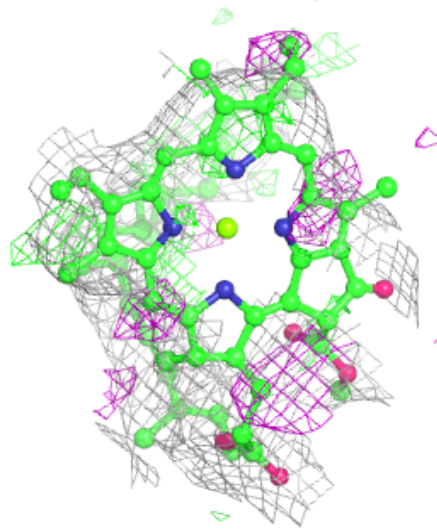
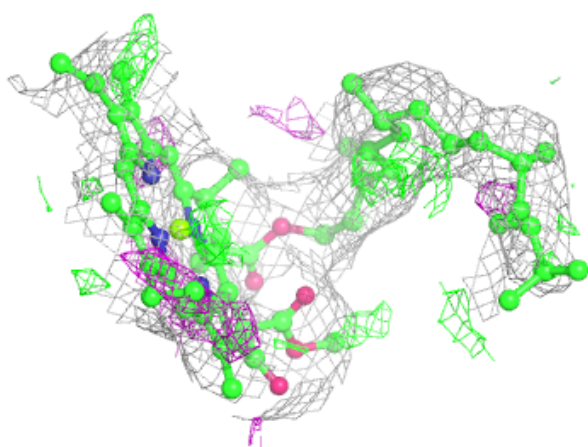
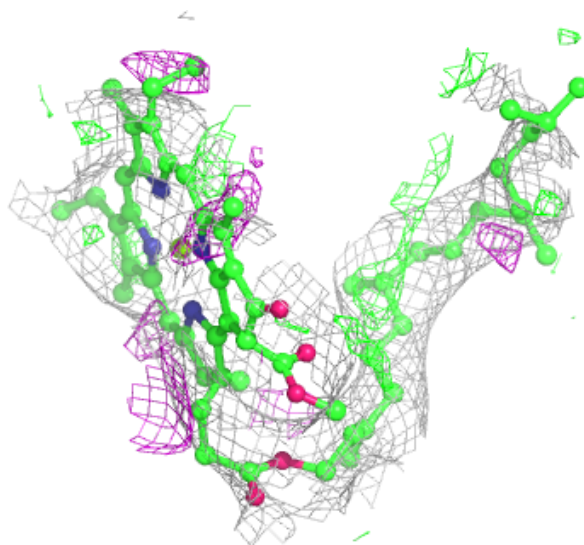
Electron density around CLA B 613:

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



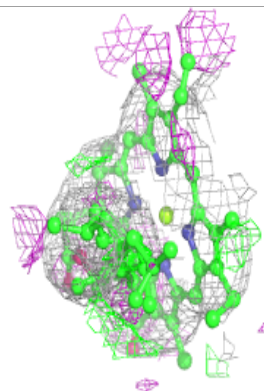
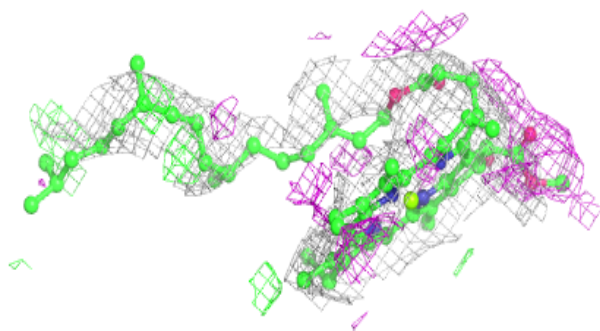
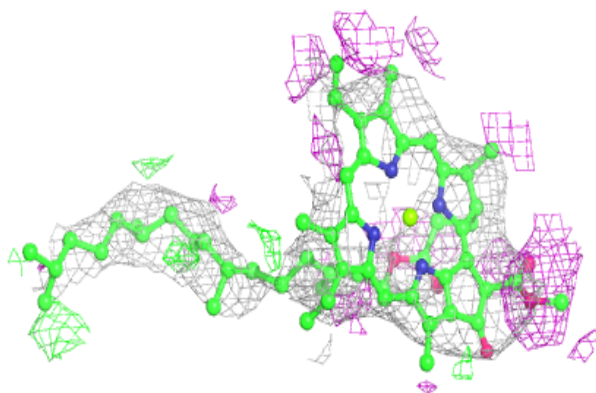
Electron density around CLA B 614:

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

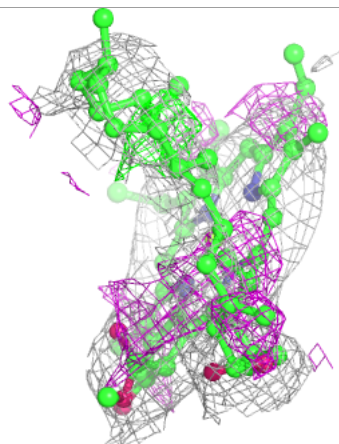
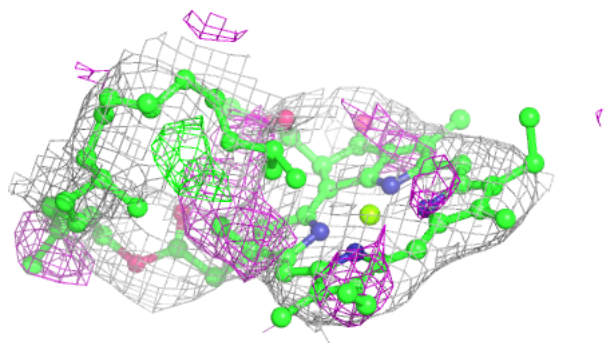
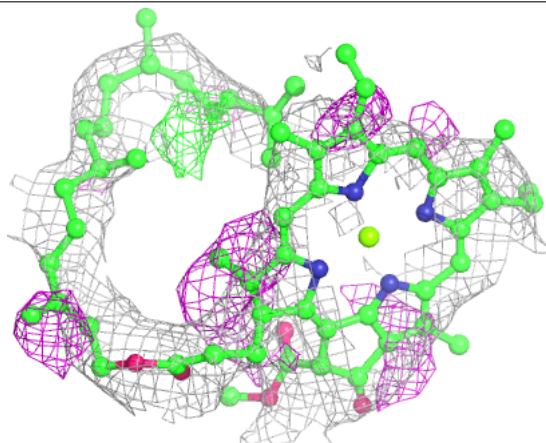


Electron density around CLA B 615:

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

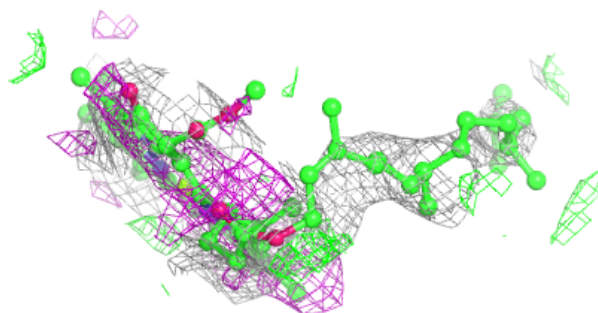
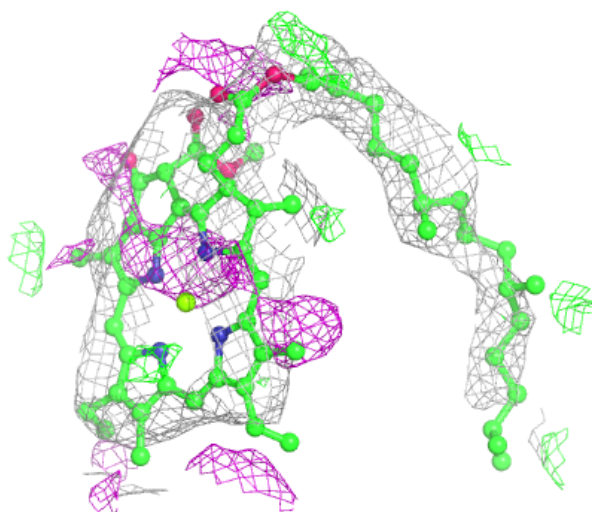
**Electron density around CLA B 616:**

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



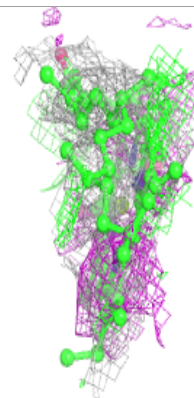
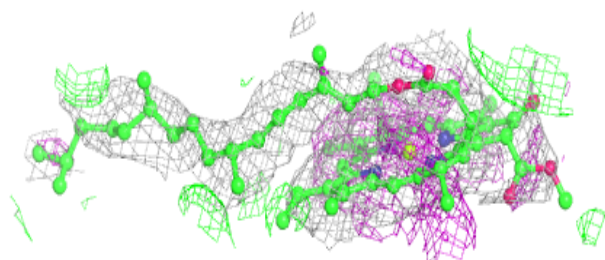
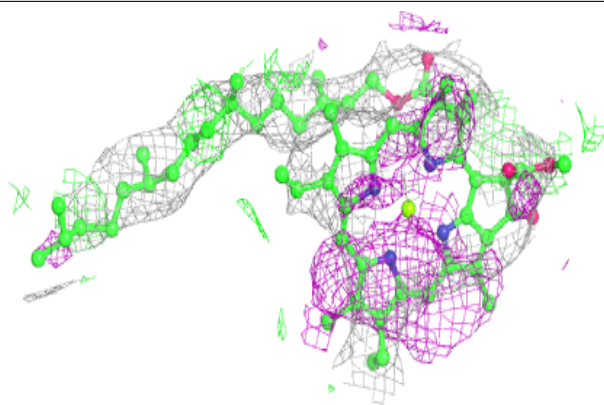
Electron density around CLA B 617:

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

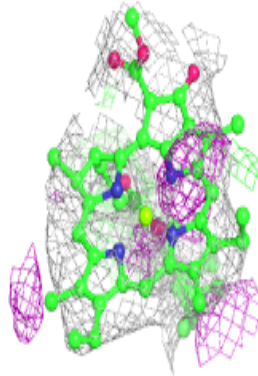
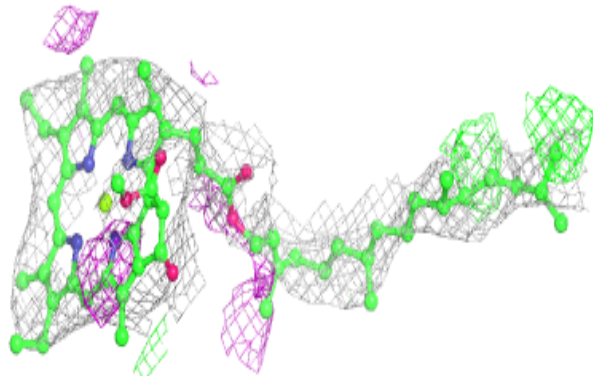
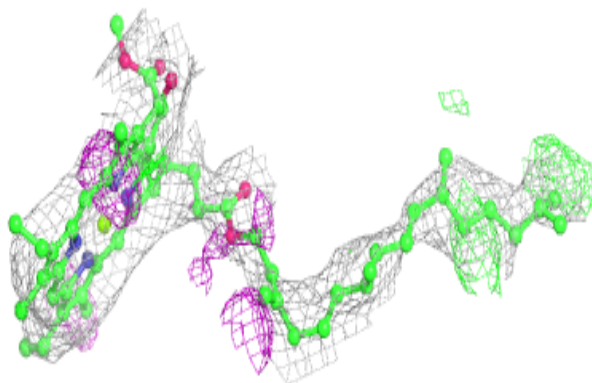


Electron density around CLA C 501:

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

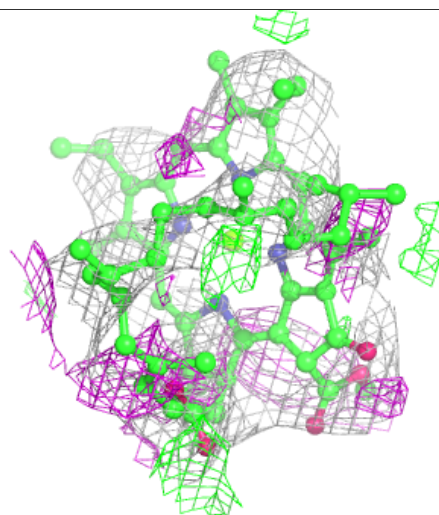
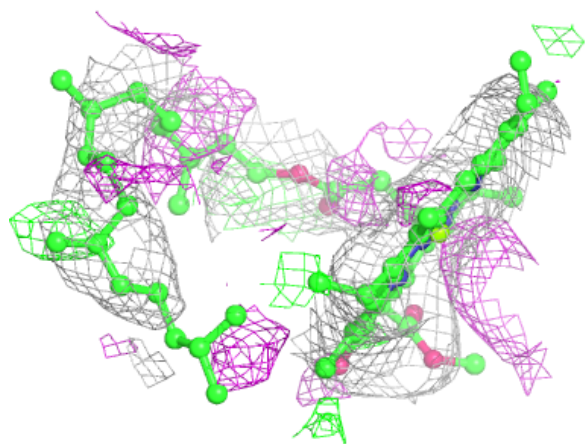
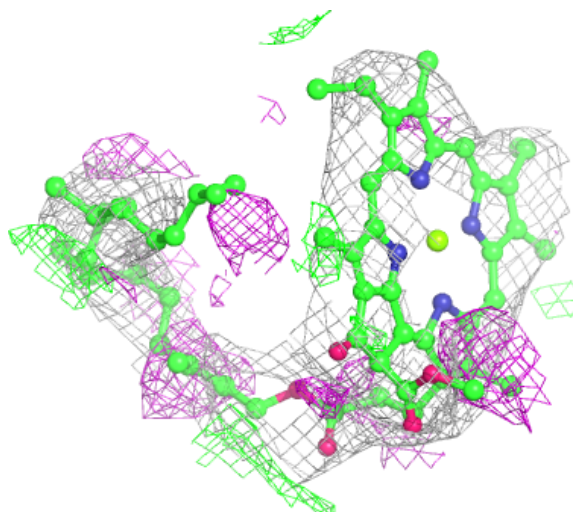
**Electron density around CLA C 502:**

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



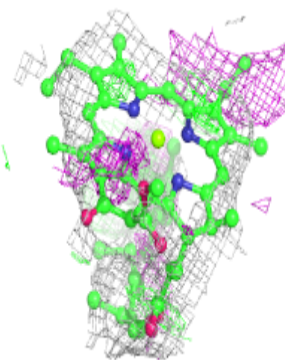
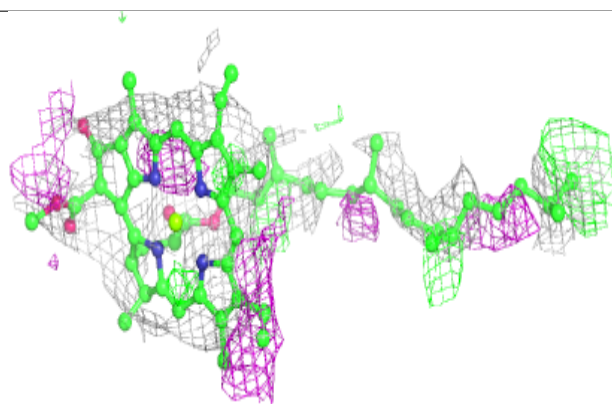
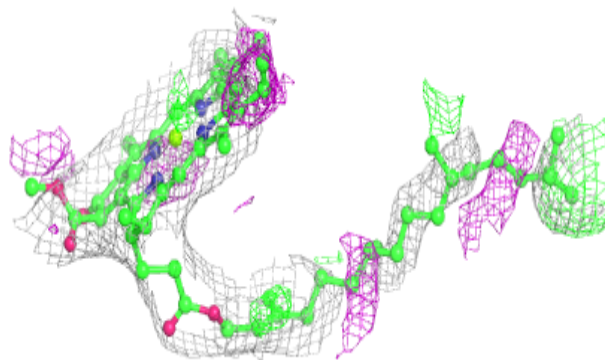
Electron density around CLA C 503:

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

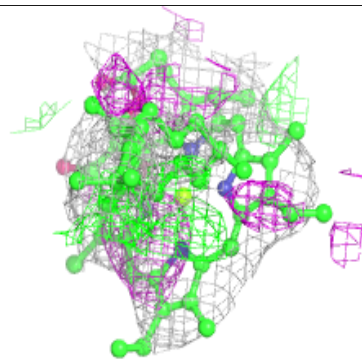
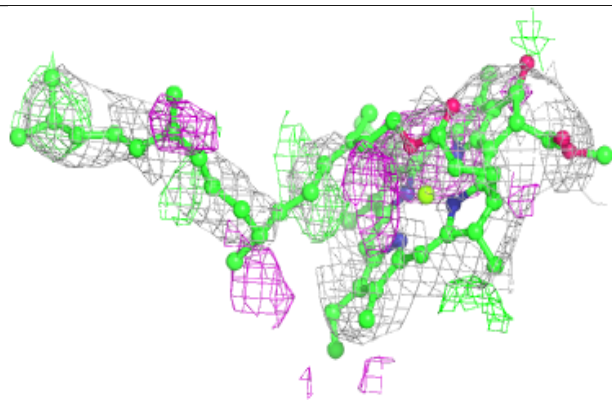
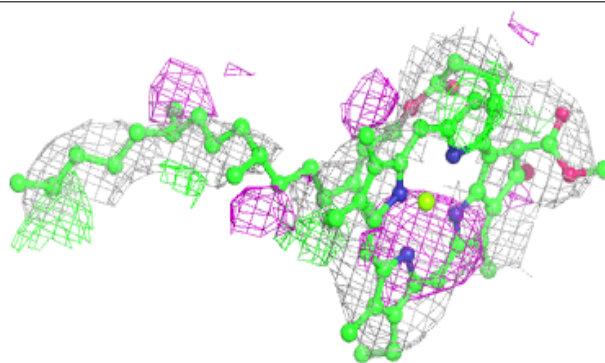


Electron density around CLA C 504:

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

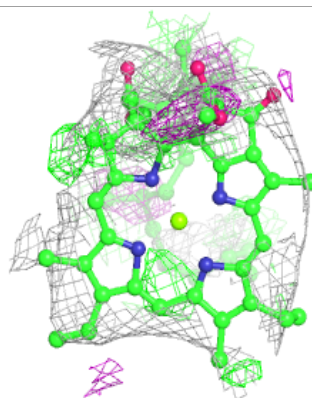
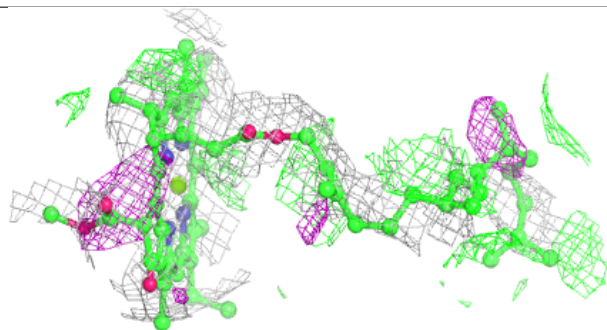
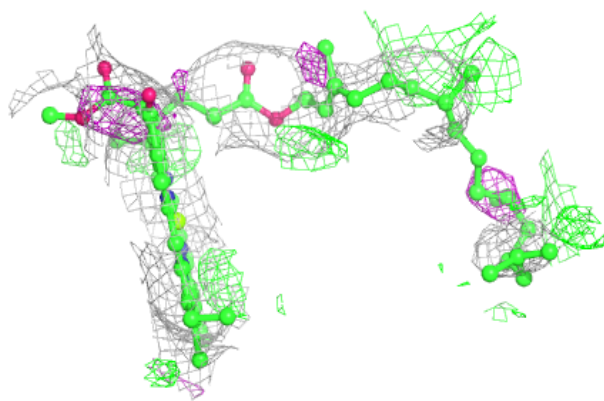
**Electron density around CLA C 505:**

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



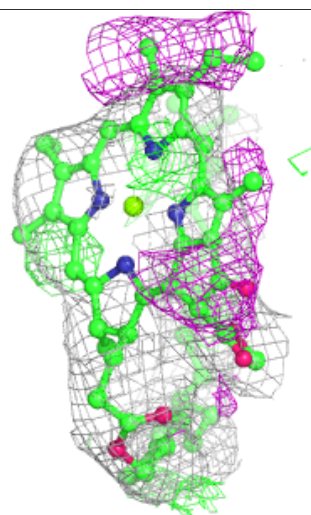
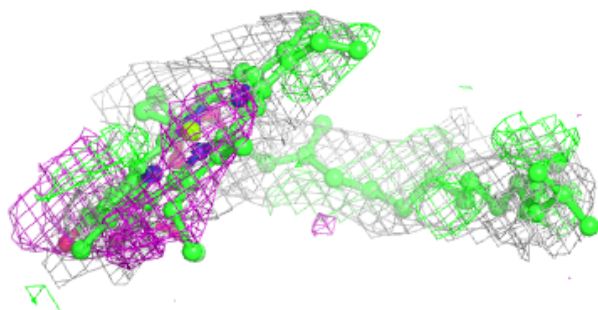
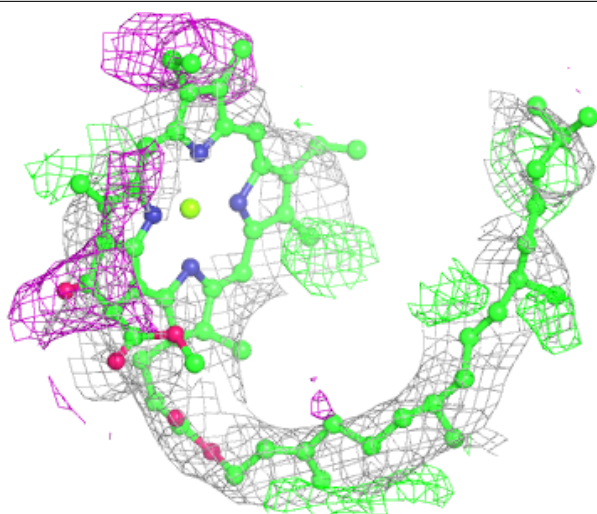
Electron density around CLA C 506:

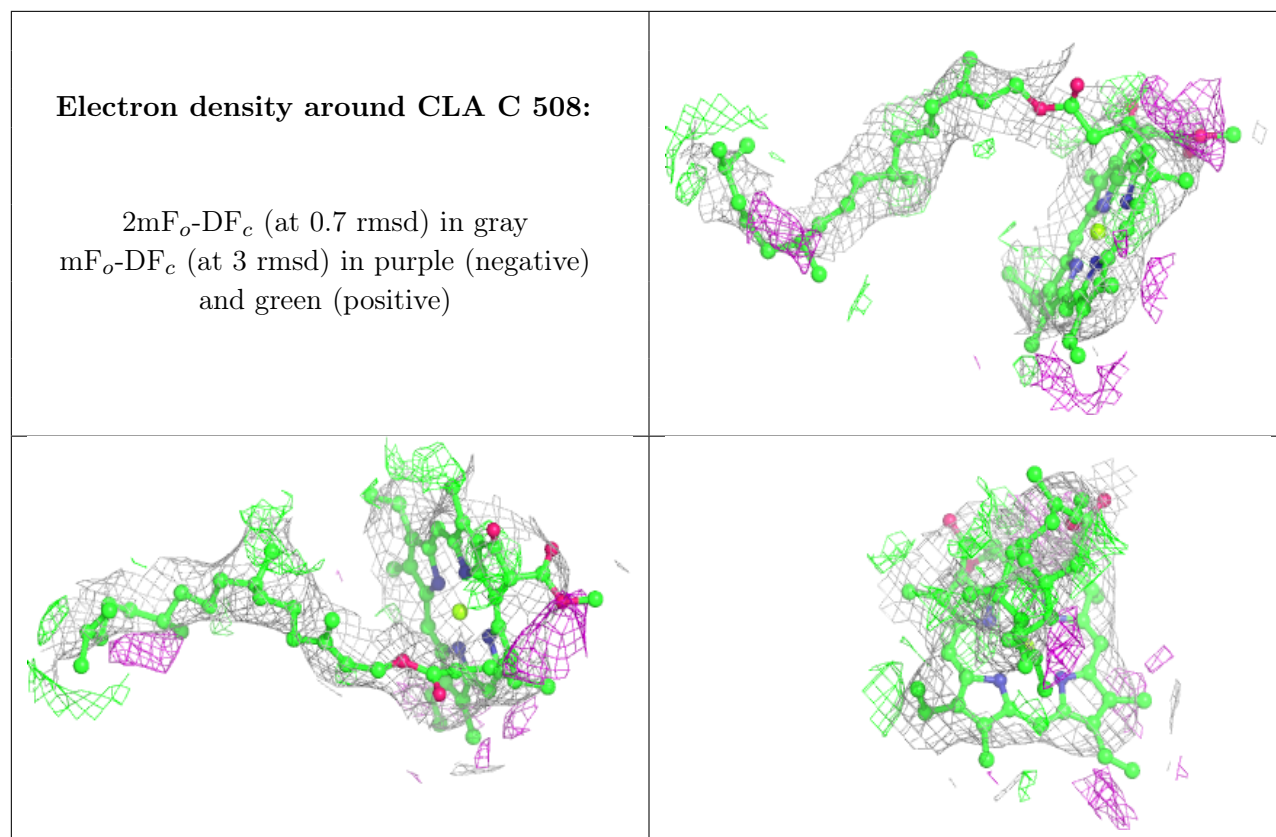
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 507:

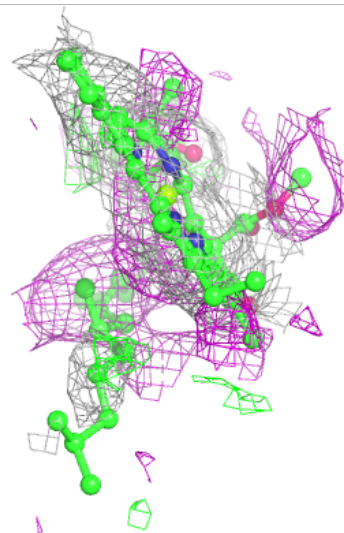
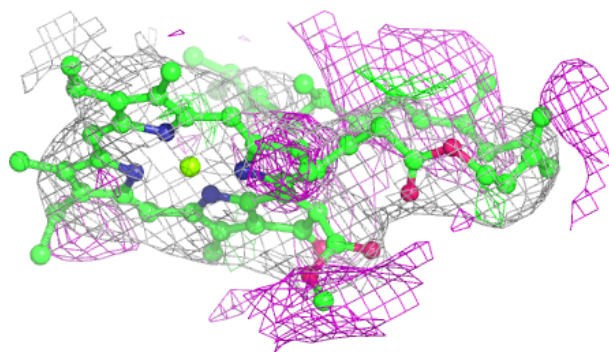
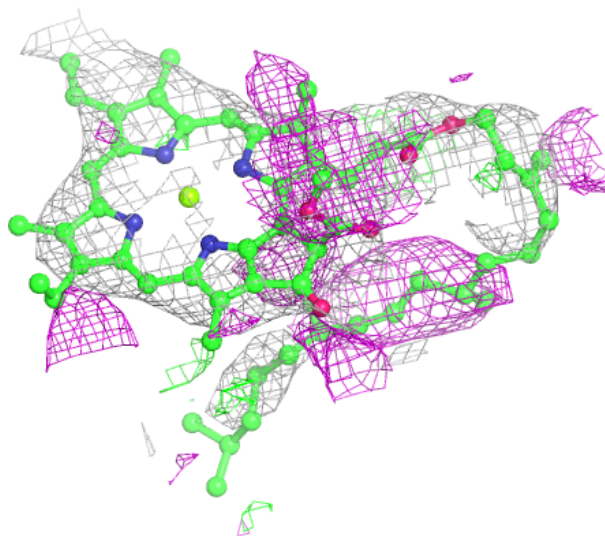
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





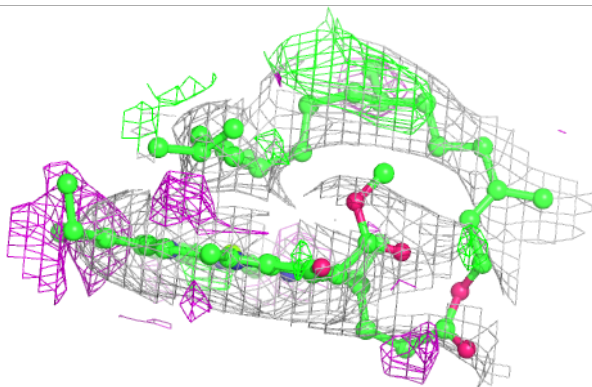
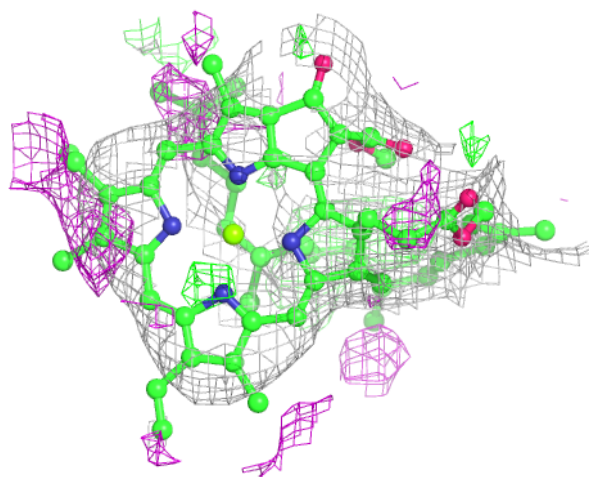
Electron density around CLA C 509:

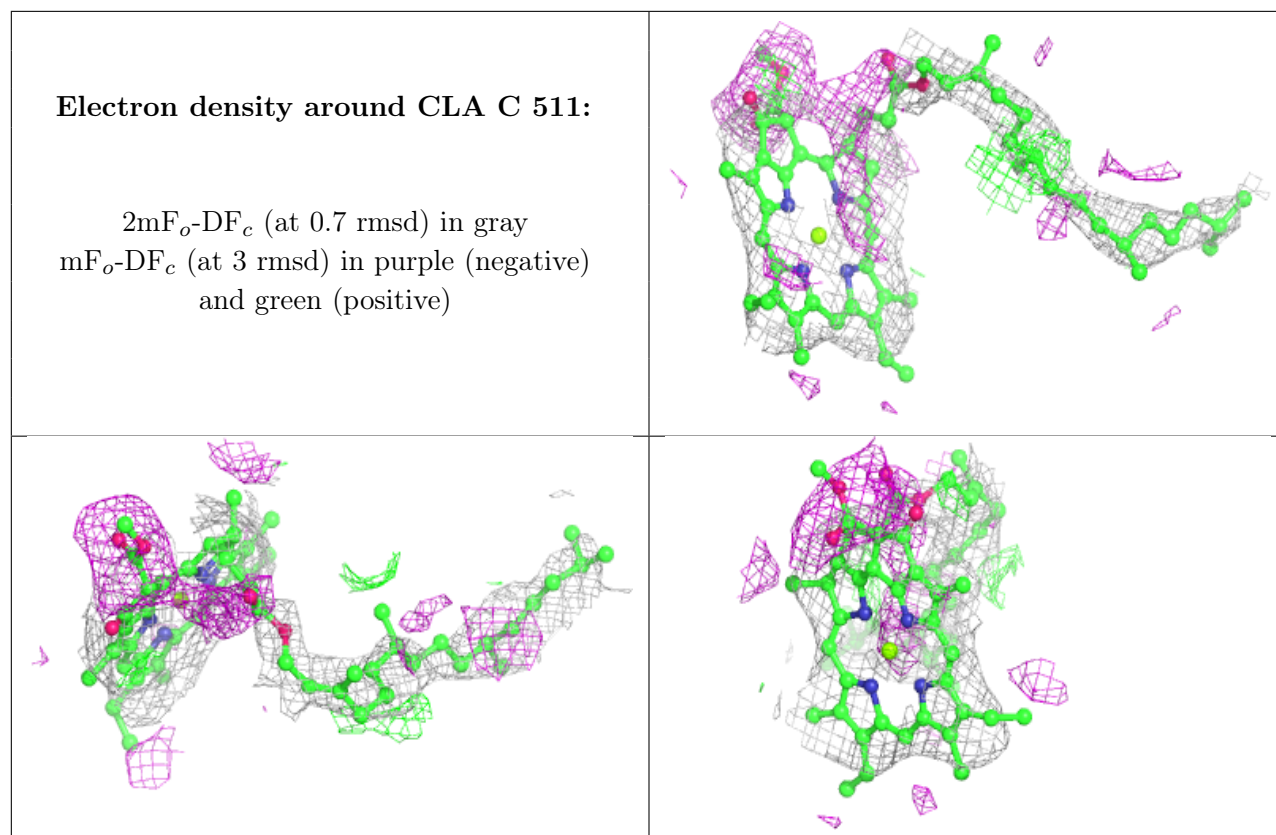
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 510:

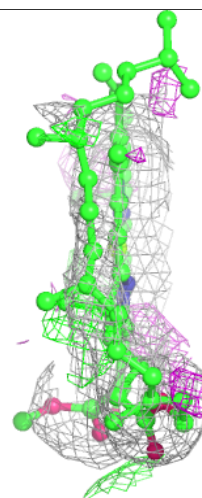
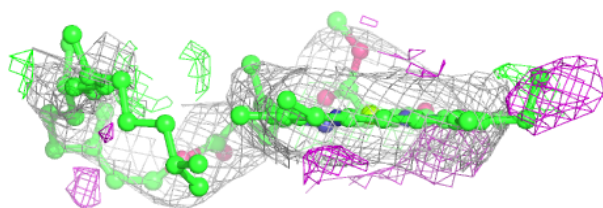
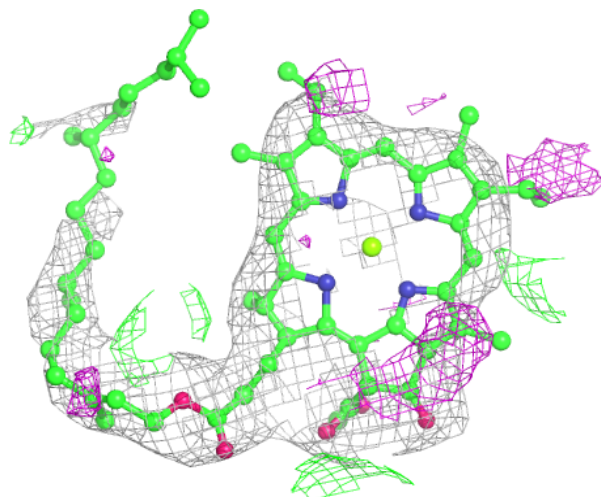
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





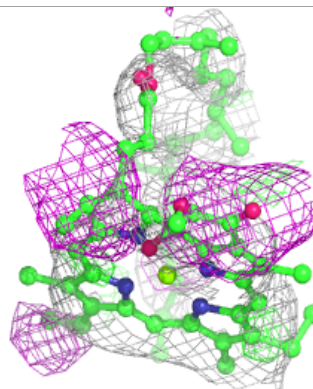
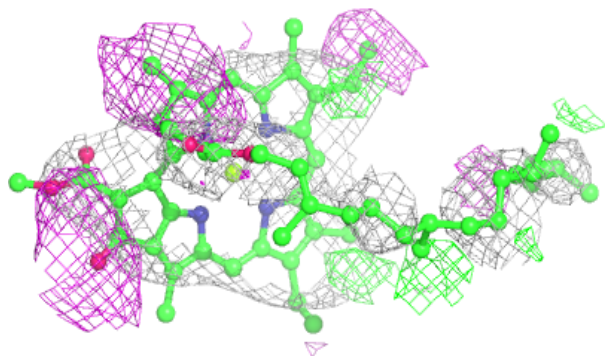
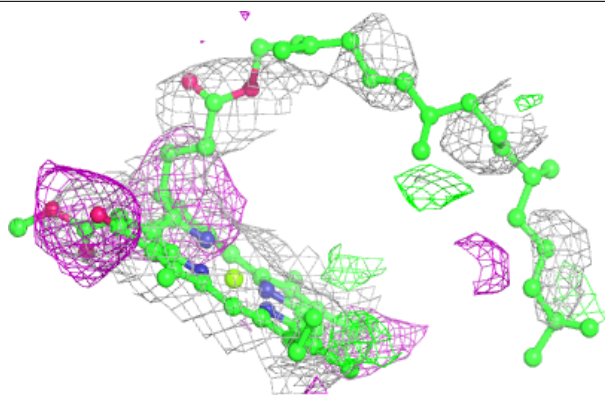
Electron density around CLA C 512:

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

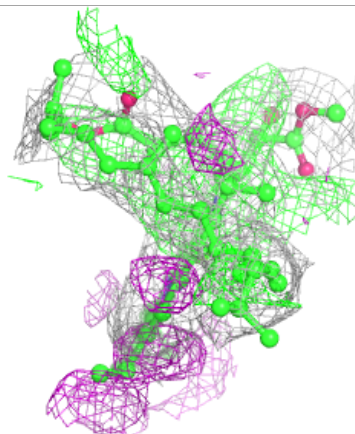
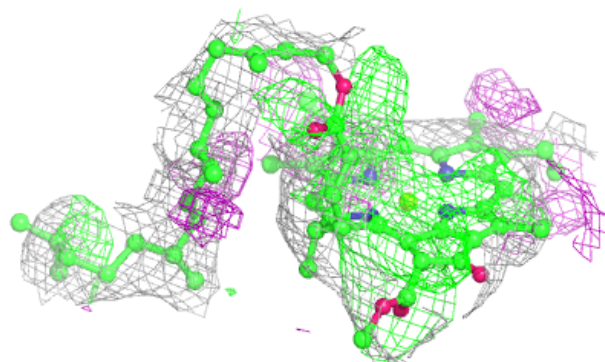
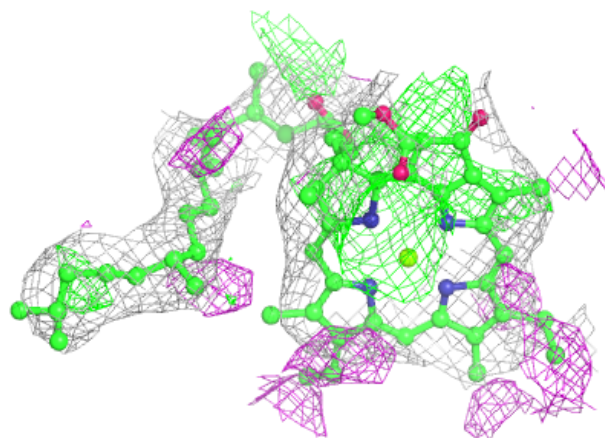


Electron density around CLA C 513:

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

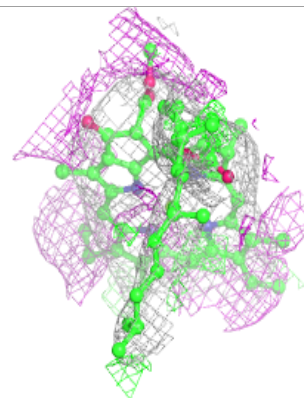
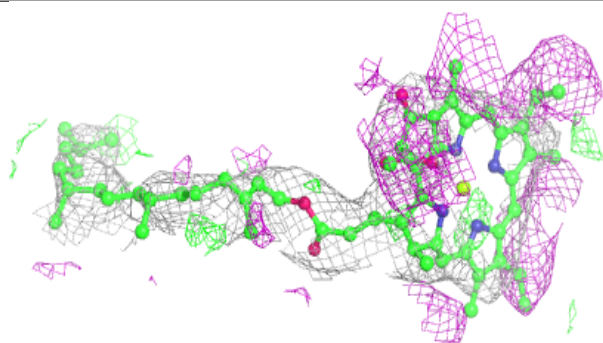
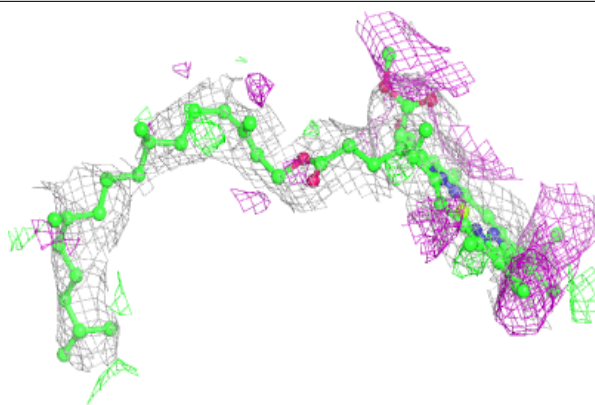
**Electron density around CLA D 402:**

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

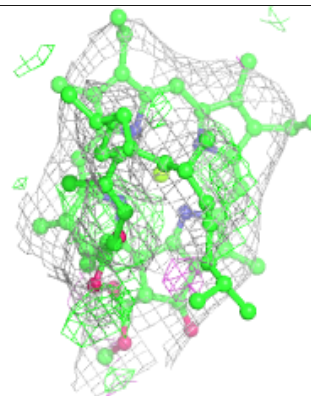
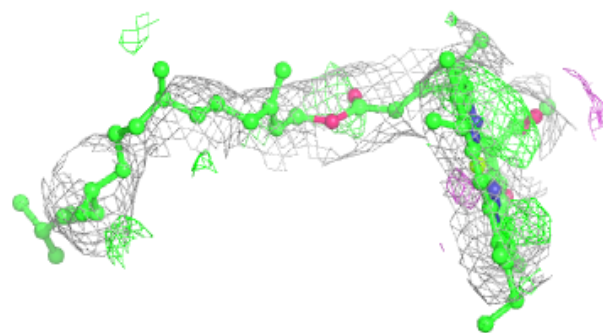
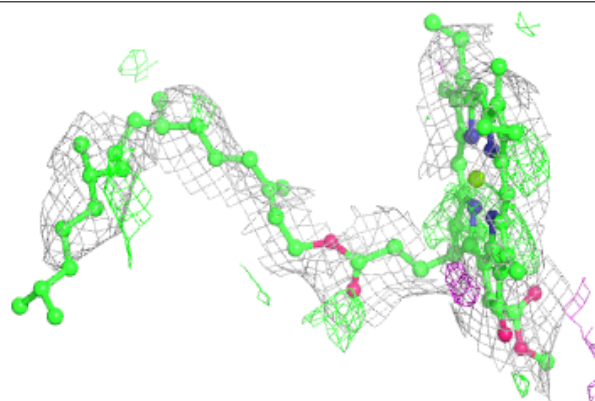


Electron density around CLA D 403:

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

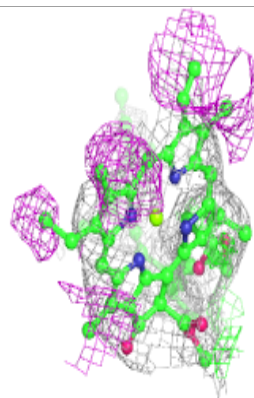
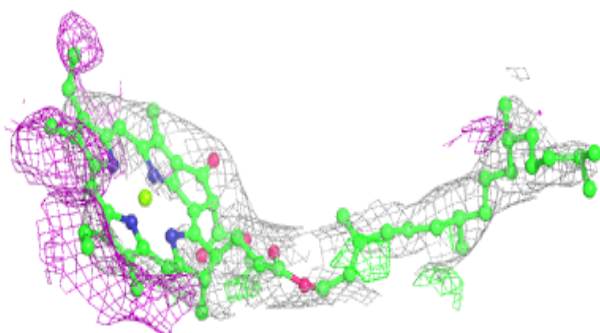
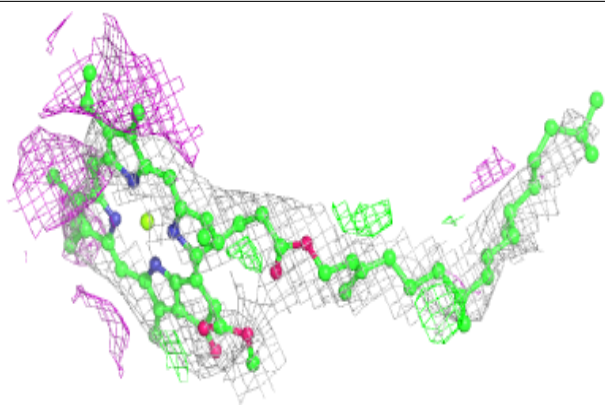
**Electron density around CLA D 404:**

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

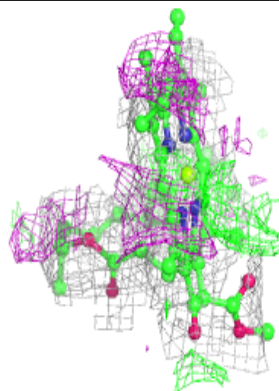
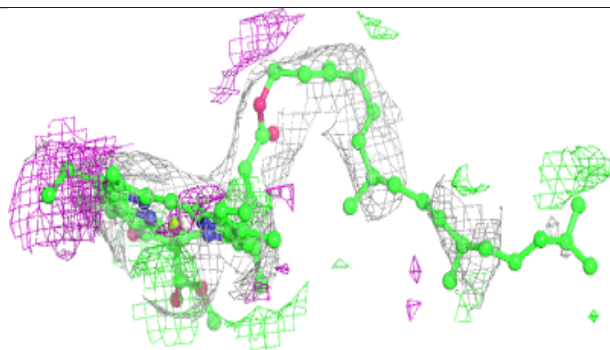
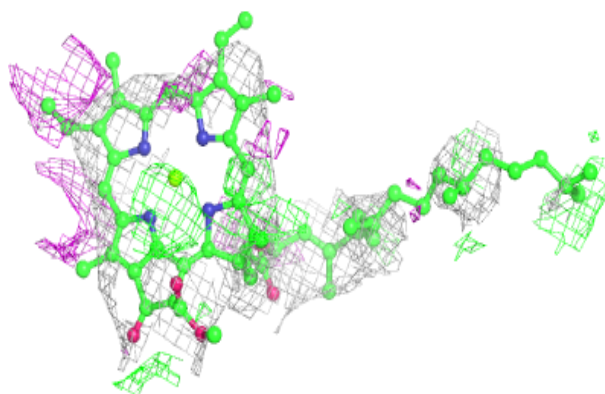


Electron density around CLA a 606:

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

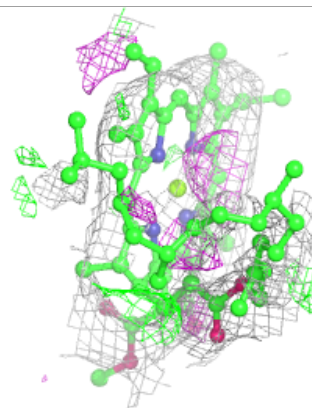
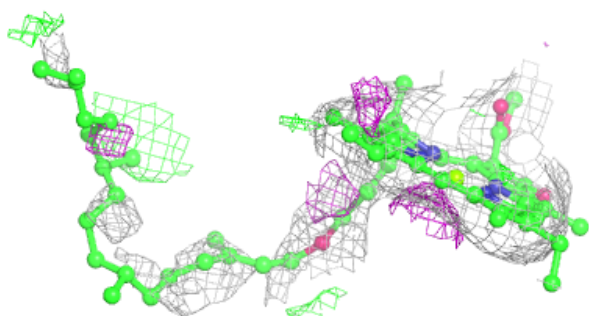
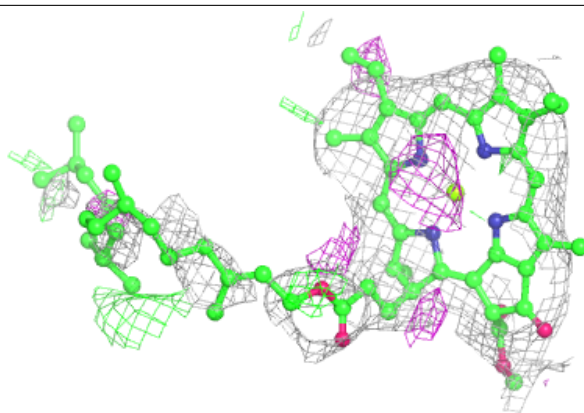
**Electron density around CLA a 607:**

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

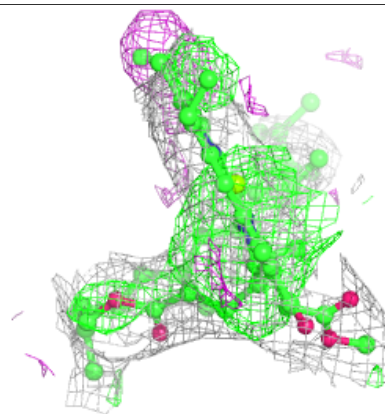
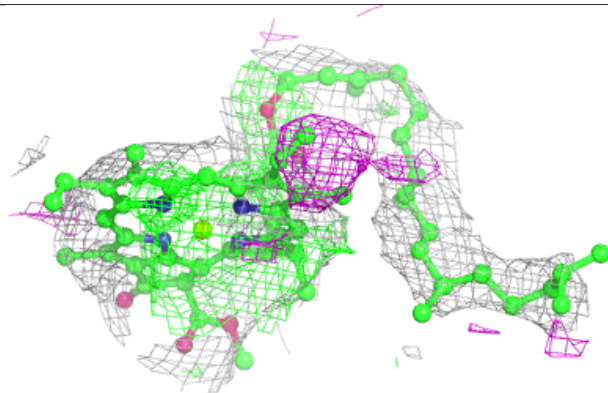
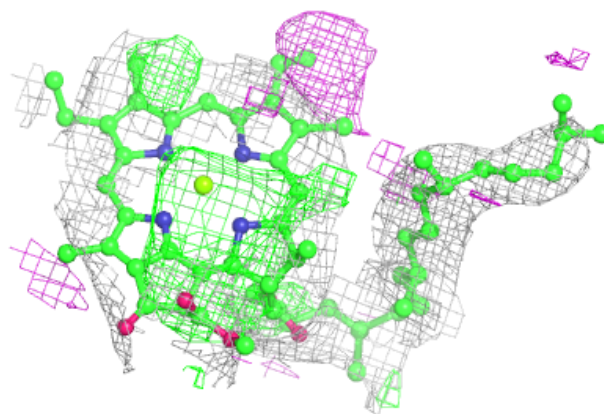


Electron density around CLA a 609:

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

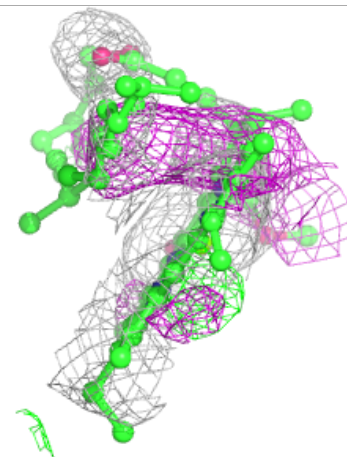
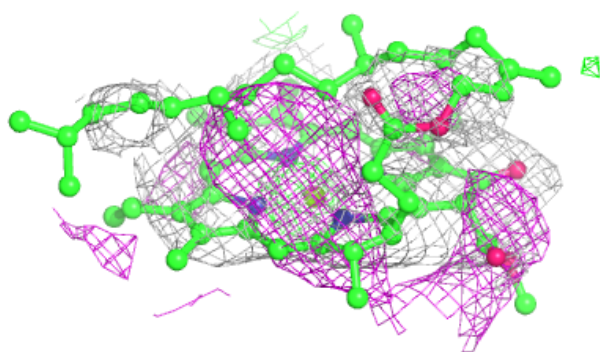
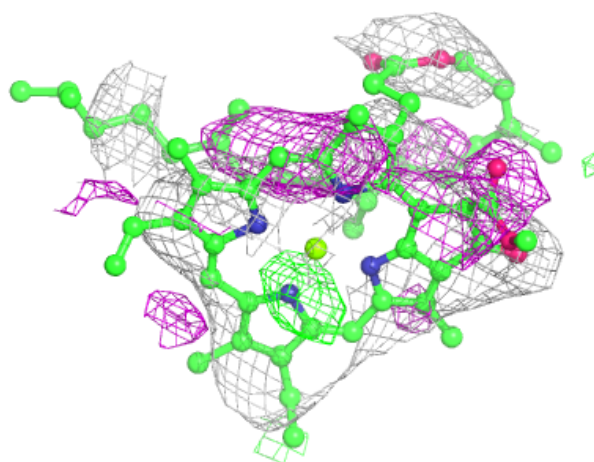
**Electron density around CLA a 615:**

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



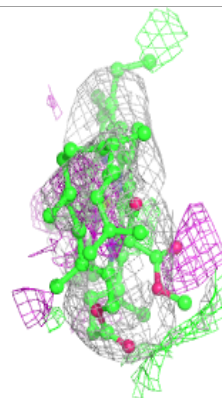
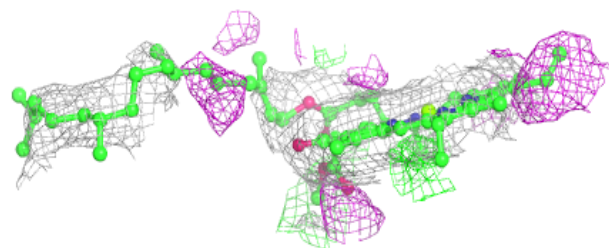
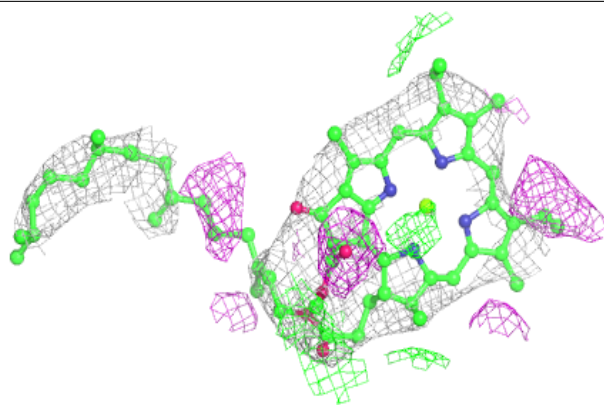
Electron density around CLA b 603:

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

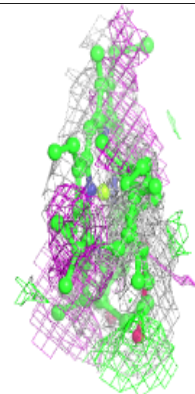
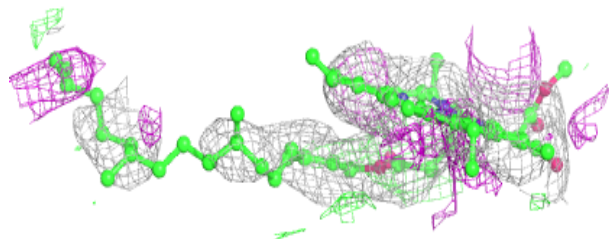
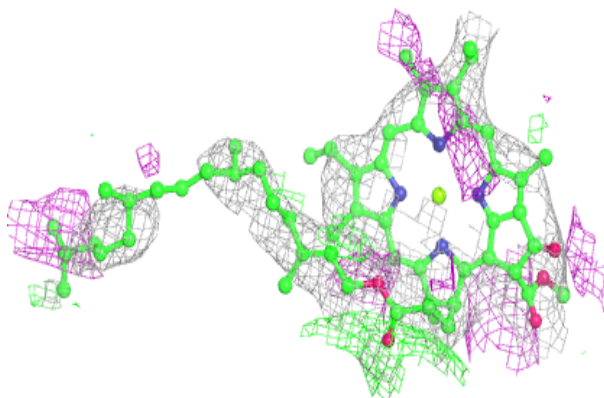


Electron density around CLA b 604:

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

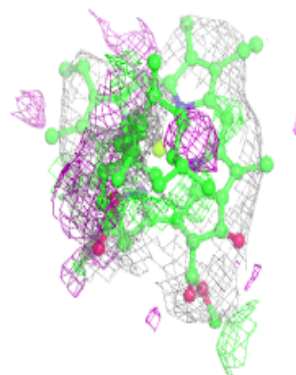
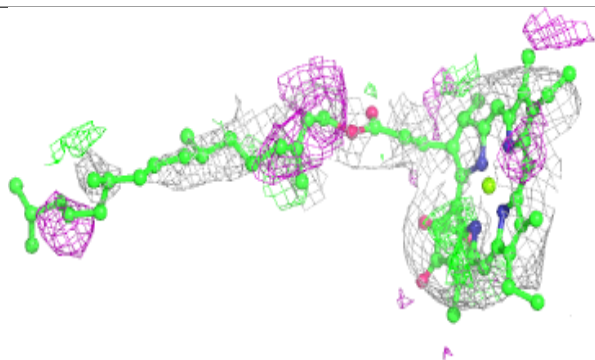
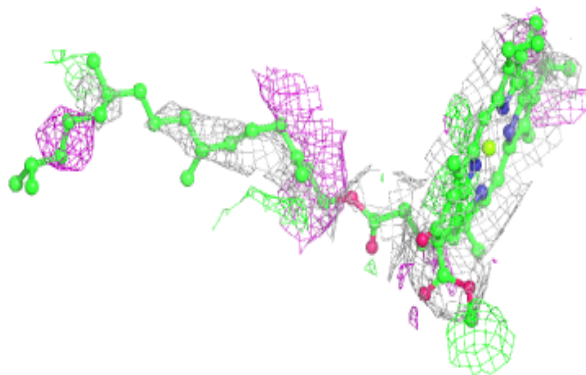
**Electron density around CLA b 605:**

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

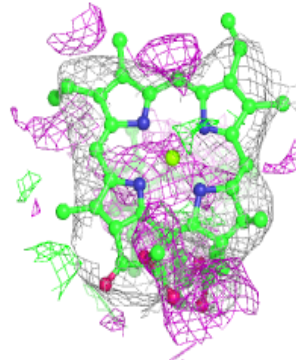
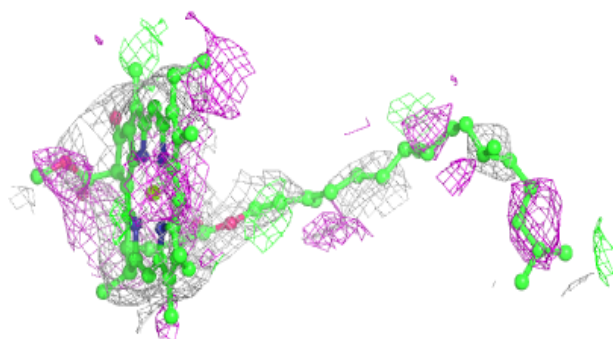
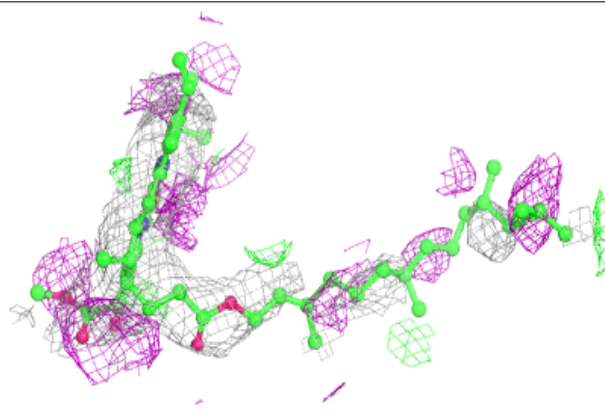


Electron density around CLA b 606:

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

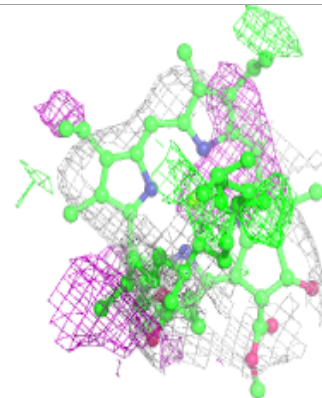
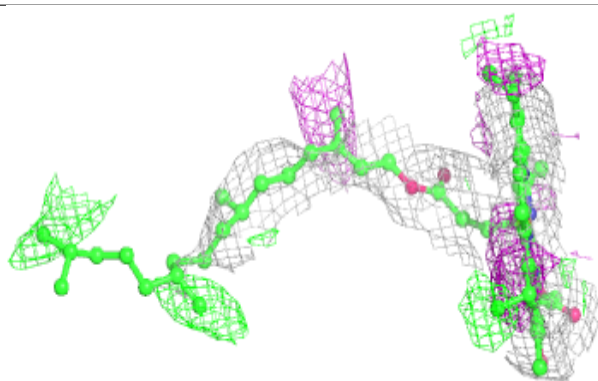
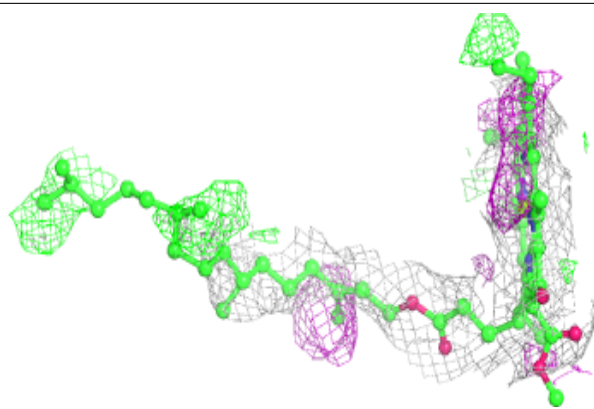
**Electron density around CLA b 607:**

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



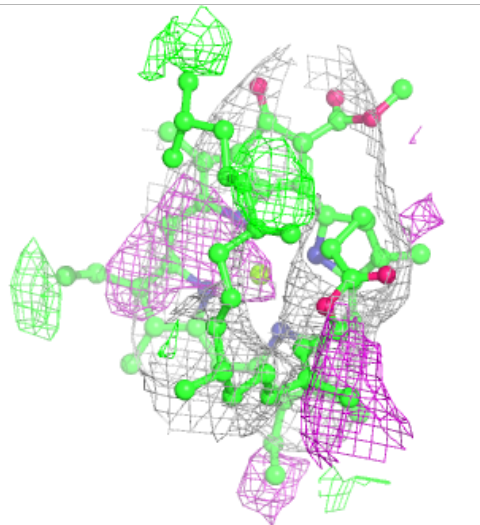
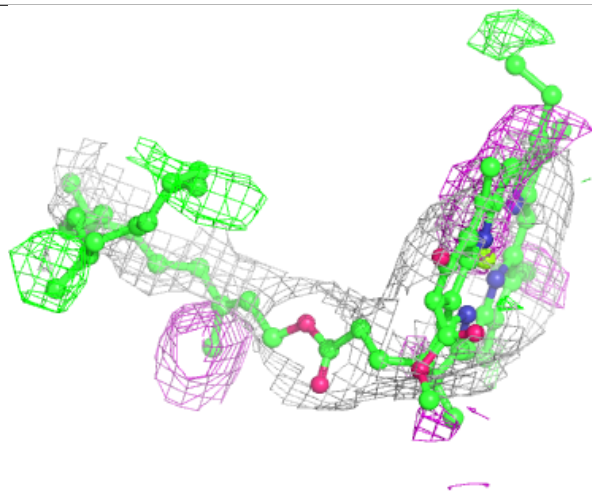
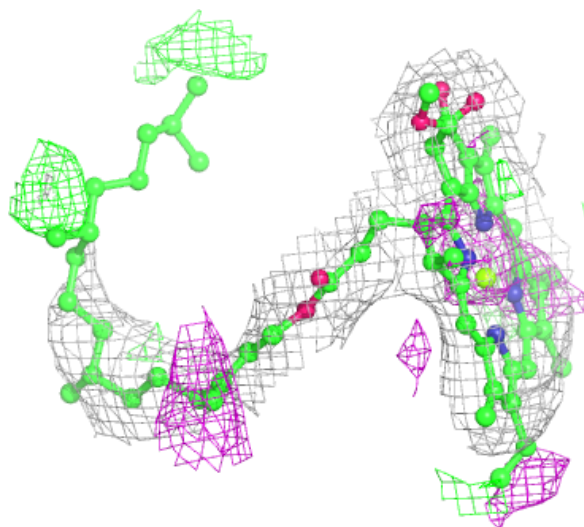
Electron density around CLA b 608 (A):

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



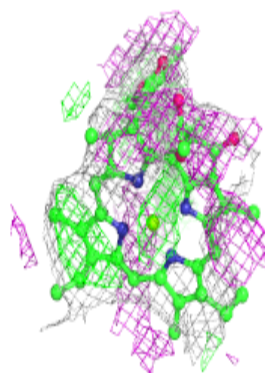
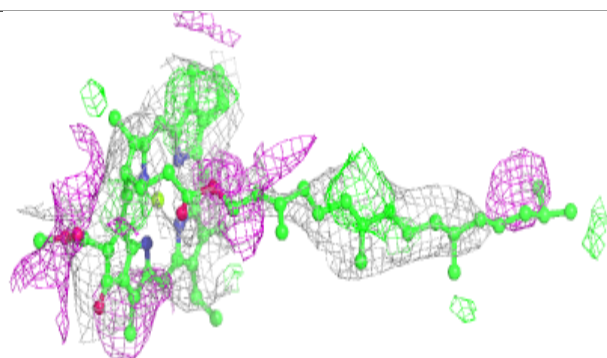
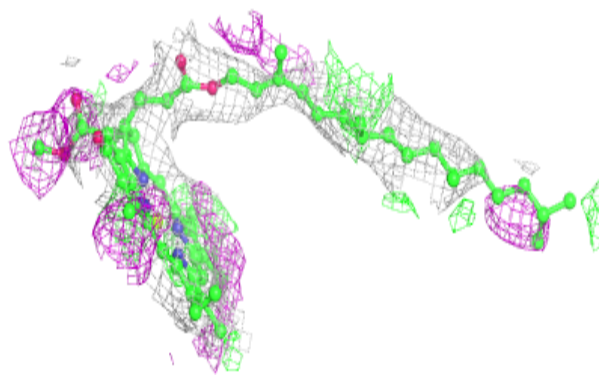
Electron density around CLA b 608 (B):

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

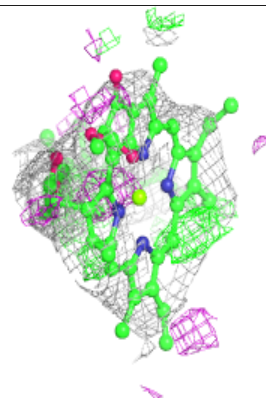
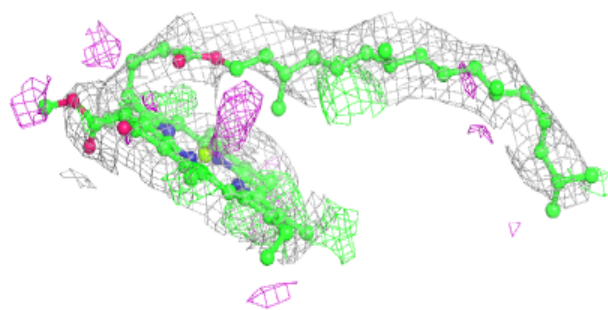
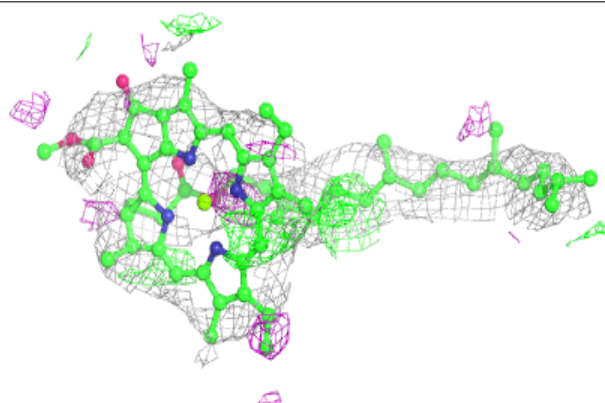


Electron density around CLA b 609:

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

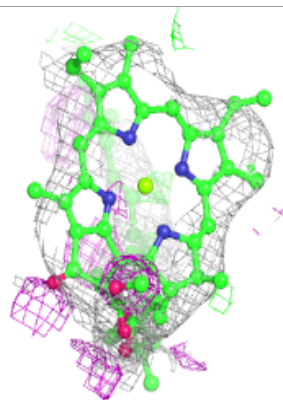
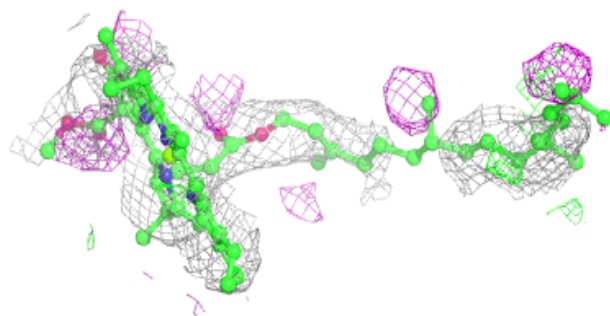
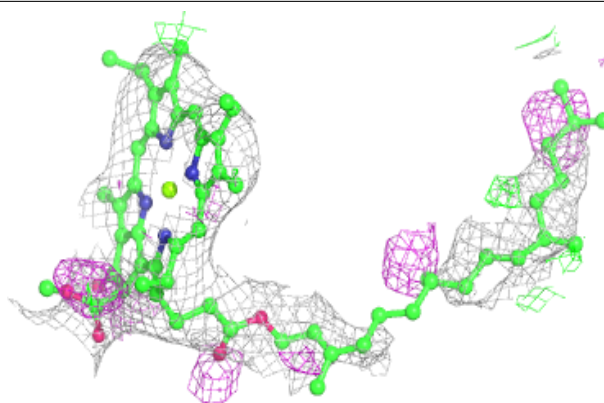
**Electron density around CLA b 610:**

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

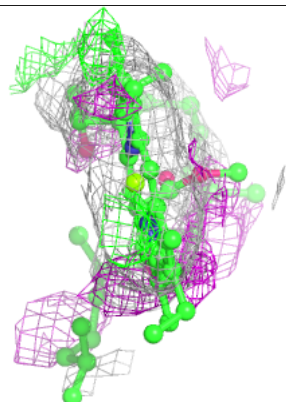
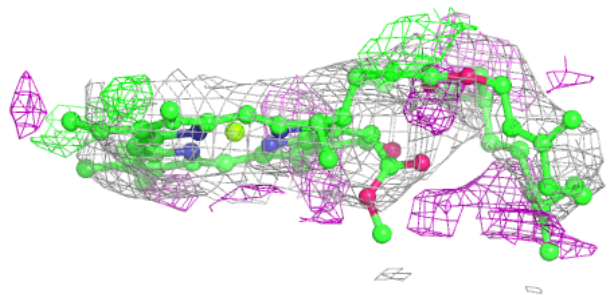
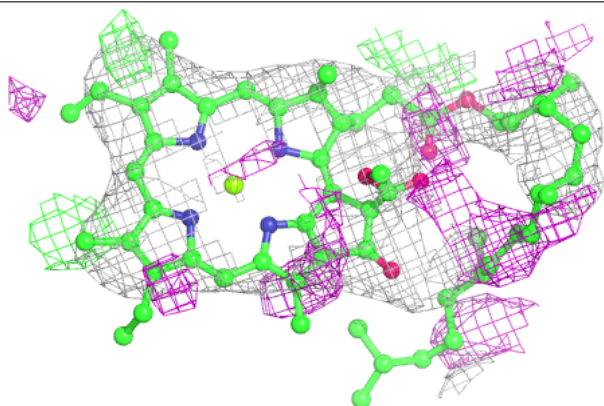


Electron density around CLA b 611:

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

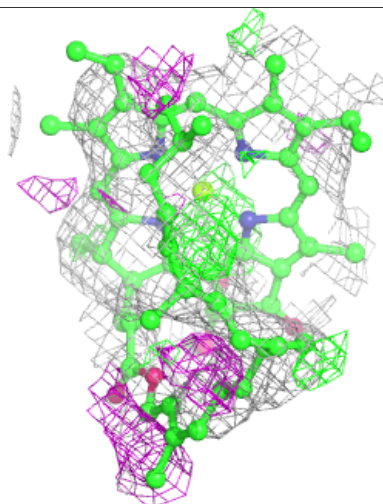
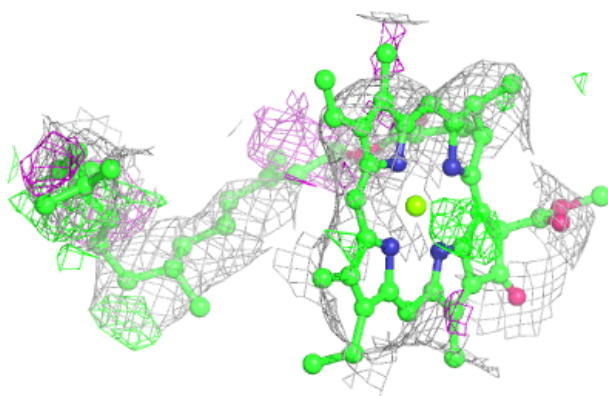
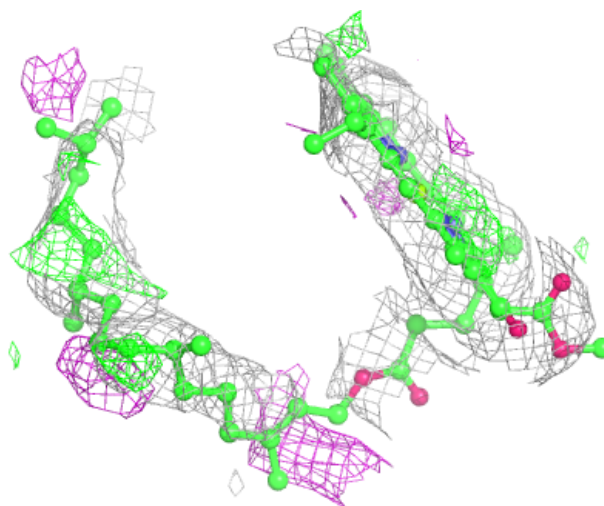
**Electron density around CLA b 612:**

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



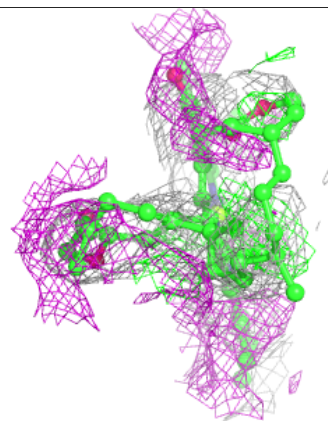
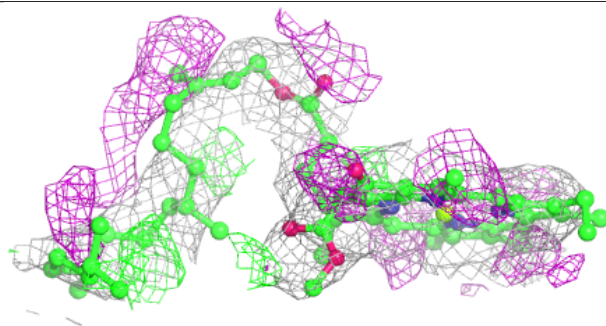
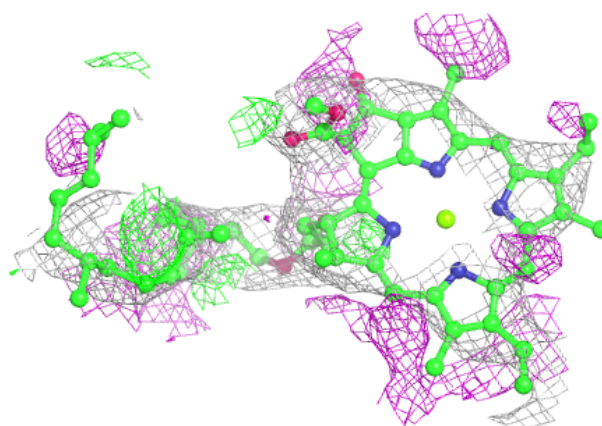
Electron density around CLA b 613:

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



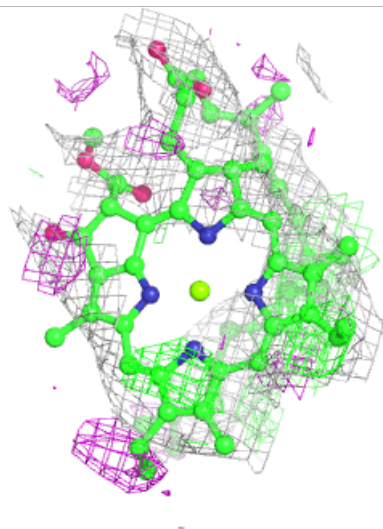
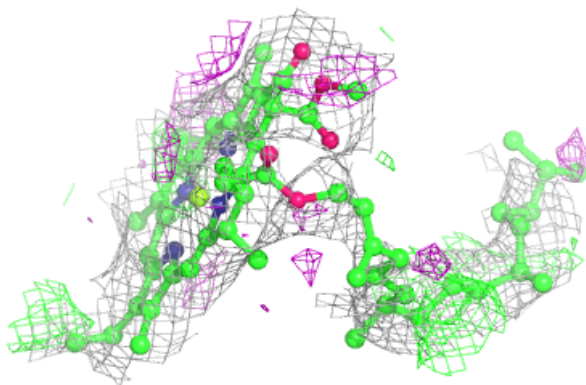
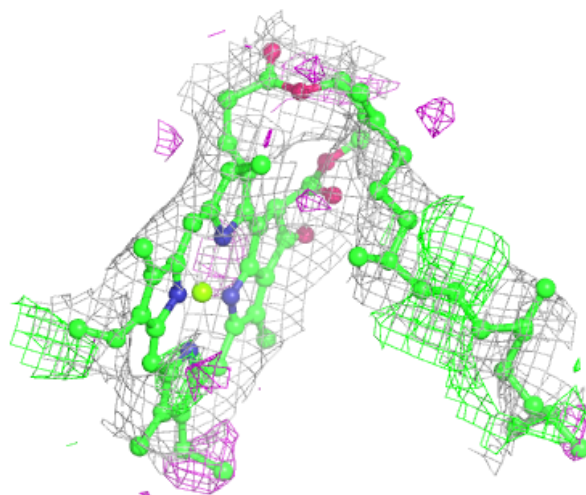
Electron density around CLA b 614:

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



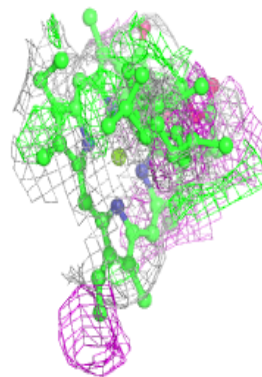
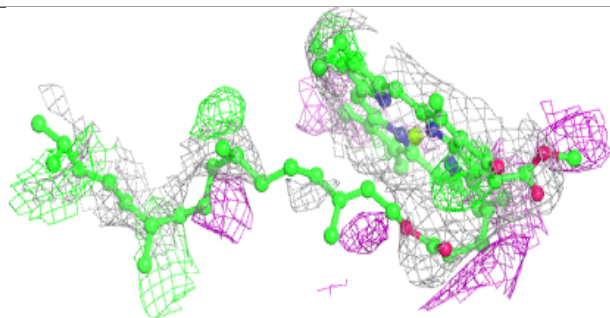
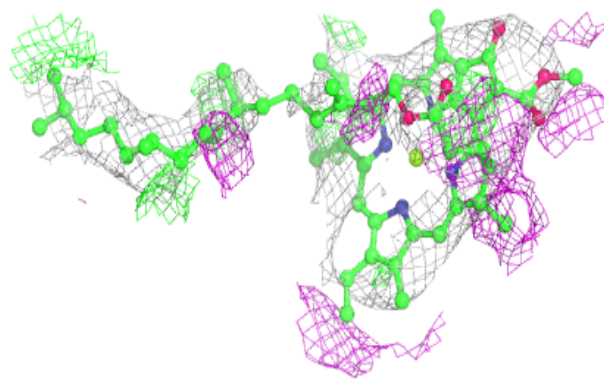
Electron density around CLA b 615:

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



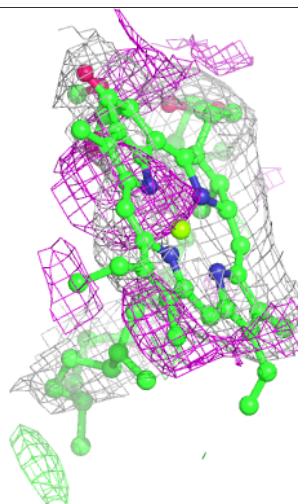
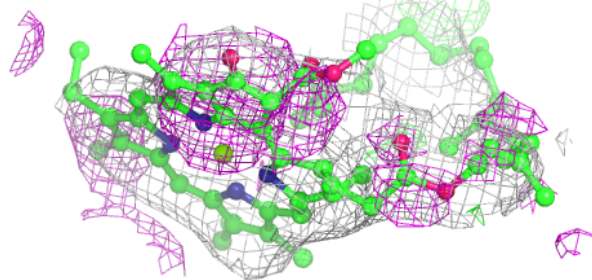
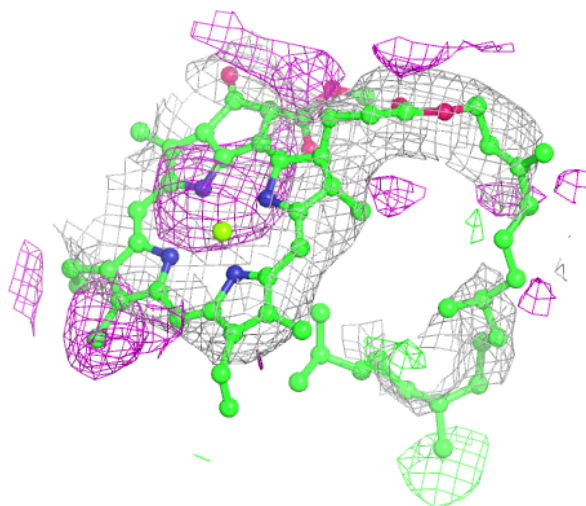
Electron density around CLA b 616:

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



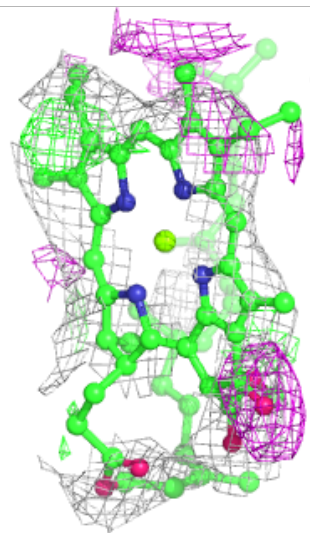
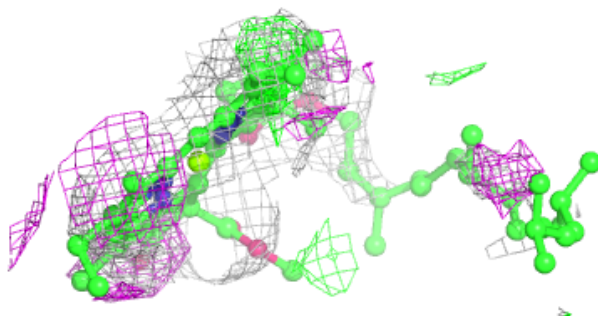
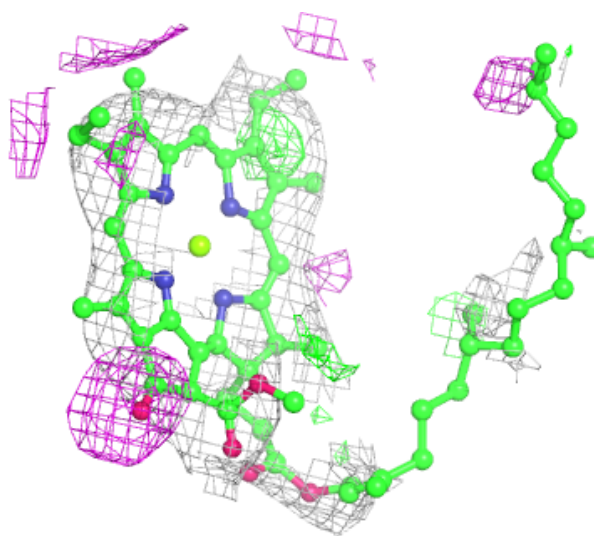
Electron density around CLA b 617:

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



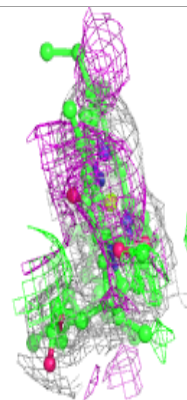
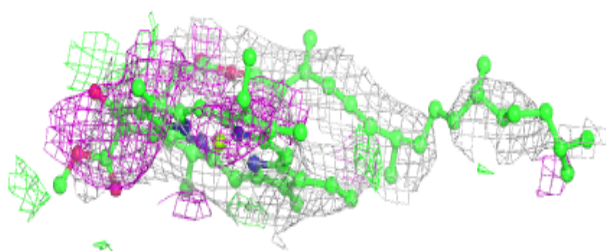
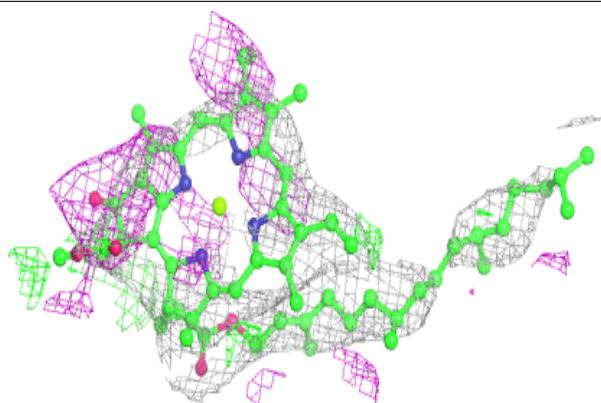
Electron density around CLA b 618:

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

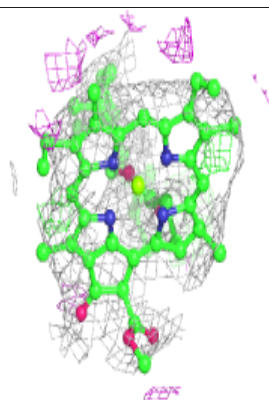
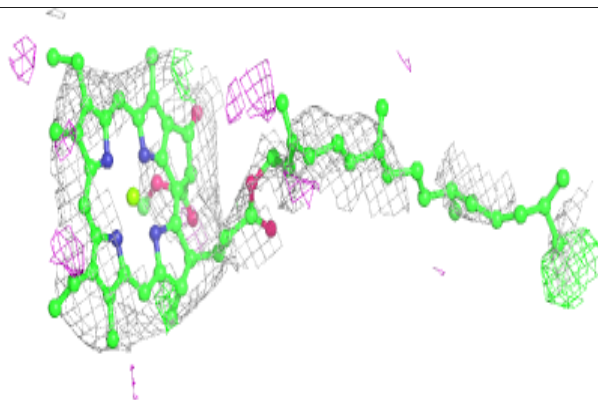
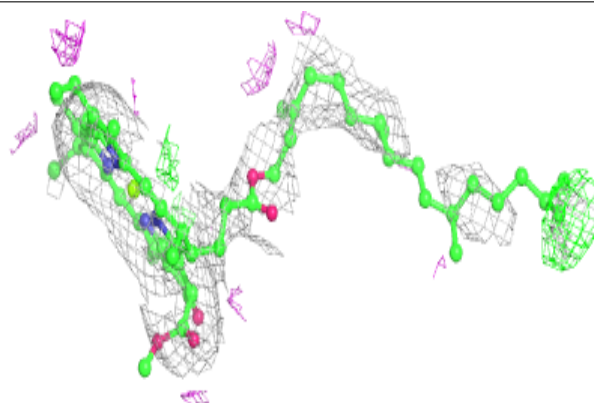


Electron density around CLA c 501:

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

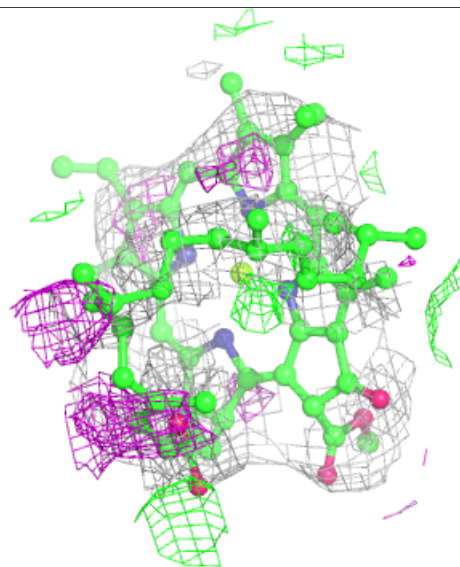
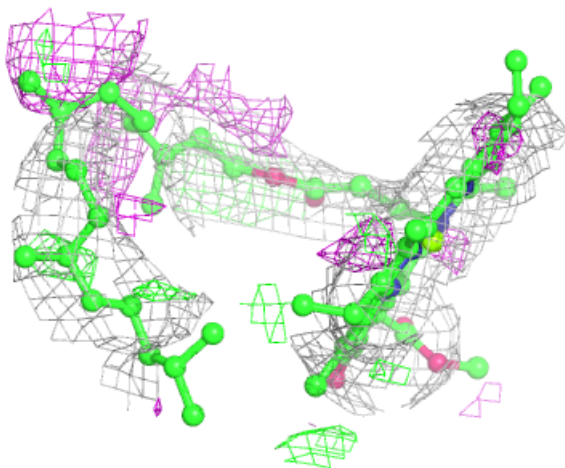
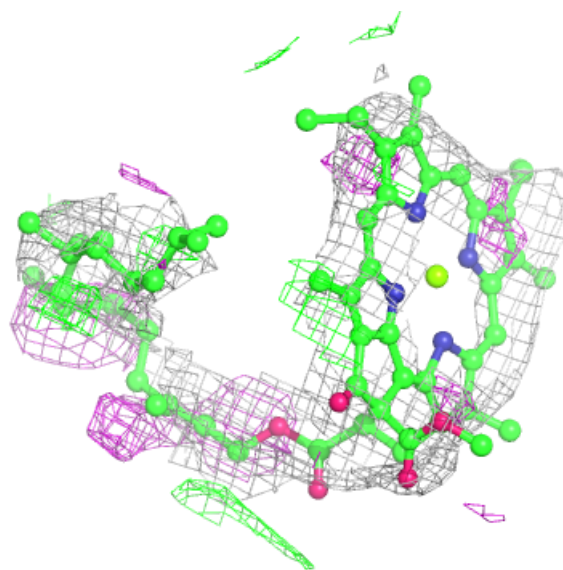
**Electron density around CLA c 502:**

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



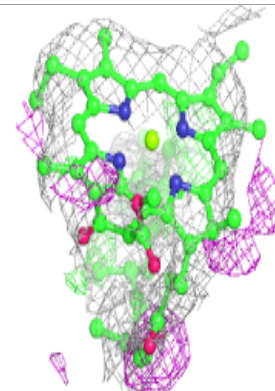
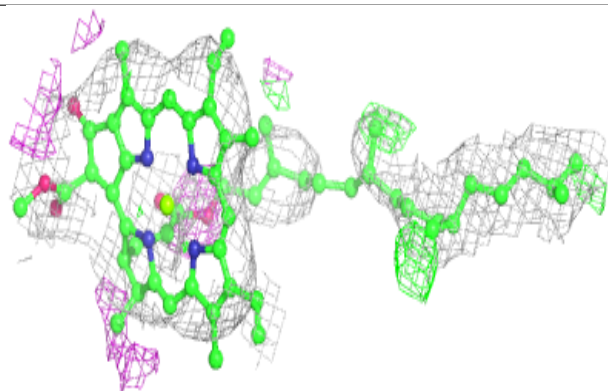
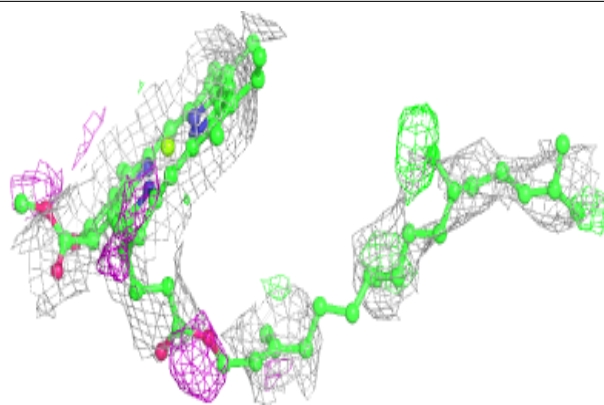
Electron density around CLA c 503:

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

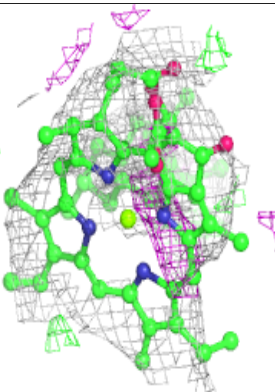
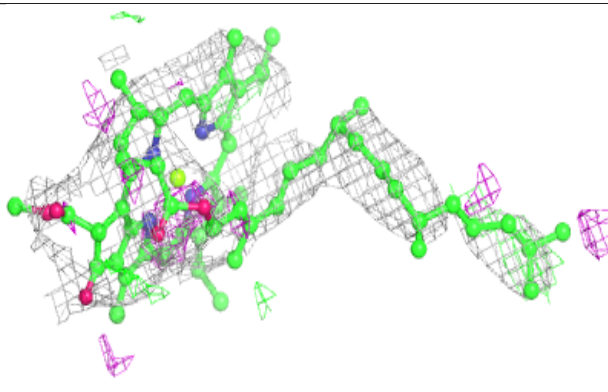
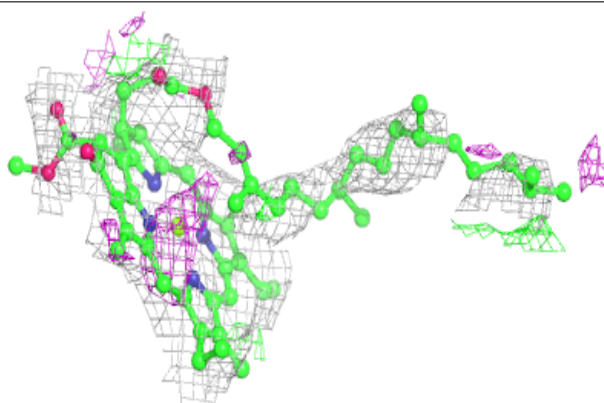


Electron density around CLA c 504:

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

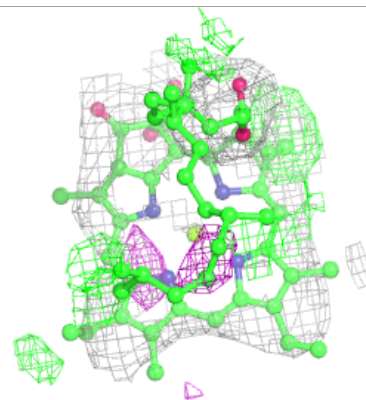
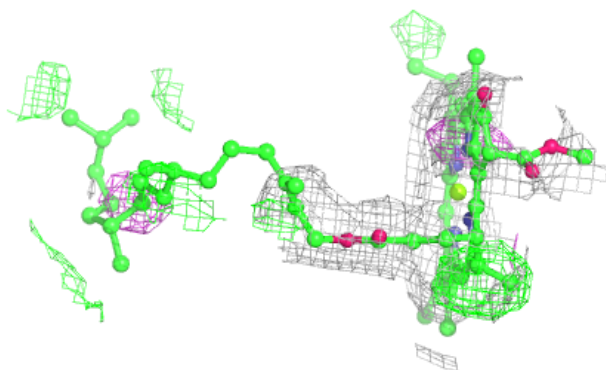
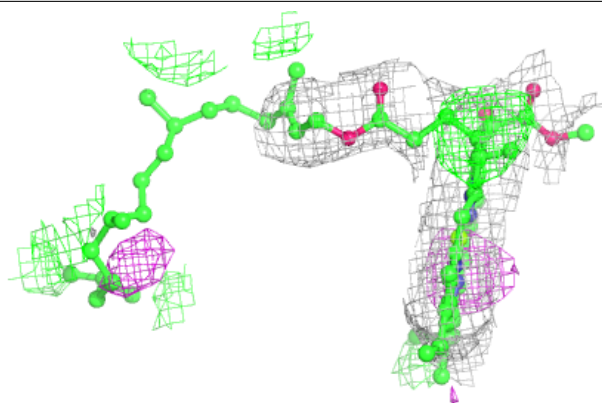
**Electron density around CLA c 505:**

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



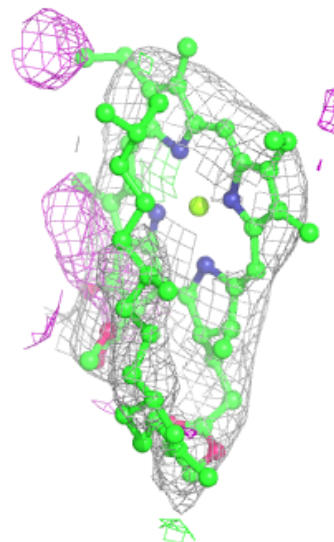
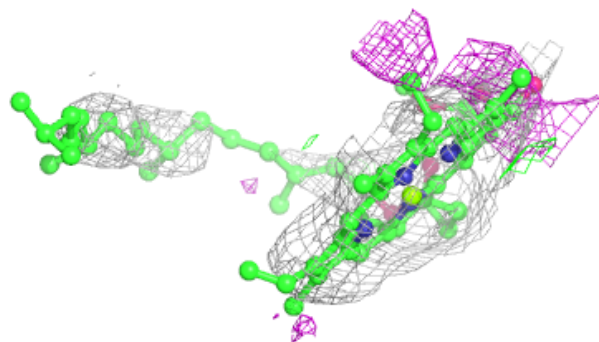
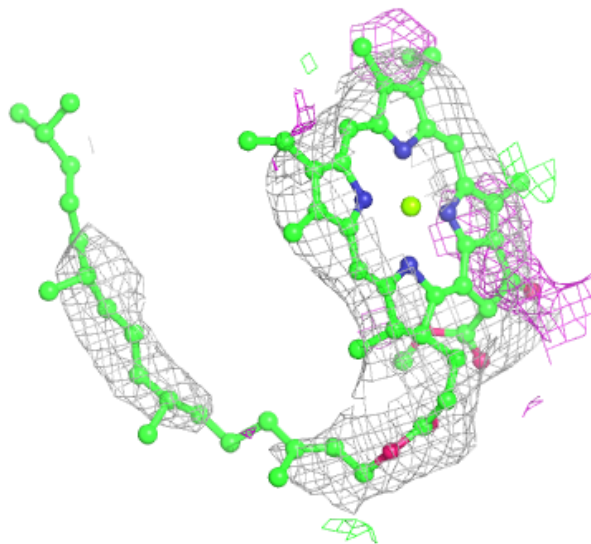
Electron density around CLA c 506:

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



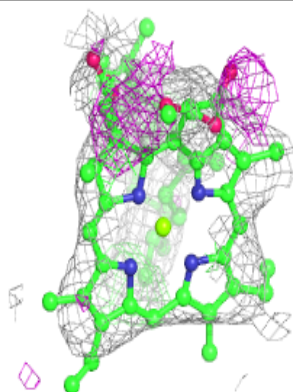
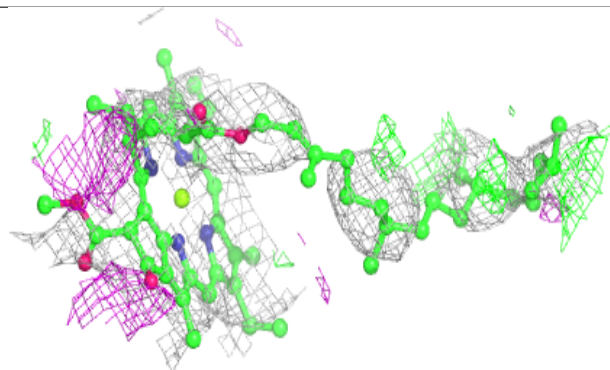
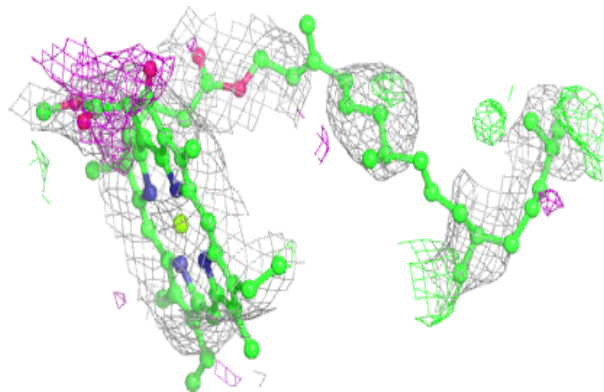
Electron density around CLA c 507:

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



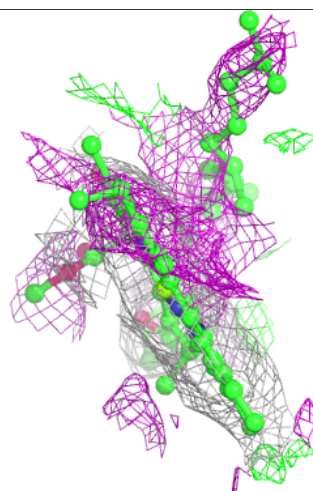
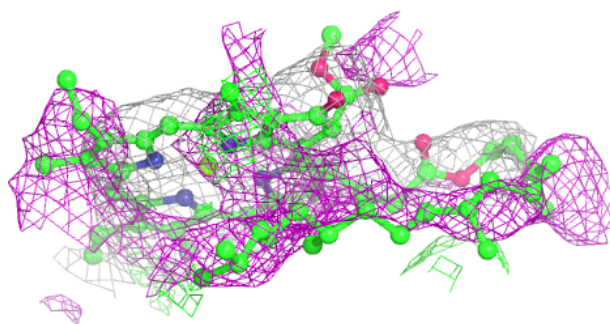
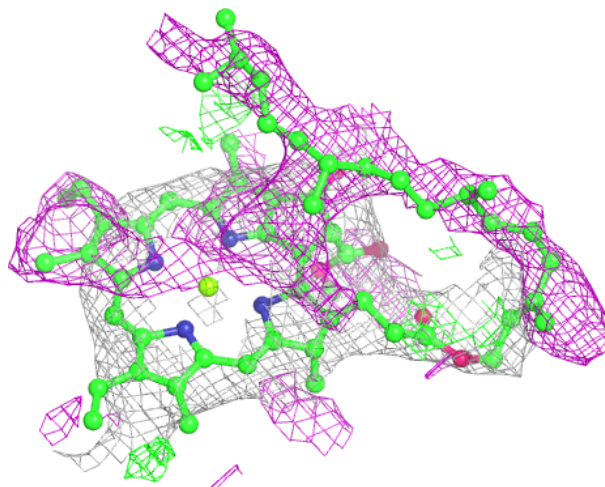
Electron density around CLA c 508:

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



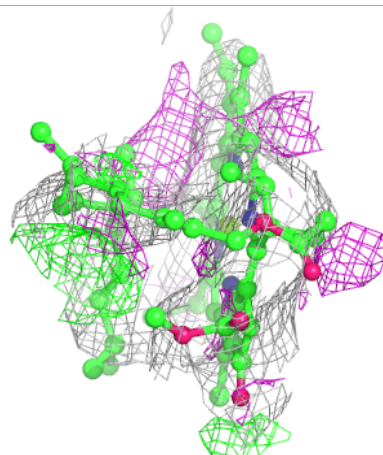
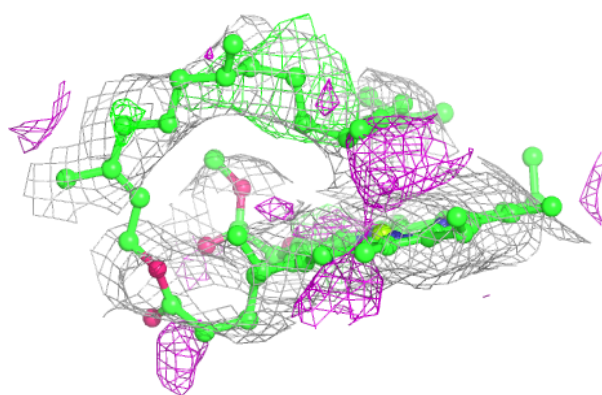
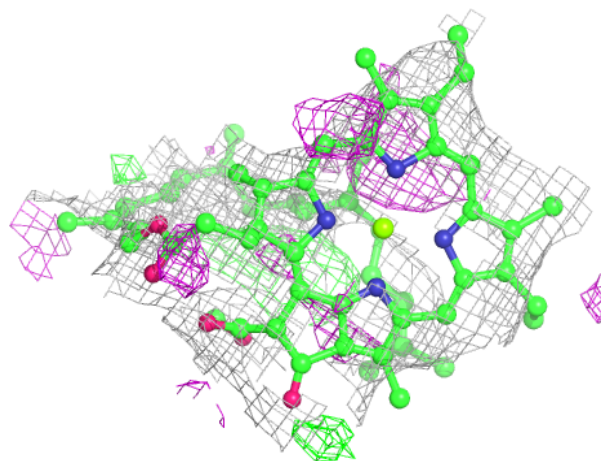
Electron density around CLA c 509:

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



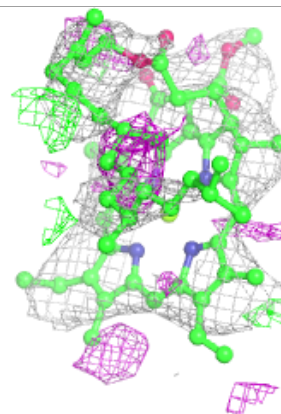
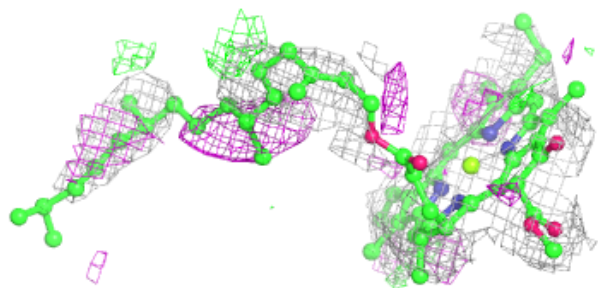
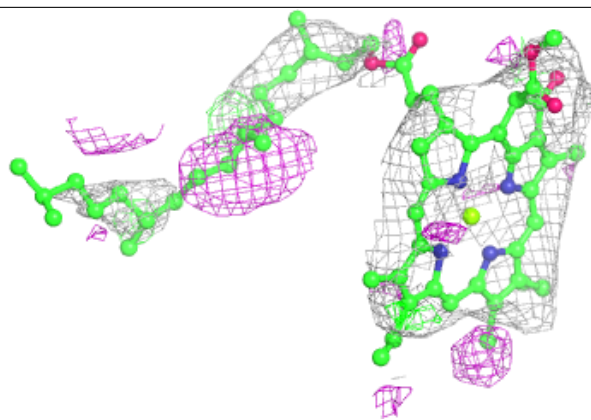
Electron density around CLA c 510:

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



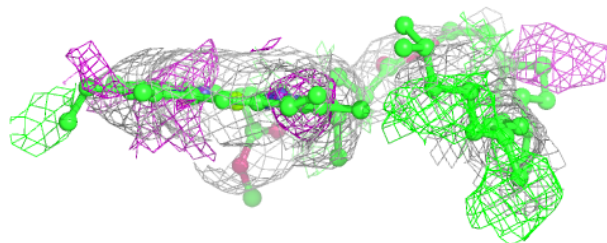
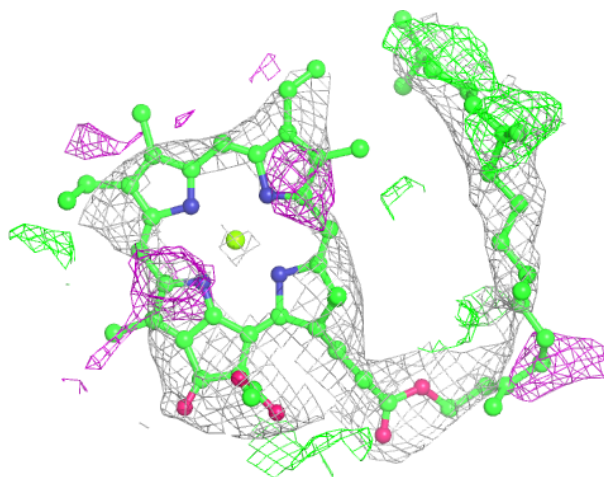
Electron density around CLA c 511:

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



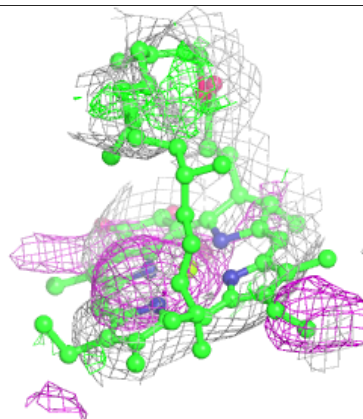
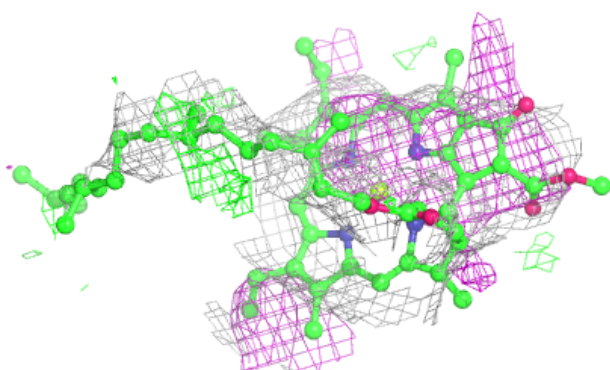
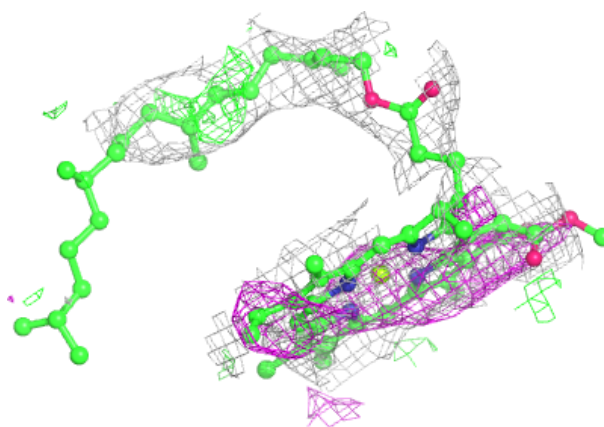
Electron density around CLA c 512:

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

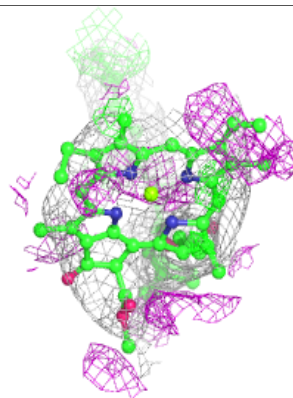
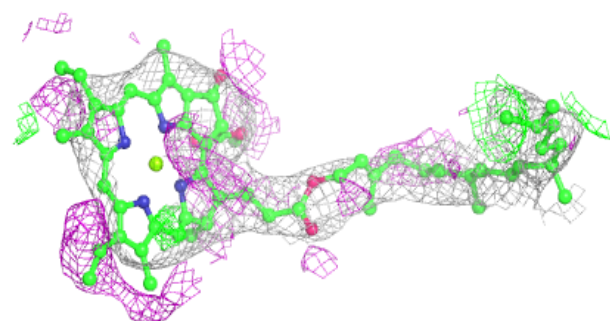
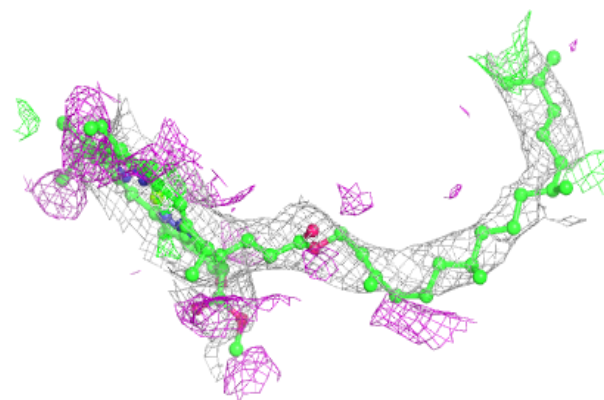


Electron density around CLA c 513:

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

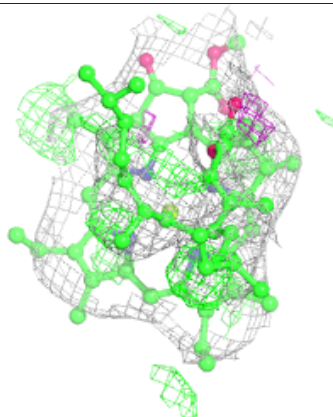
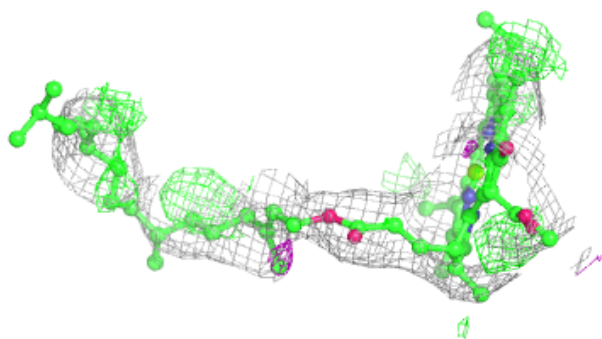
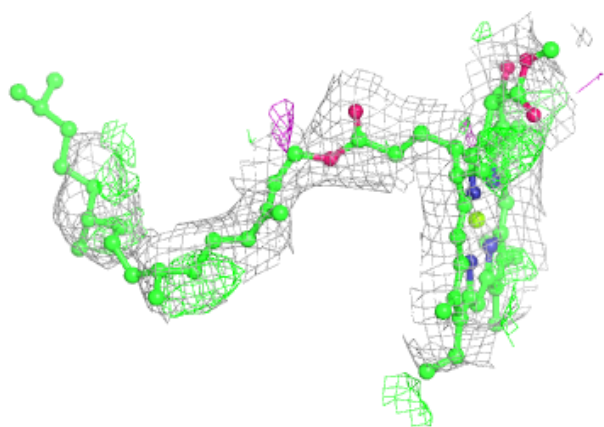
**Electron density around CLA d 402:**

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



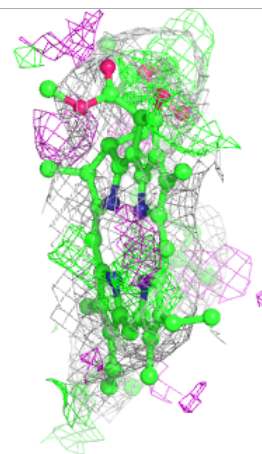
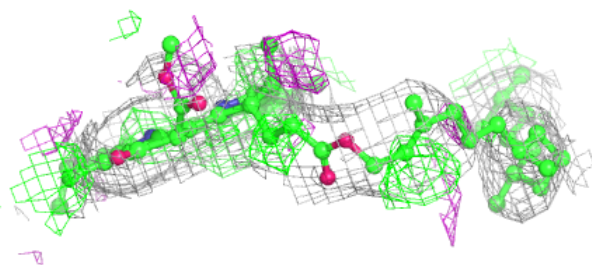
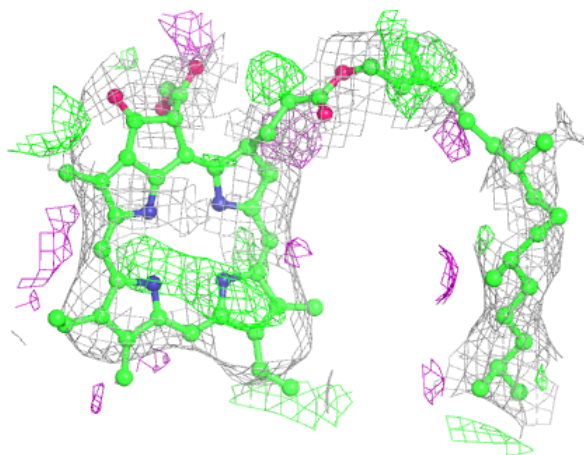
Electron density around CLA d 403:

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



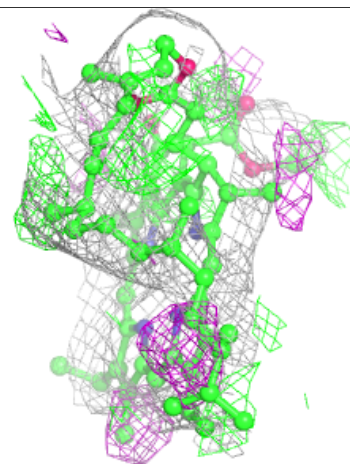
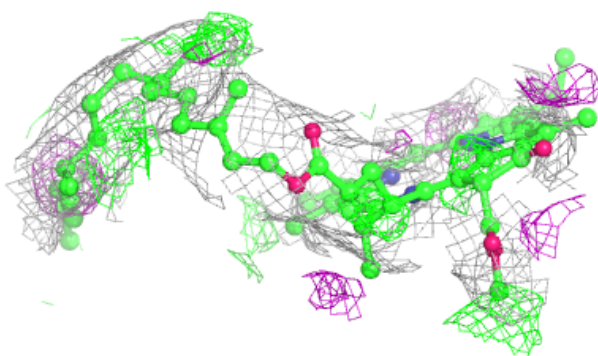
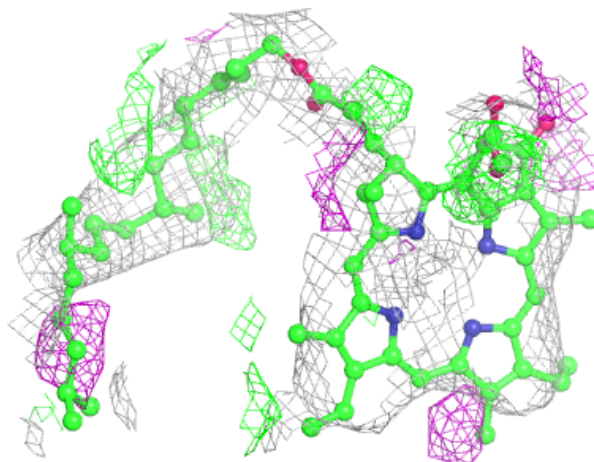
Electron density around PHO A 608:

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



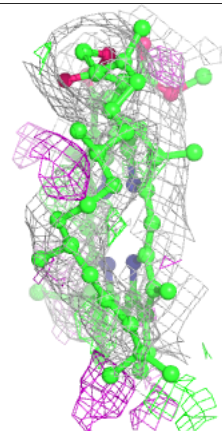
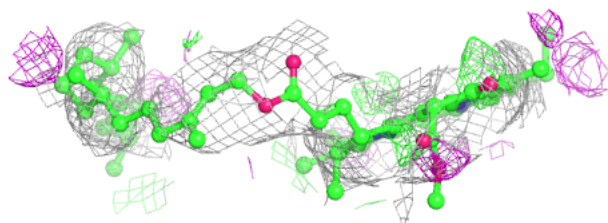
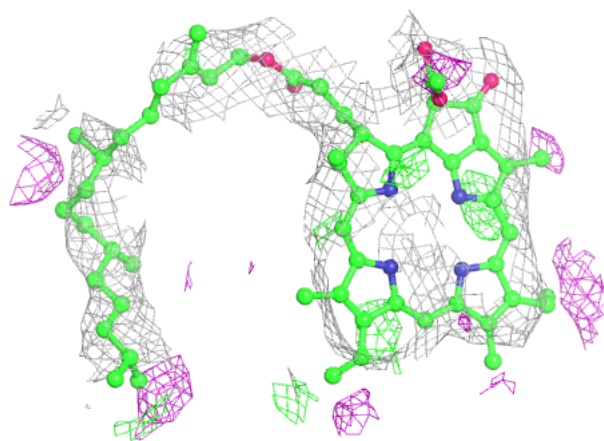
Electron density around PHO D 401:

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



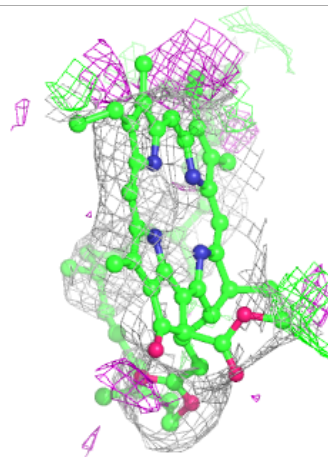
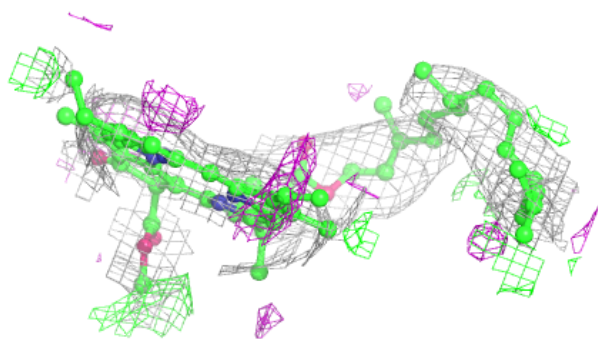
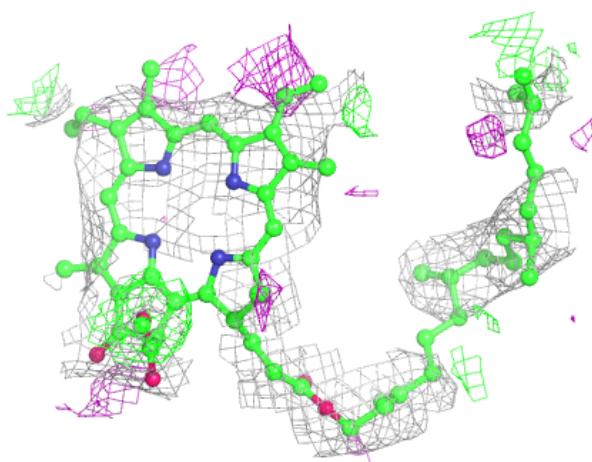
Electron density around PHO a 608:

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



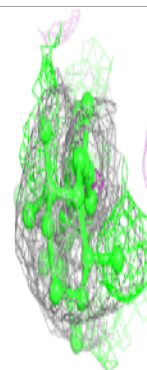
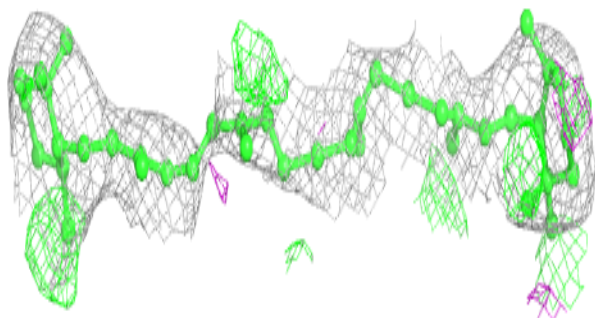
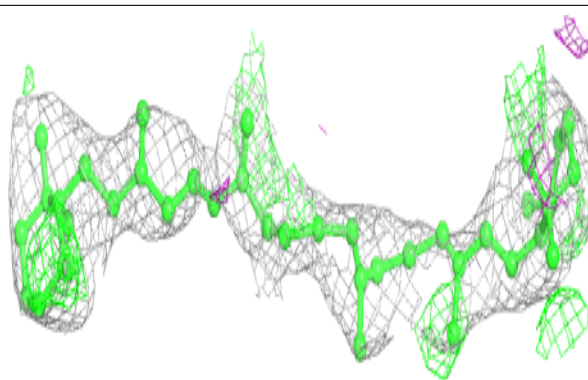
Electron density around PHO d 401:

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

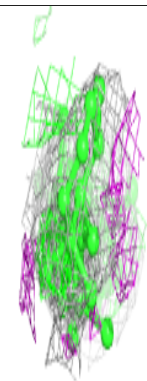
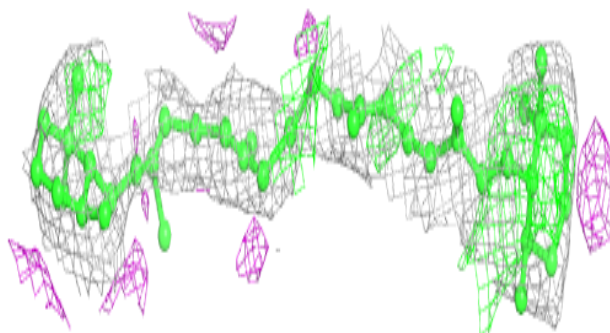
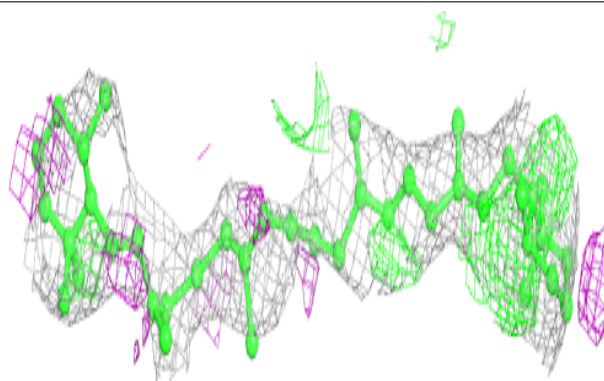


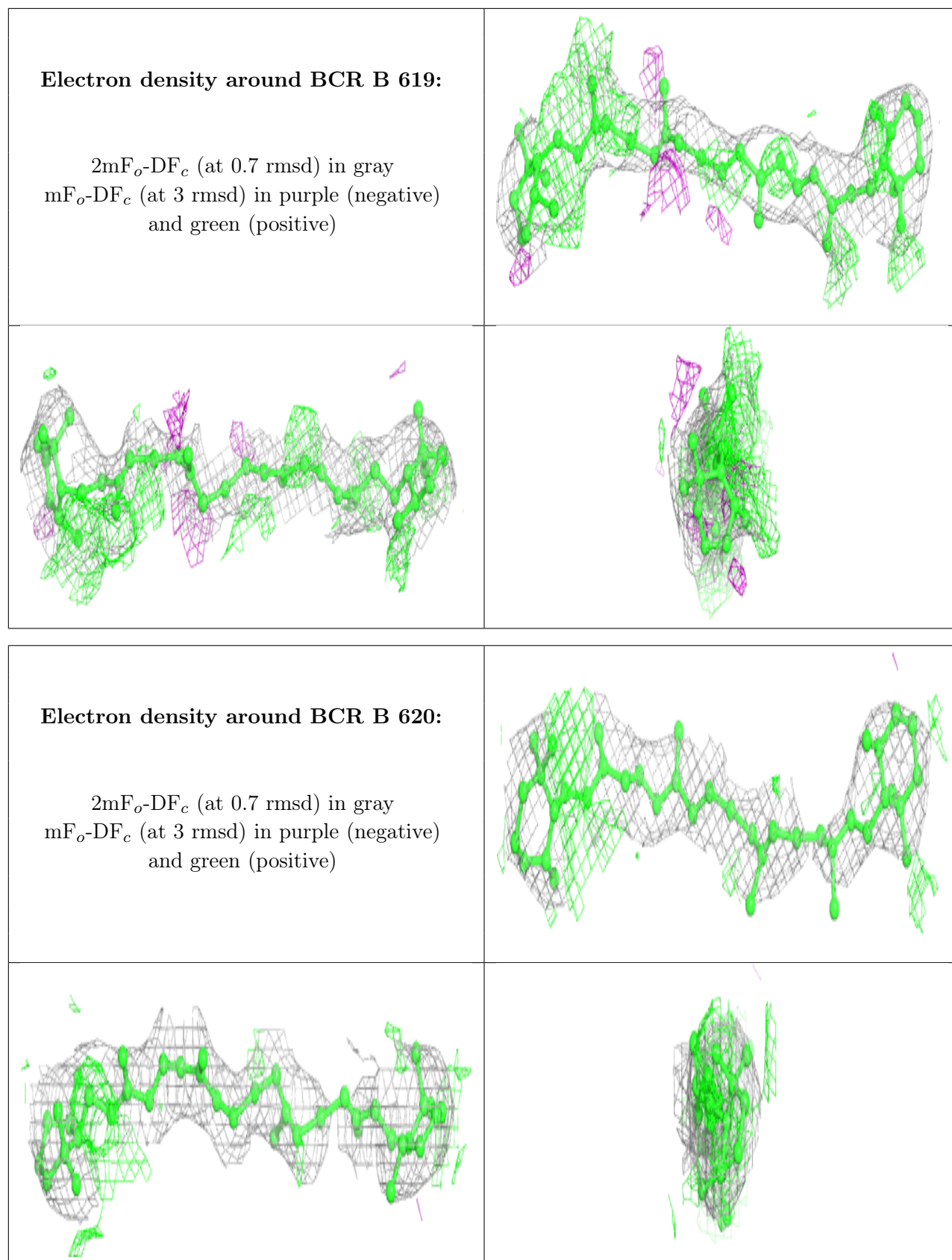
Electron density around BCR A 610:

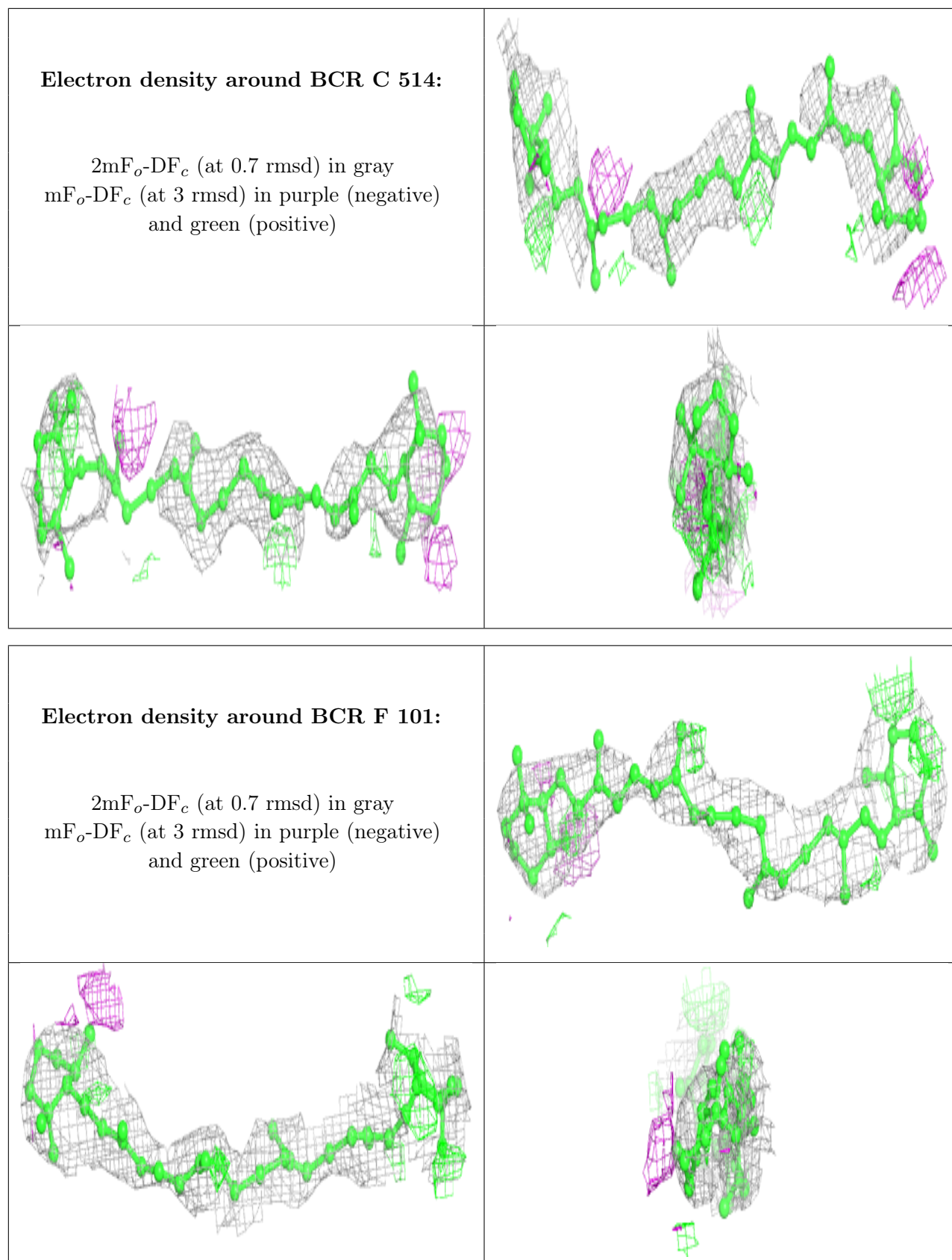
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCR B 618:**

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

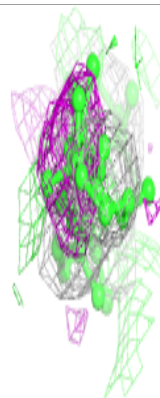
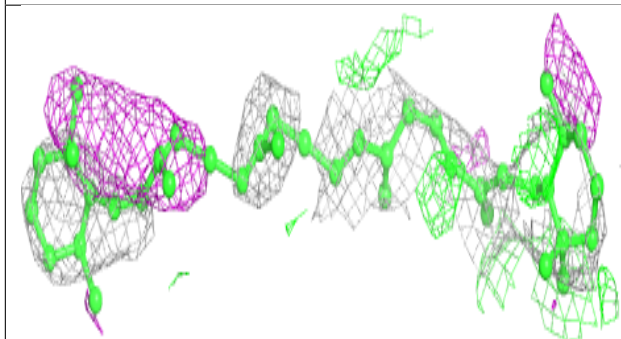
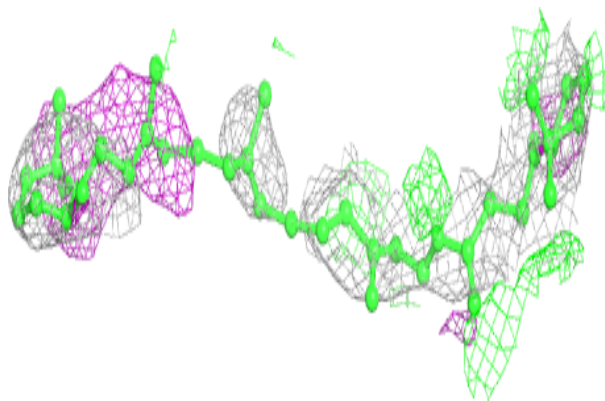




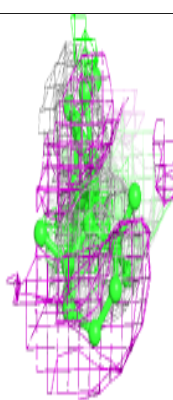
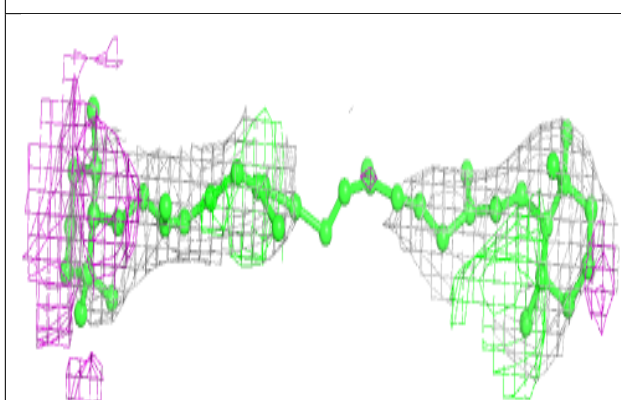
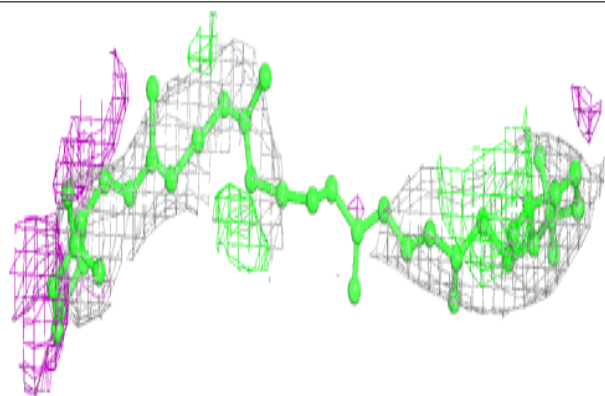


Electron density around BCR H 101:

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

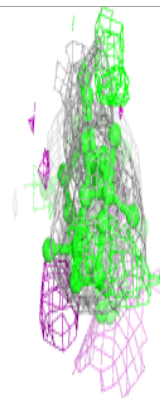
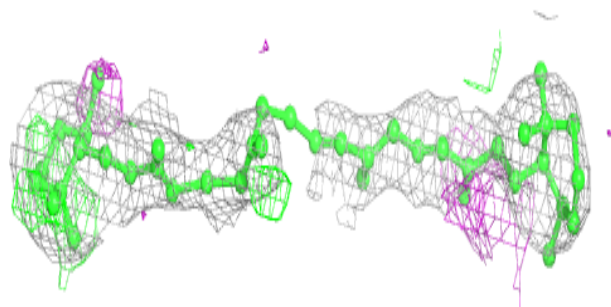
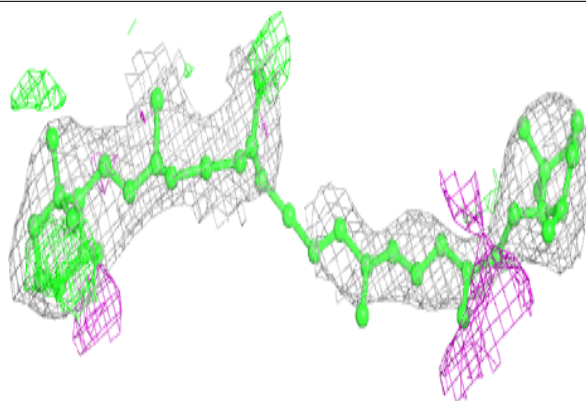
**Electron density around BCR I 101:**

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

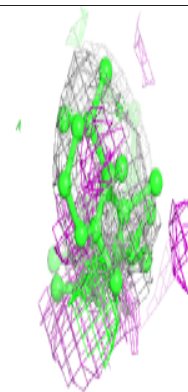
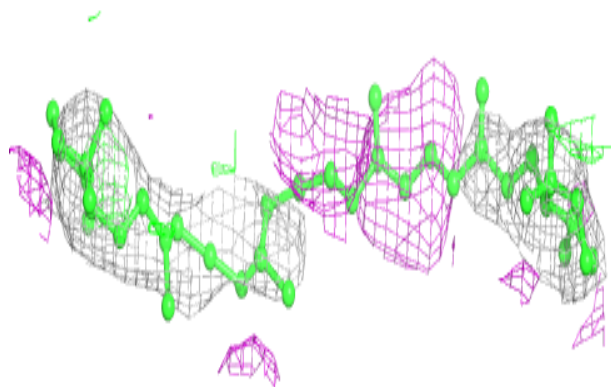
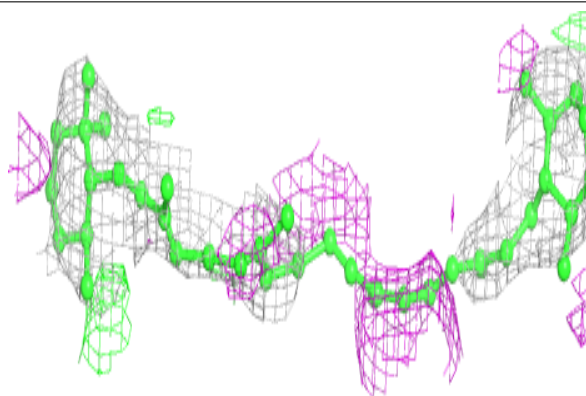


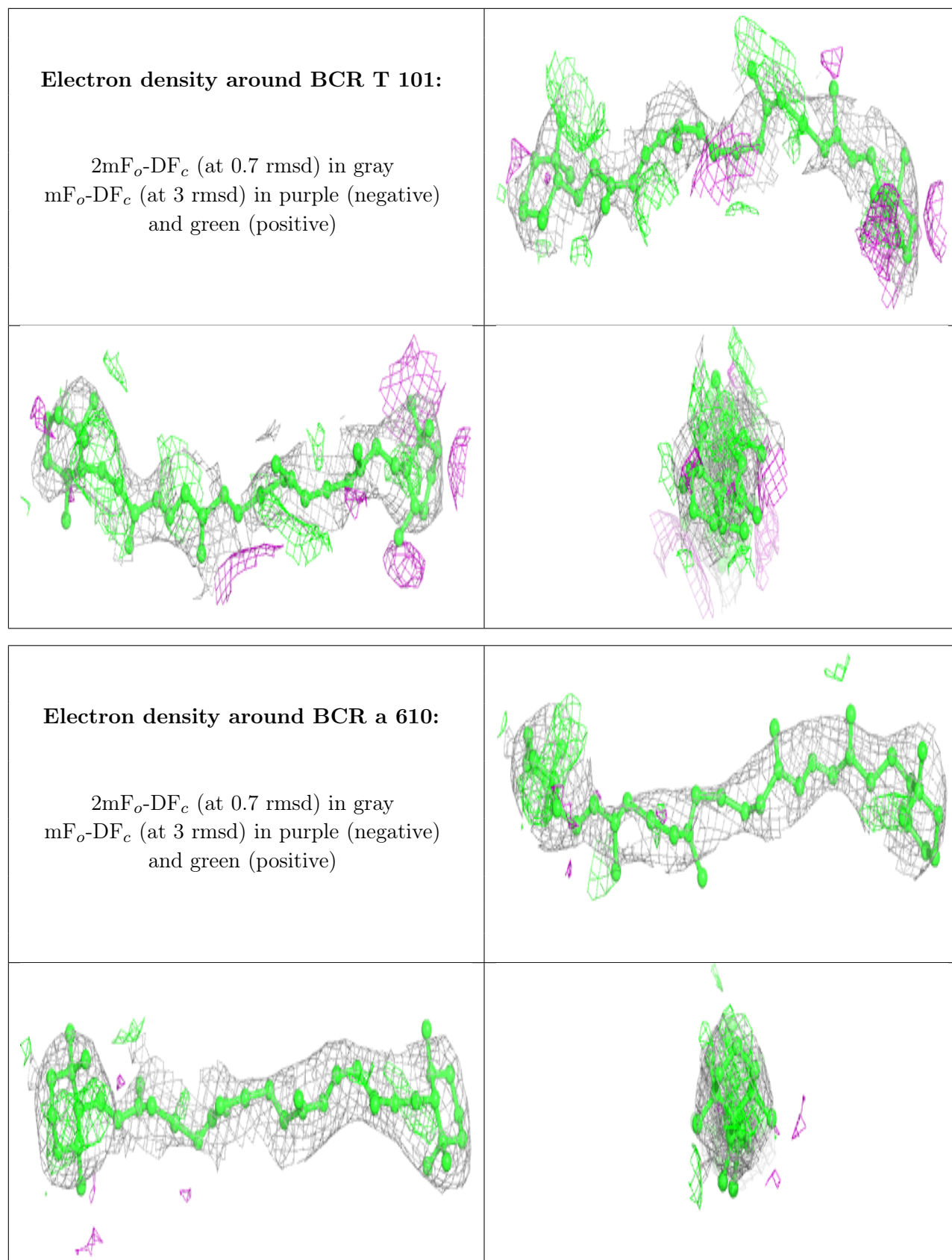
Electron density around BCR K 101:

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

**Electron density around BCR K 102:**

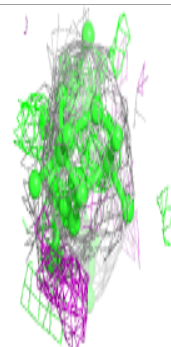
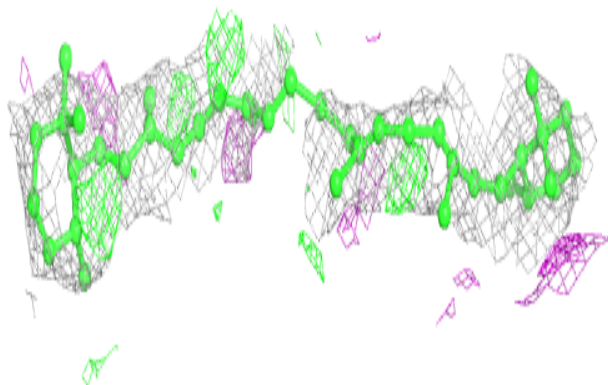
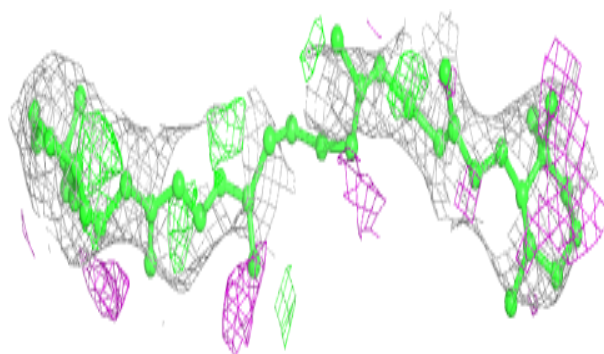
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



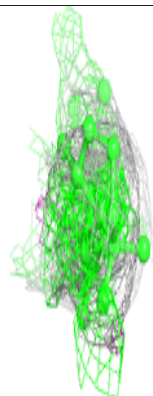
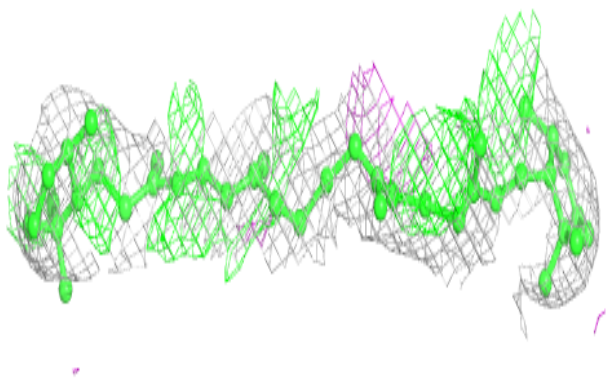
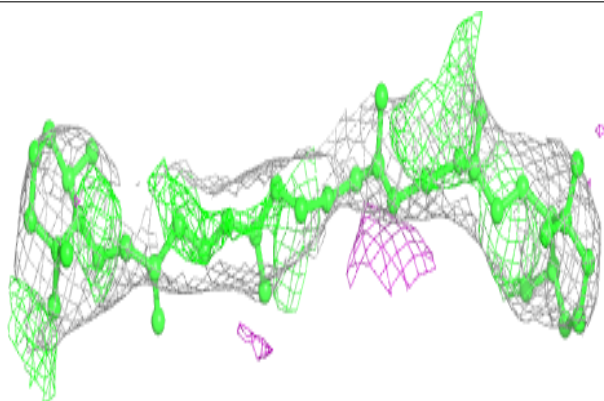


Electron density around BCR b 619:

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

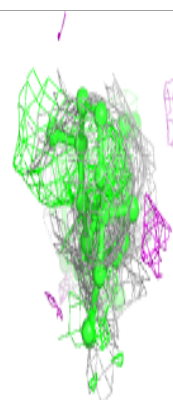
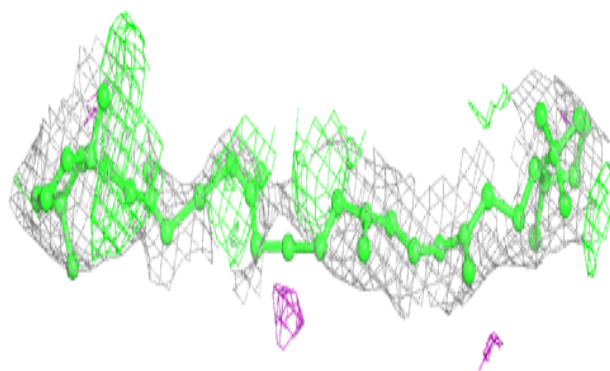
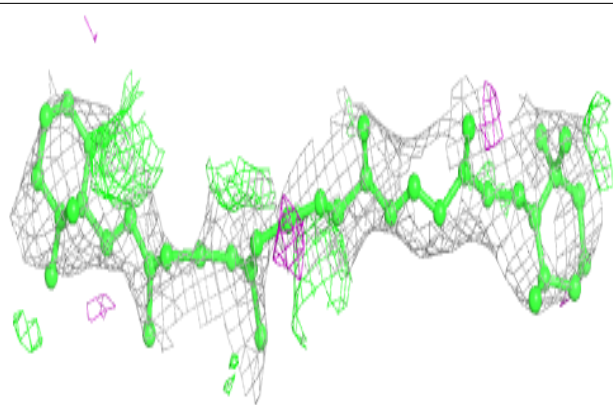
**Electron density around BCR b 620:**

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

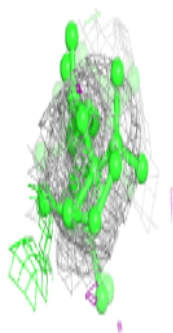
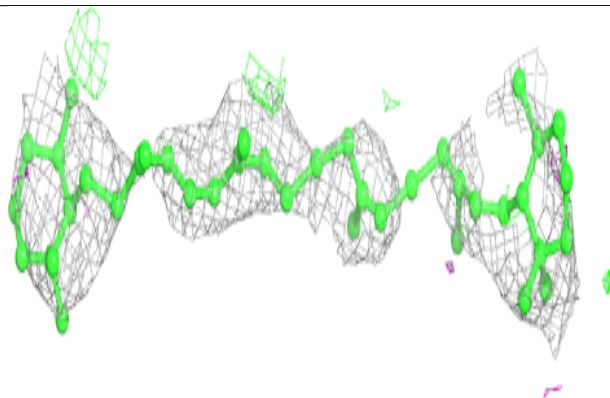
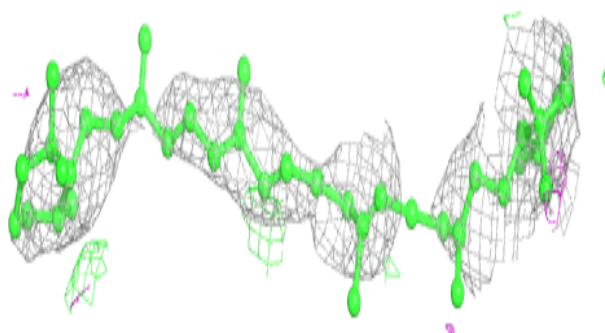


Electron density around BCR b 621:

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

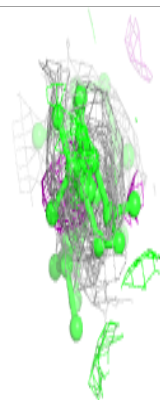
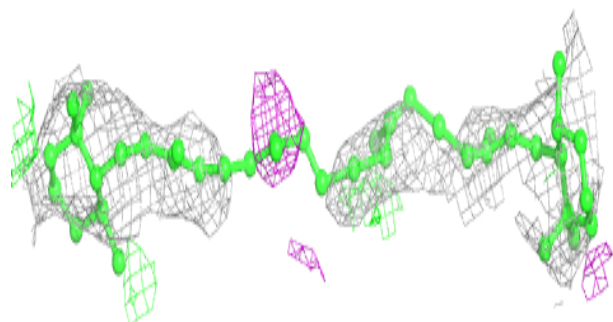
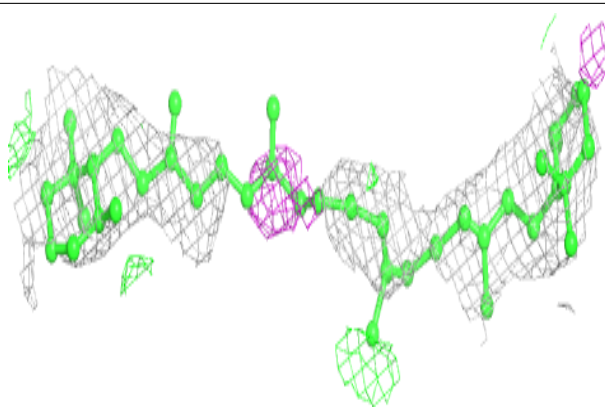
**Electron density around BCR c 514:**

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

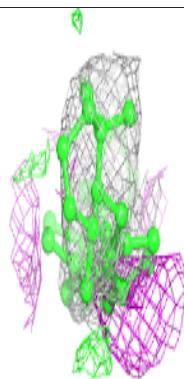
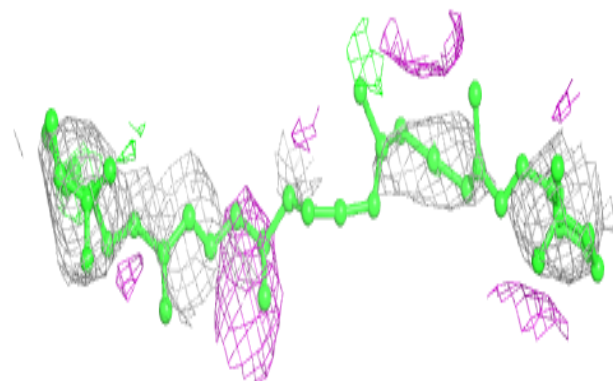
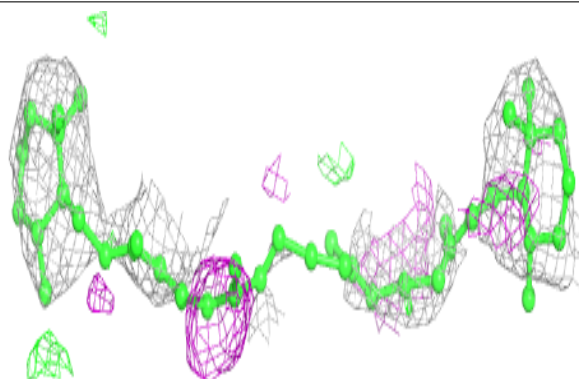


Electron density around BCR c 515:

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

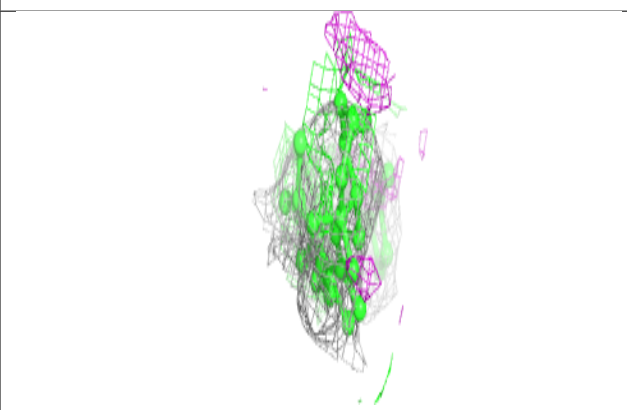
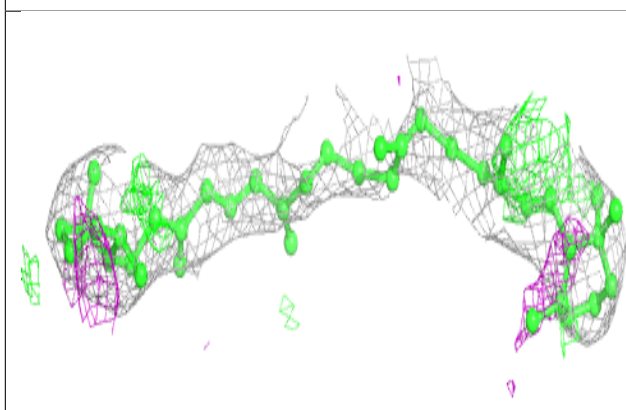
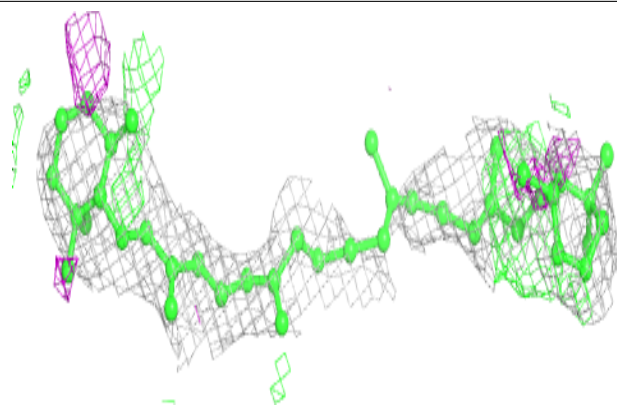
**Electron density around BCR c 521:**

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

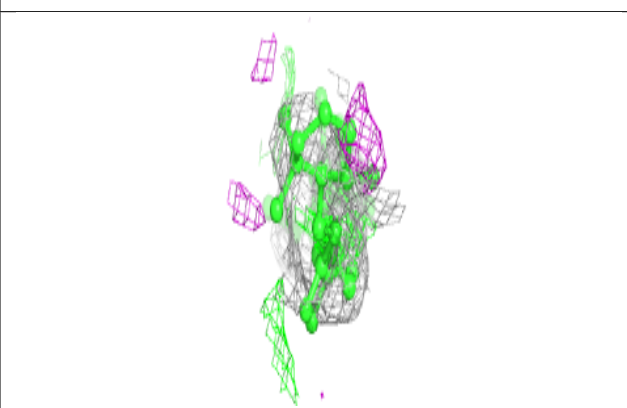
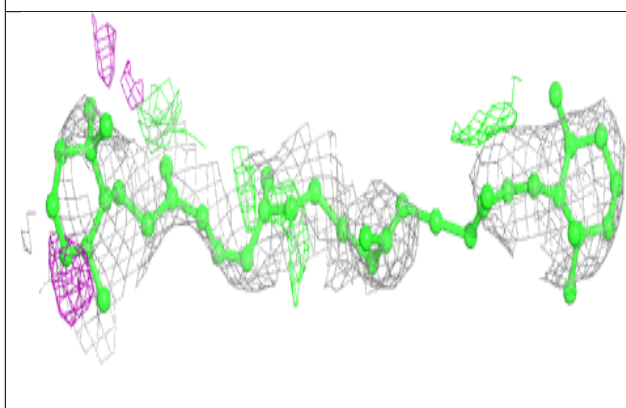
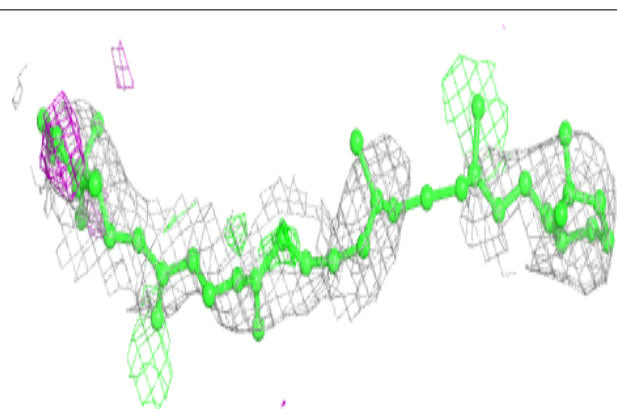


Electron density around BCR f 101:

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

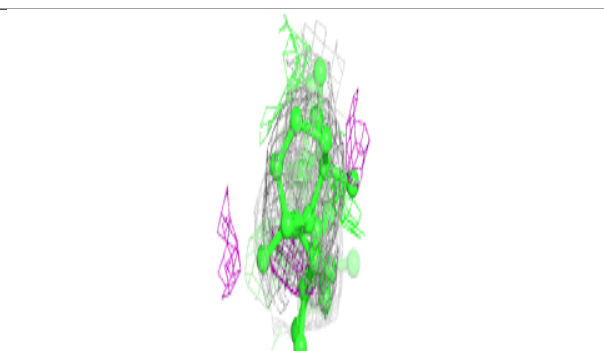
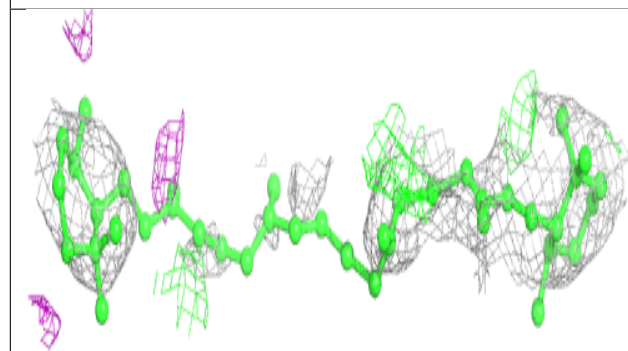
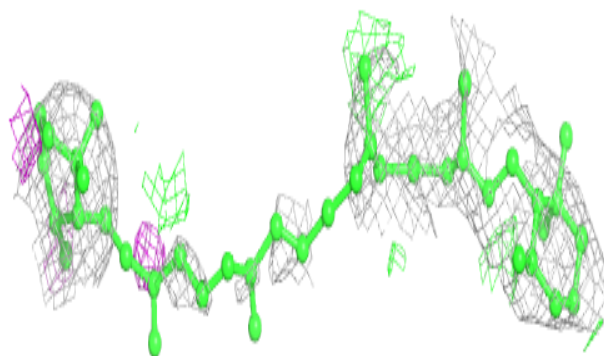
**Electron density around BCR h 101:**

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

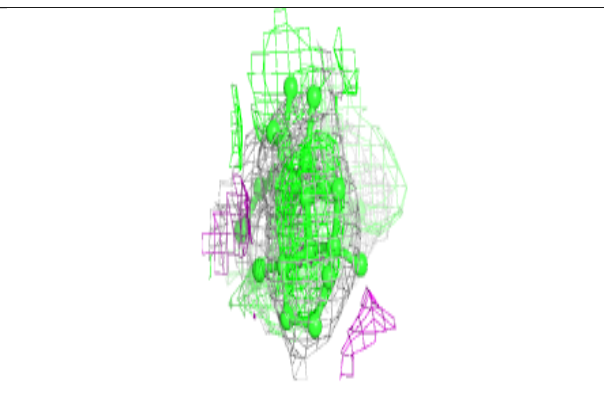
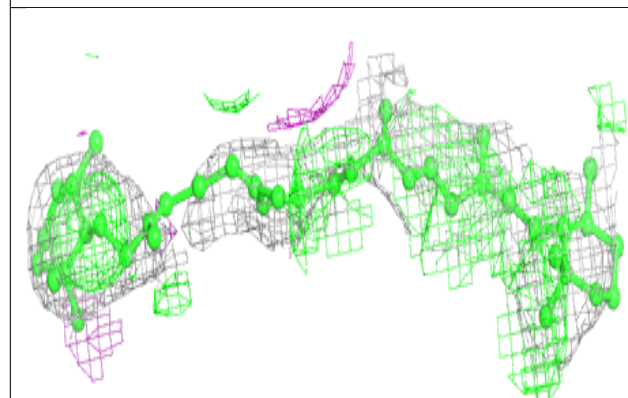
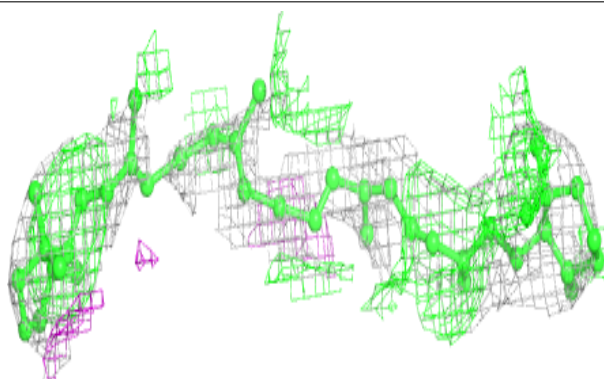


Electron density around BCR k 101:

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

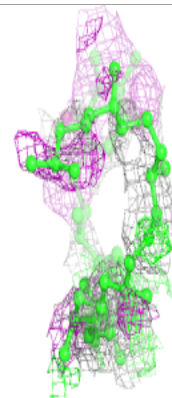
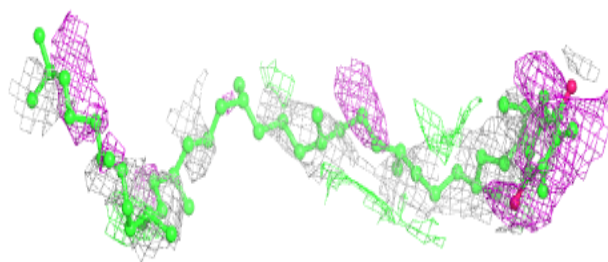
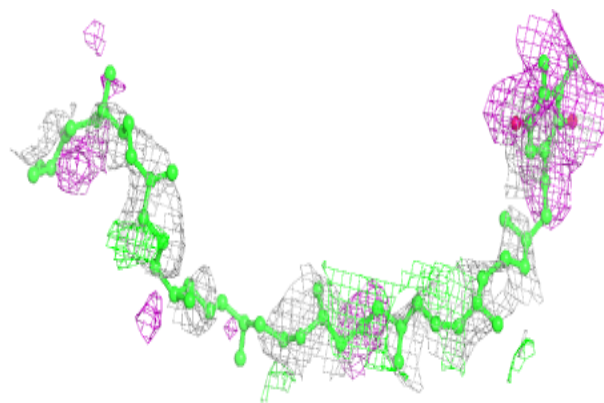
**Electron density around BCR t 101:**

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

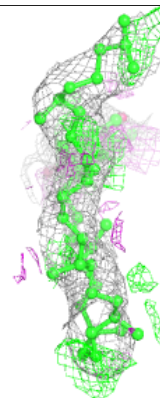
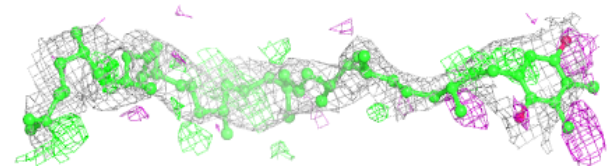
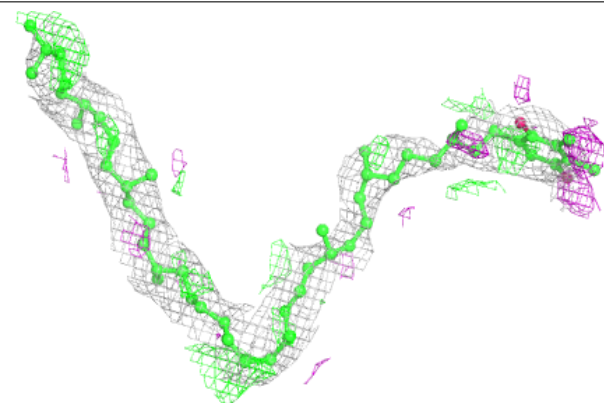


Electron density around PL9 A 611:

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

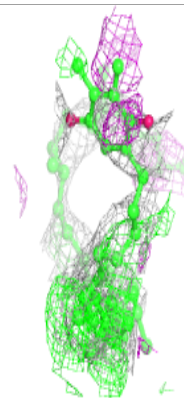
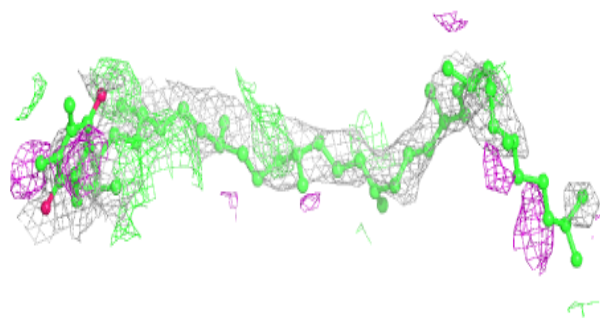
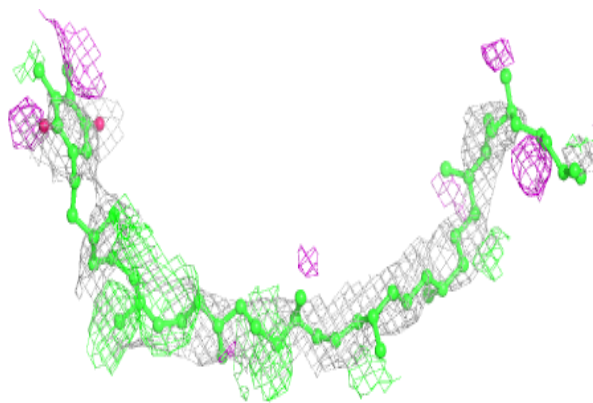
**Electron density around PL9 D 405:**

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

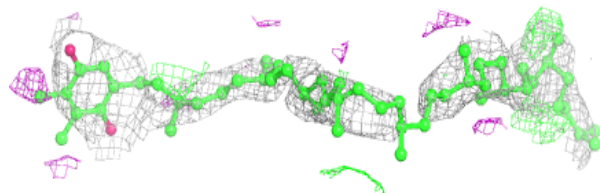
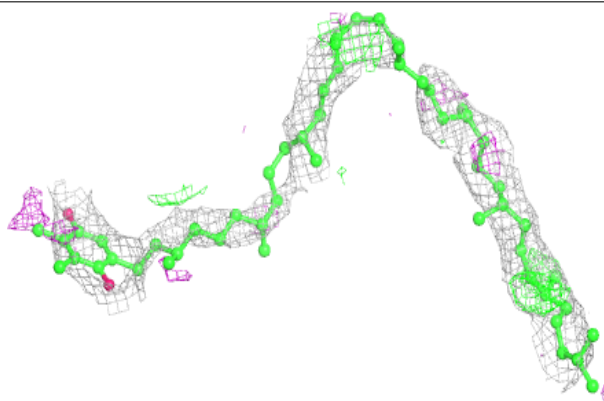


Electron density around PL9 a 611:

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

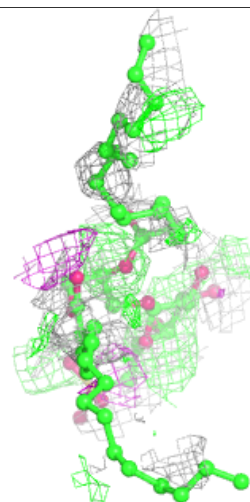
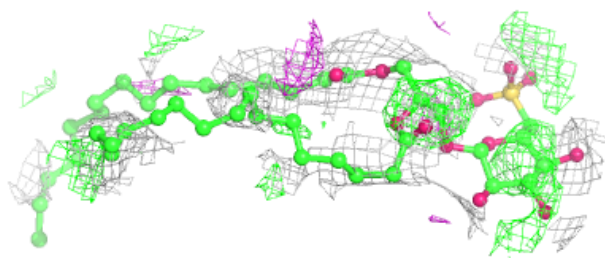
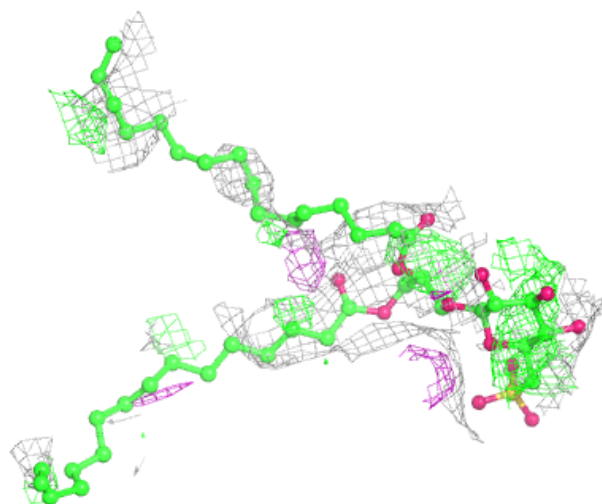
**Electron density around PL9 d 404:**

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



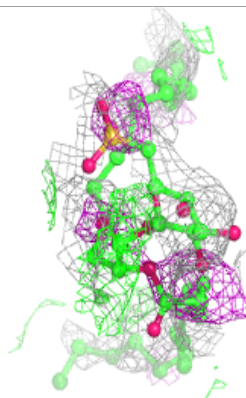
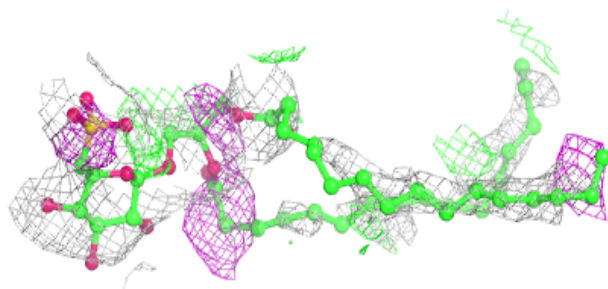
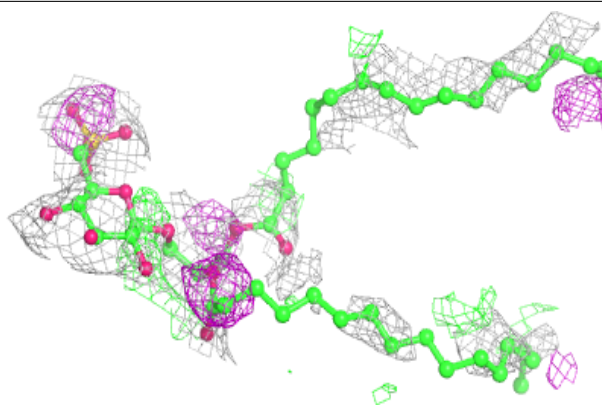
Electron density around SQD A 612:

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

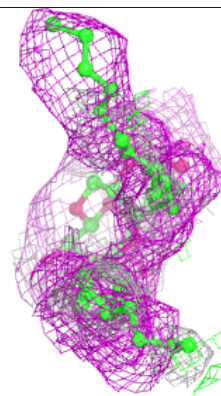
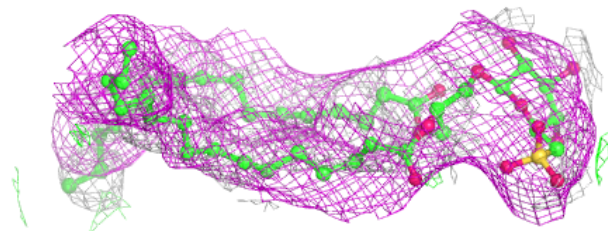
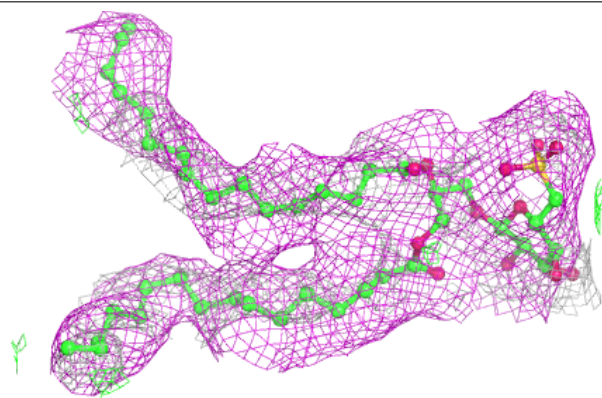


Electron density around SQD A 614:

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

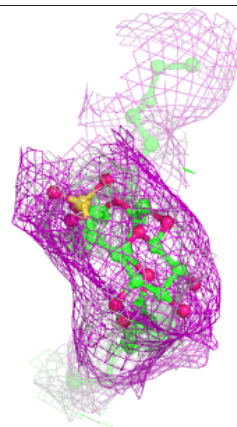
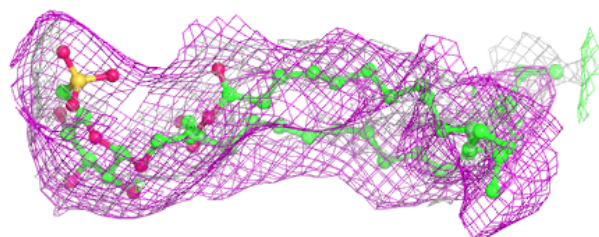
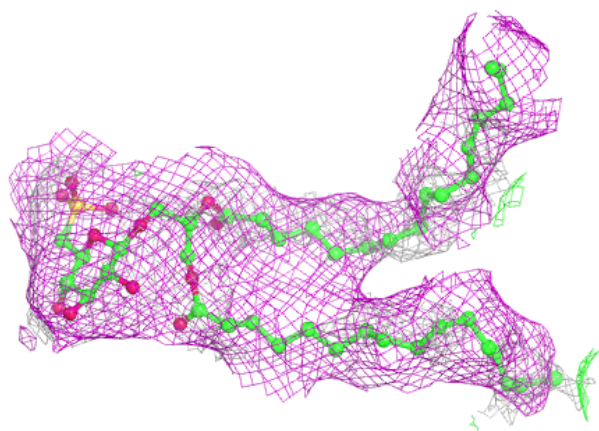
**Electron density around SQD B 622:**

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

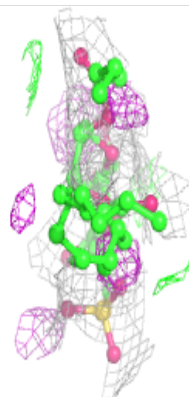
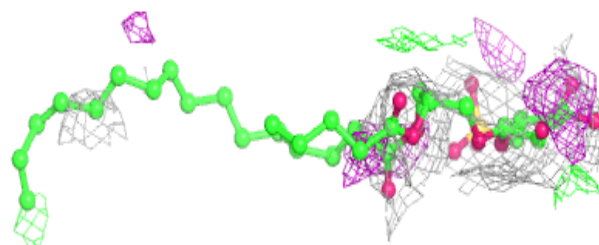
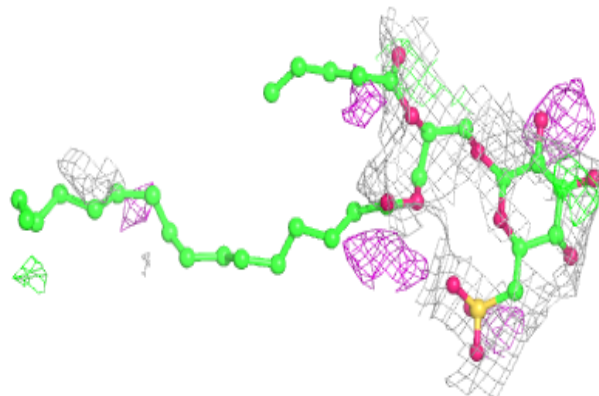


Electron density around SQD L 102:

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

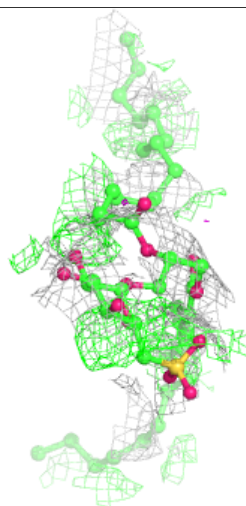
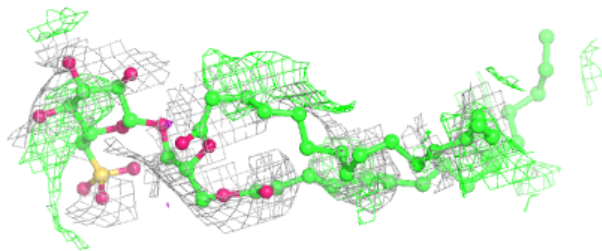
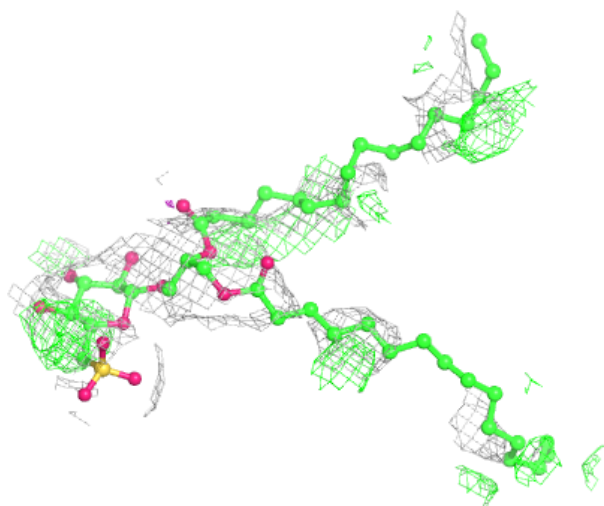
**Electron density around SQD X 101:**

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



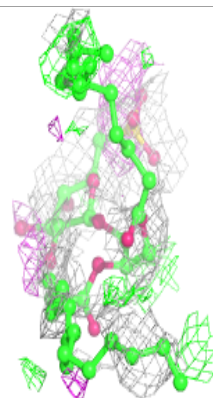
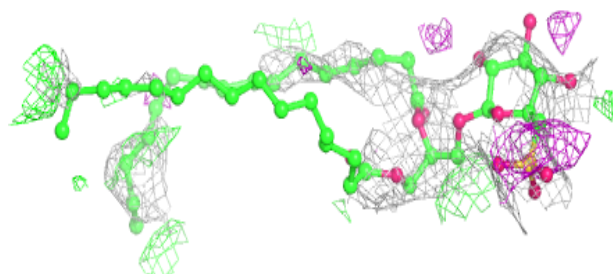
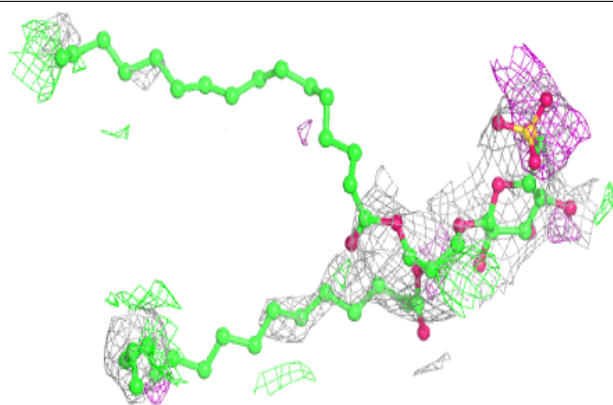
Electron density around SQD a 612:

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

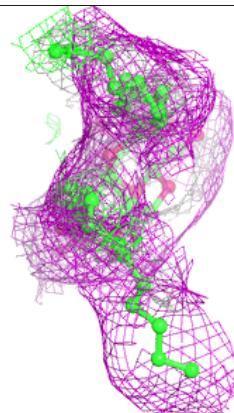
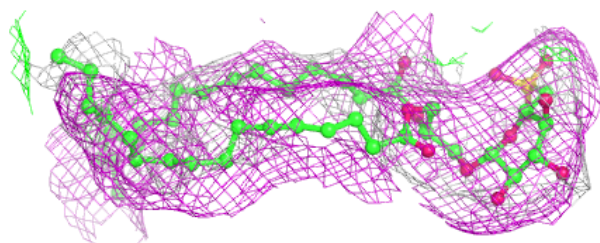
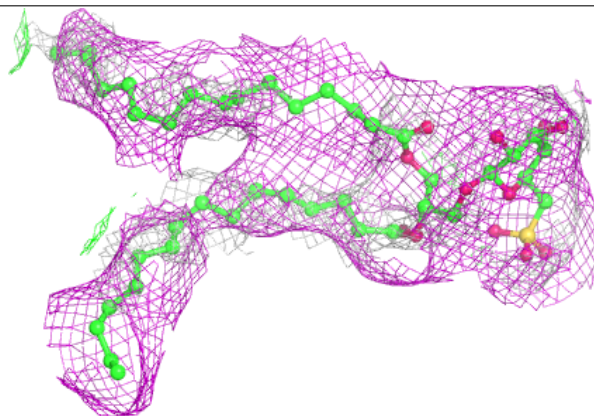


Electron density around SQD a 614:

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

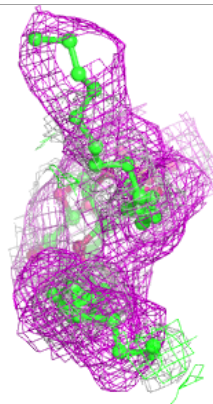
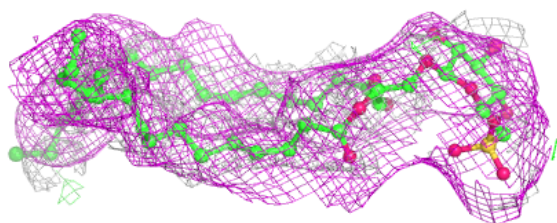
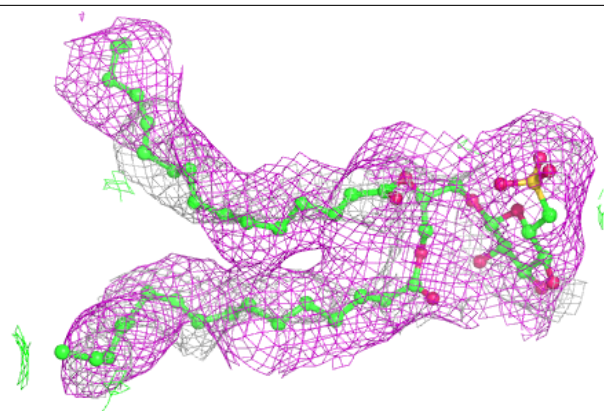
**Electron density around SQD b 601:**

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

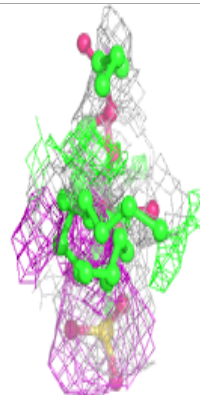
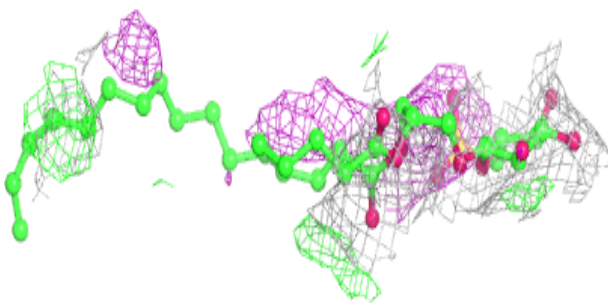
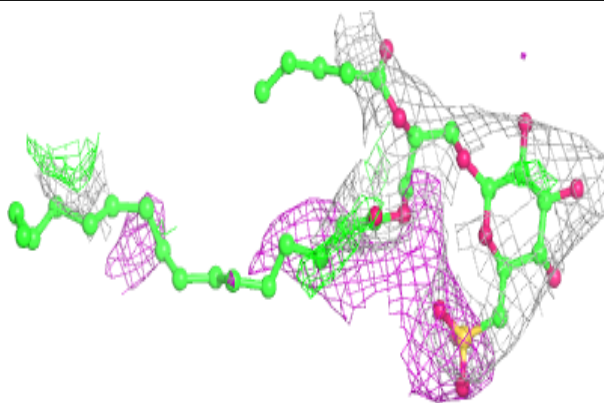


Electron density around SQD 1 101:

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

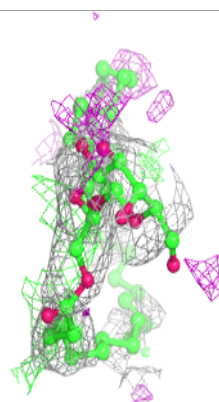
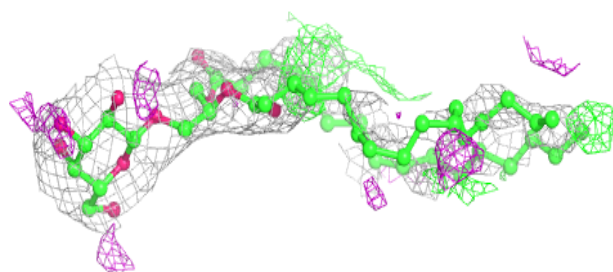
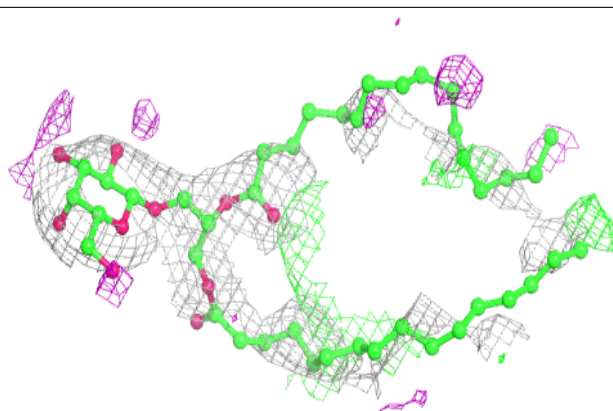
**Electron density around SQD x 101:**

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

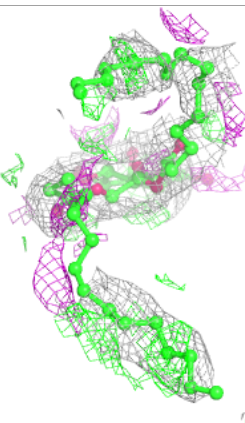
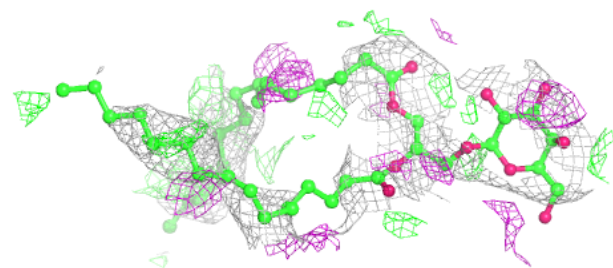
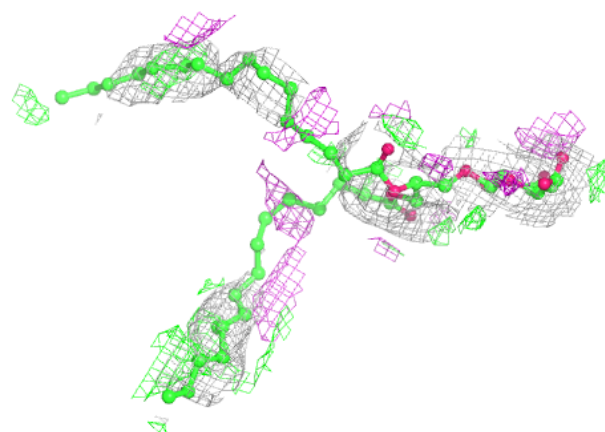


Electron density around LMG A 613:

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

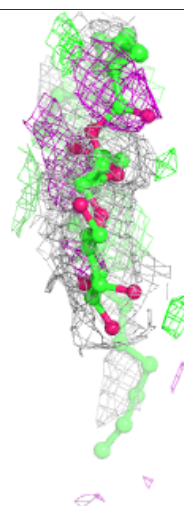
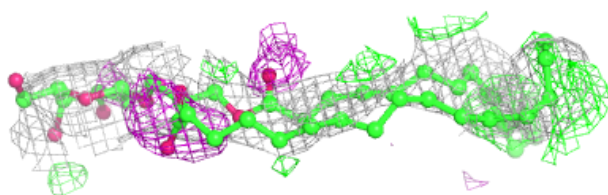
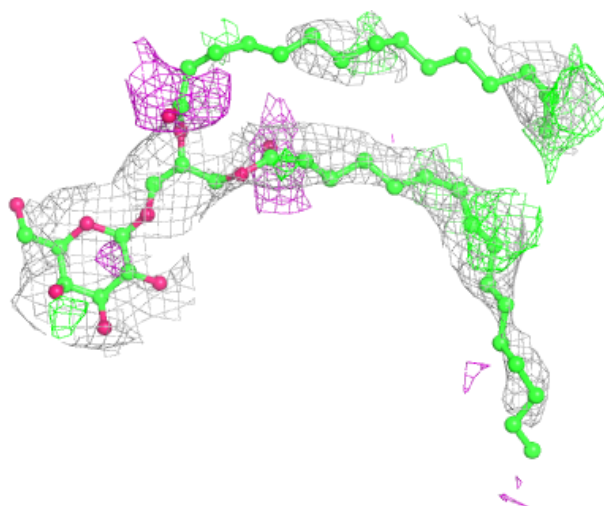
**Electron density around LMG B 621:**

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



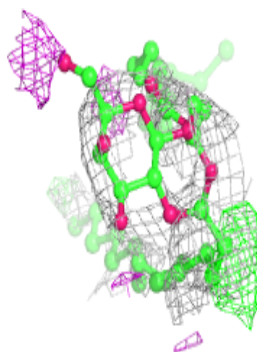
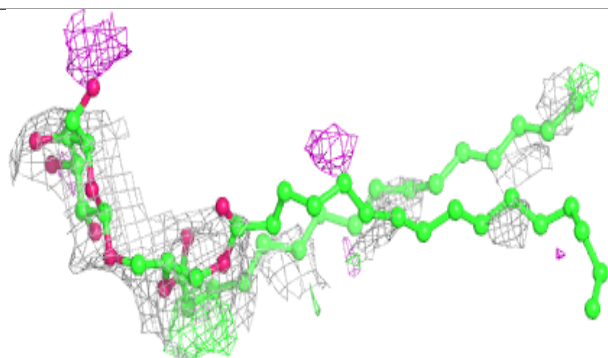
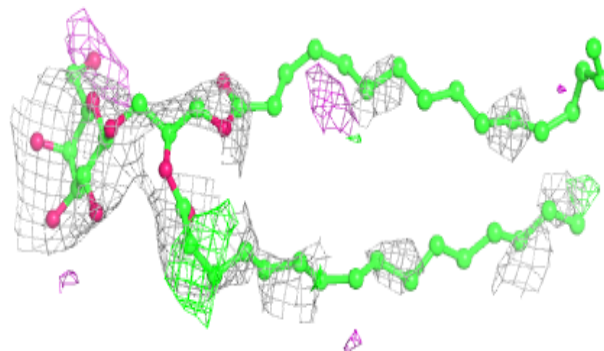
Electron density around LMG C 518:

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

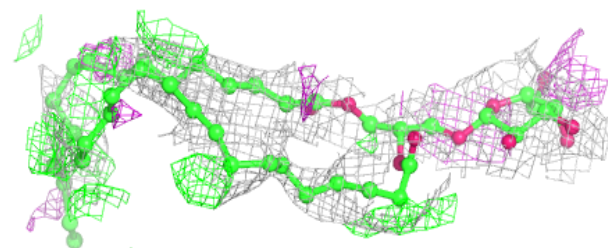
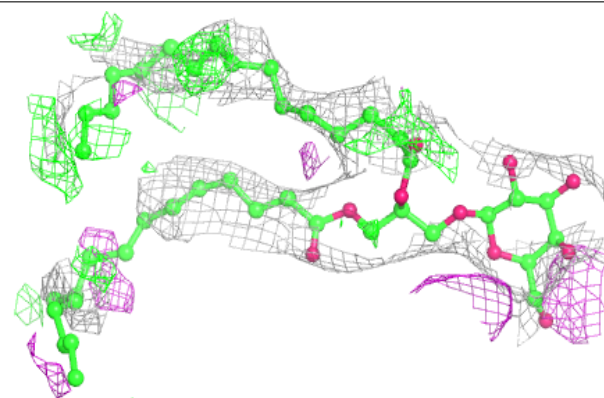


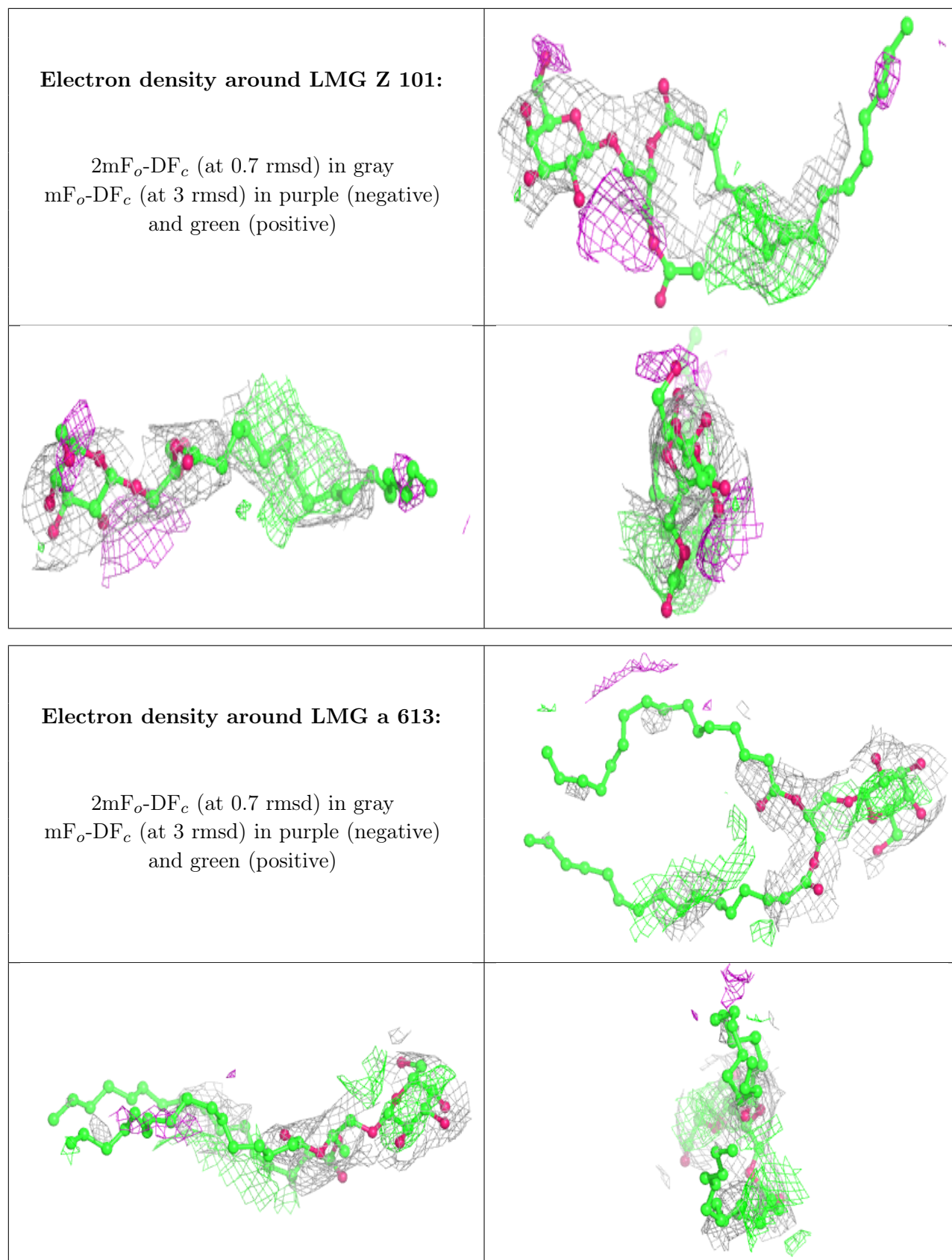
Electron density around LMG C 519:

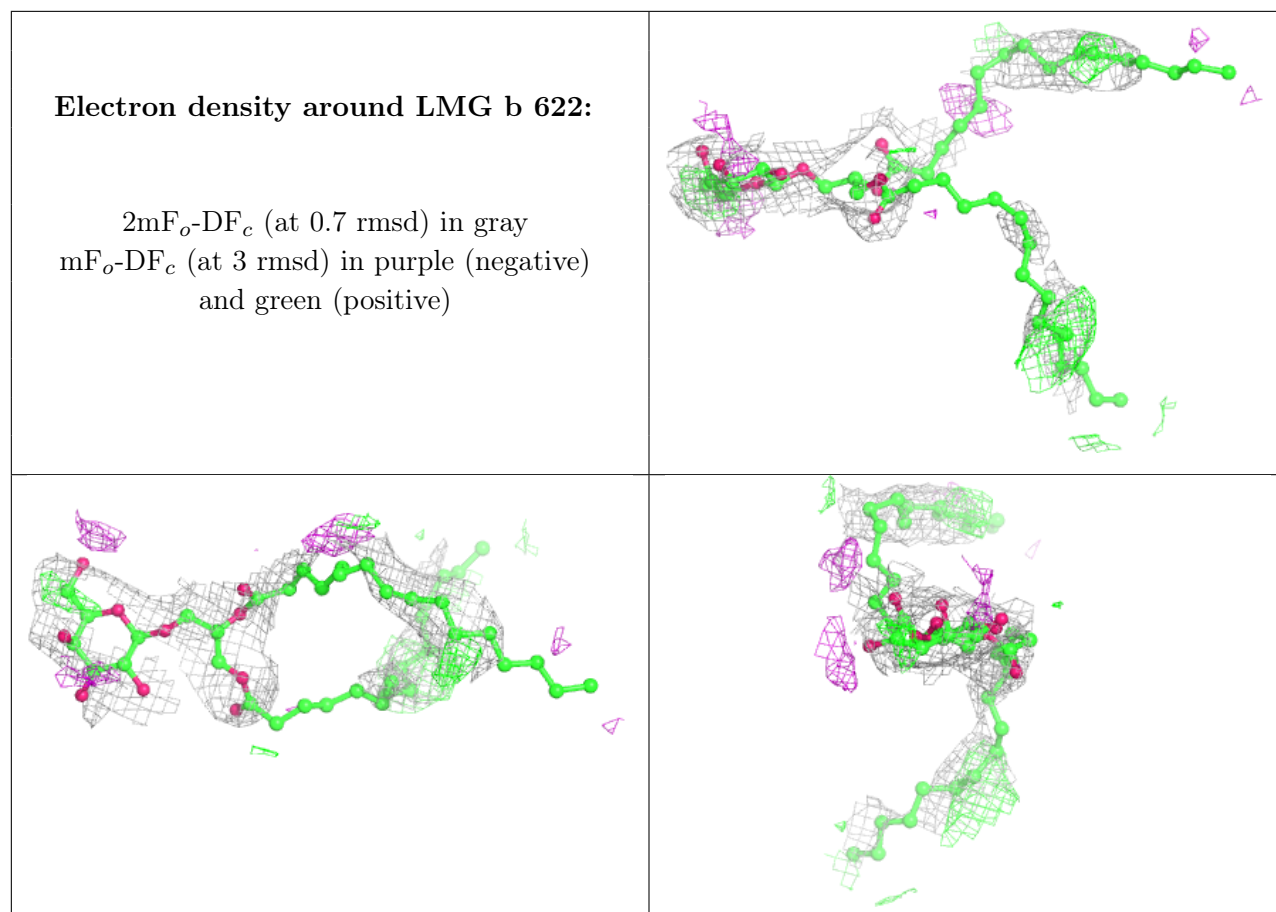
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LMG D 408:**

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

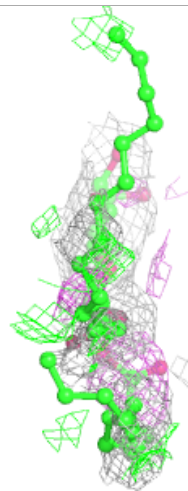
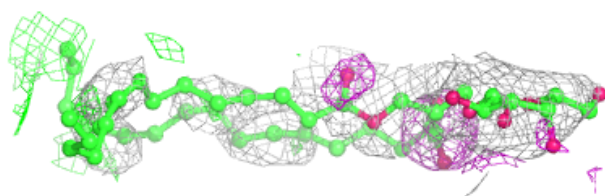
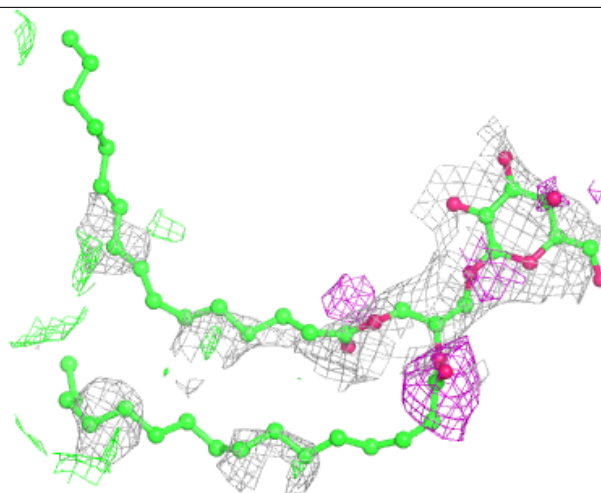






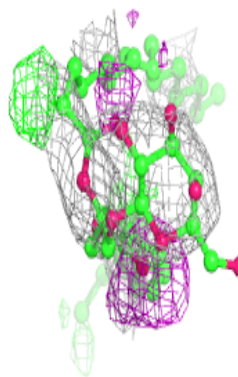
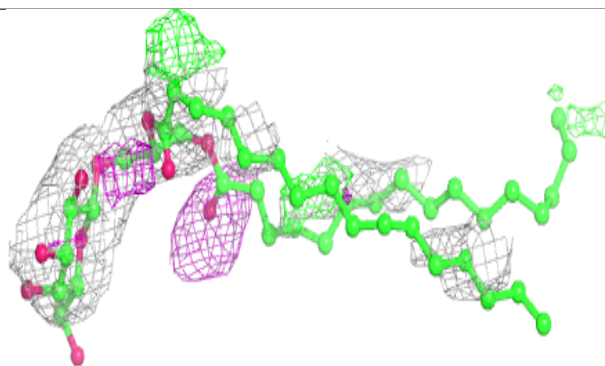
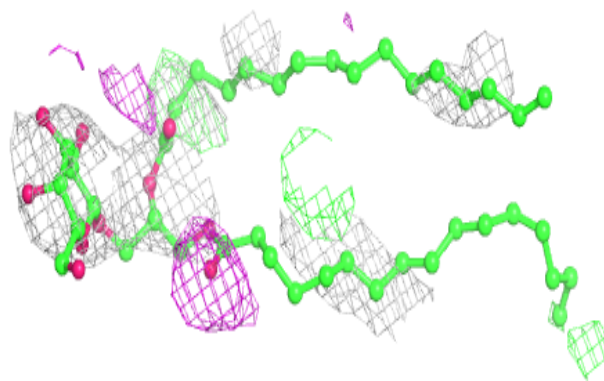
Electron density around LMG c 519:

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

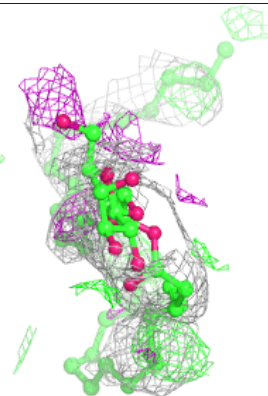
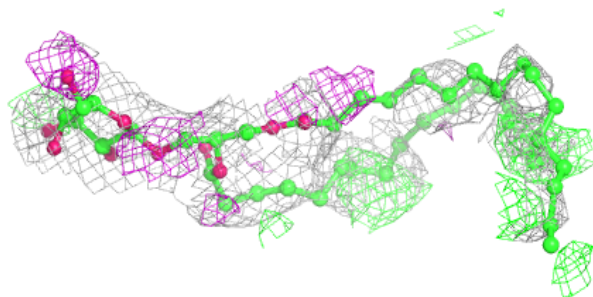
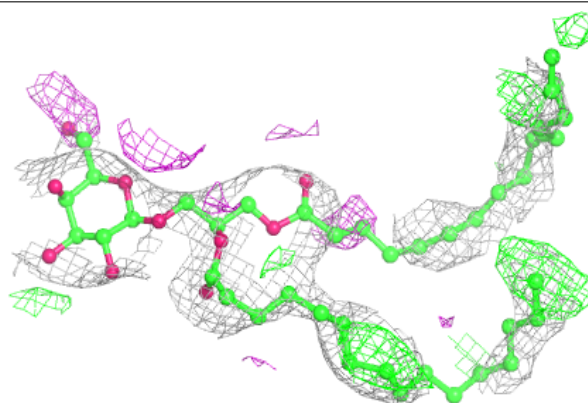


Electron density around LMG c 520:

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

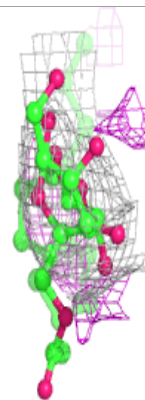
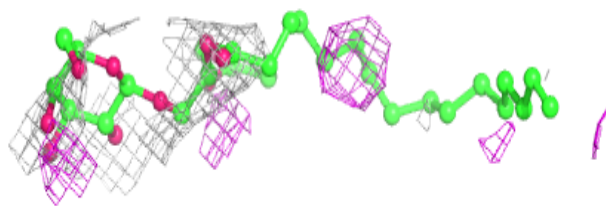
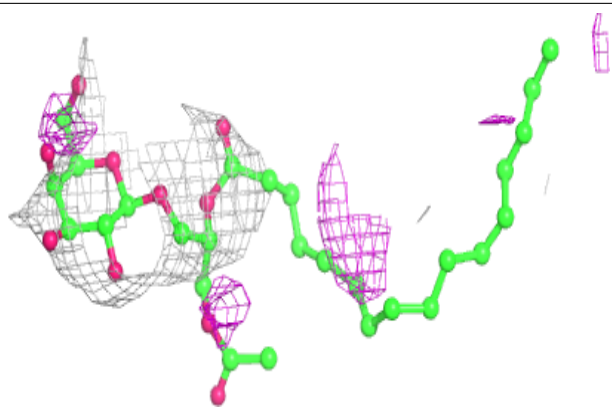
**Electron density around LMG j 101:**

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

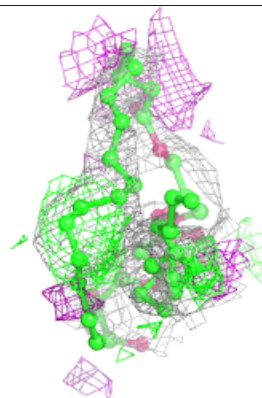
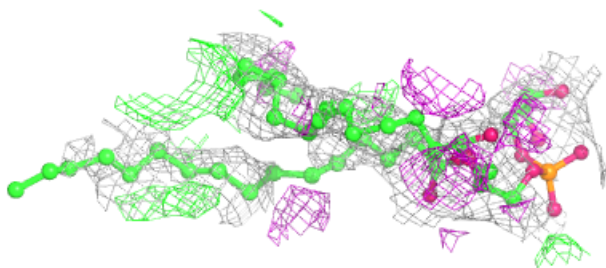
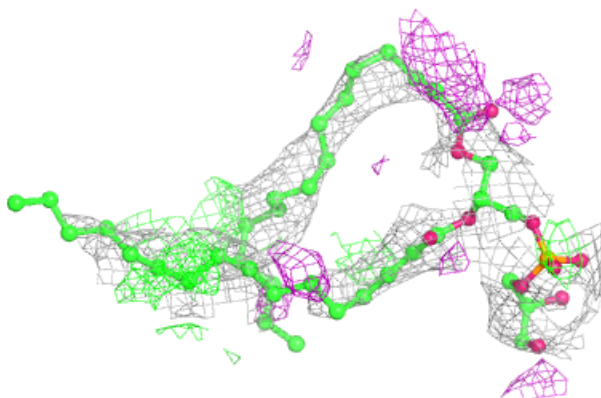


Electron density around LMG z 101:

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

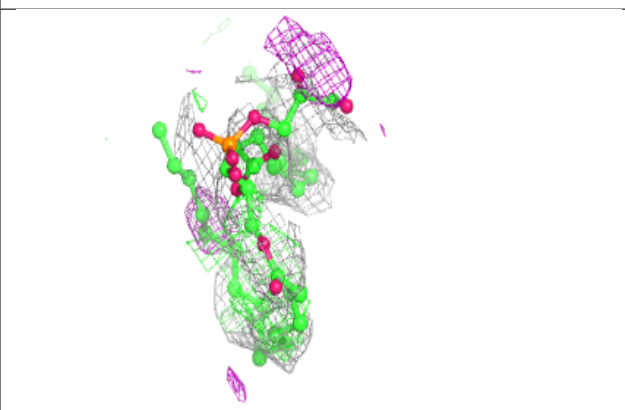
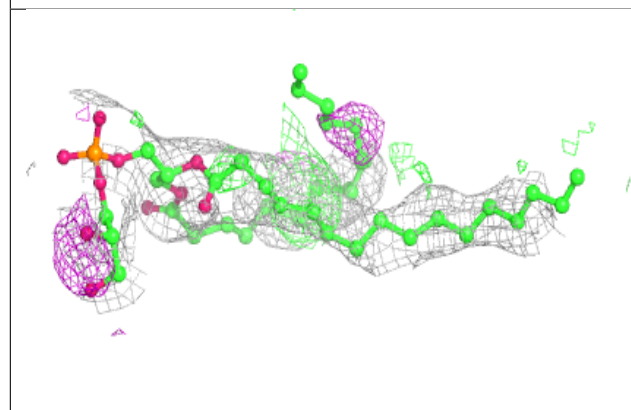
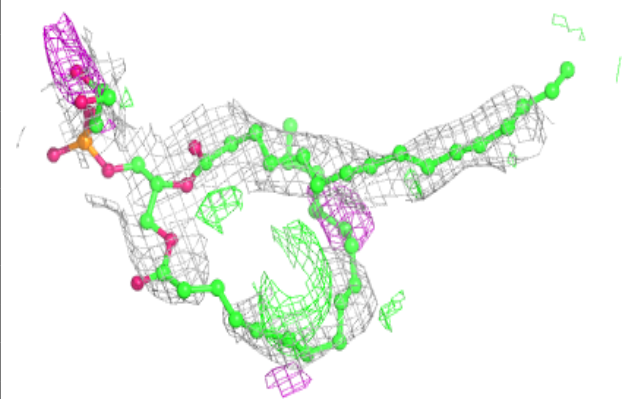
**Electron density around LHG A 615:**

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

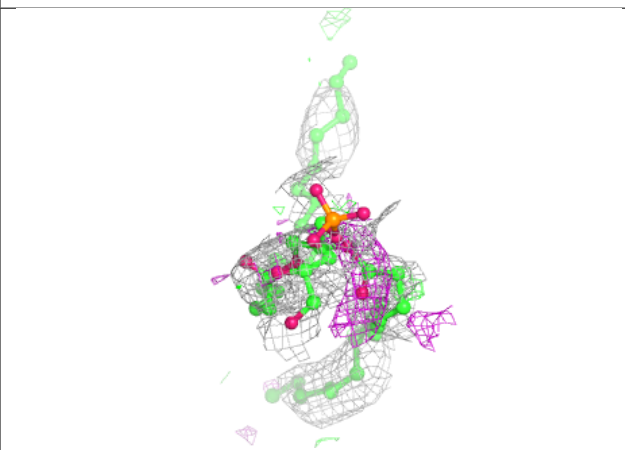
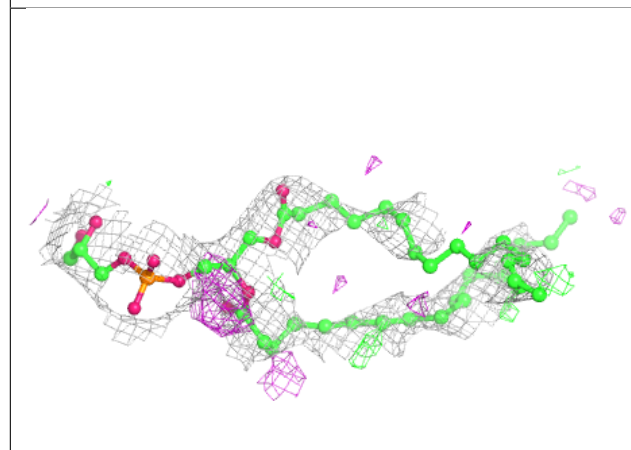
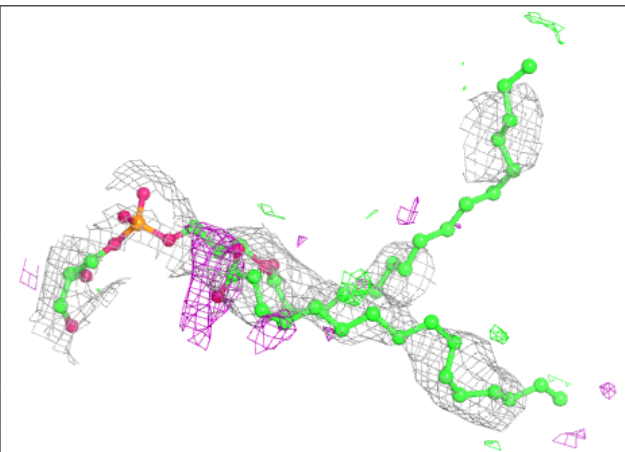


Electron density around LHG D 406:

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

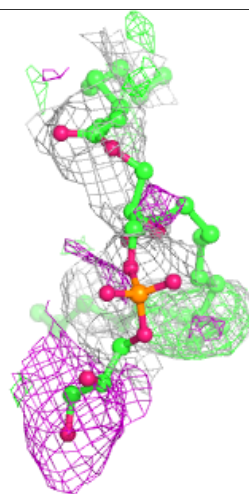
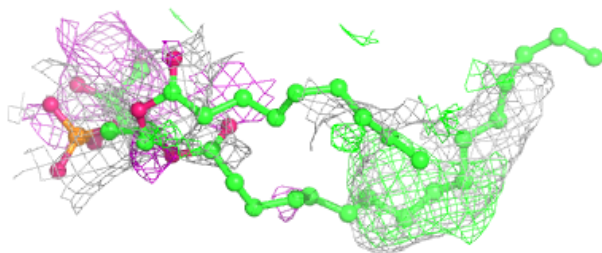
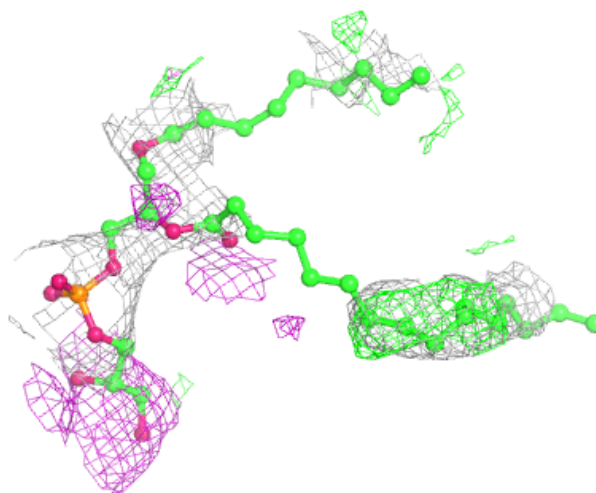
**Electron density around LHG D 407:**

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



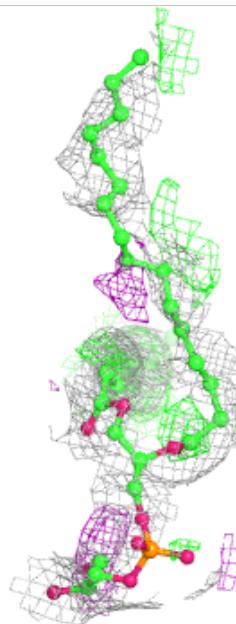
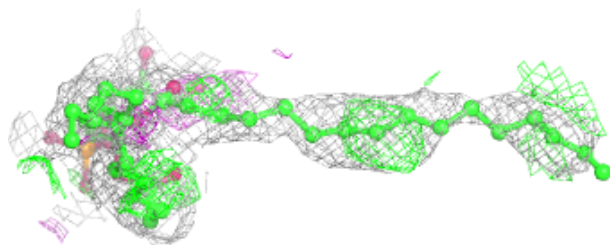
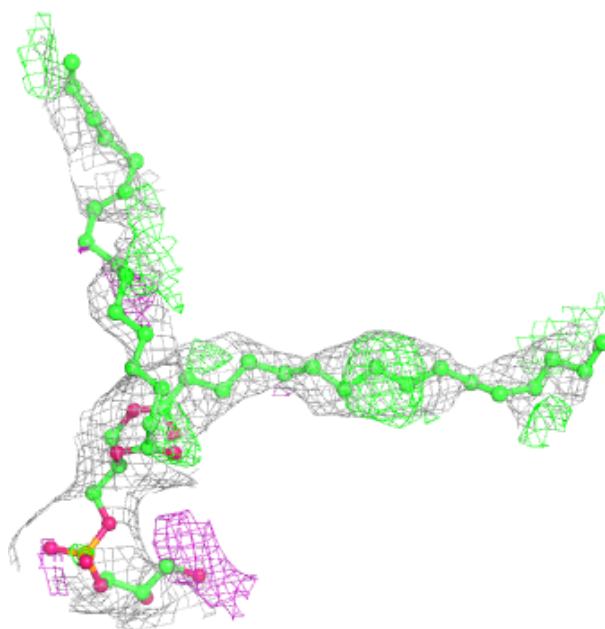
Electron density around LHG E 102:

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



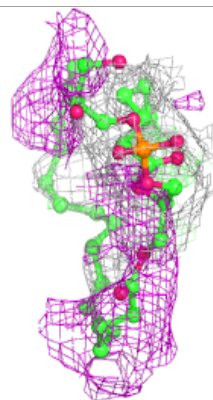
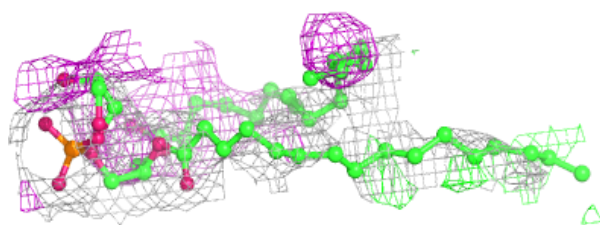
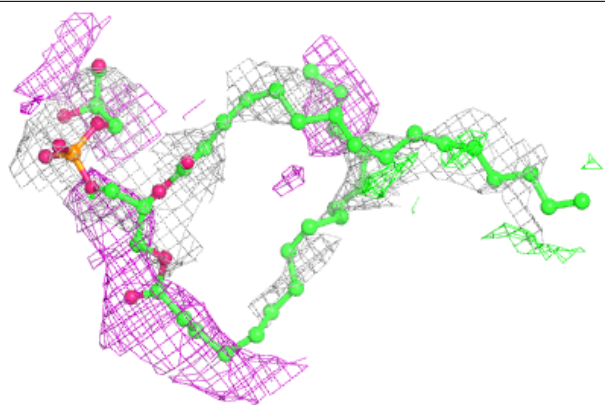
Electron density around LHG L 101:

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

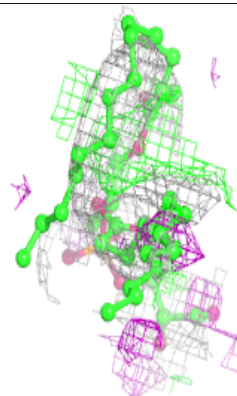
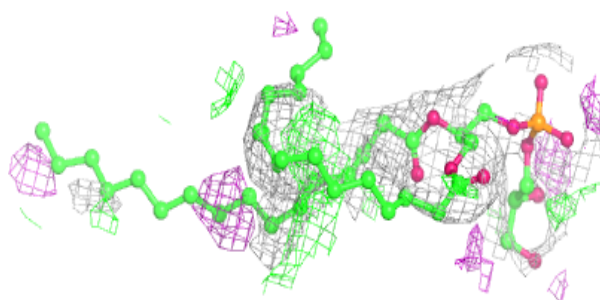
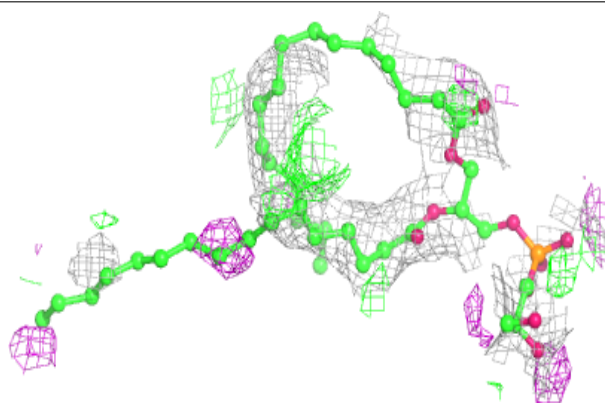


Electron density around LHG a 616:

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

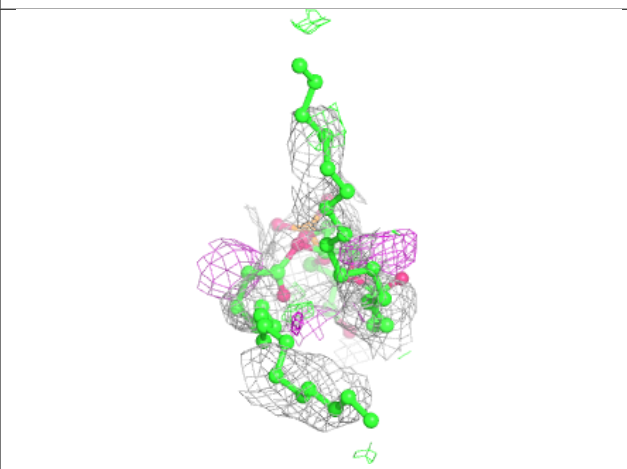
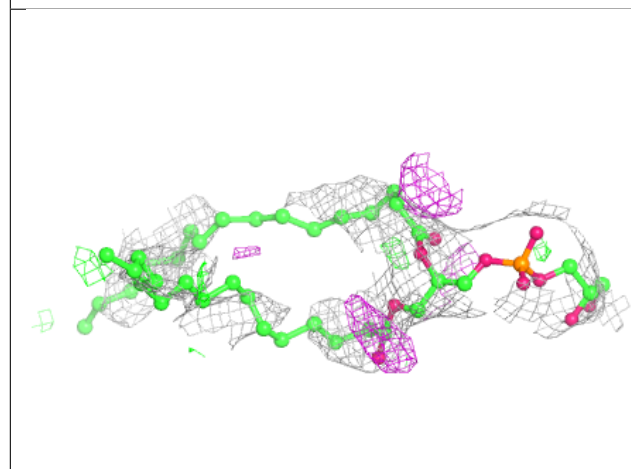
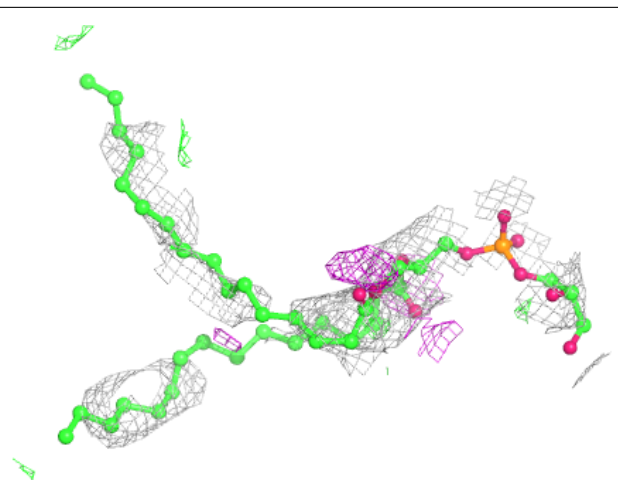
**Electron density around LHG d 406:**

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



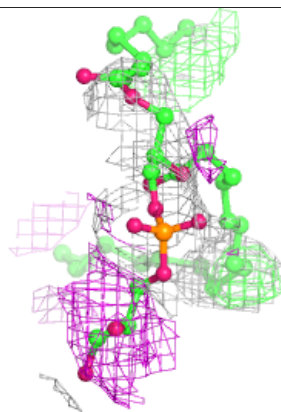
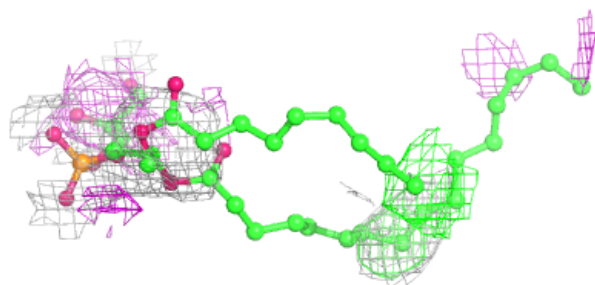
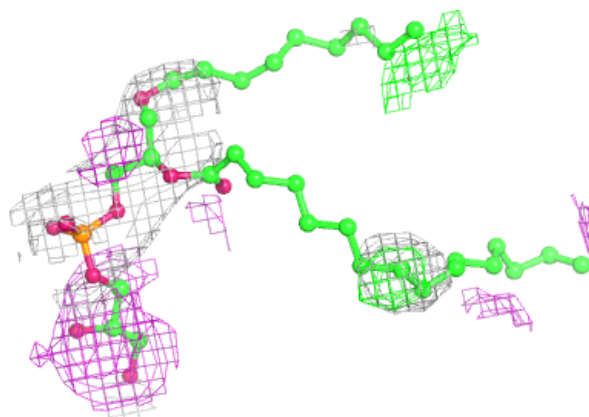
Electron density around LHG d 407:

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



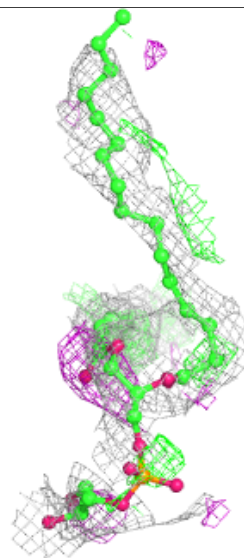
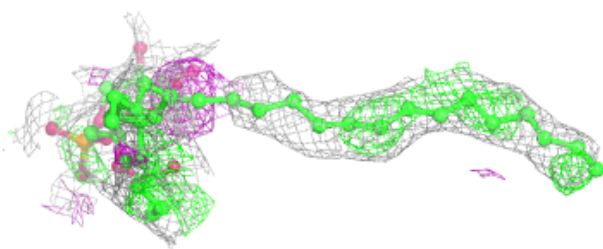
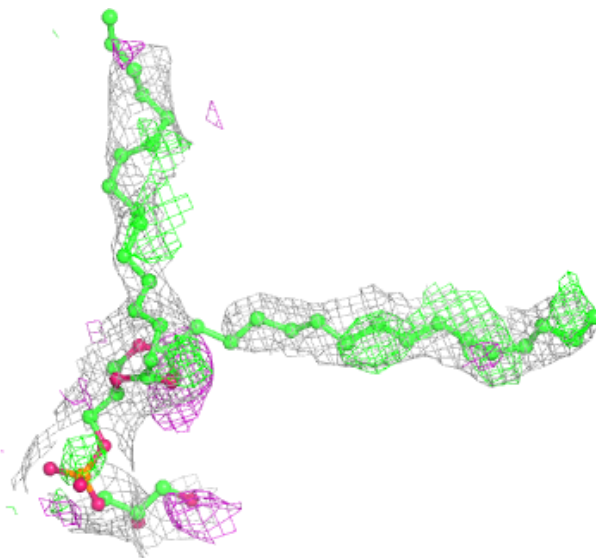
Electron density around LHG e 101:

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



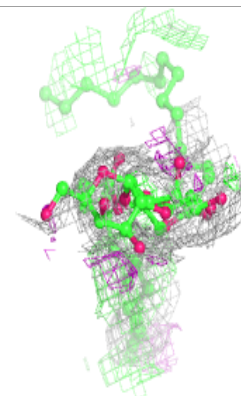
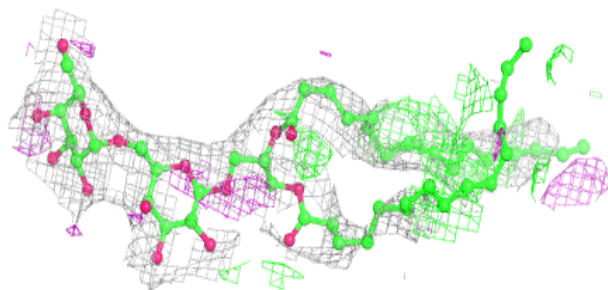
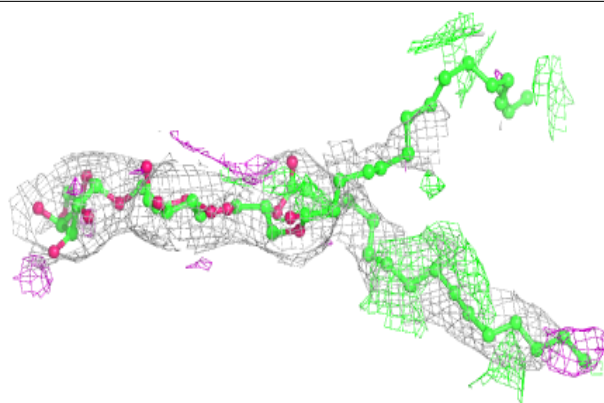
Electron density around LHG 1 102:

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

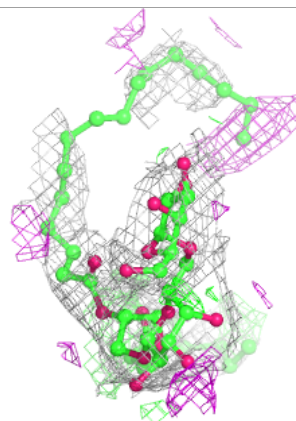
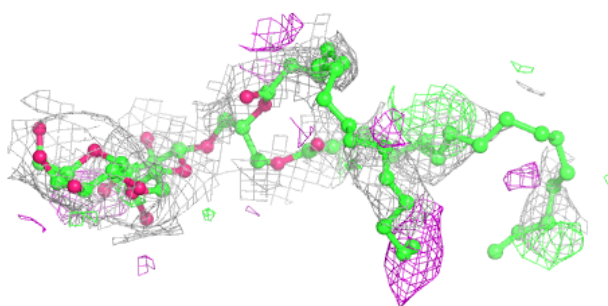
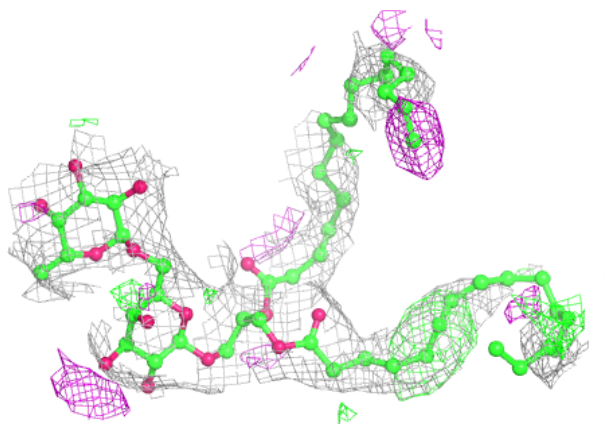


Electron density around DGD C 515:

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

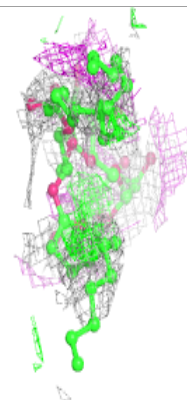
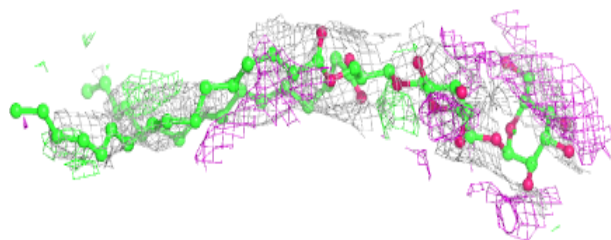
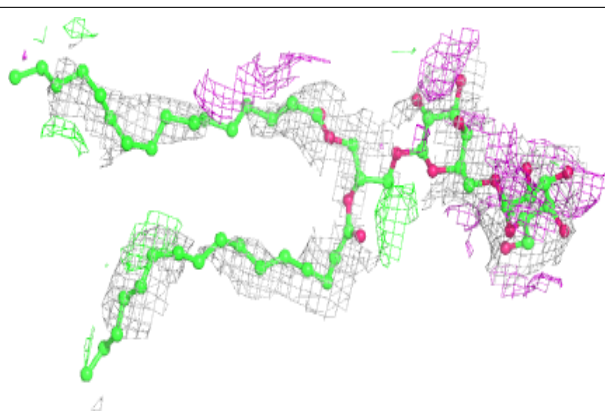
**Electron density around DGD C 516:**

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

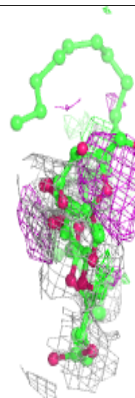
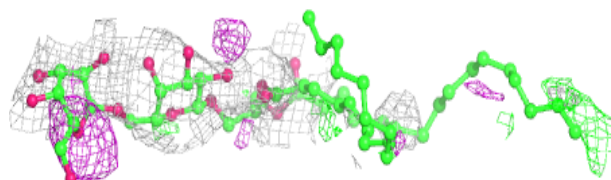
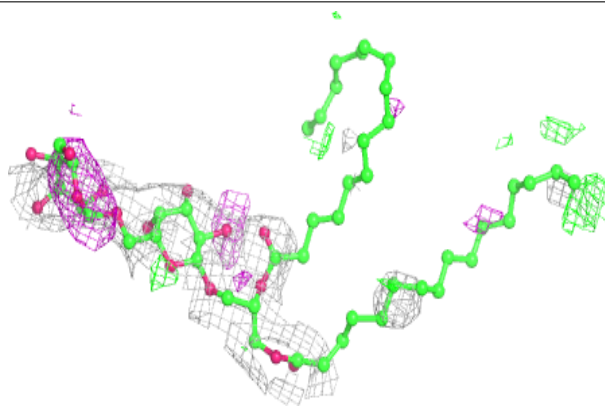


Electron density around DGD C 517:

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

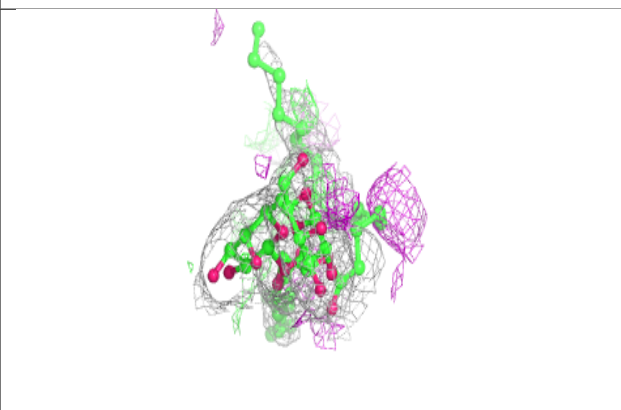
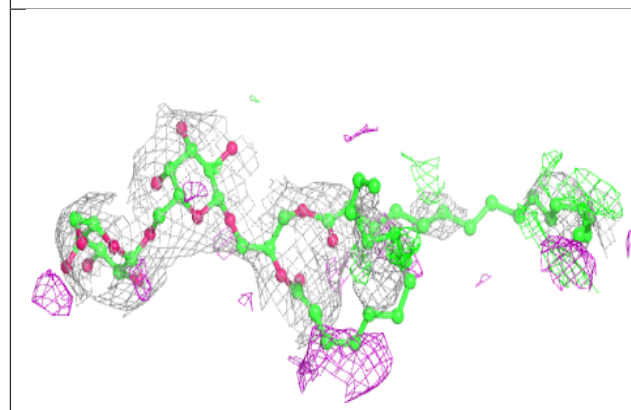
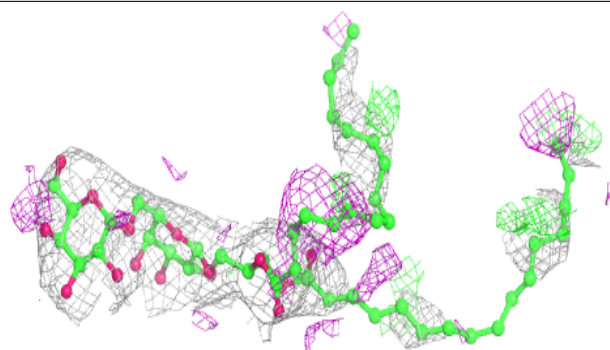
**Electron density around DGD E 101:**

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

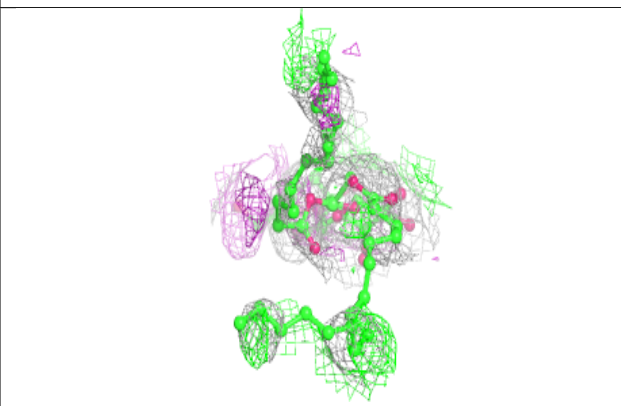
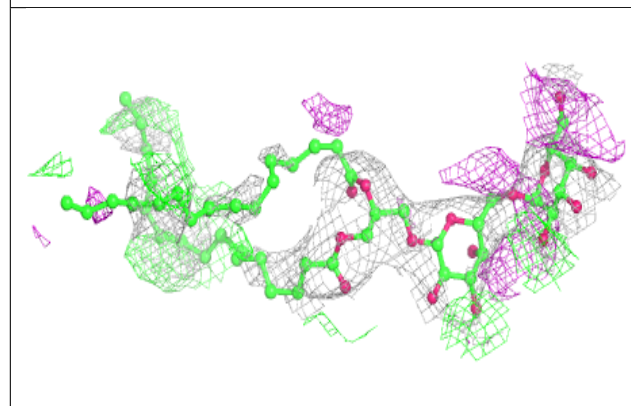
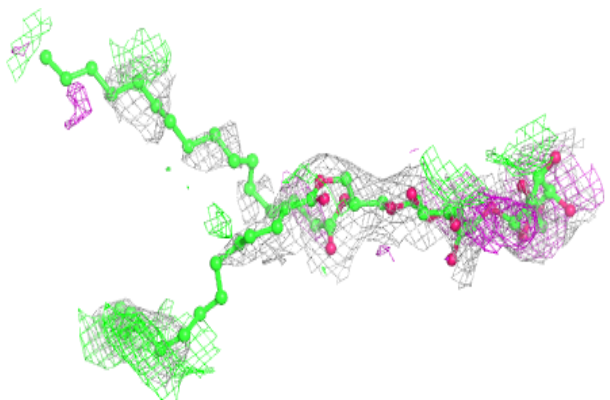


Electron density around DGD H 102:

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

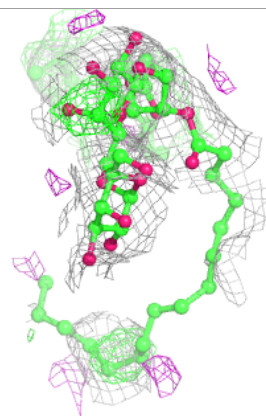
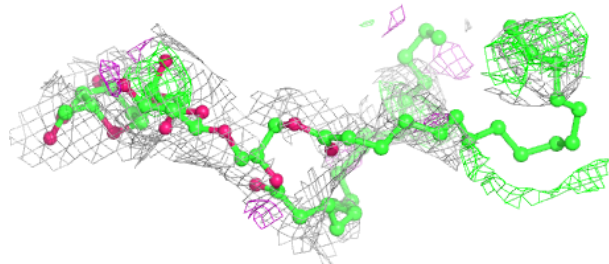
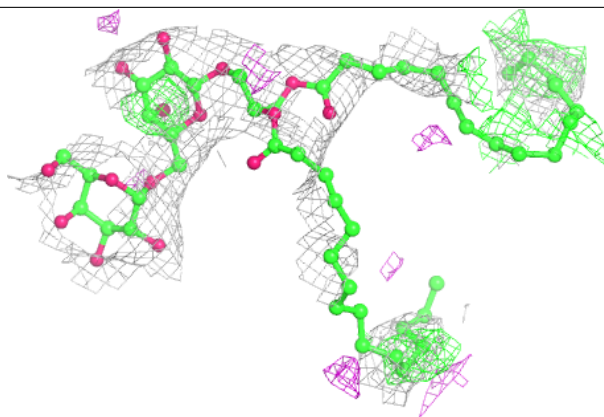
**Electron density around DGD c 516:**

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

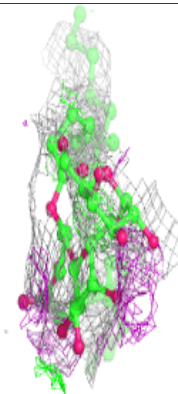
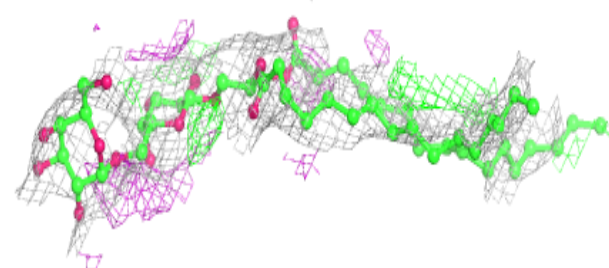
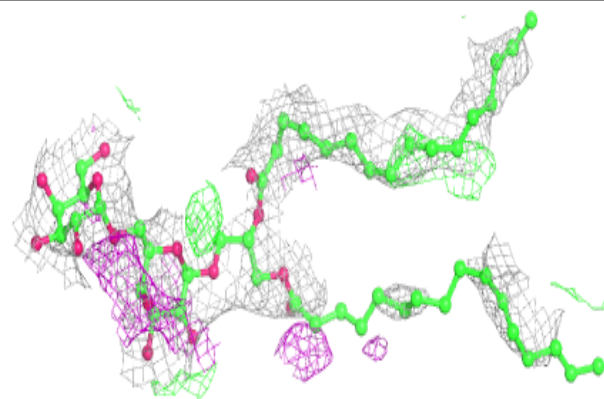


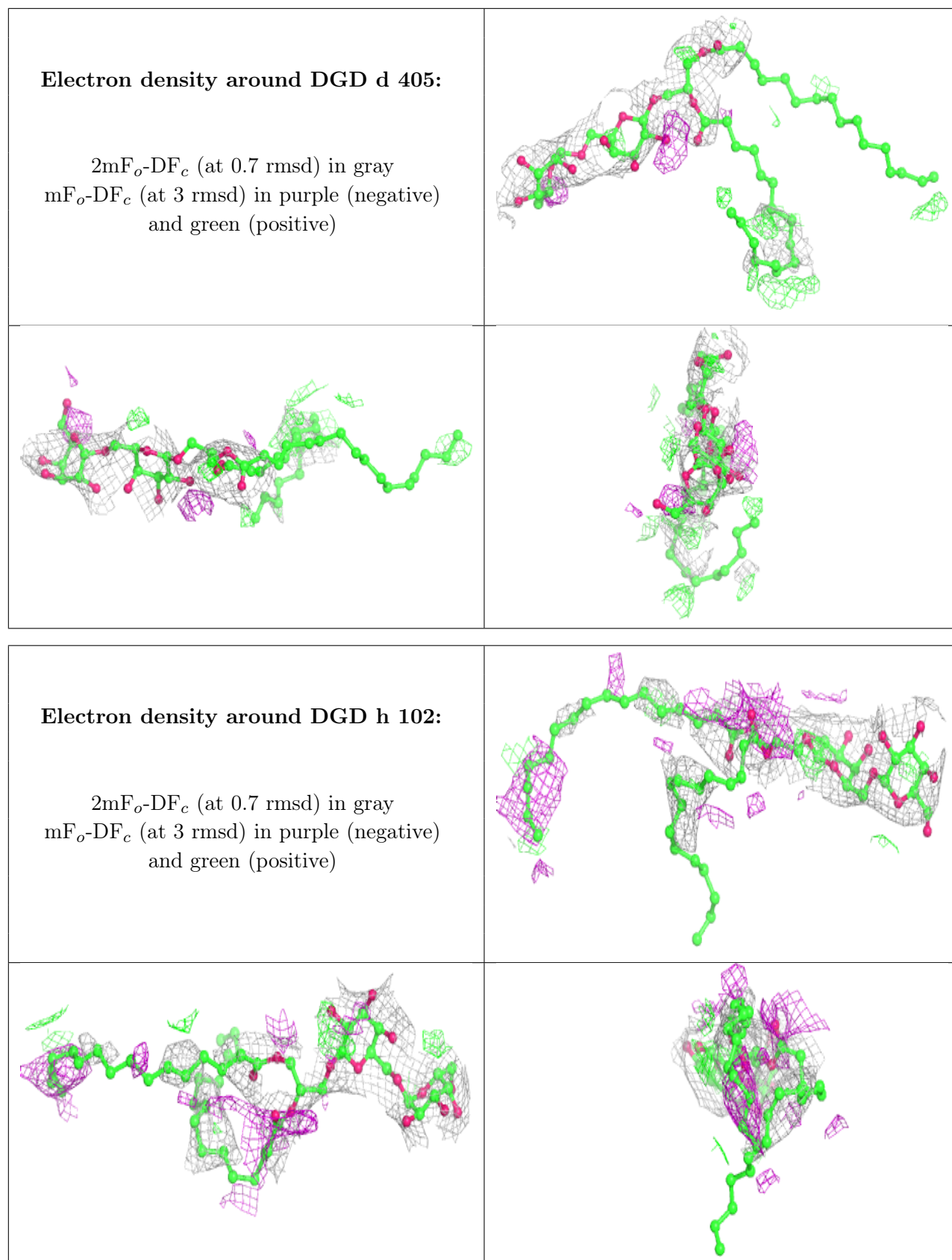
Electron density around DGD c 517:

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

**Electron density around DGD c 518:**

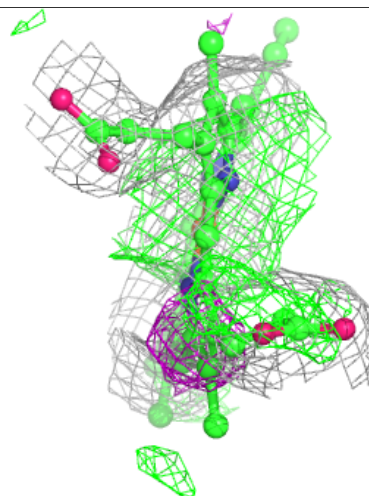
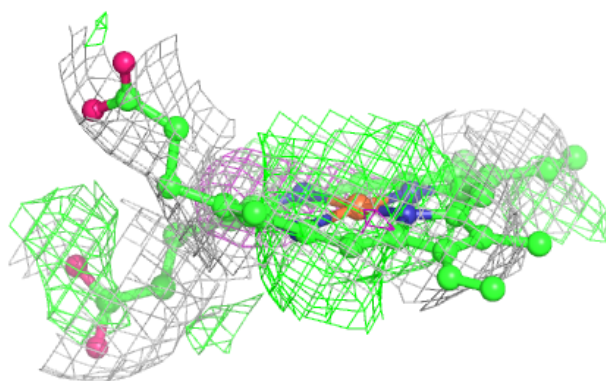
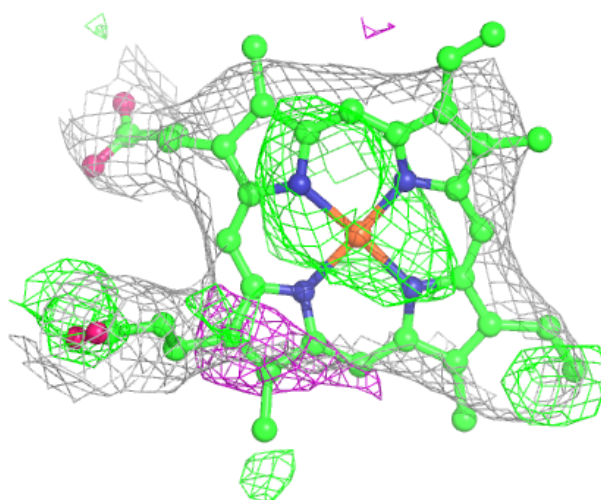
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





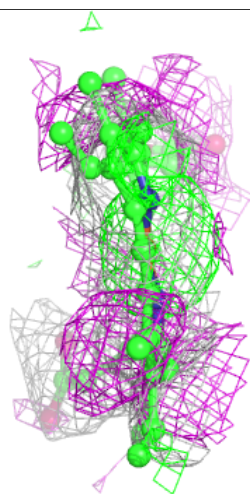
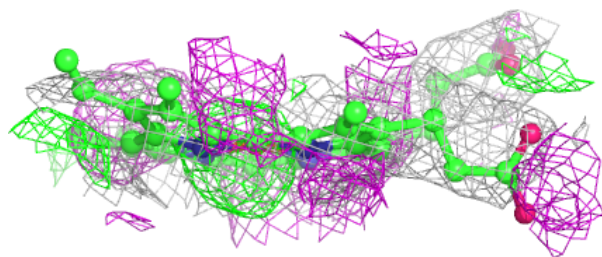
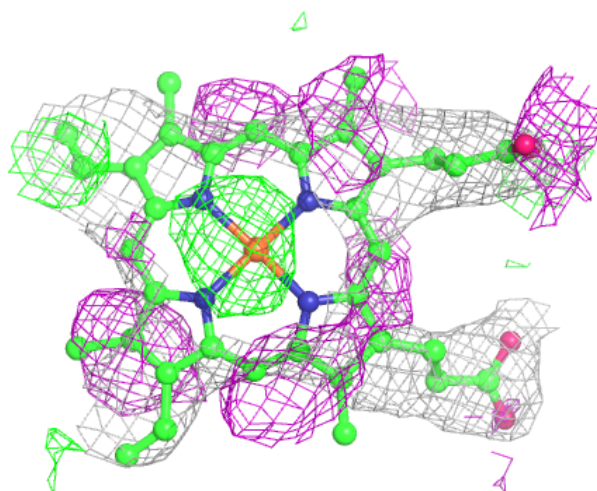
Electron density around HEM E 103:

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



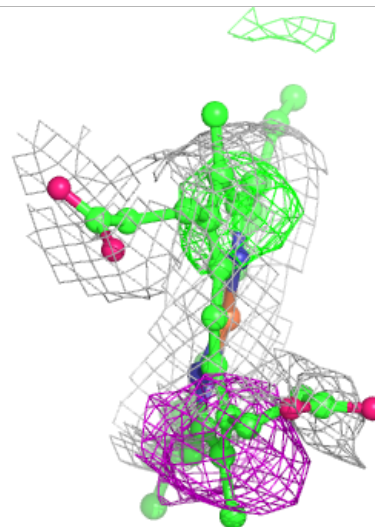
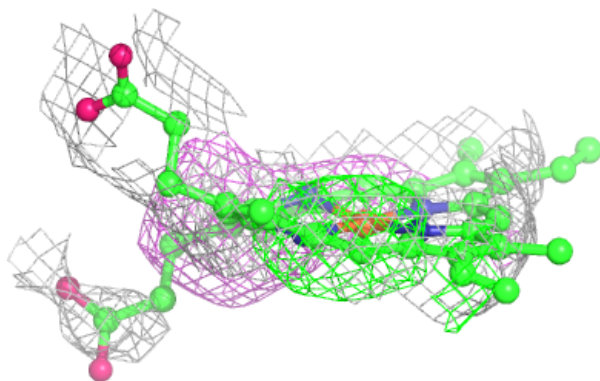
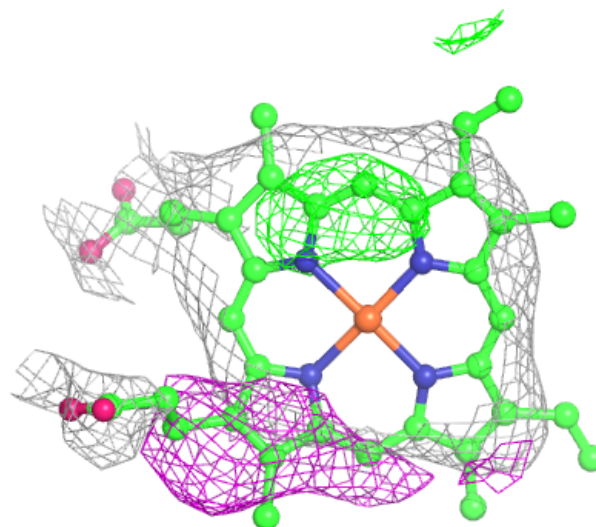
Electron density around HEM V 201:

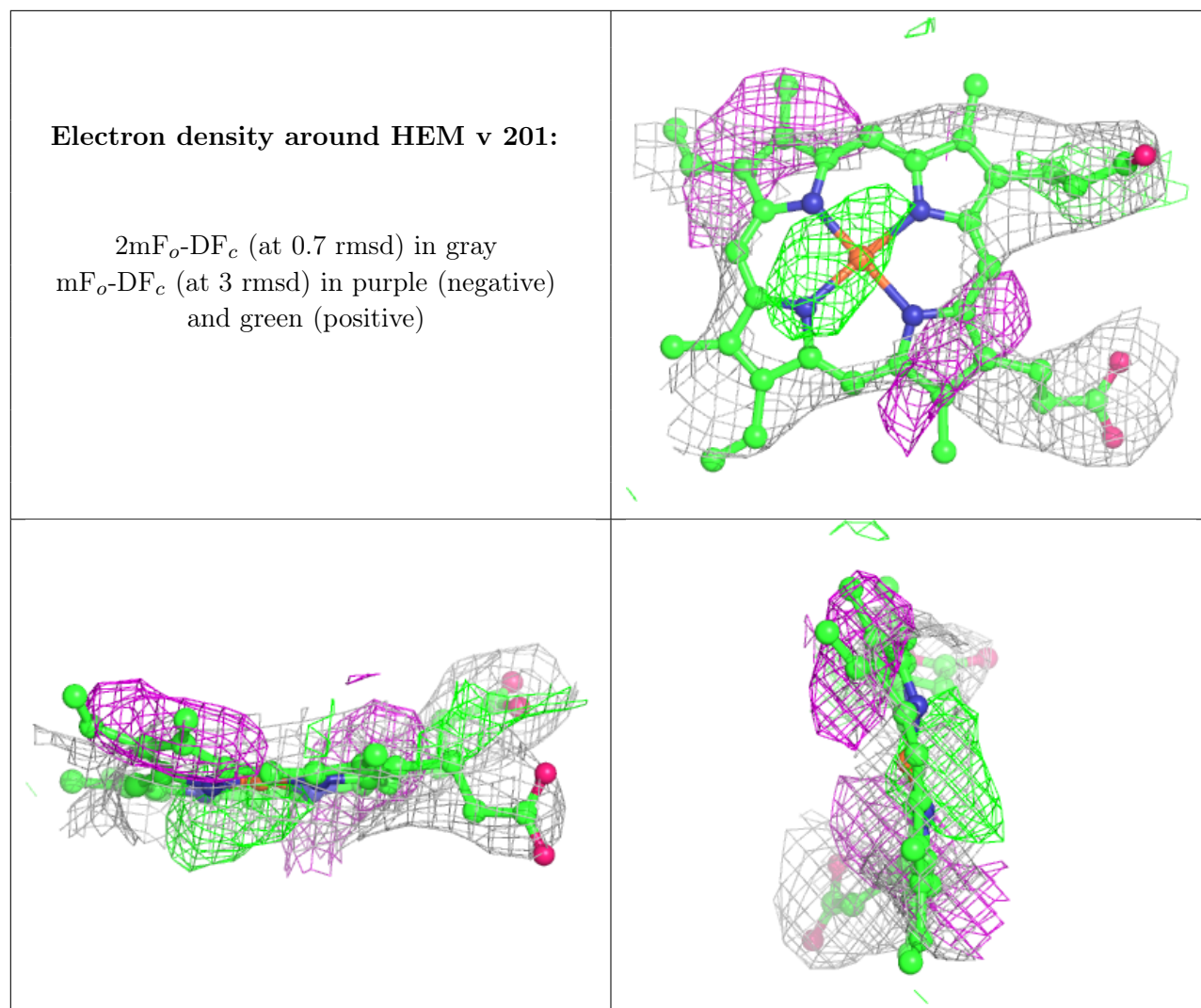
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM e 102:

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





6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.