



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:20 AM JST

PDB ID : 6IGZ / pdb_00006igz
EMDB ID : EMD-9670
Title : Structure of PSI-LHCI
Authors : Xiong, P.; Xiaochun, Q.
Deposited on : 2018-09-27
Resolution : 3.49 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

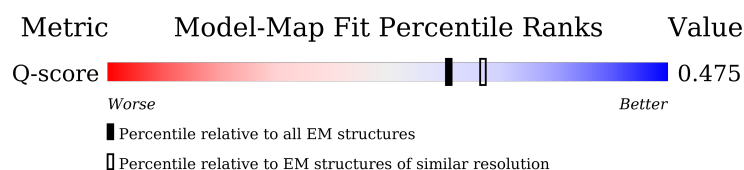
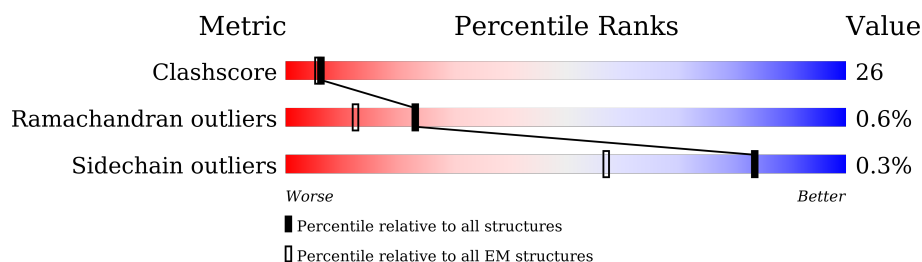
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13600 (2.99 - 3.99)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	7% 58% 40% ..
2	B	734	8% 57% 42%
3	C	81	11% 51% 47% ..
4	D	198	16% 43% 28% .. 28%

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Mol	Chain	Length	Quality of chain
5	E	91	
6	F	236	
7	G	167	
8	H	133	
9	I	36	
10	J	41	
11	K	123	
12	L	204	
13	1	226	
13	5	226	
14	2	256	
15	3	281	
16	4	248	
16	8	248	
17	6	267	
18	7	264	
19	9	222	
20	0	245	
21	M	32	

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
25	8CT	7	323	-	-	X	-
29	CHL	0	301	X	-	-	-
29	CHL	2	301	X	-	-	-
29	CHL	4	301	X	-	-	-
29	CHL	4	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	5	301	X	-	-	-
29	CHL	6	302	X	-	-	-
29	CHL	8	305	X	-	-	-
29	CHL	9	302	X	-	-	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 51585 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5819	3803	988	1006	22		

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5824	3824	979	1002	19		

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			602	370	105	116	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1109	709	193	202	5		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	61	Total	C	N	O	S	0	0
			488	308	87	92	1		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	163	Total	C	N	O	S	0	0
			1257	799	219	233	6		

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	92	Total	C	N	O	0	0
			714	462	118	134		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	88	Total	C	N	O	S	0	0
			677	426	119	131	1		

- Molecule 9 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	32	Total	C	N	O	S	0	0
			243	168	34	39	2		

- Molecule 10 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			336	232	49	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	80	Total	C	N	O	S	0	0
			558	363	92	100	3		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	155	Total	C	N	O	S	0	0
			1139	736	187	212	4		

- Molecule 13 is a protein called Lhca-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1466	942	241	271	12		
13	5	195	Total	C	N	O	S	0	0
			1484	956	243	273	12		

- Molecule 14 is a protein called Lhca-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	212	Total	C	N	O	S	0	0
			1641	1066	265	298	12		

- Molecule 15 is a protein called Lhca-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	226	Total	C	N	O	S	0	0
			1751	1132	283	326	10		

- Molecule 16 is a protein called Lhca-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	207	Total	C	N	O	S	0	0
			1589	1046	258	276	9		
16	8	205	Total	C	N	O	S	0	0
			1574	1035	256	274	9		

- Molecule 17 is a protein called Lhca-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	229	Total	C	N	O	S	0	0
			1797	1182	292	313	10		

- Molecule 18 is a protein called Lhca-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	228	Total	C	N	O	S	0	0
			1758	1137	291	319	11		

- Molecule 19 is a protein called Lhca-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	183	Total	C	N	O	S	0	0
			1416	913	235	259	9		

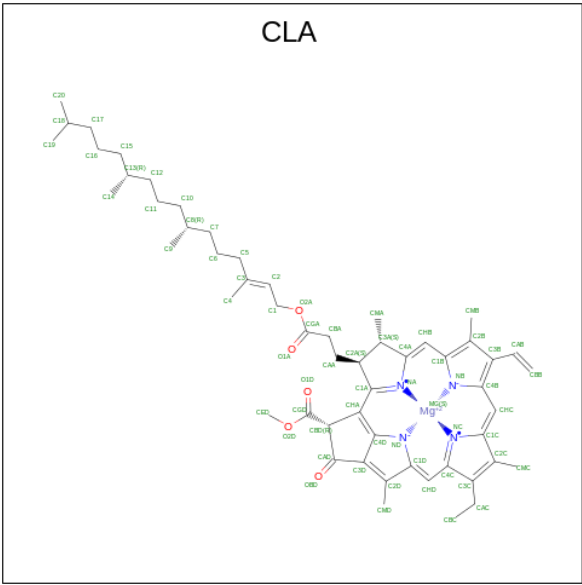
- Molecule 20 is a protein called Lhca-j.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	0	202	Total	C	N	O	S	0	0
			1560	1014	255	280	11		

- Molecule 21 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	M	31	Total	C	N	O	0	0
			238	158	37	43		

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	2	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
22	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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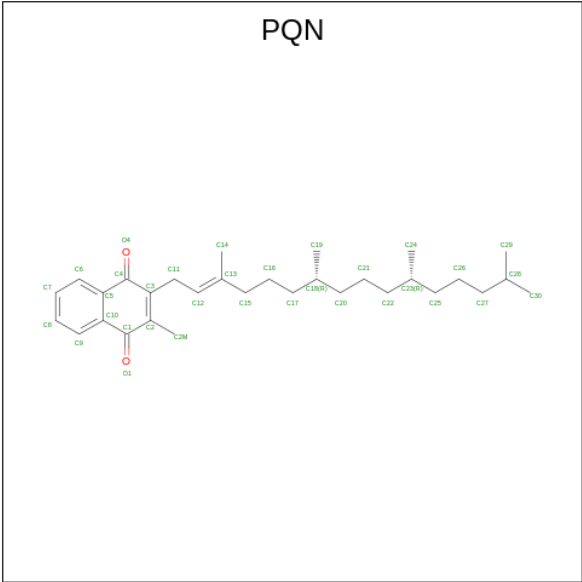
Mol	Chain	Residues	Atoms					AltConf
22	7	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
22	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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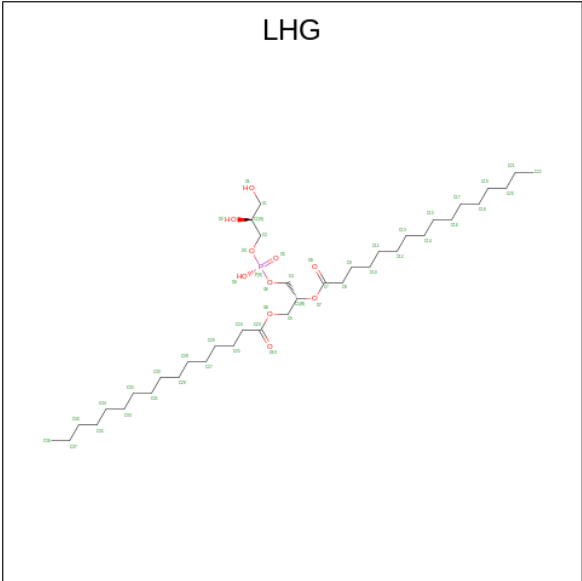
Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			33	31	2	
23	B	1	Total	C	O	0
			33	31	2	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



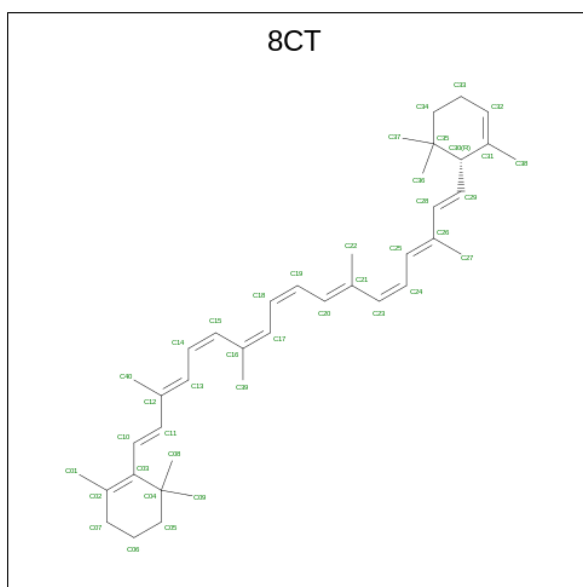
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			27	16	10	1	
24	B	1	Total	C	O	P	0
			23	12	10	1	
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	2	1	Total	C	O	P	0
			32	21	10	1	
24	3	1	Total	C	O	P	0
			20	10	9	1	
24	6	1	Total	C	O	P	0
			37	26	10	1	
24	5	1	Total	C	O	P	0
			49	38	10	1	
24	7	1	Total	C	O	P	0
			20	10	9	1	
24	9	1	Total	C	O	P	0
			49	38	10	1	
24	0	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	C	0
			40	40	

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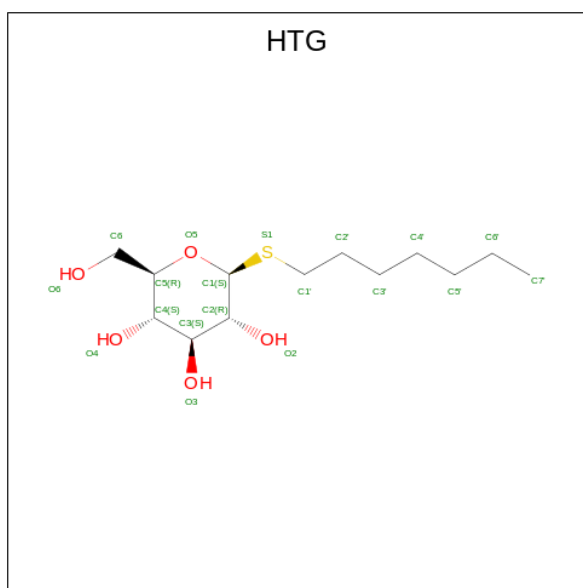
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0

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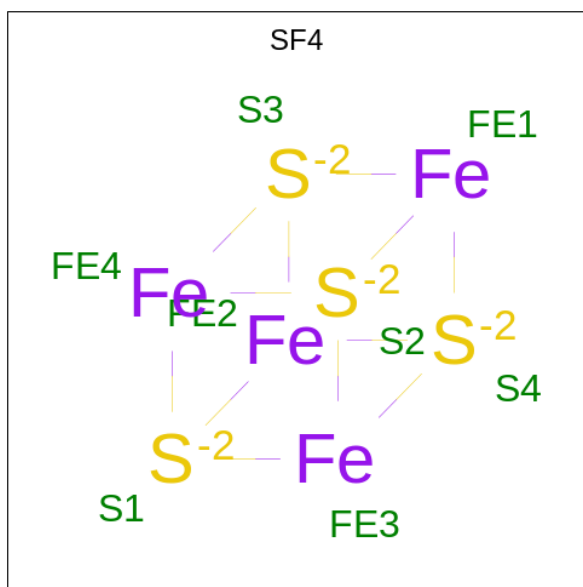
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	8	1	Total C 40 40	0

- Molecule 26 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



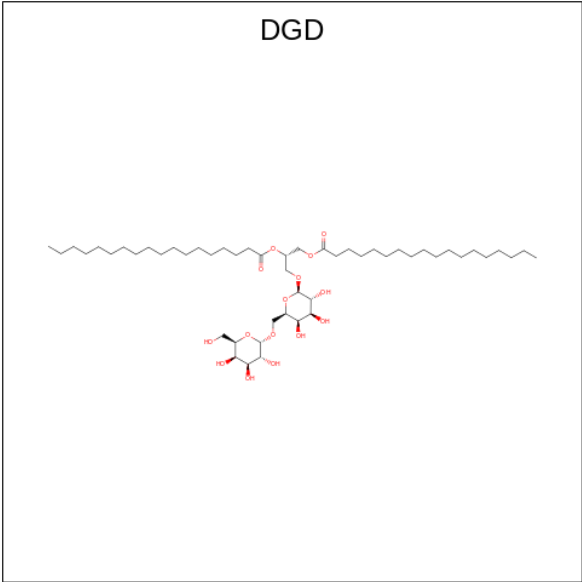
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			19	13	5	1	
26	J	1	Total	C	O	S	0
			19	13	5	1	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



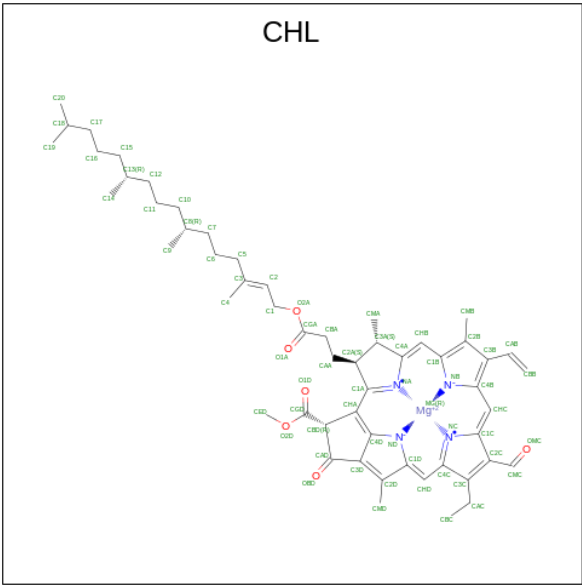
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			66	51	15	

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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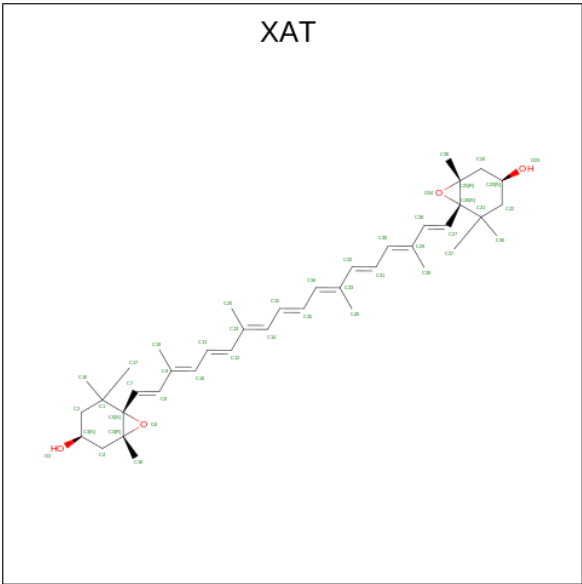
Mol	Chain	Residues	Atoms					AltConf
29	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	5	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	5	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
29	0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	0	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 30 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



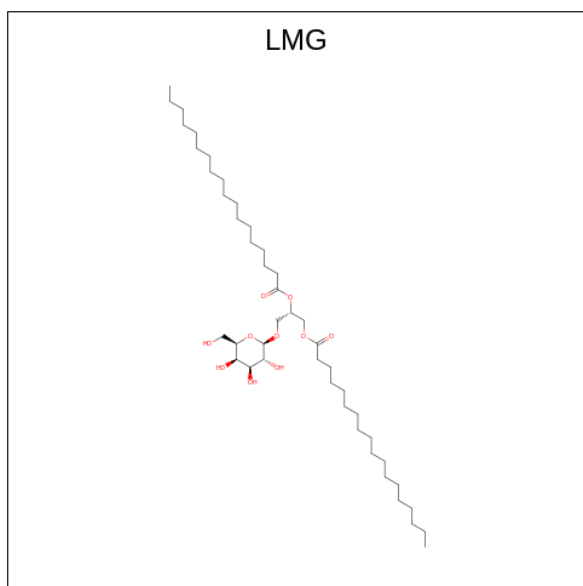
Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			44	40	4	
30	1	1	Total	C	O	0
			44	40	4	
30	2	1	Total	C	O	0
			44	40	4	
30	2	1	Total	C	O	0
			44	40	4	
30	3	1	Total	C	O	0
			44	40	4	
30	3	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	
30	6	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
30	6	1	Total	C	O	0
			44	40	4	
30	5	1	Total	C	O	0
			44	40	4	
30	5	1	Total	C	O	0
			44	40	4	
30	7	1	Total	C	O	0
			44	40	4	
30	7	1	Total	C	O	0
			44	40	4	
30	8	1	Total	C	O	0
			44	40	4	
30	8	1	Total	C	O	0
			44	40	4	
30	9	1	Total	C	O	0
			44	40	4	
30	9	1	Total	C	O	0
			44	40	4	
30	0	1	Total	C	O	0
			44	40	4	
30	0	1	Total	C	O	0
			44	40	4	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

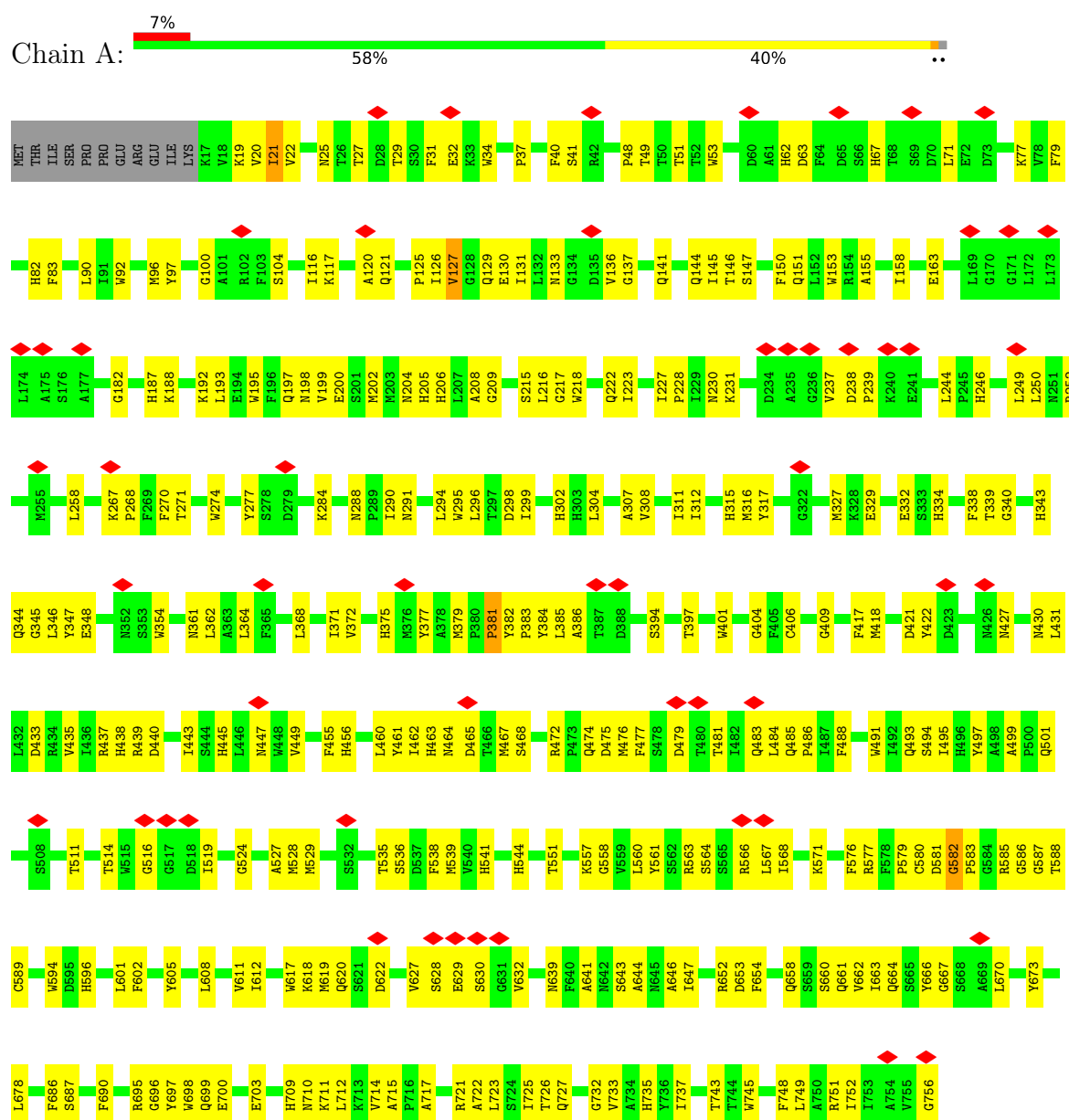


Mol	Chain	Residues	Atoms			AltConf
31	4	1	Total 44	C 34	O 10	0
31	5	1	Total 44	C 34	O 10	0
31	8	1	Total 44	C 34	O 10	0

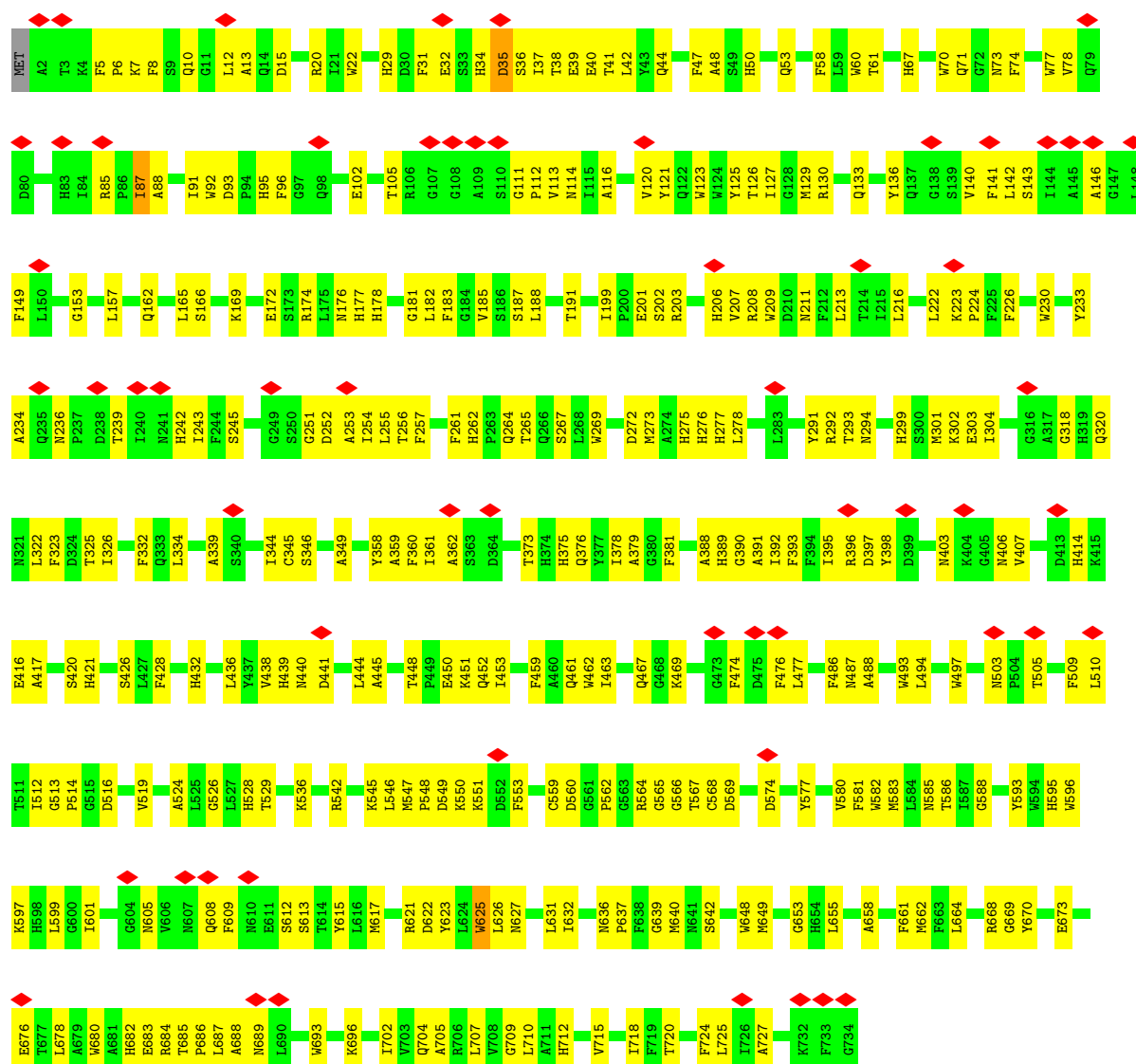
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

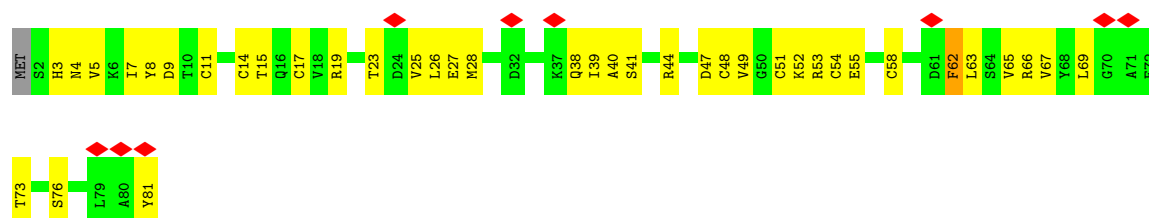
• Molecule 1: PsaA



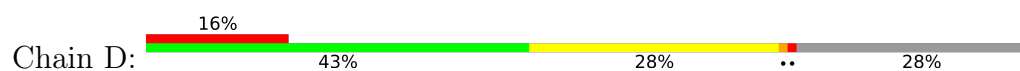
• Molecule 2: PsaB

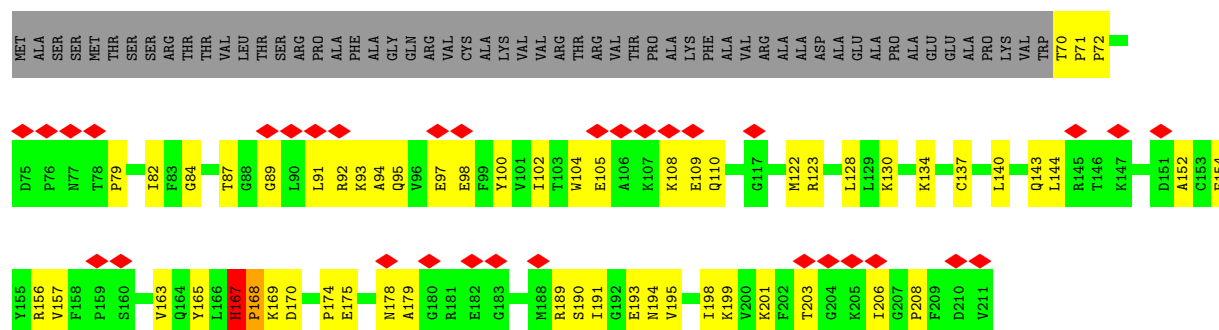


• Molecule 3: Psac

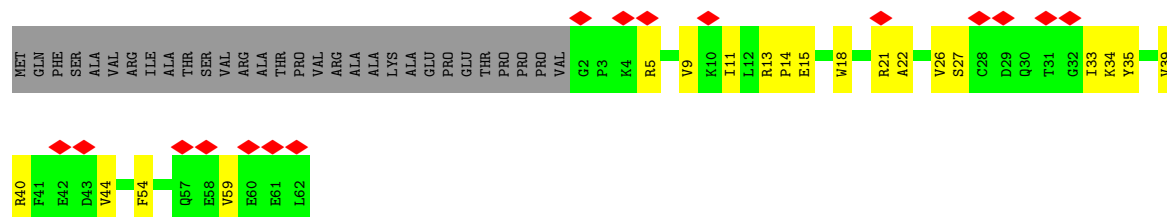


• Molecule 4: Psad

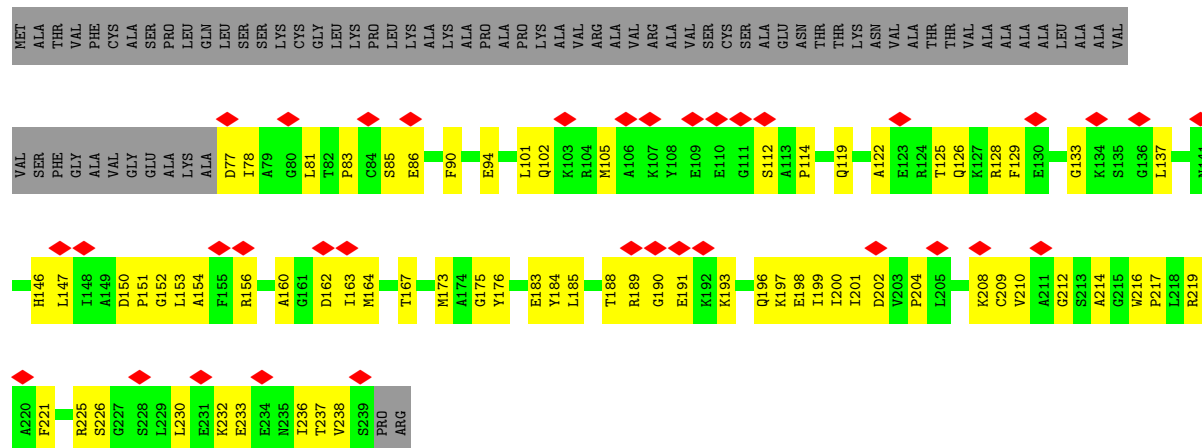




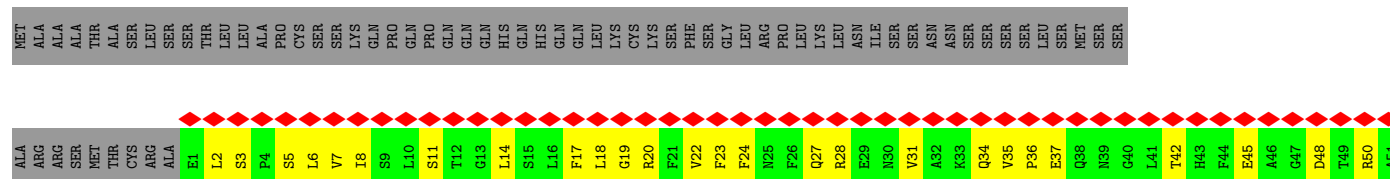
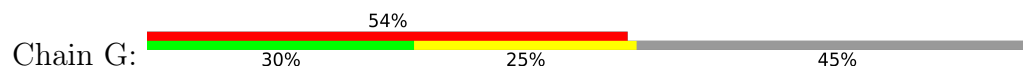
• Molecule 5: PsaE



• Molecule 6: PsaF

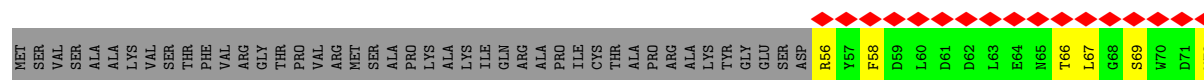


• Molecule 7: PsaG





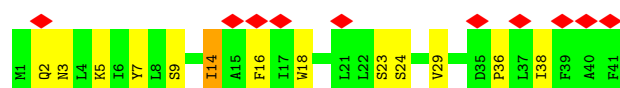
• Molecule 8: PsaH



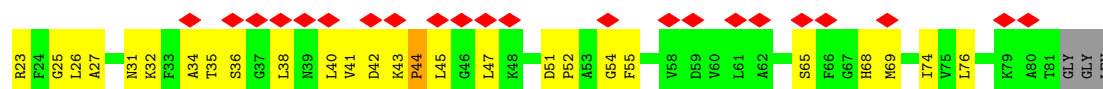
• Molecule 9: PsaI



• Molecule 10: PsaJ



• Molecule 11: PsaK

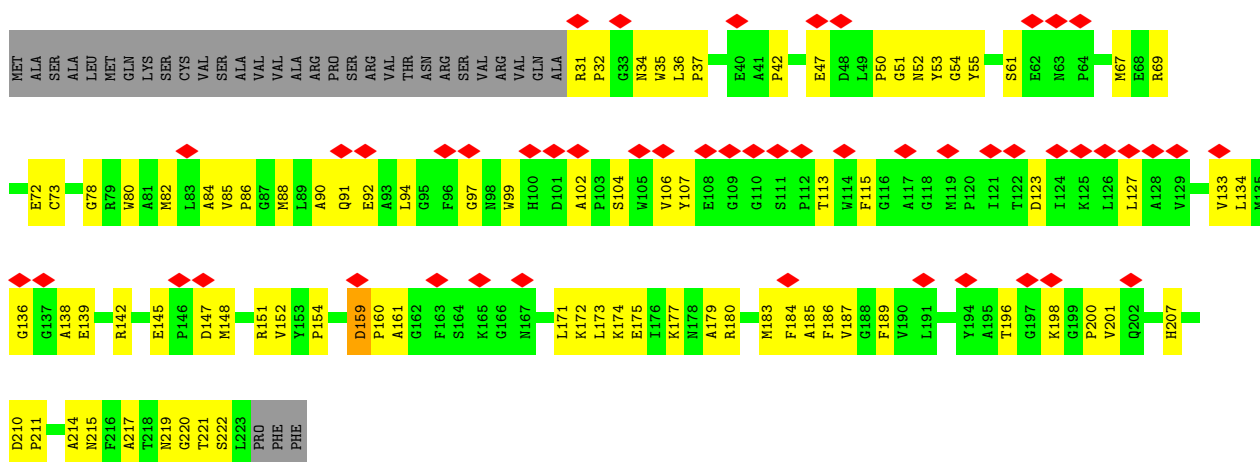


• Molecule 12: PsaL

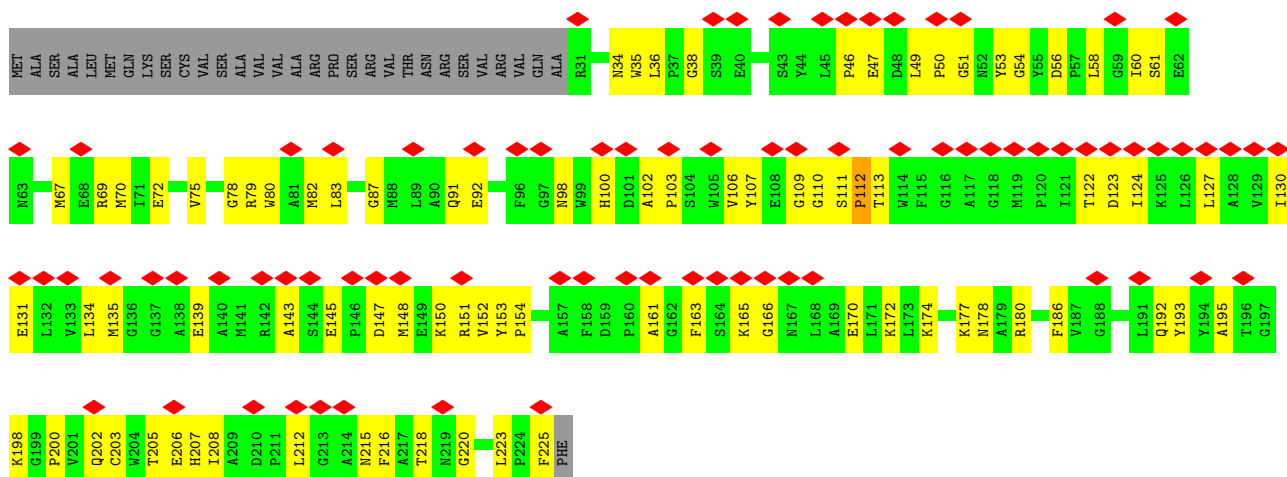




• Molecule 13: Lhca-a

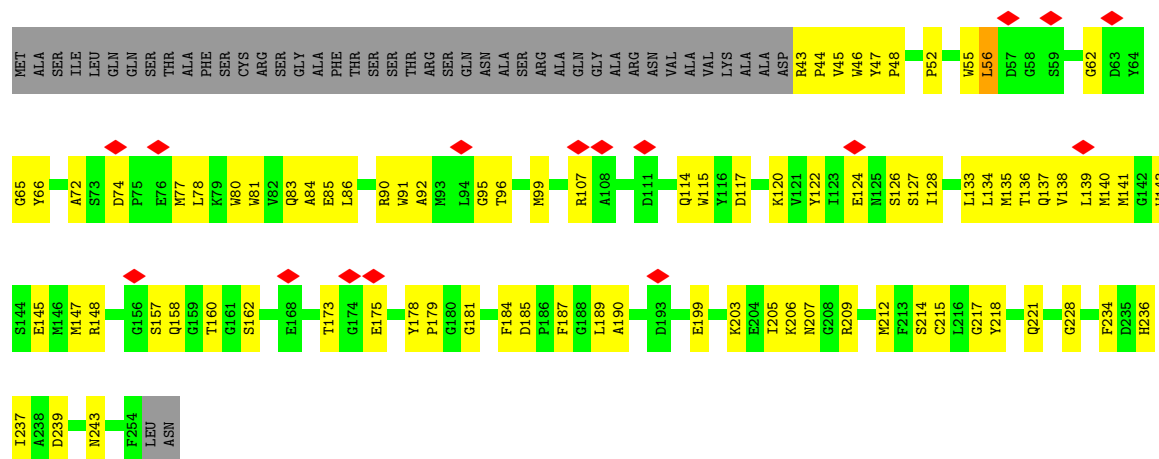


• Molecule 13: Lhca-a

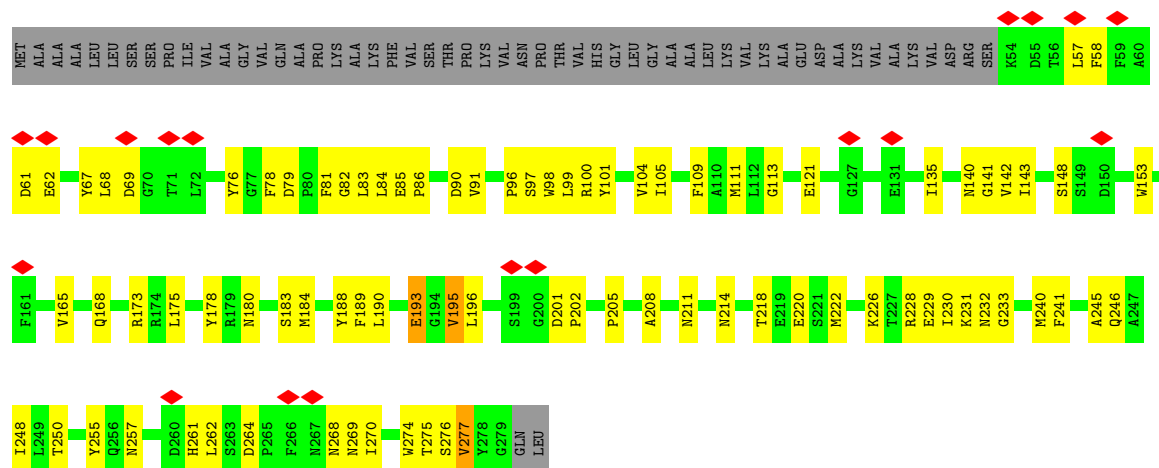


• Molecule 14: Lhca-c

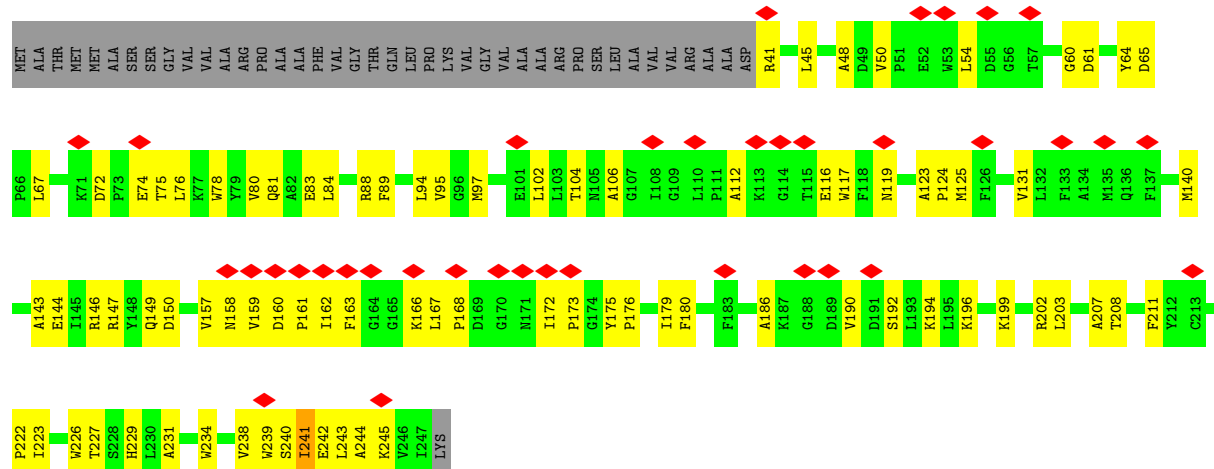




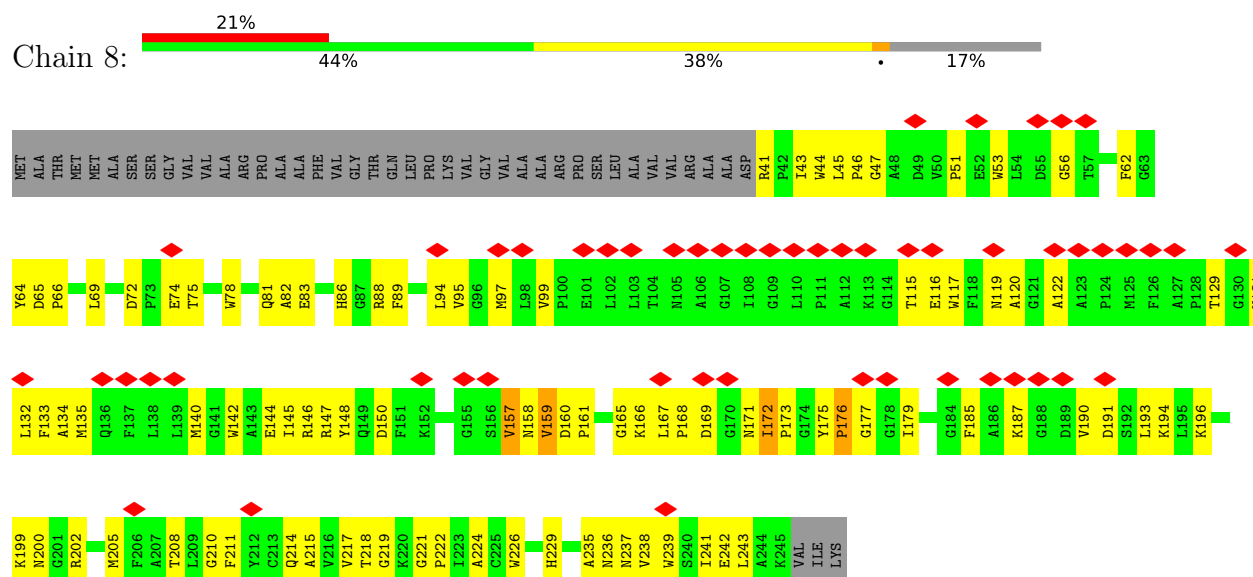
• Molecule 15: Lhca-d



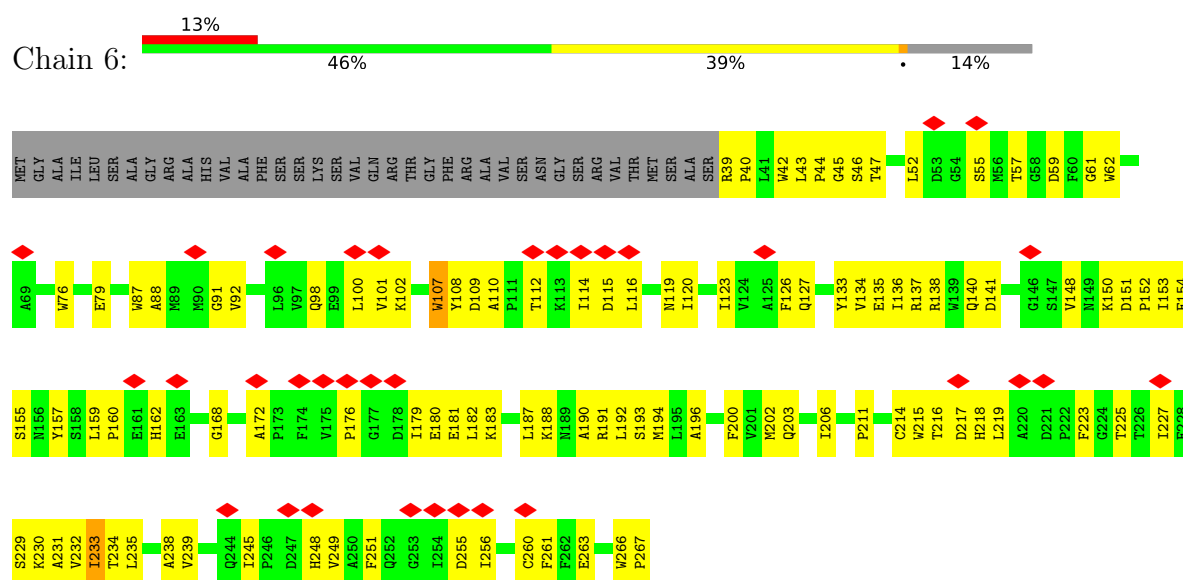
• Molecule 16: Lhca-b



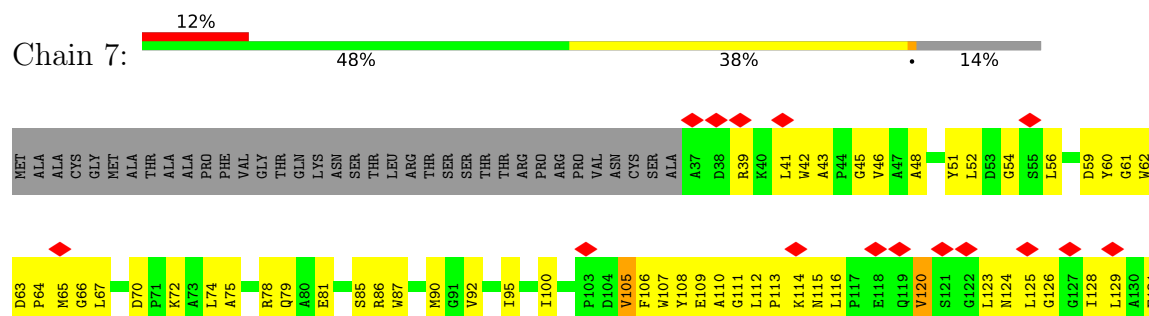
- Molecule 16: Lhca-b

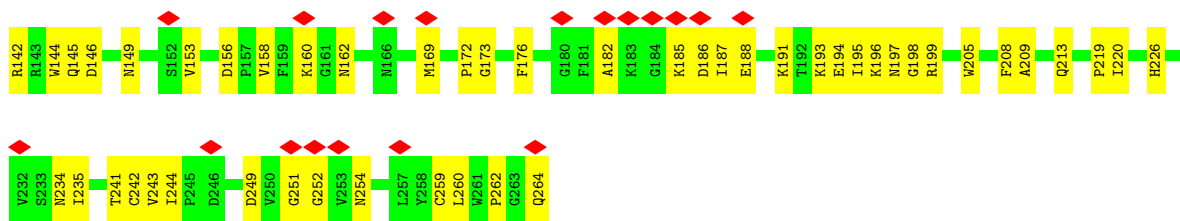


- Molecule 17: Lhca-g

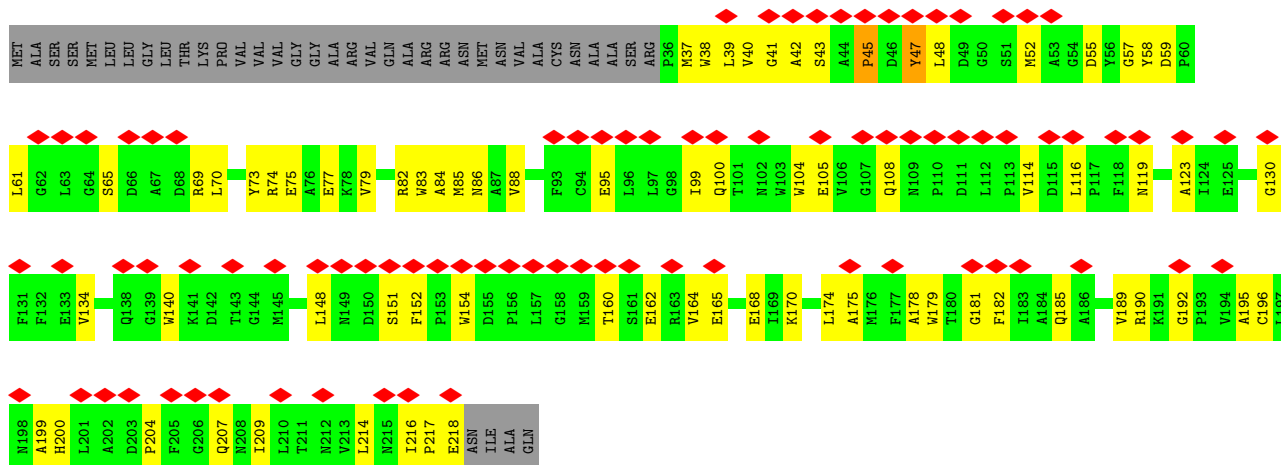


- Molecule 18: Lhca-h

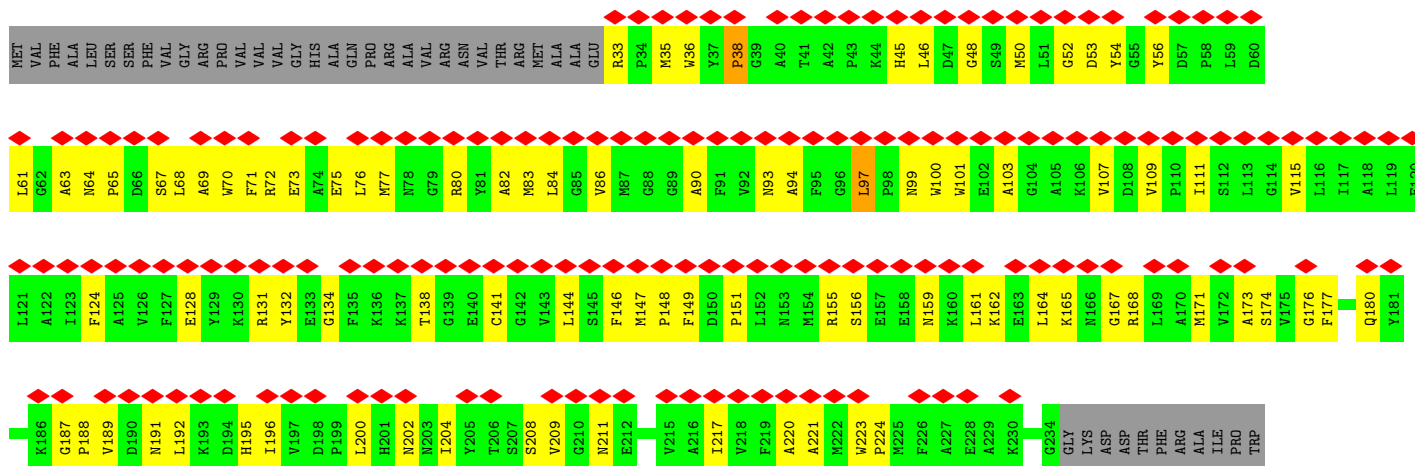




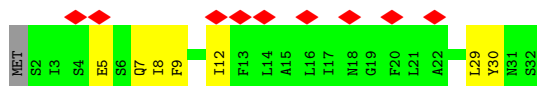
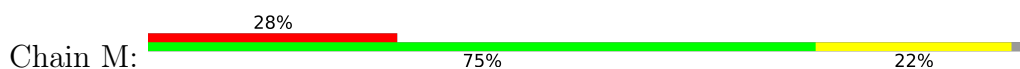
• Molecule 19: Lhca-i



• Molecule 20: Lhca-j



• Molecule 21: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59525	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.852	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.034	Depositor
Map size ($\text{\AA}$)	401.442, 401.442, 401.442	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8727, 0.8727, 0.8727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, CLA, LHG, DGD, PQN, LMG, HTG, 8CT, XAT, SF4

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	0.46	0/6015	0.50	0/8196
2	B	0.46	0/6034	0.54	0/8239
3	C	0.46	0/612	0.61	0/830
4	D	0.36	0/1135	0.58	0/1533
5	E	0.32	0/498	0.45	0/673
6	F	0.35	0/1281	0.54	0/1724
7	G	0.22	0/730	0.49	0/992
8	H	0.30	0/691	0.55	0/929
9	I	0.32	0/250	0.48	0/341
10	J	0.40	0/346	0.54	0/472
11	K	0.31	0/567	0.72	1/769 (0.1%)
12	L	0.28	0/1165	0.64	0/1591
13	1	0.33	0/1510	0.48	0/2054
13	5	0.31	0/1530	0.53	0/2082
14	2	0.43	0/1701	0.55	0/2315
15	3	0.46	0/1801	0.60	0/2444
16	4	0.40	0/1642	0.55	0/2238
16	8	0.41	0/1627	0.61	0/2217
17	6	0.37	0/1862	0.57	0/2542
18	7	0.38	0/1812	0.54	0/2468
19	9	0.34	0/1456	0.64	2/1986 (0.1%)
20	0	0.24	0/1603	0.53	0/2174
21	M	0.36	0/241	0.36	0/325
All	All	0.40	0/36109	0.55	3/49134 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	1
4	D	0	1
11	K	0	1
13	1	0	1
14	2	0	2
16	4	0	1
17	6	0	3
20	0	0	3
All	All	0	14

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	47	TYR	CA-C-N	-5.66	115.19	123.00
19	9	47	TYR	C-N-CA	-5.66	115.19	123.00
11	K	25	GLY	N-CA-C	5.17	122.24	115.47

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	0	156	SER	Peptide
20	0	38	PRO	Peptide
20	0	97	LEU	Peptide
13	1	159	ASP	Peptide
14	2	162	SER	Peptide
14	2	56	LEU	Peptide
16	4	123	ALA	Peptide
17	6	107	TRP	Peptide
17	6	109	ASP	Peptide
17	6	155	SER	Peptide
1	A	582	GLY	Peptide
3	C	62	PHE	Peptide
4	D	167	HIS	Peptide
11	K	41	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5659	289	0
2	B	5824	0	5604	353	0
3	C	602	0	591	42	0
4	D	1109	0	1124	54	0
5	E	488	0	480	15	0
6	F	1257	0	1274	63	0
7	G	714	0	708	39	0
8	H	677	0	654	59	0
9	I	243	0	258	11	0
10	J	336	0	355	16	0
11	K	558	0	591	40	0
12	L	1139	0	1147	73	0
13	1	1466	0	1411	77	0
13	5	1484	0	1427	80	0
14	2	1641	0	1537	83	0
15	3	1751	0	1684	87	0
16	4	1589	0	1570	97	0
16	8	1574	0	1550	139	0
17	6	1797	0	1752	117	0
18	7	1758	0	1701	112	0
19	9	1416	0	1367	75	0
20	0	1560	0	1540	89	0
21	M	238	0	248	8	0
22	0	572	0	542	44	0
22	1	683	0	657	69	0
22	2	596	0	548	28	0
22	3	644	0	529	37	0
22	4	539	0	476	29	0
22	5	653	0	599	55	0
22	6	785	0	741	63	0
22	7	817	0	694	71	0
22	8	539	0	477	40	0
22	9	595	0	534	38	0
22	A	2628	0	2677	187	0
22	B	2420	0	2485	213	0
22	F	45	0	33	5	0
22	G	141	0	105	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H	65	0	72	16	0
22	J	42	0	31	1	0
22	K	187	0	138	28	0
22	L	245	0	255	22	0
22	M	46	0	33	4	0
23	A	33	0	46	3	0
23	B	33	0	46	3	0
24	0	49	0	72	11	0
24	1	49	0	74	3	0
24	2	32	0	34	3	0
24	3	20	0	14	4	0
24	5	49	0	72	8	0
24	6	37	0	44	4	0
24	7	20	0	13	2	0
24	9	49	0	74	8	0
24	A	76	0	98	4	0
24	B	23	0	16	1	0
25	1	40	0	0	13	0
25	2	40	0	0	13	0
25	3	80	0	0	11	0
25	4	40	0	0	12	0
25	5	40	0	0	5	0
25	6	40	0	0	14	0
25	7	120	0	0	35	0
25	8	80	0	0	13	0
25	A	240	0	0	30	0
25	B	320	0	0	41	0
25	F	40	0	0	0	0
25	G	40	0	0	19	0
25	I	40	0	0	0	0
25	J	80	0	0	25	0
25	K	40	0	0	13	0
25	L	80	0	0	0	0
26	A	19	0	26	0	0
26	J	19	0	26	1	0
27	B	8	0	0	1	0
27	C	16	0	0	1	0
28	B	66	0	96	11	0
29	0	109	0	87	17	0
29	1	48	0	33	3	0
29	2	203	0	154	18	0
29	3	47	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	4	219	0	176	28	0
29	5	109	0	90	16	0
29	6	241	0	181	23	0
29	7	47	0	31	8	0
29	8	201	0	148	28	0
29	9	109	0	90	3	0
30	0	88	0	104	16	0
30	1	88	0	109	14	0
30	2	88	0	112	12	0
30	3	88	0	110	17	0
30	4	88	0	109	14	0
30	5	88	0	107	13	0
30	6	88	0	111	14	0
30	7	88	0	109	14	0
30	8	88	0	109	20	0
30	9	88	0	109	12	0
31	4	44	0	61	1	0
31	5	44	0	61	6	0
31	8	44	0	60	6	0
All	All	51585	0	48901	2587	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (2587) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:832:CLA:H43	25:B:848:8CT:C27	1.26	1.58
22:1:304:CLA:H3A	25:1:316:8CT:C27	1.31	1.57
22:B:840:CLA:C1C	25:B:848:8CT:C22	1.82	1.57
18:7:251:GLY:HA3	25:7:323:8CT:C01	1.35	1.54
15:3:195:VAL:CG2	15:3:208:ALA:HB3	1.44	1.48
25:A:846:8CT:C40	25:A:854:8CT:C01	1.98	1.39
22:1:304:CLA:HAA1	25:1:316:8CT:C27	1.52	1.39
15:3:189:PHE:CE1	25:3:316:8CT:C27	2.07	1.38
18:7:124:ASN:OD1	25:7:323:8CT:C08	1.71	1.37
18:7:251:GLY:CA	25:7:323:8CT:C01	2.02	1.36
25:B:843:8CT:C18	25:G:104:8CT:C08	2.00	1.36
22:G:103:CLA:C4B	25:G:104:8CT:C37	2.05	1.34
22:A:808:CLA:C2	25:J:104:8CT:C40	2.07	1.32
15:3:189:PHE:CZ	25:3:316:8CT:C27	2.11	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:809:CLA:CBB	25:J:104:8CT:C38	2.08	1.30
22:B:840:CLA:CHC	25:B:848:8CT:C22	2.08	1.29
22:7:307:CLA:C1B	25:7:323:8CT:C27	2.09	1.28
7:G:83:TYR:CD2	25:G:104:8CT:C01	2.16	1.27
16:8:179:ILE:CD1	29:8:314:CHL:HHB	1.64	1.26
22:7:307:CLA:C2B	25:7:323:8CT:C27	2.17	1.22
22:A:808:CLA:H12	25:J:104:8CT:C40	1.70	1.21
22:B:840:CLA:C2C	25:B:848:8CT:C22	2.19	1.21
22:A:808:CLA:C1	25:J:104:8CT:C40	2.17	1.20
22:A:832:CLA:C4	25:B:848:8CT:C27	2.20	1.20
22:1:304:CLA:C3A	25:1:316:8CT:C27	2.19	1.20
22:A:808:CLA:H2	25:J:104:8CT:C40	1.70	1.19
1:A:745:TRP:CG	25:A:850:8CT:C38	2.28	1.16
15:3:195:VAL:HG22	15:3:208:ALA:HB3	1.26	1.16
22:B:826:CLA:C2B	25:B:847:8CT:C22	2.24	1.14
8:H:124:ASP:HB3	8:H:127:LEU:HD12	1.16	1.13
22:G:103:CLA:CHC	25:G:104:8CT:C37	2.26	1.12
1:A:663:ILE:CG2	2:B:621:ARG:HG3	1.80	1.11
1:A:663:ILE:HG22	2:B:621:ARG:HG3	1.32	1.11
11:K:68:HIS:CE1	25:K:103:8CT:C15	2.34	1.09
1:A:745:TRP:CD1	25:A:850:8CT:C38	2.35	1.09
16:8:166:LYS:HE3	16:8:179:ILE:HG13	1.30	1.08
14:2:143:TRP:CH2	25:2:317:8CT:C09	2.36	1.08
29:4:305:CHL:NB	25:4:317:8CT:C38	2.17	1.07
22:G:103:CLA:NB	25:G:104:8CT:C37	2.17	1.07
8:H:124:ASP:CB	8:H:127:LEU:HD12	1.83	1.06
22:6:305:CLA:C4B	25:6:321:8CT:C33	2.33	1.06
17:6:133:TYR:CE2	25:6:321:8CT:C40	2.40	1.05
22:7:306:CLA:H3A	25:7:321:8CT:C25	1.85	1.05
29:4:305:CHL:C1B	25:4:317:8CT:C38	2.36	1.03
22:A:809:CLA:CAB	25:J:104:8CT:C38	2.37	1.02
22:B:826:CLA:C3B	25:B:847:8CT:C22	2.37	1.02
16:8:179:ILE:HD12	29:8:314:CHL:CHB	1.91	1.01
29:3:306:CHL:HMB1	25:3:316:8CT:C22	1.89	1.01
15:3:195:VAL:CG2	15:3:208:ALA:CB	2.39	1.00
22:1:304:CLA:CAA	25:1:316:8CT:C27	2.38	1.00
2:B:595:HIS:CD2	2:B:623:TYR:OH	2.15	0.99
29:6:307:CHL:HMA1	25:8:301:8CT:C38	1.91	0.99
22:G:102:CLA:HBB1	25:G:104:8CT:C39	1.92	0.99
15:3:195:VAL:HG23	15:3:208:ALA:HB3	1.42	0.98
13:1:134:LEU:HD11	25:1:316:8CT:C19	1.89	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:809:CLA:HBB2	25:J:104:8CT:C38	1.93	0.98
2:B:627:ASN:HB2	2:B:724:PHE:HE1	1.25	0.97
16:8:179:ILE:CD1	29:8:314:CHL:CHB	2.42	0.96
2:B:627:ASN:HD22	2:B:724:PHE:HZ	0.98	0.96
7:G:83:TYR:HD2	25:G:104:8CT:C01	1.64	0.96
19:9:39:LEU:HD12	19:9:40:VAL:H	1.28	0.96
24:6:322:LHG:HC81	25:7:321:8CT:C08	1.95	0.96
29:2:305:CHL:CHB	25:2:317:8CT:C27	2.43	0.95
29:4:307:CHL:HMB2	25:4:317:8CT:C18	1.96	0.95
22:B:850:CLA:HMA2	22:B:850:CLA:H2	1.48	0.95
25:K:103:8CT:C38	22:K:104:CLA:C2B	2.44	0.95
15:3:189:PHE:HZ	25:3:316:8CT:C27	1.69	0.95
25:J:101:8CT:C39	25:J:104:8CT:C39	2.45	0.95
18:7:251:GLY:HA2	25:7:323:8CT:C01	1.97	0.95
2:B:631:LEU:HD11	2:B:724:PHE:HA	1.48	0.94
19:9:85:MET:HE2	30:9:314:XAT:H14	1.48	0.94
22:A:809:CLA:H11	25:J:104:8CT:C39	1.95	0.94
16:8:172:ILE:H	16:8:172:ILE:HD12	1.28	0.94
19:9:37:MET:SD	19:9:42:ALA:O	2.26	0.93
22:7:306:CLA:CBA	25:7:321:8CT:C25	2.46	0.93
16:8:179:ILE:HD12	29:8:314:CHL:HHB	0.95	0.93
8:H:124:ASP:HB3	8:H:127:LEU:CD1	1.99	0.92
2:B:623:TYR:O	2:B:627:ASN:ND2	2.01	0.92
17:6:133:TYR:CD2	25:6:321:8CT:C40	2.51	0.92
16:8:166:LYS:HE2	16:8:168:PRO:HG3	1.51	0.92
2:B:395:ILE:HG23	2:B:396:ARG:HG3	1.51	0.92
15:3:189:PHE:HE1	25:3:316:8CT:C27	1.62	0.91
22:B:826:CLA:C1B	25:B:847:8CT:C22	2.48	0.91
29:4:305:CHL:CHB	25:4:317:8CT:C38	2.50	0.89
1:A:660:SER:HB3	2:B:625:TRP:CZ2	2.08	0.88
2:B:73:ASN:O	2:B:121:TYR:OH	1.90	0.88
2:B:627:ASN:HB2	2:B:724:PHE:CE1	2.09	0.88
1:A:479:ASP:O	1:A:483:GLN:NE2	2.07	0.87
22:G:102:CLA:CBB	25:G:104:8CT:C39	2.52	0.87
25:K:103:8CT:C38	22:K:104:CLA:C3B	2.53	0.87
29:6:307:CHL:CMA	25:8:301:8CT:C38	2.53	0.87
17:6:133:TYR:CZ	25:6:321:8CT:C40	2.58	0.86
22:7:307:CLA:CHB	25:7:323:8CT:C27	2.54	0.85
12:L:40:ARG:O	12:L:48:ARG:NH2	2.09	0.85
16:8:166:LYS:HZ1	16:8:179:ILE:H	1.21	0.85
16:4:150:ASP:HB2	16:4:157:VAL:HG22	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:8:176:PRO:O	22:8:309:CLA:OBD	1.95	0.84
15:3:270:ILE:HD11	22:3:311:CLA:H12	1.57	0.84
2:B:595:HIS:HD2	2:B:623:TYR:OH	1.59	0.84
20:0:124:PHE:HZ	22:0:305:CLA:HHD	1.42	0.84
14:2:141:MET:HA	25:2:317:8CT:C22	2.07	0.84
22:B:824:CLA:HBC3	25:B:846:8CT:C27	2.08	0.83
2:B:684:ARG:HD3	12:L:18:MET:HB2	1.60	0.83
22:G:103:CLA:C1C	25:G:104:8CT:C37	2.55	0.83
29:7:308:CHL:HMB1	25:7:321:8CT:C18	2.09	0.83
2:B:595:HIS:HD2	2:B:623:TYR:CE1	1.97	0.83
8:H:82:PRO:HD3	22:L:202:CLA:HMD1	1.61	0.83
18:7:86:ARG:NH1	18:7:194:GLU:OE2	2.12	0.83
17:6:134:VAL:HG23	25:6:321:8CT:C39	2.10	0.82
1:A:151:GLN:NE2	1:A:384:TYR:O	2.13	0.82
18:7:60:TYR:OH	24:7:322:LHG:O5	1.97	0.82
29:2:305:CHL:HBB	25:2:317:8CT:C27	2.09	0.82
29:3:306:CHL:CMB	25:3:316:8CT:C22	2.58	0.81
29:0:301:CHL:HAC2	24:0:315:LHG:HC41	1.62	0.81
2:B:631:LEU:HD21	2:B:727:ALA:HB3	1.60	0.81
22:6:318:CLA:HMA3	25:7:323:8CT:C39	2.09	0.81
29:6:307:CHL:H3A	25:8:301:8CT:C38	2.10	0.81
22:1:312:CLA:H93	29:4:301:CHL:H51	1.62	0.81
16:8:166:LYS:CE	16:8:179:ILE:HG13	2.11	0.81
1:A:745:TRP:CD2	25:A:850:8CT:C38	2.63	0.81
2:B:48:ALA:HB2	2:B:157:LEU:HD11	1.62	0.80
25:A:850:8CT:C22	22:B:803:CLA:H161	2.10	0.80
22:B:829:CLA:HBB1	22:B:829:CLA:HHC	1.64	0.80
14:2:145:GLU:OE1	14:2:148:ARG:NH2	2.14	0.80
16:8:166:LYS:CE	16:8:179:ILE:H	1.94	0.80
7:G:8:ILE:HD12	7:G:82:ALA:HB1	1.64	0.80
17:6:91:GLY:HA3	30:6:320:XAT:H193	1.64	0.80
16:4:146:ARG:HH12	16:4:158:ASN:HB2	1.47	0.80
16:8:166:LYS:NZ	16:8:179:ILE:H	1.79	0.80
18:7:199:ARG:HH22	22:7:303:CLA:HED2	1.45	0.80
2:B:707:LEU:HD11	28:B:849:DGD:HB41	1.64	0.79
18:7:262:PRO:HD2	22:7:317:CLA:HAA1	1.63	0.79
2:B:120:VAL:HG22	22:B:829:CLA:HAA2	1.65	0.79
14:2:114:GLN:HE21	14:2:228:GLY:HA3	1.47	0.79
16:8:166:LYS:HZ1	16:8:179:ILE:N	1.80	0.79
15:3:188:TYR:HA	15:3:193:GLU:OE1	1.82	0.79
2:B:516:ASP:OD1	2:B:593:TYR:OH	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:301:CLA:HAB	30:3:315:XAT:H32	1.64	0.78
19:9:58:TYR:HE2	30:9:315:XAT:H383	1.49	0.78
2:B:390:GLY:CA	25:B:847:8CT:C32	2.62	0.78
22:G:102:CLA:HBB1	25:G:104:8CT:C16	2.12	0.78
3:C:7:ILE:HG12	3:C:65:VAL:HG12	1.65	0.78
12:L:71:ARG:O	12:L:72:ASP:OD1	2.01	0.78
2:B:595:HIS:HD2	2:B:623:TYR:CZ	2.01	0.78
29:6:307:CHL:C3A	25:8:301:8CT:C38	2.62	0.78
22:6:310:CLA:H52	30:6:319:XAT:H30	1.66	0.78
22:B:841:CLA:HMA3	25:B:846:8CT:C40	2.15	0.77
4:D:94:ALA:HB1	8:H:67:LEU:HD22	1.67	0.77
8:H:98:ARG:H	8:H:102:ILE:HD12	1.49	0.77
13:1:113:THR:HG22	13:1:115:PHE:H	1.49	0.77
25:K:103:8CT:C38	22:K:104:CLA:C1B	2.61	0.77
13:1:91:GLN:O	13:1:97:GLY:N	2.15	0.77
17:6:232:VAL:HG12	17:6:239:VAL:HG22	1.65	0.77
29:8:305:CHL:HHC	29:8:305:CHL:HBB1	1.66	0.77
19:9:160:THR:HG22	19:9:162:GLU:H	1.49	0.77
22:K:102:CLA:HMC3	25:K:103:8CT:C09	2.14	0.77
22:B:824:CLA:CBC	25:B:846:8CT:C27	2.63	0.76
29:4:305:CHL:O2A	25:4:317:8CT:C22	2.34	0.76
1:A:121:GLN:NE2	22:A:809:CLA:OBD	2.17	0.76
2:B:562:PRO:HA	2:B:566:GLY:HA2	1.66	0.76
1:A:147:SER:OG	22:A:808:CLA:OBD	2.03	0.76
16:8:176:PRO:HD2	22:8:309:CLA:OBD	1.84	0.76
12:L:70:LEU:H	12:L:70:LEU:HD12	1.49	0.76
17:6:140:GLN:NE2	16:8:46:PRO:O	2.19	0.75
2:B:390:GLY:HA2	25:B:847:8CT:C32	2.17	0.75
22:0:309:CLA:HBC3	24:0:315:LHG:HC62	1.66	0.75
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.68	0.75
19:9:75:GLU:OE1	19:9:140:TRP:NE1	2.17	0.75
20:0:162:LYS:HD3	22:0:310:CLA:HBD	1.69	0.75
1:A:666:TYR:HD1	2:B:445:ALA:HA	1.52	0.75
22:B:813:CLA:H11	22:B:813:CLA:H92	1.67	0.75
22:5:309:CLA:HBB1	30:5:315:XAT:H10	1.67	0.75
17:6:225:THR:HA	17:6:230:LYS:HD2	1.69	0.74
19:9:38:TRP:CD1	19:9:43:SER:HB3	2.22	0.74
22:B:826:CLA:C4B	25:B:847:8CT:C22	2.65	0.74
1:A:77:LYS:NZ	22:A:811:CLA:OBD	2.21	0.74
18:7:205:TRP:CE2	30:7:320:XAT:H10	2.23	0.74
29:0:301:CHL:HHC	29:0:301:CHL:HBB1	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:158:ASN:ND2	16:4:163:PHE:HB3	2.03	0.74
13:5:106:VAL:O	13:5:110:GLY:N	2.18	0.74
2:B:339:ALA:HB2	25:B:847:8CT:C27	2.17	0.74
2:B:560:ASP:OD2	2:B:564:ARG:NH2	2.16	0.74
18:7:124:ASN:CG	25:7:323:8CT:C08	2.60	0.74
13:1:55:TYR:HE2	30:1:315:XAT:H383	1.51	0.74
16:8:172:ILE:HD12	16:8:172:ILE:N	2.01	0.74
16:8:196:LYS:O	16:8:200:ASN:ND2	2.19	0.74
29:5:301:CHL:HHC	29:5:301:CHL:HBB1	1.70	0.73
2:B:585:ASN:HD21	22:B:803:CLA:HBC2	1.53	0.73
16:8:175:TYR:HB3	22:8:309:CLA:O1D	1.87	0.73
2:B:35:ASP:OD1	2:B:36:SER:N	2.19	0.73
6:F:191:GLU:OE2	6:F:197:LYS:NZ	2.21	0.73
13:1:73:CYS:SG	22:1:302:CLA:HAA2	2.28	0.73
16:8:86:HIS:HE1	30:8:317:XAT:H15	1.54	0.73
9:I:29:TYR:OH	21:M:30:TYR:OH	2.05	0.73
20:0:36:TRP:HA	29:0:301:CHL:C4C	2.18	0.73
15:3:173:ARG:HG2	29:3:306:CHL:HBB1	1.71	0.73
16:8:179:ILE:HD11	29:8:314:CHL:H3A	1.71	0.73
1:A:21:ILE:HG22	1:A:192:LYS:HD2	1.71	0.73
13:5:46:PRO:HG2	13:5:49:LEU:HB2	1.69	0.72
18:7:173:GLY:HA2	18:7:176:PHE:HB2	1.70	0.72
1:A:577:ARG:NH1	24:A:844:LHG:O10	2.21	0.72
11:K:21:ALA:HB3	11:K:26:LEU:HD23	1.70	0.72
1:A:695:ARG:NE	2:B:565:GLY:O	2.22	0.72
2:B:627:ASN:ND2	2:B:724:PHE:HZ	1.82	0.72
2:B:627:ASN:CB	2:B:724:PHE:CE1	2.73	0.72
13:1:134:LEU:CD1	25:1:316:8CT:C19	2.65	0.72
16:4:223:ILE:HA	16:4:226:TRP:HB3	1.72	0.72
12:L:114:VAL:HG12	12:L:115:LYS:H	1.52	0.72
14:2:62:GLY:O	14:2:209:ARG:NH1	2.22	0.72
25:A:850:8CT:C05	22:B:832:CLA:HMB2	2.20	0.72
22:5:303:CLA:H102	22:5:303:CLA:H41	1.71	0.72
20:0:155:ARG:HH22	20:0:162:LYS:HD2	1.55	0.72
1:A:127:VAL:HG11	22:A:809:CLA:HAB	1.72	0.72
20:0:141:CYS:HB3	20:0:144:LEU:HB2	1.71	0.72
22:H:201:CLA:H72	12:L:88:LEU:HD11	1.71	0.71
19:9:185:GLN:NE2	19:9:196:CYS:SG	2.63	0.71
14:2:143:TRP:HH2	25:2:317:8CT:C09	2.01	0.71
13:1:174:LYS:HD3	22:1:310:CLA:HBA1	1.70	0.71
14:2:48:PRO:HB2	15:3:184:MET:HE1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:801:CLA:CGA	22:B:801:CLA:H3A	2.21	0.71
14:2:115:TRP:HB2	30:2:316:XAT:H21	1.71	0.71
18:7:113:PRO:HA	18:7:116:LEU:HD13	1.72	0.71
1:A:312:ILE:HD12	11:K:69:MET:HE2	1.72	0.71
2:B:683:GLU:HG2	4:D:92:ARG:HH11	1.55	0.71
2:B:720:THR:OG1	22:B:805:CLA:O1D	2.08	0.71
12:L:63:PRO:HG3	22:L:204:CLA:HAB	1.73	0.71
14:2:128:ILE:HD11	14:2:133:LEU:HD12	1.73	0.71
15:3:195:VAL:HG21	15:3:208:ALA:HB3	1.65	0.71
16:8:86:HIS:CE1	30:8:317:XAT:H15	2.25	0.71
1:A:587:GLY:O	2:B:668:ARG:NH1	2.24	0.70
22:B:841:CLA:HBB2	22:1:301:CLA:H41	1.73	0.70
29:2:305:CHL:HH1	29:2:305:CHL:HBB1	1.72	0.70
17:6:135:GLU:HA	17:6:138:ARG:HG2	1.73	0.70
1:A:404:GLY:HA3	1:A:608:LEU:HD11	1.73	0.70
2:B:546:LEU:HD21	2:B:567:THR:HG22	1.72	0.70
22:7:318:CLA:H43	22:7:318:CLA:H121	1.72	0.70
20:0:54:TYR:HE2	20:0:165:LYS:HZ3	1.37	0.70
1:A:100:GLY:O	1:A:104:SER:OG	2.08	0.70
1:A:268:PRO:HA	1:A:271:THR:HG22	1.72	0.70
22:A:810:CLA:H43	22:A:812:CLA:H43	1.73	0.70
4:D:100:TYR:OH	4:D:156:ARG:NH1	2.25	0.70
14:2:135:MET:HB3	16:4:239:TRP:HE3	1.56	0.70
15:3:81:PHE:HD2	30:3:315:XAT:H221	1.55	0.70
18:7:67:LEU:HD23	22:7:303:CLA:H43	1.73	0.70
22:7:318:CLA:HMA3	22:7:318:CLA:H42	1.73	0.70
1:A:567:LEU:HD23	1:A:568:ILE:HG13	1.73	0.70
22:6:305:CLA:NB	25:6:321:8CT:C33	2.53	0.70
29:7:308:CHL:HMB3	25:7:321:8CT:C19	2.22	0.70
16:8:199:LYS:NZ	22:8:310:CLA:O1D	2.24	0.70
2:B:85:ARG:HH22	8:H:142:LYS:HB3	1.55	0.70
7:G:17:PHE:HD2	7:G:18:LEU:HD12	1.56	0.70
1:A:639:ASN:HB2	1:A:643:SER:HB2	1.74	0.70
7:G:50:ARG:NH1	19:9:65:SER:OG	2.25	0.70
1:A:126:ILE:HG12	1:A:127:VAL:HG23	1.74	0.70
20:0:83:MET:HE2	20:0:167:GLY:HA3	1.74	0.69
22:A:801:CLA:HBB1	22:B:803:CLA:HED1	1.74	0.69
13:5:198:LYS:NZ	13:5:206:GLU:OE1	2.24	0.69
1:A:752:ILE:O	1:A:756:GLY:N	2.25	0.69
4:D:190:SER:OG	5:E:13:ARG:NH1	2.25	0.69
6:F:221:PHE:HB3	6:F:225:ARG:HH12	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:6:314:CLA:HAA2	18:7:131:PHE:HA	1.73	0.69
2:B:129:MET:O	2:B:208:ARG:NH2	2.26	0.69
16:4:104:THR:HG1	16:4:112:ALA:H	1.39	0.69
22:6:309:CLA:HBB1	22:6:315:CLA:HAA1	1.75	0.69
22:6:304:CLA:H141	22:6:315:CLA:H161	1.74	0.69
22:7:303:CLA:H62	22:7:304:CLA:H3A	1.74	0.69
7:G:20:ARG:NH1	7:G:62:ASP:OD2	2.24	0.69
7:G:28:ARG:NH2	7:G:70:ASP:OD2	2.25	0.69
22:B:833:CLA:HAA2	10:J:36:PRO:HG2	1.74	0.69
13:1:219:ASN:HB3	13:1:221:THR:HG22	1.73	0.69
17:6:98:GLN:HA	17:6:102:LYS:HD3	1.74	0.69
13:5:80:TRP:CE3	22:5:308:CLA:H2A	2.28	0.69
13:5:215:ASN:ND2	22:5:313:CLA:O1D	2.26	0.69
20:0:70:TRP:HZ2	22:0:307:CLA:HBA1	1.57	0.69
22:B:820:CLA:HBC2	22:B:824:CLA:H72	1.73	0.69
16:4:157:VAL:HG21	29:4:307:CHL:HMC	1.73	0.69
16:4:229:HIS:CG	22:4:312:CLA:HAA2	2.28	0.69
16:8:150:ASP:HB2	16:8:158:ASN:HD22	1.58	0.69
1:A:660:SER:HB3	2:B:625:TRP:HZ2	1.56	0.68
22:B:810:CLA:HBC1	21:M:12:ILE:HA	1.75	0.68
18:7:42:TRP:CD1	18:7:62:TRP:HB2	2.28	0.68
1:A:252:ARG:NH1	15:3:275:THR:O	2.22	0.68
1:A:620:GLN:OE1	1:A:658:GLN:NE2	2.25	0.68
14:2:66:TYR:HE2	30:2:316:XAT:H383	1.58	0.68
29:5:306:CHL:HHC	29:5:306:CHL:HBB1	1.75	0.68
13:1:69:ARG:NH1	22:1:302:CLA:O1A	2.27	0.68
16:8:83:GLU:OE2	16:8:202:ARG:NE	2.23	0.68
2:B:542:ARG:HD3	2:B:551:LYS:HB3	1.76	0.68
22:A:828:CLA:H42	25:A:850:8CT:C36	2.23	0.68
16:8:166:LYS:HG2	16:8:168:PRO:HD3	1.76	0.68
12:L:40:ARG:HB2	12:L:48:ARG:HH22	1.59	0.68
16:8:190:VAL:O	16:8:194:LYS:N	2.24	0.68
6:F:221:PHE:HB3	6:F:225:ARG:NH1	2.09	0.68
16:8:172:ILE:H	16:8:172:ILE:CD1	2.04	0.68
2:B:174:ARG:HG3	22:B:814:CLA:HBC2	1.76	0.68
2:B:693:TRP:HE1	2:B:696:LYS:HG2	1.59	0.68
6:F:237:THR:HG22	6:F:238:VAL:H	1.59	0.68
22:7:307:CLA:CMB	25:7:323:8CT:C27	2.71	0.68
11:K:23:ARG:HH11	11:K:52:PRO:HG2	1.58	0.67
14:2:141:MET:SD	25:2:317:8CT:C22	2.82	0.67
6:F:214:ALA:HB3	16:4:67:LEU:HD22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PHE:HD1	22:K:102:CLA:HBC2	1.59	0.67
22:A:803:CLA:HBB1	25:J:101:8CT:C07	2.25	0.67
16:4:83:GLU:OE2	16:4:202:ARG:NE	2.19	0.67
29:2:305:CHL:NA	25:2:317:8CT:C38	2.58	0.67
17:6:137:ARG:NH1	22:6:323:CLA:OBD	2.28	0.67
13:5:80:TRP:CZ3	22:5:308:CLA:H2A	2.29	0.67
24:0:315:LHG:H311	24:0:315:LHG:H191	1.75	0.67
14:2:203:LYS:HD3	22:2:311:CLA:HAA2	1.76	0.67
16:4:158:ASN:ND2	16:4:162:ILE:O	2.18	0.67
22:8:310:CLA:H2	22:8:311:CLA:CAD	2.24	0.67
6:F:101:LEU:HD22	6:F:122:ALA:HB2	1.77	0.67
12:L:116:THR:OG1	12:L:120:ARG:O	2.10	0.67
16:8:81:GLN:NE2	16:8:173:PRO:HB2	2.10	0.67
22:L:202:CLA:H12	22:L:202:CLA:H3A	1.76	0.67
16:4:226:TRP:HZ3	22:4:313:CLA:HAC1	1.58	0.67
13:5:83:LEU:HB3	22:5:304:CLA:HBB2	1.75	0.67
20:0:171:MET:O	20:0:174:SER:OG	2.13	0.67
1:A:460:LEU:O	1:A:464:ASN:ND2	2.27	0.67
2:B:93:ASP:HB2	2:B:96:PHE:CE2	2.29	0.67
15:3:195:VAL:HG22	15:3:208:ALA:CB	2.16	0.67
29:5:301:CHL:HBA2	24:5:318:LHG:H162	1.76	0.67
4:D:130:LYS:NZ	8:H:66:THR:O	2.27	0.66
20:0:56:TYR:N	22:0:302:CLA:OBD	2.29	0.66
2:B:582:TRP:CH2	22:B:803:CLA:HAB	2.30	0.66
20:0:195:HIS:HB2	20:0:202:ASN:HD22	1.60	0.66
1:A:284:LYS:HZ3	1:A:295:TRP:CD1	2.12	0.66
2:B:631:LEU:HD21	2:B:727:ALA:CB	2.26	0.66
15:3:195:VAL:HG23	15:3:208:ALA:CB	2.15	0.66
19:9:47:TYR:OH	19:9:59:ASP:OD2	2.13	0.66
4:D:87:THR:HA	12:L:17:GLY:O	1.95	0.66
16:8:211:PHE:CZ	30:8:316:XAT:H363	2.31	0.66
19:9:52:MET:HE1	19:9:70:LEU:HG	1.77	0.66
8:H:79:LYS:HG2	12:L:43:VAL:HG23	1.78	0.66
2:B:39:GLU:OE2	2:B:169:LYS:NZ	2.25	0.66
22:8:309:CLA:H41	22:8:311:CLA:H2	1.75	0.66
19:9:45:PRO:CG	19:9:48:LEU:HG	2.26	0.66
6:F:176:TYR:CE2	22:F:301:CLA:HBD	2.31	0.66
1:A:422:TYR:HE1	1:A:427:ASN:HD21	1.44	0.66
2:B:177:HIS:CD2	22:B:814:CLA:HMC2	2.31	0.66
11:K:23:ARG:NH1	11:K:52:PRO:HG2	2.10	0.66
19:9:119:ASN:ND2	20:0:211:ASN:OD1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:809:CLA:H91	25:J:101:8CT:C40	2.26	0.66
2:B:140:VAL:O	2:B:143:SER:OG	2.11	0.66
22:B:839:CLA:H122	22:B:840:CLA:H112	1.78	0.66
29:7:308:CHL:CMB	25:7:321:8CT:C18	2.74	0.66
8:H:124:ASP:CG	8:H:127:LEU:HD12	2.21	0.66
13:1:171:LEU:HD23	13:1:174:LYS:HD2	1.77	0.66
15:3:140:ASN:ND2	30:3:315:XAT:O3	2.28	0.66
17:6:100:LEU:HD12	17:6:101:VAL:HG23	1.78	0.65
17:6:229:SER:O	25:7:323:8CT:C09	2.45	0.65
13:5:202:GLN:O	13:5:206:GLU:N	2.25	0.65
16:8:144:GLU:OE1	16:8:147:ARG:NH2	2.29	0.65
14:2:85:GLU:OE2	14:2:209:ARG:NH2	2.29	0.65
22:2:309:CLA:H121	30:2:315:XAT:H193	1.77	0.65
13:5:147:ASP:HB3	13:5:150:LYS:HB3	1.79	0.65
22:0:302:CLA:HBB1	30:0:314:XAT:H31	1.79	0.65
2:B:684:ARG:HB3	12:L:18:MET:HE3	1.78	0.65
22:B:850:CLA:H93	6:F:153:LEU:HD22	1.78	0.65
22:6:305:CLA:C3B	25:6:321:8CT:C33	2.75	0.65
22:A:809:CLA:H122	25:J:104:8CT:C07	2.27	0.65
11:K:45:LEU:HD23	11:K:47:LEU:H	1.62	0.65
1:A:96:MET:HE2	22:A:828:CLA:HED1	1.78	0.65
1:A:133:ASN:HB3	1:A:141:GLN:HB3	1.78	0.65
1:A:514:THR:HG22	1:A:528:MET:HE2	1.79	0.65
13:1:207:HIS:CG	22:1:311:CLA:HAA2	2.32	0.65
18:7:106:PHE:CE2	18:7:108:TYR:HB3	2.31	0.65
22:A:841:CLA:HBB1	22:A:841:CLA:H92	1.78	0.65
2:B:174:ARG:NH1	22:B:808:CLA:H162	2.12	0.65
1:A:386:ALA:HB1	1:A:527:ALA:HA	1.77	0.65
16:4:175:TYR:HE2	16:4:194:LYS:HE2	1.61	0.65
17:6:92:VAL:HG23	17:6:200:PHE:CE2	2.31	0.65
20:0:80:ARG:HA	20:0:83:MET:HE3	1.77	0.65
8:H:75:GLN:HG3	12:L:34:SER:HB2	1.80	0.64
2:B:105:THR:HA	2:B:112:PRO:HA	1.77	0.64
13:1:159:ASP:O	13:1:161:ALA:N	2.30	0.64
14:2:138:VAL:HA	22:2:308:CLA:HBB2	1.79	0.64
13:5:91:GLN:HE22	22:5:304:CLA:CGD	2.11	0.64
13:1:219:ASN:OD1	13:1:220:GLY:N	2.29	0.64
16:8:166:LYS:HE3	16:8:179:ILE:H	1.60	0.64
2:B:623:TYR:O	2:B:627:ASN:CG	2.39	0.64
25:K:103:8CT:C38	22:K:104:CLA:C4B	2.76	0.64
14:2:147:MET:HG3	14:2:158:GLN:NE2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:803:CLA:HBB	22:B:805:CLA:H202	1.80	0.64
15:3:135:ILE:HD12	15:3:140:ASN:HA	1.80	0.64
16:8:237:ASN:O	16:8:241:ILE:HG12	1.98	0.64
1:A:199:VAL:HG11	22:A:825:CLA:HAC2	1.79	0.64
22:B:806:CLA:H3A	22:B:806:CLA:CGA	2.27	0.64
16:4:124:PRO:O	16:4:125:MET:HE2	1.98	0.64
13:1:139:GLU:OE1	13:1:142:ARG:NH2	2.22	0.64
22:5:309:CLA:H13	30:5:315:XAT:H203	1.78	0.64
16:8:210:GLY:O	16:8:214:GLN:N	2.22	0.64
29:5:301:CHL:HED1	16:8:146:ARG:HA	1.80	0.64
18:7:39:ARG:NH1	18:7:59:ASP:O	2.31	0.64
18:7:234:ASN:OD1	18:7:235:ILE:N	2.31	0.64
1:A:308:VAL:O	1:A:312:ILE:HG12	1.98	0.64
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.15	0.64
4:D:130:LYS:NZ	8:H:66:THR:OG1	2.20	0.64
17:6:133:TYR:CG	25:6:321:8CT:C40	2.80	0.64
2:B:397:ASP:HA	4:D:198:ILE:HD11	1.80	0.63
1:A:71:LEU:HB2	1:A:193:LEU:HD12	1.79	0.63
1:A:629:GLU:HG3	1:A:630:SER:H	1.63	0.63
22:G:102:CLA:HBB1	25:G:104:8CT:C15	2.29	0.63
1:A:544:HIS:HE1	1:A:611:VAL:HA	1.64	0.63
2:B:545:LYS:HE2	6:F:236:ILE:HG12	1.79	0.63
13:5:47:GLU:N	13:5:47:GLU:OE1	2.30	0.63
14:2:206:LYS:NZ	24:2:318:LHG:O5	2.23	0.63
17:6:107:TRP:CD1	17:6:107:TRP:H	2.16	0.63
1:A:205:HIS:O	1:A:209:GLY:N	2.27	0.63
19:9:209:ILE:N	22:9:312:CLA:O1A	2.32	0.63
7:G:7:VAL:O	7:G:11:SER:N	2.31	0.63
16:8:179:ILE:HD11	29:8:314:CHL:C3A	2.27	0.63
20:0:72:ARG:HH21	20:0:164:LEU:HD11	1.63	0.63
1:A:601:LEU:HB3	1:A:737:ILE:HD11	1.80	0.63
1:A:643:SER:OG	1:A:653:ASP:OD2	2.16	0.63
22:B:810:CLA:HBB	22:B:811:CLA:HMB3	1.80	0.63
6:F:154:ALA:HB1	6:F:160:ALA:HA	1.81	0.63
8:H:99:ARG:HH21	12:L:102:GLN:HG2	1.63	0.63
16:8:199:LYS:NZ	31:8:319:LMG:O5	2.29	0.63
19:9:52:MET:HE2	19:9:74:ARG:HD2	1.81	0.63
11:K:32:LYS:HB3	11:K:43:LYS:HG3	1.80	0.63
13:1:178:GLY:HA3	13:1:179:ALA:HB1	1.81	0.63
17:6:134:VAL:CG2	25:6:321:8CT:C39	2.77	0.63
18:7:62:TRP:CZ3	30:7:320:XAT:H383	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:0:93:ASN:HD22	20:0:188:PRO:HD2	1.63	0.63
2:B:582:TRP:HH2	22:B:803:CLA:HAB	1.64	0.62
2:B:687:LEU:N	12:L:39:TYR:OH	2.32	0.62
7:G:79:HIS:CG	25:G:104:8CT:C40	2.82	0.62
1:A:695:ARG:NH1	1:A:722:ALA:O	2.25	0.62
4:D:167:HIS:O	4:D:169:LYS:N	2.32	0.62
8:H:83:GLY:HA2	8:H:86:ASN:HB2	1.81	0.62
8:H:103:ARG:NH2	12:L:98:THR:O	2.32	0.62
22:4:311:CLA:H2A	22:4:311:CLA:O2A	1.98	0.62
16:8:89:PHE:CZ	22:8:308:CLA:HBC1	2.34	0.62
1:A:223:ILE:HA	1:A:227:ILE:HD12	1.81	0.62
1:A:491:TRP:O	1:A:494:SER:OG	2.14	0.62
16:4:238:VAL:HB	16:4:239:TRP:CD1	2.33	0.62
13:1:186:PHE:HA	13:1:189:PHE:HD2	1.65	0.62
29:0:301:CHL:H72	22:0:312:CLA:H93	1.81	0.62
2:B:398:TYR:HD2	2:B:542:ARG:HH22	1.45	0.62
2:B:595:HIS:CD2	2:B:623:TYR:CE1	2.85	0.62
22:B:806:CLA:H162	25:B:848:8CT:C18	2.29	0.62
4:D:178:ASN:OD1	4:D:179:ALA:N	2.29	0.62
22:1:303:CLA:NB	25:1:316:8CT:C36	2.63	0.62
15:3:81:PHE:CD2	30:3:315:XAT:H221	2.33	0.62
18:7:226:HIS:CG	22:7:313:CLA:HAA2	2.34	0.62
16:8:176:PRO:HD2	22:8:309:CLA:CAD	2.29	0.62
2:B:339:ALA:CB	25:B:847:8CT:C27	2.78	0.62
14:2:215:CYS:SG	30:2:316:XAT:H12	2.39	0.62
15:3:261:HIS:CG	22:3:311:CLA:HAA2	2.33	0.62
17:6:159:LEU:HD22	17:6:168:GLY:HA3	1.80	0.62
19:9:174:LEU:HD21	30:9:314:XAT:H391	1.79	0.62
22:A:840:CLA:H202	22:F:301:CLA:HBB1	1.81	0.62
2:B:676:GLU:O	3:C:81:TYR:OH	2.11	0.62
24:5:318:LHG:H282	24:5:318:LHG:HC82	1.82	0.62
22:A:826:CLA:H92	25:A:849:8CT:C40	2.30	0.62
22:B:840:CLA:NC	25:B:848:8CT:C22	2.57	0.62
11:K:65:SER:N	25:K:103:8CT:C39	2.63	0.62
13:1:55:TYR:CE2	30:1:315:XAT:H383	2.35	0.62
18:7:109:GLU:O	18:7:111:GLY:N	2.31	0.62
29:8:314:CHL:HHC	29:8:314:CHL:HBB1	1.80	0.62
19:9:45:PRO:HG2	19:9:48:LEU:HG	1.82	0.62
19:9:86:ASN:HD21	22:9:309:CLA:HAC1	1.64	0.62
1:A:125:PRO:HA	1:A:130:GLU:HB2	1.82	0.62
2:B:92:TRP:NE1	8:H:129:ILE:HG12	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:ILE:HD12	3:C:41:SER:HA	1.81	0.62
22:4:302:CLA:H2	30:4:316:XAT:O24	1.99	0.62
13:5:207:HIS:CG	22:5:312:CLA:HAA2	2.35	0.62
1:A:666:TYR:CE2	2:B:617:MET:HG2	2.35	0.61
17:6:116:LEU:HD21	17:6:120:ILE:HD11	1.82	0.61
18:7:90:MET:HB3	22:7:305:CLA:HBB2	1.82	0.61
20:0:147:MET:HG2	20:0:148:PRO:HD3	1.82	0.61
2:B:133:GLN:HE22	21:M:7:GLN:HE22	1.48	0.61
13:1:104:SER:HB2	29:1:305:CHL:C2D	2.30	0.61
18:7:78:ARG:HH22	22:7:303:CLA:HED3	1.65	0.61
22:9:303:CLA:H3A	22:9:303:CLA:CGA	2.30	0.61
20:0:75:GLU:OE2	20:0:168:ARG:NH1	2.27	0.61
2:B:223:LYS:HA	19:9:214:LEU:HG	1.82	0.61
14:2:114:GLN:NE2	14:2:228:GLY:HA3	2.16	0.61
17:6:223:PHE:HD2	18:7:123:LEU:HD22	1.65	0.61
2:B:165:LEU:HD21	2:B:169:LYS:HZ2	1.66	0.61
4:D:167:HIS:CG	4:D:168:PRO:HD3	2.36	0.61
6:F:77:ASP:N	6:F:81:LEU:O	2.33	0.61
29:6:302:CHL:HBB2	22:6:303:CLA:HBC2	1.83	0.61
20:0:83:MET:HB2	30:0:313:XAT:H15	1.82	0.61
1:A:90:LEU:HD21	22:A:805:CLA:H91	1.83	0.61
1:A:339:THR:HB	1:A:431:LEU:HD21	1.81	0.61
2:B:302:LYS:NZ	7:G:37:GLU:HG3	2.15	0.61
22:B:850:CLA:H2A	22:B:850:CLA:H12	1.82	0.61
11:K:38:LEU:HA	22:K:105:CLA:H42	1.82	0.61
13:1:53:TYR:OH	13:1:177:LYS:NZ	2.25	0.61
22:1:303:CLA:H2	25:1:316:8CT:C34	2.30	0.61
22:1:304:CLA:C2A	25:1:316:8CT:C27	2.79	0.61
14:2:66:TYR:CE2	30:2:316:XAT:H383	2.34	0.61
22:6:305:CLA:C3B	30:6:320:XAT:H163	2.30	0.61
22:1:304:CLA:H2A	22:1:304:CLA:O1A	1.99	0.61
20:0:128:GLU:HA	20:0:131:ARG:HG2	1.81	0.61
2:B:92:TRP:CZ2	9:I:8:SER:HA	2.36	0.61
22:8:310:CLA:HBC3	31:8:319:LMG:HC92	1.82	0.61
1:A:208:ALA:HB1	22:A:820:CLA:HBC3	1.81	0.60
2:B:375:HIS:HA	2:B:378:ILE:HG22	1.83	0.60
14:2:136:THR:HG22	14:2:140:MET:HE2	1.83	0.60
16:4:208:THR:HG21	30:4:316:XAT:H12	1.83	0.60
16:8:161:PRO:HB3	29:8:314:CHL:C3B	2.31	0.60
19:9:47:TYR:HE1	19:9:48:LEU:HD23	1.66	0.60
2:B:191:THR:HG23	2:B:277:HIS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ILE:HD12	2:B:332:PHE:CE1	2.37	0.60
16:8:179:ILE:CD1	29:8:314:CHL:C4A	2.79	0.60
2:B:303:GLU:OE1	7:G:34:GLN:HA	1.99	0.60
2:B:580:VAL:HB	2:B:710:LEU:HD11	1.83	0.60
22:B:840:CLA:CMC	25:B:848:8CT:C22	2.78	0.60
19:9:69:ARG:HH12	22:9:301:CLA:CGD	2.14	0.60
2:B:361:ILE:HG22	2:B:362:ALA:H	1.65	0.60
12:L:21:THR:H	12:L:24:THR:HG1	1.46	0.60
12:L:111:GLN:HG2	12:L:128:GLN:HB2	1.83	0.60
14:2:96:THR:HG21	30:2:315:XAT:H32	1.84	0.60
16:4:161:PRO:HG2	16:4:162:ILE:HD12	1.83	0.60
16:8:190:VAL:HG23	16:8:191:ASP:H	1.66	0.60
19:9:59:ASP:OD1	30:9:315:XAT:O23	2.15	0.60
29:2:306:CHL:HHC	29:2:306:CHL:HBB1	1.83	0.60
18:7:105:VAL:HG11	22:7:305:CLA:HED1	1.81	0.60
13:5:50:PRO:HB3	13:5:172:LYS:HG2	1.83	0.60
1:A:618:LYS:NZ	1:A:622:ASP:OD2	2.26	0.60
2:B:61:THR:HG21	22:B:829:CLA:H42	1.83	0.60
2:B:74:PHE:HA	2:B:121:TYR:OH	2.02	0.60
2:B:292:ARG:HD2	7:G:36:PRO:HD3	1.84	0.60
12:L:77:ALA:HA	12:L:80:THR:HG22	1.83	0.60
24:1:317:LHG:H341	29:4:301:CHL:HMB3	1.83	0.60
29:2:305:CHL:C4A	25:2:317:8CT:C38	2.80	0.60
22:4:313:CLA:O1D	22:4:313:CLA:H2A	2.01	0.60
17:6:120:ILE:HD13	25:8:301:8CT:C40	2.31	0.60
1:A:430:ASN:H	1:A:433:ASP:HB3	1.67	0.60
22:2:319:CLA:HBB1	31:4:318:LMG:H162	1.84	0.60
15:3:61:ASP:OD1	15:3:62:GLU:N	2.34	0.60
17:6:62:TRP:CD1	30:6:320:XAT:H383	2.36	0.60
19:9:58:TYR:CE2	30:9:315:XAT:H383	2.33	0.60
20:0:109:VAL:HG11	22:0:305:CLA:HBA2	1.84	0.60
1:A:307:ALA:O	1:A:311:ILE:HD12	2.02	0.60
14:2:203:LYS:O	14:2:207:ASN:ND2	2.30	0.60
15:3:190:LEU:HD13	25:3:316:8CT:C38	2.31	0.60
17:6:153:ILE:HG22	22:8:310:CLA:HAB	1.83	0.60
13:5:78:GLY:O	13:5:82:MET:N	2.27	0.60
19:9:39:LEU:CD1	19:9:40:VAL:H	2.09	0.60
1:A:725:ILE:HD11	2:B:566:GLY:HA3	1.83	0.59
16:4:159:VAL:HG13	16:4:161:PRO:HD2	1.84	0.59
29:5:301:CHL:H11	16:8:142:TRP:HE3	1.67	0.59
18:7:234:ASN:ND2	22:7:314:CLA:O1D	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:ASN:CB	2:B:724:PHE:HE1	2.04	0.59
6:F:176:TYR:OH	6:F:210:VAL:O	2.13	0.59
11:K:15:THR:HG21	11:K:68:HIS:CE1	2.37	0.59
13:1:175:GLU:HB3	22:1:308:CLA:C1B	2.33	0.59
1:A:544:HIS:CE1	1:A:611:VAL:HA	2.36	0.59
6:F:232:LYS:HG2	6:F:233:GLU:H	1.66	0.59
17:6:108:TYR:HE2	17:6:245:ILE:HG21	1.66	0.59
17:6:119:ASN:HD21	16:8:235:ALA:HB2	1.68	0.59
17:6:140:GLN:NE2	16:8:47:GLY:O	2.36	0.59
22:A:815:CLA:HBD	15:3:277:VAL:HG11	1.85	0.59
22:A:826:CLA:HAA2	22:A:827:CLA:OBD	2.02	0.59
5:E:18:TRP:HD1	5:E:21:ARG:HD2	1.66	0.59
6:F:176:TYR:CD2	22:F:301:CLA:HBD	2.37	0.59
14:2:147:MET:HG3	14:2:158:GLN:HE21	1.67	0.59
17:6:102:LYS:HD2	22:6:305:CLA:HMD2	1.83	0.59
22:7:307:CLA:C4D	25:7:323:8CT:C22	2.80	0.59
1:A:663:ILE:HG23	2:B:617:MET:HE3	1.84	0.59
10:J:16:PHE:HE1	25:J:101:8CT:C17	2.16	0.59
17:6:133:TYR:CE1	25:6:321:8CT:C40	2.86	0.59
3:C:63:LEU:HD12	3:C:66:ARG:HH21	1.67	0.59
7:G:2:LEU:HD23	7:G:3:SER:H	1.66	0.59
8:H:111:GLY:HA2	22:H:201:CLA:H13	1.84	0.59
12:L:21:THR:HB	12:L:22:PRO:HD2	1.84	0.59
29:7:308:CHL:CMB	25:7:321:8CT:C19	2.81	0.59
2:B:548:PRO:HD2	3:C:62:PHE:CE1	2.37	0.59
16:4:175:TYR:CE2	16:4:194:LYS:HE2	2.37	0.59
25:A:850:8CT:C05	22:B:832:CLA:CMB	2.81	0.59
2:B:390:GLY:HA3	25:B:847:8CT:C32	2.32	0.59
3:C:47:ASP:OD2	4:D:134:LYS:NZ	2.30	0.59
19:9:79:VAL:O	19:9:83:TRP:N	2.35	0.59
19:9:170:LYS:NZ	22:9:310:CLA:O1D	2.26	0.59
1:A:238:ASP:HB2	1:A:239:PRO:HD2	1.83	0.59
8:H:99:ARG:HB3	12:L:102:GLN:HE21	1.68	0.59
11:K:31:ASN:ND2	11:K:54:GLY:O	2.36	0.59
11:K:34:ALA:HA	22:K:105:CLA:H41	1.85	0.59
4:D:170:ASP:OD2	4:D:178:ASN:ND2	2.36	0.59
16:4:166:LYS:H	22:5:303:CLA:C3	2.16	0.59
20:0:128:GLU:HB3	20:0:132:TYR:CE2	2.38	0.59
2:B:345:CYS:SG	22:B:829:CLA:HMC2	2.43	0.58
4:D:71:PRO:HG2	4:D:72:PRO:HD3	1.85	0.58
6:F:183:GLU:HB2	6:F:209:CYS:SG	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:58:PHE:HD2	15:3:76:TYR:HB3	1.67	0.58
16:4:168:PRO:HB3	13:5:60:ILE:HG23	1.85	0.58
20:0:187:GLY:O	20:0:191:ASN:ND2	2.36	0.58
2:B:234:ALA:HA	2:B:256:THR:HG22	1.85	0.58
14:2:234:PHE:HA	14:2:237:ILE:HG22	1.84	0.58
17:6:43:LEU:HB3	17:6:46:SER:HB2	1.85	0.58
2:B:580:VAL:HG11	2:B:710:LEU:HD21	1.85	0.58
2:B:682:HIS:CE1	2:B:688:ALA:HB1	2.38	0.58
14:2:140:MET:HE3	29:2:305:CHL:HMA2	1.85	0.58
18:7:129:LEU:HD22	25:7:323:8CT:C39	2.33	0.58
16:8:86:HIS:HD1	16:8:205:MET:HE3	1.68	0.58
8:H:96:LEU:HB3	8:H:102:ILE:HG21	1.84	0.58
16:4:166:LYS:H	22:5:303:CLA:C2	2.17	0.58
1:A:364:LEU:HD12	22:A:825:CLA:HBB	1.85	0.58
8:H:96:LEU:HD22	8:H:102:ILE:HG12	1.85	0.58
22:0:308:CLA:H61	30:0:313:XAT:H11	1.84	0.58
2:B:463:ILE:O	2:B:467:GLN:HG2	2.03	0.58
22:6:318:CLA:CMA	25:7:323:8CT:C39	2.81	0.58
22:5:303:CLA:CHD	22:5:308:CLA:HAA1	2.33	0.58
19:9:99:ILE:HG12	19:9:100:GLN:H	1.69	0.58
2:B:292:ARG:NH1	7:G:34:GLN:O	2.34	0.58
3:C:5:VAL:HG22	3:C:67:VAL:HG22	1.85	0.58
16:4:160:ASP:OD1	16:4:160:ASP:N	2.36	0.58
17:6:229:SER:HA	18:7:126:GLY:HA3	1.86	0.58
13:1:99:TRP:HD1	13:1:200:PRO:HD3	1.68	0.58
17:6:231:ALA:HA	17:6:239:VAL:HG23	1.86	0.58
25:A:850:8CT:C40	2:B:438:VAL:HG11	2.33	0.58
22:B:834:CLA:HBC2	22:B:835:CLA:HAB	1.86	0.58
22:B:850:CLA:O1A	22:B:850:CLA:H3A	2.04	0.58
1:A:465:ASP:OD1	1:A:646:ALA:HB1	2.04	0.57
1:A:690:PHE:HZ	22:A:840:CLA:HBC3	1.69	0.57
2:B:322:LEU:O	2:B:326:ILE:HG12	2.04	0.57
8:H:127:LEU:HD13	8:H:129:ILE:HD12	1.86	0.57
16:4:95:VAL:HG21	30:4:315:XAT:H401	1.86	0.57
16:8:185:PHE:HA	16:8:187:LYS:HG3	1.86	0.57
22:9:303:CLA:HBC1	24:9:316:LHG:H262	1.86	0.57
1:A:329:GLU:OE1	1:A:329:GLU:N	2.36	0.57
29:2:301:CHL:H42	15:3:165:VAL:HG22	1.86	0.57
13:5:46:PRO:O	13:5:49:LEU:N	2.31	0.57
20:0:46:LEU:HD13	22:0:302:CLA:HBD	1.85	0.57
2:B:213:LEU:HD13	19:9:190:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:826:CLA:HMA1	25:B:847:8CT:C17	2.35	0.57
12:L:115:LYS:HB3	12:L:121:ASP:HA	1.85	0.57
17:6:153:ILE:HG13	17:6:154:PHE:H	1.68	0.57
13:5:195:ALA:HB2	22:5:314:CLA:HED3	1.87	0.57
6:F:102:GLN:HA	6:F:105:MET:HG2	1.85	0.57
30:3:314:XAT:H30	30:3:314:XAT:H403	1.86	0.57
18:7:199:ARG:NH2	22:7:303:CLA:HED2	2.17	0.57
19:9:116:LEU:HD23	20:0:200:LEU:HG	1.86	0.57
13:1:217:ALA:HB3	16:4:131:VAL:HG22	1.86	0.57
17:6:227:ILE:HA	17:6:230:LYS:HB2	1.85	0.57
16:8:158:ASN:HD22	29:8:307:CHL:HAC1	1.68	0.57
24:9:316:LHG:H341	24:9:316:LHG:H171	1.86	0.57
20:0:68:LEU:O	20:0:71:PHE:N	2.37	0.57
1:A:120:ALA:CB	1:A:145:ILE:HD11	2.35	0.57
22:A:805:CLA:H51	22:A:813:CLA:H12	1.86	0.57
22:B:807:CLA:O2D	22:B:807:CLA:H2A	2.03	0.57
22:B:828:CLA:HBC3	28:B:849:DGD:HBV1	1.86	0.57
7:G:42:THR:N	7:G:45:GLU:OE2	2.38	0.57
11:K:51:ASP:CG	11:K:52:PRO:HD2	2.30	0.57
18:7:125:LEU:HD23	18:7:128:ILE:HD12	1.86	0.57
16:8:81:GLN:HE22	16:8:173:PRO:HB2	1.69	0.57
1:A:40:PHE:HB2	1:A:67:HIS:CD2	2.39	0.57
1:A:92:TRP:O	1:A:96:MET:HG2	2.05	0.57
1:A:215:SER:HB3	1:A:307:ALA:HB2	1.87	0.57
1:A:687:SER:OG	1:A:732:GLY:O	2.22	0.57
2:B:102:GLU:O	2:B:105:THR:HG22	2.05	0.57
2:B:596:TRP:HB2	2:B:623:TYR:CD1	2.39	0.57
22:6:310:CLA:O1D	22:6:310:CLA:H2A	2.05	0.57
22:5:304:CLA:C2B	25:5:317:8CT:C38	2.83	0.57
1:A:97:TYR:HE1	1:A:153:TRP:HE1	1.53	0.57
1:A:151:GLN:OE1	1:A:385:LEU:HD23	2.05	0.57
22:B:850:CLA:OBD	6:F:156:ARG:NH2	2.37	0.57
11:K:68:HIS:HE1	25:K:103:8CT:C15	2.13	0.57
13:1:145:GLU:HB2	13:1:151:ARG:HD2	1.85	0.57
15:3:231:LYS:NZ	24:3:317:LHG:O5	2.38	0.57
22:A:804:CLA:H43	22:A:811:CLA:H92	1.86	0.57
2:B:392:ILE:HA	2:B:395:ILE:HG22	1.85	0.57
14:2:55:TRP:HE1	14:2:72:ALA:HB3	1.68	0.57
14:2:236:HIS:CG	22:2:312:CLA:HAA2	2.40	0.57
17:6:179:ILE:HG22	17:6:181:GLU:H	1.70	0.57
13:5:165:LYS:HG2	13:5:166:GLY:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:185:LYS:HG2	18:7:186:ASP:H	1.69	0.57
1:A:497:TYR:HB2	1:A:516:GLY:H	1.70	0.57
1:A:726:THR:OG1	24:A:844:LHG:O4	2.22	0.57
3:C:73:THR:H	3:C:76:SER:HG	1.53	0.57
4:D:93:LYS:NZ	4:D:97:GLU:HG2	2.20	0.57
15:3:141:GLY:HA2	15:3:148:SER:HA	1.87	0.57
15:3:246:GLN:HG2	15:3:257:ASN:HD22	1.70	0.57
17:6:136:ILE:HD11	22:6:323:CLA:H2A	1.86	0.57
1:A:274:TRP:CZ3	11:K:76:LEU:HD11	2.40	0.56
2:B:474:PHE:CG	22:B:850:CLA:H52	2.40	0.56
13:1:90:ALA:O	13:1:94:LEU:N	2.37	0.56
13:1:183:MET:SD	22:1:301:CLA:HBB1	2.45	0.56
17:6:92:VAL:HG23	17:6:200:PHE:HE2	1.70	0.56
22:8:308:CLA:HBB1	22:8:308:CLA:HHC	1.85	0.56
2:B:631:LEU:CD1	2:B:724:PHE:HA	2.30	0.56
16:4:104:THR:OG1	16:4:112:ALA:N	2.23	0.56
22:4:310:CLA:H2	22:4:311:CLA:HMD2	1.86	0.56
1:A:63:ASP:O	1:A:67:HIS:ND1	2.37	0.56
1:A:364:LEU:HD11	22:A:825:CLA:HMB3	1.86	0.56
1:A:417:PHE:HD2	1:A:418:MET:HE2	1.70	0.56
1:A:455:PHE:HB3	22:A:833:CLA:HBB2	1.87	0.56
2:B:10:GLN:HA	2:B:13:ALA:HB3	1.86	0.56
2:B:631:LEU:CD2	2:B:727:ALA:HB3	2.32	0.56
22:B:809:CLA:H42	22:B:809:CLA:HMA2	1.86	0.56
8:H:74:GLY:HA2	12:L:39:TYR:HB3	1.88	0.56
8:H:103:ARG:HH22	12:L:102:GLN:HG3	1.70	0.56
16:4:157:VAL:HG21	29:4:307:CHL:HAC1	1.87	0.56
13:5:103:PRO:O	13:5:107:TYR:N	2.37	0.56
13:5:130:ILE:HG23	13:5:134:LEU:HD12	1.88	0.56
22:5:304:CLA:HBB1	25:5:317:8CT:C37	2.35	0.56
18:7:95:ILE:HG12	18:7:107:TRP:NE1	2.20	0.56
29:9:307:CHL:HHC	29:9:307:CHL:HBB1	1.87	0.56
1:A:19:LYS:HE3	1:A:21:ILE:HD11	1.87	0.56
2:B:349:ALA:HB2	2:B:375:HIS:HB2	1.87	0.56
6:F:175:GLY:HA3	6:F:216:TRP:CZ2	2.40	0.56
12:L:70:LEU:HD12	12:L:70:LEU:N	2.20	0.56
16:4:94:LEU:HD22	30:4:315:XAT:H12	1.86	0.56
16:4:176:PRO:HB2	16:4:180:PHE:CD2	2.40	0.56
22:5:305:CLA:H3A	25:5:317:8CT:C26	2.36	0.56
1:A:580:CYS:HB3	1:A:589:CYS:HA	1.88	0.56
2:B:37:ILE:HD12	2:B:41:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:TYR:HD2	2:B:542:ARG:NH2	2.04	0.56
22:B:850:CLA:H71	6:F:153:LEU:HD13	1.88	0.56
17:6:202:MET:HE1	17:6:261:PHE:CD2	2.41	0.56
18:7:59:ASP:OD1	18:7:61:GLY:N	2.32	0.56
18:7:109:GLU:C	18:7:111:GLY:H	2.13	0.56
1:A:345:GLY:HA2	1:A:348:GLU:OE2	2.05	0.56
22:2:304:CLA:HBC2	22:6:301:CLA:HBC1	1.87	0.56
29:4:307:CHL:HMB2	25:4:317:8CT:C19	2.35	0.56
20:0:36:TRP:H	29:0:301:CHL:HBC3	1.71	0.56
1:A:117:LYS:HB2	1:A:136:VAL:HG13	1.86	0.56
2:B:436:LEU:O	2:B:440:ASN:ND2	2.39	0.56
12:L:66:LYS:O	12:L:71:ARG:HG2	2.06	0.56
13:1:215:ASN:HD21	22:1:312:CLA:HED2	1.69	0.56
14:2:66:TYR:HB3	22:2:302:CLA:CAD	2.35	0.56
22:3:319:CLA:HED3	18:7:264:GLN:HE22	1.70	0.56
18:7:107:TRP:HE1	30:7:320:XAT:H3	1.71	0.56
1:A:230:ASN:HD22	1:A:296:LEU:HD13	1.70	0.56
1:A:249:LEU:HD12	1:A:250:LEU:HG	1.88	0.56
1:A:304:LEU:HD21	22:A:817:CLA:C3B	2.35	0.56
15:3:195:VAL:HB	18:7:66:GLY:HA3	1.87	0.56
17:6:115:ASP:OD1	17:6:116:LEU:N	2.38	0.56
2:B:141:PHE:CZ	22:B:815:CLA:H12	2.40	0.56
2:B:349:ALA:HB3	2:B:376:GLN:HE21	1.69	0.56
4:D:191:ILE:O	4:D:194:ASN:ND2	2.38	0.56
7:G:56:SER:O	19:9:42:ALA:HB1	2.06	0.56
13:1:184:PHE:CE2	22:1:311:CLA:HAB	2.41	0.56
13:1:185:ALA:HB2	30:1:314:XAT:H192	1.88	0.56
13:5:49:LEU:HD12	13:5:50:PRO:HD2	1.87	0.56
20:0:134:GLY:O	20:0:138:THR:N	2.24	0.56
1:A:664:GLN:N	1:A:664:GLN:OE1	2.39	0.56
3:C:19:ARG:NE	4:D:175:GLU:OE2	2.39	0.56
16:4:226:TRP:CZ3	22:4:313:CLA:HAC1	2.41	0.56
17:6:79:GLU:OE2	17:6:138:ARG:NH2	2.37	0.56
22:5:312:CLA:H2A	22:5:312:CLA:O1D	2.06	0.56
1:A:361:ASN:ND2	22:A:805:CLA:OBD	2.39	0.55
2:B:224:PRO:HG2	2:B:233:TYR:OH	2.06	0.55
1:A:27:THR:OG1	1:A:187:HIS:ND1	2.39	0.55
1:A:743:THR:OG1	22:A:801:CLA:O1D	2.24	0.55
22:A:853:CLA:H121	10:J:18:TRP:HD1	1.72	0.55
22:B:830:CLA:H101	28:B:849:DGD:HAG1	1.87	0.55
13:5:223:LEU:HD11	16:8:134:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:193:LYS:HD3	22:7:312:CLA:HBD	1.87	0.55
22:7:307:CLA:C1D	25:7:323:8CT:C22	2.84	0.55
20:0:36:TRP:CH2	20:0:38:PRO:HB3	2.42	0.55
1:A:206:HIS:HE1	22:A:813:CLA:NA	2.04	0.55
1:A:745:TRP:CE2	25:A:850:8CT:C38	2.89	0.55
31:5:319:LMG:H112	29:8:306:CHL:HBB1	1.88	0.55
16:8:64:TYR:HE2	30:8:317:XAT:H383	1.71	0.55
16:8:158:ASN:HB3	29:8:307:CHL:HMC	1.87	0.55
2:B:88:ALA:HB2	2:B:116:ALA:HB2	1.88	0.55
2:B:469:LYS:NZ	2:B:509:PHE:O	2.40	0.55
22:B:806:CLA:HBC2	22:B:806:CLA:HHD	1.88	0.55
3:C:15:THR:HG22	3:C:28:MET:HG3	1.88	0.55
7:G:37:GLU:HA	7:G:42:THR:HA	1.88	0.55
16:4:84:LEU:HB3	16:4:88:ARG:NH1	2.22	0.55
20:0:53:ASP:HA	22:0:302:CLA:O2D	2.06	0.55
22:0:305:CLA:HED3	22:0:305:CLA:H2	1.86	0.55
2:B:414:HIS:ND1	2:B:414:HIS:O	2.39	0.55
22:B:841:CLA:CMA	25:B:846:8CT:C40	2.84	0.55
4:D:93:LYS:O	4:D:97:GLU:N	2.36	0.55
22:6:310:CLA:H2	30:6:319:XAT:H28	1.88	0.55
16:8:161:PRO:HD2	16:8:165:GLY:HA2	1.89	0.55
29:0:306:CHL:HHC	29:0:306:CHL:HBB1	1.88	0.55
8:H:113:ALA:HB3	22:H:201:CLA:H121	1.87	0.55
17:6:206:ILE:HD11	17:6:227:ILE:HD13	1.89	0.55
16:8:78:TRP:HZ2	22:8:308:CLA:HAA2	1.72	0.55
20:0:50:MET:HE3	20:0:69:ALA:HB2	1.88	0.55
2:B:35:ASP:CG	2:B:36:SER:H	2.14	0.55
2:B:44:GLN:HG3	2:B:162:GLN:HE21	1.70	0.55
8:H:81:TYR:CE2	12:L:43:VAL:HG21	2.41	0.55
13:5:212:LEU:HD22	16:8:131:VAL:HG11	1.87	0.55
22:8:310:CLA:C4C	31:8:319:LMG:HC71	2.36	0.55
1:A:120:ALA:HB2	1:A:145:ILE:HD11	1.89	0.55
8:H:99:ARG:HE	12:L:102:GLN:HG2	1.72	0.55
8:H:133:PRO:O	8:H:135:LYS:N	2.40	0.55
12:L:35:ASN:O	12:L:40:ARG:NH2	2.38	0.55
15:3:189:PHE:CD1	25:3:316:8CT:C38	2.89	0.55
16:4:186:ALA:HA	16:4:190:VAL:HG22	1.87	0.55
20:0:72:ARG:HH12	22:0:302:CLA:HED3	1.70	0.55
1:A:206:HIS:HE1	22:A:813:CLA:C1A	2.20	0.55
2:B:85:ARG:NH2	8:H:142:LYS:HB3	2.21	0.55
13:1:196:THR:HG22	13:1:198:LYS:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:194:MET:HE3	22:6:303:CLA:HMC2	1.88	0.55
17:6:248:HIS:ND1	17:6:255:ASP:OD1	2.36	0.55
2:B:96:PHE:O	8:H:126:THR:OG1	2.22	0.55
25:B:846:8CT:C39	25:B:846:8CT:C13	2.85	0.55
16:4:239:TRP:CD1	16:4:243:LEU:HD11	2.42	0.55
17:6:57:THR:HG21	17:6:183:LYS:HG2	1.88	0.55
16:8:142:TRP:O	16:8:146:ARG:HG2	2.07	0.55
22:A:839:CLA:HBC3	22:A:853:CLA:NC	2.22	0.54
2:B:216:LEU:HD21	19:9:216:ILE:HG12	1.88	0.54
22:B:832:CLA:HAB	22:B:833:CLA:HMB2	1.88	0.54
22:3:319:CLA:H51	22:3:319:CLA:H121	1.88	0.54
16:4:172:ILE:HD11	16:4:175:TYR:HB2	1.88	0.54
1:A:745:TRP:NE1	22:A:828:CLA:O1A	2.41	0.54
25:B:847:8CT:C27	25:B:847:8CT:C23	2.85	0.54
3:C:51:CYS:HB3	3:C:53:ARG:HG3	1.89	0.54
25:J:104:8CT:C38	25:J:104:8CT:C28	2.86	0.54
13:1:211:PRO:HB2	22:1:312:CLA:HMA2	1.87	0.54
16:8:72:ASP:OD1	16:8:75:THR:OG1	2.24	0.54
25:A:850:8CT:C11	25:A:850:8CT:C09	2.85	0.54
2:B:476:PHE:CE2	22:B:850:CLA:H11	2.42	0.54
2:B:503:ASN:O	2:B:505:THR:N	2.35	0.54
25:G:104:8CT:C15	25:G:104:8CT:C40	2.86	0.54
25:K:103:8CT:C39	25:K:103:8CT:C13	2.85	0.54
13:1:134:LEU:HD22	22:1:304:CLA:H2	1.88	0.54
22:6:301:CLA:HED2	22:6:301:CLA:H12	1.89	0.54
22:6:305:CLA:CHC	25:6:321:8CT:C33	2.84	0.54
16:8:221:GLY:H	16:8:224:ALA:HB3	1.72	0.54
1:A:687:SER:HB2	1:A:735:HIS:HB2	1.89	0.54
1:A:703:GLU:CD	2:B:545:LYS:HB2	2.32	0.54
25:A:850:8CT:C36	25:A:850:8CT:C28	2.85	0.54
25:B:843:8CT:C19	25:G:104:8CT:C08	2.77	0.54
22:2:302:CLA:O1A	22:2:302:CLA:H3A	2.07	0.54
15:3:264:ASP:HB3	15:3:268:ASN:HD22	1.73	0.54
29:7:308:CHL:HBB2	22:7:316:CLA:HMC3	1.89	0.54
25:8:301:8CT:C11	25:8:301:8CT:C09	2.86	0.54
2:B:358:TYR:HB2	2:B:361:ILE:HD12	1.88	0.54
2:B:685:THR:O	2:B:689:ASN:ND2	2.41	0.54
22:G:103:CLA:NC	25:G:104:8CT:C37	2.70	0.54
25:J:101:8CT:C37	25:J:101:8CT:C28	2.86	0.54
15:3:175:LEU:O	15:3:178:TYR:N	2.40	0.54
25:3:316:8CT:C19	25:3:316:8CT:C39	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:264:GLN:OE1	18:7:264:GLN:N	2.36	0.54
22:9:312:CLA:H93	24:9:316:LHG:H172	1.90	0.54
20:0:146:PHE:HB2	20:0:149:PHE:O	2.08	0.54
1:A:304:LEU:HD12	22:A:815:CLA:HMC3	1.90	0.54
1:A:581:ASP:OD2	3:C:53:ARG:NH2	2.24	0.54
2:B:439:HIS:CD2	2:B:453:ILE:HG12	2.43	0.54
12:L:114:VAL:HG12	12:L:115:LYS:N	2.22	0.54
13:5:153:TYR:HB3	22:5:309:CLA:HED2	1.89	0.54
22:5:302:CLA:HMB3	22:5:303:CLA:HBA2	1.88	0.54
18:7:75:ALA:O	18:7:79:GLN:HG2	2.07	0.54
25:7:323:8CT:C39	25:7:323:8CT:C19	2.85	0.54
25:7:323:8CT:C22	25:7:323:8CT:C18	2.85	0.54
16:8:144:GLU:HG3	22:8:308:CLA:C4B	2.38	0.54
29:8:307:CHL:O1A	22:8:309:CLA:HHD	2.08	0.54
1:A:566:ARG:NE	2:B:676:GLU:OE2	2.30	0.54
1:A:709:HIS:HE1	22:A:839:CLA:NA	2.06	0.54
22:A:810:CLA:HBB2	22:A:813:CLA:HMA3	1.88	0.54
25:B:846:8CT:C37	25:B:846:8CT:C28	2.85	0.54
5:E:9:VAL:CG1	5:E:59:VAL:HG13	2.38	0.54
13:1:72:GLU:HG3	13:1:152:VAL:HG22	1.88	0.54
13:1:92:GLU:OE1	13:1:201:VAL:HB	2.07	0.54
15:3:241:PHE:HD1	22:3:302:CLA:HBB2	1.72	0.54
25:A:849:8CT:C18	25:A:849:8CT:C22	2.86	0.54
22:B:807:CLA:H3A	21:M:29:LEU:HD22	1.90	0.54
22:1:311:CLA:H71	22:1:312:CLA:H91	1.89	0.54
25:1:316:8CT:C40	25:1:316:8CT:C15	2.86	0.54
15:3:69:ASP:OD1	15:3:69:ASP:N	2.38	0.54
13:5:111:SER:O	13:5:113:THR:N	2.37	0.54
1:A:663:ILE:CG2	2:B:621:ARG:CG	2.71	0.54
22:B:810:CLA:CGA	9:I:14:VAL:HG11	2.37	0.54
4:D:82:ILE:HG13	4:D:123:ARG:HE	1.73	0.54
7:G:79:HIS:CB	25:G:104:8CT:C40	2.86	0.54
8:H:98:ARG:H	8:H:102:ILE:CD1	2.21	0.54
25:J:101:8CT:C40	25:J:101:8CT:C15	2.85	0.54
13:1:134:LEU:O	13:1:138:ALA:N	2.36	0.54
17:6:176:PRO:HD2	22:6:310:CLA:O1A	2.07	0.54
22:5:307:CLA:O1D	22:5:307:CLA:H2A	2.08	0.54
18:7:162:ASN:N	18:7:162:ASN:OD1	2.41	0.54
25:8:318:8CT:C38	25:8:318:8CT:C28	2.86	0.54
25:A:849:8CT:C40	25:A:849:8CT:C15	2.85	0.54
25:1:316:8CT:C28	25:1:316:8CT:C38	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:5:310:CLA:HBC3	24:5:318:LHG:HC62	1.90	0.54
16:8:238:VAL:HG13	16:8:239:TRP:CD1	2.43	0.54
1:A:711:LYS:HE2	6:F:230:LEU:HD23	1.89	0.53
2:B:636:ASN:OD1	2:B:637:PRO:HD2	2.08	0.53
22:B:816:CLA:O1D	22:B:816:CLA:H2A	2.08	0.53
17:6:263:GLU:HG3	17:6:266:TRP:CE3	2.43	0.53
16:8:78:TRP:CZ2	22:8:308:CLA:HAA2	2.44	0.53
19:9:209:ILE:HB	22:9:312:CLA:H12	1.90	0.53
1:A:476:MET:O	1:A:481:THR:OG1	2.17	0.53
1:A:695:ARG:O	1:A:698:TRP:N	2.38	0.53
22:A:802:CLA:O1A	22:A:802:CLA:H3A	2.07	0.53
17:6:42:TRP:NE1	17:6:61:GLY:O	2.42	0.53
17:6:116:LEU:HD11	17:6:120:ILE:HG13	1.90	0.53
19:9:38:TRP:NE1	19:9:43:SER:HB3	2.22	0.53
1:A:299:ILE:O	1:A:302:HIS:HB3	2.08	0.53
1:A:433:ASP:OD1	1:A:437:ARG:HD2	2.08	0.53
2:B:206:HIS:O	2:B:211:ASN:ND2	2.39	0.53
2:B:685:THR:HG23	2:B:688:ALA:HB3	1.89	0.53
2:B:705:ALA:O	2:B:709:GLY:N	2.35	0.53
5:E:26:VAL:HG11	5:E:40:ARG:HE	1.73	0.53
25:2:317:8CT:C09	25:2:317:8CT:C11	2.86	0.53
22:6:303:CLA:HBA1	22:6:303:CLA:C4A	2.37	0.53
20:0:204:ILE:HD11	20:0:209:VAL:HG23	1.90	0.53
25:A:854:8CT:C36	25:A:854:8CT:C28	2.86	0.53
2:B:627:ASN:ND2	2:B:724:PHE:CZ	2.65	0.53
25:2:317:8CT:C27	25:2:317:8CT:C38	2.85	0.53
22:3:311:CLA:C2B	30:3:314:XAT:H183	2.38	0.53
19:9:181:GLY:O	19:9:185:GLN:HG2	2.09	0.53
20:0:73:GLU:O	20:0:77:MET:N	2.36	0.53
29:0:301:CHL:HAA1	24:0:315:LHG:H151	1.90	0.53
25:B:843:8CT:C17	25:G:104:8CT:C08	2.84	0.53
16:4:60:GLY:O	16:4:202:ARG:NH2	2.39	0.53
13:5:53:TYR:OH	13:5:177:LYS:NZ	2.33	0.53
18:7:146:ASP:OD2	29:7:308:CHL:HAC1	2.08	0.53
25:7:321:8CT:C37	25:7:321:8CT:C28	2.87	0.53
4:D:128:LEU:HD13	8:H:58:PHE:CE1	2.44	0.53
6:F:112:SER:HB3	6:F:114:PRO:HD2	1.90	0.53
14:2:46:TRP:NE1	14:2:65:GLY:O	2.36	0.53
15:3:240:MET:HE2	30:3:315:XAT:H10	1.90	0.53
25:J:101:8CT:C28	25:J:101:8CT:C36	2.86	0.53
19:9:195:ALA:O	19:9:199:ALA:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:0:174:SER:HA	20:0:177:PHE:HD2	1.74	0.53
2:B:513:GLY:H	2:B:516:ASP:HB3	1.74	0.53
6:F:137:LEU:HD21	10:J:38:ILE:HG21	1.91	0.53
15:3:85:GLU:HB2	15:3:86:PRO:HD2	1.90	0.53
19:9:104:TRP:CD1	19:9:105:GLU:HG3	2.44	0.53
1:A:364:LEU:HD12	22:A:825:CLA:HMA1	1.91	0.53
22:H:201:CLA:HBB2	9:I:15:GLY:HA3	1.91	0.53
11:K:52:PRO:HD3	22:K:104:CLA:C1D	2.39	0.53
15:3:109:PHE:O	15:3:113:GLY:N	2.34	0.53
18:7:195:ILE:O	18:7:198:GLY:N	2.42	0.53
22:7:306:CLA:HBB1	22:7:306:CLA:HMB3	1.91	0.53
16:8:115:THR:N	16:8:119:ASN:OD1	2.42	0.53
2:B:294:ASN:HD22	22:B:813:CLA:HMA1	1.74	0.53
2:B:299:HIS:HB3	2:B:304:ILE:HD11	1.91	0.53
22:B:826:CLA:NB	25:B:847:8CT:C22	2.72	0.53
6:F:150:ASP:HB2	6:F:153:LEU:HD12	1.91	0.53
2:B:707:LEU:HD22	28:B:849:DGD:HA22	1.90	0.52
22:1:302:CLA:HBB1	22:1:307:CLA:H151	1.92	0.52
14:2:157:SER:HA	14:2:160:THR:HG23	1.91	0.52
15:3:269:ASN:OD1	15:3:270:ILE:HD12	2.09	0.52
18:7:42:TRP:CE2	18:7:62:TRP:HD1	2.27	0.52
16:8:226:TRP:CD1	30:8:316:XAT:H241	2.44	0.52
13:1:88:MET:HG2	13:1:99:TRP:HB2	1.91	0.52
15:3:262:LEU:HD21	22:3:312:CLA:HMC2	1.91	0.52
1:A:126:ILE:O	1:A:129:GLN:HG2	2.10	0.52
1:A:386:ALA:CB	1:A:527:ALA:HA	2.40	0.52
25:A:850:8CT:C22	22:B:803:CLA:C16	2.85	0.52
2:B:166:SER:OG	7:G:48:ASP:N	2.42	0.52
22:B:825:CLA:H2A	22:B:825:CLA:O1A	2.08	0.52
7:G:28:ARG:HH22	7:G:67:ASN:ND2	2.07	0.52
18:7:144:TRP:CE2	22:7:315:CLA:HBC1	2.45	0.52
25:7:321:8CT:C40	25:7:321:8CT:C15	2.87	0.52
16:8:115:THR:H	16:8:119:ASN:ND2	2.07	0.52
19:9:204:PRO:HB2	22:9:313:CLA:HMA1	1.91	0.52
1:A:216:LEU:HG	1:A:307:ALA:HB1	1.92	0.52
2:B:126:THR:HG21	2:B:358:TYR:CD1	2.44	0.52
2:B:547:MET:HB2	2:B:564:ARG:HH21	1.74	0.52
4:D:140:LEU:O	4:D:143:GLN:HB3	2.09	0.52
8:H:114:LEU:HG	22:H:201:CLA:H112	1.90	0.52
10:J:9:SER:HA	10:J:14:ILE:HD11	1.91	0.52
14:2:56:LEU:HD12	14:2:56:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:116:GLU:HB2	16:4:119:ASN:HD22	1.75	0.52
25:7:323:8CT:C09	25:7:323:8CT:C11	2.86	0.52
16:8:215:ALA:O	16:8:219:GLY:N	2.43	0.52
19:9:73:TYR:HE1	22:9:304:CLA:H2	1.73	0.52
22:B:827:CLA:H171	25:B:846:8CT:C37	2.39	0.52
22:B:830:CLA:H72	28:B:849:DGD:HAV1	1.92	0.52
5:E:15:GLU:O	5:E:15:GLU:HG2	2.09	0.52
6:F:105:MET:HE1	6:F:119:GLN:HB2	1.91	0.52
16:8:169:ASP:O	16:8:171:ASN:OD1	2.27	0.52
1:A:200:GLU:HB3	1:A:317:TYR:HB3	1.92	0.52
1:A:268:PRO:HG2	1:A:277:TYR:OH	2.10	0.52
1:A:585:ARG:HG3	3:C:49:VAL:CG1	2.40	0.52
13:5:79:ARG:O	13:5:83:LEU:N	2.37	0.52
13:5:87:GLY:O	13:5:91:GLN:HG2	2.09	0.52
1:A:117:LYS:HD3	1:A:144:GLN:HE22	1.74	0.52
1:A:146:THR:HG21	1:A:749:LEU:HD22	1.92	0.52
1:A:663:ILE:HG22	2:B:621:ARG:CG	2.22	0.52
22:B:803:CLA:H112	22:B:833:CLA:HBC1	1.91	0.52
15:3:245:ALA:HA	15:3:248:ILE:HG22	1.91	0.52
18:7:235:ILE:H	18:7:235:ILE:HD12	1.75	0.52
16:8:150:ASP:HB2	16:8:158:ASN:ND2	2.24	0.52
19:9:130:GLY:HA2	22:9:308:CLA:HAB	1.92	0.52
1:A:250:LEU:HD11	22:A:816:CLA:HAC2	1.92	0.52
2:B:451:LYS:HE3	6:F:128:ARG:NH1	2.24	0.52
2:B:585:ASN:O	2:B:588:GLY:N	2.43	0.52
14:2:91:TRP:CE2	29:2:307:CHL:HED2	2.44	0.52
22:3:319:CLA:H18	18:7:264:GLN:HB2	1.91	0.52
1:A:541:HIS:HA	1:A:544:HIS:HD2	1.75	0.52
17:6:151:ASP:HB3	17:6:154:PHE:O	2.10	0.52
30:8:316:XAT:H371	30:8:316:XAT:H28	1.91	0.52
19:9:47:TYR:CE1	19:9:48:LEU:HD23	2.44	0.52
1:A:104:SER:HB2	1:A:150:PHE:HZ	1.75	0.52
2:B:292:ARG:NH1	7:G:35:VAL:HA	2.24	0.52
3:C:39:ILE:HG22	3:C:40:ALA:O	2.09	0.52
3:C:58:CYS:SG	3:C:65:VAL:HG22	2.50	0.52
13:1:50:PRO:HG3	13:1:172:LYS:HE3	1.91	0.52
29:6:302:CHL:H41	22:6:313:CLA:H161	1.91	0.52
2:B:39:GLU:HG2	2:B:165:LEU:HD11	1.92	0.51
22:1:303:CLA:C2B	30:1:315:XAT:H183	2.40	0.51
16:4:97:MET:HE1	16:4:208:THR:HG23	1.91	0.51
13:5:174:LYS:HE2	22:5:311:CLA:CGD	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:PHE:CZ	22:B:850:CLA:H72	2.45	0.51
3:C:17:CYS:HB3	3:C:26:LEU:HD12	1.91	0.51
4:D:104:TRP:HE1	4:D:122:MET:HE3	1.74	0.51
10:J:24:SER:OG	22:J:103:CLA:HAB	2.10	0.51
22:3:308:CLA:HAB	30:3:314:XAT:H403	1.92	0.51
18:7:213:GLN:HE21	18:7:259:CYS:HB2	1.74	0.51
16:8:172:ILE:HG21	16:8:175:TYR:HD1	1.75	0.51
19:9:154:TRP:HB2	22:9:309:CLA:OBD	2.10	0.51
20:0:35:MET:HA	20:0:54:TYR:HB3	1.92	0.51
25:A:850:8CT:C40	22:B:833:CLA:HMC1	2.40	0.51
2:B:526:GLY:HA3	2:B:586:THR:HB	1.92	0.51
16:4:45:LEU:HD11	16:4:48:ALA:HB2	1.92	0.51
29:4:305:CHL:CBA	25:4:317:8CT:C22	2.89	0.51
17:6:110:ALA:HB2	29:6:307:CHL:HMD1	1.92	0.51
18:7:205:TRP:CD2	30:7:320:XAT:H12	2.46	0.51
16:8:175:TYR:HB3	22:8:309:CLA:CGD	2.41	0.51
2:B:149:PHE:O	2:B:153:GLY:N	2.25	0.51
8:H:105:VAL:HG22	22:0:303:CLA:H42	1.91	0.51
14:2:135:MET:HB3	16:4:239:TRP:CE3	2.40	0.51
29:2:301:CHL:HMA3	22:3:313:CLA:OBD	2.10	0.51
15:3:78:PHE:HE2	30:3:315:XAT:H383	1.76	0.51
25:7:321:8CT:C32	25:7:321:8CT:C36	2.86	0.51
20:0:174:SER:HB2	30:0:314:XAT:H203	1.92	0.51
25:B:846:8CT:C22	25:B:846:8CT:C25	2.88	0.51
7:G:19:GLY:O	7:G:24:PHE:N	2.43	0.51
13:1:173:LEU:HD23	22:1:309:CLA:HED2	1.93	0.51
13:5:208:ILE:HD11	22:5:313:CLA:HBB1	1.91	0.51
20:0:76:LEU:O	20:0:80:ARG:N	2.30	0.51
30:0:313:XAT:H381	30:0:313:XAT:H28	1.92	0.51
1:A:49:THR:HB	5:E:44:VAL:HG21	1.91	0.51
1:A:83:PHE:HD2	1:A:182:GLY:HA2	1.75	0.51
1:A:290:ILE:HG23	1:A:291:ASN:H	1.75	0.51
2:B:712:HIS:HE1	22:B:840:CLA:NA	2.09	0.51
22:B:824:CLA:HBC2	25:B:846:8CT:C27	2.39	0.51
6:F:146:HIS:O	6:F:147:LEU:HD23	2.09	0.51
22:H:201:CLA:H102	12:L:88:LEU:HD21	1.91	0.51
10:J:5:LYS:NZ	14:2:74:ASP:OD2	2.42	0.51
22:6:317:CLA:HBC3	22:6:318:CLA:C1C	2.40	0.51
1:A:663:ILE:HG21	2:B:621:ARG:HG3	1.82	0.51
2:B:595:HIS:CD2	2:B:623:TYR:HE1	2.26	0.51
12:L:21:THR:N	12:L:24:THR:OG1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:79:ASP:OD2	15:3:82:GLY:HA2	2.10	0.51
15:3:218:THR:C	15:3:220:GLU:H	2.17	0.51
13:5:102:ALA:O	13:5:106:VAL:HG22	2.10	0.51
22:5:313:CLA:HBA2	22:5:313:CLA:H42	1.92	0.51
18:7:85:SER:HB2	18:7:198:GLY:HA3	1.93	0.51
20:0:35:MET:O	20:0:38:PRO:HD3	2.10	0.51
2:B:686:PRO:HD3	22:L:201:CLA:HBA1	1.92	0.51
22:K:105:CLA:H2	22:K:105:CLA:H2A	1.92	0.51
14:2:141:MET:HG2	22:2:308:CLA:HMC2	1.93	0.51
16:4:65:ASP:OD1	30:4:316:XAT:O23	2.21	0.51
17:6:112:THR:OG1	17:6:115:ASP:O	2.28	0.51
29:6:308:CHL:H2A	29:6:308:CHL:HED3	1.93	0.51
29:5:301:CHL:H11	16:8:142:TRP:CE3	2.46	0.51
1:A:493:GLN:NE2	22:A:836:CLA:OBD	2.36	0.51
3:C:4:ASN:ND2	4:D:206:ILE:HG21	2.26	0.51
7:G:5:SER:HA	22:G:102:CLA:OBD	2.10	0.51
17:6:43:LEU:HD23	17:6:45:GLY:H	1.76	0.51
18:7:65:MET:HG3	30:7:320:XAT:H372	1.93	0.51
22:7:304:CLA:HBC1	22:7:309:CLA:HAC1	1.93	0.51
22:A:819:CLA:HBB1	22:A:819:CLA:HMB3	1.92	0.51
2:B:676:GLU:HG2	3:C:81:TYR:CE2	2.46	0.51
14:2:181:GLY:O	14:2:185:ASP:HB3	2.11	0.51
14:2:199:GLU:OE2	14:2:203:LYS:HE2	2.10	0.51
15:3:205:PRO:HD2	22:3:308:CLA:OBD	2.10	0.51
18:7:60:TYR:OH	18:7:196:LYS:HE2	2.11	0.51
1:A:528:MET:SD	1:A:619:MET:HE1	2.51	0.50
25:A:850:8CT:C37	25:A:850:8CT:C32	2.86	0.50
8:H:103:ARG:NH1	12:L:102:GLN:OE1	2.45	0.50
14:2:178:TYR:HB3	22:2:309:CLA:HED2	1.92	0.50
16:8:243:LEU:HD22	25:8:301:8CT:C07	2.40	0.50
19:9:216:ILE:O	19:9:218:GLU:N	2.44	0.50
2:B:302:LYS:HG3	2:B:303:GLU:HG3	1.93	0.50
22:B:827:CLA:O1D	22:B:827:CLA:H2A	2.11	0.50
3:C:14:CYS:O	3:C:15:THR:OG1	2.22	0.50
14:2:120:LYS:C	14:2:124:GLU:HG2	2.36	0.50
17:6:92:VAL:HG11	17:6:193:SER:HB2	1.92	0.50
22:0:302:CLA:CGA	22:0:302:CLA:H3A	2.41	0.50
1:A:32:GLU:HA	10:J:3:ASN:ND2	2.26	0.50
1:A:334:HIS:HE1	22:A:824:CLA:HED3	1.76	0.50
2:B:174:ARG:HH11	22:B:808:CLA:H141	1.75	0.50
13:1:107:TYR:HE2	22:1:304:CLA:HAC1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:303:CLA:HBA1	22:1:304:CLA:CHD	2.41	0.50
22:6:313:CLA:C2B	30:6:319:XAT:H183	2.41	0.50
13:5:91:GLN:NE2	22:5:304:CLA:O1D	2.43	0.50
19:9:88:VAL:HG13	19:9:182:PHE:CZ	2.46	0.50
1:A:456:HIS:O	1:A:460:LEU:HG	2.12	0.50
1:A:551:THR:HG21	22:A:826:CLA:HBC3	1.93	0.50
1:A:602:PHE:CZ	1:A:733:VAL:HG22	2.46	0.50
2:B:29:HIS:HE1	22:B:807:CLA:NB	2.09	0.50
5:E:14:PRO:HG2	5:E:15:GLU:OE1	2.11	0.50
12:L:88:LEU:O	12:L:92:ILE:HD12	2.11	0.50
22:4:308:CLA:HBB1	22:4:308:CLA:HMB3	1.92	0.50
16:8:95:VAL:O	16:8:99:VAL:HG23	2.11	0.50
16:8:179:ILE:HD11	29:8:314:CHL:C4A	2.41	0.50
22:8:304:CLA:H12	29:8:305:CHL:C3D	2.40	0.50
1:A:343:HIS:HB3	1:A:346:LEU:HD12	1.94	0.50
1:A:583:PRO:HB3	2:B:559:CYS:SG	2.51	0.50
2:B:275:HIS:HE1	22:B:817:CLA:NA	2.10	0.50
2:B:617:MET:HG3	2:B:621:ARG:HB2	1.94	0.50
2:B:676:GLU:HG2	3:C:81:TYR:HE2	1.76	0.50
2:B:693:TRP:CD1	2:B:696:LYS:HA	2.46	0.50
6:F:94:GLU:HB3	6:F:129:PHE:CD2	2.47	0.50
6:F:125:THR:O	6:F:128:ARG:HG2	2.11	0.50
6:F:201:ILE:O	10:J:9:SER:HB3	2.11	0.50
22:H:201:CLA:H162	12:L:92:ILE:HD11	1.94	0.50
13:1:31:ARG:N	13:1:47:GLU:OE2	2.45	0.50
29:5:301:CHL:HED3	16:8:145:ILE:HG22	1.93	0.50
16:8:95:VAL:HG21	30:8:316:XAT:H14	1.94	0.50
1:A:51:THR:CG2	1:A:721:ARG:H	2.25	0.50
2:B:239:THR:HG23	2:B:242:HIS:N	2.26	0.50
2:B:325:THR:HG21	2:B:403:ASN:HD21	1.76	0.50
2:B:631:LEU:CD2	2:B:727:ALA:CB	2.90	0.50
8:H:81:TYR:HA	22:L:202:CLA:HMD1	1.93	0.50
29:2:305:CHL:CHB	25:2:317:8CT:C38	2.90	0.50
15:3:96:PRO:O	15:3:100:ARG:NE	2.43	0.50
16:4:238:VAL:C	16:4:240:SER:H	2.17	0.50
20:0:161:LEU:O	20:0:165:LYS:N	2.43	0.50
22:0:308:CLA:H102	30:0:313:XAT:C11	2.42	0.50
1:A:316:MET:HB3	22:A:822:CLA:HAC2	1.93	0.50
2:B:302:LYS:HZ2	7:G:37:GLU:HG3	1.77	0.50
6:F:212:GLY:O	6:F:219:ARG:NH2	2.42	0.50
7:G:56:SER:O	19:9:43:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:184:PHE:HE2	22:1:311:CLA:HAB	1.76	0.50
18:7:70:ASP:O	18:7:72:LYS:N	2.45	0.50
22:A:808:CLA:HHC	22:A:828:CLA:H142	1.94	0.50
22:A:839:CLA:H2A	22:A:839:CLA:HED3	1.94	0.50
2:B:183:PHE:CE1	22:B:814:CLA:H72	2.47	0.50
2:B:648:TRP:HZ3	25:B:848:8CT:C07	2.25	0.50
15:3:111:MET:HB3	30:3:314:XAT:C34	2.42	0.50
15:3:189:PHE:N	15:3:193:GLU:OE1	2.41	0.50
24:3:317:LHG:O3	24:3:317:LHG:O1	2.15	0.50
17:6:219:LEU:HD11	22:6:314:CLA:HMC2	1.94	0.50
18:7:62:TRP:CD1	18:7:64:PRO:HD3	2.47	0.50
18:7:242:CYS:O	18:7:244:ILE:HG12	2.12	0.50
1:A:205:HIS:CD2	22:A:813:CLA:HMC2	2.47	0.50
2:B:403:ASN:HA	2:B:406:ASN:ND2	2.27	0.50
2:B:416:GLU:O	2:B:420:SER:N	2.31	0.50
22:B:805:CLA:O1D	22:B:805:CLA:H2A	2.11	0.50
13:1:31:ARG:HH22	13:1:42:PRO:HD2	1.76	0.50
16:8:146:ARG:O	16:8:158:ASN:ND2	2.39	0.50
22:A:831:CLA:HAA1	12:L:7:ILE:HD13	1.93	0.49
6:F:216:TRP:CG	6:F:217:PRO:HD3	2.47	0.49
14:2:173:THR:HG23	14:2:175:GLU:OE1	2.12	0.49
16:8:43:ILE:HG22	16:8:44:TRP:N	2.25	0.49
16:8:190:VAL:O	16:8:194:LYS:HG2	2.12	0.49
20:0:67:SER:HB3	22:0:307:CLA:H111	1.94	0.49
29:0:301:CHL:HAA1	24:0:315:LHG:H132	1.93	0.49
1:A:218:TRP:HE1	1:A:222:GLN:NE2	2.10	0.49
3:C:8:TYR:CE2	4:D:191:ILE:HG12	2.47	0.49
22:G:103:CLA:HED2	25:G:104:8CT:C38	2.41	0.49
10:J:23:SER:HB3	25:J:104:8CT:C24	2.42	0.49
11:K:40:LEU:O	11:K:40:LEU:HD23	2.12	0.49
14:2:115:TRP:CE3	30:2:316:XAT:H172	2.47	0.49
15:3:201:ASP:HB2	15:3:202:PRO:HD2	1.94	0.49
16:4:238:VAL:HG13	22:4:312:CLA:O1A	2.11	0.49
17:6:229:SER:HB2	18:7:124:ASN:HD21	1.76	0.49
13:5:109:GLY:O	13:5:112:PRO:HD2	2.12	0.49
18:7:65:MET:HG2	30:7:320:XAT:H221	1.94	0.49
22:A:819:CLA:H13	22:A:819:CLA:HBB2	1.94	0.49
2:B:358:TYR:OH	22:B:829:CLA:OBD	2.18	0.49
2:B:553:PHE:HZ	3:C:52:LYS:HZ3	1.60	0.49
12:L:67:LEU:HA	12:L:71:ARG:HD3	1.93	0.49
22:L:202:CLA:HBD	22:L:202:CLA:H193	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:84:ALA:HB2	22:2:308:CLA:HED1	1.95	0.49
22:2:312:CLA:C2B	30:2:315:XAT:H383	2.42	0.49
17:6:151:ASP:OD1	17:6:152:PRO:HD2	2.12	0.49
17:6:231:ALA:HB1	17:6:267:PRO:O	2.12	0.49
13:5:215:ASN:OD1	16:8:131:VAL:HG22	2.12	0.49
1:A:332:GLU:HG2	1:A:344:GLN:HA	1.93	0.49
22:A:803:CLA:H91	10:J:16:PHE:HB2	1.94	0.49
22:A:812:CLA:HMB1	15:3:81:PHE:HE1	1.77	0.49
2:B:130:ARG:HH11	2:B:245:SER:HB3	1.78	0.49
2:B:549:ASP:OD2	3:C:66:ARG:NH1	2.46	0.49
4:D:201:LYS:C	4:D:203:THR:H	2.20	0.49
12:L:88:LEU:O	12:L:91:ILE:N	2.46	0.49
14:2:134:LEU:O	14:2:137:GLN:HB3	2.13	0.49
20:0:72:ARG:O	20:0:76:LEU:N	2.38	0.49
1:A:354:TRP:CE2	22:A:825:CLA:H18	2.47	0.49
1:A:417:PHE:CD2	1:A:418:MET:HE2	2.47	0.49
22:A:831:CLA:HMA2	12:L:21:THR:HG21	1.92	0.49
22:A:837:CLA:HBB1	22:A:837:CLA:HMB3	1.94	0.49
2:B:174:ARG:NH1	22:B:808:CLA:H141	2.27	0.49
2:B:174:ARG:HH12	22:B:808:CLA:H162	1.76	0.49
22:3:303:CLA:O2A	22:7:317:CLA:H11	2.11	0.49
17:6:133:TYR:CD1	25:6:321:8CT:C40	2.95	0.49
29:5:301:CHL:H51	22:5:313:CLA:H62	1.95	0.49
16:8:133:PHE:HB2	29:8:306:CHL:HBC1	1.93	0.49
16:8:211:PHE:CE1	30:8:316:XAT:H363	2.47	0.49
25:A:850:8CT:C28	25:A:850:8CT:C34	2.87	0.49
2:B:334:LEU:HD22	2:B:389:HIS:CD2	2.48	0.49
22:B:813:CLA:HHC	22:B:813:CLA:HBB1	1.94	0.49
4:D:79:PRO:HB3	8:H:56:ARG:HB3	1.94	0.49
8:H:79:LYS:HE3	12:L:44:SER:H	1.76	0.49
11:K:40:LEU:HB2	22:K:105:CLA:C2	2.43	0.49
16:4:64:TYR:HE2	30:4:316:XAT:H383	1.78	0.49
17:6:202:MET:HB3	22:6:317:CLA:HED1	1.94	0.49
22:8:309:CLA:HAB	30:8:316:XAT:H203	1.95	0.49
19:9:200:HIS:CG	22:9:312:CLA:HAA2	2.47	0.49
2:B:70:TRP:CE3	2:B:71:GLN:HG3	2.47	0.49
2:B:497:TRP:CZ3	22:B:834:CLA:HED2	2.48	0.49
3:C:51:CYS:N	27:C:101:SF4:S2	2.86	0.49
5:E:9:VAL:HG13	5:E:59:VAL:HG13	1.94	0.49
17:6:172:ALA:HB2	22:6:310:CLA:HBD	1.93	0.49
13:5:102:ALA:HB3	13:5:103:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:156:ASP:O	18:7:160:LYS:HA	2.11	0.49
22:7:312:CLA:C3B	30:7:319:XAT:H35	2.42	0.49
22:9:308:CLA:H72	22:9:308:CLA:H142	1.95	0.49
22:A:838:CLA:H71	25:A:849:8CT:C40	2.43	0.49
2:B:136:TYR:CZ	21:M:7:GLN:HB3	2.48	0.49
6:F:232:LYS:HG2	6:F:233:GLU:N	2.28	0.49
22:H:201:CLA:H143	12:L:88:LEU:HD22	1.95	0.49
13:1:36:LEU:HD21	16:4:149:GLN:HG3	1.95	0.49
30:4:315:XAT:H401	30:4:315:XAT:H35	1.50	0.49
22:0:307:CLA:H92	22:0:307:CLA:H2	1.94	0.49
1:A:666:TYR:CD1	2:B:445:ALA:HA	2.40	0.49
1:A:714:VAL:O	1:A:714:VAL:HG12	2.13	0.49
17:6:203:GLN:HE21	22:6:313:CLA:C4D	2.26	0.49
13:5:100:HIS:NE2	29:5:306:CHL:HMA3	2.28	0.49
18:7:100:ILE:HD11	18:7:220:ILE:HG21	1.94	0.49
19:9:73:TYR:CE1	22:9:304:CLA:H2	2.46	0.49
22:9:301:CLA:H11	22:9:301:CLA:CHA	2.42	0.49
20:0:159:ASN:O	20:0:162:LYS:N	2.35	0.49
1:A:483:GLN:OE1	1:A:485:GLN:NE2	2.46	0.49
25:B:848:8CT:C32	25:B:848:8CT:C36	2.90	0.49
4:D:108:LYS:HG3	4:D:110:GLN:OE1	2.12	0.49
4:D:157:VAL:HG22	4:D:163:VAL:HG22	1.94	0.49
13:1:32:PRO:O	13:1:53:TYR:HE1	1.96	0.49
13:1:91:GLN:NE2	22:1:303:CLA:HMD1	2.28	0.49
29:4:307:CHL:HMB2	25:4:317:8CT:C20	2.42	0.49
16:8:140:MET:HE2	22:8:308:CLA:HBC2	1.95	0.49
20:0:46:LEU:HB3	20:0:53:ASP:OD1	2.13	0.49
1:A:116:ILE:HG23	1:A:137:GLY:HA3	1.95	0.48
1:A:382:TYR:HB2	1:A:385:LEU:HG	1.95	0.48
1:A:745:TRP:NE1	25:A:850:8CT:C38	2.73	0.48
22:A:829:CLA:H2	25:A:847:8CT:C28	2.43	0.48
2:B:519:VAL:HG11	2:B:593:TYR:CG	2.47	0.48
25:B:847:8CT:C40	25:B:847:8CT:C15	2.90	0.48
22:1:303:CLA:H12	22:1:304:CLA:CAD	2.43	0.48
14:2:189:LEU:HD23	14:2:190:ALA:N	2.28	0.48
17:6:43:LEU:HD21	18:7:145:GLN:HG2	1.95	0.48
22:5:304:CLA:NB	25:5:317:8CT:C32	2.75	0.48
16:8:120:ALA:HB1	22:8:304:CLA:HMA1	1.95	0.48
16:8:229:HIS:CG	22:8:312:CLA:HAA2	2.47	0.48
1:A:440:ASP:OD2	1:A:566:ARG:NH2	2.38	0.48
1:A:566:ARG:HH12	4:D:89:GLY:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:850:8CT:C06	22:B:832:CLA:HMB1	2.43	0.48
2:B:318:GLY:O	2:B:407:VAL:HG23	2.13	0.48
4:D:195:VAL:CG1	4:D:199:LYS:HB3	2.44	0.48
5:E:33:ILE:HG22	5:E:35:TYR:H	1.78	0.48
11:K:42:ASP:CG	11:K:44:PRO:HD3	2.38	0.48
15:3:274:TRP:O	15:3:277:VAL:HG23	2.13	0.48
30:5:315:XAT:H391	30:5:315:XAT:H31	1.48	0.48
18:7:45:GLY:O	18:7:46:VAL:HG13	2.14	0.48
18:7:78:ARG:NH2	22:7:303:CLA:HED3	2.27	0.48
18:7:144:TRP:HB2	22:7:309:CLA:HMA1	1.95	0.48
18:7:205:TRP:NE1	30:7:320:XAT:H10	2.29	0.48
30:0:313:XAT:H391	30:0:313:XAT:H31	1.59	0.48
2:B:176:ASN:HD22	2:B:293:THR:HG23	1.78	0.48
2:B:176:ASN:ND2	2:B:291:TYR:O	2.29	0.48
6:F:94:GLU:HA	6:F:94:GLU:OE1	2.12	0.48
7:G:2:LEU:HD23	7:G:3:SER:N	2.29	0.48
15:3:153:TRP:CD1	15:3:153:TRP:H	2.31	0.48
20:0:46:LEU:HD11	22:0:302:CLA:HAA1	1.95	0.48
1:A:472:ARG:HD3	1:A:475:ASP:OD2	2.13	0.48
22:A:802:CLA:HBB1	22:A:802:CLA:HMB3	1.95	0.48
22:A:840:CLA:H11	22:A:840:CLA:C4D	2.44	0.48
13:5:69:ARG:O	13:5:72:GLU:HG2	2.13	0.48
13:5:186:PHE:CE1	30:5:316:XAT:H10	2.47	0.48
22:7:318:CLA:H122	22:7:318:CLA:H162	1.66	0.48
1:A:127:VAL:HG12	1:A:127:VAL:O	2.13	0.48
1:A:202:MET:HE1	22:A:825:CLA:H8	1.96	0.48
1:A:227:ILE:HB	1:A:228:PRO:HD3	1.96	0.48
1:A:486:PRO:HD3	1:A:538:PHE:HB2	1.95	0.48
2:B:524:ALA:O	2:B:528:HIS:HD2	1.95	0.48
22:B:833:CLA:H52	10:J:29:VAL:HG11	1.95	0.48
3:C:54:CYS:HB3	3:C:65:VAL:HG21	1.94	0.48
24:1:317:LHG:H291	24:1:317:LHG:H102	1.95	0.48
14:2:107:ARG:HD2	14:2:234:PHE:CE2	2.49	0.48
22:4:312:CLA:O1D	22:4:312:CLA:H2A	2.13	0.48
29:6:306:CHL:HMB3	22:6:309:CLA:HBC2	1.95	0.48
2:B:174:ARG:HB3	2:B:178:HIS:HD2	1.78	0.48
2:B:216:LEU:HA	22:B:816:CLA:HED1	1.94	0.48
2:B:254:ILE:HG13	2:B:255:LEU:H	1.78	0.48
25:B:848:8CT:C40	25:B:848:8CT:C15	2.91	0.48
4:D:93:LYS:HZ2	4:D:97:GLU:HG2	1.78	0.48
12:L:115:LYS:HD3	12:L:121:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:185:ALA:HB2	30:1:314:XAT:C19	2.43	0.48
15:3:98:TRP:O	15:3:101:TYR:N	2.43	0.48
15:3:228:ARG:O	15:3:232:ASN:ND2	2.37	0.48
16:4:239:TRP:CD1	16:4:239:TRP:N	2.80	0.48
17:6:260:CYS:SG	17:6:263:GLU:HB2	2.53	0.48
22:7:316:CLA:H122	22:7:316:CLA:H162	1.38	0.48
22:8:302:CLA:O1A	22:8:302:CLA:H3A	2.12	0.48
1:A:340:GLY:HA2	12:L:5:GLN:HE21	1.78	0.48
1:A:362:LEU:HD13	1:A:409:GLY:HA3	1.96	0.48
1:A:443:ILE:HD11	1:A:560:LEU:HD12	1.95	0.48
1:A:488:PHE:HE2	22:A:837:CLA:H42	1.78	0.48
22:A:839:CLA:HBC3	22:A:853:CLA:C1C	2.43	0.48
3:C:4:ASN:HD21	4:D:206:ILE:HG21	1.79	0.48
22:2:308:CLA:HHC	22:2:308:CLA:HBB1	1.94	0.48
22:4:309:CLA:CHC	30:4:315:XAT:H30	2.43	0.48
16:8:41:ARG:NH1	16:8:56:GLY:H	2.12	0.48
16:8:64:TYR:CE2	30:8:317:XAT:H383	2.48	0.48
16:8:65:ASP:OD2	16:8:69:LEU:N	2.46	0.48
1:A:195:TRP:CZ2	22:A:813:CLA:HAC2	2.48	0.48
1:A:252:ARG:NH2	15:3:277:VAL:HB	2.29	0.48
1:A:696:GLY:N	2:B:568:CYS:O	2.47	0.48
2:B:112:PRO:HG3	8:H:128:PRO:HB3	1.96	0.48
22:B:801:CLA:H3A	22:B:801:CLA:O2A	2.14	0.48
3:C:28:MET:HE3	3:C:38:GLN:HG2	1.96	0.48
30:1:314:XAT:H373	30:1:314:XAT:H23	1.70	0.48
17:6:87:TRP:CE2	29:6:308:CHL:HED2	2.48	0.48
24:6:322:LHG:H101	25:7:321:8CT:C08	2.43	0.48
18:7:51:TYR:OH	18:7:63:ASP:OD2	2.26	0.48
22:7:307:CLA:C3B	25:7:323:8CT:C27	2.87	0.48
19:9:179:TRP:CD1	30:9:315:XAT:H14	2.48	0.48
22:0:302:CLA:HHC	30:0:314:XAT:H403	1.95	0.48
1:A:338:PHE:HE1	12:L:6:VAL:HG11	1.79	0.48
2:B:474:PHE:CD2	22:B:850:CLA:H52	2.49	0.48
9:I:4:ALA:O	9:I:7:PRO:HD2	2.14	0.48
14:2:45:VAL:HG11	14:2:52:PRO:HG3	1.96	0.48
14:2:126:SER:O	14:2:127:SER:OG	2.21	0.48
15:3:67:TYR:OH	15:3:79:ASP:OD2	2.32	0.48
16:8:243:LEU:CD2	25:8:301:8CT:C07	2.92	0.48
20:0:192:LEU:O	20:0:196:ILE:HG12	2.14	0.48
21:M:5:GLU:HG2	21:M:9:PHE:HE2	1.78	0.48
22:A:835:CLA:O2D	22:A:835:CLA:H2A	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:831:CLA:HBA2	22:B:831:CLA:H3A	1.45	0.48
3:C:27:GLU:HG2	4:D:174:PRO:HB3	1.96	0.48
13:1:85:VAL:HG13	13:1:189:PHE:CZ	2.49	0.48
16:4:229:HIS:CD2	22:4:312:CLA:HAA2	2.48	0.48
16:4:238:VAL:HG12	22:4:312:CLA:C3D	2.44	0.48
22:6:304:CLA:H92	22:6:304:CLA:H61	1.72	0.48
18:7:41:LEU:HD21	18:7:48:ALA:HB2	1.95	0.48
16:8:238:VAL:O	16:8:242:GLU:HB3	2.13	0.48
1:A:62:HIS:ND1	22:A:805:CLA:HBB2	2.29	0.47
2:B:5:PHE:HB3	2:B:20:ARG:NH1	2.29	0.47
2:B:207:VAL:HA	2:B:211:ASN:HD21	1.77	0.47
6:F:160:ALA:HB1	6:F:164:MET:HB2	1.96	0.47
13:1:142:ARG:HD3	22:1:306:CLA:C1D	2.44	0.47
22:4:309:CLA:CGA	22:4:309:CLA:C4A	2.92	0.47
13:5:145:GLU:HB2	13:5:151:ARG:HB3	1.96	0.47
13:5:225:PHE:HD1	31:5:319:LMG:H212	1.78	0.47
22:5:309:CLA:H61	30:5:315:XAT:H161	1.96	0.47
16:8:211:PHE:HZ	30:8:316:XAT:H363	1.75	0.47
1:A:468:SER:HB2	1:A:476:MET:SD	2.54	0.47
1:A:558:GLY:HA2	1:A:596:HIS:CD2	2.49	0.47
22:B:830:CLA:H61	22:B:830:CLA:H41	1.54	0.47
3:C:25:VAL:HG11	3:C:48:CYS:SG	2.53	0.47
11:K:26:LEU:HD22	22:K:105:CLA:C1C	2.44	0.47
29:4:305:CHL:H41	29:4:305:CHL:H61	1.71	0.47
25:4:317:8CT:C19	25:4:317:8CT:C39	2.92	0.47
17:6:232:VAL:HB	25:7:323:8CT:C40	2.44	0.47
1:A:717:ALA:N	6:F:198:GLU:OE2	2.28	0.47
22:A:821:CLA:H2	22:A:821:CLA:H62	1.72	0.47
22:A:833:CLA:HAA2	12:L:67:LEU:O	2.14	0.47
2:B:642:SER:OG	8:H:138:GLU:OE1	2.32	0.47
2:B:680:TRP:CD1	4:D:91:LEU:HD21	2.49	0.47
6:F:226:SER:OG	16:4:74:GLU:OE2	2.22	0.47
16:4:72:ASP:N	16:4:72:ASP:OD1	2.47	0.47
17:6:44:PRO:HD2	29:6:302:CHL:O2D	2.14	0.47
1:A:206:HIS:CE1	22:A:813:CLA:NA	2.83	0.47
1:A:697:TYR:CE1	2:B:536:LYS:HD3	2.49	0.47
22:A:803:CLA:CBB	25:J:101:8CT:C07	2.92	0.47
2:B:344:ILE:HD12	22:B:819:CLA:H71	1.96	0.47
12:L:90:VAL:O	12:L:94:THR:HG23	2.14	0.47
13:1:187:VAL:HG12	22:1:311:CLA:HAC1	1.96	0.47
15:3:90:ASP:CG	15:3:91:VAL:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:9:55:ASP:CG	19:9:57:GLY:H	2.23	0.47
20:0:99:ASN:O	20:0:103:ALA:N	2.47	0.47
20:0:147:MET:CG	20:0:148:PRO:HD3	2.44	0.47
20:0:176:GLY:O	20:0:180:GLN:HG2	2.14	0.47
1:A:499:ALA:O	1:A:501:GLN:N	2.40	0.47
1:A:511:THR:HG21	22:A:827:CLA:HAB	1.96	0.47
1:A:524:GLY:O	1:A:627:VAL:N	2.36	0.47
22:A:833:CLA:H2A	22:A:833:CLA:O2D	2.15	0.47
2:B:12:LEU:HG	28:B:849:DGD:HE2	1.97	0.47
2:B:58:PHE:HB2	2:B:146:ALA:HB2	1.96	0.47
2:B:476:PHE:HE2	22:B:850:CLA:H11	1.79	0.47
2:B:514:PRO:HG3	6:F:146:HIS:CD2	2.49	0.47
2:B:715:VAL:HG22	28:B:849:DGD:HBS2	1.95	0.47
7:G:59:LYS:HB2	19:9:42:ALA:HB2	1.96	0.47
8:H:75:GLN:CG	12:L:34:SER:HB2	2.44	0.47
22:2:302:CLA:H92	22:2:302:CLA:H61	1.75	0.47
15:3:246:GLN:O	15:3:250:THR:OG1	2.29	0.47
16:4:89:PHE:CE2	29:4:307:CHL:HED2	2.49	0.47
16:4:159:VAL:HG22	16:4:160:ASP:OD1	2.14	0.47
16:4:211:PHE:CE1	16:4:222:PRO:HB3	2.50	0.47
29:4:306:CHL:HBB1	29:4:306:CHL:HHC	1.96	0.47
22:7:303:CLA:HMB2	22:7:303:CLA:H2	1.96	0.47
19:9:38:TRP:CD1	19:9:58:TYR:HA	2.50	0.47
2:B:91:ILE:HD11	2:B:114:ASN:CG	2.40	0.47
22:B:811:CLA:H142	22:B:811:CLA:H112	1.68	0.47
7:G:54:TYR:CE2	7:G:57:LEU:HB2	2.49	0.47
7:G:79:HIS:CE1	25:G:104:8CT:C17	2.98	0.47
15:3:231:LYS:HZ1	24:3:317:LHG:HC62	1.80	0.47
13:5:131:GLU:HA	22:5:305:CLA:HMA2	1.96	0.47
19:9:152:PHE:O	19:9:154:TRP:HE3	1.98	0.47
1:A:117:LYS:HB3	1:A:144:GLN:OE1	2.15	0.47
1:A:204:ASN:OD1	1:A:317:TYR:HB2	2.14	0.47
1:A:274:TRP:CD1	22:A:817:CLA:HMB1	2.50	0.47
1:A:315:HIS:CD2	25:A:854:8CT:C24	2.97	0.47
1:A:567:LEU:HB3	2:B:673:GLU:OE2	2.15	0.47
2:B:123:TRP:HA	2:B:126:THR:HG22	1.96	0.47
2:B:444:LEU:HD13	2:B:615:TYR:CD1	2.50	0.47
22:B:803:CLA:H2A	22:B:803:CLA:O1D	2.15	0.47
22:B:850:CLA:HMA3	6:F:153:LEU:HD11	1.96	0.47
12:L:66:LYS:HD3	22:L:204:CLA:HMA3	1.96	0.47
13:1:82:MET:HE3	13:1:179:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:310:CLA:HBB1	30:1:314:XAT:C14	2.43	0.47
14:2:120:LYS:O	14:2:124:GLU:HG2	2.14	0.47
15:3:109:PHE:CE1	22:3:307:CLA:HBC3	2.50	0.47
15:3:142:VAL:HG13	15:3:143:ILE:HG13	1.95	0.47
17:6:62:TRP:NE1	30:6:320:XAT:H383	2.30	0.47
17:6:154:PHE:HZ	29:6:316:CHL:HAA1	1.79	0.47
13:5:100:HIS:ND1	13:5:193:TYR:HE2	2.12	0.47
22:5:303:CLA:H2A	22:5:303:CLA:H43	1.95	0.47
22:5:303:CLA:HHD	22:5:308:CLA:HAA1	1.96	0.47
22:5:304:CLA:C4A	22:5:304:CLA:HBA2	2.44	0.47
29:5:306:CHL:HBA1	29:5:306:CHL:H3A	1.66	0.47
30:5:316:XAT:H35	30:5:316:XAT:H401	1.55	0.47
18:7:43:ALA:HB3	18:7:46:VAL:HG13	1.96	0.47
18:7:112:LEU:O	18:7:114:LYS:N	2.39	0.47
18:7:123:LEU:HB2	18:7:128:ILE:HD11	1.97	0.47
18:7:187:ILE:HG23	18:7:188:GLU:H	1.79	0.47
1:A:62:HIS:HD1	22:A:805:CLA:HBB2	1.79	0.47
1:A:244:LEU:HD13	1:A:246:HIS:HE1	1.79	0.47
2:B:191:THR:CG2	2:B:277:HIS:HB2	2.44	0.47
22:B:808:CLA:H3A	22:B:808:CLA:HBA1	1.44	0.47
22:1:311:CLA:NC	22:1:311:CLA:H43	2.30	0.47
14:2:48:PRO:HG2	29:2:301:CHL:HMD2	1.95	0.47
29:4:301:CHL:H62	29:4:301:CHL:H41	1.62	0.47
22:7:316:CLA:CBB	25:7:321:8CT:C13	2.92	0.47
22:7:317:CLA:H12	22:7:317:CLA:HBA2	1.55	0.47
16:8:89:PHE:CE1	22:8:308:CLA:HBC1	2.49	0.47
19:9:148:LEU:HD13	19:9:151:SER:O	2.15	0.47
20:0:83:MET:CB	30:0:313:XAT:H15	2.45	0.47
22:0:312:CLA:H91	22:0:312:CLA:CAD	2.45	0.47
1:A:298:ASP:O	1:A:302:HIS:N	2.48	0.47
1:A:362:LEU:HB3	1:A:406:CYS:O	2.15	0.47
2:B:451:LYS:HE3	6:F:128:ARG:HH12	1.78	0.47
22:B:819:CLA:HBA2	22:B:819:CLA:H3A	1.46	0.47
3:C:73:THR:N	3:C:76:SER:OG	2.38	0.47
17:6:52:LEU:HD22	17:6:61:GLY:HA2	1.95	0.47
17:6:215:TRP:HD1	17:6:216:THR:HG23	1.80	0.47
17:6:227:ILE:H	17:6:230:LYS:HD3	1.80	0.47
13:5:56:ASP:OD1	22:5:302:CLA:HBA2	2.14	0.47
13:5:147:ASP:OD1	13:5:148:MET:N	2.48	0.47
18:7:262:PRO:CD	22:7:317:CLA:HAA1	2.39	0.47
16:8:44:TRP:CE2	16:8:64:TYR:HD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:8:214:GLN:O	16:8:218:THR:OG1	2.23	0.47
20:0:128:GLU:HB3	20:0:132:TYR:CD2	2.50	0.47
1:A:294:LEU:HD12	1:A:381:PRO:HB3	1.97	0.47
1:A:445:HIS:O	1:A:449:VAL:HG23	2.15	0.47
1:A:663:ILE:HD11	22:A:801:CLA:CBC	2.45	0.47
22:B:829:CLA:C4A	22:B:829:CLA:HBA2	2.44	0.47
22:1:303:CLA:C4B	25:1:316:8CT:C36	2.93	0.47
14:2:187:PHE:HD2	30:2:315:XAT:H21	1.80	0.47
16:4:78:TRP:NE1	22:4:303:CLA:O1A	2.38	0.47
17:6:150:LYS:HA	17:6:157:TYR:HD1	1.80	0.47
17:6:234:THR:HG23	17:6:235:LEU:O	2.14	0.47
16:8:208:THR:HG21	30:8:317:XAT:H12	1.97	0.47
20:0:86:VAL:HG12	20:0:90:ALA:HB2	1.96	0.47
20:0:221:ALA:O	20:0:224:PRO:HD2	2.15	0.47
1:A:417:PHE:CD1	1:A:421:ASP:HB2	2.49	0.46
1:A:700:GLU:C	2:B:536:LYS:HZ1	2.24	0.46
2:B:585:ASN:HD21	22:B:803:CLA:CBC	2.26	0.46
22:B:815:CLA:H2A	22:B:815:CLA:O2D	2.15	0.46
22:B:825:CLA:H111	22:B:825:CLA:H72	1.50	0.46
5:E:5:ARG:HG2	5:E:27:SER:HA	1.97	0.46
12:L:10:ILE:HG23	12:L:11:ASN:HD22	1.80	0.46
15:3:270:ILE:HD11	22:3:311:CLA:C1	2.39	0.46
16:4:64:TYR:CE2	30:4:316:XAT:H383	2.49	0.46
22:6:312:CLA:H61	22:6:312:CLA:H41	1.54	0.46
16:8:159:VAL:CG1	16:8:167:LEU:HA	2.45	0.46
1:A:661:GLN:HG3	1:A:751:ARG:HD2	1.96	0.46
1:A:686:PHE:CE2	1:A:690:PHE:HE2	2.33	0.46
22:A:833:CLA:H3A	22:A:833:CLA:HBA2	1.48	0.46
2:B:20:ARG:HH22	9:I:30:ILE:HG22	1.80	0.46
2:B:78:VAL:HG13	2:B:125:TYR:CE1	2.50	0.46
2:B:474:PHE:CD1	22:B:850:CLA:H52	2.49	0.46
2:B:487:ASN:OD1	2:B:488:ALA:N	2.49	0.46
2:B:510:LEU:HD22	2:B:601:ILE:HD13	1.96	0.46
22:B:820:CLA:H91	22:B:820:CLA:H111	1.60	0.46
6:F:122:ALA:O	6:F:125:THR:HG22	2.16	0.46
30:3:314:XAT:H401	30:3:314:XAT:H35	1.49	0.46
16:4:72:ASP:OD1	16:4:75:THR:OG1	2.22	0.46
16:4:180:PHE:HB3	22:4:309:CLA:HMD2	1.97	0.46
30:6:319:XAT:H402	30:6:319:XAT:H31	1.79	0.46
13:5:163:PHE:HB2	22:5:309:CLA:O1A	2.15	0.46
24:5:318:LHG:H192	24:5:318:LHG:H372	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:8:301:8CT:C23	25:8:301:8CT:C27	2.93	0.46
22:8:309:CLA:H52	30:8:316:XAT:H192	1.98	0.46
1:A:712:LEU:HD12	22:A:839:CLA:HMA2	1.98	0.46
22:A:822:CLA:H2A	22:A:822:CLA:O2D	2.16	0.46
2:B:111:GLY:HA2	8:H:133:PRO:HG2	1.98	0.46
2:B:172:GLU:HG2	2:B:301:MET:HG2	1.95	0.46
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.97	0.46
2:B:242:HIS:HD2	2:B:262:HIS:CE1	2.33	0.46
6:F:85:SER:HB3	6:F:133:GLY:O	2.15	0.46
8:H:129:ILE:HG22	8:H:130:THR:HG23	1.96	0.46
22:L:203:CLA:H141	22:L:203:CLA:H162	1.62	0.46
16:4:157:VAL:CG2	29:4:307:CHL:HAC1	2.45	0.46
22:5:303:CLA:HBB1	30:5:316:XAT:H35	1.97	0.46
18:7:260:LEU:HD11	22:7:317:CLA:C1C	2.45	0.46
22:7:314:CLA:O1D	22:7:314:CLA:H2A	2.15	0.46
16:8:135:MET:HE3	29:8:305:CHL:O1D	2.16	0.46
20:0:93:ASN:OD1	20:0:94:ALA:N	2.48	0.46
20:0:111:ILE:O	20:0:115:VAL:HB	2.16	0.46
2:B:569:ASP:HA	2:B:574:ASP:OD2	2.16	0.46
22:B:820:CLA:H112	22:B:820:CLA:H152	1.72	0.46
22:B:841:CLA:H3A	22:B:841:CLA:HBA1	1.50	0.46
22:L:201:CLA:H41	22:L:201:CLA:H61	1.59	0.46
22:1:311:CLA:H121	29:4:301:CHL:H92	1.97	0.46
22:1:311:CLA:O1D	22:1:311:CLA:H2A	2.15	0.46
31:5:319:LMG:H201	16:8:129:THR:HG21	1.97	0.46
25:8:301:8CT:C40	25:8:301:8CT:C15	2.94	0.46
19:9:95:GLU:OE2	19:9:192:GLY:HA3	2.16	0.46
1:A:116:ILE:HD12	1:A:137:GLY:HA3	1.98	0.46
1:A:217:GLY:O	22:A:814:CLA:HMC3	2.16	0.46
22:A:840:CLA:H161	25:A:850:8CT:C01	2.45	0.46
2:B:174:ARG:NE	22:B:825:CLA:HMD3	2.30	0.46
3:C:3:HIS:CE1	3:C:69:LEU:HD22	2.50	0.46
11:K:26:LEU:HD12	11:K:27:ALA:N	2.30	0.46
13:1:51:GLY:O	13:1:180:ARG:NH1	2.34	0.46
14:2:143:TRP:CZ3	25:2:317:8CT:C09	2.96	0.46
17:6:190:ALA:O	17:6:193:SER:N	2.49	0.46
22:6:315:CLA:H152	22:6:315:CLA:H112	1.62	0.46
13:5:100:HIS:HE2	29:5:306:CHL:HMA3	1.81	0.46
13:5:174:LYS:NZ	22:5:311:CLA:OBD	2.34	0.46
16:8:82:ALA:O	16:8:86:HIS:N	2.35	0.46
16:8:211:PHE:CE1	30:8:316:XAT:H372	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:0:220:ALA:O	29:0:301:CHL:HMA2	2.15	0.46
21:M:5:GLU:HA	21:M:8:ILE:HD12	1.98	0.46
1:A:158:ILE:HG23	1:A:163:GLU:HB2	1.97	0.46
1:A:587:GLY:HA3	2:B:702:ILE:HD11	1.97	0.46
1:A:605:TYR:OH	22:A:801:CLA:HED3	2.15	0.46
22:A:826:CLA:CAD	22:A:836:CLA:HBB1	2.46	0.46
2:B:31:PHE:HA	2:B:34:HIS:NE2	2.30	0.46
4:D:144:LEU:HD11	4:D:152:ALA:HB2	1.97	0.46
11:K:51:ASP:OD2	11:K:55:PHE:HB3	2.16	0.46
12:L:138:SER:O	12:L:142:VAL:HG23	2.15	0.46
14:2:175:GLU:OE1	14:2:175:GLU:N	2.48	0.46
22:4:309:CLA:H62	22:4:309:CLA:H41	1.55	0.46
13:5:218:THR:C	13:5:220:GLY:H	2.23	0.46
18:7:75:ALA:HB1	18:7:169:MET:SD	2.55	0.46
24:0:315:LHG:H292	24:0:315:LHG:H171	1.97	0.46
1:A:62:HIS:HD2	22:A:830:CLA:H12	1.80	0.46
1:A:628:SER:O	1:A:629:GLU:HG2	2.16	0.46
22:A:816:CLA:HHC	22:A:816:CLA:HBB1	1.97	0.46
2:B:395:ILE:HD11	2:B:550:LYS:O	2.16	0.46
2:B:680:TRP:HD1	4:D:91:LEU:HD21	1.80	0.46
22:B:828:CLA:CGA	22:B:828:CLA:H3A	2.44	0.46
22:B:837:CLA:H61	22:B:837:CLA:H41	1.49	0.46
3:C:62:PHE:CD2	4:D:191:ILE:HD12	2.51	0.46
14:2:80:TRP:CZ2	22:2:308:CLA:HED3	2.51	0.46
22:3:310:CLA:HMB2	30:3:314:XAT:H402	1.98	0.46
25:6:321:8CT:C36	25:6:321:8CT:C32	2.93	0.46
22:5:311:CLA:HBB2	30:5:315:XAT:H393	1.96	0.46
18:7:162:ASN:HD22	22:7:316:CLA:CAD	2.29	0.46
16:8:115:THR:H	16:8:119:ASN:CG	2.23	0.46
22:8:309:CLA:H51	22:8:311:CLA:H3A	1.98	0.46
19:9:83:TRP:CZ2	22:9:308:CLA:HAC2	2.51	0.46
19:9:123:ALA:HB1	20:0:217:ILE:HG21	1.97	0.46
19:9:174:LEU:HD21	30:9:314:XAT:H30	1.97	0.46
20:0:61:LEU:HD13	22:0:302:CLA:H42	1.97	0.46
29:0:301:CHL:H52	22:0:311:CLA:H121	1.98	0.46
1:A:218:TRP:N	22:A:814:CLA:HAB	2.31	0.46
1:A:445:HIS:CD2	22:A:831:CLA:HMB1	2.50	0.46
1:A:617:TRP:HB2	1:A:654:PHE:CE1	2.51	0.46
1:A:710:ASN:OD1	1:A:715:ALA:HB2	2.16	0.46
22:A:826:CLA:HBA1	22:A:826:CLA:H3A	1.64	0.46
2:B:459:PHE:HD2	22:B:837:CLA:C3D	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:161:ALA:HB3	22:1:308:CLA:HBA2	1.97	0.46
30:1:314:XAT:H171	30:1:314:XAT:H7	1.29	0.46
15:3:140:ASN:ND2	30:3:315:XAT:HO3	2.13	0.46
22:3:319:CLA:HED1	22:3:319:CLA:H42	1.98	0.46
16:4:242:GLU:OE1	16:4:243:LEU:HB3	2.16	0.46
16:4:242:GLU:H	16:4:245:LYS:HE3	1.80	0.46
13:5:122:THR:HG23	13:5:127:LEU:HD12	1.96	0.46
13:5:139:GLU:HG3	22:5:308:CLA:C1D	2.46	0.46
22:9:309:CLA:CBB	22:9:311:CLA:H3A	2.46	0.46
20:0:45:HIS:CD2	20:0:63:ALA:HA	2.50	0.46
21:M:9:PHE:O	22:M:101:CLA:HBB1	2.16	0.46
1:A:155:ALA:HB1	22:A:819:CLA:HED1	1.97	0.46
22:B:813:CLA:C2	19:9:61:LEU:HD13	2.46	0.46
4:D:102:ILE:O	4:D:128:LEU:HA	2.16	0.46
6:F:162:ASP:OD1	6:F:163:ILE:N	2.47	0.46
22:L:202:CLA:H3A	22:L:202:CLA:HBA2	1.55	0.46
22:1:312:CLA:H3A	22:1:312:CLA:HBA1	1.32	0.46
15:3:190:LEU:CD1	25:3:316:8CT:C38	2.94	0.46
17:6:218:HIS:HE1	22:6:314:CLA:NB	2.14	0.46
18:7:249:ASP:HB3	18:7:254:ASN:H	1.80	0.46
19:9:41:GLY:O	19:9:42:ALA:C	2.58	0.46
20:0:208:SER:OG	20:0:209:VAL:N	2.49	0.46
1:A:339:THR:HG1	24:A:845:LHG:H02	1.60	0.46
1:A:585:ARG:O	2:B:668:ARG:NH1	2.49	0.46
22:A:828:CLA:H203	25:J:104:8CT:C22	2.46	0.46
5:E:11:ILE:HG12	5:E:54:PHE:CE2	2.50	0.46
7:G:20:ARG:NH1	7:G:64:VAL:HG22	2.31	0.46
16:4:146:ARG:NH1	16:4:158:ASN:HB2	2.25	0.46
13:5:145:GLU:CB	13:5:151:ARG:HB3	2.46	0.46
22:7:307:CLA:ND	25:7:323:8CT:C22	2.79	0.46
19:9:85:MET:HE1	22:9:309:CLA:HAB	1.97	0.46
1:A:362:LEU:HD23	22:A:805:CLA:HED1	1.97	0.45
22:A:828:CLA:H2A	22:A:828:CLA:O1D	2.15	0.45
2:B:254:ILE:HG13	2:B:255:LEU:N	2.31	0.45
22:B:809:CLA:H71	22:B:809:CLA:H111	1.61	0.45
22:B:813:CLA:H91	22:B:813:CLA:C1D	2.46	0.45
22:B:814:CLA:H71	22:B:814:CLA:H111	1.46	0.45
8:H:85:GLN:HE22	22:L:202:CLA:H192	1.81	0.45
22:L:202:CLA:C2D	22:L:202:CLA:H121	2.47	0.45
22:1:312:CLA:O1D	22:1:312:CLA:H2A	2.16	0.45
17:6:102:LYS:HB3	17:6:102:LYS:HE3	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:0:195:HIS:CG	22:0:311:CLA:HAA2	2.51	0.45
1:A:21:ILE:CG2	1:A:192:LYS:HD2	2.45	0.45
1:A:200:GLU:OE2	1:A:327:MET:N	2.48	0.45
1:A:519:ILE:HG22	1:A:529:MET:HB2	1.98	0.45
2:B:361:ILE:HG22	2:B:362:ALA:N	2.31	0.45
2:B:622:ASP:O	2:B:626:LEU:HG	2.15	0.45
2:B:639:GLY:C	2:B:640:MET:HE2	2.41	0.45
4:D:95:GLN:HE21	8:H:69:SER:HB2	1.82	0.45
25:J:104:8CT:C01	25:J:104:8CT:C11	2.94	0.45
22:K:105:CLA:H3A	22:K:105:CLA:HBA1	1.58	0.45
15:3:231:LYS:NZ	24:3:317:LHG:HC62	2.30	0.45
22:3:311:CLA:H2A	22:3:311:CLA:O1D	2.16	0.45
17:6:227:ILE:O	17:6:227:ILE:HG22	2.17	0.45
22:6:301:CLA:H3A	22:6:301:CLA:HBA1	1.53	0.45
13:5:92:GLU:OE1	13:5:200:PRO:HD2	2.16	0.45
16:8:44:TRP:CD1	16:8:64:TYR:HB2	2.51	0.45
16:8:74:GLU:HG2	16:8:75:THR:N	2.32	0.45
16:8:199:LYS:HD2	22:8:310:CLA:C3D	2.46	0.45
22:0:308:CLA:H2	22:0:308:CLA:CHB	2.46	0.45
1:A:34:TRP:CH2	22:A:804:CLA:H2	2.51	0.45
1:A:34:TRP:HE1	22:A:811:CLA:HBA1	1.81	0.45
2:B:230:TRP:O	22:B:817:CLA:H3A	2.15	0.45
2:B:444:LEU:HD13	2:B:615:TYR:CE1	2.51	0.45
6:F:163:ILE:O	6:F:167:THR:N	2.37	0.45
25:J:104:8CT:C22	25:J:104:8CT:C25	2.95	0.45
22:L:204:CLA:HBA1	22:L:204:CLA:H3A	1.70	0.45
14:2:122:TYR:O	14:2:126:SER:N	2.45	0.45
29:2:305:CHL:HED3	16:4:234:TRP:HH2	1.81	0.45
24:2:318:LHG:H272	24:2:318:LHG:H242	1.63	0.45
13:5:51:GLY:O	13:5:180:ARG:NH2	2.44	0.45
16:8:190:VAL:HB	16:8:194:LYS:HE2	1.99	0.45
30:0:314:XAT:H191	30:0:314:XAT:H11	1.65	0.45
1:A:270:PHE:CD1	22:K:102:CLA:HBC2	2.46	0.45
1:A:464:ASN:HB3	1:A:646:ALA:HB2	1.96	0.45
22:A:804:CLA:H61	22:A:809:CLA:H202	1.99	0.45
22:A:839:CLA:C4A	22:A:839:CLA:HBA2	2.45	0.45
25:A:850:8CT:C06	22:B:832:CLA:CMB	2.95	0.45
2:B:509:PHE:CE1	22:B:827:CLA:HBC2	2.51	0.45
22:B:812:CLA:HED3	22:B:812:CLA:HBD	1.72	0.45
6:F:176:TYR:HE2	22:F:301:CLA:HBD	1.77	0.45
22:L:204:CLA:HBA1	22:L:204:CLA:H11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:99:TRP:CD1	13:1:200:PRO:HD3	2.50	0.45
15:3:81:PHE:HB2	15:3:83:LEU:HD13	1.98	0.45
16:4:166:LYS:C	16:4:167:LEU:HG	2.42	0.45
16:4:227:THR:O	16:4:231:ALA:N	2.39	0.45
13:5:35:TRP:CG	13:5:36:LEU:H	2.34	0.45
13:5:75:VAL:HG11	13:5:152:VAL:HG21	1.98	0.45
22:7:305:CLA:C4A	22:7:305:CLA:HBA2	2.47	0.45
30:0:313:XAT:H30	30:0:313:XAT:H403	1.99	0.45
22:A:823:CLA:H12	22:A:823:CLA:CHB	2.46	0.45
2:B:595:HIS:CG	2:B:623:TYR:OH	2.66	0.45
2:B:617:MET:O	2:B:621:ARG:N	2.32	0.45
22:B:828:CLA:H3A	22:B:828:CLA:HBA2	1.62	0.45
5:E:39:VAL:HG12	5:E:40:ARG:N	2.31	0.45
8:H:78:GLN:HA	12:L:42:GLY:HA3	1.99	0.45
8:H:113:ALA:HB3	22:H:201:CLA:C12	2.47	0.45
22:H:201:CLA:H151	12:L:88:LEU:HD13	1.99	0.45
10:J:7:TYR:OH	25:J:101:8CT:C06	2.65	0.45
22:1:303:CLA:HBA1	22:1:304:CLA:C1D	2.47	0.45
22:1:303:CLA:C4A	22:1:303:CLA:HBA2	2.46	0.45
14:2:83:GLN:HE21	14:2:148:ARG:HH11	1.65	0.45
16:4:160:ASP:HA	16:4:167:LEU:HD13	1.99	0.45
17:6:200:PHE:CE1	17:6:211:PRO:HB3	2.51	0.45
17:6:232:VAL:HG13	17:6:233:ILE:N	2.31	0.45
18:7:54:GLY:HA2	18:7:59:ASP:HB3	1.98	0.45
30:0:314:XAT:H201	30:0:314:XAT:H15	1.62	0.45
30:0:314:XAT:H202	30:0:314:XAT:H10	1.98	0.45
1:A:327:MET:HB2	1:A:347:TYR:CE1	2.51	0.45
22:A:813:CLA:HAA2	22:A:825:CLA:H52	1.98	0.45
2:B:141:PHE:CZ	22:B:815:CLA:H43	2.51	0.45
22:B:812:CLA:H112	22:B:840:CLA:H12	1.98	0.45
22:B:818:CLA:H3A	22:B:818:CLA:HBA2	1.32	0.45
22:B:830:CLA:H2A	22:B:830:CLA:O1D	2.16	0.45
3:C:25:VAL:O	3:C:27:GLU:HG3	2.17	0.45
9:I:19:PRO:O	9:I:23:MET:HB2	2.17	0.45
11:K:40:LEU:N	22:K:105:CLA:H43	2.32	0.45
13:1:221:THR:HG23	13:1:222:SER:N	2.32	0.45
14:2:234:PHE:O	14:2:237:ILE:HG22	2.17	0.45
29:2:301:CHL:HED3	15:3:173:ARG:HA	1.98	0.45
29:2:307:CHL:H2A	29:2:307:CHL:HED3	1.97	0.45
22:3:319:CLA:HAA2	22:3:319:CLA:CED	2.46	0.45
22:5:309:CLA:H72	30:5:315:XAT:C9	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:7:307:CLA:HMB1	25:7:323:8CT:C27	2.47	0.45
22:0:304:CLA:H41	22:0:304:CLA:H61	1.56	0.45
1:A:463:HIS:CE1	1:A:467:MET:HG3	2.52	0.45
1:A:467:MET:HB2	1:A:476:MET:HG2	1.98	0.45
22:A:839:CLA:HBB2	22:A:839:CLA:H152	1.97	0.45
2:B:585:ASN:ND2	22:B:803:CLA:HBC2	2.26	0.45
2:B:658:ALA:CB	22:B:806:CLA:HBB2	2.47	0.45
22:B:815:CLA:C4A	22:B:815:CLA:HBA2	2.46	0.45
6:F:126:GLN:HA	6:F:129:PHE:CD2	2.51	0.45
8:H:132:GLY:HA3	8:H:133:PRO:HD3	1.79	0.45
11:K:16:GLY:O	11:K:20:ALA:HB2	2.17	0.45
11:K:68:HIS:ND1	25:K:103:8CT:C15	2.77	0.45
13:1:207:HIS:CD2	22:1:311:CLA:HAA2	2.51	0.45
22:1:308:CLA:H41	22:1:310:CLA:HMA2	1.99	0.45
14:2:212:MET:HB2	22:2:302:CLA:HMC2	1.98	0.45
14:2:239:ASP:HB3	14:2:243:ASN:ND2	2.32	0.45
18:7:116:LEU:HB3	18:7:120:VAL:HG23	1.98	0.45
18:7:249:ASP:HB2	18:7:252:GLY:O	2.16	0.45
30:7:319:XAT:H31	30:7:319:XAT:H391	1.58	0.45
16:8:43:ILE:HG22	16:8:44:TRP:H	1.81	0.45
20:0:72:ARG:HH22	22:0:302:CLA:HED3	1.81	0.45
29:0:301:CHL:H92	22:0:312:CLA:H93	1.99	0.45
22:0:311:CLA:C2B	30:0:313:XAT:H363	2.46	0.45
1:A:576:PHE:HE2	1:A:594:TRP:HD1	1.65	0.45
2:B:265:THR:HA	2:B:360:PHE:CE1	2.51	0.45
22:B:811:CLA:CGA	22:B:811:CLA:C1A	2.95	0.45
22:B:825:CLA:H161	22:B:825:CLA:H141	1.63	0.45
4:D:110:GLN:O	4:D:122:MET:HG2	2.17	0.45
14:2:187:PHE:CE1	22:6:304:CLA:H2	2.51	0.45
17:6:180:GLU:OE1	17:6:180:GLU:N	2.41	0.45
29:6:302:CHL:HBB1	29:6:302:CHL:HHC	1.99	0.45
13:5:147:ASP:HB3	13:5:150:LYS:CB	2.47	0.45
16:8:66:PRO:HD2	30:8:317:XAT:H222	1.98	0.45
16:8:196:LYS:HE2	22:8:311:CLA:HAA2	1.99	0.45
20:0:72:ARG:NH2	20:0:164:LEU:HD11	2.28	0.45
1:A:585:ARG:NH1	3:C:49:VAL:HG11	2.32	0.45
1:A:703:GLU:OE2	2:B:545:LYS:HB2	2.16	0.45
2:B:38:THR:OG1	2:B:41:THR:HG22	2.17	0.45
2:B:47:PHE:HA	2:B:50:HIS:HD2	1.82	0.45
2:B:597:LYS:HD2	22:B:836:CLA:HBC1	1.97	0.45
22:B:807:CLA:C4A	22:B:807:CLA:HBA2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:21:ALA:C	11:K:26:LEU:HG	2.41	0.45
14:2:86:LEU:HB3	14:2:90:ARG:NH1	2.32	0.45
16:4:76:LEU:O	16:4:80:VAL:HG23	2.17	0.45
16:4:196:LYS:HE3	22:4:311:CLA:HAA2	1.99	0.45
17:6:88:ALA:O	17:6:92:VAL:HG12	2.17	0.45
22:6:303:CLA:HBC1	24:6:322:LHG:H261	1.99	0.45
13:5:35:TRP:NE1	13:5:54:GLY:O	2.50	0.45
22:7:316:CLA:H2	22:7:316:CLA:H61	1.58	0.45
16:8:196:LYS:HE3	22:8:311:CLA:HBD	1.99	0.45
30:8:316:XAT:H191	30:8:316:XAT:H11	1.42	0.45
22:A:801:CLA:H2	22:A:801:CLA:H61	1.79	0.45
22:A:811:CLA:H143	22:A:811:CLA:H161	1.62	0.45
22:A:841:CLA:HMD3	25:B:848:8CT:C36	2.47	0.45
2:B:441:ASP:OD1	2:B:615:TYR:HB2	2.17	0.45
2:B:612:SER:HA	2:B:615:TYR:CE1	2.52	0.45
22:B:823:CLA:H92	22:B:823:CLA:H61	1.73	0.45
6:F:184:TYR:CZ	6:F:188:THR:HG21	2.51	0.45
7:G:14:LEU:HG	13:1:133:VAL:HG22	1.99	0.45
22:G:102:CLA:H2A	22:G:102:CLA:CED	2.46	0.45
8:H:98:ARG:N	8:H:102:ILE:HD12	2.26	0.45
30:1:315:XAT:H35	30:1:315:XAT:H401	1.65	0.45
22:3:319:CLA:HED2	22:3:319:CLA:HBD	1.47	0.45
22:4:311:CLA:H61	22:4:311:CLA:H41	1.71	0.45
13:5:135:MET:HG2	22:5:308:CLA:OBD	2.17	0.45
16:8:89:PHE:HZ	29:8:305:CHL:HAB	1.81	0.45
16:8:97:MET:HB2	16:8:117:TRP:CB	2.47	0.45
22:8:308:CLA:HHC	22:8:308:CLA:CBB	2.46	0.45
19:9:216:ILE:N	19:9:217:PRO:HD3	2.31	0.45
22:A:826:CLA:C9	25:A:849:8CT:C40	2.95	0.44
22:A:828:CLA:H161	22:A:828:CLA:H202	1.64	0.44
2:B:70:TRP:HE1	9:I:3:ALA:HB3	1.82	0.44
2:B:257:PHE:HE2	2:B:493:TRP:CE3	2.35	0.44
7:G:61:ASN:ND2	22:G:103:CLA:OBD	2.51	0.44
22:G:101:CLA:HAA2	29:1:305:CHL:HBC2	1.99	0.44
9:I:16:LEU:C	9:I:19:PRO:HD2	2.42	0.44
13:1:215:ASN:ND2	22:1:312:CLA:O1D	2.50	0.44
16:4:158:ASN:OD1	16:4:162:ILE:HB	2.17	0.44
17:6:55:SER:N	17:6:59:ASP:OD2	2.49	0.44
13:5:34:ASN:ND2	13:5:36:LEU:O	2.50	0.44
13:5:36:LEU:HD12	13:5:38:GLY:H	1.82	0.44
22:7:317:CLA:HBA2	22:7:317:CLA:O2D	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:8:148:TYR:HB2	22:8:308:CLA:CMA	2.47	0.44
29:8:307:CHL:HMA1	25:8:318:8CT:C39	2.47	0.44
19:9:114:VAL:HB	22:9:306:CLA:HMD1	1.99	0.44
29:0:301:CHL:HBB1	29:0:301:CHL:CHC	2.42	0.44
1:A:379:MET:SD	22:A:818:CLA:HAA2	2.58	0.44
22:B:837:CLA:H143	22:B:837:CLA:H112	1.80	0.44
28:B:849:DGD:HAV2	28:B:849:DGD:HAF1	1.67	0.44
22:B:850:CLA:C3D	6:F:152:GLY:HA3	2.47	0.44
8:H:72:MET:HA	12:L:117:LEU:HD21	1.99	0.44
15:3:277:VAL:O	15:3:277:VAL:HG12	2.17	0.44
16:4:41:ARG:HH12	16:4:50:VAL:HG11	1.82	0.44
22:6:311:CLA:H61	22:6:311:CLA:H121	1.99	0.44
13:5:205:THR:HA	13:5:208:ILE:HG22	1.99	0.44
19:9:82:ARG:HG3	22:9:309:CLA:C4C	2.47	0.44
20:0:84:LEU:HD13	22:0:304:CLA:HBB2	1.98	0.44
22:0:311:CLA:H121	24:0:315:LHG:H172	1.99	0.44
1:A:209:GLY:HA3	22:A:813:CLA:HBB1	2.00	0.44
1:A:652:ARG:HB2	2:B:632:ILE:CG2	2.46	0.44
22:A:807:CLA:H171	22:A:807:CLA:H13	1.50	0.44
22:A:830:CLA:H61	22:A:830:CLA:H92	1.65	0.44
22:A:853:CLA:H142	22:A:853:CLA:H111	1.76	0.44
2:B:438:VAL:HG22	22:B:803:CLA:C2	2.47	0.44
12:L:85:SER:HA	12:L:88:LEU:HG	1.98	0.44
14:2:86:LEU:CD2	14:2:205:ILE:HD11	2.47	0.44
16:4:150:ASP:CB	16:4:157:VAL:HG22	2.40	0.44
17:6:45:GLY:O	18:7:149:ASN:ND2	2.49	0.44
17:6:52:LEU:HD21	17:6:59:ASP:HB2	1.97	0.44
17:6:182:LEU:HD21	22:6:310:CLA:O1A	2.17	0.44
17:6:214:CYS:HA	17:6:217:ASP:HB2	1.98	0.44
22:7:303:CLA:H41	22:7:303:CLA:H61	1.41	0.44
16:8:132:LEU:HD21	29:8:305:CHL:CHD	2.47	0.44
22:8:304:CLA:C2B	30:8:317:XAT:H183	2.48	0.44
19:9:164:VAL:HG11	22:9:309:CLA:H12	1.99	0.44
22:A:840:CLA:C4A	22:A:840:CLA:HBA2	2.47	0.44
23:A:842:PQN:H261	23:A:842:PQN:H243	1.72	0.44
2:B:581:PHE:O	2:B:585:ASN:ND2	2.51	0.44
2:B:658:ALA:HB3	22:B:806:CLA:HBB2	1.99	0.44
22:B:836:CLA:H62	22:B:836:CLA:H41	1.63	0.44
22:2:302:CLA:H3A	22:2:302:CLA:CGA	2.48	0.44
22:3:311:CLA:HBB1	22:3:311:CLA:H8	1.99	0.44
16:4:102:LEU:O	16:4:106:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:307:CHL:CMB	25:4:317:8CT:C18	2.83	0.44
13:5:123:ASP:O	13:5:127:LEU:N	2.38	0.44
18:7:51:TYR:CE2	18:7:52:LEU:HG	2.52	0.44
16:8:229:HIS:ND1	16:8:236:ASN:O	2.50	0.44
19:9:69:ARG:NH1	22:9:301:CLA:O2D	2.24	0.44
1:A:20:VAL:HG12	1:A:22:VAL:HG13	2.00	0.44
1:A:193:LEU:HG	1:A:197:GLN:HE21	1.82	0.44
22:A:826:CLA:H91	22:A:826:CLA:H112	1.64	0.44
2:B:61:THR:OG1	2:B:142:LEU:HD13	2.17	0.44
2:B:448:THR:HB	2:B:450:GLU:HG2	2.00	0.44
2:B:477:LEU:HD13	22:B:834:CLA:HMD1	1.99	0.44
22:B:803:CLA:H111	22:B:803:CLA:H91	1.55	0.44
22:B:813:CLA:HBA2	22:B:813:CLA:H3A	1.73	0.44
8:H:110:GLY:O	22:H:201:CLA:H142	2.18	0.44
22:2:304:CLA:H43	25:2:317:8CT:C34	2.47	0.44
22:3:301:CLA:H3A	22:3:301:CLA:CGA	2.48	0.44
17:6:120:ILE:O	17:6:123:ILE:N	2.50	0.44
22:6:310:CLA:H52	30:6:319:XAT:C30	2.43	0.44
22:6:315:CLA:H2	22:6:315:CLA:H61	1.64	0.44
13:5:123:ASP:OD1	13:5:124:ILE:N	2.47	0.44
13:5:180:ARG:HD3	22:5:302:CLA:CHD	2.48	0.44
29:5:301:CHL:H102	22:5:313:CLA:H71	1.98	0.44
20:0:100:TRP:HB2	30:0:314:XAT:H41	1.99	0.44
1:A:217:GLY:C	22:A:814:CLA:HAB	2.43	0.44
1:A:381:PRO:HG3	22:A:819:CLA:HBA1	1.99	0.44
1:A:447:ASN:ND2	2:B:678:LEU:HD21	2.33	0.44
1:A:464:ASN:ND2	1:A:539:MET:HE1	2.33	0.44
2:B:92:TRP:HB2	22:B:810:CLA:HED1	2.00	0.44
2:B:126:THR:HG21	2:B:358:TYR:HD1	1.82	0.44
2:B:224:PRO:HG2	2:B:233:TYR:CZ	2.52	0.44
6:F:90:PHE:O	6:F:94:GLU:HG2	2.18	0.44
6:F:237:THR:HG22	6:F:238:VAL:N	2.30	0.44
11:K:40:LEU:HB2	22:K:105:CLA:C3	2.48	0.44
22:K:102:CLA:HMB1	22:K:102:CLA:HBB1	2.00	0.44
13:1:73:CYS:SG	22:1:302:CLA:HBD	2.57	0.44
22:1:301:CLA:HBC2	29:4:301:CHL:HBB2	1.99	0.44
14:2:99:MET:HE1	14:2:215:CYS:SG	2.58	0.44
22:3:307:CLA:H3A	22:3:307:CLA:HBA2	1.66	0.44
13:5:216:PHE:HD1	22:5:312:CLA:H12	1.82	0.44
30:7:319:XAT:H15	30:7:319:XAT:H201	1.77	0.44
20:0:173:ALA:HA	22:0:311:CLA:HBB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:808:CLA:H2A	22:A:808:CLA:O2D	2.17	0.44
22:A:818:CLA:HBA2	22:A:818:CLA:H3A	1.41	0.44
22:A:826:CLA:H141	22:A:826:CLA:H161	1.73	0.44
2:B:545:LYS:CE	6:F:236:ILE:HG12	2.47	0.44
2:B:655:LEU:CD2	22:B:840:CLA:HAB	2.48	0.44
22:B:813:CLA:CGA	22:B:813:CLA:C1A	2.95	0.44
12:L:36:LEU:HD23	22:L:203:CLA:HBD	1.99	0.44
12:L:71:ARG:C	12:L:72:ASP:OD1	2.60	0.44
22:2:304:CLA:H8	22:2:304:CLA:H122	1.41	0.44
15:3:104:VAL:HG22	15:3:230:ILE:HD11	2.00	0.44
16:4:54:LEU:HD21	16:4:61:ASP:OD1	2.18	0.44
16:4:176:PRO:HG2	22:4:309:CLA:OBD	2.18	0.44
16:4:238:VAL:O	16:4:240:SER:N	2.50	0.44
17:6:159:LEU:HD12	17:6:160:PRO:HD2	1.99	0.44
17:6:232:VAL:HG13	17:6:233:ILE:H	1.82	0.44
29:6:307:CHL:HHC	29:6:307:CHL:HBB1	2.00	0.44
13:5:61:SER:HB2	13:5:67:MET:HB2	1.99	0.44
22:0:307:CLA:H92	22:0:307:CLA:H61	1.68	0.44
1:A:31:PHE:O	1:A:32:GLU:C	2.59	0.44
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.52	0.44
22:A:829:CLA:H72	22:A:829:CLA:H112	1.83	0.44
2:B:71:GLN:NE2	22:B:810:CLA:O1D	2.42	0.44
2:B:203:ARG:NE	2:B:251:GLY:O	2.51	0.44
2:B:345:CYS:HB2	2:B:379:ALA:HB2	1.98	0.44
2:B:609:PHE:O	2:B:613:SER:N	2.49	0.44
6:F:199:ILE:HG22	6:F:200:ILE:HG13	1.98	0.44
8:H:124:ASP:HB3	8:H:127:LEU:CG	2.47	0.44
22:1:312:CLA:H2	22:1:312:CLA:HAA1	2.00	0.44
22:3:301:CLA:H2A	22:3:301:CLA:CED	2.47	0.44
16:4:241:ILE:HD12	16:4:241:ILE:O	2.17	0.44
17:6:159:LEU:HD23	17:6:162:HIS:ND1	2.33	0.44
13:5:192:GLN:HE21	22:5:312:CLA:C4D	2.31	0.44
16:8:43:ILE:HG23	16:8:62:PHE:O	2.18	0.44
20:0:146:PHE:CD1	20:0:151:PRO:HD2	2.53	0.44
1:A:217:GLY:O	22:A:814:CLA:HHC	2.18	0.44
1:A:437:ARG:HH22	4:D:84:GLY:C	2.25	0.44
1:A:439:ARG:NH1	1:A:560:LEU:O	2.50	0.44
2:B:8:PHE:HB2	2:B:34:HIS:ND1	2.33	0.44
2:B:32:GLU:HG3	2:B:42:LEU:HD11	2.00	0.44
2:B:60:TRP:HA	22:B:810:CLA:HAB	2.00	0.44
2:B:233:TYR:O	2:B:253:ALA:HB1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:GLN:O	2:B:406:ASN:ND2	2.51	0.44
22:B:834:CLA:H122	22:B:834:CLA:H161	1.90	0.44
9:I:11:VAL:HA	9:I:14:VAL:HG12	1.99	0.44
25:K:103:8CT:C38	22:K:104:CLA:NB	2.80	0.44
13:1:123:ASP:O	13:1:127:LEU:HB2	2.17	0.44
22:1:308:CLA:H112	22:1:308:CLA:H91	1.60	0.44
17:6:154:PHE:CZ	29:6:316:CHL:HAA1	2.52	0.44
29:9:302:CHL:HBB1	29:9:302:CHL:HHC	2.00	0.44
29:0:301:CHL:H3A	24:0:315:LHG:H321	1.99	0.44
11:K:38:LEU:HB3	22:K:105:CLA:O2A	2.18	0.43
17:6:87:TRP:CE2	22:6:309:CLA:HBC3	2.53	0.43
29:6:306:CHL:HBB2	29:6:307:CHL:CBB	2.48	0.43
24:5:318:LHG:H321	24:5:318:LHG:H352	1.72	0.43
18:7:67:LEU:CD2	22:7:303:CLA:H43	2.45	0.43
16:8:159:VAL:HG12	16:8:160:ASP:N	2.33	0.43
1:A:198:ASN:HD22	22:A:812:CLA:CED	2.31	0.43
22:A:803:CLA:H2A	22:A:803:CLA:O1D	2.19	0.43
22:A:806:CLA:H192	22:A:806:CLA:H161	1.75	0.43
2:B:50:HIS:CE1	22:B:808:CLA:NA	2.85	0.43
22:B:806:CLA:H72	22:B:840:CLA:HBB2	2.00	0.43
22:1:311:CLA:H122	22:1:311:CLA:H161	1.72	0.43
22:1:311:CLA:H41	22:1:311:CLA:H61	1.46	0.43
30:1:314:XAT:H181	30:1:314:XAT:C8	2.48	0.43
30:2:315:XAT:H15	30:2:315:XAT:H201	1.79	0.43
24:2:318:LHG:H142	22:3:313:CLA:HED1	1.99	0.43
22:5:303:CLA:H141	22:5:303:CLA:H161	1.83	0.43
29:7:308:CHL:OMC	22:7:316:CLA:HMC1	2.17	0.43
22:7:312:CLA:H12	22:7:312:CLA:H52	1.85	0.43
24:9:316:LHG:H192	24:9:316:LHG:H361	2.01	0.43
20:0:82:ALA:HA	30:0:314:XAT:H11	2.00	0.43
20:0:93:ASN:HA	20:0:97:LEU:HD23	2.00	0.43
22:0:312:CLA:H92	22:0:312:CLA:H61	1.77	0.43
1:A:346:LEU:HD21	22:A:824:CLA:HBC3	1.99	0.43
2:B:6:PRO:HG2	2:B:13:ALA:HA	1.99	0.43
2:B:182:LEU:HD12	22:B:814:CLA:CHB	2.47	0.43
2:B:222:LEU:HB3	2:B:226:PHE:CD2	2.52	0.43
2:B:272:ASP:OD1	22:B:818:CLA:HHB	2.18	0.43
2:B:438:VAL:HG22	22:B:803:CLA:H2	1.99	0.43
6:F:147:LEU:HD22	6:F:162:ASP:HB2	2.01	0.43
12:L:60:VAL:O	12:L:63:PRO:HD2	2.17	0.43
13:1:154:PRO:HB3	22:1:306:CLA:HBC2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:168:GLN:HE22	22:3:313:CLA:C4D	2.31	0.43
15:3:211:ASN:ND2	15:3:214:ASN:HA	2.33	0.43
15:3:269:ASN:OD1	15:3:270:ILE:N	2.46	0.43
22:3:319:CLA:H41	22:3:319:CLA:H61	1.71	0.43
16:4:146:ARG:HA	29:4:301:CHL:HED1	1.99	0.43
22:6:309:CLA:H3A	22:6:309:CLA:HBA1	1.60	0.43
22:5:312:CLA:H2	22:5:313:CLA:OBD	2.18	0.43
18:7:241:THR:HA	18:7:264:GLN:O	2.18	0.43
22:9:312:CLA:H72	22:9:313:CLA:HMD3	2.00	0.43
29:0:301:CHL:O2A	24:0:315:LHG:H182	2.19	0.43
1:A:97:TYR:HD1	1:A:153:TRP:CZ2	2.36	0.43
1:A:202:MET:HB2	22:A:813:CLA:HBC3	2.00	0.43
1:A:617:TRP:CZ3	1:A:644:ALA:HB2	2.52	0.43
2:B:126:THR:HB	2:B:359:ALA:H	1.83	0.43
22:B:823:CLA:HAB	25:B:846:8CT:C08	2.48	0.43
22:B:834:CLA:H142	22:B:834:CLA:H111	1.72	0.43
5:E:9:VAL:O	5:E:22:ALA:HA	2.18	0.43
12:L:38:ALA:HB2	22:L:203:CLA:OBD	2.19	0.43
12:L:127:LEU:HD21	12:L:133:TRP:CE3	2.53	0.43
13:1:127:LEU:HD11	22:1:304:CLA:C2D	2.49	0.43
15:3:180:ASN:HB3	15:3:183:SER:HB3	2.01	0.43
17:6:249:VAL:HG11	29:6:307:CHL:O2D	2.17	0.43
22:6:318:CLA:H2A	22:6:318:CLA:O2D	2.18	0.43
30:6:320:XAT:H15	30:6:320:XAT:H201	1.65	0.43
19:9:85:MET:HA	19:9:175:ALA:HB1	1.99	0.43
22:9:312:CLA:H72	22:9:312:CLA:H2	2.01	0.43
1:A:379:MET:HE1	22:A:827:CLA:HHC	1.99	0.43
1:A:670:LEU:HB2	1:A:673:TYR:HD2	1.84	0.43
2:B:188:LEU:HB3	22:B:816:CLA:HBB2	1.99	0.43
2:B:493:TRP:HE1	22:B:834:CLA:HED1	1.83	0.43
4:D:137:CYS:SG	4:D:154:PHE:CG	3.08	0.43
16:4:192:SER:O	16:4:196:LYS:HG3	2.17	0.43
13:5:139:GLU:O	13:5:143:ALA:N	2.52	0.43
22:7:310:CLA:CGA	22:7:310:CLA:C4A	2.96	0.43
22:9:306:CLA:H61	22:9:306:CLA:H41	1.81	0.43
1:A:536:SER:HB3	1:A:641:ALA:HA	2.01	0.43
1:A:586:GLY:O	2:B:668:ARG:HD3	2.19	0.43
22:A:838:CLA:O2D	22:A:838:CLA:H2A	2.18	0.43
22:A:840:CLA:H62	22:A:840:CLA:H41	1.80	0.43
2:B:687:LEU:N	12:L:39:TYR:HH	2.16	0.43
22:B:805:CLA:H62	22:B:805:CLA:H2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:809:CLA:H61	22:B:809:CLA:H92	1.72	0.43
3:C:23:THR:O	4:D:134:LYS:HE2	2.18	0.43
10:J:2:GLN:NE2	14:2:74:ASP:OD1	2.51	0.43
22:K:102:CLA:H3A	22:K:102:CLA:HBA1	1.65	0.43
13:1:37:PRO:HG3	16:4:162:ILE:HG21	2.00	0.43
14:2:117:ASP:OD1	14:2:120:LYS:HB2	2.19	0.43
14:2:217:GLY:O	14:2:221:GLN:HG2	2.19	0.43
17:6:215:TRP:HE3	30:6:319:XAT:H21	1.82	0.43
13:5:152:VAL:C	13:5:154:PRO:HD3	2.43	0.43
29:5:301:CHL:C2C	24:5:318:LHG:HC81	2.48	0.43
18:7:56:LEU:HD11	18:7:74:LEU:HD21	2.01	0.43
18:7:197:ASN:HD22	22:7:310:CLA:CBB	2.31	0.43
22:7:302:CLA:HAC2	24:7:322:LHG:HC32	2.01	0.43
16:8:221:GLY:N	16:8:224:ALA:HB3	2.33	0.43
22:0:307:CLA:H13	22:0:307:CLA:H172	1.79	0.43
1:A:48:PRO:HG3	6:F:199:ILE:HD11	2.00	0.43
22:A:806:CLA:H62	22:A:806:CLA:H102	1.81	0.43
2:B:178:HIS:HE1	22:B:814:CLA:NA	2.17	0.43
2:B:302:LYS:HE2	2:B:323:PHE:CD2	2.53	0.43
22:B:833:CLA:H102	6:F:173:MET:HE1	2.01	0.43
3:C:27:GLU:OE2	3:C:44:ARG:NH1	2.47	0.43
13:1:171:LEU:HD13	22:1:308:CLA:O1A	2.18	0.43
22:1:313:CLA:HBA1	22:1:313:CLA:H3A	1.47	0.43
14:2:74:ASP:HB3	14:2:77:MET:HB3	2.01	0.43
15:3:97:SER:HA	15:3:100:ARG:HH21	1.84	0.43
22:3:311:CLA:HBA2	22:3:311:CLA:H3A	1.63	0.43
17:6:114:ILE:HG12	22:6:305:CLA:HAA1	2.01	0.43
17:6:251:PHE:HB3	17:6:256:ILE:HD12	2.00	0.43
29:6:307:CHL:CBA	25:8:301:8CT:C37	2.97	0.43
13:5:92:GLU:HB2	13:5:98:ASN:HA	2.01	0.43
29:5:301:CHL:H111	29:5:301:CHL:H91	1.67	0.43
18:7:81:GLU:OE2	18:7:199:ARG:NH2	2.50	0.43
18:7:105:VAL:HG23	18:7:115:ASN:CG	2.44	0.43
18:7:226:HIS:NE2	22:7:313:CLA:HBA1	2.34	0.43
22:7:318:CLA:HAA2	22:7:318:CLA:HBD	1.99	0.43
16:8:158:ASN:ND2	29:8:307:CHL:HAC1	2.32	0.43
16:8:168:PRO:HG2	16:8:177:GLY:O	2.18	0.43
22:0:302:CLA:HBC1	24:0:315:LHG:H271	2.00	0.43
1:A:394:SER:OG	22:A:828:CLA:HBB	2.18	0.43
22:A:840:CLA:H141	22:F:301:CLA:HMC2	1.99	0.43
2:B:393:PHE:HA	2:B:397:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:ASN:OD1	2:B:452:GLN:HB3	2.18	0.43
2:B:595:HIS:CD2	2:B:623:TYR:CZ	2.88	0.43
22:B:808:CLA:H62	22:B:808:CLA:H2	1.64	0.43
8:H:89:PHE:CD1	12:L:50:VAL:HG21	2.54	0.43
11:K:6:THR:HA	11:K:9:LEU:HD12	2.01	0.43
11:K:38:LEU:C	22:K:105:CLA:H11	2.43	0.43
17:6:123:ILE:O	17:6:127:GLN:N	2.46	0.43
22:6:311:CLA:CBB	25:7:321:8CT:C01	2.96	0.43
18:7:92:VAL:HA	18:7:208:PHE:HE2	1.82	0.43
16:8:44:TRP:CE3	16:8:45:LEU:HB2	2.53	0.43
16:8:51:PRO:HB3	16:8:53:TRP:CH2	2.54	0.43
16:8:193:LEU:HD22	22:8:309:CLA:H3A	2.01	0.43
16:8:211:PHE:CE1	16:8:222:PRO:HB3	2.54	0.43
16:8:236:ASN:O	16:8:237:ASN:ND2	2.51	0.43
22:9:312:CLA:H71	24:9:316:LHG:H181	2.01	0.43
1:A:343:HIS:ND1	1:A:431:LEU:HD12	2.34	0.43
1:A:596:HIS:CE1	2:B:670:TYR:HD1	2.37	0.43
1:A:667:GLY:N	2:B:445:ALA:O	2.41	0.43
22:A:808:CLA:H193	22:A:808:CLA:H162	1.76	0.43
22:A:832:CLA:HAA2	25:B:851:8CT:C17	2.49	0.43
2:B:278:LEU:HD21	22:B:817:CLA:HAB	2.00	0.43
2:B:428:PHE:HE2	22:B:832:CLA:C2D	2.32	0.43
2:B:486:PHE:HA	2:B:494:LEU:HD11	2.01	0.43
2:B:553:PHE:HZ	3:C:52:LYS:NZ	2.16	0.43
2:B:599:LEU:HD11	2:B:623:TYR:HE1	1.84	0.43
22:B:818:CLA:H93	22:B:818:CLA:H62	1.69	0.43
22:B:840:CLA:H42	23:B:842:PQN:H271	2.01	0.43
8:H:131:VAL:O	8:H:134:GLN:HG3	2.18	0.43
22:1:301:CLA:H3A	22:1:301:CLA:CGA	2.49	0.43
17:6:100:LEU:CD1	17:6:101:VAL:HG23	2.46	0.43
17:6:153:ILE:HG13	17:6:154:PHE:N	2.34	0.43
29:6:302:CHL:H91	29:6:302:CHL:H111	1.64	0.43
13:5:178:ASN:HD22	22:5:309:CLA:HAB	1.83	0.43
18:7:153:VAL:O	18:7:153:VAL:HG13	2.18	0.43
18:7:208:PHE:CD1	18:7:219:PRO:HB3	2.54	0.43
18:7:260:LEU:HD21	22:7:317:CLA:C4C	2.49	0.43
19:9:189:VAL:HG11	22:9:312:CLA:HED1	2.01	0.43
22:9:310:CLA:HBC3	24:9:316:LHG:HC62	2.00	0.43
20:0:141:CYS:HB3	20:0:144:LEU:HD12	2.00	0.43
20:0:189:VAL:HA	20:0:192:LEU:HD12	1.99	0.43
29:0:301:CHL:C3B	24:0:315:LHG:H301	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PRO:HB2	1:A:53:TRP:HH2	1.84	0.43
1:A:439:ARG:NH2	1:A:564:SER:O	2.50	0.43
2:B:632:ILE:HD11	22:B:805:CLA:HBC1	2.00	0.43
22:B:809:CLA:H3A	22:B:809:CLA:HBA1	1.42	0.43
7:G:3:SER:HA	7:G:6:LEU:HB2	2.00	0.43
12:L:9:PRO:HA	12:L:19:LEU:HB2	2.00	0.43
12:L:29:VAL:HG13	22:L:201:CLA:H43	2.00	0.43
22:L:201:CLA:H2	22:L:203:CLA:H72	1.99	0.43
22:1:303:CLA:C1B	25:1:316:8CT:C36	2.97	0.43
17:6:46:SER:OG	17:6:47:THR:N	2.52	0.43
22:6:323:CLA:HBB1	31:8:319:LMG:H162	2.00	0.43
16:8:146:ARG:NE	29:8:307:CHL:OMC	2.40	0.43
22:8:310:CLA:C4A	31:8:319:LMG:HC4	2.49	0.43
22:A:825:CLA:H161	22:A:825:CLA:H141	1.64	0.42
22:A:853:CLA:H71	22:A:853:CLA:H112	1.75	0.42
2:B:417:ALA:O	2:B:421:HIS:HD2	2.02	0.42
2:B:438:VAL:HG13	22:B:803:CLA:H62	2.01	0.42
15:3:222:MET:HG3	15:3:226:LYS:HE3	2.00	0.42
22:4:314:CLA:H61	22:4:314:CLA:H2	1.85	0.42
13:5:170:GLU:OE2	13:5:174:LYS:HD2	2.18	0.42
24:5:318:LHG:H341	24:5:318:LHG:H172	1.99	0.42
31:5:319:LMG:O4	31:5:319:LMG:O5	2.34	0.42
18:7:42:TRP:CD1	18:7:42:TRP:H	2.37	0.42
18:7:209:ALA:O	18:7:213:GLN:HB2	2.19	0.42
19:9:84:ALA:HB2	30:9:315:XAT:C13	2.48	0.42
1:A:371:ILE:HG12	22:A:826:CLA:HED3	2.00	0.42
22:A:805:CLA:H3A	22:A:805:CLA:HBA1	1.71	0.42
22:A:810:CLA:H111	22:A:810:CLA:H152	1.77	0.42
2:B:177:HIS:O	2:B:181:GLY:N	2.48	0.42
4:D:189:ARG:HB2	4:D:193:GLU:HB2	2.00	0.42
8:H:115:LEU:HD21	9:I:13:LEU:HB2	2.01	0.42
30:2:316:XAT:H15	30:2:316:XAT:H201	1.83	0.42
17:6:141:ASP:OD2	29:6:308:CHL:HBC1	2.18	0.42
13:5:203:CYS:HA	13:5:206:GLU:HB3	2.00	0.42
18:7:87:TRP:CE2	29:7:308:CHL:HED2	2.54	0.42
22:9:303:CLA:O2D	22:9:303:CLA:H2A	2.18	0.42
1:A:375:HIS:HE1	22:A:827:CLA:NB	2.17	0.42
22:A:810:CLA:H62	22:A:810:CLA:H2	1.80	0.42
23:A:842:PQN:H292	23:A:842:PQN:H262	1.84	0.42
2:B:44:GLN:NE2	2:B:162:GLN:HG3	2.35	0.42
2:B:686:PRO:HG2	22:L:203:CLA:H41	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:814:CLA:H142	22:B:814:CLA:H112	1.75	0.42
22:B:829:CLA:HHC	22:B:829:CLA:CBB	2.42	0.42
4:D:98:GLU:OE1	4:D:156:ARG:HD3	2.19	0.42
22:H:201:CLA:H2	22:H:201:CLA:H61	1.79	0.42
12:L:91:ILE:O	12:L:94:THR:OG1	2.37	0.42
13:1:80:TRP:CD1	22:1:307:CLA:HMD3	2.54	0.42
15:3:229:GLU:HG3	22:3:308:CLA:C1B	2.49	0.42
16:4:202:ARG:HD2	22:4:302:CLA:C4C	2.49	0.42
29:4:307:CHL:O1A	22:4:309:CLA:HHD	2.19	0.42
16:8:115:THR:H	16:8:119:ASN:HD21	1.66	0.42
16:8:172:ILE:HB	16:8:175:TYR:O	2.20	0.42
1:A:563:ARG:O	1:A:571:LYS:HB3	2.20	0.42
22:B:806:CLA:H161	22:B:806:CLA:H141	1.66	0.42
22:B:840:CLA:HMC1	25:B:848:8CT:C22	2.49	0.42
4:D:104:TRP:HD1	4:D:105:GLU:O	2.01	0.42
8:H:114:LEU:HG	22:H:201:CLA:H152	2.02	0.42
14:2:72:ALA:HB1	14:2:78:LEU:HD13	2.01	0.42
14:2:99:MET:HG2	14:2:115:TRP:CB	2.50	0.42
30:4:316:XAT:H27	30:4:316:XAT:H30	1.70	0.42
17:6:119:ASN:HB3	17:6:120:ILE:H	1.61	0.42
13:5:147:ASP:CG	13:5:150:LYS:H	2.27	0.42
18:7:182:ALA:HB3	22:7:310:CLA:HAA2	2.01	0.42
22:7:306:CLA:HBC2	22:7:307:CLA:HBC3	2.01	0.42
19:9:77:GLU:HB2	22:9:303:CLA:C1B	2.49	0.42
20:0:68:LEU:HD12	20:0:69:ALA:N	2.34	0.42
1:A:40:PHE:CD1	1:A:41:SER:N	2.87	0.42
1:A:79:PHE:HA	1:A:82:HIS:HD2	1.85	0.42
1:A:312:ILE:HG21	22:A:817:CLA:H162	2.02	0.42
1:A:484:LEU:O	1:A:535:THR:HG22	2.18	0.42
2:B:5:PHE:O	2:B:7:LYS:N	2.52	0.42
2:B:209:TRP:NE1	22:B:815:CLA:H11	2.35	0.42
25:J:104:8CT:C37	25:J:104:8CT:C32	2.98	0.42
22:K:105:CLA:HBB	22:K:105:CLA:HMA1	1.85	0.42
12:L:18:MET:HG2	12:L:19:LEU:N	2.34	0.42
12:L:127:LEU:HD21	12:L:133:TRP:HE3	1.84	0.42
13:1:61:SER:OG	13:1:67:MET:HB2	2.19	0.42
13:1:210:ASP:O	13:1:214:ALA:HB3	2.20	0.42
30:4:315:XAT:H31	30:4:315:XAT:H391	1.79	0.42
22:6:323:CLA:H3A	22:6:323:CLA:HBA1	1.55	0.42
13:5:35:TRP:CG	13:5:36:LEU:N	2.88	0.42
31:5:319:LMG:H331	31:5:319:LMG:H152	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:109:GLU:HA	22:7:307:CLA:O1D	2.19	0.42
18:7:208:PHE:CE1	30:7:319:XAT:H362	2.54	0.42
16:8:88:ARG:NH1	16:8:175:TYR:CD2	2.88	0.42
1:A:557:LYS:HG3	1:A:561:TYR:HD2	1.85	0.42
2:B:509:PHE:CD1	22:B:827:CLA:HBC2	2.53	0.42
2:B:582:TRP:O	2:B:586:THR:HG22	2.19	0.42
22:B:805:CLA:H52	22:B:805:CLA:H8	1.81	0.42
23:B:842:PQN:H241	23:B:842:PQN:H262	1.78	0.42
3:C:28:MET:HB3	3:C:38:GLN:HE21	1.84	0.42
11:K:2:PHE:CE2	11:K:8:ASN:HB2	2.53	0.42
30:1:314:XAT:H31	30:1:314:XAT:H391	1.47	0.42
22:3:312:CLA:O2D	22:3:312:CLA:H2A	2.19	0.42
16:4:97:MET:HG2	16:4:117:TRP:HB2	2.01	0.42
29:4:305:CHL:C4A	25:4:317:8CT:C38	2.95	0.42
22:6:305:CLA:C1B	25:6:321:8CT:C33	2.97	0.42
13:5:61:SER:HA	13:5:70:MET:HE1	2.02	0.42
18:7:226:HIS:ND1	22:7:313:CLA:HAA2	2.35	0.42
16:8:122:ALA:N	29:8:306:CHL:O1D	2.53	0.42
1:A:131:ILE:HD11	1:A:667:GLY:O	2.20	0.42
2:B:29:HIS:CE1	22:B:807:CLA:NB	2.87	0.42
22:B:827:CLA:H41	22:B:827:CLA:H62	1.76	0.42
22:B:832:CLA:H143	22:B:832:CLA:H112	1.74	0.42
22:B:832:CLA:HAA1	22:B:832:CLA:HBD	2.00	0.42
6:F:78:ILE:HD13	6:F:78:ILE:HA	1.87	0.42
11:K:21:ALA:HB3	11:K:26:LEU:CD2	2.43	0.42
11:K:35:THR:HG22	11:K:36:SER:N	2.34	0.42
13:1:147:ASP:OD1	13:1:148:MET:N	2.53	0.42
14:2:179:PRO:HB2	14:2:184:PHE:HD2	1.85	0.42
22:2:303:CLA:H91	22:2:303:CLA:H111	1.75	0.42
15:3:121:GLU:HG2	15:3:255:TYR:HB3	2.02	0.42
15:3:196:LEU:HD23	15:3:196:LEU:HA	1.83	0.42
16:4:172:ILE:HD12	16:4:173:PRO:O	2.19	0.42
22:4:314:CLA:H3A	22:4:314:CLA:HBA1	1.57	0.42
17:6:39:ARG:HB2	17:6:40:PRO:HD2	2.02	0.42
17:6:159:LEU:HD22	17:6:168:GLY:CA	2.48	0.42
22:5:302:CLA:H51	22:5:303:CLA:H3A	2.02	0.42
22:8:312:CLA:HMD1	22:8:315:CLA:HBC3	2.02	0.42
22:9:303:CLA:H2	30:9:315:XAT:O24	2.20	0.42
20:0:33:ARG:O	20:0:35:MET:HG2	2.20	0.42
20:0:223:TRP:HB3	20:0:224:PRO:HD3	2.01	0.42
1:A:699:GLN:O	1:A:703:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:820:CLA:HMB3	22:A:820:CLA:HBB1	2.00	0.42
22:A:836:CLA:HBC2	22:A:836:CLA:HHD	2.02	0.42
2:B:95:HIS:HE1	22:H:201:CLA:NA	2.17	0.42
2:B:207:VAL:O	2:B:208:ARG:HD3	2.20	0.42
2:B:273:MET:O	2:B:276:HIS:HB3	2.20	0.42
2:B:559:CYS:HB3	27:B:802:SF4:S3	2.59	0.42
22:B:824:CLA:H112	22:B:824:CLA:H143	1.82	0.42
22:B:827:CLA:H151	22:B:827:CLA:H18	1.77	0.42
22:B:829:CLA:H192	22:B:829:CLA:H162	1.81	0.42
7:G:22:VAL:HG13	7:G:23:PHE:N	2.35	0.42
8:H:124:ASP:CB	8:H:127:LEU:CD1	2.73	0.42
11:K:18:CYS:SG	22:K:105:CLA:HBB2	2.59	0.42
22:K:105:CLA:H2	22:K:105:CLA:CMA	2.50	0.42
22:L:202:CLA:H203	22:L:202:CLA:H122	2.01	0.42
16:4:41:ARG:NH1	16:4:50:VAL:HG11	2.35	0.42
22:4:314:CLA:O2D	22:4:314:CLA:H2A	2.19	0.42
29:6:302:CHL:H101	22:6:314:CLA:C1D	2.50	0.42
22:6:310:CLA:H62	22:6:310:CLA:H41	1.69	0.42
18:7:188:GLU:HA	18:7:191:LYS:HB2	2.02	0.42
30:7:319:XAT:H11	30:7:319:XAT:H191	1.52	0.42
2:B:53:GLN:HE22	22:B:809:CLA:C4D	2.32	0.42
2:B:397:ASP:HA	4:D:198:ILE:CD1	2.49	0.42
2:B:662:MET:HE3	22:B:840:CLA:HBC2	2.02	0.42
22:B:828:CLA:H141	22:B:830:CLA:H162	2.02	0.42
22:B:850:CLA:HBC2	6:F:151:PRO:HG2	2.01	0.42
11:K:31:ASN:C	11:K:43:LYS:HA	2.45	0.42
13:1:31:ARG:HB2	13:1:52:ASN:O	2.20	0.42
22:1:301:CLA:HBB2	30:1:315:XAT:H34	2.02	0.42
15:3:68:LEU:HD12	15:3:84:LEU:HD22	2.02	0.42
16:4:157:VAL:HG11	29:4:307:CHL:HMC	2.02	0.42
17:6:126:PHE:HD1	22:8:313:CLA:HBA1	1.83	0.42
17:6:233:ILE:HG12	17:6:238:ALA:HB1	2.02	0.42
29:5:301:CHL:C1C	24:5:318:LHG:HC81	2.49	0.42
16:8:166:LYS:HE3	16:8:179:ILE:N	2.32	0.42
19:9:178:ALA:HA	22:9:312:CLA:CBB	2.49	0.42
20:0:36:TRP:CD1	20:0:56:TYR:HB2	2.55	0.42
20:0:52:GLY:H	20:0:161:LEU:HD12	1.85	0.42
1:A:474:GLN:HG3	1:A:475:ASP:OD1	2.20	0.42
22:A:806:CLA:H12	22:A:806:CLA:HBA2	1.75	0.42
22:A:809:CLA:H162	22:A:809:CLA:H141	1.75	0.42
2:B:5:PHE:HB3	2:B:20:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ILE:HG12	2:B:113:VAL:HG21	2.02	0.42
2:B:680:TRP:CE2	2:B:684:ARG:HD2	2.54	0.42
22:B:813:CLA:H93	22:9:301:CLA:O2A	2.20	0.42
5:E:39:VAL:HG12	5:E:40:ARG:H	1.85	0.42
7:G:22:VAL:HG13	7:G:23:PHE:CD2	2.55	0.42
7:G:69:VAL:HA	7:G:72:LEU:HD12	2.01	0.42
10:J:24:SER:HA	25:J:101:8CT:C27	2.49	0.42
13:1:80:TRP:CE2	22:1:306:CLA:HED2	2.55	0.42
13:1:134:LEU:HD13	22:1:304:CLA:H51	2.02	0.42
14:2:46:TRP:CE3	14:2:47:TYR:HB2	2.55	0.42
16:4:144:GLU:OE2	16:4:147:ARG:NH2	2.44	0.42
17:6:187:LEU:HB3	17:6:191:ARG:HD3	2.01	0.42
20:0:48:GLY:N	20:0:53:ASP:OD2	2.53	0.42
1:A:126:ILE:HG23	1:A:127:VAL:HG23	2.01	0.41
1:A:379:MET:HG3	1:A:379:MET:O	2.19	0.41
22:A:819:CLA:H3A	22:A:819:CLA:HBA2	1.31	0.41
22:A:827:CLA:H61	22:A:827:CLA:H2	1.67	0.41
22:A:828:CLA:H13	22:A:828:CLA:H102	1.27	0.41
22:A:837:CLA:H162	22:A:837:CLA:H121	1.75	0.41
2:B:92:TRP:O	2:B:93:ASP:C	2.62	0.41
2:B:494:LEU:HD23	2:B:494:LEU:HA	1.89	0.41
2:B:608:GLN:O	2:B:612:SER:OG	2.37	0.41
22:B:810:CLA:H92	22:B:810:CLA:H61	1.81	0.41
22:B:828:CLA:O1D	22:B:829:CLA:HBB	2.20	0.41
11:K:3:ILE:HA	11:K:8:ASN:HD22	1.85	0.41
22:1:307:CLA:HBA2	22:1:307:CLA:H3A	1.39	0.41
14:2:86:LEU:HB3	14:2:90:ARG:HH12	1.85	0.41
14:2:189:LEU:HD22	22:2:309:CLA:CGA	2.50	0.41
29:3:306:CHL:HMB2	25:3:316:8CT:C22	2.48	0.41
16:4:199:LYS:HE2	16:4:199:LYS:HB2	1.79	0.41
22:6:305:CLA:C4B	30:6:320:XAT:H163	2.50	0.41
22:6:317:CLA:HBC3	22:6:318:CLA:CHC	2.50	0.41
18:7:142:ARG:HH22	18:7:153:VAL:HG21	1.85	0.41
22:8:310:CLA:H2	22:8:311:CLA:C3D	2.50	0.41
19:9:165:GLU:O	19:9:168:GLU:HB3	2.20	0.41
20:0:131:ARG:NH2	20:0:132:TYR:OH	2.53	0.41
1:A:237:VAL:HG12	1:A:238:ASP:H	1.85	0.41
1:A:267:LYS:HD2	1:A:267:LYS:HA	1.86	0.41
1:A:666:TYR:HE2	2:B:617:MET:HG2	1.84	0.41
1:A:690:PHE:HA	23:A:842:PQN:O1	2.20	0.41
22:A:817:CLA:H2	22:K:101:CLA:HED1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:833:CLA:H203	22:A:833:CLA:H141	2.01	0.41
2:B:222:LEU:HD11	22:B:816:CLA:C3D	2.51	0.41
2:B:236:ASN:HD22	2:B:252:ASP:HB3	1.85	0.41
2:B:381:PHE:CE1	2:B:583:MET:HE1	2.55	0.41
22:B:824:CLA:HBC3	25:B:846:8CT:C26	2.48	0.41
22:B:837:CLA:H3A	22:B:837:CLA:HBA2	1.74	0.41
3:C:9:ASP:OD2	5:E:34:LYS:NZ	2.53	0.41
4:D:195:VAL:O	4:D:208:PRO:HB3	2.21	0.41
22:H:201:CLA:H203	22:H:201:CLA:H161	1.81	0.41
11:K:34:ALA:CA	22:K:105:CLA:H41	2.48	0.41
22:L:202:CLA:H3A	22:L:202:CLA:CGA	2.45	0.41
13:1:85:VAL:HG11	30:1:314:XAT:C11	2.50	0.41
22:1:308:CLA:CGA	22:1:308:CLA:C4A	2.98	0.41
14:2:77:MET:HG2	14:2:81:TRP:NE1	2.35	0.41
14:2:189:LEU:HD23	14:2:190:ALA:H	1.85	0.41
30:2:315:XAT:H27	30:2:315:XAT:H371	1.81	0.41
15:3:230:ILE:O	15:3:233:GLY:N	2.54	0.41
17:6:76:TRP:CE2	22:6:309:CLA:HED1	2.56	0.41
17:6:223:PHE:CD2	18:7:123:LEU:HD22	2.50	0.41
17:6:227:ILE:HD12	22:6:313:CLA:HMD3	2.01	0.41
22:5:307:CLA:HED3	22:5:309:CLA:HAC2	2.01	0.41
22:7:317:CLA:H2	22:7:317:CLA:O1D	2.20	0.41
22:8:315:CLA:H152	22:8:315:CLA:C2	2.50	0.41
22:9:309:CLA:C2	30:9:314:XAT:H7	2.50	0.41
22:0:310:CLA:H3A	22:0:310:CLA:HBA1	1.24	0.41
1:A:268:PRO:HG2	1:A:277:TYR:CZ	2.56	0.41
1:A:723:LEU:HD22	1:A:727:GLN:HG2	2.01	0.41
22:A:806:CLA:H172	22:A:829:CLA:HBB2	2.02	0.41
22:A:807:CLA:H8	22:A:807:CLA:H51	1.85	0.41
22:A:813:CLA:H142	22:A:813:CLA:C2B	2.51	0.41
22:A:820:CLA:CBB	25:K:103:8CT:C40	2.98	0.41
22:A:822:CLA:H2A	11:K:34:ALA:HB3	2.02	0.41
22:A:834:CLA:NB	25:A:849:8CT:C07	2.83	0.41
22:A:841:CLA:H203	22:A:841:CLA:H162	1.79	0.41
2:B:605:ASN:HB3	2:B:608:GLN:OE1	2.19	0.41
2:B:683:GLU:HG2	4:D:92:ARG:NH1	2.28	0.41
22:B:817:CLA:H93	22:B:817:CLA:H61	1.75	0.41
3:C:3:HIS:HD2	3:C:48:CYS:O	2.04	0.41
4:D:109:GLU:HG2	4:D:123:ARG:C	2.45	0.41
6:F:190:GLY:O	6:F:191:GLU:HG3	2.20	0.41
11:K:35:THR:HG22	11:K:36:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:311:CLA:H111	22:1:311:CLA:H72	1.63	0.41
16:4:207:ALA:HB1	30:4:315:XAT:H181	2.02	0.41
16:4:239:TRP:HA	16:4:244:ALA:HB3	2.02	0.41
29:6:302:CHL:HAA1	24:6:322:LHG:H122	2.01	0.41
18:7:86:ARG:HB3	22:7:310:CLA:CAC	2.50	0.41
18:7:144:TRP:HB2	22:7:309:CLA:CMA	2.50	0.41
18:7:235:ILE:HG13	22:7:313:CLA:CAD	2.50	0.41
18:7:241:THR:HB	18:7:243:VAL:HG13	2.02	0.41
22:8:302:CLA:HAB	30:8:317:XAT:H32	2.03	0.41
30:9:315:XAT:H15	30:9:315:XAT:H201	1.76	0.41
1:A:237:VAL:HG12	1:A:238:ASP:N	2.36	0.41
1:A:377:TYR:HE1	1:A:619:MET:CE	2.34	0.41
22:A:809:CLA:H91	22:A:809:CLA:H111	1.88	0.41
22:A:837:CLA:H41	22:A:837:CLA:H62	1.67	0.41
2:B:77:TRP:CD2	2:B:121:TYR:HE1	2.38	0.41
2:B:261:PHE:O	2:B:269:TRP:NE1	2.54	0.41
2:B:302:LYS:HE2	2:B:302:LYS:HB3	1.84	0.41
2:B:346:SER:OG	22:B:826:CLA:OBD	2.38	0.41
2:B:693:TRP:HE3	22:B:839:CLA:HMD3	1.85	0.41
22:B:833:CLA:HBA1	22:B:833:CLA:H3A	1.87	0.41
24:B:852:LHG:O3	24:B:852:LHG:O1	2.38	0.41
13:1:82:MET:HB3	30:1:314:XAT:C40	2.50	0.41
14:2:43:ARG:HA	14:2:44:PRO:HD3	1.83	0.41
22:2:308:CLA:HHC	22:2:308:CLA:CBB	2.50	0.41
22:3:307:CLA:HBB1	22:3:313:CLA:HBB1	2.03	0.41
22:3:308:CLA:HAB	30:3:314:XAT:C40	2.50	0.41
30:3:315:XAT:H35	30:3:315:XAT:H401	1.91	0.41
16:4:60:GLY:O	22:4:302:CLA:HED3	2.21	0.41
30:6:320:XAT:H23	30:6:320:XAT:H373	1.83	0.41
22:5:302:CLA:H72	30:5:316:XAT:H30	2.02	0.41
30:5:316:XAT:H15	30:5:316:XAT:H201	1.91	0.41
22:7:313:CLA:O1D	22:7:313:CLA:H2A	2.21	0.41
16:8:94:LEU:HG	16:8:211:PHE:CE2	2.55	0.41
16:8:157:VAL:O	16:8:159:VAL:HG23	2.21	0.41
19:9:200:HIS:ND1	19:9:207:GLN:O	2.51	0.41
20:0:195:HIS:ND1	22:0:311:CLA:HAA2	2.36	0.41
22:A:827:CLA:H111	22:A:827:CLA:H151	1.39	0.41
2:B:41:THR:HA	2:B:44:GLN:HG2	2.02	0.41
22:B:817:CLA:H43	7:G:88:THR:HG22	2.02	0.41
22:B:826:CLA:HMB3	22:B:826:CLA:HBB1	2.01	0.41
22:1:301:CLA:HED2	22:1:301:CLA:H2A	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:310:CLA:O2D	22:1:310:CLA:HBA2	2.20	0.41
14:2:173:THR:HG22	14:2:178:TYR:O	2.20	0.41
15:3:274:TRP:C	15:3:276:SER:N	2.78	0.41
17:6:176:PRO:HG2	22:6:310:CLA:H42	2.02	0.41
22:5:302:CLA:CMB	22:5:303:CLA:HBA2	2.50	0.41
16:8:161:PRO:HD2	16:8:166:LYS:H	1.85	0.41
29:8:306:CHL:HBB1	29:8:306:CHL:HHC	2.03	0.41
1:A:104:SER:HA	1:A:120:ALA:HA	2.03	0.41
1:A:291:ASN:HB3	1:A:383:PRO:HA	2.02	0.41
22:A:822:CLA:H2	22:K:105:CLA:HBB	2.03	0.41
22:A:827:CLA:H62	22:A:827:CLA:H102	1.93	0.41
22:A:829:CLA:H18	22:A:829:CLA:H152	1.85	0.41
2:B:130:ARG:NH2	2:B:201:GLU:OE2	2.54	0.41
2:B:187:SER:OG	2:B:277:HIS:O	2.37	0.41
2:B:233:TYR:HB3	2:B:254:ILE:HG13	2.02	0.41
2:B:277:HIS:HE1	22:B:819:CLA:NA	2.19	0.41
22:B:801:CLA:H92	22:B:801:CLA:H62	1.66	0.41
22:B:803:CLA:HMB3	22:B:805:CLA:H202	2.01	0.41
7:G:8:ILE:HD11	7:G:86:LEU:HD12	2.03	0.41
12:L:64:PHE:HB3	12:L:82:GLY:HA2	2.02	0.41
22:1:306:CLA:H141	22:1:306:CLA:H162	1.57	0.41
14:2:139:LEU:HD23	22:4:313:CLA:O2A	2.20	0.41
22:2:309:CLA:H3A	22:2:309:CLA:O1A	2.20	0.41
22:2:312:CLA:H2A	22:2:312:CLA:O1D	2.21	0.41
16:4:222:PRO:O	16:4:226:TRP:N	2.33	0.41
17:6:98:GLN:HE22	22:6:305:CLA:CGD	2.33	0.41
17:6:192:LEU:HD21	30:6:319:XAT:H191	2.02	0.41
18:7:205:TRP:O	18:7:208:PHE:HB2	2.21	0.41
22:7:313:CLA:HBA2	22:7:313:CLA:H3A	1.31	0.41
30:7:319:XAT:H373	30:7:319:XAT:H23	1.63	0.41
19:9:105:GLU:O	19:9:108:GLN:HB3	2.20	0.41
20:0:155:ARG:HH22	20:0:162:LYS:CD	2.30	0.41
1:A:252:ARG:HH21	15:3:277:VAL:HB	1.84	0.41
22:A:814:CLA:HBA1	22:A:814:CLA:H3A	1.92	0.41
22:A:817:CLA:O2D	22:A:817:CLA:H2A	2.20	0.41
22:A:839:CLA:H111	22:A:839:CLA:H142	1.79	0.41
2:B:432:HIS:O	2:B:436:LEU:HG	2.20	0.41
2:B:461:GLN:HG3	2:B:512:ILE:HD11	2.02	0.41
2:B:661:PHE:HB2	22:B:806:CLA:HMC2	2.00	0.41
11:K:74:ILE:HA	22:K:101:CLA:HBB1	2.02	0.41
22:2:302:CLA:H61	22:2:302:CLA:H41	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:314:XAT:H15	30:3:314:XAT:H201	1.52	0.41
16:4:140:MET:O	16:4:143:ALA:N	2.54	0.41
29:4:301:CHL:HAA1	29:4:301:CHL:HBD	2.03	0.41
17:6:267:PRO:HB3	22:6:318:CLA:CBB	2.51	0.41
18:7:260:LEU:HD21	22:7:317:CLA:C3C	2.51	0.41
24:9:316:LHG:H111	24:9:316:LHG:HC82	1.66	0.41
20:0:64:ASN:N	20:0:65:PRO:HD3	2.35	0.41
20:0:189:VAL:HG22	20:0:192:LEU:HD12	2.02	0.41
22:M:101:CLA:CED	22:M:101:CLA:H2A	2.50	0.41
1:A:368:LEU:O	1:A:372:VAL:HG23	2.20	0.41
1:A:397:THR:O	1:A:401:TRP:HD1	2.04	0.41
1:A:465:ASP:OD2	1:A:647:ILE:HB	2.21	0.41
22:A:801:CLA:H202	22:A:801:CLA:H162	1.87	0.41
22:A:802:CLA:H2	2:B:655:LEU:HD13	2.02	0.41
2:B:388:ALA:O	2:B:391:ALA:N	2.54	0.41
2:B:662:MET:HB2	22:B:806:CLA:C1C	2.50	0.41
22:B:815:CLA:H102	22:B:815:CLA:H61	1.65	0.41
12:L:40:ARG:HH22	22:L:202:CLA:C3C	2.34	0.41
13:1:31:ARG:HH22	13:1:54:GLY:HA3	1.85	0.41
13:1:102:ALA:O	13:1:106:VAL:HG23	2.20	0.41
14:2:90:ARG:HD2	29:2:307:CHL:OBD	2.20	0.41
14:2:214:SER:O	14:2:217:GLY:N	2.50	0.41
15:3:57:LEU:O	15:3:58:PHE:C	2.63	0.41
16:4:81:GLN:HE21	16:4:147:ARG:HH11	1.69	0.41
17:6:110:ALA:O	17:6:112:THR:HG23	2.21	0.41
22:6:304:CLA:H92	22:6:304:CLA:H41	2.02	0.41
13:5:106:VAL:HB	13:5:110:GLY:O	2.21	0.41
29:5:301:CHL:HBB1	29:5:301:CHL:CHC	2.45	0.41
22:5:311:CLA:CGA	22:5:311:CLA:H3A	2.51	0.41
25:5:317:8CT:C38	25:5:317:8CT:C28	2.99	0.41
31:5:319:LMG:H242	31:5:319:LMG:H272	1.68	0.41
29:9:302:CHL:C1C	24:9:316:LHG:HC81	2.51	0.41
29:0:306:CHL:HBC3	29:0:306:CHL:HMC	2.02	0.41
1:A:628:SER:OG	1:A:632:VAL:N	2.54	0.41
1:A:662:VAL:HG13	1:A:663:ILE:HG13	2.02	0.41
22:A:803:CLA:H101	10:J:16:PHE:HD1	1.85	0.41
22:A:807:CLA:HMB3	22:A:808:CLA:H3A	2.03	0.41
22:A:831:CLA:HAA1	12:L:7:ILE:CD1	2.51	0.41
22:A:841:CLA:H72	22:A:841:CLA:H111	1.64	0.41
24:A:844:LHG:H281	24:A:844:LHG:H252	1.87	0.41
2:B:92:TRP:O	2:B:92:TRP:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ALA:HA	2:B:256:THR:CG2	2.50	0.41
2:B:243:ILE:HD12	2:B:264:GLN:HE21	1.84	0.41
2:B:658:ALA:O	22:B:806:CLA:HAB	2.21	0.41
22:B:823:CLA:HBA2	22:B:823:CLA:H11	1.78	0.41
22:B:826:CLA:HAA2	22:B:827:CLA:OBD	2.20	0.41
3:C:11:CYS:HB2	3:C:39:ILE:CD1	2.51	0.41
3:C:55:GLU:OE2	3:C:66:ARG:HD3	2.21	0.41
4:D:102:ILE:HG12	4:D:137:CYS:SG	2.61	0.41
6:F:202:ASP:HA	26:J:102:HTG:O2	2.21	0.41
8:H:103:ARG:HG2	8:H:107:PHE:CE2	2.56	0.41
8:H:113:ALA:O	22:H:201:CLA:H91	2.21	0.41
13:1:84:ALA:HA	22:1:303:CLA:HBB1	2.03	0.41
29:2:305:CHL:HBC2	29:2:306:CHL:HHD	2.03	0.41
15:3:105:ILE:HD12	22:3:307:CLA:HED2	2.03	0.41
30:3:315:XAT:H11	30:3:315:XAT:H191	1.98	0.41
22:3:319:CLA:H142	22:3:319:CLA:H112	1.86	0.41
16:4:147:ARG:NH2	22:4:308:CLA:O1D	2.42	0.41
16:4:179:ILE:HA	13:5:58:LEU:HD22	2.03	0.41
16:4:243:LEU:HD12	16:4:244:ALA:N	2.36	0.41
17:6:188:LYS:HD2	22:6:311:CLA:C3D	2.51	0.41
18:7:109:GLU:C	18:7:111:GLY:N	2.76	0.41
18:7:182:ALA:CB	22:7:310:CLA:HAA2	2.51	0.41
18:7:195:ILE:HD13	18:7:195:ILE:HA	1.88	0.41
18:7:235:ILE:HG13	22:7:313:CLA:C3D	2.50	0.41
22:7:304:CLA:OBD	22:7:309:CLA:HBA2	2.21	0.41
22:7:317:CLA:H12	22:7:317:CLA:O2D	2.20	0.41
16:8:166:LYS:HE2	16:8:168:PRO:CG	2.37	0.41
16:8:238:VAL:HG13	16:8:239:TRP:HD1	1.83	0.41
29:8:314:CHL:HBB1	29:8:314:CHL:CHC	2.46	0.41
30:8:317:XAT:H35	30:8:317:XAT:H401	1.70	0.41
19:9:69:ARG:NH1	22:9:301:CLA:CGD	2.83	0.41
20:0:100:TRP:CE2	20:0:101:TRP:HE3	2.39	0.41
20:0:124:PHE:CZ	22:0:305:CLA:HAC2	2.56	0.41
20:0:162:LYS:NZ	22:0:309:CLA:HBD	2.36	0.41
22:0:311:CLA:H62	22:0:311:CLA:H93	1.80	0.41
1:A:267:LYS:O	1:A:271:THR:N	2.31	0.41
1:A:460:LEU:HD22	1:A:477:PHE:CE2	2.55	0.41
1:A:462:ILE:HG23	22:A:802:CLA:H61	2.03	0.41
22:A:832:CLA:H72	22:A:832:CLA:H111	1.83	0.41
2:B:438:VAL:HG12	22:B:833:CLA:HAC1	2.03	0.41
2:B:577:TYR:OH	2:B:664:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:718:ILE:HD12	28:B:849:DGD:HBV2	2.02	0.41
22:B:814:CLA:H2	22:B:814:CLA:H61	1.81	0.41
22:B:824:CLA:HBB	22:B:841:CLA:O1D	2.21	0.41
22:B:830:CLA:H42	28:B:849:DGD:HB42	2.02	0.41
22:B:837:CLA:HMB1	22:B:837:CLA:HBB1	2.03	0.41
23:B:842:PQN:H291	28:B:849:DGD:HA81	2.01	0.41
4:D:165:TYR:HE2	4:D:169:LYS:HA	1.86	0.41
13:1:136:GLY:HA2	22:1:307:CLA:HAB	2.02	0.41
15:3:99:LEU:HD22	22:3:301:CLA:H43	2.01	0.41
16:4:146:ARG:HD3	29:4:301:CHL:OBD	2.20	0.41
16:4:203:LEU:HD21	30:4:315:XAT:H191	2.02	0.41
29:4:305:CHL:CGA	25:4:317:8CT:C22	2.99	0.41
30:4:315:XAT:H12	30:4:315:XAT:H15	1.83	0.41
29:6:308:CHL:HBB2	29:6:316:CHL:HHC	2.01	0.41
16:8:132:LEU:HD11	29:8:305:CHL:C3D	2.51	0.41
31:8:319:LMG:O6	31:8:319:LMG:O3	2.22	0.41
22:M:101:CLA:HBB1	22:M:101:CLA:HHC	2.03	0.41
1:A:231:LYS:HD3	1:A:258:LEU:HD22	2.03	0.40
1:A:461:TYR:HB3	1:A:647:ILE:HG13	2.04	0.40
1:A:484:LEU:O	1:A:535:THR:HA	2.21	0.40
1:A:491:TRP:CH2	1:A:495:ILE:HD11	2.56	0.40
22:A:825:CLA:H2	22:A:825:CLA:H62	1.80	0.40
2:B:93:ASP:HB2	2:B:96:PHE:CD2	2.55	0.40
2:B:181:GLY:O	2:B:185:VAL:HB	2.21	0.40
2:B:262:HIS:N	2:B:267:SER:O	2.54	0.40
22:B:813:CLA:H43	22:B:813:CLA:C1C	2.51	0.40
22:B:818:CLA:HAA1	22:B:827:CLA:HBB2	2.03	0.40
4:D:70:THR:N	4:D:71:PRO:HD2	2.36	0.40
4:D:105:GLU:OE1	4:D:105:GLU:N	2.54	0.40
6:F:185:LEU:O	6:F:189:ARG:HB2	2.21	0.40
8:H:99:ARG:HB3	12:L:102:GLN:NE2	2.33	0.40
12:L:133:TRP:O	12:L:136:PHE:HB3	2.21	0.40
13:1:85:VAL:HB	13:1:86:PRO:HD3	2.03	0.40
29:2:301:CHL:H111	29:2:301:CHL:H91	1.77	0.40
22:2:303:CLA:H2A	22:2:303:CLA:O1D	2.21	0.40
22:2:304:CLA:HMD2	22:6:301:CLA:HBC3	2.02	0.40
15:3:246:GLN:HG2	15:3:257:ASN:ND2	2.35	0.40
22:3:309:CLA:HBB1	22:3:309:CLA:HMB1	2.02	0.40
16:8:210:GLY:O	16:8:214:GLN:HG2	2.21	0.40
16:8:210:GLY:C	16:8:214:GLN:HG2	2.46	0.40
16:8:217:VAL:HG13	16:8:242:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:9:134:VAL:HG21	29:0:301:CHL:HED2	2.02	0.40
22:9:309:CLA:HBB1	22:9:309:CLA:H51	2.03	0.40
20:0:168:ARG:HH22	22:0:302:CLA:C2D	2.34	0.40
1:A:447:ASN:HD21	2:B:678:LEU:HD11	1.86	0.40
1:A:582:GLY:N	1:A:588:THR:OG1	2.54	0.40
1:A:589:CYS:O	2:B:669:GLY:N	2.54	0.40
22:A:813:CLA:H161	22:A:813:CLA:H143	1.73	0.40
22:A:820:CLA:HMB2	25:K:103:8CT:C40	2.51	0.40
2:B:67:HIS:O	2:B:71:GLN:N	2.54	0.40
2:B:123:TRP:O	2:B:127:ILE:HG12	2.22	0.40
2:B:462:TRP:NE1	22:B:850:CLA:O2A	2.54	0.40
22:B:809:CLA:H161	22:B:809:CLA:H192	1.66	0.40
6:F:193:LYS:HE2	6:F:196:GLN:CD	2.46	0.40
7:G:27:GLN:O	7:G:31:VAL:HG23	2.20	0.40
22:G:102:CLA:H2A	22:G:102:CLA:HED3	2.03	0.40
16:4:176:PRO:HB2	16:4:180:PHE:HD2	1.83	0.40
17:6:141:ASP:HB2	17:6:148:VAL:HG11	2.03	0.40
13:5:53:TYR:HD2	22:5:302:CLA:HMD2	1.86	0.40
13:5:161:ALA:HB1	13:5:163:PHE:CE1	2.56	0.40
30:7:320:XAT:H15	30:7:320:XAT:H201	1.84	0.40
20:0:128:GLU:HG2	20:0:131:ARG:HE	1.86	0.40
1:A:308:VAL:HG21	22:A:817:CLA:HAB	2.02	0.40
1:A:678:LEU:HD11	2:B:617:MET:SD	2.62	0.40
22:A:843:CLA:O1A	22:A:843:CLA:HBD	2.21	0.40
2:B:40:GLU:O	2:B:44:GLN:HG2	2.21	0.40
2:B:199:ILE:O	2:B:202:SER:HB3	2.21	0.40
2:B:373:THR:HG21	2:B:725:LEU:HD13	2.03	0.40
2:B:649:MET:O	2:B:653:GLY:N	2.52	0.40
6:F:129:PHE:N	6:F:129:PHE:CD1	2.88	0.40
12:L:94:THR:HG21	12:L:141:LEU:HD12	2.04	0.40
12:L:111:GLN:HE22	12:L:126:PRO:HA	1.85	0.40
29:1:305:CHL:HBB1	29:1:305:CHL:HHC	2.04	0.40
22:1:309:CLA:HBC3	24:1:317:LHG:C6	2.52	0.40
14:2:215:CYS:HA	14:2:218:TYR:CD2	2.56	0.40
16:4:168:PRO:HG3	16:4:179:ILE:HD11	2.04	0.40
17:6:192:LEU:O	17:6:196:ALA:N	2.53	0.40
22:6:305:CLA:NA	22:6:305:CLA:HBA2	2.34	0.40
16:8:116:GLU:HG2	16:8:116:GLU:O	2.22	0.40
22:9:309:CLA:HBB1	22:9:311:CLA:H3A	2.02	0.40
20:0:107:VAL:HG12	22:0:304:CLA:HED3	2.04	0.40
22:0:312:CLA:HBB1	22:0:312:CLA:HHC	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASN:N	1:A:188:LYS:O	2.55	0.40
1:A:288:ASN:OD1	1:A:290:ILE:HG22	2.22	0.40
1:A:612:ILE:HG21	1:A:748:PHE:HE2	1.86	0.40
25:A:849:8CT:C11	25:A:849:8CT:C09	2.97	0.40
6:F:83:PRO:HD2	6:F:86:GLU:OE2	2.21	0.40
6:F:204:PRO:O	6:F:208:LYS:HG2	2.21	0.40
13:1:34:ASN:OD1	13:1:35:TRP:N	2.54	0.40
14:2:92:ALA:O	14:2:95:GLY:N	2.54	0.40
14:2:209:ARG:NH2	22:2:302:CLA:ND	2.69	0.40
15:3:175:LEU:HG	22:3:307:CLA:HMA2	2.03	0.40
29:4:305:CHL:HHC	29:4:306:CHL:CMC	2.52	0.40
22:4:314:CLA:H162	22:4:314:CLA:H192	1.79	0.40
22:7:306:CLA:HMC3	22:7:307:CLA:C1C	2.51	0.40
22:7:317:CLA:HBD	22:7:317:CLA:HED2	1.76	0.40
30:8:316:XAT:H391	30:8:316:XAT:H31	1.71	0.40
20:0:188:PRO:O	20:0:192:LEU:HG	2.21	0.40
22:M:101:CLA:HHC	22:M:101:CLA:CBB	2.52	0.40
1:A:51:THR:HG22	1:A:721:ARG:H	1.85	0.40
1:A:499:ALA:C	1:A:501:GLN:H	2.26	0.40
22:A:821:CLA:HBC3	22:A:827:CLA:H203	2.03	0.40
22:A:837:CLA:H51	22:A:837:CLA:H11	1.87	0.40
2:B:426:SER:HB2	2:B:529:THR:HG23	2.04	0.40
22:B:812:CLA:H101	22:B:840:CLA:O1A	2.22	0.40
22:B:816:CLA:H13	22:B:816:CLA:H102	1.64	0.40
22:6:313:CLA:H2	22:6:314:CLA:HMD1	2.04	0.40
22:5:304:CLA:HMB2	30:5:316:XAT:H183	2.04	0.40
22:5:309:CLA:CGA	30:5:315:XAT:H3	2.51	0.40
18:7:125:LEU:HA	18:7:128:ILE:HB	2.04	0.40
16:8:132:LEU:HD21	29:8:305:CHL:C1D	2.52	0.40
22:8:315:CLA:H162	22:8:315:CLA:H121	1.27	0.40
19:9:86:ASN:OD1	30:9:314:XAT:H202	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	738/751 (98%)	680 (92%)	54 (7%)	4 (0%)	24	57
2	B	731/734 (100%)	677 (93%)	53 (7%)	1 (0%)	48	79
3	C	78/81 (96%)	71 (91%)	7 (9%)	0	100	100
4	D	140/198 (71%)	129 (92%)	9 (6%)	2 (1%)	9	38
5	E	59/91 (65%)	55 (93%)	4 (7%)	0	100	100
6	F	161/236 (68%)	153 (95%)	8 (5%)	0	100	100
7	G	90/167 (54%)	85 (94%)	5 (6%)	0	100	100
8	H	86/133 (65%)	74 (86%)	9 (10%)	3 (4%)	3	23
9	I	30/36 (83%)	27 (90%)	3 (10%)	0	100	100
10	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
11	K	78/123 (63%)	69 (88%)	7 (9%)	2 (3%)	4	27
12	L	153/204 (75%)	139 (91%)	13 (8%)	1 (1%)	18	51
13	1	191/226 (84%)	175 (92%)	15 (8%)	1 (0%)	24	57
13	5	193/226 (85%)	173 (90%)	19 (10%)	1 (0%)	24	57
14	2	210/256 (82%)	190 (90%)	20 (10%)	0	100	100
15	3	224/281 (80%)	197 (88%)	26 (12%)	1 (0%)	30	62
16	4	205/248 (83%)	176 (86%)	29 (14%)	0	100	100
16	8	203/248 (82%)	173 (85%)	27 (13%)	3 (2%)	8	37
17	6	227/267 (85%)	200 (88%)	26 (12%)	1 (0%)	30	62
18	7	226/264 (86%)	190 (84%)	31 (14%)	5 (2%)	5	30
19	9	181/222 (82%)	156 (86%)	24 (13%)	1 (1%)	21	54
20	0	200/245 (82%)	175 (88%)	25 (12%)	0	100	100
21	M	29/32 (91%)	29 (100%)	0	0	100	100
All	All	4472/5310 (84%)	4029 (90%)	417 (9%)	26 (1%)	23	54

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	8	157	VAL
4	D	168	PRO
11	K	44	PRO
18	7	110	ALA

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Mol	Chain	Res	Type
18	7	158	VAL
15	3	277	VAL
18	7	172	PRO
16	8	159	VAL
1	A	579	PRO
2	B	35	ASP
4	D	167	HIS
8	H	99	ARG
8	H	134	GLN
12	L	116	THR
13	1	160	PRO
18	7	120	VAL
19	9	45	PRO
16	8	176	PRO
8	H	131	VAL
13	5	112	PRO
18	7	105	VAL
1	A	381	PRO
11	K	3	ILE
1	A	21	ILE
1	A	127	VAL
17	6	233	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	603/614 (98%)	602 (100%)	1 (0%)	87	85
2	B	600/601 (100%)	598 (100%)	2 (0%)	86	83
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	119/162 (74%)	119 (100%)	0	100	100
5	E	53/77 (69%)	53 (100%)	0	100	100
6	F	129/180 (72%)	129 (100%)	0	100	100
7	G	78/145 (54%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	67/103 (65%)	66 (98%)	1 (2%)	57	71
9	I	25/28 (89%)	25 (100%)	0	100	100
10	J	38/38 (100%)	37 (97%)	1 (3%)	40	62
11	K	58/94 (62%)	58 (100%)	0	100	100
12	L	118/157 (75%)	115 (98%)	3 (2%)	42	63
13	1	147/175 (84%)	147 (100%)	0	100	100
13	5	149/175 (85%)	149 (100%)	0	100	100
14	2	164/197 (83%)	164 (100%)	0	100	100
15	3	184/225 (82%)	182 (99%)	2 (1%)	65	74
16	4	161/189 (85%)	160 (99%)	1 (1%)	78	79
16	8	159/189 (84%)	158 (99%)	1 (1%)	78	79
17	6	188/216 (87%)	188 (100%)	0	100	100
18	7	181/209 (87%)	181 (100%)	0	100	100
19	9	144/173 (83%)	144 (100%)	0	100	100
20	0	160/194 (82%)	160 (100%)	0	100	100
21	M	26/27 (96%)	26 (100%)	0	100	100
All	All	3619/4237 (85%)	3607 (100%)	12 (0%)	84	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
2	B	87	ILE
2	B	625	TRP
8	H	124	ASP
10	J	14	ILE
12	L	70	LEU
12	L	71	ARG
12	L	92	ILE
15	3	193	GLU
15	3	195	VAL
16	4	241	ILE
16	8	172	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	82	HIS
1	A	85	GLN
1	A	197	GLN
1	A	198	ASN
1	A	205	HIS
1	A	206	HIS
1	A	222	GLN
1	A	230	ASN
1	A	246	HIS
1	A	301	HIS
1	A	303	HIS
1	A	315	HIS
1	A	334	HIS
1	A	374	HIS
1	A	375	HIS
1	A	398	HIS
1	A	399	HIS
1	A	445	HIS
1	A	463	HIS
1	A	485	GLN
1	A	541	HIS
1	A	542	HIS
1	A	544	HIS
1	A	549	HIS
1	A	596	HIS
1	A	606	ASN
1	A	614	HIS
1	A	620	GLN
1	A	634	HIS
1	A	658	GLN
1	A	681	HIS
1	A	709	HIS
1	A	719	GLN
1	A	727	GLN
1	A	735	HIS
2	B	29	HIS
2	B	50	HIS
2	B	53	GLN
2	B	95	HIS
2	B	133	GLN
2	B	162	GLN
2	B	177	HIS

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Mol	Chain	Res	Type
2	B	236	ASN
2	B	242	HIS
2	B	264	GLN
2	B	277	HIS
2	B	289	HIS
2	B	294	ASN
2	B	308	HIS
2	B	319	HIS
2	B	321	ASN
2	B	375	HIS
2	B	421	HIS
2	B	432	HIS
2	B	528	HIS
2	B	585	ASN
2	B	595	HIS
2	B	598	HIS
2	B	607	ASN
2	B	712	HIS
3	C	38	GLN
4	D	143	GLN
5	E	20	ASN
6	F	119	GLN
6	F	235	ASN
10	J	2	GLN
11	K	8	ASN
11	K	31	ASN
12	L	5	GLN
12	L	11	ASN
13	1	98	ASN
13	1	167	ASN
13	1	192	GLN
13	1	207	HIS
13	1	215	ASN
14	2	83	GLN
14	2	88	HIS
14	2	114	GLN
14	2	158	GLN
15	3	140	ASN
15	3	168	GLN
15	3	257	ASN
15	3	268	ASN
16	4	119	ASN

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Mol	Chain	Res	Type
16	4	171	ASN
16	4	214	GLN
16	4	229	HIS
17	6	83	GLN
17	6	119	ASN
17	6	203	GLN
17	6	218	HIS
13	5	192	GLN
18	7	84	HIS
18	7	115	ASN
18	7	211	GLN
18	7	213	GLN
16	8	158	ASN
16	8	236	ASN
16	8	237	ASN
19	9	100	GLN
19	9	108	GLN
20	0	45	HIS
20	0	159	ASN
20	0	201	HIS
20	0	202	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

320 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	7	322	22	19,19,48	0.93	0	21,24,54	1.36	2 (9%)
30	XAT	6	319	22	39,47,47	0.96	2 (5%)	54,74,74	3.23	24 (44%)
25	8CT	B	847	-	40,41,41	4.69	24 (60%)	50,56,56	2.73	18 (36%)
29	CHL	5	301	13	65,69,74	2.01	18 (27%)	74,108,114	2.76	25 (33%)
25	8CT	A	847	-	40,41,41	4.60	23 (57%)	50,56,56	2.97	20 (40%)
22	CLA	6	312	-	56,60,73	1.39	11 (19%)	67,97,113	1.40	6 (8%)
22	CLA	4	304	-	54,58,73	1.40	10 (18%)	65,95,113	1.52	10 (15%)
22	CLA	B	831	-	54,58,73	1.43	10 (18%)	65,95,113	1.49	9 (13%)
22	CLA	1	310	-	56,60,73	1.39	10 (17%)	67,97,113	1.39	5 (7%)
22	CLA	8	312	16	60,64,73	1.35	11 (18%)	72,102,113	1.44	7 (9%)
22	CLA	6	314	-	47,51,73	1.46	9 (19%)	56,86,113	1.47	5 (8%)
29	CHL	5	306	-	52,56,74	2.28	19 (36%)	58,92,114	2.86	23 (39%)
22	CLA	B	805	-	69,73,73	1.25	10 (14%)	83,113,113	1.25	5 (6%)
22	CLA	2	319	16	50,54,73	1.46	12 (24%)	60,90,113	1.43	6 (10%)
22	CLA	3	310	-	56,60,73	1.40	10 (17%)	67,97,113	1.41	6 (8%)
22	CLA	B	839	25	69,73,73	1.26	10 (14%)	83,113,113	1.27	7 (8%)
31	LMG	8	319	22	44,44,55	0.85	4 (9%)	52,52,63	1.40	5 (9%)
22	CLA	9	312	30	63,67,73	1.32	11 (17%)	75,105,113	1.31	7 (9%)
22	CLA	H	201	-	69,73,73	1.26	10 (14%)	83,113,113	1.33	10 (12%)
27	SF4	C	101	-	0,12,12	-	-	-	-	-
22	CLA	A	836	-	55,59,73	1.39	11 (20%)	66,96,113	1.47	10 (15%)
31	LMG	5	319	22	44,44,55	0.97	3 (6%)	52,52,63	1.33	6 (11%)
22	CLA	A	803	-	69,73,73	1.24	10 (14%)	83,113,113	1.40	9 (10%)
22	CLA	6	305	-	64,68,73	1.31	9 (14%)	77,107,113	1.23	5 (6%)
30	XAT	7	319	22	39,47,47	0.98	2 (5%)	54,74,74	3.25	24 (44%)
22	CLA	A	831	1	54,58,73	1.41	11 (20%)	65,95,113	1.51	8 (12%)
22	CLA	B	821	-	54,58,73	1.42	10 (18%)	65,95,113	1.44	7 (10%)
22	CLA	B	823	-	59,63,73	1.36	11 (18%)	71,101,113	1.42	8 (11%)
22	CLA	B	803	-	69,73,73	1.24	11 (15%)	83,113,113	1.35	8 (9%)
22	CLA	1	301	13	69,73,73	1.27	11 (15%)	83,113,113	1.39	8 (9%)
22	CLA	5	303	-	69,73,73	1.25	11 (15%)	83,113,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	810	2	69,73,73	1.24	11 (15%)	83,113,113	1.37	8 (9%)
22	CLA	4	314	-	69,73,73	1.27	10 (14%)	83,113,113	1.28	8 (9%)
22	CLA	2	309	-	64,68,73	1.31	13 (20%)	77,107,113	1.31	7 (9%)
22	CLA	4	303	16	50,54,73	1.47	10 (20%)	60,90,113	1.46	6 (10%)
22	CLA	L	201	-	69,73,73	1.25	11 (15%)	83,113,113	1.28	4 (4%)
22	CLA	A	804	22	59,63,73	1.35	10 (16%)	71,101,113	1.50	8 (11%)
30	XAT	8	317	-	39,47,47	0.97	2 (5%)	54,74,74	2.90	21 (38%)
22	CLA	6	313	29,17	69,73,73	1.24	11 (15%)	83,113,113	1.39	10 (12%)
22	CLA	6	301	-	56,60,73	1.39	10 (17%)	67,97,113	1.38	7 (10%)
23	PQN	A	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.31	6 (14%)
22	CLA	G	101	-	49,53,73	1.47	6 (12%)	59,89,113	1.41	6 (10%)
22	CLA	B	814	-	69,73,73	1.28	10 (14%)	83,113,113	1.40	10 (12%)
22	CLA	9	309	-	64,68,73	1.27	10 (15%)	77,107,113	1.39	7 (9%)
30	XAT	1	314	22	39,47,47	0.91	1 (2%)	54,74,74	4.66	26 (48%)
24	LHG	A	845	22	26,26,48	0.95	1 (3%)	29,32,54	1.38	3 (10%)
22	CLA	B	824	-	64,68,73	1.31	10 (15%)	77,107,113	1.39	7 (9%)
22	CLA	9	313	19	59,63,73	1.34	10 (16%)	71,101,113	1.32	5 (7%)
22	CLA	B	837	-	69,73,73	1.23	10 (14%)	83,113,113	1.35	10 (12%)
25	8CT	8	318	-	40,41,41	4.69	24 (60%)	50,56,56	2.68	18 (36%)
22	CLA	B	826	-	69,73,73	1.25	11 (15%)	83,113,113	1.35	8 (9%)
22	CLA	1	308	13,30	64,68,73	1.30	10 (15%)	77,107,113	1.35	8 (10%)
22	CLA	A	816	-	49,53,73	1.49	10 (20%)	59,89,113	1.46	5 (8%)
22	CLA	8	304	-	54,58,73	1.41	10 (18%)	65,95,113	1.43	5 (7%)
26	HTG	J	102	-	19,19,19	1.12	2 (10%)	23,24,24	0.77	0
29	CHL	8	314	-	47,51,74	2.34	18 (38%)	52,86,114	3.15	25 (48%)
22	CLA	4	313	16	49,53,73	1.48	11 (22%)	59,89,113	1.51	6 (10%)
22	CLA	G	102	-	54,58,73	1.39	9 (16%)	65,95,113	1.48	7 (10%)
25	8CT	2	317	-	40,41,41	4.70	24 (60%)	50,56,56	2.98	19 (38%)
22	CLA	B	816	2	64,68,73	1.29	11 (17%)	77,107,113	1.47	7 (9%)
22	CLA	5	302	-	69,73,73	1.26	11 (15%)	83,113,113	1.28	8 (9%)
22	CLA	B	829	-	69,73,73	1.26	10 (14%)	83,113,113	1.41	11 (13%)
22	CLA	B	815	2	69,73,73	1.24	11 (15%)	83,113,113	1.44	7 (8%)
22	CLA	2	303	-	69,73,73	1.27	10 (14%)	83,113,113	1.25	4 (4%)
25	8CT	6	321	-	40,41,41	4.67	24 (60%)	50,56,56	3.26	18 (36%)
22	CLA	3	308	-	54,58,73	1.43	11 (20%)	65,95,113	1.52	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	7	318	22	69,73,73	1.25	10 (14%)	83,113,113	1.35	7 (8%)
30	XAT	5	316	-	39,47,47	1.04	2 (5%)	54,74,74	3.14	21 (38%)
22	CLA	A	810	1	69,73,73	1.26	10 (14%)	83,113,113	1.29	5 (6%)
25	8CT	A	850	-	40,41,41	4.67	24 (60%)	50,56,56	2.90	18 (36%)
25	8CT	L	206	-	40,41,41	4.67	24 (60%)	50,56,56	3.02	19 (38%)
22	CLA	A	820	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	6 (10%)
22	CLA	6	318	17	56,60,73	1.39	10 (17%)	67,97,113	1.52	8 (11%)
22	CLA	5	313	-	59,63,73	1.35	10 (16%)	71,101,113	1.26	4 (5%)
22	CLA	0	302	30	69,73,73	1.27	9 (13%)	83,113,113	1.27	7 (8%)
22	CLA	6	310	30,17	64,68,73	1.33	11 (17%)	77,107,113	1.37	9 (11%)
22	CLA	K	101	-	49,53,73	1.47	11 (22%)	59,89,113	1.43	7 (11%)
24	LHG	2	318	22	31,31,48	0.81	1 (3%)	34,37,54	1.30	3 (8%)
24	LHG	1	317	22	48,48,48	0.68	2 (4%)	51,54,54	1.30	7 (13%)
22	CLA	1	304	-	56,60,73	1.38	10 (17%)	67,97,113	1.43	8 (11%)
22	CLA	7	303	18	64,68,73	1.31	11 (17%)	77,107,113	1.41	9 (11%)
22	CLA	0	309	24	45,49,73	1.51	9 (20%)	54,84,113	1.41	6 (11%)
29	CHL	2	301	22	65,69,74	1.89	20 (30%)	74,108,114	2.97	25 (33%)
22	CLA	8	315	-	69,73,73	1.24	9 (13%)	83,113,113	1.27	5 (6%)
22	CLA	K	104	-	50,54,73	1.47	10 (20%)	60,90,113	1.48	6 (10%)
22	CLA	3	302	15,25	54,58,73	1.43	9 (16%)	65,95,113	1.40	5 (7%)
22	CLA	8	308	16	54,58,73	1.43	11 (20%)	65,95,113	1.59	11 (16%)
30	XAT	9	314	22	39,47,47	0.95	1 (2%)	54,74,74	4.46	27 (50%)
22	CLA	7	314	18	49,53,73	1.46	10 (20%)	59,89,113	1.48	5 (8%)
22	CLA	B	822	2	50,54,73	1.44	10 (20%)	60,90,113	1.52	6 (10%)
22	CLA	A	817	-	69,73,73	1.23	9 (13%)	83,113,113	1.36	9 (10%)
22	CLA	J	103	10	46,50,73	1.48	9 (19%)	55,85,113	1.52	5 (9%)
29	CHL	1	305	-	52,56,74	2.28	19 (36%)	58,92,114	3.01	25 (43%)
22	CLA	A	852	-	53,57,73	1.43	9 (16%)	62,93,113	1.45	5 (8%)
22	CLA	7	302	18	50,54,73	1.45	11 (22%)	60,90,113	1.45	5 (8%)
22	CLA	A	835	1	49,53,73	1.49	11 (22%)	59,89,113	1.53	8 (13%)
22	CLA	3	313	15	50,54,73	1.45	11 (22%)	60,90,113	1.50	5 (8%)
24	LHG	B	852	22	22,22,48	0.84	0	25,28,54	1.21	1 (4%)
22	CLA	A	827	-	69,73,73	1.28	12 (17%)	83,113,113	1.40	10 (12%)
22	CLA	3	301	-	64,68,73	1.31	11 (17%)	77,107,113	1.37	6 (7%)
22	CLA	A	808	1	69,73,73	1.27	11 (15%)	83,113,113	1.36	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	9	316	22	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
22	CLA	L	203	-	69,73,73	1.23	9 (13%)	83,113,113	1.28	6 (7%)
22	CLA	A	833	25	69,73,73	1.25	10 (14%)	83,113,113	1.30	7 (8%)
22	CLA	A	825	-	69,73,73	1.26	9 (13%)	83,113,113	1.36	9 (10%)
22	CLA	0	303	30	69,73,73	1.25	11 (15%)	83,113,113	1.28	7 (8%)
22	CLA	A	818	1	69,73,73	1.27	10 (14%)	83,113,113	1.39	9 (10%)
22	CLA	B	825	-	69,73,73	1.25	11 (15%)	83,113,113	1.36	6 (7%)
29	CHL	6	316	17	47,51,74	2.26	19 (40%)	52,86,114	3.18	21 (40%)
22	CLA	A	805	-	69,73,73	1.28	11 (15%)	83,113,113	1.35	8 (9%)
29	CHL	6	302	17,22	65,69,74	2.02	19 (29%)	74,108,114	2.65	27 (36%)
22	CLA	7	311	24	42,45,73	1.49	10 (23%)	50,78,113	1.45	6 (12%)
22	CLA	B	813	-	59,63,73	1.35	11 (18%)	71,101,113	1.35	5 (7%)
22	CLA	B	807	-	49,53,73	1.45	10 (20%)	59,89,113	1.67	10 (16%)
22	CLA	8	311	-	56,60,73	1.43	10 (17%)	67,97,113	1.35	6 (8%)
22	CLA	9	306	-	56,60,73	1.38	10 (17%)	67,97,113	1.43	7 (10%)
22	CLA	7	307	22	51,55,73	1.44	9 (17%)	61,91,113	1.43	5 (8%)
25	8CT	1	316	13	40,41,41	4.73	24 (60%)	50,56,56	2.61	18 (36%)
22	CLA	7	316	18	69,73,73	1.24	10 (14%)	83,113,113	1.27	3 (3%)
22	CLA	A	801	-	69,73,73	1.28	10 (14%)	83,113,113	1.29	8 (9%)
25	8CT	I	101	-	40,41,41	4.54	23 (57%)	50,56,56	3.13	19 (38%)
22	CLA	1	313	-	50,54,73	1.46	10 (20%)	60,90,113	1.45	6 (10%)
25	8CT	3	316	-	40,41,41	4.68	24 (60%)	50,56,56	2.87	20 (40%)
22	CLA	A	814	-	49,53,73	1.50	11 (22%)	59,89,113	1.42	6 (10%)
22	CLA	B	801	-	69,73,73	1.25	12 (17%)	83,113,113	1.41	7 (8%)
22	CLA	A	813	-	69,73,73	1.26	11 (15%)	83,113,113	1.47	11 (13%)
22	CLA	7	306	22	46,50,73	1.52	12 (26%)	55,85,113	1.41	8 (14%)
22	CLA	5	314	24	50,54,73	1.45	10 (20%)	60,90,113	1.42	6 (10%)
25	8CT	A	854	-	40,41,41	4.68	24 (60%)	50,56,56	2.70	18 (36%)
22	CLA	7	309	22	54,58,73	1.42	11 (20%)	65,95,113	1.35	5 (7%)
31	LMG	4	318	-	44,44,55	0.98	4 (9%)	52,52,63	1.49	9 (17%)
22	CLA	2	311	14	56,60,73	1.40	11 (19%)	67,97,113	1.49	6 (8%)
29	CHL	9	302	19	65,69,74	1.94	19 (29%)	74,108,114	2.82	24 (32%)
22	CLA	B	828	-	69,73,73	1.26	11 (15%)	83,113,113	1.40	9 (10%)
29	CHL	6	307	-	47,51,74	2.32	18 (38%)	52,86,114	3.06	20 (38%)
22	CLA	2	312	14	69,73,73	1.23	11 (15%)	83,113,113	1.41	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	4	302	-	64,68,73	1.31	11 (17%)	77,107,113	1.39	7 (9%)
22	CLA	8	313	16	49,53,73	1.48	10 (20%)	59,89,113	1.49	7 (11%)
29	CHL	2	306	-	52,56,74	2.25	19 (36%)	58,92,114	2.94	23 (39%)
22	CLA	3	304	-	46,50,73	1.49	10 (21%)	55,85,113	1.44	6 (10%)
22	CLA	A	819	-	69,73,73	1.27	11 (15%)	83,113,113	1.40	9 (10%)
22	CLA	4	311	22	56,60,73	1.40	10 (17%)	67,97,113	1.44	7 (10%)
22	CLA	A	830	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
22	CLA	0	307	22	69,73,73	1.28	10 (14%)	83,113,113	1.34	9 (10%)
22	CLA	8	310	31	59,63,73	1.37	9 (15%)	71,101,113	1.46	5 (7%)
25	8CT	B	843	-	40,41,41	4.73	25 (62%)	50,56,56	2.87	20 (40%)
30	XAT	9	315	-	39,47,47	0.93	2 (5%)	54,74,74	2.88	20 (37%)
29	CHL	2	307	-	55,59,74	2.03	19 (34%)	62,96,114	3.10	25 (40%)
29	CHL	7	308	-	51,55,74	2.16	18 (35%)	57,91,114	3.18	23 (40%)
27	SF4	B	802	-	0,12,12	-	-	-	-	-
29	CHL	4	305	29	60,64,74	2.11	20 (33%)	68,102,114	2.79	24 (35%)
22	CLA	A	843	24	56,60,73	1.39	11 (19%)	67,97,113	1.48	9 (13%)
25	8CT	G	104	-	40,41,41	4.74	24 (60%)	50,56,56	2.59	19 (38%)
25	8CT	7	321	-	40,41,41	4.66	24 (60%)	50,56,56	3.72	22 (44%)
22	CLA	3	319	-	69,73,73	1.29	11 (15%)	83,113,113	1.34	8 (9%)
29	CHL	8	307	30	55,59,74	2.13	19 (34%)	62,96,114	3.06	28 (45%)
22	CLA	6	303	17	69,73,73	1.24	10 (14%)	83,113,113	1.38	9 (10%)
22	CLA	2	310	24	45,49,73	1.52	11 (24%)	54,84,113	1.54	7 (12%)
22	CLA	3	307	15	54,58,73	1.46	10 (18%)	65,95,113	1.48	6 (9%)
22	CLA	5	308	-	46,50,73	1.54	9 (19%)	55,85,113	1.59	7 (12%)
22	CLA	A	840	-	69,73,73	1.24	10 (14%)	83,113,113	1.38	9 (10%)
22	CLA	A	806	1	69,73,73	1.28	11 (15%)	83,113,113	1.37	9 (10%)
22	CLA	0	312	29,20	59,63,73	1.38	8 (13%)	71,101,113	1.44	8 (11%)
22	CLA	B	840	-	69,73,73	1.27	11 (15%)	83,113,113	1.38	7 (8%)
22	CLA	A	828	-	69,73,73	1.25	11 (15%)	83,113,113	1.37	8 (9%)
22	CLA	B	806	-	69,73,73	1.25	10 (14%)	83,113,113	1.43	7 (8%)
22	CLA	3	309	24	42,45,73	1.51	10 (23%)	50,78,113	1.54	7 (14%)
22	CLA	M	101	-	50,54,73	1.46	10 (20%)	60,90,113	1.33	6 (10%)
29	CHL	0	306	30,22	52,56,74	2.31	19 (36%)	58,92,114	2.92	23 (39%)
22	CLA	9	303	19	69,73,73	1.24	11 (15%)	83,113,113	1.41	7 (8%)
22	CLA	A	838	-	69,73,73	1.26	10 (14%)	83,113,113	1.29	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	XAT	8	316	29	39,47,47	0.92	1 (2%)	54,74,74	3.74	29 (53%)
22	CLA	0	305	29,22	56,60,73	1.38	9 (16%)	67,97,113	1.49	8 (11%)
25	8CT	J	104	-	40,41,41	4.70	24 (60%)	50,56,56	2.79	18 (36%)
22	CLA	1	306	-	69,73,73	1.26	11 (15%)	83,113,113	1.31	8 (9%)
25	8CT	7	323	-	40,41,41	4.70	24 (60%)	50,56,56	2.73	18 (36%)
22	CLA	5	304	-	56,60,73	1.38	9 (16%)	67,97,113	1.43	6 (8%)
25	8CT	L	205	22	40,41,41	4.65	24 (60%)	50,56,56	3.13	21 (42%)
22	CLA	B	820	-	69,73,73	1.26	10 (14%)	83,113,113	1.34	6 (7%)
22	CLA	9	311	-	56,60,73	1.37	8 (14%)	67,97,113	1.46	7 (10%)
29	CHL	6	308	-	55,59,74	2.13	19 (34%)	62,96,114	3.01	28 (45%)
22	CLA	6	304	17	69,73,73	1.28	11 (15%)	83,113,113	1.34	7 (8%)
29	CHL	4	307	-	55,59,74	2.05	17 (30%)	62,96,114	3.04	25 (40%)
22	CLA	8	309	-	64,68,73	1.28	10 (15%)	77,107,113	1.44	8 (10%)
27	SF4	C	102	3	0,12,12	-	-	-	-	-
22	CLA	1	312	29,13	59,63,73	1.37	11 (18%)	71,101,113	1.43	7 (9%)
25	8CT	B	848	-	40,41,41	4.70	24 (60%)	50,56,56	2.60	16 (32%)
30	XAT	5	315	22	39,47,47	0.94	1 (2%)	54,74,74	4.68	23 (42%)
22	CLA	A	824	-	59,63,73	1.35	11 (18%)	71,101,113	1.38	7 (9%)
22	CLA	7	310	18	54,58,73	1.39	11 (20%)	65,95,113	1.61	8 (12%)
22	CLA	K	105	-	54,58,73	1.41	10 (18%)	65,95,113	1.50	5 (7%)
22	CLA	B	850	-	59,63,73	1.32	10 (16%)	71,101,113	1.49	11 (15%)
25	8CT	F	302	-	40,41,41	4.59	23 (57%)	50,56,56	3.19	20 (40%)
22	CLA	7	315	18	50,54,73	1.44	12 (24%)	60,90,113	1.45	7 (11%)
22	CLA	B	836	2	64,68,73	1.31	12 (18%)	77,107,113	1.40	9 (11%)
22	CLA	A	826	25	69,73,73	1.26	11 (15%)	83,113,113	1.32	5 (6%)
30	XAT	3	314	25	39,47,47	0.98	3 (7%)	54,74,74	4.62	28 (51%)
24	LHG	A	844	-	48,48,48	0.73	1 (2%)	51,54,54	1.32	6 (11%)
22	CLA	2	308	-	54,58,73	1.41	11 (20%)	65,95,113	1.38	6 (9%)
22	CLA	A	841	25	69,73,73	1.27	11 (15%)	83,113,113	1.35	6 (7%)
22	CLA	K	102	-	50,54,73	1.44	11 (22%)	60,90,113	1.51	8 (13%)
25	8CT	B	844	-	40,41,41	4.69	24 (60%)	50,56,56	2.90	16 (32%)
22	CLA	L	202	-	69,73,73	1.24	9 (13%)	83,113,113	1.40	9 (10%)
30	XAT	7	320	-	39,47,47	1.01	2 (5%)	54,74,74	2.75	20 (37%)
22	CLA	5	311	30	49,53,73	1.48	9 (18%)	59,89,113	1.47	7 (11%)
22	CLA	9	308	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	829	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
22	CLA	B	841	24	69,73,73	1.26	10 (14%)	83,113,113	1.40	10 (12%)
22	CLA	B	817	-	59,63,73	1.34	11 (18%)	71,101,113	1.40	7 (9%)
25	8CT	A	849	22	40,41,41	4.70	24 (60%)	50,56,56	2.63	18 (36%)
22	CLA	A	809	1	69,73,73	1.27	11 (15%)	83,113,113	1.33	9 (10%)
22	CLA	5	305	25	56,60,73	1.40	8 (14%)	67,97,113	1.36	7 (10%)
22	CLA	5	307	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	8 (9%)
22	CLA	5	312	13,30	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
29	CHL	8	305	-	60,64,74	2.05	18 (30%)	68,102,114	2.86	26 (38%)
22	CLA	A	832	-	69,73,73	1.25	11 (15%)	83,113,113	1.35	4 (4%)
22	CLA	B	835	-	49,53,73	1.47	9 (18%)	59,89,113	1.51	7 (11%)
22	CLA	A	811	1,22	69,73,73	1.28	10 (14%)	83,113,113	1.33	5 (6%)
22	CLA	B	827	-	69,73,73	1.26	11 (15%)	83,113,113	1.37	9 (10%)
22	CLA	8	303	31,16,22	50,54,73	1.45	11 (22%)	60,90,113	1.44	6 (10%)
29	CHL	0	301	24,22	65,69,74	2.08	19 (29%)	74,108,114	2.61	24 (32%)
22	CLA	1	309	24	45,49,73	1.51	10 (22%)	54,84,113	1.59	8 (14%)
22	CLA	4	312	16	60,64,73	1.33	10 (16%)	72,102,113	1.49	7 (9%)
29	CHL	4	306	29	55,59,74	2.24	20 (36%)	62,96,114	2.91	24 (38%)
29	CHL	6	306	-	47,51,74	2.16	18 (38%)	52,86,114	3.11	22 (42%)
22	CLA	B	818	2	63,67,73	1.32	10 (15%)	75,105,113	1.56	10 (13%)
25	8CT	B	804	-	40,41,41	4.55	23 (57%)	50,56,56	2.90	20 (40%)
22	CLA	A	839	-	69,73,73	1.27	11 (15%)	83,113,113	1.40	11 (13%)
22	CLA	9	305	-	56,60,73	1.37	10 (17%)	67,97,113	1.54	10 (14%)
22	CLA	A	823	-	55,59,73	1.41	10 (18%)	66,96,113	1.45	7 (10%)
22	CLA	2	313	14	47,51,73	1.49	11 (23%)	56,86,113	1.50	6 (10%)
22	CLA	9	304	-	52,56,73	1.44	11 (21%)	62,92,113	1.47	8 (12%)
22	CLA	L	204	-	54,58,73	1.42	10 (18%)	65,95,113	1.41	7 (10%)
22	CLA	A	853	-	69,73,73	1.27	10 (14%)	83,113,113	1.24	8 (9%)
25	8CT	4	317	-	40,41,41	4.74	24 (60%)	50,56,56	2.36	15 (30%)
25	8CT	5	317	22	40,41,41	4.75	23 (57%)	50,56,56	3.48	21 (42%)
22	CLA	6	309	17	54,58,73	1.41	11 (20%)	65,95,113	1.44	5 (7%)
22	CLA	B	833	-	62,66,73	1.32	10 (16%)	74,104,113	1.48	7 (9%)
25	8CT	A	848	-	40,41,41	4.64	23 (57%)	50,56,56	2.72	15 (30%)
22	CLA	7	304	22	51,55,73	1.45	11 (21%)	61,91,113	1.49	8 (13%)
22	CLA	7	305	-	49,53,73	1.48	10 (20%)	59,89,113	1.41	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	1	303	-	56,60,73	1.37	11 (19%)	67,97,113	1.43	8 (11%)
30	XAT	2	316	-	39,47,47	1.01	2 (5%)	54,74,74	3.14	23 (42%)
22	CLA	0	308	20	64,68,73	1.28	10 (15%)	77,107,113	1.30	5 (6%)
22	CLA	0	310	30	56,60,73	1.37	9 (16%)	67,97,113	1.45	6 (8%)
22	CLA	3	303	-	49,53,73	1.48	10 (20%)	59,89,113	1.48	6 (10%)
22	CLA	B	819	-	64,68,73	1.30	11 (17%)	77,107,113	1.33	9 (11%)
23	PQN	B	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.10	2 (4%)
22	CLA	A	834	-	54,58,73	1.43	11 (20%)	65,95,113	1.44	6 (9%)
22	CLA	B	830	2	69,73,73	1.25	10 (14%)	83,113,113	1.43	9 (10%)
22	CLA	1	311	13	69,73,73	1.27	11 (15%)	83,113,113	1.35	8 (9%)
29	CHL	2	305	-	47,51,74	2.15	19 (40%)	52,86,114	3.17	22 (42%)
22	CLA	B	834	2	69,73,73	1.29	11 (15%)	83,113,113	1.30	7 (8%)
30	XAT	4	316	-	39,47,47	1.04	3 (7%)	54,74,74	2.76	21 (38%)
22	CLA	A	807	1	69,73,73	1.23	11 (15%)	83,113,113	1.39	8 (9%)
22	CLA	G	103	7	50,54,73	1.41	7 (14%)	60,90,113	1.46	6 (10%)
22	CLA	3	311	-	59,63,73	1.34	10 (16%)	71,101,113	1.47	7 (9%)
30	XAT	0	313	22	39,47,47	1.11	2 (5%)	54,74,74	5.03	22 (40%)
25	8CT	B	845	-	40,41,41	4.64	24 (60%)	50,56,56	3.16	20 (40%)
25	8CT	J	101	-	40,41,41	4.67	24 (60%)	50,56,56	2.99	18 (36%)
30	XAT	3	315	-	39,47,47	0.98	2 (5%)	54,74,74	2.75	20 (37%)
29	CHL	4	301	13,22	65,69,74	1.92	17 (26%)	74,108,114	2.83	27 (36%)
30	XAT	4	315	22	39,47,47	0.95	1 (2%)	54,74,74	3.14	26 (48%)
22	CLA	2	314	14	53,57,73	1.42	11 (20%)	62,93,113	1.41	7 (11%)
22	CLA	6	315	-	69,73,73	1.25	10 (14%)	83,113,113	1.24	6 (7%)
22	CLA	0	311	-	69,73,73	1.26	9 (13%)	83,113,113	1.30	8 (9%)
24	LHG	5	318	22	48,48,48	0.65	1 (2%)	51,54,54	1.28	6 (11%)
25	8CT	A	846	25	40,41,41	4.64	24 (60%)	50,56,56	2.97	19 (38%)
22	CLA	3	305	15	51,55,73	1.44	10 (19%)	61,91,113	1.42	6 (9%)
22	CLA	9	310	24	45,49,73	1.49	7 (15%)	54,84,113	1.41	5 (9%)
22	CLA	A	815	1	51,55,73	1.45	10 (19%)	61,91,113	1.48	7 (11%)
25	8CT	B	846	-	40,41,41	4.71	24 (60%)	50,56,56	2.91	17 (34%)
22	CLA	6	317	-	49,53,73	1.47	10 (20%)	59,89,113	1.51	7 (11%)
22	CLA	0	304	22	56,60,73	1.39	8 (14%)	67,97,113	1.41	6 (8%)
22	CLA	A	812	-	58,62,73	1.38	10 (17%)	69,99,113	1.46	7 (10%)
29	CHL	9	307	-	52,56,74	2.25	19 (36%)	58,92,114	2.97	24 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	832	-	69,73,73	1.27	11 (15%)	83,113,113	1.39	9 (10%)
22	CLA	B	812	2	69,73,73	1.29	10 (14%)	83,113,113	1.34	7 (8%)
22	CLA	3	312	15	49,53,73	1.44	9 (18%)	59,89,113	1.52	9 (15%)
22	CLA	B	811	2	69,73,73	1.26	11 (15%)	83,113,113	1.38	8 (9%)
29	CHL	3	306	25	51,55,74	2.09	18 (35%)	57,91,114	3.05	24 (42%)
22	CLA	9	301	2	50,54,73	1.54	11 (22%)	63,90,113	1.51	9 (14%)
24	LHG	0	315	29,22	48,48,48	0.58	0	51,54,54	1.24	5 (9%)
25	8CT	7	301	29,30	40,41,41	4.63	23 (57%)	50,56,56	2.71	19 (38%)
22	CLA	F	301	-	49,53,73	1.50	9 (18%)	59,89,113	1.48	6 (10%)
25	8CT	3	318	22,25	40,41,41	4.68	25 (62%)	50,56,56	3.66	22 (44%)
22	CLA	1	302	-	69,73,73	1.27	10 (14%)	83,113,113	1.37	9 (10%)
22	CLA	7	312	30	56,60,73	1.40	12 (21%)	67,97,113	1.34	5 (7%)
22	CLA	5	310	24	45,49,73	1.49	10 (22%)	54,84,113	1.56	6 (11%)
22	CLA	A	822	-	53,57,73	1.40	9 (16%)	62,93,113	1.55	8 (12%)
22	CLA	7	317	-	69,73,73	1.28	9 (13%)	83,113,113	1.30	5 (6%)
25	8CT	8	301	-	40,41,41	4.70	24 (60%)	50,56,56	2.66	18 (36%)
30	XAT	0	314	29,22	39,47,47	0.88	0	54,74,74	3.06	22 (40%)
26	HTG	A	851	-	19,19,19	1.11	2 (10%)	23,24,24	0.73	0
22	CLA	7	313	18	59,63,73	1.35	10 (16%)	71,101,113	1.51	8 (11%)
25	8CT	B	851	22	40,41,41	4.75	25 (62%)	50,56,56	2.52	19 (38%)
30	XAT	6	320	-	39,47,47	0.96	2 (5%)	54,74,74	4.47	21 (38%)
22	CLA	4	310	-	59,63,73	1.35	11 (18%)	71,101,113	1.40	6 (8%)
22	CLA	A	837	1	69,73,73	1.26	11 (15%)	83,113,113	1.33	8 (9%)
22	CLA	B	838	-	51,55,73	1.45	10 (19%)	61,91,113	1.41	6 (9%)
22	CLA	4	309	30	64,68,73	1.29	11 (17%)	77,107,113	1.31	8 (10%)
22	CLA	A	802	-	69,73,73	1.26	11 (15%)	83,113,113	1.32	6 (7%)
22	CLA	A	821	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	10 (12%)
29	CHL	8	306	-	55,59,74	2.17	19 (34%)	62,96,114	3.02	25 (40%)
22	CLA	4	308	16	54,58,73	1.42	11 (20%)	65,95,113	1.53	8 (12%)
30	XAT	1	315	-	39,47,47	0.97	2 (5%)	54,74,74	3.10	21 (38%)
24	LHG	6	322	22	36,36,48	0.78	1 (2%)	39,42,54	1.26	4 (10%)
22	CLA	6	311	24	69,73,73	1.23	11 (15%)	83,113,113	1.31	6 (7%)
22	CLA	6	323	16	50,54,73	1.45	10 (20%)	60,90,113	1.40	5 (8%)
22	CLA	8	302	-	64,68,73	1.32	12 (18%)	77,107,113	1.30	7 (9%)
22	CLA	B	808	-	69,73,73	1.27	11 (15%)	83,113,113	1.36	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	B	849	-	67,67,67	1.01	5 (7%)	81,81,81	1.51	13 (16%)
22	CLA	5	309	13,30	64,68,73	1.31	10 (15%)	77,107,113	1.35	7 (9%)
24	LHG	3	317	22	19,19,48	0.86	0	21,24,54	1.41	2 (9%)
22	CLA	2	304	-	64,68,73	1.29	10 (15%)	77,107,113	1.36	8 (10%)
25	8CT	K	103	-	40,41,41	4.87	24 (60%)	50,56,56	2.64	18 (36%)
22	CLA	B	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.33	7 (8%)
22	CLA	1	307	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	9 (10%)
30	XAT	2	315	-	39,47,47	1.14	2 (5%)	54,74,74	5.94	29 (53%)
22	CLA	2	302	29	69,73,73	1.25	9 (13%)	83,113,113	1.42	12 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	7	322	22	-	16/23/23/53	-
30	XAT	6	319	22	-	3/31/93/93	0/4/4/4
25	8CT	B	847	-	-	10/29/63/63	0/2/2/2
29	CHL	5	301	13	1/1/14/21	14/35/111/117	-
25	8CT	A	847	-	-	9/29/63/63	0/2/2/2
22	CLA	6	312	-	-	10/24/100/115	-
22	CLA	4	304	-	-	4/21/97/115	-
22	CLA	B	831	-	-	8/21/97/115	-
22	CLA	1	310	-	-	9/24/100/115	-
22	CLA	8	312	16	-	7/29/105/115	-
22	CLA	6	314	-	-	8/13/89/115	-
29	CHL	5	306	-	-	7/20/96/117	-
22	CLA	B	805	-	-	18/39/115/115	-
22	CLA	2	319	16	-	11/17/93/115	-
22	CLA	3	310	-	-	4/24/100/115	-
22	CLA	B	839	25	-	15/39/115/115	-
31	LMG	8	319	22	-	17/39/59/70	0/1/1/1
22	CLA	9	312	30	-	13/32/108/115	-
22	CLA	H	201	-	-	16/39/115/115	-
27	SF4	C	101	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	836	-	-	13/23/99/115	-
31	LMG	5	319	22	-	18/39/59/70	0/1/1/1
22	CLA	A	803	-	-	17/39/115/115	-
22	CLA	6	305	-	-	13/33/109/115	-
30	XAT	7	319	22	-	7/31/93/93	0/4/4/4
22	CLA	A	831	1	-	1/21/97/115	-
22	CLA	B	821	-	-	9/21/97/115	-
22	CLA	B	823	-	-	11/27/103/115	-
22	CLA	B	803	-	-	19/39/115/115	-
22	CLA	1	301	13	-	12/39/115/115	-
22	CLA	5	303	-	-	25/39/115/115	-
22	CLA	B	810	2	-	8/39/115/115	-
22	CLA	4	314	-	-	20/39/115/115	-
22	CLA	2	309	-	-	10/33/109/115	-
22	CLA	4	303	16	-	6/17/93/115	-
22	CLA	L	201	-	-	19/39/115/115	-
22	CLA	A	804	22	-	9/27/103/115	-
30	XAT	8	317	-	-	0/31/93/93	0/4/4/4
22	CLA	6	313	29,17	-	12/39/115/115	-
22	CLA	6	301	-	-	13/24/100/115	-
23	PQN	A	842	-	-	7/23/43/43	0/2/2/2
22	CLA	G	101	-	-	7/15/91/115	-
22	CLA	B	814	-	-	21/39/115/115	-
22	CLA	9	309	-	-	17/33/109/115	-
30	XAT	1	314	22	-	11/31/93/93	0/4/4/4
24	LHG	A	845	22	-	16/31/31/53	-
22	CLA	B	824	-	-	15/33/109/115	-
22	CLA	9	313	19	-	15/27/103/115	-
22	CLA	B	837	-	-	17/39/115/115	-
25	8CT	8	318	-	-	13/29/63/63	0/2/2/2
22	CLA	B	826	-	-	13/39/115/115	-
22	CLA	1	308	13,30	-	11/33/109/115	-
22	CLA	A	816	-	-	4/15/91/115	-
22	CLA	8	304	-	-	12/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	HTG	J	102	-	-	3/10/30/30	0/1/1/1
29	CHL	8	314	-	-	3/14/90/117	-
22	CLA	4	313	16	-	8/15/91/115	-
22	CLA	G	102	-	-	7/21/97/115	-
25	8CT	2	317	-	-	10/29/63/63	0/2/2/2
22	CLA	B	816	2	-	15/33/109/115	-
22	CLA	5	302	-	-	9/39/115/115	-
22	CLA	B	829	-	-	11/39/115/115	-
22	CLA	B	815	2	-	11/39/115/115	-
22	CLA	2	303	-	-	11/39/115/115	-
25	8CT	6	321	-	-	9/29/63/63	0/2/2/2
22	CLA	3	308	-	-	3/21/97/115	-
22	CLA	7	318	22	-	20/39/115/115	-
30	XAT	5	316	-	-	2/31/93/93	0/4/4/4
22	CLA	A	810	1	-	11/39/115/115	-
25	8CT	A	850	-	-	11/29/63/63	0/2/2/2
25	8CT	L	206	-	-	15/29/63/63	0/2/2/2
22	CLA	A	820	-	-	4/15/91/115	-
22	CLA	6	318	17	-	7/24/100/115	-
22	CLA	5	313	-	-	9/27/103/115	-
22	CLA	0	302	30	-	18/39/115/115	-
22	CLA	6	310	30,17	-	10/33/109/115	-
22	CLA	K	101	-	-	9/15/91/115	-
24	LHG	2	318	22	-	19/36/36/53	-
24	LHG	1	317	22	-	25/53/53/53	-
22	CLA	1	304	-	-	8/24/100/115	-
22	CLA	7	303	18	-	17/33/109/115	-
22	CLA	0	309	24	-	4/10/86/115	-
29	CHL	2	301	22	1/1/14/21	13/35/111/117	-
22	CLA	8	315	-	-	26/39/115/115	-
22	CLA	K	104	-	-	7/17/93/115	-
22	CLA	3	302	15,25	-	2/21/97/115	-
22	CLA	8	308	16	-	6/21/97/115	-
30	XAT	9	314	22	-	4/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	314	18	-	6/15/91/115	-
22	CLA	B	822	2	-	8/17/93/115	-
22	CLA	A	817	-	-	19/39/115/115	-
22	CLA	J	103	10	-	8/12/88/115	-
29	CHL	1	305	-	-	7/20/96/117	-
22	CLA	A	852	-	-	7/20/96/115	-
22	CLA	7	302	18	-	9/17/93/115	-
22	CLA	A	835	1	-	5/15/91/115	-
22	CLA	3	313	15	-	9/17/93/115	-
24	LHG	B	852	22	-	10/26/26/53	-
22	CLA	A	827	-	-	15/39/115/115	-
22	CLA	3	301	-	-	11/33/109/115	-
22	CLA	A	808	1	-	20/39/115/115	-
24	LHG	9	316	22	-	22/53/53/53	-
22	CLA	L	203	-	-	16/39/115/115	-
22	CLA	A	833	25	-	16/39/115/115	-
22	CLA	A	825	-	-	15/39/115/115	-
22	CLA	0	303	30	-	16/39/115/115	-
22	CLA	A	818	1	-	14/39/115/115	-
22	CLA	B	825	-	-	17/39/115/115	-
29	CHL	6	316	17	-	10/14/90/117	-
22	CLA	A	805	-	-	16/39/115/115	-
29	CHL	6	302	17,22	1/1/14/21	14/35/111/117	-
22	CLA	7	311	24	-	2/4/76/115	-
22	CLA	B	813	-	-	7/27/103/115	-
22	CLA	B	807	-	-	5/15/91/115	-
22	CLA	8	311	-	-	7/24/100/115	-
22	CLA	9	306	-	-	8/24/100/115	-
22	CLA	7	307	22	-	5/18/94/115	-
25	8CT	1	316	13	-	11/29/63/63	0/2/2/2
22	CLA	7	316	18	-	20/39/115/115	-
22	CLA	A	801	-	-	10/39/115/115	-
25	8CT	I	101	-	-	10/29/63/63	0/2/2/2
22	CLA	1	313	-	-	9/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	3	316	-	-	12/29/63/63	0/2/2/2
22	CLA	A	814	-	-	12/15/91/115	-
22	CLA	B	801	-	-	10/39/115/115	-
22	CLA	A	813	-	-	16/39/115/115	-
22	CLA	7	306	22	-	4/12/88/115	-
22	CLA	5	314	24	-	11/17/93/115	-
25	8CT	A	854	-	-	12/29/63/63	0/2/2/2
22	CLA	7	309	22	-	6/21/97/115	-
31	LMG	4	318	-	-	19/39/59/70	0/1/1/1
22	CLA	2	311	14	-	7/24/100/115	-
29	CHL	9	302	19	1/1/14/21	11/35/111/117	-
22	CLA	B	828	-	-	16/39/115/115	-
29	CHL	6	307	-	-	6/14/90/117	-
22	CLA	2	312	14	-	15/39/115/115	-
22	CLA	4	302	-	-	10/33/109/115	-
22	CLA	8	313	16	-	3/15/91/115	-
29	CHL	2	306	-	-	8/20/96/117	-
22	CLA	3	304	-	-	5/12/88/115	-
22	CLA	A	819	-	-	14/39/115/115	-
22	CLA	4	311	22	-	10/24/100/115	-
22	CLA	A	830	1	-	11/39/115/115	-
22	CLA	0	307	22	-	28/39/115/115	-
22	CLA	8	310	31	-	8/27/103/115	-
25	8CT	B	843	-	-	16/29/63/63	0/2/2/2
30	XAT	9	315	-	-	0/31/93/93	0/4/4/4
29	CHL	2	307	-	-	11/23/99/117	-
29	CHL	7	308	-	-	10/19/95/117	-
27	SF4	B	802	-	-	-	0/6/5/5
29	CHL	4	305	29	1/1/13/21	13/29/105/117	-
22	CLA	A	843	24	-	11/24/100/115	-
25	8CT	G	104	-	-	13/29/63/63	0/2/2/2
25	8CT	7	321	-	-	10/29/63/63	0/2/2/2
22	CLA	3	319	-	-	23/39/115/115	-
29	CHL	8	307	30	-	9/23/99/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	303	17	-	16/39/115/115	-
22	CLA	2	310	24	-	5/10/86/115	-
22	CLA	3	307	15	-	10/21/97/115	-
22	CLA	5	308	-	-	4/12/88/115	-
22	CLA	A	840	-	-	16/39/115/115	-
22	CLA	A	806	1	-	22/39/115/115	-
22	CLA	0	312	29,20	-	10/27/103/115	-
22	CLA	B	840	-	-	15/39/115/115	-
22	CLA	A	828	-	-	18/39/115/115	-
22	CLA	B	806	-	-	17/39/115/115	-
22	CLA	3	309	24	-	0/4/76/115	-
22	CLA	M	101	-	-	8/17/93/115	-
29	CHL	0	306	30,22	-	5/20/96/117	-
22	CLA	9	303	19	-	14/39/115/115	-
22	CLA	A	838	-	-	16/39/115/115	-
30	XAT	8	316	29	-	7/31/93/93	0/4/4/4
22	CLA	0	305	29,22	-	10/24/100/115	-
25	8CT	J	104	-	-	7/29/63/63	0/2/2/2
22	CLA	1	306	-	-	14/39/115/115	-
25	8CT	7	323	-	-	14/29/63/63	0/2/2/2
22	CLA	5	304	-	-	10/24/100/115	-
25	8CT	L	205	22	-	13/29/63/63	0/2/2/2
22	CLA	B	820	-	-	11/39/115/115	-
22	CLA	9	311	-	-	6/24/100/115	-
29	CHL	6	308	-	-	8/23/99/117	-
22	CLA	6	304	17	-	17/39/115/115	-
29	CHL	4	307	-	-	5/23/99/117	-
22	CLA	8	309	-	-	9/33/109/115	-
27	SF4	C	102	3	-	-	0/6/5/5
22	CLA	1	312	29,13	-	10/27/103/115	-
25	8CT	B	848	-	-	10/29/63/63	0/2/2/2
30	XAT	5	315	22	-	6/31/93/93	0/4/4/4
22	CLA	A	824	-	-	10/27/103/115	-
22	CLA	7	310	18	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	105	-	-	11/21/97/115	-
22	CLA	B	850	-	-	11/27/103/115	-
25	8CT	F	302	-	-	9/29/63/63	0/2/2/2
22	CLA	7	315	18	-	4/17/93/115	-
22	CLA	B	836	2	-	13/33/109/115	-
22	CLA	A	826	25	-	15/39/115/115	-
30	XAT	3	314	25	-	4/31/93/93	0/4/4/4
24	LHG	A	844	-	-	25/53/53/53	-
22	CLA	2	308	-	-	5/21/97/115	-
22	CLA	A	841	25	-	15/39/115/115	-
22	CLA	K	102	-	-	9/17/93/115	-
25	8CT	B	844	-	-	15/29/63/63	0/2/2/2
22	CLA	L	202	-	-	15/39/115/115	-
30	XAT	7	320	-	-	0/31/93/93	0/4/4/4
22	CLA	5	311	30	-	1/15/91/115	-
22	CLA	9	308	-	-	18/39/115/115	-
22	CLA	A	829	-	-	10/39/115/115	-
22	CLA	B	841	24	-	15/39/115/115	-
22	CLA	B	817	-	-	12/27/103/115	-
25	8CT	A	849	22	-	11/29/63/63	0/2/2/2
22	CLA	A	809	1	-	15/39/115/115	-
22	CLA	5	305	25	-	8/24/100/115	-
22	CLA	5	307	-	-	18/39/115/115	-
22	CLA	5	312	13,30	-	12/39/115/115	-
29	CHL	8	305	-	1/1/13/21	9/29/105/117	-
22	CLA	A	832	-	-	18/39/115/115	-
22	CLA	B	835	-	-	5/15/91/115	-
22	CLA	A	811	1,22	-	20/39/115/115	-
22	CLA	B	827	-	-	18/39/115/115	-
29	CHL	0	301	24,22	1/1/14/21	17/35/111/117	-
22	CLA	8	303	31,16,22	-	5/17/93/115	-
22	CLA	1	309	24	-	4/10/86/115	-
22	CLA	4	312	16	-	8/29/105/115	-
29	CHL	4	306	29	-	7/23/99/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	6	306	-	-	2/14/90/117	-
22	CLA	B	818	2	-	14/32/108/115	-
25	8CT	B	804	-	-	15/29/63/63	0/2/2/2
22	CLA	A	839	-	-	19/39/115/115	-
22	CLA	9	305	-	-	8/24/100/115	-
22	CLA	A	823	-	-	7/23/99/115	-
22	CLA	2	313	14	-	4/13/89/115	-
22	CLA	9	304	-	-	8/19/95/115	-
22	CLA	L	204	-	-	11/21/97/115	-
22	CLA	A	853	-	-	16/39/115/115	-
25	8CT	4	317	-	-	8/29/63/63	0/2/2/2
25	8CT	5	317	22	-	10/29/63/63	0/2/2/2
22	CLA	6	309	17	-	10/21/97/115	-
22	CLA	B	833	-	-	15/31/107/115	-
25	8CT	A	848	-	-	6/29/63/63	0/2/2/2
22	CLA	7	304	22	-	8/18/94/115	-
22	CLA	7	305	-	-	10/15/91/115	-
22	CLA	1	303	-	-	10/24/100/115	-
30	XAT	2	316	-	-	3/31/93/93	0/4/4/4
22	CLA	0	308	20	-	16/33/109/115	-
22	CLA	0	310	30	-	4/24/100/115	-
22	CLA	3	303	-	-	7/15/91/115	-
22	CLA	B	819	-	-	19/33/109/115	-
23	PQN	B	842	-	-	5/23/43/43	0/2/2/2
22	CLA	A	834	-	-	3/21/97/115	-
22	CLA	B	830	2	-	9/39/115/115	-
22	CLA	1	311	13	-	15/39/115/115	-
29	CHL	2	305	-	-	3/14/90/117	-
22	CLA	B	834	2	-	18/39/115/115	-
30	XAT	4	316	-	-	3/31/93/93	0/4/4/4
22	CLA	A	807	1	-	15/39/115/115	-
22	CLA	G	103	7	-	9/17/93/115	-
22	CLA	3	311	-	-	13/27/103/115	-
30	XAT	0	313	22	-	16/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	B	845	-	-	12/29/63/63	0/2/2/2
25	8CT	J	101	-	-	9/29/63/63	0/2/2/2
30	XAT	3	315	-	-	0/31/93/93	0/4/4/4
29	CHL	4	301	13,22	1/1/14/21	11/35/111/117	-
30	XAT	4	315	22	-	8/31/93/93	0/4/4/4
22	CLA	2	314	14	-	9/20/96/115	-
22	CLA	6	315	-	-	16/39/115/115	-
22	CLA	0	311	-	-	16/39/115/115	-
24	LHG	5	318	22	-	29/53/53/53	-
25	8CT	A	846	25	-	13/29/63/63	0/2/2/2
22	CLA	3	305	15	-	10/18/94/115	-
22	CLA	9	310	24	-	6/10/86/115	-
22	CLA	A	815	1	-	3/18/94/115	-
25	8CT	B	846	-	-	13/29/63/63	0/2/2/2
22	CLA	6	317	-	-	7/15/91/115	-
22	CLA	0	304	22	-	13/24/100/115	-
22	CLA	A	812	-	-	3/26/102/115	-
29	CHL	9	307	-	-	10/20/96/117	-
22	CLA	B	832	-	-	14/39/115/115	-
22	CLA	B	812	2	-	13/39/115/115	-
22	CLA	3	312	15	-	7/15/91/115	-
22	CLA	B	811	2	-	11/39/115/115	-
29	CHL	3	306	25	-	3/19/95/117	-
22	CLA	9	301	2	-	6/16/92/115	-
24	LHG	0	315	29,22	-	27/53/53/53	-
25	8CT	7	301	29,30	-	11/29/63/63	0/2/2/2
22	CLA	F	301	-	-	10/15/91/115	-
25	8CT	3	318	22,25	-	6/29/63/63	0/2/2/2
22	CLA	1	302	-	-	23/39/115/115	-
22	CLA	7	312	30	-	5/24/100/115	-
22	CLA	5	310	24	-	5/10/86/115	-
22	CLA	A	822	-	-	12/20/96/115	-
22	CLA	7	317	-	-	21/39/115/115	-
25	8CT	8	301	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	XAT	0	314	29,22	-	8/31/93/93	0/4/4/4
26	HTG	A	851	-	-	4/10/30/30	0/1/1/1
22	CLA	7	313	18	-	15/27/103/115	-
25	8CT	B	851	22	-	15/29/63/63	0/2/2/2
30	XAT	6	320	-	-	4/31/93/93	0/4/4/4
22	CLA	4	310	-	-	9/27/103/115	-
22	CLA	A	837	1	-	19/39/115/115	-
22	CLA	B	838	-	-	4/18/94/115	-
22	CLA	4	309	30	-	14/33/109/115	-
22	CLA	A	802	-	-	8/39/115/115	-
22	CLA	A	821	-	-	9/39/115/115	-
29	CHL	8	306	-	-	9/23/99/117	-
22	CLA	4	308	16	-	1/21/97/115	-
30	XAT	1	315	-	-	1/31/93/93	0/4/4/4
24	LHG	6	322	22	-	22/41/41/53	-
22	CLA	6	311	24	-	22/39/115/115	-
22	CLA	6	323	16	-	13/17/93/115	-
22	CLA	8	302	-	-	7/33/109/115	-
22	CLA	B	808	-	-	18/39/115/115	-
28	DGD	B	849	-	-	31/55/95/95	0/2/2/2
22	CLA	5	309	13,30	-	10/33/109/115	-
24	LHG	3	317	22	-	12/23/23/53	-
22	CLA	2	304	-	-	16/33/109/115	-
25	8CT	K	103	-	-	12/29/63/63	0/2/2/2
22	CLA	B	809	2	-	20/39/115/115	-
22	CLA	1	307	-	-	18/39/115/115	-
30	XAT	2	315	-	-	2/31/93/93	0/4/4/4
22	CLA	2	302	29	-	17/39/115/115	-

All (3601) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	318	8CT	C02-C03	14.68	1.59	1.34
25	5	317	8CT	C02-C03	14.38	1.59	1.34
25	K	103	8CT	C32-C31	14.37	1.61	1.32
25	7	301	8CT	C02-C03	14.33	1.59	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	316	8CT	C02-C03	14.33	1.59	1.34
25	B	844	8CT	C02-C03	14.33	1.59	1.34
25	J	101	8CT	C02-C03	14.29	1.59	1.34
25	8	301	8CT	C02-C03	14.29	1.59	1.34
25	L	205	8CT	C02-C03	14.29	1.59	1.34
25	A	847	8CT	C02-C03	14.28	1.59	1.34
25	A	848	8CT	C02-C03	14.28	1.59	1.34
25	B	851	8CT	C02-C03	14.28	1.59	1.34
25	A	854	8CT	C02-C03	14.27	1.59	1.34
25	B	847	8CT	C02-C03	14.27	1.59	1.34
25	G	104	8CT	C02-C03	14.26	1.59	1.34
25	L	206	8CT	C02-C03	14.25	1.59	1.34
25	B	848	8CT	C02-C03	14.25	1.59	1.34
25	4	317	8CT	C02-C03	14.22	1.59	1.34
25	8	318	8CT	C02-C03	14.17	1.59	1.34
25	A	849	8CT	C02-C03	14.17	1.59	1.34
25	B	846	8CT	C02-C03	14.16	1.59	1.34
25	2	317	8CT	C02-C03	14.14	1.58	1.34
25	F	302	8CT	C02-C03	14.14	1.58	1.34
25	J	104	8CT	C02-C03	14.14	1.58	1.34
25	7	323	8CT	C02-C03	14.14	1.58	1.34
25	3	316	8CT	C02-C03	14.11	1.58	1.34
25	6	321	8CT	C02-C03	14.08	1.58	1.34
25	K	103	8CT	C02-C03	14.07	1.58	1.34
25	I	101	8CT	C02-C03	14.07	1.58	1.34
25	A	846	8CT	C02-C03	14.04	1.58	1.34
25	7	321	8CT	C02-C03	14.03	1.58	1.34
25	B	845	8CT	C02-C03	14.03	1.58	1.34
25	A	850	8CT	C02-C03	14.02	1.58	1.34
25	B	804	8CT	C02-C03	14.00	1.58	1.34
25	B	843	8CT	C02-C03	14.00	1.58	1.34
25	4	317	8CT	C32-C31	13.97	1.60	1.32
25	L	205	8CT	C32-C31	13.93	1.60	1.32
25	B	843	8CT	C32-C31	13.89	1.60	1.32
25	G	104	8CT	C32-C31	13.86	1.60	1.32
25	7	323	8CT	C32-C31	13.85	1.60	1.32
25	1	316	8CT	C32-C31	13.84	1.59	1.32
25	A	850	8CT	C32-C31	13.82	1.59	1.32
25	A	849	8CT	C32-C31	13.82	1.59	1.32
25	J	104	8CT	C32-C31	13.82	1.59	1.32
25	5	317	8CT	C32-C31	13.82	1.59	1.32
25	3	318	8CT	C32-C31	13.82	1.59	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	318	8CT	C32-C31	13.80	1.59	1.32
25	B	848	8CT	C32-C31	13.79	1.59	1.32
25	6	321	8CT	C32-C31	13.78	1.59	1.32
25	8	301	8CT	C32-C31	13.75	1.59	1.32
25	B	851	8CT	C32-C31	13.73	1.59	1.32
25	2	317	8CT	C32-C31	13.73	1.59	1.32
25	B	847	8CT	C32-C31	13.73	1.59	1.32
25	3	316	8CT	C32-C31	13.73	1.59	1.32
25	7	321	8CT	C32-C31	13.72	1.59	1.32
25	A	854	8CT	C32-C31	13.72	1.59	1.32
25	B	845	8CT	C32-C31	13.69	1.59	1.32
25	B	846	8CT	C32-C31	13.69	1.59	1.32
25	L	206	8CT	C32-C31	13.62	1.59	1.32
25	B	804	8CT	C32-C31	13.58	1.59	1.32
25	J	101	8CT	C32-C31	13.52	1.59	1.32
25	7	301	8CT	C32-C31	13.45	1.59	1.32
25	F	302	8CT	C32-C31	13.44	1.59	1.32
25	A	847	8CT	C32-C31	13.43	1.59	1.32
25	A	846	8CT	C32-C31	13.42	1.59	1.32
25	A	848	8CT	C32-C31	13.38	1.59	1.32
25	B	844	8CT	C32-C31	13.29	1.58	1.32
25	I	101	8CT	C32-C31	13.19	1.58	1.32
25	A	847	8CT	C34-C35	-8.55	1.36	1.54
25	B	843	8CT	C34-C35	-8.25	1.37	1.54
25	B	851	8CT	C34-C35	-8.25	1.37	1.54
25	F	302	8CT	C34-C35	-8.21	1.37	1.54
25	3	318	8CT	C34-C35	-8.20	1.37	1.54
25	L	205	8CT	C34-C35	-8.14	1.37	1.54
25	B	804	8CT	C34-C35	-8.07	1.37	1.54
25	A	849	8CT	C34-C35	-8.06	1.37	1.54
25	A	850	8CT	C34-C35	-8.02	1.37	1.54
25	A	848	8CT	C34-C35	-8.02	1.37	1.54
25	8	301	8CT	C34-C35	-8.01	1.37	1.54
25	B	845	8CT	C34-C35	-8.01	1.37	1.54
25	7	323	8CT	C34-C35	-7.98	1.37	1.54
25	7	321	8CT	C34-C35	-7.98	1.37	1.54
25	8	318	8CT	C34-C35	-7.98	1.37	1.54
25	3	316	8CT	C34-C35	-7.97	1.37	1.54
25	A	854	8CT	C34-C35	-7.97	1.37	1.54
25	I	101	8CT	C34-C35	-7.96	1.37	1.54
25	4	317	8CT	C34-C35	-7.94	1.37	1.54
25	1	316	8CT	C34-C35	-7.94	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	847	8CT	C34-C35	-7.93	1.37	1.54
25	B	846	8CT	C34-C35	-7.91	1.37	1.54
25	B	848	8CT	C34-C35	-7.91	1.37	1.54
25	7	301	8CT	C34-C35	-7.91	1.37	1.54
25	J	104	8CT	C34-C35	-7.90	1.37	1.54
25	B	844	8CT	C34-C35	-7.88	1.37	1.54
25	2	317	8CT	C34-C35	-7.88	1.37	1.54
25	A	846	8CT	C34-C35	-7.86	1.38	1.54
25	6	321	8CT	C34-C35	-7.86	1.38	1.54
25	G	104	8CT	C34-C35	-7.86	1.38	1.54
25	L	206	8CT	C34-C35	-7.70	1.38	1.54
25	5	317	8CT	C34-C35	-7.63	1.38	1.54
25	J	101	8CT	C34-C35	-7.62	1.38	1.54
25	K	103	8CT	C34-C35	-7.42	1.38	1.54
23	B	842	PQN	C3-C2	7.19	1.48	1.35
23	A	842	PQN	C3-C2	7.16	1.48	1.35
25	K	103	8CT	C28-C26	6.85	1.60	1.45
25	B	851	8CT	C15-C16	6.81	1.60	1.45
25	F	302	8CT	C05-C06	-6.80	1.35	1.52
25	3	318	8CT	C05-C06	-6.77	1.35	1.52
25	7	301	8CT	C05-C06	-6.73	1.36	1.52
25	A	847	8CT	C05-C06	-6.71	1.36	1.52
25	5	317	8CT	C28-C26	6.70	1.60	1.45
25	B	843	8CT	C05-C06	-6.68	1.36	1.52
25	4	317	8CT	C15-C16	6.66	1.60	1.45
25	L	205	8CT	C05-C06	-6.65	1.36	1.52
25	I	101	8CT	C05-C06	-6.64	1.36	1.52
25	A	846	8CT	C05-C06	-6.60	1.36	1.52
25	B	844	8CT	C05-C06	-6.59	1.36	1.52
25	B	845	8CT	C05-C06	-6.57	1.36	1.52
25	B	851	8CT	C05-C06	-6.56	1.36	1.52
25	K	103	8CT	C23-C21	6.56	1.60	1.45
25	B	844	8CT	C15-C16	6.55	1.60	1.45
25	B	846	8CT	C15-C16	6.55	1.60	1.45
25	G	104	8CT	C15-C16	6.55	1.60	1.45
25	K	103	8CT	C15-C16	6.53	1.60	1.45
25	1	316	8CT	C15-C16	6.53	1.60	1.45
25	L	206	8CT	C05-C06	-6.53	1.36	1.52
25	J	101	8CT	C05-C06	-6.51	1.36	1.52
25	J	104	8CT	C05-C06	-6.46	1.36	1.52
25	8	318	8CT	C05-C06	-6.46	1.36	1.52
25	A	849	8CT	C05-C06	-6.45	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	317	8CT	C15-C16	6.45	1.59	1.45
25	6	321	8CT	C05-C06	-6.44	1.36	1.52
25	4	317	8CT	C05-C06	-6.44	1.36	1.52
25	8	301	8CT	C15-C16	6.44	1.59	1.45
25	8	318	8CT	C15-C16	6.42	1.59	1.45
25	B	804	8CT	C05-C06	-6.42	1.36	1.52
25	B	847	8CT	C05-C06	-6.42	1.36	1.52
25	B	848	8CT	C05-C06	-6.42	1.36	1.52
25	3	316	8CT	C15-C16	6.41	1.59	1.45
25	A	854	8CT	C05-C06	-6.41	1.36	1.52
25	1	316	8CT	C05-C06	-6.41	1.36	1.52
25	A	848	8CT	C05-C06	-6.41	1.36	1.52
25	J	101	8CT	C15-C16	6.40	1.59	1.45
25	B	848	8CT	C15-C16	6.40	1.59	1.45
25	8	301	8CT	C05-C06	-6.40	1.36	1.52
25	B	843	8CT	C15-C16	6.40	1.59	1.45
25	3	316	8CT	C05-C06	-6.40	1.36	1.52
25	1	316	8CT	C28-C26	6.39	1.59	1.45
25	B	846	8CT	C05-C06	-6.39	1.36	1.52
25	A	850	8CT	C05-C06	-6.38	1.36	1.52
25	F	302	8CT	C04-C03	-6.38	1.45	1.53
25	2	317	8CT	C05-C06	-6.38	1.36	1.52
25	5	317	8CT	C05-C06	-6.38	1.36	1.52
25	7	323	8CT	C05-C06	-6.38	1.36	1.52
25	J	104	8CT	C15-C16	6.37	1.59	1.45
25	7	321	8CT	C05-C06	-6.37	1.36	1.52
25	G	104	8CT	C28-C26	6.37	1.59	1.45
25	B	847	8CT	C15-C16	6.35	1.59	1.45
25	4	317	8CT	C28-C26	6.35	1.59	1.45
25	K	103	8CT	C05-C06	-6.35	1.36	1.52
25	A	849	8CT	C15-C16	6.35	1.59	1.45
25	6	321	8CT	C15-C16	6.34	1.59	1.45
25	B	846	8CT	C28-C26	6.33	1.59	1.45
25	A	854	8CT	C15-C16	6.33	1.59	1.45
25	5	317	8CT	C15-C16	6.33	1.59	1.45
25	2	317	8CT	C28-C26	6.31	1.59	1.45
25	L	206	8CT	C28-C26	6.31	1.59	1.45
25	7	323	8CT	C15-C16	6.31	1.59	1.45
25	7	321	8CT	C15-C16	6.30	1.59	1.45
25	7	323	8CT	C28-C26	6.30	1.59	1.45
25	B	845	8CT	C15-C16	6.30	1.59	1.45
25	B	843	8CT	C28-C26	6.29	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	104	8CT	C05-C06	-6.29	1.37	1.52
25	A	849	8CT	C28-C26	6.28	1.59	1.45
25	B	851	8CT	C23-C21	6.28	1.59	1.45
25	A	850	8CT	C15-C16	6.28	1.59	1.45
25	A	848	8CT	C15-C16	6.27	1.59	1.45
25	J	104	8CT	C28-C26	6.25	1.59	1.45
25	B	847	8CT	C28-C26	6.25	1.59	1.45
25	8	301	8CT	C28-C26	6.25	1.59	1.45
25	A	846	8CT	C15-C16	6.23	1.59	1.45
25	B	851	8CT	C28-C26	6.22	1.59	1.45
25	A	850	8CT	C28-C26	6.22	1.59	1.45
25	A	854	8CT	C28-C26	6.22	1.59	1.45
25	3	316	8CT	C28-C26	6.21	1.59	1.45
25	J	101	8CT	C28-C26	6.21	1.59	1.45
25	8	318	8CT	C28-C26	6.19	1.59	1.45
25	7	321	8CT	C28-C26	6.16	1.59	1.45
25	6	321	8CT	C28-C26	6.16	1.59	1.45
25	7	301	8CT	C15-C16	6.14	1.59	1.45
25	B	848	8CT	C28-C26	6.13	1.59	1.45
25	L	206	8CT	C15-C16	6.10	1.59	1.45
25	A	847	8CT	C15-C16	6.05	1.58	1.45
25	B	843	8CT	C23-C21	6.04	1.58	1.45
25	L	205	8CT	C28-C26	6.04	1.58	1.45
25	B	844	8CT	C23-C21	6.02	1.58	1.45
25	3	318	8CT	C15-C16	5.98	1.58	1.45
25	B	845	8CT	C28-C26	5.98	1.58	1.45
25	A	847	8CT	C28-C26	5.97	1.58	1.45
25	G	104	8CT	C23-C21	5.96	1.58	1.45
25	A	848	8CT	C28-C26	5.96	1.58	1.45
25	B	848	8CT	C23-C21	5.95	1.58	1.45
25	B	804	8CT	C15-C16	5.94	1.58	1.45
25	B	845	8CT	C23-C21	5.94	1.58	1.45
25	2	317	8CT	C23-C21	5.94	1.58	1.45
25	F	302	8CT	C28-C26	5.93	1.58	1.45
25	I	101	8CT	C15-C16	5.93	1.58	1.45
25	4	317	8CT	C23-C21	5.92	1.58	1.45
25	B	844	8CT	C28-C26	5.92	1.58	1.45
25	A	846	8CT	C28-C26	5.91	1.58	1.45
25	1	316	8CT	C23-C21	5.89	1.58	1.45
25	L	205	8CT	C15-C16	5.89	1.58	1.45
25	B	804	8CT	C28-C26	5.88	1.58	1.45
25	J	104	8CT	C23-C21	5.88	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	847	8CT	C23-C21	5.87	1.58	1.45
25	3	316	8CT	C23-C21	5.86	1.58	1.45
25	L	206	8CT	C23-C21	5.86	1.58	1.45
25	8	318	8CT	C23-C21	5.86	1.58	1.45
25	7	323	8CT	C23-C21	5.85	1.58	1.45
25	J	101	8CT	C23-C21	5.84	1.58	1.45
25	8	301	8CT	C23-C21	5.84	1.58	1.45
25	7	301	8CT	C28-C26	5.83	1.58	1.45
25	A	849	8CT	C23-C21	5.83	1.58	1.45
25	3	318	8CT	C28-C26	5.82	1.58	1.45
25	B	804	8CT	C04-C03	-5.80	1.45	1.53
25	6	321	8CT	C23-C21	5.80	1.58	1.45
25	A	848	8CT	C23-C21	5.79	1.58	1.45
25	A	850	8CT	C23-C21	5.77	1.58	1.45
25	A	854	8CT	C23-C21	5.76	1.58	1.45
25	B	846	8CT	C23-C21	5.76	1.58	1.45
25	5	317	8CT	C23-C21	5.76	1.58	1.45
25	K	103	8CT	C34-C33	5.75	1.66	1.52
25	7	321	8CT	C23-C21	5.75	1.58	1.45
25	5	317	8CT	C34-C33	5.72	1.66	1.52
25	I	101	8CT	C04-C03	-5.70	1.45	1.53
25	A	846	8CT	C04-C03	-5.70	1.45	1.53
25	B	843	8CT	C04-C03	-5.69	1.46	1.53
25	7	323	8CT	C04-C03	-5.67	1.46	1.53
25	6	321	8CT	C04-C03	-5.67	1.46	1.53
25	A	849	8CT	C04-C03	-5.67	1.46	1.53
25	F	302	8CT	C15-C16	5.67	1.58	1.45
25	J	101	8CT	C34-C33	5.66	1.65	1.52
25	A	846	8CT	C23-C21	5.65	1.58	1.45
25	A	847	8CT	C04-C03	-5.64	1.46	1.53
25	L	206	8CT	C04-C03	-5.64	1.46	1.53
25	B	845	8CT	C04-C03	-5.63	1.46	1.53
25	I	101	8CT	C28-C26	5.63	1.58	1.45
25	L	206	8CT	C34-C33	5.62	1.65	1.52
25	3	318	8CT	C23-C21	5.62	1.58	1.45
25	7	301	8CT	C23-C21	5.62	1.58	1.45
25	L	205	8CT	C23-C21	5.61	1.58	1.45
25	B	844	8CT	C34-C33	5.60	1.65	1.52
25	B	847	8CT	C34-C33	5.60	1.65	1.52
25	7	321	8CT	C04-C03	-5.58	1.46	1.53
25	K	103	8CT	C04-C03	-5.58	1.46	1.53
25	J	104	8CT	C34-C33	5.58	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	848	8CT	C34-C33	5.57	1.65	1.52
25	I	101	8CT	C34-C33	5.55	1.65	1.52
25	G	104	8CT	C34-C33	5.54	1.65	1.52
25	A	850	8CT	C34-C33	5.54	1.65	1.52
25	F	302	8CT	C23-C21	5.54	1.57	1.45
25	6	321	8CT	C34-C33	5.53	1.65	1.52
25	A	850	8CT	C04-C03	-5.52	1.46	1.53
25	J	104	8CT	C04-C03	-5.52	1.46	1.53
25	G	104	8CT	C04-C03	-5.50	1.46	1.53
25	B	846	8CT	C34-C33	5.50	1.65	1.52
25	B	848	8CT	C04-C03	-5.49	1.46	1.53
25	A	846	8CT	C34-C33	5.49	1.65	1.52
25	7	321	8CT	C34-C33	5.48	1.65	1.52
25	J	101	8CT	C04-C03	-5.48	1.46	1.53
25	8	318	8CT	C04-C03	-5.48	1.46	1.53
25	B	846	8CT	C04-C03	-5.47	1.46	1.53
25	A	854	8CT	C04-C03	-5.47	1.46	1.53
25	2	317	8CT	C04-C03	-5.47	1.46	1.53
25	3	316	8CT	C34-C33	5.46	1.65	1.52
25	1	316	8CT	C34-C33	5.46	1.65	1.52
25	2	317	8CT	C34-C33	5.45	1.65	1.52
25	4	317	8CT	C34-C33	5.45	1.65	1.52
25	8	301	8CT	C34-C33	5.45	1.65	1.52
25	8	318	8CT	C34-C33	5.44	1.65	1.52
25	5	317	8CT	C04-C03	-5.44	1.46	1.53
25	4	317	8CT	C04-C03	-5.43	1.46	1.53
25	A	854	8CT	C34-C33	5.43	1.65	1.52
25	I	101	8CT	C23-C21	5.42	1.57	1.45
25	3	316	8CT	C04-C03	-5.42	1.46	1.53
25	3	318	8CT	C04-C03	-5.41	1.46	1.53
25	8	301	8CT	C04-C03	-5.40	1.46	1.53
25	B	844	8CT	C04-C03	-5.40	1.46	1.53
25	7	323	8CT	C34-C33	5.40	1.65	1.52
25	A	848	8CT	C04-C03	-5.39	1.46	1.53
29	1	305	CHL	O2D-CGD	5.38	1.46	1.33
29	3	306	CHL	C3D-C4D	-5.38	1.32	1.44
25	A	849	8CT	C34-C33	5.37	1.65	1.52
29	7	308	CHL	C3D-C4D	-5.35	1.32	1.44
25	1	316	8CT	C04-C03	-5.34	1.46	1.53
25	B	804	8CT	C23-C21	5.34	1.57	1.45
25	B	847	8CT	C04-C03	-5.33	1.46	1.53
25	B	804	8CT	C34-C33	5.33	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	301	8CT	C34-C33	5.32	1.65	1.52
25	B	845	8CT	C34-C33	5.28	1.65	1.52
25	G	104	8CT	C05-C04	5.25	1.66	1.54
25	A	847	8CT	C23-C21	5.25	1.57	1.45
25	L	205	8CT	C34-C33	5.25	1.64	1.52
25	B	851	8CT	C04-C03	-5.24	1.46	1.53
29	2	306	CHL	C3D-C4D	-5.24	1.32	1.44
25	A	848	8CT	C05-C04	5.22	1.66	1.54
29	8	314	CHL	O2D-CGD	5.21	1.45	1.33
25	A	848	8CT	C34-C33	5.20	1.64	1.52
25	A	850	8CT	C05-C04	5.20	1.66	1.54
25	B	847	8CT	C05-C04	5.20	1.66	1.54
29	2	307	CHL	C3D-C4D	-5.19	1.32	1.44
25	7	321	8CT	C05-C04	5.18	1.66	1.54
29	5	301	CHL	C3D-C4D	-5.17	1.32	1.44
29	6	316	CHL	O2D-CGD	5.16	1.45	1.33
25	5	317	8CT	C05-C04	5.16	1.66	1.54
29	2	305	CHL	C3D-C4D	-5.15	1.32	1.44
25	1	316	8CT	C05-C04	5.15	1.66	1.54
29	5	306	CHL	O2D-CGD	5.14	1.45	1.33
25	A	854	8CT	C05-C04	5.14	1.66	1.54
25	8	318	8CT	C05-C04	5.13	1.66	1.54
25	B	843	8CT	C34-C33	5.11	1.64	1.52
25	B	848	8CT	C05-C04	5.11	1.65	1.54
25	B	846	8CT	C05-C04	5.11	1.65	1.54
25	J	101	8CT	C05-C04	5.10	1.65	1.54
25	K	103	8CT	C05-C04	5.10	1.65	1.54
29	4	305	CHL	C3D-C4D	-5.10	1.32	1.44
25	A	849	8CT	C05-C04	5.09	1.65	1.54
25	8	301	8CT	C05-C04	5.09	1.65	1.54
25	F	302	8CT	C34-C33	5.09	1.64	1.52
25	6	321	8CT	C05-C04	5.09	1.65	1.54
29	4	301	CHL	C3D-C4D	-5.09	1.32	1.44
25	2	317	8CT	C05-C04	5.08	1.65	1.54
25	3	316	8CT	C05-C04	5.06	1.65	1.54
29	4	306	CHL	C3D-C4D	-5.05	1.32	1.44
25	B	845	8CT	C05-C04	5.05	1.65	1.54
29	9	307	CHL	O2D-CGD	5.05	1.45	1.33
29	4	307	CHL	C3D-C4D	-5.05	1.32	1.44
29	8	306	CHL	O2D-CGD	5.04	1.45	1.33
29	0	301	CHL	O2D-CGD	5.04	1.45	1.33
29	2	301	CHL	C3D-C4D	-5.03	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	306	CHL	O2D-CGD	5.03	1.45	1.33
25	3	318	8CT	C34-C33	5.02	1.64	1.52
29	0	306	CHL	O2D-CGD	5.02	1.45	1.33
29	8	307	CHL	C3D-C4D	-5.02	1.32	1.44
25	7	323	8CT	C05-C04	5.02	1.65	1.54
25	A	847	8CT	C34-C33	5.01	1.64	1.52
25	B	851	8CT	C34-C33	5.01	1.64	1.52
25	7	301	8CT	C05-C04	5.01	1.65	1.54
25	J	104	8CT	C05-C04	5.01	1.65	1.54
29	6	307	CHL	C3D-C4D	-5.01	1.32	1.44
29	6	306	CHL	C3D-C4D	-5.00	1.32	1.44
29	6	302	CHL	C3D-C4D	-5.00	1.32	1.44
25	L	206	8CT	C05-C04	4.99	1.65	1.54
25	4	317	8CT	C05-C04	4.99	1.65	1.54
29	4	305	CHL	O2D-CGD	4.98	1.45	1.33
29	6	308	CHL	C3D-C4D	-4.97	1.33	1.44
29	8	306	CHL	C3D-C4D	-4.97	1.33	1.44
29	2	306	CHL	O2D-CGD	4.96	1.45	1.33
29	8	314	CHL	C3D-C4D	-4.95	1.33	1.44
29	9	307	CHL	C3D-C4D	-4.95	1.33	1.44
29	8	305	CHL	C3D-C4D	-4.95	1.33	1.44
29	6	316	CHL	C3D-C4D	-4.95	1.33	1.44
29	1	305	CHL	C3D-C4D	-4.94	1.33	1.44
29	9	302	CHL	O2D-CGD	4.94	1.45	1.33
25	B	844	8CT	C05-C04	4.94	1.65	1.54
29	0	306	CHL	C3D-C4D	-4.91	1.33	1.44
25	B	851	8CT	C05-C04	4.91	1.65	1.54
25	L	205	8CT	C05-C04	4.91	1.65	1.54
25	L	205	8CT	C04-C03	-4.91	1.47	1.53
25	B	804	8CT	C05-C04	4.90	1.65	1.54
29	6	307	CHL	O2D-CGD	4.89	1.45	1.33
29	6	302	CHL	O2D-CGD	4.88	1.45	1.33
29	0	301	CHL	C3D-C4D	-4.87	1.33	1.44
29	9	302	CHL	C3D-C4D	-4.86	1.33	1.44
25	A	846	8CT	C05-C04	4.85	1.65	1.54
25	7	301	8CT	C04-C03	-4.84	1.47	1.53
25	B	843	8CT	C05-C04	4.84	1.65	1.54
29	8	307	CHL	O2D-CGD	4.81	1.44	1.33
29	4	306	CHL	O2D-CGD	4.81	1.44	1.33
25	3	318	8CT	C05-C04	4.80	1.65	1.54
29	2	301	CHL	O2D-CGD	4.77	1.44	1.33
29	3	306	CHL	O2D-CGD	4.77	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	308	CHL	O2D-CGD	4.77	1.44	1.33
25	I	101	8CT	C05-C04	4.75	1.65	1.54
29	8	305	CHL	O2D-CGD	4.74	1.44	1.33
25	K	103	8CT	C06-C07	4.72	1.67	1.52
25	7	301	8CT	C19-C20	4.72	1.58	1.43
29	5	306	CHL	C3D-C4D	-4.72	1.33	1.44
29	6	308	CHL	O2D-CGD	4.72	1.44	1.33
25	J	104	8CT	C06-C07	4.70	1.67	1.52
25	B	846	8CT	C06-C07	4.69	1.67	1.52
25	B	851	8CT	C19-C20	4.69	1.58	1.43
25	7	323	8CT	C06-C07	4.68	1.67	1.52
25	G	104	8CT	C06-C07	4.68	1.67	1.52
25	B	848	8CT	C06-C07	4.68	1.67	1.52
29	0	306	CHL	C2C-C3C	4.67	1.46	1.36
29	0	301	CHL	CHC-C1C	4.66	1.48	1.38
25	A	850	8CT	C06-C07	4.66	1.67	1.52
25	1	316	8CT	C06-C07	4.66	1.67	1.52
25	A	847	8CT	C05-C04	4.65	1.64	1.54
25	5	317	8CT	C06-C07	4.65	1.67	1.52
25	6	321	8CT	C06-C07	4.64	1.67	1.52
29	5	301	CHL	O2D-CGD	4.64	1.44	1.33
25	4	317	8CT	C19-C20	4.63	1.57	1.43
25	B	844	8CT	C19-C20	4.62	1.57	1.43
25	B	847	8CT	C06-C07	4.62	1.67	1.52
25	7	321	8CT	C06-C07	4.62	1.67	1.52
25	8	318	8CT	C06-C07	4.62	1.67	1.52
25	A	849	8CT	C06-C07	4.61	1.67	1.52
25	3	316	8CT	C06-C07	4.61	1.67	1.52
29	4	306	CHL	CHD-C1D	4.60	1.47	1.38
25	2	317	8CT	C06-C07	4.60	1.67	1.52
25	B	844	8CT	C06-C07	4.60	1.67	1.52
25	B	804	8CT	C06-C07	4.60	1.67	1.52
25	8	301	8CT	C06-C07	4.59	1.66	1.52
25	A	854	8CT	C06-C07	4.59	1.66	1.52
25	B	843	8CT	C19-C20	4.59	1.57	1.43
25	A	848	8CT	C06-C07	4.58	1.66	1.52
25	4	317	8CT	C06-C07	4.58	1.66	1.52
25	F	302	8CT	C05-C04	4.58	1.64	1.54
29	6	307	CHL	CHC-C1C	4.58	1.47	1.38
25	1	316	8CT	C19-C20	4.58	1.57	1.43
29	4	307	CHL	O2D-CGD	4.56	1.44	1.33
25	G	104	8CT	C19-C20	4.56	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	103	8CT	C28-C29	4.56	1.43	1.32
29	4	306	CHL	CHC-C1C	4.56	1.47	1.38
29	5	306	CHL	C2C-C3C	4.55	1.46	1.36
29	5	301	CHL	CHC-C1C	4.53	1.47	1.38
25	8	318	8CT	C19-C20	4.52	1.57	1.43
25	8	301	8CT	C19-C20	4.52	1.57	1.43
25	A	846	8CT	C06-C07	4.52	1.66	1.52
29	2	306	CHL	CHC-C1C	4.52	1.47	1.38
25	I	101	8CT	C06-C07	4.51	1.66	1.52
25	J	101	8CT	C06-C07	4.51	1.66	1.52
25	J	104	8CT	C19-C20	4.51	1.57	1.43
25	K	103	8CT	C24-C25	4.51	1.57	1.43
29	9	307	CHL	C2C-C3C	4.50	1.46	1.36
29	2	307	CHL	O2D-CGD	4.50	1.44	1.33
25	7	323	8CT	C19-C20	4.50	1.57	1.43
29	1	305	CHL	CHC-C1C	4.50	1.47	1.38
29	0	301	CHL	C2C-C3C	4.50	1.46	1.36
25	B	851	8CT	C06-C07	4.49	1.66	1.52
29	0	306	CHL	CHD-C1D	4.49	1.47	1.38
25	B	848	8CT	C19-C20	4.49	1.57	1.43
25	A	854	8CT	C19-C20	4.49	1.57	1.43
29	2	305	CHL	O2D-CGD	4.49	1.44	1.33
25	L	206	8CT	C06-C07	4.48	1.66	1.52
25	3	316	8CT	C19-C20	4.48	1.57	1.43
25	L	206	8CT	C19-C20	4.48	1.57	1.43
25	K	103	8CT	C19-C20	4.47	1.57	1.43
25	B	845	8CT	C06-C07	4.47	1.66	1.52
25	5	317	8CT	C24-C25	4.46	1.57	1.43
25	J	101	8CT	C19-C20	4.46	1.57	1.43
25	B	843	8CT	C06-C07	4.46	1.66	1.52
25	B	847	8CT	C19-C20	4.46	1.57	1.43
25	A	849	8CT	C19-C20	4.45	1.57	1.43
25	B	846	8CT	C19-C20	4.45	1.57	1.43
29	4	305	CHL	O2A-CGA	4.44	1.46	1.33
25	A	846	8CT	C19-C20	4.44	1.57	1.43
25	A	847	8CT	C06-C07	4.43	1.66	1.52
29	6	302	CHL	CHC-C1C	4.43	1.47	1.38
25	A	850	8CT	C19-C20	4.43	1.57	1.43
29	4	306	CHL	C2C-C3C	4.42	1.46	1.36
25	5	317	8CT	C19-C20	4.41	1.57	1.43
25	7	321	8CT	C19-C20	4.40	1.57	1.43
29	0	301	CHL	O2A-CGA	4.40	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	321	8CT	C19-C20	4.40	1.57	1.43
29	8	305	CHL	O2A-CGA	4.40	1.46	1.33
25	L	205	8CT	C06-C07	4.40	1.66	1.52
25	A	848	8CT	C19-C20	4.39	1.57	1.43
29	4	301	CHL	O2A-CGA	4.39	1.46	1.33
29	8	306	CHL	O2A-CGA	4.38	1.46	1.33
25	F	302	8CT	C06-C07	4.38	1.66	1.52
25	7	301	8CT	C06-C07	4.38	1.66	1.52
29	9	307	CHL	CHC-C1C	4.37	1.47	1.38
29	6	308	CHL	CHC-C1C	4.37	1.47	1.38
25	2	317	8CT	C19-C20	4.37	1.57	1.43
29	1	305	CHL	O2A-CGA	4.37	1.46	1.33
29	0	301	CHL	CHD-C1D	4.37	1.46	1.38
25	3	318	8CT	C06-C07	4.37	1.66	1.52
29	5	301	CHL	C2C-C3C	4.36	1.46	1.36
25	B	843	8CT	C24-C25	4.35	1.56	1.43
29	8	314	CHL	CHC-C1C	4.35	1.47	1.38
29	5	306	CHL	CHD-C1D	4.34	1.46	1.38
29	0	306	CHL	O2A-CGA	4.34	1.46	1.33
29	6	302	CHL	C2C-C3C	4.34	1.46	1.36
29	6	307	CHL	C2C-C3C	4.34	1.46	1.36
29	6	316	CHL	C2C-C3C	4.34	1.46	1.36
29	8	314	CHL	C2C-C3C	4.34	1.46	1.36
29	9	307	CHL	O2A-CGA	4.33	1.46	1.33
25	B	804	8CT	C19-C20	4.33	1.56	1.43
29	4	301	CHL	O2D-CGD	4.33	1.43	1.33
29	2	301	CHL	O2A-CGA	4.33	1.46	1.33
29	4	307	CHL	O2A-CGA	4.33	1.46	1.33
25	L	205	8CT	C19-C20	4.32	1.56	1.43
25	A	846	8CT	C24-C25	4.32	1.56	1.43
29	6	316	CHL	CHC-C1C	4.31	1.47	1.38
25	B	845	8CT	C19-C20	4.31	1.56	1.43
29	9	307	CHL	CHD-C1D	4.31	1.46	1.38
29	8	305	CHL	CHC-C1C	4.31	1.47	1.38
29	1	305	CHL	CHD-C1D	4.30	1.46	1.38
29	6	308	CHL	O2A-CGA	4.30	1.45	1.33
25	L	205	8CT	C24-C25	4.29	1.56	1.43
29	6	307	CHL	CHD-C1D	4.28	1.46	1.38
29	4	305	CHL	CHC-C1C	4.27	1.47	1.38
25	B	851	8CT	C24-C25	4.27	1.56	1.43
29	5	306	CHL	O2A-CGA	4.27	1.45	1.33
29	8	306	CHL	CHC-C1C	4.27	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	308	CHL	CHC-C1C	4.27	1.47	1.38
25	3	318	8CT	C19-C20	4.27	1.56	1.43
29	5	301	CHL	O2A-CGA	4.26	1.45	1.33
29	6	308	CHL	C2C-C3C	4.25	1.45	1.36
29	5	306	CHL	CHC-C1C	4.25	1.47	1.38
29	8	305	CHL	C2C-C3C	4.25	1.45	1.36
25	B	846	8CT	C24-C25	4.24	1.56	1.43
29	6	316	CHL	CHD-C1D	4.24	1.46	1.38
29	9	302	CHL	O2A-CGA	4.24	1.45	1.33
25	4	317	8CT	C24-C25	4.24	1.56	1.43
25	B	844	8CT	C24-C25	4.23	1.56	1.43
29	6	302	CHL	O2A-CGA	4.22	1.45	1.33
29	8	307	CHL	CHD-C1D	4.22	1.46	1.38
29	2	306	CHL	O2A-CGA	4.22	1.45	1.33
29	8	314	CHL	CHD-C1D	4.21	1.46	1.38
25	I	101	8CT	C19-C20	4.21	1.56	1.43
25	G	104	8CT	C24-C25	4.21	1.56	1.43
29	2	307	CHL	O2A-CGA	4.20	1.45	1.33
25	A	847	8CT	C19-C20	4.20	1.56	1.43
29	4	305	CHL	C2C-C3C	4.20	1.45	1.36
29	4	301	CHL	C2C-C3C	4.19	1.45	1.36
25	1	316	8CT	C24-C25	4.19	1.56	1.43
25	8	318	8CT	C24-C25	4.19	1.56	1.43
25	A	848	8CT	C24-C25	4.18	1.56	1.43
29	0	306	CHL	CHC-C1C	4.18	1.47	1.38
29	8	307	CHL	C2C-C3C	4.18	1.45	1.36
22	B	814	CLA	C4D-ND	-4.18	1.32	1.37
25	2	317	8CT	C24-C25	4.17	1.56	1.43
29	4	306	CHL	O2A-CGA	4.17	1.45	1.33
25	B	848	8CT	C24-C25	4.17	1.56	1.43
25	3	316	8CT	C24-C25	4.16	1.56	1.43
25	B	845	8CT	C24-C25	4.16	1.56	1.43
29	9	302	CHL	CHC-C1C	4.16	1.47	1.38
25	F	302	8CT	C19-C20	4.16	1.56	1.43
25	A	854	8CT	C24-C25	4.16	1.56	1.43
25	B	847	8CT	C24-C25	4.16	1.56	1.43
25	J	104	8CT	C24-C25	4.15	1.56	1.43
29	4	305	CHL	CHD-C1D	4.15	1.46	1.38
29	9	302	CHL	C2C-C3C	4.14	1.45	1.36
25	L	206	8CT	C24-C25	4.14	1.56	1.43
25	7	323	8CT	C24-C25	4.14	1.56	1.43
25	8	301	8CT	C24-C25	4.14	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	101	8CT	C24-C25	4.12	1.56	1.43
22	A	805	CLA	C4D-ND	-4.12	1.32	1.37
29	2	306	CHL	C2C-C3C	4.12	1.45	1.36
29	2	306	CHL	CHD-C1D	4.11	1.46	1.38
23	B	842	PQN	C10-C5	4.10	1.47	1.40
29	6	302	CHL	CHD-C1D	4.10	1.46	1.38
25	A	849	8CT	C24-C25	4.10	1.56	1.43
29	8	306	CHL	C2C-C3C	4.09	1.45	1.36
29	4	301	CHL	CHC-C1C	4.09	1.46	1.38
29	7	308	CHL	C2C-C3C	4.09	1.45	1.36
29	1	305	CHL	C2C-C3C	4.09	1.45	1.36
25	A	850	8CT	C24-C25	4.07	1.56	1.43
22	5	308	CLA	C1D-ND	4.07	1.42	1.37
29	2	305	CHL	C2C-C3C	4.07	1.45	1.36
29	0	306	CHL	CHD-C4C	4.06	1.48	1.39
25	7	321	8CT	C24-C25	4.06	1.56	1.43
29	8	307	CHL	CHC-C1C	4.06	1.46	1.38
25	7	301	8CT	C24-C25	4.06	1.56	1.43
29	4	307	CHL	CHC-C1C	4.06	1.46	1.38
26	J	102	HTG	C1'-S1	-4.06	1.76	1.81
29	2	305	CHL	CHC-C1C	4.05	1.46	1.38
25	B	844	8CT	C14-C13	4.05	1.56	1.43
29	8	306	CHL	CHD-C1D	4.05	1.46	1.38
25	6	321	8CT	C24-C25	4.05	1.56	1.43
29	6	306	CHL	CHD-C1D	4.05	1.46	1.38
29	5	301	CHL	CHD-C1D	4.04	1.46	1.38
22	7	317	CLA	C4D-ND	-4.03	1.32	1.37
29	4	307	CHL	C2C-C3C	4.02	1.45	1.36
29	2	307	CHL	CHC-C1C	4.02	1.46	1.38
29	5	306	CHL	CHD-C4C	4.01	1.48	1.39
29	8	307	CHL	O2A-CGA	4.01	1.45	1.33
29	8	305	CHL	CHD-C1D	4.00	1.46	1.38
25	K	103	8CT	C25-C26	4.00	1.41	1.35
29	6	306	CHL	C2C-C3C	4.00	1.45	1.36
22	B	808	CLA	C4D-ND	-3.98	1.32	1.37
29	6	306	CHL	CHC-C1C	3.97	1.46	1.38
25	B	851	8CT	C14-C13	3.97	1.55	1.43
29	9	307	CHL	CHD-C4C	3.96	1.48	1.39
25	3	318	8CT	C24-C25	3.96	1.55	1.43
29	0	301	CHL	CHD-C4C	3.96	1.48	1.39
22	B	826	CLA	C4D-ND	-3.96	1.32	1.37
29	9	302	CHL	CHD-C1D	3.96	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	837	CLA	C4D-ND	-3.93	1.32	1.37
22	A	813	CLA	C4D-ND	-3.93	1.32	1.37
25	A	848	8CT	C14-C13	3.92	1.55	1.43
29	3	306	CHL	CHC-C1C	3.92	1.46	1.38
29	2	301	CHL	CHD-C1D	3.92	1.46	1.38
23	A	842	PQN	C10-C5	3.92	1.47	1.40
25	5	317	8CT	C28-C29	3.89	1.41	1.32
22	B	838	CLA	C4D-ND	-3.89	1.32	1.37
22	A	814	CLA	C4D-ND	-3.89	1.32	1.37
29	7	308	CHL	O2A-CGA	3.89	1.45	1.33
26	A	851	HTG	C1'-S1	-3.89	1.76	1.81
29	6	308	CHL	CHD-C1D	3.89	1.45	1.38
29	4	306	CHL	CHD-C4C	3.88	1.48	1.39
29	8	314	CHL	CHD-C4C	3.88	1.48	1.39
25	I	101	8CT	C24-C25	3.88	1.55	1.43
25	K	103	8CT	C30-C29	3.88	1.56	1.50
25	G	104	8CT	C14-C13	3.87	1.55	1.43
29	6	316	CHL	CHD-C4C	3.87	1.48	1.39
25	B	843	8CT	C14-C13	3.87	1.55	1.43
25	F	302	8CT	C24-C25	3.86	1.55	1.43
22	1	312	CLA	C1D-ND	3.86	1.42	1.37
25	J	101	8CT	C14-C13	3.86	1.55	1.43
25	2	317	8CT	C14-C13	3.86	1.55	1.43
29	3	306	CHL	O2A-CGA	3.86	1.45	1.33
25	B	804	8CT	C24-C25	3.86	1.55	1.43
22	0	307	CLA	C1D-ND	3.85	1.42	1.37
22	B	806	CLA	C4D-ND	-3.85	1.32	1.37
25	B	846	8CT	C14-C13	3.85	1.55	1.43
22	B	827	CLA	C4D-ND	-3.85	1.32	1.37
25	3	316	8CT	C14-C13	3.85	1.55	1.43
25	5	317	8CT	C11-C12	3.85	1.54	1.45
25	4	317	8CT	C14-C13	3.85	1.55	1.43
25	B	848	8CT	C14-C13	3.85	1.55	1.43
30	2	315	XAT	O4-C5	-3.84	1.40	1.46
25	G	104	8CT	C11-C12	3.84	1.54	1.45
25	1	316	8CT	C14-C13	3.84	1.55	1.43
22	4	303	CLA	C4D-ND	-3.84	1.32	1.37
25	7	301	8CT	C14-C13	3.84	1.55	1.43
22	B	812	CLA	C4D-ND	-3.84	1.32	1.37
25	A	846	8CT	C14-C13	3.84	1.55	1.43
22	0	302	CLA	C4D-ND	-3.84	1.32	1.37
25	A	849	8CT	C14-C13	3.84	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	103	8CT	C14-C13	3.84	1.55	1.43
25	1	316	8CT	C11-C12	3.84	1.54	1.45
25	8	318	8CT	C14-C13	3.83	1.55	1.43
25	B	847	8CT	C14-C13	3.83	1.55	1.43
29	1	305	CHL	CHD-C4C	3.82	1.48	1.39
22	B	809	CLA	C4D-ND	-3.82	1.32	1.37
22	A	815	CLA	C4D-ND	-3.82	1.32	1.37
25	8	301	8CT	C14-C13	3.82	1.55	1.43
22	B	820	CLA	C4D-ND	-3.81	1.32	1.37
29	5	301	CHL	CHC-C4B	3.81	1.48	1.39
25	8	301	8CT	C11-C12	3.81	1.54	1.45
22	B	828	CLA	C4D-ND	-3.81	1.32	1.37
25	5	317	8CT	C14-C13	3.81	1.55	1.43
22	A	809	CLA	C4D-ND	-3.81	1.32	1.37
29	8	306	CHL	CHD-C4C	3.80	1.47	1.39
22	B	836	CLA	C4D-ND	-3.80	1.32	1.37
22	3	305	CLA	C4D-ND	-3.79	1.32	1.37
25	B	847	8CT	C11-C12	3.79	1.54	1.45
22	2	310	CLA	C4D-ND	-3.79	1.32	1.37
22	A	811	CLA	C4D-ND	-3.79	1.32	1.37
22	L	201	CLA	C4D-ND	-3.79	1.32	1.37
22	7	315	CLA	C4D-ND	-3.79	1.32	1.37
25	J	104	8CT	C11-C12	3.79	1.54	1.45
25	7	323	8CT	C14-C13	3.79	1.55	1.43
22	7	304	CLA	C4D-ND	-3.78	1.32	1.37
22	2	303	CLA	C4D-ND	-3.78	1.32	1.37
25	B	851	8CT	C28-C29	3.78	1.41	1.32
25	4	317	8CT	C28-C29	3.77	1.41	1.32
22	3	307	CLA	C4D-ND	-3.77	1.32	1.37
25	A	854	8CT	C14-C13	3.77	1.55	1.43
22	6	304	CLA	C4D-ND	-3.76	1.32	1.37
25	2	317	8CT	C11-C12	3.76	1.54	1.45
22	5	302	CLA	C4D-ND	-3.76	1.32	1.37
29	8	307	CHL	CHD-C4C	3.76	1.47	1.39
29	8	314	CHL	OBD-CAD	3.76	1.29	1.22
25	4	317	8CT	C11-C12	3.76	1.54	1.45
25	B	846	8CT	C11-C12	3.75	1.54	1.45
29	0	306	CHL	OBD-CAD	3.75	1.28	1.22
25	8	318	8CT	C11-C12	3.75	1.54	1.45
30	0	313	XAT	O24-C25	-3.75	1.40	1.46
25	7	321	8CT	C14-C13	3.75	1.55	1.43
25	6	321	8CT	C14-C13	3.74	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	839	CLA	C4D-ND	-3.74	1.32	1.37
22	2	308	CLA	C4D-ND	-3.74	1.32	1.37
22	B	817	CLA	C4D-ND	-3.74	1.32	1.37
25	L	206	8CT	C14-C13	3.74	1.55	1.43
25	J	101	8CT	C11-C12	3.74	1.54	1.45
29	4	305	CHL	CHD-C4C	3.74	1.47	1.39
29	2	306	CHL	CHD-C4C	3.73	1.47	1.39
25	B	848	8CT	C11-C12	3.73	1.54	1.45
25	J	104	8CT	C14-C13	3.73	1.55	1.43
29	5	301	CHL	CHD-C4C	3.73	1.47	1.39
25	7	323	8CT	C11-C12	3.73	1.54	1.45
22	A	812	CLA	C4D-ND	-3.73	1.32	1.37
22	B	837	CLA	C4D-ND	-3.73	1.32	1.37
22	0	312	CLA	C1D-ND	3.72	1.42	1.37
22	B	821	CLA	C4D-ND	-3.72	1.32	1.37
22	7	305	CLA	C4D-ND	-3.72	1.32	1.37
22	A	808	CLA	C4D-ND	-3.72	1.32	1.37
25	A	854	8CT	C11-C12	3.72	1.53	1.45
22	4	309	CLA	C4D-ND	-3.72	1.32	1.37
29	9	307	CHL	OBD-CAD	3.71	1.28	1.22
22	A	828	CLA	C4D-ND	-3.71	1.32	1.37
29	6	307	CHL	CHD-C4C	3.71	1.47	1.39
29	2	301	CHL	CHD-C4C	3.71	1.47	1.39
29	4	306	CHL	CHC-C4B	3.71	1.47	1.39
29	6	308	CHL	CHD-C4C	3.71	1.47	1.39
22	6	323	CLA	C4D-ND	-3.71	1.32	1.37
25	K	103	8CT	C11-C12	3.70	1.53	1.45
22	3	302	CLA	C4D-ND	-3.70	1.32	1.37
25	A	849	8CT	C11-C12	3.70	1.53	1.45
29	0	301	CHL	CHC-C4B	3.70	1.47	1.39
29	4	301	CHL	CHD-C1D	3.70	1.45	1.38
25	7	301	8CT	C11-C12	3.70	1.53	1.45
22	B	824	CLA	C4D-ND	-3.70	1.32	1.37
25	A	850	8CT	C14-C13	3.70	1.54	1.43
22	B	819	CLA	C4D-ND	-3.70	1.32	1.37
25	B	845	8CT	C14-C13	3.70	1.54	1.43
22	3	301	CLA	C4D-ND	-3.69	1.32	1.37
25	6	321	8CT	C11-C12	3.69	1.53	1.45
22	3	319	CLA	C4D-ND	-3.69	1.32	1.37
22	6	310	CLA	C4D-ND	-3.69	1.32	1.37
25	A	847	8CT	C24-C25	3.69	1.54	1.43
22	1	313	CLA	C4D-ND	-3.69	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	310	CLA	C4D-ND	-3.69	1.32	1.37
22	G	101	CLA	C1D-ND	3.69	1.42	1.37
22	4	311	CLA	C4D-ND	-3.68	1.32	1.37
25	B	851	8CT	C11-C12	3.68	1.53	1.45
25	A	848	8CT	C11-C12	3.68	1.53	1.45
29	1	305	CHL	OBD-CAD	3.68	1.28	1.22
25	B	846	8CT	C28-C29	3.68	1.41	1.32
25	2	317	8CT	C28-C29	3.68	1.41	1.32
29	0	301	CHL	CHB-C1B	3.68	1.47	1.39
22	4	308	CLA	C4D-ND	-3.68	1.32	1.37
22	3	308	CLA	C4D-ND	-3.68	1.32	1.37
22	8	308	CLA	C4D-ND	-3.68	1.32	1.37
22	A	838	CLA	C4D-ND	-3.68	1.32	1.37
25	B	844	8CT	C11-C12	3.68	1.53	1.45
22	A	840	CLA	C4D-ND	-3.68	1.32	1.37
25	F	302	8CT	C14-C13	3.67	1.54	1.43
29	5	306	CHL	OBD-CAD	3.67	1.28	1.22
22	4	310	CLA	C4D-ND	-3.67	1.32	1.37
25	B	843	8CT	C11-C12	3.67	1.53	1.45
22	5	305	CLA	C1D-ND	3.67	1.42	1.37
22	F	301	CLA	C4D-ND	-3.67	1.32	1.37
25	G	104	8CT	C28-C29	3.66	1.41	1.32
22	3	304	CLA	C4D-ND	-3.66	1.32	1.37
22	2	313	CLA	C4D-ND	-3.66	1.32	1.37
22	A	853	CLA	C4D-ND	-3.66	1.32	1.37
25	3	318	8CT	C28-C29	3.65	1.40	1.32
29	6	302	CHL	CHD-C4C	3.65	1.47	1.39
25	A	850	8CT	C11-C12	3.65	1.53	1.45
22	A	826	CLA	C4D-ND	-3.65	1.32	1.37
22	7	310	CLA	C4D-ND	-3.65	1.32	1.37
22	8	303	CLA	C4D-ND	-3.65	1.32	1.37
29	6	302	CHL	CHC-C4B	3.64	1.47	1.39
25	I	101	8CT	C14-C13	3.64	1.54	1.43
25	7	321	8CT	C11-C12	3.64	1.53	1.45
22	2	302	CLA	C4D-ND	-3.64	1.32	1.37
25	L	206	8CT	C28-C29	3.64	1.40	1.32
22	8	311	CLA	C1D-ND	3.64	1.42	1.37
22	A	831	CLA	C4D-ND	-3.64	1.32	1.37
22	L	204	CLA	C1D-ND	3.64	1.42	1.37
29	6	307	CHL	CHC-C4B	3.64	1.47	1.39
25	3	316	8CT	C11-C12	3.64	1.53	1.45
22	A	830	CLA	C4D-ND	-3.64	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	846	8CT	C11-C12	3.64	1.53	1.45
22	B	835	CLA	C4D-ND	-3.63	1.32	1.37
22	B	840	CLA	C4D-ND	-3.63	1.32	1.37
22	A	852	CLA	C4D-ND	-3.63	1.32	1.37
22	B	841	CLA	C4D-ND	-3.63	1.32	1.37
22	2	312	CLA	C4D-ND	-3.63	1.32	1.37
29	2	301	CHL	C2C-C3C	3.63	1.44	1.36
29	8	314	CHL	CHB-C1B	3.63	1.47	1.39
22	A	827	CLA	C4D-ND	-3.62	1.32	1.37
25	L	205	8CT	C14-C13	3.62	1.54	1.43
22	H	201	CLA	C4D-ND	-3.62	1.32	1.37
22	A	834	CLA	C4D-ND	-3.62	1.32	1.37
22	A	836	CLA	C4D-ND	-3.62	1.32	1.37
22	3	310	CLA	C4D-ND	-3.62	1.32	1.37
22	7	309	CLA	C4D-ND	-3.62	1.32	1.37
22	6	305	CLA	C4D-ND	-3.62	1.32	1.37
29	2	306	CHL	CHC-C4B	3.62	1.47	1.39
25	3	318	8CT	C14-C13	3.62	1.54	1.43
25	7	323	8CT	C28-C29	3.62	1.40	1.32
25	J	104	8CT	C28-C29	3.61	1.40	1.32
25	3	316	8CT	C28-C29	3.61	1.40	1.32
22	A	803	CLA	C4D-ND	-3.61	1.32	1.37
29	7	308	CHL	CHD-C1D	3.61	1.45	1.38
22	8	311	CLA	C4D-ND	-3.61	1.32	1.37
22	A	833	CLA	C4D-ND	-3.61	1.32	1.37
25	1	316	8CT	C28-C29	3.61	1.40	1.32
22	2	309	CLA	C4D-ND	-3.61	1.32	1.37
29	2	307	CHL	CHD-C1D	3.60	1.45	1.38
29	3	306	CHL	C2C-C3C	3.60	1.44	1.36
25	A	847	8CT	C14-C13	3.60	1.54	1.43
22	A	819	CLA	C4D-ND	-3.60	1.32	1.37
29	9	302	CHL	CHD-C4C	3.59	1.47	1.39
25	A	846	8CT	C28-C29	3.59	1.40	1.32
25	B	848	8CT	C28-C29	3.59	1.40	1.32
25	L	205	8CT	C28-C29	3.59	1.40	1.32
29	9	302	CHL	OBD-CAD	3.59	1.28	1.22
22	B	831	CLA	C4D-ND	-3.59	1.32	1.37
25	B	804	8CT	C14-C13	3.59	1.54	1.43
29	2	305	CHL	CHD-C1D	3.59	1.45	1.38
25	8	301	8CT	C28-C29	3.59	1.40	1.32
22	A	802	CLA	C4D-ND	-3.59	1.32	1.37
29	2	301	CHL	CHC-C1C	3.58	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	305	CHL	CHD-C4C	3.58	1.47	1.39
22	1	303	CLA	C4D-ND	-3.58	1.32	1.37
25	L	206	8CT	C11-C12	3.58	1.53	1.45
25	A	854	8CT	C28-C29	3.58	1.40	1.32
29	8	305	CHL	CHC-C4B	3.57	1.47	1.39
22	4	304	CLA	C4D-ND	-3.57	1.32	1.37
22	0	312	CLA	C4B-NB	3.57	1.42	1.37
22	A	824	CLA	C4D-ND	-3.57	1.32	1.37
29	2	307	CHL	CHD-C4C	3.57	1.47	1.39
22	A	829	CLA	C4D-ND	-3.57	1.32	1.37
22	A	843	CLA	C4D-ND	-3.57	1.32	1.37
25	B	844	8CT	C28-C29	3.57	1.40	1.32
22	M	101	CLA	C4D-ND	-3.56	1.32	1.37
22	0	309	CLA	C1D-ND	3.56	1.42	1.37
22	A	820	CLA	C4D-ND	-3.56	1.32	1.37
25	A	850	8CT	C28-C29	3.56	1.40	1.32
29	8	314	CHL	CHC-C4B	3.56	1.47	1.39
25	A	849	8CT	C28-C29	3.56	1.40	1.32
25	B	843	8CT	C28-C29	3.56	1.40	1.32
22	1	309	CLA	C4D-ND	-3.55	1.32	1.37
29	7	308	CHL	CHC-C4B	3.55	1.47	1.39
25	7	321	8CT	C28-C29	3.55	1.40	1.32
29	6	306	CHL	CHD-C4C	3.55	1.47	1.39
29	8	307	CHL	OBD-CAD	3.54	1.28	1.22
22	3	313	CLA	C4D-ND	-3.54	1.32	1.37
29	4	305	CHL	OBD-CAD	3.54	1.28	1.22
25	B	847	8CT	C28-C29	3.53	1.40	1.32
22	6	318	CLA	C1D-ND	3.53	1.42	1.37
22	0	304	CLA	C1D-ND	3.53	1.42	1.37
22	B	811	CLA	C1D-ND	3.53	1.42	1.37
25	6	321	8CT	C28-C29	3.53	1.40	1.32
29	5	306	CHL	CHC-C4B	3.53	1.47	1.39
22	9	304	CLA	C4D-ND	-3.53	1.32	1.37
22	A	823	CLA	C4D-ND	-3.53	1.32	1.37
22	B	829	CLA	C4D-ND	-3.53	1.32	1.37
22	L	203	CLA	C4D-ND	-3.53	1.32	1.37
29	5	301	CHL	OBD-CAD	3.53	1.28	1.22
22	B	822	CLA	C4D-ND	-3.52	1.32	1.37
29	4	307	CHL	CHD-C1D	3.52	1.45	1.38
25	J	101	8CT	C28-C29	3.52	1.40	1.32
22	6	313	CLA	C4D-ND	-3.52	1.32	1.37
29	7	308	CHL	CHD-C4C	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	317	8CT	C30-C29	3.52	1.55	1.50
29	8	306	CHL	OBD-CAD	3.52	1.28	1.22
22	B	823	CLA	C4D-ND	-3.51	1.32	1.37
29	4	305	CHL	CHC-C4B	3.51	1.47	1.39
22	8	312	CLA	C4D-ND	-3.51	1.32	1.37
22	1	306	CLA	C1D-ND	3.51	1.42	1.37
22	9	310	CLA	C1D-ND	3.51	1.42	1.37
22	A	818	CLA	C4D-ND	-3.51	1.32	1.37
22	A	821	CLA	C4D-ND	-3.51	1.32	1.37
22	6	315	CLA	C4D-ND	-3.51	1.32	1.37
22	7	302	CLA	C4D-ND	-3.51	1.32	1.37
22	8	302	CLA	C4D-ND	-3.51	1.32	1.37
22	B	834	CLA	C4D-ND	-3.50	1.32	1.37
22	6	309	CLA	C4D-ND	-3.50	1.32	1.37
29	4	307	CHL	CHD-C4C	3.50	1.47	1.39
22	1	301	CLA	C4D-ND	-3.50	1.32	1.37
22	7	310	CLA	C1D-ND	3.50	1.42	1.37
22	8	309	CLA	C4D-ND	-3.50	1.32	1.37
22	2	311	CLA	C4D-ND	-3.50	1.32	1.37
22	B	818	CLA	C4D-ND	-3.50	1.32	1.37
22	B	801	CLA	C4D-ND	-3.49	1.32	1.37
22	7	303	CLA	C4D-ND	-3.49	1.32	1.37
22	6	301	CLA	C1D-ND	3.49	1.42	1.37
22	A	816	CLA	C4D-ND	-3.49	1.32	1.37
29	6	316	CHL	OBD-CAD	3.49	1.28	1.22
29	8	306	CHL	CHC-C4B	3.49	1.47	1.39
22	A	806	CLA	C4D-ND	-3.49	1.32	1.37
29	4	301	CHL	CHD-C4C	3.48	1.47	1.39
29	0	306	CHL	CHB-C1B	3.48	1.47	1.39
25	7	301	8CT	C28-C29	3.48	1.40	1.32
29	6	316	CHL	CHC-C4B	3.48	1.47	1.39
22	B	805	CLA	C4D-ND	-3.48	1.32	1.37
22	K	104	CLA	C4D-ND	-3.48	1.32	1.37
22	5	311	CLA	C1D-ND	3.48	1.42	1.37
22	1	307	CLA	C4D-ND	-3.47	1.32	1.37
22	9	312	CLA	C1D-ND	3.47	1.42	1.37
22	0	310	CLA	C1D-ND	3.47	1.42	1.37
29	4	301	CHL	OBD-CAD	3.46	1.28	1.22
22	6	318	CLA	C4D-ND	-3.46	1.32	1.37
22	5	313	CLA	C4D-ND	-3.46	1.32	1.37
25	B	843	8CT	C30-C29	3.46	1.55	1.50
22	6	312	CLA	C4D-ND	-3.46	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	830	CLA	C4D-ND	-3.46	1.32	1.37
22	1	311	CLA	C4D-ND	-3.46	1.32	1.37
22	9	311	CLA	C4D-ND	-3.46	1.32	1.37
25	A	848	8CT	C28-C29	3.46	1.40	1.32
22	B	813	CLA	C4D-ND	-3.45	1.32	1.37
22	B	803	CLA	C4D-ND	-3.45	1.32	1.37
29	3	306	CHL	CHD-C1D	3.45	1.45	1.38
22	6	317	CLA	C4D-ND	-3.45	1.32	1.37
25	I	101	8CT	C01-C02	3.45	1.56	1.50
25	A	846	8CT	C30-C29	3.45	1.55	1.50
29	4	306	CHL	OBD-CAD	3.45	1.28	1.22
22	4	314	CLA	C1D-ND	3.45	1.42	1.37
22	7	307	CLA	C4D-ND	-3.45	1.33	1.37
22	B	825	CLA	C4D-ND	-3.45	1.33	1.37
22	G	101	CLA	C4B-NB	3.44	1.42	1.37
22	3	319	CLA	C1D-ND	3.44	1.42	1.37
22	0	311	CLA	C1D-ND	3.44	1.42	1.37
29	2	307	CHL	C2C-C3C	3.44	1.44	1.36
22	1	310	CLA	C4D-ND	-3.44	1.33	1.37
22	4	313	CLA	C4D-ND	-3.44	1.33	1.37
22	B	832	CLA	C4D-ND	-3.43	1.33	1.37
22	2	319	CLA	C4D-ND	-3.43	1.33	1.37
29	1	305	CHL	CHC-C4B	3.43	1.47	1.39
22	2	304	CLA	C4D-ND	-3.43	1.33	1.37
22	9	301	CLA	C4D-ND	-3.43	1.33	1.37
22	7	318	CLA	C4D-ND	-3.43	1.33	1.37
29	0	301	CHL	OBD-CAD	3.43	1.28	1.22
22	5	314	CLA	C1D-ND	3.43	1.42	1.37
22	5	314	CLA	C4D-ND	-3.42	1.33	1.37
22	7	313	CLA	C4D-ND	-3.42	1.33	1.37
25	A	847	8CT	C28-C29	3.42	1.40	1.32
22	B	833	CLA	C4D-ND	-3.42	1.33	1.37
22	5	304	CLA	C4D-ND	-3.42	1.33	1.37
29	6	302	CHL	OBD-CAD	3.42	1.28	1.22
22	9	309	CLA	C1D-ND	3.42	1.42	1.37
22	7	318	CLA	C1D-ND	3.42	1.42	1.37
25	8	318	8CT	C28-C29	3.42	1.40	1.32
25	B	846	8CT	C01-C02	3.42	1.56	1.50
22	3	311	CLA	C4D-ND	-3.42	1.33	1.37
22	8	304	CLA	C4D-ND	-3.41	1.33	1.37
22	0	303	CLA	C1D-ND	3.41	1.42	1.37
22	0	311	CLA	C4D-ND	-3.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	308	CHL	OBD-CAD	3.41	1.28	1.22
25	3	318	8CT	C01-C02	3.41	1.56	1.50
22	A	801	CLA	C4D-ND	-3.41	1.33	1.37
22	3	303	CLA	C4D-ND	-3.41	1.33	1.37
22	0	308	CLA	C1D-ND	3.40	1.42	1.37
22	B	807	CLA	C4D-ND	-3.40	1.33	1.37
22	A	807	CLA	C4D-ND	-3.40	1.33	1.37
22	2	314	CLA	C4D-ND	-3.40	1.33	1.37
25	7	323	8CT	C01-C02	3.40	1.56	1.50
29	8	305	CHL	OBD-CAD	3.40	1.28	1.22
22	1	308	CLA	C1D-ND	3.40	1.42	1.37
22	9	308	CLA	C1D-ND	3.40	1.42	1.37
22	K	101	CLA	C4D-ND	-3.40	1.33	1.37
25	F	302	8CT	C28-C29	3.40	1.40	1.32
25	7	321	8CT	C01-C02	3.39	1.56	1.50
22	4	314	CLA	C4D-ND	-3.39	1.33	1.37
25	B	843	8CT	C35-C30	3.39	1.65	1.56
25	F	302	8CT	C01-C02	3.39	1.56	1.50
22	6	314	CLA	C4D-ND	-3.39	1.33	1.37
22	A	804	CLA	C4D-ND	-3.39	1.33	1.37
22	B	815	CLA	C4D-ND	-3.39	1.33	1.37
22	7	311	CLA	C4D-ND	-3.39	1.33	1.37
22	9	312	CLA	C4D-ND	-3.39	1.33	1.37
25	B	845	8CT	C28-C29	3.39	1.40	1.32
22	1	307	CLA	C1D-ND	3.39	1.41	1.37
22	4	313	CLA	C1D-ND	3.39	1.41	1.37
22	8	315	CLA	C4D-ND	-3.38	1.33	1.37
25	A	847	8CT	C11-C12	3.38	1.53	1.45
29	2	305	CHL	OBD-CAD	3.38	1.28	1.22
22	A	801	CLA	C1D-ND	3.38	1.41	1.37
22	A	823	CLA	C1D-ND	3.38	1.41	1.37
22	M	101	CLA	C1D-ND	3.38	1.41	1.37
22	9	301	CLA	CAB-C3B	-3.38	1.43	1.50
22	A	832	CLA	C4D-ND	-3.38	1.33	1.37
25	B	845	8CT	C11-C12	3.38	1.53	1.45
22	K	102	CLA	C4D-ND	-3.38	1.33	1.37
22	A	822	CLA	C1D-ND	3.38	1.41	1.37
29	2	305	CHL	CHC-C4B	3.38	1.47	1.39
29	6	307	CHL	OBD-CAD	3.38	1.28	1.22
22	B	839	CLA	C4D-ND	-3.38	1.33	1.37
22	3	307	CLA	C1D-ND	3.38	1.41	1.37
22	A	833	CLA	C1D-ND	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	311	CLA	C1D-ND	3.37	1.41	1.37
22	2	304	CLA	C1D-ND	3.37	1.41	1.37
29	9	307	CHL	CHC-C4B	3.37	1.47	1.39
22	7	316	CLA	C4D-ND	-3.37	1.33	1.37
29	2	301	CHL	OBD-CAD	3.37	1.28	1.22
22	B	816	CLA	C4D-ND	-3.37	1.33	1.37
25	1	316	8CT	C01-C02	3.36	1.56	1.50
29	3	306	CHL	CHD-C4C	3.36	1.46	1.39
29	2	306	CHL	CHB-C1B	3.36	1.47	1.39
25	B	848	8CT	C01-C02	3.36	1.56	1.50
22	G	102	CLA	C1D-ND	3.36	1.41	1.37
25	3	316	8CT	C01-C02	3.36	1.56	1.50
22	9	313	CLA	C1D-ND	3.36	1.41	1.37
22	5	312	CLA	C4D-ND	-3.36	1.33	1.37
22	1	304	CLA	C4D-ND	-3.35	1.33	1.37
22	A	835	CLA	C4D-ND	-3.35	1.33	1.37
22	5	307	CLA	C1D-ND	3.35	1.41	1.37
22	K	105	CLA	C4D-ND	-3.35	1.33	1.37
22	7	312	CLA	C4D-ND	-3.34	1.33	1.37
22	5	309	CLA	C1D-ND	3.34	1.41	1.37
22	6	310	CLA	C1D-ND	3.34	1.41	1.37
25	3	318	8CT	C11-C12	3.34	1.53	1.45
29	6	307	CHL	CHB-C1B	3.34	1.46	1.39
22	6	305	CLA	C1D-ND	3.34	1.41	1.37
22	9	305	CLA	C4D-ND	-3.34	1.33	1.37
22	0	305	CLA	C1D-ND	3.33	1.41	1.37
22	3	309	CLA	C4D-ND	-3.33	1.33	1.37
25	6	321	8CT	C01-C02	3.33	1.56	1.50
22	7	306	CLA	C4D-ND	-3.33	1.33	1.37
22	B	841	CLA	C1D-ND	3.33	1.41	1.37
22	8	313	CLA	C4D-ND	-3.33	1.33	1.37
25	5	317	8CT	C01-C02	3.33	1.56	1.50
25	B	851	8CT	C18-C17	3.33	1.53	1.43
22	A	825	CLA	C4D-ND	-3.33	1.33	1.37
25	8	301	8CT	C01-C02	3.33	1.56	1.50
25	J	101	8CT	C01-C02	3.32	1.56	1.50
22	5	307	CLA	C4D-ND	-3.32	1.33	1.37
25	G	104	8CT	C01-C02	3.32	1.56	1.50
25	K	103	8CT	C01-C02	3.32	1.56	1.50
22	H	201	CLA	C1D-ND	3.32	1.41	1.37
25	K	103	8CT	C35-C30	3.32	1.65	1.56
29	6	306	CHL	OBD-CAD	3.32	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	302	CHL	CHB-C1B	3.31	1.46	1.39
22	9	303	CLA	C1D-ND	3.31	1.41	1.37
22	1	308	CLA	C4D-ND	-3.31	1.33	1.37
29	4	306	CHL	CHB-C1B	3.31	1.46	1.39
29	5	306	CHL	CHB-C1B	3.31	1.46	1.39
22	0	304	CLA	C4B-NB	3.31	1.41	1.37
25	J	104	8CT	C01-C02	3.31	1.56	1.50
25	L	206	8CT	C35-C30	3.31	1.65	1.56
25	A	849	8CT	C01-C02	3.31	1.56	1.50
22	9	313	CLA	C4D-ND	-3.31	1.33	1.37
25	I	101	8CT	C11-C12	3.31	1.53	1.45
22	6	314	CLA	C1D-ND	3.30	1.41	1.37
25	A	854	8CT	C01-C02	3.30	1.56	1.50
22	1	311	CLA	C1D-ND	3.30	1.41	1.37
22	7	314	CLA	C1D-ND	3.30	1.41	1.37
22	A	810	CLA	C1D-ND	3.30	1.41	1.37
22	0	312	CLA	C4D-ND	-3.30	1.33	1.37
25	4	317	8CT	C18-C17	3.30	1.53	1.43
22	B	818	CLA	C1D-ND	3.30	1.41	1.37
22	L	204	CLA	C4D-ND	-3.29	1.33	1.37
22	1	310	CLA	C1D-ND	3.29	1.41	1.37
22	A	810	CLA	C4D-ND	-3.29	1.33	1.37
25	4	317	8CT	C01-C02	3.29	1.56	1.50
22	9	306	CLA	C4D-ND	-3.29	1.33	1.37
22	5	310	CLA	C4D-ND	-3.29	1.33	1.37
22	5	309	CLA	C4D-ND	-3.29	1.33	1.37
22	A	841	CLA	C4D-ND	-3.29	1.33	1.37
22	B	822	CLA	C1D-ND	3.28	1.41	1.37
25	8	318	8CT	C01-C02	3.28	1.56	1.50
29	2	305	CHL	CHD-C4C	3.28	1.46	1.39
22	2	311	CLA	C1D-ND	3.28	1.41	1.37
22	B	811	CLA	C4D-ND	-3.28	1.33	1.37
22	A	820	CLA	C1D-ND	3.28	1.41	1.37
22	A	843	CLA	C1D-ND	3.28	1.41	1.37
22	B	810	CLA	C4D-ND	-3.27	1.33	1.37
29	6	306	CHL	CHC-C4B	3.27	1.46	1.39
22	A	822	CLA	C4D-ND	-3.27	1.33	1.37
25	L	205	8CT	C11-C12	3.27	1.53	1.45
22	1	309	CLA	C1D-ND	3.27	1.41	1.37
22	0	309	CLA	C4D-ND	-3.27	1.33	1.37
29	9	307	CHL	CHB-C1B	3.26	1.46	1.39
22	1	302	CLA	C4D-ND	-3.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	312	CLA	C4B-NB	3.26	1.41	1.37
25	L	206	8CT	C01-C02	3.26	1.56	1.50
22	7	305	CLA	C1D-ND	3.26	1.41	1.37
25	A	850	8CT	C01-C02	3.26	1.56	1.50
25	B	804	8CT	C11-C12	3.26	1.52	1.45
22	6	311	CLA	C1D-ND	3.26	1.41	1.37
29	6	308	CHL	CHC-C4B	3.26	1.46	1.39
22	8	315	CLA	C1D-ND	3.26	1.41	1.37
22	4	302	CLA	C4D-ND	-3.26	1.33	1.37
29	4	307	CHL	CHC-C4B	3.26	1.46	1.39
22	L	202	CLA	C4D-ND	-3.25	1.33	1.37
25	B	844	8CT	C01-C02	3.25	1.56	1.50
25	B	851	8CT	C01-C02	3.25	1.56	1.50
22	A	819	CLA	C1D-ND	3.25	1.41	1.37
22	8	312	CLA	C1D-ND	3.25	1.41	1.37
25	B	804	8CT	C28-C29	3.25	1.40	1.32
29	9	302	CHL	CHC-C4B	3.25	1.46	1.39
25	A	848	8CT	C01-C02	3.25	1.56	1.50
22	G	103	CLA	C1D-ND	3.25	1.41	1.37
22	5	312	CLA	C1D-ND	3.25	1.41	1.37
22	1	306	CLA	C4D-ND	-3.25	1.33	1.37
22	5	311	CLA	C4D-ND	-3.25	1.33	1.37
22	3	312	CLA	C4D-ND	-3.25	1.33	1.37
22	J	103	CLA	C1D-ND	3.25	1.41	1.37
22	1	302	CLA	C1D-ND	3.25	1.41	1.37
22	9	309	CLA	C4D-ND	-3.25	1.33	1.37
22	7	307	CLA	C1D-ND	3.24	1.41	1.37
25	B	847	8CT	C01-C02	3.24	1.56	1.50
22	5	308	CLA	C4D-ND	-3.24	1.33	1.37
22	B	839	CLA	C1D-ND	3.24	1.41	1.37
22	7	314	CLA	C4D-ND	-3.24	1.33	1.37
22	5	305	CLA	C4D-ND	-3.24	1.33	1.37
29	1	305	CHL	CHB-C1B	3.24	1.46	1.39
22	1	313	CLA	C1D-ND	3.23	1.41	1.37
22	6	312	CLA	C1D-ND	3.23	1.41	1.37
25	2	317	8CT	C01-C02	3.23	1.56	1.50
22	2	314	CLA	C1D-ND	3.23	1.41	1.37
25	A	847	8CT	C01-C02	3.23	1.56	1.50
22	8	310	CLA	C1D-ND	3.23	1.41	1.37
29	0	306	CHL	CHC-C4B	3.23	1.46	1.39
25	F	302	8CT	C11-C12	3.22	1.52	1.45
24	A	844	LHG	O7-C5	-3.22	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	301	8CT	C35-C30	3.22	1.65	1.56
29	7	308	CHL	OBD-CAD	3.22	1.28	1.22
25	B	851	8CT	C35-C30	3.22	1.65	1.56
22	4	312	CLA	C4D-ND	-3.22	1.33	1.37
25	A	846	8CT	C35-C30	3.22	1.65	1.56
22	9	308	CLA	C4D-ND	-3.22	1.33	1.37
22	0	302	CLA	C1D-ND	3.21	1.41	1.37
22	5	303	CLA	C4D-ND	-3.21	1.33	1.37
22	B	815	CLA	C1D-ND	3.21	1.41	1.37
22	B	816	CLA	C1D-ND	3.21	1.41	1.37
22	9	312	CLA	C4B-NB	3.21	1.41	1.37
22	3	302	CLA	C1D-ND	3.21	1.41	1.37
22	A	814	CLA	C1D-ND	3.21	1.41	1.37
22	7	306	CLA	C1D-ND	3.21	1.41	1.37
22	A	817	CLA	C4D-ND	-3.20	1.33	1.37
22	B	850	CLA	C4D-ND	-3.20	1.33	1.37
22	B	835	CLA	C1D-ND	3.20	1.41	1.37
22	5	310	CLA	C1D-ND	3.20	1.41	1.37
22	9	301	CLA	C1D-ND	3.20	1.41	1.37
25	A	846	8CT	C01-C02	3.20	1.56	1.50
22	B	833	CLA	C1D-ND	3.20	1.41	1.37
29	3	306	CHL	CHB-C1B	3.20	1.46	1.39
22	3	312	CLA	C1D-ND	3.20	1.41	1.37
22	9	306	CLA	C1D-ND	3.20	1.41	1.37
25	G	104	8CT	C18-C17	3.20	1.53	1.43
22	L	203	CLA	C1D-ND	3.19	1.41	1.37
22	7	316	CLA	C1D-ND	3.19	1.41	1.37
22	3	311	CLA	C1D-ND	3.19	1.41	1.37
22	6	304	CLA	C1D-ND	3.19	1.41	1.37
22	J	103	CLA	C4D-ND	-3.19	1.33	1.37
22	A	853	CLA	C1D-ND	3.19	1.41	1.37
22	A	817	CLA	C1D-ND	3.19	1.41	1.37
22	K	104	CLA	C1D-ND	3.19	1.41	1.37
22	3	309	CLA	C1D-ND	3.19	1.41	1.37
29	4	305	CHL	CHB-C1B	3.19	1.46	1.39
22	K	105	CLA	C1D-ND	3.19	1.41	1.37
25	B	845	8CT	C01-C02	3.19	1.56	1.50
22	A	835	CLA	C1D-ND	3.19	1.41	1.37
22	2	319	CLA	C1D-ND	3.18	1.41	1.37
29	8	305	CHL	CHB-C1B	3.18	1.46	1.39
29	9	302	CHL	CHB-C1B	3.18	1.46	1.39
22	6	317	CLA	C1D-ND	3.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	313	CLA	C1D-ND	3.18	1.41	1.37
22	A	834	CLA	C1D-ND	3.18	1.41	1.37
22	5	304	CLA	C1D-ND	3.18	1.41	1.37
22	G	103	CLA	C4D-ND	-3.18	1.33	1.37
22	0	308	CLA	C4D-ND	-3.17	1.33	1.37
22	A	832	CLA	C1D-ND	3.17	1.41	1.37
22	8	313	CLA	C1D-ND	3.17	1.41	1.37
25	B	846	8CT	C30-C29	3.17	1.55	1.50
25	B	848	8CT	C18-C17	3.17	1.53	1.43
22	4	303	CLA	C1D-ND	3.17	1.41	1.37
25	A	846	8CT	C18-C17	3.17	1.53	1.43
29	2	305	CHL	CHB-C1B	3.17	1.46	1.39
25	2	317	8CT	C18-C17	3.17	1.53	1.43
22	2	310	CLA	C1D-ND	3.17	1.41	1.37
29	4	301	CHL	CHC-C4B	3.17	1.46	1.39
29	8	307	CHL	CHC-C4B	3.17	1.46	1.39
25	L	205	8CT	C01-C02	3.17	1.56	1.50
22	1	312	CLA	C4D-ND	-3.16	1.33	1.37
22	9	303	CLA	C4D-ND	-3.16	1.33	1.37
29	2	307	CHL	OBD-CAD	3.16	1.27	1.22
25	1	316	8CT	C18-C17	3.16	1.53	1.43
25	L	206	8CT	C18-C17	3.16	1.53	1.43
25	L	205	8CT	C35-C30	3.16	1.65	1.56
22	8	302	CLA	C1D-ND	3.16	1.41	1.37
25	B	851	8CT	C30-C29	3.16	1.54	1.50
22	B	832	CLA	C1D-ND	3.16	1.41	1.37
22	4	312	CLA	C1D-ND	3.16	1.41	1.37
25	5	317	8CT	C35-C30	3.16	1.65	1.56
25	I	101	8CT	C35-C30	3.16	1.65	1.56
22	7	313	CLA	C1D-ND	3.15	1.41	1.37
22	A	827	CLA	C1D-ND	3.15	1.41	1.37
22	B	819	CLA	C1D-ND	3.15	1.41	1.37
22	2	302	CLA	C1D-ND	3.15	1.41	1.37
22	4	311	CLA	C1D-ND	3.15	1.41	1.37
25	A	847	8CT	C30-C29	3.15	1.54	1.50
22	6	311	CLA	C4D-ND	-3.15	1.33	1.37
25	I	101	8CT	C28-C29	3.15	1.39	1.32
25	B	846	8CT	C35-C30	3.15	1.65	1.56
25	A	849	8CT	C18-C17	3.15	1.53	1.43
22	8	304	CLA	C1D-ND	3.14	1.41	1.37
25	7	301	8CT	C01-C02	3.14	1.56	1.50
22	A	825	CLA	C1D-ND	3.14	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	815	CLA	C1D-ND	3.14	1.41	1.37
22	B	823	CLA	C1D-ND	3.14	1.41	1.37
25	B	847	8CT	C18-C17	3.14	1.53	1.43
25	3	316	8CT	C18-C17	3.14	1.53	1.43
25	B	846	8CT	C18-C17	3.14	1.53	1.43
25	8	301	8CT	C18-C17	3.14	1.53	1.43
22	1	301	CLA	C1D-ND	3.14	1.41	1.37
25	J	101	8CT	C18-C17	3.14	1.53	1.43
25	A	854	8CT	C18-C17	3.13	1.53	1.43
29	8	314	CHL	MG-NA	-3.13	1.98	2.06
25	8	318	8CT	C18-C17	3.13	1.53	1.43
22	K	101	CLA	C1D-ND	3.13	1.41	1.37
25	A	848	8CT	C18-C17	3.13	1.53	1.43
22	6	303	CLA	C4D-ND	-3.13	1.33	1.37
25	K	103	8CT	C18-C17	3.12	1.53	1.43
25	G	104	8CT	C35-C30	3.12	1.65	1.56
29	3	306	CHL	CHC-C4B	3.12	1.46	1.39
22	A	841	CLA	C1D-ND	3.12	1.41	1.37
22	B	834	CLA	C4B-NB	3.12	1.41	1.37
30	5	315	XAT	O24-C25	-3.12	1.41	1.46
25	J	104	8CT	C18-C17	3.12	1.53	1.43
25	7	323	8CT	C18-C17	3.12	1.53	1.43
22	9	305	CLA	C1D-ND	3.12	1.41	1.37
22	A	852	CLA	C1D-ND	3.11	1.41	1.37
22	5	308	CLA	C4B-NB	3.11	1.41	1.37
25	7	321	8CT	C18-C17	3.11	1.53	1.43
25	A	847	8CT	C35-C30	3.11	1.65	1.56
22	L	202	CLA	C1D-ND	3.11	1.41	1.37
22	4	314	CLA	C4B-NB	3.11	1.41	1.37
25	2	317	8CT	C35-C30	3.11	1.65	1.56
22	2	312	CLA	C1D-ND	3.11	1.41	1.37
22	3	310	CLA	C1D-ND	3.10	1.41	1.37
29	8	306	CHL	CHB-C1B	3.10	1.46	1.39
22	A	807	CLA	C1D-ND	3.10	1.41	1.37
22	0	303	CLA	C4B-NB	3.10	1.41	1.37
22	7	316	CLA	C4B-NB	3.09	1.41	1.37
22	6	301	CLA	C4D-ND	-3.09	1.33	1.37
22	0	303	CLA	C4D-ND	-3.09	1.33	1.37
22	A	811	CLA	C1D-ND	3.09	1.41	1.37
22	1	306	CLA	C4B-NB	3.09	1.41	1.37
25	7	301	8CT	C07-C02	-3.09	1.44	1.51
29	4	307	CHL	OBD-CAD	3.09	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	306	CHL	OBD-CAD	3.09	1.27	1.22
22	G	102	CLA	C4D-ND	-3.09	1.33	1.37
22	B	838	CLA	C1D-ND	3.09	1.41	1.37
22	3	308	CLA	C1D-ND	3.09	1.41	1.37
22	K	104	CLA	C4B-NB	3.08	1.41	1.37
22	0	305	CLA	C4D-ND	-3.08	1.33	1.37
22	A	821	CLA	C1D-ND	3.08	1.41	1.37
22	K	105	CLA	C4B-NB	3.08	1.41	1.37
22	3	313	CLA	C1D-ND	3.08	1.41	1.37
29	2	307	CHL	CHC-C4B	3.08	1.46	1.39
22	3	303	CLA	C1D-ND	3.08	1.41	1.37
25	B	843	8CT	C01-C02	3.08	1.56	1.50
29	0	301	CHL	MG-NA	-3.08	1.99	2.06
22	K	102	CLA	C1D-ND	3.08	1.41	1.37
25	A	854	8CT	C35-C30	3.08	1.64	1.56
22	8	311	CLA	C4B-NB	3.08	1.41	1.37
22	9	305	CLA	C4B-NB	3.08	1.41	1.37
22	0	302	CLA	C4B-NB	3.08	1.41	1.37
22	B	850	CLA	C1D-ND	3.07	1.41	1.37
22	1	304	CLA	C1D-ND	3.07	1.41	1.37
22	7	306	CLA	C4B-NB	3.07	1.41	1.37
22	M	101	CLA	C4B-NB	3.07	1.41	1.37
25	A	849	8CT	C35-C30	3.07	1.64	1.56
25	3	316	8CT	C35-C30	3.07	1.64	1.56
25	7	301	8CT	C10-C03	3.07	1.56	1.45
25	B	804	8CT	C01-C02	3.07	1.56	1.50
22	B	813	CLA	C1D-ND	3.07	1.41	1.37
29	0	301	CHL	C3D-C2D	3.07	1.47	1.39
25	B	845	8CT	C18-C17	3.07	1.52	1.43
29	6	306	CHL	CHB-C1B	3.07	1.46	1.39
22	A	816	CLA	C1D-ND	3.07	1.41	1.37
25	5	317	8CT	C18-C17	3.06	1.52	1.43
22	4	304	CLA	C1D-ND	3.06	1.41	1.37
25	3	318	8CT	C35-C30	3.06	1.64	1.56
25	A	848	8CT	C35-C30	3.06	1.64	1.56
29	4	307	CHL	CHB-C1B	3.06	1.46	1.39
29	2	307	CHL	CHB-C1B	3.06	1.46	1.39
22	A	839	CLA	C1D-ND	3.05	1.41	1.37
22	6	323	CLA	C1D-ND	3.05	1.41	1.37
22	0	304	CLA	C4D-ND	-3.05	1.33	1.37
25	1	316	8CT	C35-C30	3.05	1.64	1.56
25	B	844	8CT	C18-C17	3.05	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	850	8CT	C18-C17	3.05	1.52	1.43
25	G	104	8CT	C30-C29	3.05	1.54	1.50
22	6	309	CLA	C1D-ND	3.05	1.41	1.37
22	B	808	CLA	C1D-ND	3.05	1.41	1.37
22	B	831	CLA	C1D-ND	3.05	1.41	1.37
29	0	306	CHL	C3D-C2D	3.05	1.47	1.39
22	K	101	CLA	C4B-NB	3.05	1.41	1.37
29	4	306	CHL	C3D-C2D	3.05	1.47	1.39
25	4	317	8CT	C35-C30	3.04	1.64	1.56
22	9	310	CLA	C4D-ND	-3.04	1.33	1.37
22	1	301	CLA	C4B-NB	3.04	1.41	1.37
22	9	304	CLA	C1D-ND	3.04	1.41	1.37
22	0	309	CLA	C4B-NB	3.04	1.41	1.37
25	8	318	8CT	C35-C30	3.04	1.64	1.56
22	6	301	CLA	C4B-NB	3.04	1.41	1.37
22	7	311	CLA	C1D-ND	3.04	1.41	1.37
25	6	321	8CT	C35-C30	3.03	1.64	1.56
29	4	301	CHL	C1B-NB	-3.03	1.34	1.37
25	8	301	8CT	C10-C03	3.03	1.55	1.45
25	1	316	8CT	C10-C03	3.03	1.55	1.45
22	8	313	CLA	C4B-NB	3.03	1.41	1.37
22	4	302	CLA	C1D-ND	3.03	1.41	1.37
25	A	848	8CT	C10-C03	3.03	1.55	1.45
25	7	323	8CT	C35-C30	3.03	1.64	1.56
22	G	101	CLA	C4D-ND	-3.02	1.33	1.37
22	6	315	CLA	C1D-ND	3.02	1.41	1.37
25	B	844	8CT	C10-C03	3.02	1.55	1.45
22	L	202	CLA	C4B-NB	3.02	1.41	1.37
25	6	321	8CT	C18-C17	3.02	1.52	1.43
22	7	306	CLA	C3B-C4B	3.02	1.49	1.42
22	5	303	CLA	C1D-ND	3.02	1.41	1.37
22	5	313	CLA	C4B-NB	3.02	1.41	1.37
29	6	307	CHL	C3D-C2D	3.02	1.47	1.39
29	5	306	CHL	C3D-C2D	3.02	1.47	1.39
29	6	307	CHL	MG-NA	-3.02	1.99	2.06
22	8	309	CLA	C1D-ND	3.02	1.41	1.37
22	5	308	CLA	C3B-C4B	3.02	1.49	1.42
29	2	301	CHL	CHC-C4B	3.01	1.46	1.39
25	B	848	8CT	C35-C30	3.01	1.64	1.56
25	B	847	8CT	C10-C03	3.01	1.55	1.45
25	L	205	8CT	C18-C17	3.01	1.52	1.43
25	5	317	8CT	C10-C03	3.01	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	802	CLA	C1D-ND	3.01	1.41	1.37
22	B	810	CLA	C1D-ND	3.01	1.41	1.37
22	0	307	CLA	C4B-NB	3.01	1.41	1.37
25	B	843	8CT	C18-C17	3.00	1.52	1.43
22	4	310	CLA	C1D-ND	3.00	1.41	1.37
25	2	317	8CT	C10-C03	3.00	1.55	1.45
25	B	848	8CT	C10-C03	3.00	1.55	1.45
25	4	317	8CT	C10-C03	3.00	1.55	1.45
25	8	301	8CT	C35-C30	3.00	1.64	1.56
25	A	846	8CT	C10-C03	3.00	1.55	1.45
22	5	305	CLA	C4B-NB	3.00	1.41	1.37
22	0	310	CLA	C4D-ND	-3.00	1.33	1.37
22	B	834	CLA	C1D-ND	2.99	1.41	1.37
25	J	101	8CT	C35-C30	2.99	1.64	1.56
25	G	104	8CT	C10-C03	2.99	1.55	1.45
22	6	315	CLA	C4B-NB	2.99	1.41	1.37
25	4	317	8CT	C30-C29	2.99	1.54	1.50
29	6	316	CHL	CHB-C1B	2.99	1.46	1.39
22	A	809	CLA	C1D-ND	2.99	1.41	1.37
29	2	301	CHL	CHB-C1B	2.99	1.46	1.39
25	3	318	8CT	C07-C02	-2.99	1.45	1.51
22	A	830	CLA	CMB-C2B	-2.99	1.44	1.50
29	9	307	CHL	C3D-C2D	2.98	1.47	1.39
22	7	302	CLA	C1D-ND	2.98	1.41	1.37
22	0	312	CLA	C3B-C4B	2.98	1.49	1.42
22	0	307	CLA	C4D-ND	-2.98	1.33	1.37
25	7	321	8CT	C35-C30	2.98	1.64	1.56
29	6	302	CHL	MG-NA	-2.98	1.99	2.06
22	6	305	CLA	C4B-NB	2.97	1.41	1.37
29	6	302	CHL	C3D-C2D	2.97	1.47	1.39
22	8	308	CLA	C1D-ND	2.97	1.41	1.37
25	K	103	8CT	C10-C03	2.97	1.55	1.45
29	4	306	CHL	C1B-NB	-2.97	1.34	1.37
25	J	104	8CT	C35-C30	2.97	1.64	1.56
22	A	816	CLA	C3B-C4B	2.97	1.49	1.42
22	5	309	CLA	C4B-NB	2.97	1.41	1.37
25	3	318	8CT	C18-C17	2.97	1.52	1.43
29	1	305	CHL	C3D-C2D	2.97	1.47	1.39
22	8	303	CLA	C1D-ND	2.97	1.41	1.37
29	6	308	CHL	CHB-C1B	2.97	1.46	1.39
25	B	845	8CT	C07-C02	-2.97	1.45	1.51
25	8	318	8CT	C10-C03	2.97	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	301	8CT	C18-C17	2.96	1.52	1.43
22	A	806	CLA	C1D-ND	2.96	1.41	1.37
22	9	310	CLA	C4B-NB	2.96	1.41	1.37
29	4	305	CHL	C4B-NB	-2.96	1.34	1.37
22	G	101	CLA	C3B-C4B	2.96	1.49	1.42
25	J	104	8CT	C10-C03	2.96	1.55	1.45
29	4	307	CHL	C1B-NB	-2.96	1.34	1.37
29	6	307	CHL	C1D-ND	-2.96	1.34	1.37
22	9	301	CLA	C4B-NB	2.96	1.41	1.37
25	F	302	8CT	C18-C17	2.96	1.52	1.43
25	B	846	8CT	C10-C03	2.96	1.55	1.45
22	A	824	CLA	C1D-ND	2.95	1.41	1.37
22	F	301	CLA	C1D-ND	2.95	1.41	1.37
25	B	851	8CT	C10-C03	2.95	1.55	1.45
25	3	318	8CT	C10-C03	2.95	1.55	1.45
25	A	850	8CT	C35-C30	2.95	1.64	1.56
22	7	303	CLA	C1D-ND	2.95	1.41	1.37
29	4	301	CHL	CHB-C1B	2.95	1.46	1.39
22	2	309	CLA	C1D-ND	2.95	1.41	1.37
22	0	308	CLA	C4B-NB	2.95	1.41	1.37
22	1	303	CLA	C1D-ND	2.95	1.41	1.37
22	2	303	CLA	C1D-ND	2.95	1.41	1.37
22	B	803	CLA	C1D-ND	2.94	1.41	1.37
22	3	303	CLA	C4B-NB	2.94	1.41	1.37
22	A	808	CLA	C1D-ND	2.94	1.41	1.37
22	A	831	CLA	C1D-ND	2.94	1.41	1.37
22	A	811	CLA	C4B-NB	2.94	1.41	1.37
22	7	312	CLA	C1D-ND	2.94	1.41	1.37
25	B	845	8CT	C30-C29	2.94	1.54	1.50
22	7	312	CLA	C3B-C4B	2.94	1.49	1.42
22	3	304	CLA	C1D-ND	2.94	1.41	1.37
22	8	311	CLA	C3B-C4B	2.94	1.49	1.42
22	A	837	CLA	C1D-ND	2.94	1.41	1.37
22	B	817	CLA	C1D-ND	2.94	1.41	1.37
22	2	313	CLA	C1D-ND	2.94	1.41	1.37
22	B	824	CLA	C4B-NB	2.94	1.41	1.37
25	B	843	8CT	C10-C03	2.93	1.55	1.45
29	0	306	CHL	MG-NA	-2.93	1.99	2.06
22	3	307	CLA	CMB-C2B	-2.93	1.44	1.50
22	A	812	CLA	C1D-ND	2.93	1.41	1.37
29	5	301	CHL	CHB-C1B	2.93	1.46	1.39
22	G	102	CLA	C4B-NB	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	854	8CT	C10-C03	2.93	1.55	1.45
22	1	302	CLA	C4B-NB	2.93	1.41	1.37
29	8	314	CHL	C3D-C2D	2.93	1.47	1.39
25	3	316	8CT	C10-C03	2.93	1.55	1.45
22	B	812	CLA	C1D-ND	2.92	1.41	1.37
29	8	306	CHL	C3D-C2D	2.92	1.47	1.39
25	L	205	8CT	C07-C02	-2.92	1.45	1.51
22	A	834	CLA	C4B-NB	2.92	1.41	1.37
29	4	305	CHL	C1B-NB	-2.92	1.34	1.37
22	B	825	CLA	C1D-ND	2.92	1.41	1.37
25	5	317	8CT	C25-C26	2.92	1.39	1.35
22	B	821	CLA	C4B-NB	2.92	1.41	1.37
25	L	205	8CT	C10-C03	2.92	1.55	1.45
29	6	316	CHL	C3D-C2D	2.92	1.47	1.39
22	1	308	CLA	C3B-C4B	2.91	1.49	1.42
22	B	827	CLA	C1D-ND	2.91	1.41	1.37
22	5	307	CLA	C3B-C4B	2.91	1.49	1.42
22	8	315	CLA	C4B-NB	2.91	1.41	1.37
25	A	850	8CT	C30-C29	2.91	1.54	1.50
25	J	101	8CT	C10-C03	2.91	1.55	1.45
22	A	829	CLA	C1D-ND	2.91	1.41	1.37
22	8	312	CLA	C4B-NB	2.91	1.41	1.37
22	A	830	CLA	C4B-NB	2.91	1.41	1.37
22	B	830	CLA	C1D-ND	2.91	1.41	1.37
22	A	806	CLA	MG-NB	-2.91	2.00	2.05
22	0	307	CLA	C3B-C4B	2.91	1.49	1.42
25	A	847	8CT	C18-C17	2.91	1.52	1.43
22	A	804	CLA	C1D-ND	2.91	1.41	1.37
22	B	820	CLA	C1D-ND	2.91	1.41	1.37
22	8	310	CLA	C4B-NB	2.91	1.41	1.37
22	7	307	CLA	C4B-NB	2.90	1.41	1.37
25	A	849	8CT	C10-C03	2.90	1.55	1.45
22	A	843	CLA	C4B-NB	2.90	1.41	1.37
22	A	839	CLA	MG-NB	-2.90	2.00	2.05
22	A	826	CLA	C1D-ND	2.90	1.41	1.37
28	B	849	DGD	O2G-C2G	-2.90	1.39	1.46
25	7	323	8CT	C10-C03	2.90	1.55	1.45
25	A	850	8CT	C10-C03	2.90	1.55	1.45
22	0	311	CLA	C3B-C4B	2.90	1.49	1.42
25	B	804	8CT	C18-C17	2.90	1.52	1.43
25	7	321	8CT	C10-C03	2.90	1.55	1.45
25	2	317	8CT	C30-C29	2.90	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	847	8CT	C35-C30	2.90	1.64	1.56
22	B	812	CLA	MG-NB	-2.90	2.00	2.05
22	B	839	CLA	C4B-NB	2.90	1.41	1.37
25	A	847	8CT	C10-C03	2.90	1.55	1.45
29	2	306	CHL	C1B-NB	-2.89	1.34	1.37
22	4	308	CLA	CMD-C2D	-2.89	1.44	1.50
22	7	317	CLA	C1D-ND	2.89	1.41	1.37
22	B	807	CLA	C1D-ND	2.89	1.41	1.37
22	5	304	CLA	C4B-NB	2.89	1.41	1.37
22	6	303	CLA	MG-NB	-2.88	2.00	2.05
22	G	103	CLA	C4B-NB	2.88	1.41	1.37
22	0	311	CLA	C4B-NB	2.88	1.41	1.37
29	2	301	CHL	C1B-NB	-2.88	1.34	1.37
22	5	312	CLA	C4B-NB	2.88	1.41	1.37
25	A	848	8CT	C07-C02	-2.88	1.45	1.51
25	I	101	8CT	C18-C17	2.88	1.52	1.43
29	7	308	CHL	CHB-C1B	2.88	1.45	1.39
22	0	304	CLA	C3B-C4B	2.88	1.49	1.42
22	A	813	CLA	C1D-ND	2.88	1.41	1.37
22	1	304	CLA	MG-NB	-2.88	2.00	2.05
22	L	204	CLA	C3B-C4B	2.87	1.49	1.42
22	A	835	CLA	C3B-C4B	2.87	1.49	1.42
22	6	305	CLA	C3B-C4B	2.87	1.49	1.42
22	F	301	CLA	MG-NB	-2.87	2.00	2.05
25	1	316	8CT	C30-C29	2.87	1.54	1.50
22	A	818	CLA	C1D-ND	2.87	1.41	1.37
22	9	313	CLA	C4B-NB	2.87	1.41	1.37
25	L	206	8CT	C30-C29	2.87	1.54	1.50
31	4	318	LMG	O6-C5	-2.87	1.37	1.44
22	3	307	CLA	C4B-NB	2.86	1.41	1.37
29	4	306	CHL	MG-NA	-2.86	1.99	2.06
25	B	845	8CT	C35-C30	2.86	1.64	1.56
22	1	301	CLA	C3B-C4B	2.86	1.49	1.42
22	0	309	CLA	C3B-C4B	2.86	1.49	1.42
25	6	321	8CT	C10-C03	2.86	1.55	1.45
28	B	849	DGD	O1G-C1G	-2.86	1.38	1.45
25	7	323	8CT	C30-C29	2.86	1.54	1.50
22	5	307	CLA	C4B-NB	2.86	1.41	1.37
22	3	305	CLA	C1D-ND	2.86	1.41	1.37
22	A	810	CLA	C4B-NB	2.86	1.41	1.37
22	A	835	CLA	C4B-NB	2.86	1.41	1.37
25	F	302	8CT	C30-C29	2.85	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	827	CLA	MG-NB	-2.85	2.00	2.05
25	A	847	8CT	C07-C02	-2.85	1.45	1.51
25	A	854	8CT	C30-C29	2.85	1.54	1.50
22	2	302	CLA	MG-NB	-2.85	2.00	2.05
22	B	829	CLA	C1D-ND	2.84	1.41	1.37
25	F	302	8CT	C35-C30	2.84	1.64	1.56
22	6	303	CLA	C1D-ND	2.84	1.41	1.37
25	8	318	8CT	C30-C29	2.84	1.54	1.50
29	6	307	CHL	C1B-NB	-2.84	1.34	1.37
22	B	840	CLA	C1D-ND	2.84	1.41	1.37
22	7	304	CLA	C1D-ND	2.84	1.41	1.37
22	B	816	CLA	C4B-NB	2.84	1.41	1.37
22	B	824	CLA	C1D-ND	2.84	1.41	1.37
29	2	306	CHL	C3D-C2D	2.84	1.46	1.39
22	6	313	CLA	MG-NB	-2.83	2.00	2.05
29	2	307	CHL	C1B-NB	-2.83	1.34	1.37
29	6	308	CHL	C1B-NB	-2.83	1.34	1.37
22	B	831	CLA	MG-NB	-2.83	2.00	2.05
22	3	301	CLA	C1D-ND	2.83	1.41	1.37
25	B	847	8CT	C07-C02	-2.83	1.45	1.51
22	A	841	CLA	CMD-C2D	-2.83	1.44	1.50
22	A	838	CLA	C1D-ND	2.83	1.41	1.37
22	0	308	CLA	C3B-C4B	2.83	1.49	1.42
22	8	304	CLA	C4B-NB	2.83	1.41	1.37
25	L	205	8CT	C30-C29	2.83	1.54	1.50
22	3	302	CLA	C3B-C4B	2.82	1.49	1.42
22	J	103	CLA	C4B-NB	2.82	1.41	1.37
25	J	101	8CT	C30-C29	2.82	1.54	1.50
22	2	303	CLA	MG-NB	-2.82	2.00	2.05
29	9	307	CHL	C1D-C2D	2.82	1.50	1.45
22	8	302	CLA	MG-NB	-2.82	2.00	2.05
29	6	316	CHL	C1D-C2D	2.82	1.50	1.45
29	8	305	CHL	C3D-C2D	2.82	1.46	1.39
25	B	844	8CT	C30-C29	2.82	1.54	1.50
22	A	805	CLA	MG-NB	-2.82	2.00	2.05
22	3	319	CLA	C4B-NB	2.82	1.41	1.37
22	B	813	CLA	C3B-C4B	2.82	1.49	1.42
25	8	301	8CT	C30-C29	2.82	1.54	1.50
22	B	813	CLA	C4B-NB	2.82	1.41	1.37
22	L	203	CLA	C4B-NB	2.82	1.41	1.37
25	3	316	8CT	C30-C29	2.82	1.54	1.50
25	A	848	8CT	C30-C29	2.82	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	826	CLA	MG-NB	-2.82	2.00	2.05
22	4	308	CLA	MG-NB	-2.82	2.00	2.05
22	A	819	CLA	MG-NB	-2.81	2.00	2.05
22	B	818	CLA	CMB-C2B	-2.81	1.44	1.50
29	5	306	CHL	MG-NA	-2.81	1.99	2.06
22	3	303	CLA	C3B-C4B	2.81	1.49	1.42
25	A	850	8CT	C07-C02	-2.81	1.45	1.51
22	L	204	CLA	C4B-NB	2.81	1.41	1.37
22	B	850	CLA	C3B-C4B	2.81	1.49	1.42
22	5	314	CLA	C4B-NB	2.80	1.41	1.37
22	L	202	CLA	C3B-C4B	2.80	1.49	1.42
22	0	302	CLA	C3B-C4B	2.80	1.49	1.42
29	8	306	CHL	MG-NA	-2.80	1.99	2.06
22	5	311	CLA	C4B-NB	2.80	1.41	1.37
22	7	315	CLA	C1D-ND	2.80	1.41	1.37
22	7	309	CLA	C1D-ND	2.80	1.41	1.37
25	7	321	8CT	C07-C02	-2.80	1.45	1.51
22	2	314	CLA	C4B-NB	2.80	1.41	1.37
22	9	311	CLA	C4B-NB	2.80	1.41	1.37
25	I	101	8CT	C07-C02	-2.80	1.45	1.51
22	4	309	CLA	C1D-ND	2.80	1.41	1.37
22	6	304	CLA	C4B-NB	2.79	1.41	1.37
22	B	809	CLA	C1D-ND	2.79	1.41	1.37
22	9	308	CLA	C4B-NB	2.79	1.41	1.37
29	1	305	CHL	C4B-NB	-2.79	1.34	1.37
22	A	852	CLA	C4B-NB	2.79	1.41	1.37
22	7	303	CLA	C4B-NB	2.79	1.41	1.37
22	9	306	CLA	C4B-NB	2.79	1.41	1.37
22	B	836	CLA	MG-NB	-2.79	2.00	2.05
25	B	843	8CT	C07-C02	-2.79	1.45	1.51
25	B	804	8CT	C35-C30	2.79	1.64	1.56
25	L	206	8CT	C10-C03	2.79	1.55	1.45
29	2	306	CHL	C1D-ND	-2.79	1.34	1.37
22	3	308	CLA	C3B-C4B	2.79	1.49	1.42
22	7	307	CLA	C3B-C4B	2.79	1.49	1.42
22	B	832	CLA	C1B-NB	-2.78	1.34	1.37
22	6	315	CLA	C3B-C4B	2.78	1.49	1.42
22	4	308	CLA	C1D-ND	2.78	1.41	1.37
29	5	301	CHL	MG-NA	-2.78	1.99	2.06
22	8	309	CLA	C3B-C4B	2.78	1.49	1.42
22	B	823	CLA	MG-NB	-2.78	2.00	2.05
29	0	306	CHL	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	840	CLA	MG-NB	-2.78	2.00	2.05
22	B	834	CLA	C3B-C4B	2.78	1.49	1.42
22	3	301	CLA	C3B-C4B	2.78	1.49	1.42
22	6	310	CLA	C3B-C4B	2.77	1.49	1.42
25	2	317	8CT	C07-C02	-2.77	1.45	1.51
29	8	314	CHL	C1D-C2D	2.77	1.50	1.45
25	7	301	8CT	C30-C29	2.77	1.54	1.50
22	A	805	CLA	C1D-ND	2.77	1.41	1.37
22	3	309	CLA	C4B-NB	2.77	1.41	1.37
22	A	813	CLA	C3B-C4B	2.77	1.49	1.42
22	4	304	CLA	MG-NB	-2.77	2.00	2.05
22	7	304	CLA	MG-NB	-2.77	2.00	2.05
22	2	309	CLA	C3B-C4B	2.77	1.49	1.42
22	3	312	CLA	C4B-NB	2.77	1.41	1.37
22	6	310	CLA	C4B-NB	2.77	1.41	1.37
29	1	305	CHL	C1B-NB	-2.77	1.34	1.37
25	A	849	8CT	C30-C29	2.77	1.54	1.50
22	9	312	CLA	C3B-C4B	2.77	1.49	1.42
25	F	302	8CT	C07-C02	-2.77	1.45	1.51
29	9	302	CHL	C3D-C2D	2.77	1.46	1.39
22	4	302	CLA	MG-NB	-2.77	2.00	2.05
22	A	832	CLA	MG-NB	-2.76	2.00	2.05
29	8	307	CHL	C3D-C2D	2.76	1.46	1.39
29	6	316	CHL	C1B-NB	-2.76	1.34	1.37
29	0	306	CHL	C4C-C3C	2.76	1.49	1.45
25	B	844	8CT	C35-C30	2.76	1.64	1.56
22	2	308	CLA	MG-NB	-2.76	2.00	2.05
25	A	846	8CT	C07-C02	-2.76	1.45	1.51
22	3	302	CLA	C4B-NB	2.76	1.41	1.37
22	1	312	CLA	C3B-C4B	2.76	1.49	1.42
22	A	812	CLA	C4B-NB	2.76	1.41	1.37
22	A	852	CLA	C3B-C4B	2.76	1.49	1.42
22	1	303	CLA	C3B-C4B	2.76	1.49	1.42
22	A	838	CLA	C3B-C4B	2.76	1.49	1.42
22	6	309	CLA	C4B-NB	2.75	1.41	1.37
22	A	838	CLA	MG-NB	-2.75	2.00	2.05
25	B	851	8CT	C07-C02	-2.75	1.45	1.51
25	J	104	8CT	C30-C29	2.75	1.54	1.50
22	B	806	CLA	MG-NB	-2.75	2.00	2.05
22	2	308	CLA	C3B-C4B	2.75	1.49	1.42
29	4	305	CHL	C3D-C2D	2.75	1.46	1.39
22	1	313	CLA	C3B-C4B	2.75	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	840	CLA	C1D-ND	2.75	1.41	1.37
22	L	201	CLA	C1D-ND	2.75	1.41	1.37
22	B	809	CLA	MG-NB	-2.75	2.00	2.05
29	8	307	CHL	C1B-NB	-2.75	1.34	1.37
22	9	304	CLA	MG-NB	-2.75	2.00	2.05
22	A	838	CLA	C4B-NB	2.75	1.41	1.37
22	3	313	CLA	MG-NB	-2.75	2.00	2.05
22	B	834	CLA	CMB-C2B	-2.75	1.45	1.50
22	A	831	CLA	MG-NB	-2.75	2.00	2.05
29	8	314	CHL	C1D-ND	-2.75	1.34	1.37
22	B	821	CLA	MG-NB	-2.75	2.00	2.05
29	0	306	CHL	C1D-C2D	2.74	1.50	1.45
22	3	310	CLA	C4B-NB	2.74	1.41	1.37
29	6	308	CHL	MG-NA	-2.74	1.99	2.06
25	B	845	8CT	C10-C03	2.74	1.54	1.45
25	B	848	8CT	C30-C29	2.74	1.54	1.50
22	A	816	CLA	C4B-NB	2.74	1.41	1.37
22	B	831	CLA	C4B-NB	2.74	1.41	1.37
22	4	313	CLA	C3B-C4B	2.74	1.49	1.42
22	B	821	CLA	C1D-ND	2.74	1.41	1.37
29	3	306	CHL	C1D-ND	-2.74	1.34	1.37
22	B	830	CLA	MG-NB	-2.74	2.00	2.05
22	A	808	CLA	MG-NB	-2.74	2.00	2.05
22	A	808	CLA	C3B-C4B	2.74	1.49	1.42
25	F	302	8CT	C10-C03	2.74	1.54	1.45
22	7	316	CLA	C3B-C4B	2.74	1.49	1.42
29	6	306	CHL	C3D-C2D	2.74	1.46	1.39
22	8	313	CLA	C3B-C4B	2.74	1.49	1.42
22	A	809	CLA	MG-NB	-2.74	2.00	2.05
29	0	301	CHL	C1D-ND	-2.74	1.34	1.37
22	3	304	CLA	MG-NB	-2.74	2.00	2.05
29	1	305	CHL	MG-NA	-2.74	1.99	2.06
22	4	309	CLA	C3B-C4B	2.73	1.49	1.42
22	B	830	CLA	CMB-C2B	-2.73	1.45	1.50
25	I	101	8CT	C10-C03	2.73	1.54	1.45
22	A	820	CLA	MG-NB	-2.73	2.00	2.05
22	8	302	CLA	C3B-C4B	2.73	1.49	1.42
22	9	310	CLA	C3B-C4B	2.73	1.49	1.42
29	8	305	CHL	C1D-C2D	2.73	1.50	1.45
22	J	103	CLA	C3B-C4B	2.73	1.49	1.42
29	0	306	CHL	C1B-NB	-2.73	1.34	1.37
22	H	201	CLA	MG-NB	-2.73	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	316	8CT	C07-C02	-2.73	1.45	1.51
22	5	310	CLA	C4B-NB	2.72	1.41	1.37
29	6	302	CHL	C1B-NB	-2.72	1.34	1.37
22	1	306	CLA	C3B-C4B	2.72	1.49	1.42
22	2	319	CLA	MG-NB	-2.72	2.00	2.05
29	8	307	CHL	CHB-C1B	2.72	1.45	1.39
22	7	318	CLA	C4B-NB	2.72	1.41	1.37
22	A	803	CLA	MG-NB	-2.72	2.00	2.05
22	A	843	CLA	C3B-C4B	2.72	1.49	1.42
29	8	307	CHL	C4B-NB	-2.72	1.34	1.37
22	A	818	CLA	MG-NB	-2.72	2.00	2.05
22	A	830	CLA	MG-NB	-2.72	2.00	2.05
22	8	310	CLA	MG-NB	-2.72	2.00	2.05
22	2	310	CLA	C4B-NB	2.72	1.41	1.37
22	A	815	CLA	C3B-C4B	2.72	1.49	1.42
22	6	301	CLA	C3B-C4B	2.72	1.49	1.42
22	5	302	CLA	MG-NB	-2.72	2.00	2.05
22	1	313	CLA	C4B-NB	2.72	1.41	1.37
22	5	302	CLA	C1D-ND	2.72	1.41	1.37
22	2	302	CLA	C3B-C4B	2.72	1.49	1.42
22	5	309	CLA	C3B-C4B	2.72	1.49	1.42
22	4	309	CLA	MG-NB	-2.71	2.00	2.05
22	B	850	CLA	C4B-NB	2.71	1.41	1.37
29	5	301	CHL	C3B-C4B	2.71	1.49	1.42
29	9	302	CHL	C1D-C2D	2.71	1.50	1.45
22	B	835	CLA	MG-NB	-2.71	2.00	2.05
22	B	839	CLA	C3B-C4B	2.71	1.49	1.42
25	A	854	8CT	C07-C02	-2.71	1.45	1.51
25	B	847	8CT	C30-C29	2.71	1.54	1.50
25	8	301	8CT	C07-C02	-2.71	1.45	1.51
22	3	319	CLA	C3B-C4B	2.71	1.49	1.42
29	8	314	CHL	C1B-C2B	2.71	1.49	1.43
29	8	306	CHL	C1D-C2D	2.71	1.50	1.45
22	9	303	CLA	C4B-NB	2.71	1.41	1.37
22	0	305	CLA	C4B-NB	2.70	1.41	1.37
22	A	834	CLA	CMB-C2B	-2.70	1.45	1.50
22	A	825	CLA	C4B-NB	2.70	1.41	1.37
22	B	820	CLA	C4B-NB	2.70	1.41	1.37
22	6	312	CLA	C3B-C4B	2.70	1.49	1.42
29	5	301	CHL	C3D-C2D	2.70	1.46	1.39
22	6	318	CLA	C4B-NB	2.70	1.41	1.37
22	A	836	CLA	C1D-ND	2.70	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	308	CLA	C4B-NB	2.70	1.41	1.37
25	4	317	8CT	C07-C02	-2.70	1.45	1.51
22	1	309	CLA	C4B-NB	2.70	1.41	1.37
22	9	309	CLA	C3B-C4B	2.70	1.49	1.42
22	B	832	CLA	MG-NB	-2.70	2.00	2.05
22	B	837	CLA	C1D-ND	2.70	1.41	1.37
22	A	853	CLA	C4B-NB	2.70	1.41	1.37
29	4	306	CHL	C1D-ND	-2.70	1.34	1.37
22	5	312	CLA	C3B-C4B	2.70	1.49	1.42
22	B	821	CLA	C3B-C4B	2.69	1.49	1.42
22	F	301	CLA	C3B-C4B	2.69	1.49	1.42
22	A	841	CLA	CMB-C2B	-2.69	1.45	1.50
22	5	304	CLA	C3B-C4B	2.69	1.49	1.42
22	4	310	CLA	C4B-NB	2.69	1.41	1.37
24	1	317	LHG	O7-C5	-2.69	1.39	1.46
29	0	306	CHL	C4B-NB	-2.69	1.34	1.37
25	6	321	8CT	C30-C29	2.69	1.54	1.50
22	0	310	CLA	C3B-C4B	2.69	1.49	1.42
22	A	815	CLA	C4B-NB	2.69	1.41	1.37
22	H	201	CLA	C3B-C4B	2.69	1.49	1.42
25	8	318	8CT	C07-C02	-2.69	1.45	1.51
22	A	833	CLA	MG-NB	-2.69	2.00	2.05
22	5	303	CLA	MG-NB	-2.69	2.00	2.05
22	B	806	CLA	CMC-C2C	-2.69	1.45	1.50
22	A	808	CLA	C4B-NB	2.69	1.41	1.37
22	B	805	CLA	C1D-ND	2.68	1.41	1.37
29	4	306	CHL	C1D-C2D	2.68	1.50	1.45
22	8	309	CLA	MG-NB	-2.68	2.00	2.05
22	7	311	CLA	C4B-NB	2.68	1.41	1.37
25	K	103	8CT	C07-C02	-2.68	1.45	1.51
22	B	809	CLA	C4B-NB	2.68	1.41	1.37
22	7	314	CLA	MG-NB	-2.68	2.00	2.05
22	6	313	CLA	C1D-ND	2.68	1.41	1.37
22	B	812	CLA	CMB-C2B	-2.68	1.45	1.50
22	B	805	CLA	C4B-NB	2.68	1.41	1.37
22	7	314	CLA	C4B-NB	2.68	1.41	1.37
25	J	101	8CT	C07-C02	-2.68	1.45	1.51
22	3	305	CLA	MG-NB	-2.67	2.00	2.05
22	9	311	CLA	C3B-C4B	2.67	1.49	1.42
22	6	314	CLA	C3B-C4B	2.67	1.49	1.42
22	A	837	CLA	MG-NB	-2.67	2.00	2.05
22	B	820	CLA	MG-NB	-2.67	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	313	CLA	C3B-C4B	2.67	1.49	1.42
25	A	849	8CT	C07-C02	-2.67	1.45	1.51
22	B	824	CLA	MG-NB	-2.67	2.00	2.05
22	K	101	CLA	C3B-C4B	2.67	1.49	1.42
22	B	825	CLA	C4B-NB	2.67	1.41	1.37
22	M	101	CLA	C3B-C4B	2.67	1.49	1.42
22	1	312	CLA	MG-NB	-2.67	2.00	2.05
29	6	308	CHL	C3D-C2D	2.67	1.46	1.39
22	B	812	CLA	C4B-NB	2.67	1.41	1.37
22	B	815	CLA	C3B-C4B	2.67	1.49	1.42
22	B	817	CLA	MG-NB	-2.67	2.00	2.05
25	7	321	8CT	C30-C29	2.66	1.54	1.50
22	1	303	CLA	C4B-NB	2.66	1.41	1.37
22	0	303	CLA	C3B-C4B	2.66	1.49	1.42
22	B	803	CLA	MG-NB	-2.66	2.00	2.05
22	2	314	CLA	C3B-C4B	2.66	1.49	1.42
22	A	828	CLA	C1D-ND	2.66	1.41	1.37
22	B	801	CLA	C1D-ND	2.66	1.41	1.37
25	5	317	8CT	C07-C02	-2.66	1.45	1.51
22	A	827	CLA	C3B-C4B	2.66	1.49	1.42
29	4	301	CHL	C1D-ND	-2.66	1.34	1.37
22	G	102	CLA	C3B-C4B	2.66	1.49	1.42
22	2	303	CLA	C4B-NB	2.66	1.41	1.37
22	B	810	CLA	MG-NB	-2.66	2.00	2.05
29	9	307	CHL	MG-NA	-2.66	2.00	2.06
22	A	818	CLA	C1B-NB	-2.66	1.34	1.37
29	7	308	CHL	C1D-ND	-2.66	1.34	1.37
22	4	303	CLA	MG-NB	-2.66	2.00	2.05
22	A	821	CLA	MG-NB	-2.66	2.00	2.05
22	B	814	CLA	CMC-C2C	-2.65	1.45	1.50
22	A	819	CLA	C3B-C4B	2.65	1.49	1.42
22	1	307	CLA	C4B-NB	2.65	1.41	1.37
22	9	310	CLA	C1B-C2B	2.65	1.49	1.43
22	5	311	CLA	C3B-C4B	2.65	1.49	1.42
22	6	323	CLA	MG-NB	-2.65	2.00	2.05
29	7	308	CHL	C1B-NB	-2.65	1.34	1.37
22	G	103	CLA	C3B-C4B	2.65	1.49	1.42
22	7	309	CLA	MG-NB	-2.65	2.00	2.05
22	7	317	CLA	MG-NB	-2.65	2.00	2.05
22	8	310	CLA	C1B-C2B	2.65	1.49	1.43
22	B	837	CLA	C4B-NB	2.65	1.41	1.37
22	K	105	CLA	C3B-C4B	2.65	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	304	CLA	MG-NB	-2.65	2.00	2.05
25	B	846	8CT	C07-C02	-2.65	1.45	1.51
29	1	305	CHL	C1D-C2D	2.65	1.50	1.45
22	A	829	CLA	C3B-C4B	2.65	1.49	1.42
22	A	827	CLA	MG-NB	-2.65	2.00	2.05
22	K	104	CLA	MG-NB	-2.65	2.00	2.05
22	0	305	CLA	C1B-C2B	2.65	1.49	1.43
31	4	318	LMG	O1-C7	-2.65	1.38	1.43
29	7	308	CHL	C4B-NB	-2.65	1.34	1.37
22	B	834	CLA	MG-NB	-2.64	2.00	2.05
22	9	305	CLA	C3B-C4B	2.64	1.49	1.42
22	1	310	CLA	C4B-NB	2.64	1.41	1.37
22	9	306	CLA	MG-NB	-2.64	2.00	2.05
22	A	837	CLA	C3B-C4B	2.64	1.48	1.42
22	6	312	CLA	C4B-NB	2.64	1.41	1.37
22	7	303	CLA	MG-NB	-2.64	2.00	2.05
22	A	802	CLA	MG-NB	-2.64	2.00	2.05
22	A	813	CLA	MG-NB	-2.64	2.00	2.05
22	B	841	CLA	MG-NB	-2.64	2.00	2.05
29	2	305	CHL	C1D-ND	-2.64	1.34	1.37
22	A	841	CLA	MG-NB	-2.64	2.00	2.05
25	1	316	8CT	C07-C02	-2.64	1.45	1.51
22	L	203	CLA	C3B-C4B	2.64	1.48	1.42
22	B	831	CLA	CMB-C2B	-2.64	1.45	1.50
25	B	844	8CT	C07-C02	-2.64	1.45	1.51
22	K	102	CLA	MG-NB	-2.64	2.00	2.05
22	B	814	CLA	C3B-C4B	2.64	1.48	1.42
22	A	840	CLA	MG-NB	-2.64	2.00	2.05
22	0	310	CLA	C4B-NB	2.64	1.41	1.37
22	4	311	CLA	MG-NB	-2.63	2.00	2.05
22	6	314	CLA	C4B-NB	2.63	1.41	1.37
22	A	810	CLA	C3B-C4B	2.63	1.48	1.42
22	B	809	CLA	C3B-C4B	2.63	1.48	1.42
22	B	805	CLA	MG-NB	-2.63	2.00	2.05
22	8	308	CLA	C3B-C4B	2.63	1.48	1.42
26	A	851	HTG	C1-S1	-2.63	1.76	1.80
29	6	316	CHL	C1D-ND	-2.63	1.34	1.37
29	0	301	CHL	C1B-NB	-2.63	1.34	1.37
22	5	313	CLA	C3B-C4B	2.63	1.48	1.42
22	A	803	CLA	C1D-ND	2.63	1.41	1.37
22	A	823	CLA	C4B-NB	2.63	1.41	1.37
22	3	305	CLA	C4B-NB	2.63	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	104	8CT	C07-C02	-2.63	1.45	1.51
22	7	304	CLA	C4B-NB	2.63	1.41	1.37
22	B	814	CLA	MG-NB	-2.63	2.00	2.05
22	3	301	CLA	MG-NB	-2.63	2.00	2.05
22	2	313	CLA	C4B-NB	2.63	1.41	1.37
29	4	301	CHL	C4B-NB	-2.63	1.34	1.37
22	A	804	CLA	CMD-C2D	-2.63	1.45	1.50
22	B	811	CLA	C4B-NB	2.63	1.41	1.37
22	B	829	CLA	MG-NB	-2.63	2.00	2.05
22	A	834	CLA	MG-NB	-2.63	2.00	2.05
25	B	804	8CT	C07-C02	-2.62	1.45	1.51
22	B	833	CLA	C4B-NB	2.62	1.41	1.37
29	5	306	CHL	C4B-NB	-2.62	1.34	1.37
29	3	306	CHL	OBD-CAD	2.62	1.27	1.22
24	5	318	LHG	O7-C5	-2.62	1.40	1.46
22	B	812	CLA	C3B-C4B	2.62	1.48	1.42
22	8	308	CLA	C4B-NB	2.62	1.41	1.37
22	A	828	CLA	MG-NB	-2.62	2.00	2.05
22	K	104	CLA	C3B-C4B	2.62	1.48	1.42
22	A	836	CLA	MG-NB	-2.62	2.00	2.05
22	2	312	CLA	MG-NB	-2.62	2.00	2.05
22	B	840	CLA	CMB-C2B	-2.62	1.45	1.50
22	A	814	CLA	MG-NB	-2.62	2.00	2.05
22	2	313	CLA	MG-NB	-2.62	2.00	2.05
22	3	310	CLA	C3B-C4B	2.62	1.48	1.42
22	B	832	CLA	C3B-C4B	2.62	1.48	1.42
22	A	822	CLA	C3B-C4B	2.61	1.48	1.42
22	7	306	CLA	MG-NB	-2.61	2.00	2.05
22	B	829	CLA	C1B-NB	-2.61	1.34	1.37
22	B	827	CLA	C3B-C4B	2.61	1.48	1.42
22	B	829	CLA	CMB-C2B	-2.61	1.45	1.50
22	A	853	CLA	C3B-C4B	2.61	1.48	1.42
25	L	206	8CT	C07-C02	-2.61	1.45	1.51
22	A	817	CLA	MG-NB	-2.61	2.00	2.05
25	B	848	8CT	C07-C02	-2.61	1.45	1.51
25	6	321	8CT	C07-C02	-2.61	1.45	1.51
25	7	323	8CT	C07-C02	-2.61	1.45	1.51
22	4	314	CLA	C3B-C4B	2.61	1.48	1.42
29	3	306	CHL	C1B-NB	-2.61	1.34	1.37
22	1	302	CLA	MG-NB	-2.61	2.00	2.05
22	B	811	CLA	C3B-C4B	2.61	1.48	1.42
22	7	313	CLA	MG-NB	-2.61	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	821	CLA	C3B-C4B	2.61	1.48	1.42
22	7	315	CLA	C3B-C4B	2.61	1.48	1.42
22	7	315	CLA	MG-NB	-2.61	2.00	2.05
22	B	801	CLA	MG-NB	-2.61	2.00	2.05
25	J	104	8CT	C07-C02	-2.61	1.45	1.51
22	A	818	CLA	C4B-NB	2.60	1.41	1.37
22	A	826	CLA	C4B-NB	2.60	1.41	1.37
29	4	305	CHL	C1D-ND	-2.60	1.34	1.37
22	B	808	CLA	MG-NB	-2.60	2.00	2.05
22	6	303	CLA	C4B-NB	2.60	1.41	1.37
22	A	801	CLA	CMD-C2D	-2.60	1.45	1.50
22	A	805	CLA	CMB-C2B	-2.60	1.45	1.50
22	A	824	CLA	MG-NB	-2.60	2.00	2.05
29	6	302	CHL	C1D-ND	-2.60	1.34	1.37
29	2	306	CHL	MG-NA	-2.60	2.00	2.06
22	9	303	CLA	MG-NB	-2.60	2.00	2.05
22	B	820	CLA	C3B-C4B	2.60	1.48	1.42
22	6	318	CLA	MG-NB	-2.60	2.00	2.05
22	7	302	CLA	C3B-C4B	2.60	1.48	1.42
22	2	309	CLA	C4B-NB	2.60	1.41	1.37
22	2	309	CLA	CMC-C2C	-2.60	1.45	1.50
22	B	807	CLA	C3B-C4B	2.60	1.48	1.42
22	B	824	CLA	C3B-C4B	2.60	1.48	1.42
22	3	312	CLA	C3B-C4B	2.60	1.48	1.42
22	B	822	CLA	MG-NB	-2.60	2.00	2.05
22	5	302	CLA	CMB-C2B	-2.60	1.45	1.50
22	2	310	CLA	C3B-C4B	2.60	1.48	1.42
22	8	310	CLA	C3B-C4B	2.60	1.48	1.42
22	6	310	CLA	MG-NB	-2.60	2.00	2.05
22	7	305	CLA	MG-NB	-2.60	2.00	2.05
25	B	804	8CT	C10-C03	2.60	1.54	1.45
22	9	313	CLA	MG-NB	-2.60	2.00	2.05
22	B	810	CLA	C4B-NB	2.59	1.41	1.37
22	2	308	CLA	C1D-ND	2.59	1.41	1.37
22	1	309	CLA	MG-NB	-2.59	2.00	2.05
29	2	306	CHL	C4B-NB	-2.59	1.34	1.37
22	B	829	CLA	C3B-C4B	2.59	1.48	1.42
22	B	825	CLA	CMD-C2D	-2.59	1.45	1.50
22	A	829	CLA	MG-NB	-2.59	2.00	2.05
29	2	307	CHL	C1D-ND	-2.59	1.34	1.37
29	6	307	CHL	C4B-NB	-2.59	1.34	1.37
22	8	315	CLA	C3B-C4B	2.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	306	CHL	C1B-NB	-2.59	1.34	1.37
22	B	836	CLA	C1D-ND	2.59	1.41	1.37
29	5	301	CHL	C1D-ND	-2.59	1.34	1.37
25	3	318	8CT	C30-C29	2.59	1.54	1.50
22	1	307	CLA	MG-NB	-2.59	2.00	2.05
22	M	101	CLA	MG-NB	-2.59	2.00	2.05
22	A	801	CLA	MG-NB	-2.59	2.00	2.05
22	B	833	CLA	C1B-C2B	2.58	1.49	1.43
22	9	303	CLA	C1B-C2B	2.58	1.49	1.43
22	1	312	CLA	C4B-NB	2.58	1.41	1.37
22	9	309	CLA	C4B-NB	2.58	1.41	1.37
22	B	816	CLA	MG-NB	-2.58	2.00	2.05
22	5	310	CLA	MG-NB	-2.58	2.00	2.05
22	L	201	CLA	MG-NB	-2.58	2.00	2.05
22	6	311	CLA	MG-NB	-2.58	2.00	2.05
22	4	304	CLA	C3B-C4B	2.58	1.48	1.42
22	5	302	CLA	C3B-C4B	2.58	1.48	1.42
29	8	307	CHL	C1D-ND	-2.58	1.34	1.37
22	B	828	CLA	C3B-C4B	2.58	1.48	1.42
22	F	301	CLA	CMB-C2B	-2.58	1.45	1.50
22	6	312	CLA	MG-NB	-2.58	2.00	2.05
22	1	302	CLA	C3B-C4B	2.58	1.48	1.42
22	3	308	CLA	C4B-NB	2.58	1.41	1.37
22	A	811	CLA	MG-NB	-2.58	2.00	2.05
22	2	314	CLA	MG-NB	-2.58	2.00	2.05
22	B	816	CLA	C3B-C4B	2.58	1.48	1.42
22	3	308	CLA	CMD-C2D	-2.58	1.45	1.50
22	3	303	CLA	CMB-C2B	-2.58	1.45	1.50
22	L	202	CLA	C1B-C2B	2.58	1.49	1.43
22	A	830	CLA	C1D-ND	2.58	1.41	1.37
29	8	314	CHL	C4B-NB	-2.58	1.34	1.37
22	A	825	CLA	CMD-C2D	-2.58	1.45	1.50
22	1	303	CLA	MG-NB	-2.57	2.00	2.05
22	3	310	CLA	MG-NB	-2.57	2.00	2.05
22	4	304	CLA	C4B-NB	2.57	1.40	1.37
22	7	305	CLA	C4B-NB	2.57	1.40	1.37
22	9	304	CLA	C4B-NB	2.57	1.40	1.37
22	3	305	CLA	C3B-C4B	2.57	1.48	1.42
22	B	826	CLA	C1B-NB	-2.57	1.34	1.37
29	2	307	CHL	MG-NA	-2.57	2.00	2.06
22	3	304	CLA	C4B-NB	2.57	1.40	1.37
22	3	302	CLA	MG-NB	-2.57	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	840	CLA	C4B-NB	2.57	1.40	1.37
29	6	308	CHL	C1D-C2D	2.57	1.50	1.45
29	6	308	CHL	C4B-NB	-2.57	1.34	1.37
22	7	310	CLA	MG-NB	-2.57	2.00	2.05
22	B	828	CLA	C1D-ND	2.57	1.40	1.37
29	5	301	CHL	C1B-NB	-2.57	1.34	1.37
22	7	311	CLA	MG-NB	-2.57	2.00	2.05
29	4	307	CHL	MG-NA	-2.57	2.00	2.06
29	6	302	CHL	C4B-NB	-2.57	1.34	1.37
22	A	807	CLA	C4B-NB	2.56	1.40	1.37
22	2	311	CLA	C4B-NB	2.56	1.40	1.37
22	2	311	CLA	MG-NB	-2.56	2.00	2.05
29	6	306	CHL	C1D-C2D	2.56	1.50	1.45
22	0	302	CLA	MG-NB	-2.56	2.00	2.05
22	B	831	CLA	CMD-C2D	-2.56	1.45	1.50
22	4	312	CLA	MG-NB	-2.56	2.00	2.05
22	4	312	CLA	C4B-NB	2.56	1.40	1.37
29	0	301	CHL	C4B-NB	-2.56	1.34	1.37
22	A	824	CLA	C3B-C4B	2.56	1.48	1.42
22	A	829	CLA	C4B-NB	2.56	1.40	1.37
22	B	819	CLA	CMD-C2D	-2.56	1.45	1.50
25	B	804	8CT	C30-C29	2.56	1.54	1.50
22	1	309	CLA	C3B-C4B	2.56	1.48	1.42
29	1	305	CHL	C1D-ND	-2.56	1.34	1.37
29	5	306	CHL	C1D-C2D	2.56	1.50	1.45
22	A	825	CLA	CMB-C2B	-2.56	1.45	1.50
29	5	306	CHL	C3B-C4B	2.56	1.48	1.42
22	8	308	CLA	MG-NB	-2.56	2.00	2.05
22	B	808	CLA	C3B-C4B	2.56	1.48	1.42
22	B	838	CLA	C4B-NB	2.56	1.40	1.37
22	7	315	CLA	C4B-NB	2.56	1.40	1.37
22	6	311	CLA	C3B-C4B	2.56	1.48	1.42
22	5	310	CLA	C3B-C4B	2.56	1.48	1.42
29	6	307	CHL	C3B-C4B	2.56	1.48	1.42
29	4	305	CHL	MG-NA	-2.56	2.00	2.06
22	B	841	CLA	C3B-C4B	2.56	1.48	1.42
22	6	310	CLA	CMB-C2B	-2.56	1.45	1.50
22	B	835	CLA	C3B-C4B	2.55	1.48	1.42
29	0	301	CHL	C1D-C2D	2.55	1.50	1.45
24	2	318	LHG	O7-C5	-2.55	1.40	1.46
22	A	810	CLA	MG-NB	-2.55	2.00	2.05
22	2	311	CLA	C3B-C4B	2.55	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	310	CLA	MG-NB	-2.55	2.00	2.05
25	F	302	8CT	C33-C32	-2.55	1.43	1.50
29	8	305	CHL	C1B-NB	-2.55	1.34	1.37
22	7	313	CLA	C3B-C4B	2.55	1.48	1.42
22	6	323	CLA	C4B-NB	2.55	1.40	1.37
22	7	302	CLA	C4B-NB	2.55	1.40	1.37
22	2	310	CLA	CMB-C2B	-2.55	1.45	1.50
22	B	819	CLA	MG-NB	-2.55	2.00	2.05
22	4	313	CLA	C4B-NB	2.55	1.40	1.37
29	2	306	CHL	C1D-C2D	2.55	1.50	1.45
22	A	827	CLA	CMC-C2C	-2.55	1.45	1.50
22	A	804	CLA	MG-NB	-2.55	2.00	2.05
22	A	836	CLA	C4B-NB	2.55	1.40	1.37
25	B	844	8CT	C25-C26	2.55	1.39	1.35
22	A	853	CLA	MG-NB	-2.55	2.00	2.05
22	0	304	CLA	C1B-C2B	2.54	1.49	1.43
22	5	303	CLA	C4B-NB	2.54	1.40	1.37
22	1	313	CLA	MG-NB	-2.54	2.00	2.05
22	1	307	CLA	C1B-C2B	2.54	1.49	1.43
22	A	827	CLA	C4B-NB	2.54	1.40	1.37
22	B	823	CLA	C4B-NB	2.54	1.40	1.37
29	5	301	CHL	C4B-NB	-2.54	1.34	1.37
22	B	811	CLA	MG-NB	-2.54	2.00	2.05
22	3	309	CLA	C3B-C4B	2.54	1.48	1.42
22	A	818	CLA	C3B-C4B	2.54	1.48	1.42
29	9	302	CHL	MG-NA	-2.54	2.00	2.06
22	A	817	CLA	C4B-NB	2.54	1.40	1.37
22	A	803	CLA	C3B-C4B	2.54	1.48	1.42
22	1	301	CLA	CMB-C2B	-2.54	1.45	1.50
22	1	311	CLA	MG-NB	-2.54	2.00	2.05
22	8	312	CLA	MG-NB	-2.54	2.00	2.05
22	A	833	CLA	C3B-C4B	2.54	1.48	1.42
29	2	301	CHL	MG-NA	-2.54	2.00	2.06
22	4	303	CLA	C3B-C4B	2.54	1.48	1.42
22	8	304	CLA	C3B-C4B	2.54	1.48	1.42
22	4	311	CLA	C4B-NB	2.54	1.40	1.37
22	3	311	CLA	CMD-C2D	-2.54	1.45	1.50
29	6	316	CHL	MG-NA	-2.54	2.00	2.06
29	8	307	CHL	MG-NA	-2.54	2.00	2.06
22	5	313	CLA	C1B-C2B	2.53	1.49	1.43
22	8	311	CLA	MG-NB	-2.53	2.00	2.05
22	8	303	CLA	C4B-NB	2.53	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	101	CLA	C1B-C2B	2.53	1.49	1.43
29	5	301	CHL	C1D-C2D	2.53	1.50	1.45
22	B	819	CLA	C3B-C4B	2.53	1.48	1.42
22	B	823	CLA	C3B-C4B	2.53	1.48	1.42
22	3	303	CLA	MG-NB	-2.53	2.00	2.05
22	7	318	CLA	C3B-C4B	2.53	1.48	1.42
29	8	307	CHL	C1D-C2D	2.53	1.50	1.45
22	A	823	CLA	C3B-C4B	2.53	1.48	1.42
22	1	310	CLA	C3B-C4B	2.53	1.48	1.42
22	B	812	CLA	CMD-C2D	-2.53	1.45	1.50
29	4	307	CHL	C1D-ND	-2.53	1.34	1.37
22	A	822	CLA	MG-NB	-2.53	2.00	2.05
22	5	309	CLA	C1B-C2B	2.53	1.49	1.43
22	8	315	CLA	MG-NB	-2.53	2.00	2.05
22	B	820	CLA	CMC-C2C	-2.53	1.45	1.50
22	7	314	CLA	C3B-C4B	2.53	1.48	1.42
22	8	312	CLA	C3B-C4B	2.52	1.48	1.42
22	B	818	CLA	C4B-NB	2.52	1.40	1.37
22	A	823	CLA	MG-NB	-2.52	2.00	2.05
22	B	825	CLA	C3B-C4B	2.52	1.48	1.42
29	4	306	CHL	C3B-C4B	2.52	1.48	1.42
22	A	826	CLA	C1B-C2B	2.52	1.49	1.43
22	2	304	CLA	C4B-NB	2.52	1.40	1.37
22	A	814	CLA	C3B-C4B	2.52	1.48	1.42
22	A	822	CLA	C4B-NB	2.52	1.40	1.37
22	6	304	CLA	C3B-C4B	2.52	1.48	1.42
22	3	305	CLA	C1B-C2B	2.52	1.49	1.43
22	6	309	CLA	MG-NB	-2.52	2.00	2.05
22	6	304	CLA	MG-NB	-2.52	2.00	2.05
22	5	311	CLA	CMD-C2D	-2.52	1.45	1.50
25	A	847	8CT	C33-C32	-2.52	1.43	1.50
22	A	807	CLA	MG-NB	-2.52	2.00	2.05
22	2	304	CLA	C3B-C4B	2.52	1.48	1.42
22	B	806	CLA	CMD-C2D	-2.52	1.45	1.50
22	A	809	CLA	C4B-NB	2.52	1.40	1.37
22	B	806	CLA	MG-ND	-2.52	2.00	2.05
22	2	309	CLA	MG-NB	-2.52	2.00	2.05
22	7	312	CLA	MG-NB	-2.52	2.00	2.05
29	9	307	CHL	C3B-C4B	2.52	1.48	1.42
22	B	837	CLA	MG-NB	-2.52	2.00	2.05
22	B	837	CLA	C3B-C4B	2.52	1.48	1.42
22	A	821	CLA	C4B-NB	2.52	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	822	CLA	C4B-NB	2.51	1.40	1.37
22	A	834	CLA	C3B-C4B	2.51	1.48	1.42
22	B	839	CLA	MG-NB	-2.51	2.00	2.05
22	K	102	CLA	C4B-NB	2.51	1.40	1.37
22	B	833	CLA	CMD-C2D	-2.51	1.45	1.50
29	6	306	CHL	C1D-ND	-2.51	1.34	1.37
22	B	830	CLA	C3B-C4B	2.51	1.48	1.42
22	F	301	CLA	C4B-NB	2.51	1.40	1.37
22	7	317	CLA	C3B-C4B	2.51	1.48	1.42
22	A	837	CLA	C4B-NB	2.51	1.40	1.37
29	6	302	CHL	C1D-C2D	2.51	1.50	1.45
22	5	312	CLA	MG-NB	-2.51	2.00	2.05
22	B	838	CLA	MG-NB	-2.51	2.00	2.05
22	6	323	CLA	C3B-C4B	2.51	1.48	1.42
22	6	305	CLA	MG-NB	-2.51	2.00	2.05
25	B	851	8CT	C25-C26	2.51	1.39	1.35
29	5	306	CHL	C1D-ND	-2.51	1.34	1.37
22	B	839	CLA	CMB-C2B	-2.51	1.45	1.50
22	6	317	CLA	C4B-NB	2.51	1.40	1.37
22	9	308	CLA	C3B-C4B	2.51	1.48	1.42
25	B	846	8CT	C25-C26	2.51	1.39	1.35
22	A	840	CLA	C4B-NB	2.51	1.40	1.37
22	8	303	CLA	MG-NB	-2.51	2.00	2.05
22	2	319	CLA	C4B-NB	2.51	1.40	1.37
22	3	301	CLA	C4B-NB	2.51	1.40	1.37
22	B	833	CLA	CMC-C2C	-2.50	1.45	1.50
22	4	303	CLA	CMD-C2D	-2.50	1.45	1.50
22	B	836	CLA	CMD-C2D	-2.50	1.45	1.50
22	5	314	CLA	C3B-C4B	2.50	1.48	1.42
22	A	816	CLA	MG-NB	-2.50	2.00	2.05
22	6	311	CLA	C4B-NB	2.50	1.40	1.37
29	8	306	CHL	C1D-ND	-2.50	1.34	1.37
22	7	317	CLA	C1B-C2B	2.50	1.49	1.43
22	5	314	CLA	CMD-C2D	-2.50	1.45	1.50
22	7	307	CLA	C1B-C2B	2.50	1.49	1.43
22	3	302	CLA	CMB-C2B	-2.50	1.45	1.50
22	4	310	CLA	C3B-C4B	2.50	1.48	1.42
22	A	830	CLA	C3B-C4B	2.50	1.48	1.42
22	7	304	CLA	CMD-C2D	-2.50	1.45	1.50
22	B	831	CLA	C3B-C4B	2.50	1.48	1.42
22	K	102	CLA	C3B-C4B	2.50	1.48	1.42
22	9	305	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	814	CLA	C1D-ND	2.50	1.40	1.37
22	6	304	CLA	CMB-C2B	-2.50	1.45	1.50
22	1	301	CLA	MG-NB	-2.50	2.00	2.05
22	0	310	CLA	MG-NB	-2.50	2.00	2.05
22	5	302	CLA	C4B-NB	2.50	1.40	1.37
22	K	105	CLA	CMC-C2C	-2.50	1.45	1.50
22	G	103	CLA	C1B-C2B	2.50	1.49	1.43
22	A	843	CLA	MG-NB	-2.49	2.00	2.05
22	B	815	CLA	MG-NB	-2.49	2.00	2.05
22	8	308	CLA	CAC-C3C	-2.49	1.44	1.51
22	3	312	CLA	MG-NB	-2.49	2.00	2.05
22	L	204	CLA	MG-NB	-2.49	2.00	2.05
22	4	314	CLA	MG-NB	-2.49	2.00	2.05
22	0	307	CLA	C1B-C2B	2.49	1.49	1.43
22	5	314	CLA	MG-NB	-2.49	2.00	2.05
22	2	303	CLA	CMB-C2B	-2.49	1.45	1.50
22	4	303	CLA	C4B-NB	2.49	1.40	1.37
22	A	806	CLA	C3B-C4B	2.49	1.48	1.42
29	8	305	CHL	C3B-C4B	2.49	1.48	1.42
22	A	812	CLA	CMB-C2B	-2.49	1.45	1.50
22	A	812	CLA	MG-NB	-2.49	2.00	2.05
22	B	836	CLA	C3B-C4B	2.49	1.48	1.42
22	A	841	CLA	C4B-NB	2.49	1.40	1.37
22	B	808	CLA	CMC-C2C	-2.48	1.45	1.50
29	6	306	CHL	C1B-NB	-2.48	1.34	1.37
22	3	311	CLA	C4B-NB	2.48	1.40	1.37
22	2	303	CLA	C3B-C4B	2.48	1.48	1.42
22	A	802	CLA	C4B-NB	2.48	1.40	1.37
29	4	306	CHL	C4B-NB	-2.48	1.34	1.37
22	A	831	CLA	CMD-C2D	-2.48	1.45	1.50
31	4	318	LMG	O7-C8	-2.48	1.40	1.46
22	8	309	CLA	C4B-NB	2.48	1.40	1.37
29	8	306	CHL	C4B-NB	-2.48	1.34	1.37
30	2	315	XAT	O24-C25	-2.48	1.42	1.46
22	B	806	CLA	C1D-ND	2.48	1.40	1.37
22	A	835	CLA	MG-NB	-2.48	2.00	2.05
22	A	839	CLA	C3B-C4B	2.48	1.48	1.42
29	7	308	CHL	MG-NA	-2.48	2.00	2.06
22	2	304	CLA	MG-NB	-2.48	2.00	2.05
22	A	815	CLA	MG-NB	-2.47	2.00	2.05
22	A	812	CLA	C3B-C4B	2.47	1.48	1.42
22	A	802	CLA	CMC-C2C	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	311	CLA	MG-NB	-2.47	2.00	2.05
22	B	831	CLA	C1B-NB	-2.47	1.34	1.37
29	6	308	CHL	C1D-ND	-2.47	1.34	1.37
22	B	821	CLA	CMD-C2D	-2.47	1.45	1.50
22	4	310	CLA	MG-NB	-2.47	2.00	2.05
22	L	201	CLA	C4B-NB	2.47	1.40	1.37
22	2	310	CLA	MG-NB	-2.47	2.00	2.05
22	7	313	CLA	C4B-NB	2.47	1.40	1.37
22	7	303	CLA	C3B-C4B	2.47	1.48	1.42
22	A	817	CLA	C3B-C4B	2.47	1.48	1.42
22	4	310	CLA	CMB-C2B	-2.47	1.45	1.50
22	A	853	CLA	C1B-C2B	2.47	1.49	1.43
22	0	308	CLA	C1B-C2B	2.47	1.49	1.43
24	6	322	LHG	O7-C5	-2.47	1.40	1.46
22	B	822	CLA	C3B-C4B	2.47	1.48	1.42
22	B	832	CLA	C4B-NB	2.47	1.40	1.37
29	2	305	CHL	C1B-NB	-2.47	1.34	1.37
22	2	319	CLA	CMD-C2D	-2.47	1.45	1.50
22	4	311	CLA	C3B-C4B	2.47	1.48	1.42
29	8	314	CHL	C3B-C4B	2.47	1.48	1.42
29	8	307	CHL	CHB-C4A	-2.47	1.31	1.37
22	A	820	CLA	CMD-C2D	-2.47	1.45	1.50
22	0	303	CLA	C1B-C2B	2.46	1.49	1.43
22	A	825	CLA	MG-NB	-2.46	2.00	2.05
22	9	301	CLA	MG-NB	-2.46	2.00	2.05
22	6	313	CLA	CMD-C2D	-2.46	1.45	1.50
25	4	317	8CT	C25-C26	2.46	1.39	1.35
26	J	102	HTG	C1-S1	-2.46	1.76	1.80
22	6	315	CLA	MG-NB	-2.46	2.00	2.05
22	1	303	CLA	C1B-C2B	2.46	1.49	1.43
22	7	309	CLA	CMB-C2B	-2.46	1.45	1.50
22	A	809	CLA	C1B-C2B	2.46	1.49	1.43
29	2	301	CHL	C1D-ND	-2.46	1.34	1.37
22	5	305	CLA	MG-NB	-2.46	2.00	2.05
22	7	305	CLA	C3B-C4B	2.46	1.48	1.42
22	B	827	CLA	CMD-C2D	-2.46	1.45	1.50
29	8	314	CHL	C1B-NB	-2.46	1.34	1.37
22	L	201	CLA	C1B-C2B	2.46	1.49	1.43
22	7	309	CLA	CMD-C2D	-2.46	1.45	1.50
22	B	814	CLA	C4B-NB	2.46	1.40	1.37
22	1	304	CLA	C4B-NB	2.46	1.40	1.37
22	B	818	CLA	MG-NB	-2.46	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	304	CLA	CMD-C2D	-2.46	1.45	1.50
22	B	819	CLA	C4B-NB	2.46	1.40	1.37
22	B	815	CLA	C1B-C2B	2.46	1.49	1.43
22	A	829	CLA	CMD-C2D	-2.46	1.45	1.50
29	2	305	CHL	C3B-C4B	2.45	1.48	1.42
22	A	803	CLA	CMB-C2B	-2.45	1.45	1.50
25	3	318	8CT	C22-C21	2.45	1.56	1.50
22	4	312	CLA	CMB-C2B	-2.45	1.45	1.50
22	4	314	CLA	CMD-C2D	-2.45	1.45	1.50
22	7	302	CLA	MG-NB	-2.45	2.00	2.05
29	9	307	CHL	C4B-NB	-2.45	1.34	1.37
22	A	811	CLA	C3B-C4B	2.45	1.48	1.42
22	6	301	CLA	C1B-C2B	2.45	1.49	1.43
22	A	803	CLA	CMD-C2D	-2.45	1.45	1.50
22	5	303	CLA	C3B-C4B	2.45	1.48	1.42
22	0	305	CLA	MG-NB	-2.45	2.00	2.05
25	I	101	8CT	C33-C32	-2.45	1.43	1.50
22	A	804	CLA	C3B-C4B	2.45	1.48	1.42
22	A	828	CLA	C3B-C4B	2.45	1.48	1.42
22	K	101	CLA	MG-NB	-2.45	2.00	2.05
22	A	840	CLA	C3B-C4B	2.45	1.48	1.42
22	B	826	CLA	C3B-C4B	2.45	1.48	1.42
22	6	304	CLA	CMD-C2D	-2.45	1.45	1.50
22	7	304	CLA	C3B-C4B	2.45	1.48	1.42
22	4	313	CLA	CMD-C2D	-2.45	1.45	1.50
22	6	318	CLA	C3B-C4B	2.45	1.48	1.42
22	B	807	CLA	MG-NB	-2.45	2.00	2.05
22	B	826	CLA	CMD-C2D	-2.45	1.45	1.50
22	B	836	CLA	C4B-NB	2.45	1.40	1.37
22	A	831	CLA	CMB-C2B	-2.45	1.45	1.50
29	5	301	CHL	CHB-C4A	-2.45	1.31	1.37
22	A	832	CLA	CMB-C2B	-2.45	1.45	1.50
22	6	305	CLA	CMB-C2B	-2.45	1.45	1.50
22	1	313	CLA	C1B-C2B	2.45	1.49	1.43
22	B	810	CLA	C3B-C4B	2.44	1.48	1.42
22	9	312	CLA	MG-NB	-2.44	2.00	2.05
22	B	827	CLA	C4B-NB	2.44	1.40	1.37
22	5	313	CLA	MG-NB	-2.44	2.00	2.05
22	1	304	CLA	CMB-C2B	-2.44	1.45	1.50
22	A	818	CLA	CMB-C2B	-2.44	1.45	1.50
22	1	306	CLA	MG-NB	-2.44	2.00	2.05
22	3	307	CLA	MG-NB	-2.44	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	805	CLA	C3B-C4B	2.44	1.48	1.42
22	3	313	CLA	C3B-C4B	2.44	1.48	1.42
22	7	310	CLA	C3B-C4B	2.44	1.48	1.42
22	K	104	CLA	C1B-C2B	2.44	1.49	1.43
22	B	801	CLA	CMD-C2D	-2.44	1.45	1.50
22	B	828	CLA	CMC-C2C	-2.44	1.45	1.50
22	A	806	CLA	C4B-NB	2.44	1.40	1.37
22	A	830	CLA	C1B-NB	-2.44	1.34	1.37
22	4	314	CLA	C1B-C2B	2.44	1.49	1.43
28	B	849	DGD	O3G-C3G	-2.44	1.39	1.43
22	B	801	CLA	CMC-C2C	-2.44	1.45	1.50
22	6	309	CLA	C1B-C2B	2.44	1.49	1.43
25	K	103	8CT	C24-C23	2.44	1.40	1.34
22	B	841	CLA	CMD-C2D	-2.43	1.45	1.50
22	A	803	CLA	C4B-NB	2.43	1.40	1.37
29	9	302	CHL	C1B-NB	-2.43	1.34	1.37
22	9	306	CLA	C3B-C4B	2.43	1.48	1.42
22	A	820	CLA	C3B-C4B	2.43	1.48	1.42
22	6	317	CLA	MG-NB	-2.43	2.01	2.05
22	2	311	CLA	CMC-C2C	-2.43	1.45	1.50
22	3	301	CLA	CMD-C2D	-2.43	1.45	1.50
22	3	309	CLA	C1B-C2B	2.43	1.49	1.43
22	7	317	CLA	C4B-NB	2.43	1.40	1.37
22	1	304	CLA	MG-ND	-2.43	2.01	2.05
22	2	314	CLA	CMD-C2D	-2.43	1.45	1.50
22	3	319	CLA	MG-NB	-2.43	2.01	2.05
22	5	305	CLA	C3B-C4B	2.43	1.48	1.42
22	B	834	CLA	CMD-C2D	-2.43	1.45	1.50
22	A	801	CLA	C1B-C2B	2.43	1.49	1.43
22	9	301	CLA	CMB-C2B	-2.43	1.45	1.50
22	1	307	CLA	C3B-C4B	2.43	1.48	1.42
22	A	822	CLA	C1B-C2B	2.43	1.49	1.43
22	7	307	CLA	MG-NB	-2.43	2.01	2.05
22	B	828	CLA	MG-NB	-2.43	2.01	2.05
22	3	308	CLA	MG-NB	-2.43	2.01	2.05
22	8	302	CLA	C4B-NB	2.43	1.40	1.37
22	B	835	CLA	C1B-C2B	2.43	1.49	1.43
22	3	304	CLA	CMD-C2D	-2.43	1.45	1.50
22	8	313	CLA	CMD-C2D	-2.43	1.45	1.50
29	4	305	CHL	C1D-C2D	2.43	1.50	1.45
22	B	805	CLA	CMD-C2D	-2.42	1.45	1.50
22	L	202	CLA	MG-NB	-2.42	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	840	CLA	CMD-C2D	-2.42	1.45	1.50
22	A	827	CLA	CMD-C2D	-2.42	1.45	1.50
22	2	313	CLA	CMD-C2D	-2.42	1.45	1.50
22	B	828	CLA	C1B-NB	-2.42	1.34	1.37
22	A	824	CLA	C4B-NB	2.42	1.40	1.37
22	B	813	CLA	MG-NB	-2.42	2.01	2.05
30	3	315	XAT	O4-C5	-2.42	1.42	1.46
22	7	309	CLA	C3B-C4B	2.42	1.48	1.42
29	0	301	CHL	C3B-C4B	2.42	1.48	1.42
22	A	806	CLA	C1B-NB	-2.42	1.34	1.37
22	3	311	CLA	C3B-C4B	2.42	1.48	1.42
22	5	304	CLA	MG-NB	-2.42	2.01	2.05
22	B	807	CLA	CMD-C2D	-2.42	1.45	1.50
22	4	311	CLA	CMD-C2D	-2.42	1.45	1.50
22	B	823	CLA	CMB-C2B	-2.42	1.45	1.50
22	4	309	CLA	CMD-C2D	-2.42	1.45	1.50
22	7	303	CLA	CMB-C2B	-2.42	1.45	1.50
29	9	302	CHL	C1D-ND	-2.42	1.34	1.37
22	A	833	CLA	CMB-C2B	-2.42	1.45	1.50
29	2	301	CHL	C1D-C2D	2.41	1.50	1.45
22	1	310	CLA	CMD-C2D	-2.41	1.45	1.50
29	5	306	CHL	C1B-C2B	2.41	1.48	1.43
22	A	819	CLA	CMD-C2D	-2.41	1.45	1.50
22	B	830	CLA	CMC-C2C	-2.41	1.45	1.50
22	1	311	CLA	C4B-NB	2.41	1.40	1.37
22	B	807	CLA	CMB-C2B	-2.41	1.45	1.50
25	1	316	8CT	C25-C26	2.41	1.39	1.35
22	1	304	CLA	C3B-C4B	2.41	1.48	1.42
22	J	103	CLA	C1B-C2B	2.41	1.48	1.43
22	0	303	CLA	MG-NB	-2.41	2.01	2.05
22	A	805	CLA	CMC-C2C	-2.41	1.45	1.50
22	A	814	CLA	C4B-NB	2.41	1.40	1.37
22	A	810	CLA	C1B-C2B	2.41	1.48	1.43
22	B	829	CLA	C4B-NB	2.41	1.40	1.37
29	2	306	CHL	C3B-C4B	2.41	1.48	1.42
22	3	308	CLA	CMC-C2C	-2.41	1.45	1.50
22	6	317	CLA	C1B-C2B	2.41	1.48	1.43
22	5	303	CLA	CMB-C2B	-2.41	1.45	1.50
22	B	815	CLA	C4B-NB	2.41	1.40	1.37
22	7	307	CLA	CMC-C2C	-2.41	1.45	1.50
22	2	308	CLA	CMB-C2B	-2.41	1.45	1.50
22	A	831	CLA	C4B-NB	2.41	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	311	CLA	MG-NB	-2.41	2.01	2.05
22	B	809	CLA	CMB-C2B	-2.41	1.45	1.50
29	1	305	CHL	C3B-C4B	2.41	1.48	1.42
29	2	307	CHL	C4B-NB	-2.41	1.34	1.37
22	B	827	CLA	MG-ND	-2.41	2.01	2.05
22	1	311	CLA	C3B-C4B	2.41	1.48	1.42
22	B	814	CLA	C1B-NB	-2.41	1.34	1.37
22	A	803	CLA	MG-ND	-2.41	2.01	2.05
22	A	801	CLA	C4B-NB	2.41	1.40	1.37
22	J	103	CLA	MG-NB	-2.41	2.01	2.05
22	A	833	CLA	C4B-NB	2.40	1.40	1.37
22	6	303	CLA	C3B-C4B	2.40	1.48	1.42
22	B	828	CLA	C4B-NB	2.40	1.40	1.37
22	3	313	CLA	CMC-C2C	-2.40	1.45	1.50
22	5	309	CLA	MG-NB	-2.40	2.01	2.05
22	L	201	CLA	C3B-C4B	2.40	1.48	1.42
22	L	203	CLA	C1B-C2B	2.40	1.48	1.43
22	A	806	CLA	CMB-C2B	-2.40	1.45	1.50
22	A	837	CLA	CMD-C2D	-2.40	1.45	1.50
22	8	308	CLA	CMD-C2D	-2.40	1.45	1.50
22	7	313	CLA	CMD-C2D	-2.40	1.45	1.50
22	8	304	CLA	CMB-C2B	-2.40	1.45	1.50
22	7	318	CLA	MG-NB	-2.40	2.01	2.05
25	L	206	8CT	C25-C26	2.40	1.39	1.35
22	B	820	CLA	CMB-C2B	-2.40	1.45	1.50
22	B	833	CLA	MG-NB	-2.40	2.01	2.05
22	7	316	CLA	CMC-C2C	-2.40	1.45	1.50
22	2	308	CLA	C4B-NB	2.40	1.40	1.37
22	7	309	CLA	C4B-NB	2.40	1.40	1.37
22	2	303	CLA	CMD-C2D	-2.40	1.45	1.50
22	5	302	CLA	CMD-C2D	-2.40	1.45	1.50
22	5	308	CLA	CMB-C2B	-2.40	1.45	1.50
22	A	823	CLA	CMD-C2D	-2.40	1.45	1.50
22	2	304	CLA	CMB-C2B	-2.40	1.45	1.50
22	2	308	CLA	CMD-C2D	-2.40	1.45	1.50
22	8	311	CLA	CMD-C2D	-2.40	1.45	1.50
22	B	825	CLA	MG-NB	-2.40	2.01	2.05
22	A	813	CLA	CMC-C2C	-2.39	1.45	1.50
29	2	307	CHL	C3D-C2D	2.39	1.45	1.39
22	4	312	CLA	C3B-C4B	2.39	1.48	1.42
22	2	319	CLA	C1B-NB	-2.39	1.34	1.37
22	A	809	CLA	MG-ND	-2.39	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	811	CLA	CMC-C2C	-2.39	1.45	1.50
22	1	306	CLA	CMD-C2D	-2.39	1.45	1.50
22	B	839	CLA	CMD-C2D	-2.39	1.45	1.50
22	B	801	CLA	C3B-C4B	2.39	1.48	1.42
22	7	303	CLA	CMC-C2C	-2.39	1.45	1.50
22	4	313	CLA	MG-NB	-2.39	2.01	2.05
22	A	832	CLA	CMD-C2D	-2.39	1.45	1.50
25	3	318	8CT	C33-C32	-2.39	1.43	1.50
22	9	308	CLA	MG-NB	-2.39	2.01	2.05
22	9	311	CLA	MG-NB	-2.39	2.01	2.05
22	6	318	CLA	CMB-C2B	-2.39	1.45	1.50
30	3	315	XAT	O24-C25	-2.39	1.42	1.46
22	8	303	CLA	C3B-C4B	2.39	1.48	1.42
22	B	803	CLA	MG-ND	-2.39	2.01	2.05
22	6	313	CLA	C4B-NB	2.39	1.40	1.37
22	B	810	CLA	CMD-C2D	-2.39	1.45	1.50
22	7	309	CLA	CMC-C2C	-2.39	1.45	1.50
22	B	840	CLA	C3B-C4B	2.39	1.48	1.42
22	H	201	CLA	C4B-NB	2.39	1.40	1.37
22	A	817	CLA	C1B-C2B	2.39	1.48	1.43
22	A	812	CLA	CMD-C2D	-2.39	1.45	1.50
22	A	821	CLA	CMB-C2B	-2.39	1.45	1.50
22	B	816	CLA	CMB-C2B	-2.39	1.45	1.50
22	B	806	CLA	C3B-C4B	2.39	1.48	1.42
22	B	813	CLA	CMD-C2D	-2.39	1.45	1.50
22	4	312	CLA	CMD-C2D	-2.39	1.45	1.50
22	7	304	CLA	CMB-C2B	-2.39	1.45	1.50
29	5	306	CHL	C1B-NB	-2.39	1.34	1.37
22	B	826	CLA	MG-ND	-2.38	2.01	2.05
22	4	308	CLA	C1B-NB	-2.38	1.34	1.37
22	A	832	CLA	C3B-C4B	2.38	1.48	1.42
22	7	303	CLA	CMD-C2D	-2.38	1.45	1.50
22	B	808	CLA	C4B-NB	2.38	1.40	1.37
22	7	317	CLA	MG-ND	-2.38	2.01	2.05
22	A	824	CLA	CMD-C2D	-2.38	1.45	1.50
22	0	309	CLA	C1B-C2B	2.38	1.48	1.43
22	B	835	CLA	C4B-NB	2.38	1.40	1.37
22	9	313	CLA	C1B-C2B	2.38	1.48	1.43
22	B	801	CLA	C4B-NB	2.38	1.40	1.37
22	F	301	CLA	MG-ND	-2.38	2.01	2.05
22	A	852	CLA	CMD-C2D	-2.38	1.45	1.50
29	6	316	CHL	C4B-NB	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	104	8CT	C25-C26	2.38	1.38	1.35
22	A	828	CLA	CMD-C2D	-2.38	1.45	1.50
22	A	831	CLA	C3B-C4B	2.38	1.48	1.42
22	B	813	CLA	CMB-C2B	-2.38	1.45	1.50
22	3	309	CLA	MG-NB	-2.38	2.01	2.05
22	7	310	CLA	C4B-NB	2.38	1.40	1.37
22	A	840	CLA	MG-ND	-2.38	2.01	2.05
22	A	801	CLA	C3B-C4B	2.38	1.48	1.42
22	0	302	CLA	CMC-C2C	-2.38	1.45	1.50
22	2	311	CLA	CMD-C2D	-2.38	1.45	1.50
22	0	312	CLA	C1B-C2B	2.38	1.48	1.43
22	4	302	CLA	CMD-C2D	-2.37	1.45	1.50
29	2	305	CHL	C3D-C2D	2.37	1.45	1.39
22	6	323	CLA	C1B-C2B	2.37	1.48	1.43
22	3	302	CLA	CMD-C2D	-2.37	1.45	1.50
22	B	823	CLA	CMD-C2D	-2.37	1.45	1.50
22	A	828	CLA	C4B-NB	2.37	1.40	1.37
22	K	105	CLA	C1B-C2B	2.37	1.48	1.43
22	7	313	CLA	C1B-C2B	2.37	1.48	1.43
22	4	311	CLA	CMB-C2B	-2.37	1.45	1.50
22	6	314	CLA	MG-NB	-2.37	2.01	2.05
22	3	310	CLA	C1B-C2B	2.37	1.48	1.43
22	3	308	CLA	CMB-C2B	-2.37	1.45	1.50
22	4	308	CLA	C3B-C4B	2.37	1.48	1.42
22	8	313	CLA	MG-NB	-2.37	2.01	2.05
22	A	830	CLA	CMC-C2C	-2.37	1.45	1.50
22	5	310	CLA	C1B-C2B	2.37	1.48	1.43
22	8	308	CLA	C1B-NB	-2.37	1.34	1.37
22	1	306	CLA	CMB-C2B	-2.37	1.45	1.50
22	A	810	CLA	CMB-C2B	-2.37	1.45	1.50
22	3	313	CLA	CMD-C2D	-2.37	1.45	1.50
22	3	307	CLA	CMD-C2D	-2.37	1.45	1.50
25	B	844	8CT	C33-C32	-2.37	1.43	1.50
29	6	308	CHL	CHB-C4A	-2.37	1.32	1.37
29	8	305	CHL	MG-NA	-2.37	2.00	2.06
22	5	304	CLA	C1B-C2B	2.37	1.48	1.43
22	7	302	CLA	C1B-C2B	2.37	1.48	1.43
22	2	302	CLA	CMC-C2C	-2.37	1.45	1.50
22	A	807	CLA	C3B-C4B	2.37	1.48	1.42
22	5	311	CLA	C1B-C2B	2.37	1.48	1.43
22	K	101	CLA	C1B-C2B	2.36	1.48	1.43
22	B	801	CLA	C1B-NB	-2.36	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	302	CLA	C1B-NB	-2.36	1.34	1.37
22	4	304	CLA	C1B-NB	-2.36	1.34	1.37
22	2	319	CLA	C3B-C4B	2.36	1.48	1.42
22	A	820	CLA	C1B-C2B	2.36	1.48	1.43
22	3	308	CLA	C1B-NB	-2.36	1.34	1.37
22	4	302	CLA	C4B-NB	2.36	1.40	1.37
22	A	819	CLA	CMB-C2B	-2.36	1.45	1.50
31	8	319	LMG	O8-C9	-2.36	1.39	1.45
22	1	309	CLA	CMD-C2D	-2.36	1.45	1.50
22	B	838	CLA	CMD-C2D	-2.36	1.45	1.50
22	8	303	CLA	CMC-C2C	-2.36	1.45	1.50
22	A	804	CLA	MG-ND	-2.36	2.01	2.05
22	A	813	CLA	C1B-NB	-2.36	1.34	1.37
22	A	837	CLA	C1B-NB	-2.36	1.34	1.37
22	B	836	CLA	C1B-NB	-2.36	1.34	1.37
22	A	826	CLA	C3B-C4B	2.36	1.48	1.42
22	A	832	CLA	C4B-NB	2.36	1.40	1.37
22	A	839	CLA	C4B-NB	2.36	1.40	1.37
22	A	816	CLA	CMB-C2B	-2.36	1.45	1.50
22	B	840	CLA	MG-ND	-2.36	2.01	2.05
29	9	307	CHL	C1B-NB	-2.36	1.34	1.37
22	A	816	CLA	C1B-C2B	2.36	1.48	1.43
22	B	818	CLA	C3B-C4B	2.36	1.48	1.42
22	6	309	CLA	C3B-C4B	2.36	1.48	1.42
29	9	302	CHL	C4B-NB	-2.36	1.34	1.37
22	A	825	CLA	C3B-C4B	2.36	1.48	1.42
22	0	309	CLA	MG-NB	-2.36	2.01	2.05
22	8	315	CLA	C1B-C2B	2.36	1.48	1.43
22	A	829	CLA	CMB-C2B	-2.36	1.45	1.50
22	1	310	CLA	CMB-C2B	-2.36	1.45	1.50
22	8	308	CLA	CMB-C2B	-2.36	1.45	1.50
22	3	301	CLA	CMB-C2B	-2.35	1.45	1.50
22	9	310	CLA	MG-NB	-2.35	2.01	2.05
22	5	307	CLA	MG-NB	-2.35	2.01	2.05
22	B	830	CLA	CMD-C2D	-2.35	1.45	1.50
22	3	319	CLA	CMB-C2B	-2.35	1.45	1.50
31	8	319	LMG	O1-C7	-2.35	1.39	1.43
22	A	828	CLA	CMC-C2C	-2.35	1.45	1.50
22	B	826	CLA	C4B-NB	2.35	1.40	1.37
22	B	825	CLA	C1B-C2B	2.35	1.48	1.43
22	K	102	CLA	CMD-C2D	-2.35	1.45	1.50
25	A	848	8CT	C33-C32	-2.35	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	825	CLA	C1B-C2B	2.35	1.48	1.43
29	8	305	CHL	C1D-ND	-2.35	1.34	1.37
29	4	301	CHL	C3D-C2D	2.35	1.45	1.39
22	A	809	CLA	CMD-C2D	-2.35	1.45	1.50
22	9	308	CLA	CMD-C2D	-2.35	1.45	1.50
22	8	304	CLA	C1B-C2B	2.35	1.48	1.43
22	A	801	CLA	CMC-C2C	-2.35	1.45	1.50
22	8	303	CLA	MG-ND	-2.35	2.01	2.05
22	B	825	CLA	CMB-C2B	-2.35	1.45	1.50
22	6	317	CLA	CMD-C2D	-2.35	1.45	1.50
22	B	805	CLA	C1B-C2B	2.35	1.48	1.43
29	6	302	CHL	C3B-C4B	2.35	1.48	1.42
22	1	310	CLA	C1B-C2B	2.35	1.48	1.43
22	9	304	CLA	C3B-C4B	2.35	1.48	1.42
22	1	301	CLA	CMD-C2D	-2.34	1.45	1.50
30	7	320	XAT	O4-C5	-2.34	1.42	1.46
22	A	805	CLA	CMD-C2D	-2.34	1.45	1.50
22	A	826	CLA	CMB-C2B	-2.34	1.45	1.50
22	2	302	CLA	C4B-NB	2.34	1.40	1.37
22	5	303	CLA	C1B-NB	-2.34	1.34	1.37
29	0	306	CHL	C1D-ND	-2.34	1.34	1.37
22	A	811	CLA	CMC-C2C	-2.34	1.45	1.50
22	1	311	CLA	CMD-C2D	-2.34	1.45	1.50
22	A	809	CLA	C3B-C4B	2.34	1.48	1.42
22	A	801	CLA	CMB-C2B	-2.34	1.45	1.50
22	A	818	CLA	CMC-C2C	-2.34	1.45	1.50
22	A	828	CLA	MG-ND	-2.34	2.01	2.05
25	G	104	8CT	C25-C26	2.34	1.38	1.35
22	G	103	CLA	MG-NB	-2.34	2.01	2.05
22	1	302	CLA	C1B-C2B	2.34	1.48	1.43
22	1	303	CLA	CMC-C2C	-2.34	1.45	1.50
22	K	105	CLA	MG-NB	-2.34	2.01	2.05
22	A	831	CLA	MG-ND	-2.34	2.01	2.05
29	2	301	CHL	C3D-C2D	2.34	1.45	1.39
22	A	811	CLA	CMD-C2D	-2.34	1.45	1.50
22	7	309	CLA	C1B-C2B	2.34	1.48	1.43
22	B	831	CLA	MG-ND	-2.34	2.01	2.05
22	B	829	CLA	CMC-C2C	-2.34	1.45	1.50
29	6	307	CHL	C1D-C2D	2.34	1.49	1.45
22	A	841	CLA	MG-ND	-2.34	2.01	2.05
22	9	309	CLA	MG-NB	-2.34	2.01	2.05
22	B	829	CLA	CMD-C2D	-2.34	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	102	CLA	C1B-C2B	2.34	1.48	1.43
22	A	815	CLA	CMD-C2D	-2.34	1.45	1.50
22	7	302	CLA	CMB-C2B	-2.34	1.45	1.50
22	7	310	CLA	CMD-C2D	-2.34	1.45	1.50
22	2	314	CLA	C1B-C2B	2.34	1.48	1.43
30	6	320	XAT	O4-C5	-2.34	1.42	1.46
22	A	804	CLA	C4B-NB	2.34	1.40	1.37
22	B	814	CLA	CMD-C2D	-2.34	1.45	1.50
22	4	310	CLA	CMD-C2D	-2.34	1.45	1.50
22	5	312	CLA	C1B-C2B	2.34	1.48	1.43
22	A	837	CLA	CMB-C2B	-2.34	1.45	1.50
22	B	814	CLA	CMB-C2B	-2.34	1.45	1.50
22	7	302	CLA	CMD-C2D	-2.34	1.45	1.50
22	G	102	CLA	MG-NB	-2.34	2.01	2.05
22	4	308	CLA	MG-ND	-2.34	2.01	2.05
29	2	305	CHL	MG-NA	-2.34	2.00	2.06
22	B	838	CLA	C3B-C4B	2.33	1.48	1.42
22	8	315	CLA	CMD-C2D	-2.33	1.45	1.50
29	4	307	CHL	C1D-C2D	2.33	1.49	1.45
22	9	301	CLA	C4B-C3B	2.33	1.48	1.43
22	8	312	CLA	CMC-C2C	-2.33	1.45	1.50
22	5	308	CLA	MG-NB	-2.33	2.01	2.05
22	A	814	CLA	CMB-C2B	-2.33	1.45	1.50
22	B	819	CLA	CMB-C2B	-2.33	1.45	1.50
22	4	303	CLA	CMB-C2B	-2.33	1.45	1.50
22	5	303	CLA	CMD-C2D	-2.33	1.45	1.50
22	0	311	CLA	CMD-C2D	-2.33	1.45	1.50
22	3	313	CLA	CMB-C2B	-2.33	1.45	1.50
22	A	820	CLA	C1B-NB	-2.33	1.34	1.37
22	7	318	CLA	CMD-C2D	-2.33	1.45	1.50
22	6	309	CLA	CMD-C2D	-2.33	1.45	1.50
22	8	313	CLA	C1B-C2B	2.33	1.48	1.43
22	A	827	CLA	CMB-C2B	-2.33	1.45	1.50
22	2	309	CLA	CMD-C2D	-2.33	1.45	1.50
22	6	301	CLA	MG-NB	-2.33	2.01	2.05
22	4	302	CLA	CMB-C2B	-2.33	1.45	1.50
24	A	845	LHG	O7-C5	-2.33	1.40	1.46
22	A	826	CLA	MG-NB	-2.33	2.01	2.05
31	5	319	LMG	O1-C1	2.33	1.44	1.40
22	A	807	CLA	CMB-C2B	-2.33	1.45	1.50
22	3	304	CLA	C1B-C2B	2.33	1.48	1.43
22	A	853	CLA	CMD-C2D	-2.33	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	818	CLA	CMC-C2C	-2.33	1.45	1.50
22	6	312	CLA	CMD-C2D	-2.33	1.45	1.50
22	B	824	CLA	CMD-C2D	-2.33	1.45	1.50
22	5	303	CLA	C1B-C2B	2.33	1.48	1.43
29	2	301	CHL	C1B-C2B	2.33	1.48	1.43
22	8	302	CLA	CMD-C2D	-2.32	1.45	1.50
22	A	852	CLA	CMB-C2B	-2.32	1.45	1.50
22	7	311	CLA	C3B-C4B	2.32	1.48	1.42
22	G	102	CLA	CHC-C1C	2.32	1.43	1.38
22	B	817	CLA	C1B-NB	-2.32	1.34	1.37
29	4	305	CHL	C3B-C4B	2.32	1.48	1.42
22	9	308	CLA	C1B-C2B	2.32	1.48	1.43
22	B	803	CLA	C3B-C4B	2.32	1.48	1.42
22	2	314	CLA	CMB-C2B	-2.32	1.45	1.50
22	5	314	CLA	C1B-C2B	2.32	1.48	1.43
29	4	307	CHL	C3D-C2D	2.32	1.45	1.39
22	B	824	CLA	C1B-C2B	2.32	1.48	1.43
22	3	304	CLA	C3B-C4B	2.32	1.48	1.42
22	6	304	CLA	CMC-C2C	-2.32	1.45	1.50
22	A	836	CLA	MG-ND	-2.32	2.01	2.05
22	A	822	CLA	CMD-C2D	-2.32	1.45	1.50
22	L	204	CLA	C1B-C2B	2.32	1.48	1.43
22	7	304	CLA	CMC-C2C	-2.32	1.45	1.50
22	A	802	CLA	MG-ND	-2.32	2.01	2.05
22	9	304	CLA	MG-ND	-2.32	2.01	2.05
22	A	811	CLA	CMB-C2B	-2.32	1.45	1.50
22	7	316	CLA	CMB-C2B	-2.32	1.45	1.50
22	8	303	CLA	C1B-NB	-2.32	1.34	1.37
22	0	311	CLA	MG-NB	-2.32	2.01	2.05
31	8	319	LMG	O6-C5	-2.32	1.38	1.44
22	2	304	CLA	CMD-C2D	-2.32	1.45	1.50
25	2	317	8CT	C25-C26	2.32	1.38	1.35
30	2	316	XAT	O24-C25	-2.32	1.42	1.46
25	B	845	8CT	C33-C32	-2.32	1.44	1.50
22	A	832	CLA	C1B-C2B	2.32	1.48	1.43
22	6	303	CLA	C1B-C2B	2.32	1.48	1.43
22	A	806	CLA	MG-ND	-2.32	2.01	2.05
22	B	801	CLA	CMB-C2B	-2.32	1.45	1.50
29	6	306	CHL	C3B-C4B	2.32	1.48	1.42
22	6	314	CLA	C1B-C2B	2.31	1.48	1.43
22	A	802	CLA	C1B-NB	-2.31	1.34	1.37
22	1	302	CLA	CMD-C2D	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	307	CHL	C1B-C2B	2.31	1.48	1.43
22	A	804	CLA	CMB-C2B	-2.31	1.45	1.50
22	9	305	CLA	MG-NB	-2.31	2.01	2.05
22	5	305	CLA	C1B-C2B	2.31	1.48	1.43
22	A	852	CLA	CMC-C2C	-2.31	1.45	1.50
25	7	301	8CT	C33-C32	-2.31	1.44	1.50
22	A	808	CLA	CMC-C2C	-2.31	1.45	1.50
22	8	312	CLA	CMD-C2D	-2.31	1.45	1.50
29	2	305	CHL	CHB-C4A	-2.31	1.32	1.37
29	8	306	CHL	C3B-C4B	2.31	1.48	1.42
22	A	808	CLA	C1B-NB	-2.31	1.34	1.37
22	6	313	CLA	MG-ND	-2.31	2.01	2.05
22	A	806	CLA	CMC-C2C	-2.31	1.45	1.50
22	B	810	CLA	CMB-C2B	-2.31	1.45	1.50
22	L	202	CLA	CMD-C2D	-2.31	1.45	1.50
22	6	323	CLA	CMD-C2D	-2.31	1.45	1.50
22	7	314	CLA	C1B-C2B	2.31	1.48	1.43
22	B	803	CLA	CMD-C2D	-2.31	1.45	1.50
22	B	820	CLA	CMD-C2D	-2.31	1.45	1.50
22	6	303	CLA	CMB-C2B	-2.31	1.45	1.50
22	A	809	CLA	C1B-NB	-2.31	1.34	1.37
22	B	826	CLA	C1D-ND	2.31	1.40	1.37
22	1	311	CLA	C1B-NB	-2.31	1.34	1.37
22	B	820	CLA	MG-ND	-2.31	2.01	2.05
22	A	811	CLA	MG-ND	-2.31	2.01	2.05
22	A	833	CLA	CMD-C2D	-2.31	1.45	1.50
22	A	840	CLA	CMC-C2C	-2.31	1.45	1.50
22	3	301	CLA	C1B-NB	-2.31	1.34	1.37
22	3	301	CLA	CMC-C2C	-2.31	1.45	1.50
22	2	312	CLA	CMB-C2B	-2.31	1.45	1.50
22	A	819	CLA	C4B-NB	2.31	1.40	1.37
22	A	811	CLA	C1B-C2B	2.31	1.48	1.43
22	7	315	CLA	CMD-C2D	-2.31	1.45	1.50
29	8	306	CHL	CHB-C4A	-2.31	1.32	1.37
22	7	312	CLA	CHC-C1C	2.31	1.43	1.38
29	7	308	CHL	CHB-C4A	-2.31	1.32	1.37
22	B	817	CLA	CMD-C2D	-2.30	1.45	1.50
22	8	312	CLA	CMB-C2B	-2.30	1.45	1.50
22	L	204	CLA	CMB-C2B	-2.30	1.45	1.50
22	B	825	CLA	MG-ND	-2.30	2.01	2.05
22	3	312	CLA	C1B-C2B	2.30	1.48	1.43
22	B	817	CLA	CMC-C2C	-2.30	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	311	CLA	CMC-C2C	-2.30	1.45	1.50
22	A	802	CLA	C3B-C4B	2.30	1.48	1.42
22	A	808	CLA	CMB-C2B	-2.30	1.45	1.50
22	B	808	CLA	CMB-C2B	-2.30	1.45	1.50
22	B	841	CLA	CMB-C2B	-2.30	1.45	1.50
22	4	302	CLA	C3B-C4B	2.30	1.48	1.42
25	B	804	8CT	C33-C32	-2.30	1.44	1.50
22	B	805	CLA	CMB-C2B	-2.30	1.45	1.50
22	B	850	CLA	MG-NB	-2.30	2.01	2.05
22	B	809	CLA	CMC-C2C	-2.30	1.45	1.50
22	A	814	CLA	CMC-C2C	-2.30	1.45	1.50
22	K	104	CLA	CMB-C2B	-2.30	1.45	1.50
22	1	307	CLA	CMD-C2D	-2.30	1.45	1.50
22	6	311	CLA	CMD-C2D	-2.30	1.45	1.50
22	9	309	CLA	CMB-C2B	-2.30	1.45	1.50
22	A	839	CLA	CMB-C2B	-2.30	1.45	1.50
22	4	304	CLA	CMD-C2D	-2.30	1.45	1.50
30	5	316	XAT	O4-C5	-2.30	1.42	1.46
22	7	312	CLA	CMD-C2D	-2.30	1.45	1.50
22	0	310	CLA	C1B-C2B	2.30	1.48	1.43
22	B	803	CLA	CMC-C2C	-2.30	1.45	1.50
22	G	102	CLA	C1B-C2B	2.30	1.48	1.43
22	B	808	CLA	C1B-C2B	2.30	1.48	1.43
22	A	836	CLA	CMB-C2B	-2.30	1.45	1.50
22	1	301	CLA	CMC-C2C	-2.30	1.45	1.50
22	3	311	CLA	C1B-C2B	2.30	1.48	1.43
22	7	307	CLA	CMD-C2D	-2.30	1.45	1.50
22	2	309	CLA	CMB-C2B	-2.30	1.45	1.50
22	A	828	CLA	C1B-C2B	2.30	1.48	1.43
22	4	302	CLA	C1B-NB	-2.30	1.35	1.37
22	B	840	CLA	CMC-C2C	-2.30	1.45	1.50
22	A	812	CLA	MG-ND	-2.29	2.01	2.05
22	5	307	CLA	C1B-C2B	2.29	1.48	1.43
22	A	825	CLA	CMC-C2C	-2.29	1.45	1.50
22	B	807	CLA	C4B-NB	2.29	1.40	1.37
22	B	806	CLA	C1B-C2B	2.29	1.48	1.43
29	2	301	CHL	C3B-C4B	2.29	1.48	1.42
22	A	839	CLA	CMD-C2D	-2.29	1.45	1.50
22	B	803	CLA	CMB-C2B	-2.29	1.45	1.50
22	B	811	CLA	CMB-C2B	-2.29	1.45	1.50
22	9	306	CLA	CMD-C2D	-2.29	1.45	1.50
25	B	843	8CT	C25-C26	2.29	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	303	CLA	CMD-C2D	-2.29	1.45	1.50
22	A	827	CLA	C1B-NB	-2.29	1.35	1.37
22	9	311	CLA	C1B-C2B	2.29	1.48	1.43
22	A	805	CLA	C3B-C4B	2.29	1.48	1.42
29	0	306	CHL	C3B-C4B	2.29	1.48	1.42
22	A	838	CLA	C1B-C2B	2.29	1.48	1.43
30	4	316	XAT	O24-C25	-2.29	1.42	1.46
29	6	302	CHL	C1B-C2B	2.29	1.48	1.43
22	A	814	CLA	MG-ND	-2.29	2.01	2.05
22	3	307	CLA	C3B-C4B	2.29	1.48	1.42
22	7	311	CLA	CMD-C2D	-2.29	1.45	1.50
22	A	836	CLA	C3B-C4B	2.29	1.48	1.42
29	3	306	CHL	MG-NA	-2.29	2.00	2.06
22	A	852	CLA	MG-NB	-2.29	2.01	2.05
22	7	306	CLA	CMC-C2C	-2.29	1.45	1.50
25	3	316	8CT	C25-C26	2.29	1.38	1.35
29	8	305	CHL	CHB-C4A	-2.29	1.32	1.37
22	A	816	CLA	CMC-C2C	-2.29	1.46	1.50
22	A	836	CLA	CMD-C2D	-2.29	1.46	1.50
22	B	840	CLA	CMD-C2D	-2.29	1.46	1.50
22	7	318	CLA	C1B-C2B	2.29	1.48	1.43
22	9	312	CLA	C1B-C2B	2.29	1.48	1.43
22	A	814	CLA	CMD-C2D	-2.29	1.46	1.50
22	6	318	CLA	CMD-C2D	-2.29	1.46	1.50
22	3	319	CLA	C1B-C2B	2.29	1.48	1.43
22	0	308	CLA	MG-NB	-2.29	2.01	2.05
22	H	201	CLA	CMD-C2D	-2.29	1.46	1.50
30	7	319	XAT	O24-C25	-2.29	1.42	1.46
22	2	312	CLA	CMC-C2C	-2.29	1.46	1.50
22	4	313	CLA	CMB-C2B	-2.29	1.46	1.50
22	2	308	CLA	MG-ND	-2.29	2.01	2.05
22	7	318	CLA	MG-ND	-2.29	2.01	2.05
29	3	306	CHL	C4B-NB	-2.28	1.35	1.37
22	1	308	CLA	C1B-C2B	2.28	1.48	1.43
22	A	806	CLA	CMD-C2D	-2.28	1.46	1.50
29	1	305	CHL	C1B-C2B	2.28	1.48	1.43
22	A	835	CLA	CMB-C2B	-2.28	1.46	1.50
22	6	313	CLA	C1B-C2B	2.28	1.48	1.43
22	0	302	CLA	C1B-C2B	2.28	1.48	1.43
29	4	305	CHL	C1B-C2B	2.28	1.48	1.43
29	4	301	CHL	MG-NA	-2.28	2.00	2.06
22	B	821	CLA	MG-ND	-2.28	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	316	CLA	MG-NB	-2.28	2.01	2.05
22	B	820	CLA	C1B-C2B	2.28	1.48	1.43
22	B	836	CLA	CMB-C2B	-2.28	1.46	1.50
22	1	312	CLA	CMD-C2D	-2.28	1.46	1.50
22	L	201	CLA	C1B-NB	-2.28	1.35	1.37
22	A	815	CLA	CMC-C2C	-2.28	1.46	1.50
22	B	805	CLA	CMC-C2C	-2.28	1.46	1.50
30	6	320	XAT	O24-C25	-2.28	1.43	1.46
22	A	841	CLA	C1B-C2B	2.28	1.48	1.43
22	3	313	CLA	C4B-NB	2.28	1.40	1.37
22	B	832	CLA	CMB-C2B	-2.28	1.46	1.50
22	B	817	CLA	C3B-C4B	2.28	1.48	1.42
22	0	302	CLA	CMD-C2D	-2.28	1.46	1.50
25	8	301	8CT	C25-C26	2.28	1.38	1.35
22	6	315	CLA	CMB-C2B	-2.28	1.46	1.50
22	9	310	CLA	CMD-C2D	-2.28	1.46	1.50
22	B	830	CLA	MG-ND	-2.28	2.01	2.05
22	4	308	CLA	CMB-C2B	-2.28	1.46	1.50
22	8	309	CLA	CMD-C2D	-2.28	1.46	1.50
22	A	818	CLA	MG-ND	-2.28	2.01	2.05
22	B	836	CLA	MG-ND	-2.28	2.01	2.05
22	B	816	CLA	CMC-C2C	-2.28	1.46	1.50
22	B	828	CLA	CMD-C2D	-2.28	1.46	1.50
29	3	306	CHL	CHB-C4A	-2.27	1.32	1.37
30	1	314	XAT	O4-C5	-2.27	1.43	1.46
22	B	838	CLA	MG-ND	-2.27	2.01	2.05
22	A	820	CLA	C4B-NB	2.27	1.40	1.37
22	7	311	CLA	C1B-C2B	2.27	1.48	1.43
22	1	308	CLA	MG-NB	-2.27	2.01	2.05
22	6	317	CLA	MG-ND	-2.27	2.01	2.05
22	9	303	CLA	C3B-C4B	2.27	1.48	1.42
22	3	313	CLA	MG-ND	-2.27	2.01	2.05
22	A	802	CLA	CMB-C2B	-2.27	1.46	1.50
22	1	308	CLA	CMC-C2C	-2.27	1.46	1.50
22	A	831	CLA	C1B-NB	-2.27	1.35	1.37
22	6	315	CLA	CMD-C2D	-2.27	1.46	1.50
22	8	302	CLA	CMB-C2B	-2.27	1.46	1.50
22	0	311	CLA	C1B-C2B	2.27	1.48	1.43
22	B	809	CLA	CMD-C2D	-2.27	1.46	1.50
22	B	837	CLA	CMB-C2B	-2.27	1.46	1.50
22	3	319	CLA	CMD-C2D	-2.27	1.46	1.50
22	B	821	CLA	C1B-C2B	2.27	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	316	CLA	C1B-C2B	2.27	1.48	1.43
22	A	834	CLA	CMD-C2D	-2.27	1.46	1.50
22	9	301	CLA	C1B-C2B	2.27	1.48	1.43
22	A	809	CLA	CMB-C2B	-2.27	1.46	1.50
22	B	837	CLA	CMD-C2D	-2.27	1.46	1.50
25	B	843	8CT	C33-C32	-2.27	1.44	1.50
22	L	201	CLA	MG-ND	-2.27	2.01	2.05
22	9	304	CLA	CMB-C2B	-2.27	1.46	1.50
22	7	310	CLA	C1B-C2B	2.27	1.48	1.43
22	9	309	CLA	C1B-C2B	2.27	1.48	1.43
22	4	302	CLA	MG-ND	-2.27	2.01	2.05
29	7	308	CHL	C3D-C2D	2.27	1.45	1.39
22	L	203	CLA	MG-NB	-2.26	2.01	2.05
22	A	835	CLA	CMD-C2D	-2.26	1.46	1.50
22	B	828	CLA	CMB-C2B	-2.26	1.46	1.50
22	B	828	CLA	CHC-C1C	2.26	1.43	1.38
22	1	309	CLA	C1B-C2B	2.26	1.48	1.43
22	B	827	CLA	CMB-C2B	-2.26	1.46	1.50
22	A	833	CLA	C1B-C2B	2.26	1.48	1.43
22	A	824	CLA	CMB-C2B	-2.26	1.46	1.50
22	7	314	CLA	CMD-C2D	-2.26	1.46	1.50
22	B	838	CLA	CMC-C2C	-2.26	1.46	1.50
22	6	310	CLA	C1B-C2B	2.26	1.48	1.43
29	4	301	CHL	CHB-C4A	-2.26	1.32	1.37
29	2	305	CHL	C1D-C2D	2.26	1.49	1.45
22	A	836	CLA	CMC-C2C	-2.26	1.46	1.50
22	A	816	CLA	CMD-C2D	-2.26	1.46	1.50
29	9	302	CHL	C1B-C2B	2.26	1.48	1.43
22	7	317	CLA	CMD-C2D	-2.26	1.46	1.50
22	A	838	CLA	CMD-C2D	-2.26	1.46	1.50
22	8	303	CLA	C1B-C2B	2.26	1.48	1.43
22	B	837	CLA	C1B-C2B	2.26	1.48	1.43
22	B	833	CLA	C3B-C4B	2.26	1.48	1.42
22	4	310	CLA	MG-ND	-2.26	2.01	2.05
22	M	101	CLA	C1B-C2B	2.26	1.48	1.43
22	A	836	CLA	C1B-C2B	2.26	1.48	1.43
22	2	312	CLA	C1B-NB	-2.26	1.35	1.37
22	1	313	CLA	CMD-C2D	-2.26	1.46	1.50
22	5	314	CLA	CMB-C2B	-2.26	1.46	1.50
22	2	303	CLA	MG-ND	-2.26	2.01	2.05
22	9	306	CLA	CMB-C2B	-2.26	1.46	1.50
22	A	814	CLA	C1B-NB	-2.26	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	835	CLA	C1B-NB	-2.26	1.35	1.37
22	6	305	CLA	C1B-C2B	2.26	1.48	1.43
22	A	822	CLA	CMB-C2B	-2.26	1.46	1.50
22	6	313	CLA	CMC-C2C	-2.26	1.46	1.50
22	B	850	CLA	C1B-C2B	2.25	1.48	1.43
22	B	822	CLA	CMD-C2D	-2.25	1.46	1.50
22	A	826	CLA	MG-ND	-2.25	2.01	2.05
22	A	818	CLA	CMD-C2D	-2.25	1.46	1.50
22	4	309	CLA	CMB-C2B	-2.25	1.46	1.50
22	B	812	CLA	CMC-C2C	-2.25	1.46	1.50
22	6	310	CLA	MG-ND	-2.25	2.01	2.05
22	A	826	CLA	CMD-C2D	-2.25	1.46	1.50
22	8	303	CLA	CMD-C2D	-2.25	1.46	1.50
29	7	308	CHL	C1D-C2D	2.25	1.49	1.45
29	3	306	CHL	C3B-C4B	2.25	1.48	1.42
22	A	840	CLA	CMB-C2B	-2.25	1.46	1.50
25	8	318	8CT	C25-C26	2.25	1.38	1.35
22	A	809	CLA	CMC-C2C	-2.25	1.46	1.50
22	B	813	CLA	C1B-C2B	2.25	1.48	1.43
29	9	307	CHL	C1B-C2B	2.25	1.48	1.43
22	K	102	CLA	C1B-NB	-2.25	1.35	1.37
29	6	316	CHL	CHB-C4A	-2.25	1.32	1.37
22	3	310	CLA	CMB-C2B	-2.25	1.46	1.50
22	3	311	CLA	CMC-C2C	-2.25	1.46	1.50
22	A	837	CLA	C1B-C2B	2.25	1.48	1.43
22	7	306	CLA	MG-ND	-2.25	2.01	2.05
22	6	318	CLA	C1B-C2B	2.25	1.48	1.43
22	1	303	CLA	MG-ND	-2.25	2.01	2.05
22	4	302	CLA	C1B-C2B	2.25	1.48	1.43
30	3	314	XAT	O24-C25	-2.25	1.43	1.46
22	6	317	CLA	C3B-C4B	2.25	1.48	1.42
22	9	306	CLA	C1B-C2B	2.25	1.48	1.43
29	6	316	CHL	C3B-C4B	2.25	1.48	1.42
22	6	314	CLA	CMB-C2B	-2.24	1.46	1.50
22	A	803	CLA	C1B-NB	-2.24	1.35	1.37
22	2	311	CLA	C1B-NB	-2.24	1.35	1.37
22	A	802	CLA	C1B-C2B	2.24	1.48	1.43
22	A	823	CLA	CMB-C2B	-2.24	1.46	1.50
22	A	823	CLA	C1B-C2B	2.24	1.48	1.43
22	A	821	CLA	CMD-C2D	-2.24	1.46	1.50
22	5	309	CLA	CMC-C2C	-2.24	1.46	1.50
25	B	851	8CT	C33-C32	-2.24	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	821	CLA	CMB-C2B	-2.24	1.46	1.50
22	B	835	CLA	CMC-C2C	-2.24	1.46	1.50
22	K	102	CLA	CMB-C2B	-2.24	1.46	1.50
30	4	315	XAT	O4-C5	-2.24	1.43	1.46
22	B	824	CLA	CMC-C2C	-2.24	1.46	1.50
22	7	304	CLA	MG-ND	-2.24	2.01	2.05
22	B	808	CLA	C1B-NB	-2.24	1.35	1.37
22	2	313	CLA	C1B-C2B	2.24	1.48	1.43
22	6	301	CLA	CMB-C2B	-2.24	1.46	1.50
22	7	306	CLA	CMD-C2D	-2.24	1.46	1.50
22	3	311	CLA	CMB-C2B	-2.24	1.46	1.50
22	0	308	CLA	CMD-C2D	-2.24	1.46	1.50
22	2	313	CLA	C3B-C4B	2.24	1.48	1.42
22	B	822	CLA	CMB-C2B	-2.24	1.46	1.50
22	9	305	CLA	CMB-C2B	-2.24	1.46	1.50
22	A	843	CLA	C1B-C2B	2.24	1.48	1.43
22	H	201	CLA	C1B-C2B	2.24	1.48	1.43
22	9	312	CLA	CMB-C2B	-2.24	1.46	1.50
22	A	810	CLA	CMC-C2C	-2.24	1.46	1.50
22	4	308	CLA	C1B-C2B	2.24	1.48	1.43
22	1	313	CLA	MG-ND	-2.23	2.01	2.05
22	4	304	CLA	CMC-C2C	-2.23	1.46	1.50
22	2	313	CLA	CMB-C2B	-2.23	1.46	1.50
22	8	302	CLA	CMC-C2C	-2.23	1.46	1.50
29	9	307	CHL	C1D-ND	-2.23	1.35	1.37
22	5	302	CLA	C1B-C2B	2.23	1.48	1.43
22	A	830	CLA	MG-ND	-2.23	2.01	2.05
29	0	301	CHL	C1B-C2B	2.23	1.48	1.43
22	4	303	CLA	CMC-C2C	-2.23	1.46	1.50
22	5	303	CLA	CMC-C2C	-2.23	1.46	1.50
22	3	305	CLA	MG-ND	-2.23	2.01	2.05
29	3	306	CHL	C3D-C2D	2.23	1.45	1.39
22	A	820	CLA	MG-ND	-2.23	2.01	2.05
22	B	830	CLA	C4B-NB	2.23	1.40	1.37
22	K	101	CLA	CMC-C2C	-2.23	1.46	1.50
22	1	302	CLA	CMB-C2B	-2.23	1.46	1.50
22	3	303	CLA	CMD-C2D	-2.23	1.46	1.50
22	2	312	CLA	CMD-C2D	-2.23	1.46	1.50
22	3	309	CLA	CMD-C2D	-2.23	1.46	1.50
22	4	313	CLA	CMC-C2C	-2.23	1.46	1.50
22	6	310	CLA	C1B-NB	-2.23	1.35	1.37
22	0	308	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	0	307	CLA	CHC-C1C	2.23	1.43	1.38
22	9	301	CLA	CMD-C2D	-2.23	1.46	1.50
30	8	317	XAT	O4-C5	-2.23	1.43	1.46
22	A	808	CLA	MG-ND	-2.23	2.01	2.05
22	6	303	CLA	MG-ND	-2.23	2.01	2.05
22	B	810	CLA	C1B-C2B	2.23	1.48	1.43
22	A	835	CLA	CMC-C2C	-2.23	1.46	1.50
22	6	313	CLA	C3B-C4B	2.23	1.48	1.42
30	4	316	XAT	C22-C21	-2.23	1.51	1.54
25	3	316	8CT	C33-C32	-2.23	1.44	1.50
22	B	824	CLA	CMB-C2B	-2.23	1.46	1.50
22	A	841	CLA	C3B-C4B	2.23	1.48	1.42
22	B	812	CLA	MG-ND	-2.23	2.01	2.05
22	A	835	CLA	CHC-C1C	2.22	1.43	1.38
22	1	308	CLA	CMB-C2B	-2.22	1.46	1.50
22	3	304	CLA	CMB-C2B	-2.22	1.46	1.50
25	B	848	8CT	C25-C26	2.22	1.38	1.35
22	5	312	CLA	CMD-C2D	-2.22	1.46	1.50
22	B	817	CLA	MG-ND	-2.22	2.01	2.05
22	0	305	CLA	C3B-C4B	2.22	1.48	1.42
22	A	807	CLA	CMC-C2C	-2.22	1.46	1.50
25	7	323	8CT	C25-C26	2.22	1.38	1.35
22	B	841	CLA	CMC-C2C	-2.22	1.46	1.50
22	1	302	CLA	CMC-C2C	-2.22	1.46	1.50
22	B	803	CLA	C4B-NB	2.22	1.40	1.37
22	8	311	CLA	C1B-C2B	2.22	1.48	1.43
22	A	817	CLA	CMB-C2B	-2.22	1.46	1.50
22	9	306	CLA	MG-ND	-2.22	2.01	2.05
29	6	302	CHL	CHB-C4A	-2.22	1.32	1.37
22	A	815	CLA	C1B-C2B	2.22	1.48	1.43
22	B	835	CLA	CMB-C2B	-2.22	1.46	1.50
22	F	301	CLA	CMC-C2C	-2.22	1.46	1.50
22	B	834	CLA	C1B-C2B	2.22	1.48	1.43
22	0	304	CLA	MG-NB	-2.22	2.01	2.05
22	5	305	CLA	CMB-C2B	-2.22	1.46	1.50
25	B	845	8CT	C25-C26	2.22	1.38	1.35
22	9	303	CLA	C1B-NB	-2.22	1.35	1.37
22	5	302	CLA	CMC-C2C	-2.22	1.46	1.50
22	B	840	CLA	C1B-NB	-2.22	1.35	1.37
22	4	309	CLA	C1B-NB	-2.22	1.35	1.37
29	2	307	CHL	C1D-C2D	2.22	1.49	1.45
29	2	301	CHL	C1C-NC	-2.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	312	CLA	MG-ND	-2.22	2.01	2.05
22	6	313	CLA	C1B-NB	-2.22	1.35	1.37
22	A	808	CLA	CMD-C2D	-2.22	1.46	1.50
22	2	312	CLA	C3B-C4B	2.22	1.48	1.42
22	A	805	CLA	C1B-C2B	2.22	1.48	1.43
22	1	311	CLA	CMC-C2C	-2.22	1.46	1.50
22	6	312	CLA	CMB-C2B	-2.22	1.46	1.50
22	3	305	CLA	CMD-C2D	-2.22	1.46	1.50
22	B	841	CLA	C4B-NB	2.22	1.40	1.37
22	K	102	CLA	CMC-C2C	-2.22	1.46	1.50
22	7	305	CLA	MG-ND	-2.21	2.01	2.05
22	A	840	CLA	C1B-C2B	2.21	1.48	1.43
22	7	306	CLA	CHC-C1C	2.21	1.43	1.38
22	B	811	CLA	CMD-C2D	-2.21	1.46	1.50
22	A	819	CLA	CMC-C2C	-2.21	1.46	1.50
22	5	305	CLA	CMD-C2D	-2.21	1.46	1.50
22	3	304	CLA	MG-ND	-2.21	2.01	2.05
22	B	817	CLA	C4B-NB	2.21	1.40	1.37
22	3	310	CLA	CMD-C2D	-2.21	1.46	1.50
22	8	313	CLA	CMB-C2B	-2.21	1.46	1.50
22	L	201	CLA	CMD-C2D	-2.21	1.46	1.50
22	B	831	CLA	CMC-C2C	-2.21	1.46	1.50
22	4	314	CLA	CMB-C2B	-2.21	1.46	1.50
22	B	821	CLA	CMC-C2C	-2.21	1.46	1.50
22	3	309	CLA	CMC-C2C	-2.21	1.46	1.50
25	B	847	8CT	C25-C26	2.21	1.38	1.35
22	5	310	CLA	CMD-C2D	-2.21	1.46	1.50
22	K	102	CLA	MG-ND	-2.21	2.01	2.05
22	4	303	CLA	MG-ND	-2.21	2.01	2.05
22	B	818	CLA	C1B-NB	-2.21	1.35	1.37
22	2	312	CLA	MG-ND	-2.21	2.01	2.05
22	2	314	CLA	MG-ND	-2.21	2.01	2.05
22	A	824	CLA	CMC-C2C	-2.21	1.46	1.50
29	6	306	CHL	MG-NA	-2.21	2.01	2.06
22	A	812	CLA	CMC-C2C	-2.21	1.46	1.50
22	0	309	CLA	CHC-C1C	2.21	1.43	1.38
29	4	301	CHL	C3B-C4B	2.21	1.47	1.42
25	A	846	8CT	C33-C32	-2.21	1.44	1.50
22	6	312	CLA	C1B-C2B	2.21	1.48	1.43
22	A	824	CLA	C1B-NB	-2.21	1.35	1.37
22	A	803	CLA	CMC-C2C	-2.21	1.46	1.50
22	2	302	CLA	CMB-C2B	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	304	CLA	CMC-C2C	-2.21	1.46	1.50
22	B	803	CLA	C1B-NB	-2.21	1.35	1.37
22	6	311	CLA	C1B-NB	-2.21	1.35	1.37
22	A	824	CLA	MG-ND	-2.21	2.01	2.05
22	7	309	CLA	MG-ND	-2.21	2.01	2.05
22	4	303	CLA	C1B-C2B	2.21	1.48	1.43
22	B	811	CLA	C1B-NB	-2.21	1.35	1.37
22	4	311	CLA	C1B-C2B	2.20	1.48	1.43
22	B	832	CLA	CMC-C2C	-2.20	1.46	1.50
22	B	834	CLA	CMC-C2C	-2.20	1.46	1.50
22	7	305	CLA	C1B-C2B	2.20	1.48	1.43
22	A	841	CLA	CMC-C2C	-2.20	1.46	1.50
22	G	101	CLA	CHC-C1C	2.20	1.43	1.38
22	A	843	CLA	CMD-C2D	-2.20	1.46	1.50
22	4	312	CLA	CMC-C2C	-2.20	1.46	1.50
22	5	312	CLA	CMB-C2B	-2.20	1.46	1.50
22	8	309	CLA	C1B-C2B	2.20	1.48	1.43
22	2	311	CLA	CMB-C2B	-2.20	1.46	1.50
22	9	301	CLA	CMC-C2C	-2.20	1.46	1.50
22	0	312	CLA	MG-NB	-2.20	2.01	2.05
22	A	807	CLA	CMD-C2D	-2.20	1.46	1.50
22	1	312	CLA	CMB-C2B	-2.20	1.46	1.50
22	0	303	CLA	CMD-C2D	-2.20	1.46	1.50
22	B	850	CLA	CHC-C1C	2.20	1.43	1.38
22	A	826	CLA	CMC-C2C	-2.20	1.46	1.50
22	A	838	CLA	CMB-C2B	-2.20	1.46	1.50
22	4	311	CLA	MG-ND	-2.20	2.01	2.05
22	B	815	CLA	CMD-C2D	-2.20	1.46	1.50
22	6	303	CLA	CMC-C2C	-2.20	1.46	1.50
22	9	303	CLA	CMB-C2B	-2.20	1.46	1.50
29	2	307	CHL	CHB-C4A	-2.20	1.32	1.37
22	7	311	CLA	MG-ND	-2.20	2.01	2.05
29	9	302	CHL	C3B-C4B	2.20	1.47	1.42
22	A	802	CLA	CMD-C2D	-2.20	1.46	1.50
22	B	815	CLA	CMC-C2C	-2.20	1.46	1.50
22	B	850	CLA	CMD-C2D	-2.20	1.46	1.50
22	6	314	CLA	CMD-C2D	-2.20	1.46	1.50
22	7	307	CLA	CMB-C2B	-2.20	1.46	1.50
22	8	312	CLA	C1B-C2B	2.20	1.48	1.43
22	2	312	CLA	C4B-NB	2.20	1.40	1.37
22	9	308	CLA	CMB-C2B	-2.20	1.46	1.50
22	A	813	CLA	C4B-NB	2.20	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	305	CHL	C4B-NB	-2.20	1.35	1.37
22	1	307	CLA	CMC-C2C	-2.20	1.46	1.50
22	3	312	CLA	CMD-C2D	-2.20	1.46	1.50
22	1	310	CLA	MG-ND	-2.20	2.01	2.05
22	A	814	CLA	C1B-C2B	2.20	1.48	1.43
22	2	319	CLA	CMC-C2C	-2.20	1.46	1.50
22	7	305	CLA	CMD-C2D	-2.20	1.46	1.50
24	9	316	LHG	O7-C5	-2.20	1.41	1.46
22	B	823	CLA	C1B-NB	-2.20	1.35	1.37
22	B	806	CLA	C1B-NB	-2.19	1.35	1.37
22	2	319	CLA	CMB-C2B	-2.19	1.46	1.50
22	7	317	CLA	CMB-C2B	-2.19	1.46	1.50
22	A	829	CLA	MG-ND	-2.19	2.01	2.05
22	2	309	CLA	C1B-C2B	2.19	1.48	1.43
22	A	813	CLA	CMB-C2B	-2.19	1.46	1.50
22	B	828	CLA	MG-ND	-2.19	2.01	2.05
22	A	807	CLA	C1B-C2B	2.19	1.48	1.43
22	5	302	CLA	MG-ND	-2.19	2.01	2.05
22	5	308	CLA	CHC-C1C	2.19	1.43	1.38
22	3	307	CLA	CMC-C2C	-2.19	1.46	1.50
22	B	840	CLA	C1B-C2B	2.19	1.48	1.43
30	9	314	XAT	O4-C5	-2.19	1.43	1.46
22	9	304	CLA	C1B-NB	-2.19	1.35	1.37
22	M	101	CLA	CMB-C2B	-2.19	1.46	1.50
22	B	830	CLA	C1B-NB	-2.19	1.35	1.37
22	7	316	CLA	CMD-C2D	-2.19	1.46	1.50
25	A	849	8CT	C25-C26	2.19	1.38	1.35
22	6	312	CLA	C1B-NB	-2.19	1.35	1.37
22	B	816	CLA	CMD-C2D	-2.19	1.46	1.50
22	B	826	CLA	CMC-C2C	-2.19	1.46	1.50
22	H	201	CLA	CMB-C2B	-2.19	1.46	1.50
22	J	103	CLA	CMD-C2D	-2.19	1.46	1.50
22	7	310	CLA	CMC-C2C	-2.19	1.46	1.50
25	L	205	8CT	C33-C32	-2.19	1.44	1.50
29	6	316	CHL	C4C-C3C	2.19	1.48	1.45
22	6	310	CLA	CMC-C2C	-2.19	1.46	1.50
22	B	838	CLA	CMB-C2B	-2.18	1.46	1.50
22	B	850	CLA	CMB-C2B	-2.18	1.46	1.50
22	A	804	CLA	CMC-C2C	-2.18	1.46	1.50
22	5	309	CLA	CMB-C2B	-2.18	1.46	1.50
22	7	306	CLA	CMB-C2B	-2.18	1.46	1.50
29	4	305	CHL	C4C-C3C	2.18	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	313	CLA	CMC-C2C	-2.18	1.46	1.50
22	8	311	CLA	CMC-C2C	-2.18	1.46	1.50
22	9	311	CLA	CMB-C2B	-2.18	1.46	1.50
22	B	837	CLA	CMC-C2C	-2.18	1.46	1.50
25	J	101	8CT	C25-C26	2.18	1.38	1.35
22	8	311	CLA	CMB-C2B	-2.18	1.46	1.50
29	5	306	CHL	C4C-C3C	2.18	1.48	1.45
22	A	826	CLA	C1B-NB	-2.18	1.35	1.37
22	6	310	CLA	CMD-C2D	-2.18	1.46	1.50
22	2	309	CLA	C1B-NB	-2.18	1.35	1.37
22	1	311	CLA	C1B-C2B	2.18	1.48	1.43
22	1	309	CLA	MG-ND	-2.18	2.01	2.05
22	2	308	CLA	CMC-C2C	-2.18	1.46	1.50
22	3	305	CLA	CMB-C2B	-2.18	1.46	1.50
22	9	304	CLA	CMC-C2C	-2.18	1.46	1.50
22	0	304	CLA	CMD-C2D	-2.18	1.46	1.50
22	6	323	CLA	CMC-C2C	-2.18	1.46	1.50
22	8	310	CLA	CMD-C2D	-2.18	1.46	1.50
22	5	307	CLA	CHC-C1C	2.18	1.42	1.38
25	7	321	8CT	C25-C26	2.18	1.38	1.35
22	B	826	CLA	CMB-C2B	-2.18	1.46	1.50
22	1	303	CLA	CHC-C1C	2.18	1.42	1.38
22	B	822	CLA	C1B-C2B	2.18	1.48	1.43
22	4	312	CLA	MG-ND	-2.18	2.01	2.05
22	A	813	CLA	CMD-C2D	-2.18	1.46	1.50
22	A	828	CLA	CMB-C2B	-2.18	1.46	1.50
29	8	307	CHL	C3B-C4B	2.18	1.47	1.42
30	4	316	XAT	O4-C5	-2.18	1.43	1.46
22	A	804	CLA	C1B-C2B	2.18	1.48	1.43
30	7	320	XAT	O24-C25	-2.17	1.43	1.46
22	A	819	CLA	C1B-NB	-2.17	1.35	1.37
22	6	315	CLA	C1B-C2B	2.17	1.48	1.43
22	8	315	CLA	CMB-C2B	-2.17	1.46	1.50
22	A	821	CLA	C1B-C2B	2.17	1.48	1.43
22	8	304	CLA	MG-ND	-2.17	2.01	2.05
22	B	836	CLA	CMC-C2C	-2.17	1.46	1.50
22	5	313	CLA	CMD-C2D	-2.17	1.46	1.50
25	2	317	8CT	C33-C32	-2.17	1.44	1.50
22	7	315	CLA	C1B-C2B	2.17	1.48	1.43
22	3	305	CLA	CMC-C2C	-2.17	1.46	1.50
29	3	306	CHL	C1D-C2D	2.17	1.49	1.45
22	A	828	CLA	C1B-NB	-2.17	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	305	CHL	C4B-NB	-2.17	1.35	1.37
22	2	310	CLA	CMD-C2D	-2.17	1.46	1.50
22	M	101	CLA	CMC-C2C	-2.17	1.46	1.50
22	6	315	CLA	CMC-C2C	-2.17	1.46	1.50
22	6	318	CLA	CMC-C2C	-2.17	1.46	1.50
22	A	813	CLA	MG-ND	-2.17	2.01	2.05
22	2	313	CLA	MG-ND	-2.17	2.01	2.05
22	1	311	CLA	CMB-C2B	-2.17	1.46	1.50
22	8	309	CLA	CMB-C2B	-2.17	1.46	1.50
30	8	317	XAT	O24-C25	-2.17	1.43	1.46
22	B	809	CLA	MG-ND	-2.17	2.01	2.05
25	L	205	8CT	C25-C26	2.17	1.38	1.35
31	8	319	LMG	O7-C8	-2.17	1.41	1.46
29	6	307	CHL	CHB-C4A	-2.17	1.32	1.37
22	A	829	CLA	CMC-C2C	-2.17	1.46	1.50
22	5	314	CLA	CMC-C2C	-2.17	1.46	1.50
22	5	310	CLA	CMB-C2B	-2.16	1.46	1.50
22	3	307	CLA	MG-ND	-2.16	2.01	2.05
22	3	308	CLA	MG-ND	-2.16	2.01	2.05
22	8	315	CLA	MG-ND	-2.16	2.01	2.05
22	B	838	CLA	C1B-C2B	2.16	1.48	1.43
29	4	305	CHL	CHB-C4A	-2.16	1.32	1.37
22	9	312	CLA	MG-ND	-2.16	2.01	2.05
22	B	823	CLA	C1B-C2B	2.16	1.48	1.43
22	B	808	CLA	CMD-C2D	-2.16	1.46	1.50
22	1	309	CLA	CMB-C2B	-2.16	1.46	1.50
22	8	303	CLA	CMB-C2B	-2.16	1.46	1.50
22	8	308	CLA	CMC-C2C	-2.16	1.46	1.50
22	2	310	CLA	MG-ND	-2.16	2.01	2.05
22	B	825	CLA	CMC-C2C	-2.16	1.46	1.50
22	1	304	CLA	C1B-C2B	2.16	1.48	1.43
22	L	202	CLA	CMC-C2C	-2.16	1.46	1.50
29	6	306	CHL	C4B-NB	-2.16	1.35	1.37
22	B	813	CLA	CMC-C2C	-2.16	1.46	1.50
22	7	312	CLA	CMB-C2B	-2.16	1.46	1.50
22	6	309	CLA	MG-ND	-2.16	2.01	2.05
29	4	307	CHL	CHB-C4A	-2.16	1.32	1.37
22	6	309	CLA	CMB-C2B	-2.16	1.46	1.50
22	L	203	CLA	CMB-C2B	-2.16	1.46	1.50
22	L	204	CLA	CMD-C2D	-2.16	1.46	1.50
22	A	805	CLA	C4B-NB	2.16	1.40	1.37
22	B	839	CLA	C1B-NB	-2.16	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	315	CLA	MG-ND	-2.16	2.01	2.05
22	8	310	CLA	MG-ND	-2.16	2.01	2.05
22	A	839	CLA	C1B-C2B	2.16	1.48	1.43
22	0	303	CLA	CMB-C2B	-2.16	1.46	1.50
25	A	850	8CT	C25-C26	2.16	1.38	1.35
22	6	323	CLA	CMB-C2B	-2.16	1.46	1.50
30	5	316	XAT	O24-C25	-2.16	1.43	1.46
22	5	307	CLA	CMB-C2B	-2.16	1.46	1.50
22	4	309	CLA	CMC-C2C	-2.15	1.46	1.50
22	A	812	CLA	C1B-NB	-2.15	1.35	1.37
22	A	852	CLA	C1B-C2B	2.15	1.48	1.43
22	6	301	CLA	CMD-C2D	-2.15	1.46	1.50
22	5	304	CLA	CMD-C2D	-2.15	1.46	1.50
22	A	831	CLA	C1B-C2B	2.15	1.48	1.43
22	4	314	CLA	MG-ND	-2.15	2.01	2.05
22	A	817	CLA	CMD-C2D	-2.15	1.46	1.50
22	A	853	CLA	CMC-C2C	-2.15	1.46	1.50
22	7	315	CLA	CMC-C2C	-2.15	1.46	1.50
29	6	308	CHL	C3B-C4B	2.15	1.47	1.42
29	2	306	CHL	CHB-C4A	-2.15	1.32	1.37
22	L	201	CLA	CMB-C2B	-2.15	1.46	1.50
22	7	314	CLA	CMC-C2C	-2.15	1.46	1.50
29	9	307	CHL	CHB-C4A	-2.15	1.32	1.37
29	8	306	CHL	C1B-C2B	2.15	1.48	1.43
22	B	819	CLA	CMC-C2C	-2.15	1.46	1.50
22	9	313	CLA	CMB-C2B	-2.15	1.46	1.50
30	0	313	XAT	O4-C5	-2.15	1.43	1.46
22	A	843	CLA	CMB-C2B	-2.15	1.46	1.50
22	6	309	CLA	CMC-C2C	-2.15	1.46	1.50
22	6	313	CLA	CMB-C2B	-2.15	1.46	1.50
22	7	311	CLA	CMC-C2C	-2.15	1.46	1.50
22	K	105	CLA	CMD-C2D	-2.15	1.46	1.50
22	2	310	CLA	C1B-C2B	2.15	1.48	1.43
22	B	808	CLA	MG-ND	-2.15	2.01	2.05
22	B	819	CLA	MG-ND	-2.15	2.01	2.05
22	A	832	CLA	C1B-NB	-2.15	1.35	1.37
22	L	203	CLA	CMD-C2D	-2.15	1.46	1.50
22	7	302	CLA	MG-ND	-2.15	2.01	2.05
22	B	827	CLA	CMC-C2C	-2.15	1.46	1.50
22	6	311	CLA	CMC-C2C	-2.15	1.46	1.50
22	7	305	CLA	CMC-C2C	-2.15	1.46	1.50
22	3	313	CLA	C1B-NB	-2.15	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	304	CLA	C1B-NB	-2.15	1.35	1.37
22	A	822	CLA	CMC-C2C	-2.15	1.46	1.50
22	F	301	CLA	CMD-C2D	-2.15	1.46	1.50
25	B	846	8CT	C33-C32	-2.15	1.44	1.50
22	A	829	CLA	CHC-C1C	2.15	1.42	1.38
22	B	819	CLA	C1B-NB	-2.15	1.35	1.37
22	5	302	CLA	C1B-NB	-2.15	1.35	1.37
22	6	311	CLA	CMB-C2B	-2.14	1.46	1.50
22	7	314	CLA	CMB-C2B	-2.14	1.46	1.50
22	6	311	CLA	C1B-C2B	2.14	1.48	1.43
22	2	311	CLA	C1B-C2B	2.14	1.48	1.43
22	6	317	CLA	CMB-C2B	-2.14	1.46	1.50
22	B	818	CLA	CMD-C2D	-2.14	1.46	1.50
22	6	304	CLA	C1B-NB	-2.14	1.35	1.37
22	7	310	CLA	MG-ND	-2.14	2.01	2.05
30	7	319	XAT	O4-C5	-2.14	1.43	1.46
22	A	836	CLA	C1B-NB	-2.14	1.35	1.37
22	1	307	CLA	CMB-C2B	-2.14	1.46	1.50
22	2	314	CLA	CMC-C2C	-2.14	1.46	1.50
22	9	312	CLA	CMD-C2D	-2.14	1.46	1.50
29	6	306	CHL	CHB-C4A	-2.14	1.32	1.37
22	0	307	CLA	MG-NB	-2.14	2.01	2.05
22	7	315	CLA	CMB-C2B	-2.14	1.46	1.50
22	B	836	CLA	CHC-C1C	2.14	1.42	1.38
22	A	805	CLA	MG-ND	-2.14	2.01	2.05
22	7	306	CLA	C1B-C2B	2.14	1.48	1.43
22	0	312	CLA	CMB-C2B	-2.14	1.46	1.50
22	0	312	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	810	CLA	CMC-C2C	-2.14	1.46	1.50
22	B	823	CLA	CMC-C2C	-2.14	1.46	1.50
25	8	318	8CT	C33-C32	-2.14	1.44	1.50
22	7	318	CLA	CMB-C2B	-2.14	1.46	1.50
25	3	318	8CT	C25-C26	2.14	1.38	1.35
22	A	819	CLA	CHC-C1C	2.14	1.42	1.38
22	A	838	CLA	MG-ND	-2.14	2.01	2.05
22	A	808	CLA	C1B-C2B	2.14	1.48	1.43
22	B	817	CLA	C1B-C2B	2.13	1.48	1.43
22	1	312	CLA	CMC-C2C	-2.13	1.46	1.50
30	1	315	XAT	O24-C25	-2.13	1.43	1.46
22	5	310	CLA	MG-ND	-2.13	2.01	2.05
22	7	312	CLA	C1B-C2B	2.13	1.48	1.43
22	B	827	CLA	C1B-NB	-2.13	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	301	8CT	C33-C32	-2.13	1.44	1.50
22	A	821	CLA	MG-ND	-2.13	2.01	2.05
22	2	311	CLA	MG-ND	-2.13	2.01	2.05
22	4	304	CLA	CMB-C2B	-2.13	1.46	1.50
22	B	819	CLA	C1B-C2B	2.13	1.48	1.43
22	1	307	CLA	MG-ND	-2.13	2.01	2.05
30	9	315	XAT	O24-C25	-2.13	1.43	1.46
22	B	832	CLA	CMD-C2D	-2.13	1.46	1.50
22	3	312	CLA	CMB-C2B	-2.13	1.46	1.50
22	2	319	CLA	C1B-C2B	2.13	1.48	1.43
22	7	311	CLA	CMB-C2B	-2.13	1.46	1.50
22	9	311	CLA	CMD-C2D	-2.13	1.46	1.50
22	6	301	CLA	CHC-C1C	2.13	1.42	1.38
22	9	304	CLA	C1B-C2B	2.13	1.48	1.43
22	3	309	CLA	MG-ND	-2.13	2.01	2.05
22	1	301	CLA	CHC-C1C	2.13	1.42	1.38
29	7	308	CHL	C3B-C4B	2.13	1.47	1.42
22	0	304	CLA	CMB-C2B	-2.13	1.46	1.50
22	0	309	CLA	CMB-C2B	-2.13	1.46	1.50
22	B	813	CLA	C1B-NB	-2.13	1.35	1.37
22	1	304	CLA	C1B-NB	-2.13	1.35	1.37
22	6	312	CLA	CMC-C2C	-2.13	1.46	1.50
25	1	316	8CT	C33-C32	-2.13	1.44	1.50
22	B	801	CLA	CAC-C3C	-2.13	1.45	1.51
22	A	827	CLA	MG-ND	-2.13	2.01	2.05
22	4	304	CLA	MG-ND	-2.13	2.01	2.05
22	A	834	CLA	CMC-C2C	-2.13	1.46	1.50
22	A	820	CLA	CMC-C2C	-2.12	1.46	1.50
22	3	302	CLA	MG-ND	-2.12	2.01	2.05
29	1	305	CHL	CHB-C4A	-2.12	1.32	1.37
22	B	822	CLA	MG-ND	-2.12	2.01	2.05
22	1	313	CLA	CMB-C2B	-2.12	1.46	1.50
22	A	823	CLA	MG-ND	-2.12	2.01	2.05
22	5	309	CLA	CMD-C2D	-2.12	1.46	1.50
22	1	308	CLA	CMD-C2D	-2.12	1.46	1.50
22	4	302	CLA	CMC-C2C	-2.12	1.46	1.50
22	A	839	CLA	MG-ND	-2.12	2.01	2.05
22	A	843	CLA	MG-ND	-2.12	2.01	2.05
22	3	303	CLA	CMC-C2C	-2.12	1.46	1.50
22	3	311	CLA	MG-ND	-2.12	2.01	2.05
22	7	312	CLA	C1B-NB	-2.12	1.35	1.37
22	B	827	CLA	C1B-C2B	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	323	CLA	MG-ND	-2.12	2.01	2.05
22	9	309	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	815	CLA	C1B-NB	-2.12	1.35	1.37
22	B	815	CLA	MG-ND	-2.12	2.01	2.05
22	A	843	CLA	CMC-C2C	-2.12	1.46	1.50
22	7	313	CLA	CMB-C2B	-2.12	1.46	1.50
22	1	310	CLA	CMC-C2C	-2.12	1.46	1.50
22	2	304	CLA	CMC-C2C	-2.12	1.46	1.50
22	0	305	CLA	CMB-C2B	-2.12	1.46	1.50
22	7	303	CLA	C1B-C2B	2.12	1.48	1.43
22	9	309	CLA	CHC-C1C	2.12	1.42	1.38
22	A	807	CLA	MG-ND	-2.12	2.01	2.05
22	K	101	CLA	CMD-C2D	-2.12	1.46	1.50
22	5	310	CLA	CMC-C2C	-2.12	1.46	1.50
25	A	849	8CT	C33-C32	-2.12	1.44	1.50
22	A	835	CLA	MG-ND	-2.12	2.01	2.05
22	2	319	CLA	MG-ND	-2.12	2.01	2.05
22	7	303	CLA	MG-ND	-2.12	2.01	2.05
22	2	309	CLA	MG-ND	-2.12	2.01	2.05
29	2	306	CHL	C1B-C2B	2.11	1.48	1.43
22	3	303	CLA	C1B-NB	-2.11	1.35	1.37
22	2	310	CLA	CMC-C2C	-2.11	1.46	1.50
22	4	309	CLA	C4B-NB	2.11	1.40	1.37
22	K	104	CLA	MG-ND	-2.11	2.01	2.05
31	4	318	LMG	O8-C9	-2.11	1.40	1.45
22	B	807	CLA	CMC-C2C	-2.11	1.46	1.50
22	A	834	CLA	MG-ND	-2.11	2.01	2.05
22	B	801	CLA	MG-ND	-2.11	2.01	2.05
22	8	302	CLA	MG-ND	-2.11	2.01	2.05
30	6	319	XAT	O24-C25	-2.11	1.43	1.46
22	B	806	CLA	CMB-C2B	-2.11	1.46	1.50
22	5	309	CLA	CHC-C1C	2.11	1.42	1.38
30	6	319	XAT	O4-C5	-2.11	1.43	1.46
22	8	304	CLA	CMC-C2C	-2.11	1.46	1.50
25	6	321	8CT	C25-C26	2.11	1.38	1.35
22	7	310	CLA	CMB-C2B	-2.11	1.46	1.50
22	4	308	CLA	C4B-NB	2.11	1.40	1.37
22	7	305	CLA	CMB-C2B	-2.11	1.46	1.50
22	0	305	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	805	CLA	MG-ND	-2.11	2.01	2.05
22	B	814	CLA	MG-ND	-2.11	2.01	2.05
25	L	206	8CT	C33-C32	-2.11	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	308	CHL	C1B-C2B	2.11	1.48	1.43
22	A	837	CLA	CMC-C2C	-2.11	1.46	1.50
25	I	101	8CT	C30-C29	2.11	1.53	1.50
22	3	313	CLA	C1B-C2B	2.11	1.48	1.43
22	B	839	CLA	C1B-C2B	2.11	1.48	1.43
22	A	832	CLA	CMC-C2C	-2.10	1.46	1.50
22	A	819	CLA	MG-ND	-2.10	2.01	2.05
22	B	809	CLA	C1B-NB	-2.10	1.35	1.37
22	B	837	CLA	MG-ND	-2.10	2.01	2.05
22	3	301	CLA	MG-ND	-2.10	2.01	2.05
22	A	834	CLA	C1B-NB	-2.10	1.35	1.37
25	B	851	8CT	C24-C23	2.10	1.40	1.34
22	A	831	CLA	CMC-C2C	-2.10	1.46	1.50
22	B	803	CLA	C1B-C2B	2.10	1.48	1.43
22	3	304	CLA	CMC-C2C	-2.10	1.46	1.50
22	B	839	CLA	MG-ND	-2.10	2.01	2.05
25	A	854	8CT	C25-C26	2.10	1.38	1.35
29	4	306	CHL	CHB-C4A	-2.10	1.32	1.37
22	5	314	CLA	MG-ND	-2.10	2.01	2.05
22	A	839	CLA	C1B-NB	-2.10	1.35	1.37
22	6	318	CLA	MG-ND	-2.10	2.01	2.05
22	A	817	CLA	CMC-C2C	-2.10	1.46	1.50
25	A	854	8CT	C33-C32	-2.10	1.44	1.50
22	A	810	CLA	MG-ND	-2.10	2.01	2.05
22	8	304	CLA	CMD-C2D	-2.10	1.46	1.50
29	8	314	CHL	C1C-NC	-2.10	1.34	1.37
22	0	310	CLA	CMC-C2C	-2.10	1.46	1.50
22	1	306	CLA	C1B-C2B	2.10	1.48	1.43
22	A	815	CLA	CMB-C2B	-2.10	1.46	1.50
22	B	835	CLA	CMD-C2D	-2.10	1.46	1.50
22	8	309	CLA	MG-ND	-2.10	2.01	2.05
25	7	321	8CT	C33-C32	-2.10	1.44	1.50
22	6	317	CLA	CMC-C2C	-2.10	1.46	1.50
22	9	312	CLA	CMC-C2C	-2.10	1.46	1.50
22	L	204	CLA	CHC-C1C	2.10	1.42	1.38
22	B	829	CLA	MG-ND	-2.10	2.01	2.05
22	0	310	CLA	CMB-C2B	-2.10	1.46	1.50
22	A	830	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	822	CLA	CMC-C2C	-2.10	1.46	1.50
22	4	309	CLA	MG-ND	-2.10	2.01	2.05
22	B	841	CLA	MG-ND	-2.09	2.01	2.05
22	L	202	CLA	MG-ND	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	311	CLA	CHC-C1C	2.09	1.42	1.38
22	7	309	CLA	C1B-NB	-2.09	1.35	1.37
22	A	853	CLA	CMB-C2B	-2.09	1.46	1.50
22	5	313	CLA	CMC-C2C	-2.09	1.46	1.50
22	9	313	CLA	CMD-C2D	-2.09	1.46	1.50
25	7	323	8CT	C33-C32	-2.09	1.44	1.50
22	3	319	CLA	CMC-C2C	-2.09	1.46	1.50
22	0	307	CLA	CMD-C2D	-2.09	1.46	1.50
22	7	312	CLA	MG-ND	-2.09	2.01	2.05
22	9	308	CLA	MG-ND	-2.09	2.01	2.05
30	1	315	XAT	O4-C5	-2.09	1.43	1.46
22	B	807	CLA	C1B-NB	-2.09	1.35	1.37
22	2	303	CLA	C1B-C2B	2.09	1.48	1.43
22	A	810	CLA	CMD-C2D	-2.09	1.46	1.50
22	K	104	CLA	CMD-C2D	-2.09	1.46	1.50
22	7	318	CLA	CMC-C2C	-2.09	1.46	1.50
29	6	316	CHL	C1B-C2B	2.09	1.48	1.43
22	A	827	CLA	CHC-C1C	2.09	1.42	1.38
22	2	313	CLA	CMC-C2C	-2.09	1.46	1.50
22	K	105	CLA	CMB-C2B	-2.09	1.46	1.50
22	9	303	CLA	CMC-C2C	-2.09	1.46	1.50
22	B	816	CLA	C1B-NB	-2.09	1.35	1.37
22	H	201	CLA	CMC-C2C	-2.09	1.46	1.50
22	A	827	CLA	C1B-C2B	2.09	1.48	1.43
22	3	301	CLA	C1B-C2B	2.09	1.48	1.43
22	1	303	CLA	CMB-C2B	-2.09	1.46	1.50
22	M	101	CLA	CMD-C2D	-2.09	1.46	1.50
22	0	303	CLA	CHC-C1C	2.09	1.42	1.38
22	1	302	CLA	MG-ND	-2.08	2.01	2.05
22	B	807	CLA	MG-ND	-2.08	2.01	2.05
22	8	302	CLA	CHC-C1C	2.08	1.42	1.38
22	B	810	CLA	MG-ND	-2.08	2.01	2.05
22	5	311	CLA	MG-ND	-2.08	2.01	2.05
22	9	313	CLA	MG-ND	-2.08	2.01	2.05
22	1	306	CLA	CMC-C2C	-2.08	1.46	1.50
22	0	307	CLA	CMB-C2B	-2.08	1.46	1.50
22	6	304	CLA	MG-ND	-2.08	2.01	2.05
29	2	305	CHL	C1B-C2B	2.08	1.48	1.43
22	2	303	CLA	CMC-C2C	-2.08	1.46	1.50
22	0	310	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	816	CLA	C1B-C2B	2.08	1.48	1.43
22	G	102	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	311	CLA	CMB-C2B	-2.08	1.46	1.50
31	5	319	LMG	C1-C2	2.08	1.58	1.52
22	4	310	CLA	CMC-C2C	-2.08	1.46	1.50
22	A	823	CLA	CMC-C2C	-2.08	1.46	1.50
22	A	807	CLA	C1B-NB	-2.08	1.35	1.37
22	5	312	CLA	CMC-C2C	-2.08	1.46	1.50
22	5	303	CLA	MG-ND	-2.08	2.01	2.05
22	1	308	CLA	CHC-C1C	2.08	1.42	1.38
28	B	849	DGD	O6E-C5E	-2.08	1.39	1.44
22	1	312	CLA	C1B-C2B	2.08	1.48	1.43
22	7	304	CLA	C1B-C2B	2.08	1.48	1.43
22	1	313	CLA	CMC-C2C	-2.08	1.46	1.50
22	3	307	CLA	C1B-C2B	2.08	1.48	1.43
22	B	850	CLA	CMC-C2C	-2.07	1.46	1.50
22	2	308	CLA	C1B-NB	-2.07	1.35	1.37
29	4	307	CHL	C3B-C4B	2.07	1.47	1.42
22	3	319	CLA	MG-ND	-2.07	2.01	2.05
22	A	820	CLA	CMB-C2B	-2.07	1.46	1.50
22	9	312	CLA	CHC-C1C	2.07	1.42	1.38
22	1	304	CLA	CMD-C2D	-2.07	1.46	1.50
22	6	305	CLA	CMC-C2C	-2.07	1.46	1.50
22	6	315	CLA	MG-ND	-2.07	2.01	2.05
22	B	833	CLA	MG-ND	-2.07	2.01	2.05
22	5	304	CLA	CMB-C2B	-2.07	1.46	1.50
22	A	832	CLA	MG-ND	-2.07	2.01	2.05
25	J	104	8CT	C33-C32	-2.07	1.44	1.50
22	6	311	CLA	MG-ND	-2.07	2.01	2.05
28	B	849	DGD	O4D-C4D	-2.07	1.38	1.43
22	8	308	CLA	MG-ND	-2.07	2.01	2.05
30	3	314	XAT	O4-C5	-2.07	1.43	1.46
29	2	307	CHL	C1B-C2B	2.07	1.48	1.43
22	5	313	CLA	CMB-C2B	-2.07	1.46	1.50
22	3	308	CLA	CAC-C3C	-2.07	1.45	1.51
22	2	310	CLA	C1B-NB	-2.07	1.35	1.37
29	2	301	CHL	C4B-NB	-2.07	1.35	1.37
22	1	312	CLA	C1B-NB	-2.06	1.35	1.37
22	7	306	CLA	C1B-NB	-2.06	1.35	1.37
22	9	303	CLA	MG-ND	-2.06	2.01	2.05
22	B	841	CLA	C1B-C2B	2.06	1.48	1.43
22	L	201	CLA	CMC-C2C	-2.06	1.46	1.50
22	5	308	CLA	C1B-C2B	2.06	1.48	1.43
22	K	104	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	834	CLA	MG-ND	-2.06	2.01	2.05
22	4	309	CLA	C1B-C2B	2.06	1.48	1.43
22	7	303	CLA	C1B-NB	-2.06	1.35	1.37
29	4	306	CHL	C4C-C3C	2.06	1.48	1.45
22	1	303	CLA	CMD-C2D	-2.06	1.46	1.50
22	3	310	CLA	CMC-C2C	-2.06	1.46	1.50
24	1	317	LHG	O8-C6	-2.06	1.40	1.45
22	5	308	CLA	CMD-C2D	-2.06	1.46	1.50
22	0	308	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	833	CLA	MG-ND	-2.06	2.01	2.05
22	B	825	CLA	C1B-NB	-2.06	1.35	1.37
22	6	314	CLA	CMC-C2C	-2.06	1.46	1.50
22	0	311	CLA	CMC-C2C	-2.06	1.46	1.50
29	6	306	CHL	C1B-C2B	2.06	1.48	1.43
25	G	104	8CT	C33-C32	-2.06	1.44	1.50
22	B	826	CLA	C1B-C2B	2.06	1.48	1.43
22	5	307	CLA	CMD-C2D	-2.06	1.46	1.50
22	0	309	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	853	CLA	MG-ND	-2.06	2.01	2.05
22	5	313	CLA	CHC-C1C	2.06	1.42	1.38
22	7	314	CLA	MG-ND	-2.06	2.01	2.05
22	6	303	CLA	CMD-C2D	-2.06	1.46	1.50
22	8	310	CLA	CMB-C2B	-2.06	1.46	1.50
22	2	312	CLA	C1B-C2B	2.06	1.48	1.43
25	J	101	8CT	C33-C32	-2.06	1.44	1.50
22	1	306	CLA	MG-ND	-2.06	2.01	2.05
22	4	313	CLA	CHC-C1C	2.05	1.42	1.38
22	0	311	CLA	CHC-C1C	2.05	1.42	1.38
22	B	813	CLA	MG-ND	-2.05	2.01	2.05
22	B	823	CLA	MG-ND	-2.05	2.01	2.05
22	K	105	CLA	MG-ND	-2.05	2.01	2.05
22	1	309	CLA	CMC-C2C	-2.05	1.46	1.50
22	A	821	CLA	CMC-C2C	-2.05	1.46	1.50
25	A	846	8CT	C25-C26	2.05	1.38	1.35
22	2	313	CLA	CHC-C1C	2.05	1.42	1.38
22	2	304	CLA	C1B-C2B	2.05	1.48	1.43
22	9	306	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	818	CLA	MG-ND	-2.05	2.01	2.05
22	0	303	CLA	CMC-C2C	-2.05	1.46	1.50
22	7	315	CLA	C1B-NB	-2.05	1.35	1.37
22	K	101	CLA	MG-ND	-2.05	2.01	2.05
22	K	101	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	0	302	CLA	MG-ND	-2.04	2.01	2.05
22	B	811	CLA	C1B-C2B	2.04	1.48	1.43
22	0	308	CLA	CHC-C1C	2.04	1.42	1.38
22	2	309	CLA	CHC-C1C	2.04	1.42	1.38
22	B	815	CLA	CMB-C2B	-2.04	1.46	1.50
22	4	308	CLA	CMC-C2C	-2.04	1.46	1.50
22	1	311	CLA	MG-ND	-2.04	2.01	2.05
22	B	812	CLA	C1B-NB	-2.04	1.35	1.37
22	6	301	CLA	CMC-C2C	-2.04	1.46	1.50
22	9	305	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	824	CLA	C1B-C2B	2.04	1.48	1.43
22	4	310	CLA	C1B-NB	-2.04	1.35	1.37
22	B	832	CLA	C1B-C2B	2.04	1.48	1.43
30	9	315	XAT	O4-C5	-2.04	1.43	1.46
22	9	305	CLA	CMC-C2C	-2.04	1.46	1.50
22	3	312	CLA	CMC-C2C	-2.04	1.46	1.50
25	4	317	8CT	C33-C32	-2.04	1.44	1.50
22	J	103	CLA	CHC-C1C	2.04	1.42	1.38
22	3	302	CLA	CMC-C2C	-2.04	1.46	1.50
22	4	314	CLA	CMC-C2C	-2.04	1.46	1.50
22	A	805	CLA	CAC-C3C	-2.04	1.45	1.51
22	7	302	CLA	C1B-NB	-2.04	1.35	1.37
22	8	312	CLA	C1B-NB	-2.04	1.35	1.37
22	J	103	CLA	CMB-C2B	-2.04	1.46	1.50
22	9	301	CLA	MG-ND	-2.04	2.01	2.05
22	A	837	CLA	MG-ND	-2.04	2.01	2.05
22	B	801	CLA	C1B-C2B	2.04	1.48	1.43
22	A	816	CLA	MG-ND	-2.04	2.01	2.05
22	B	817	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	833	CLA	CMB-C2B	-2.04	1.46	1.50
22	3	319	CLA	CHC-C1C	2.04	1.42	1.38
22	1	306	CLA	CHC-C1C	2.03	1.42	1.38
22	8	302	CLA	C1B-C2B	2.03	1.48	1.43
22	B	836	CLA	C1B-C2B	2.03	1.48	1.43
29	2	307	CHL	C3B-C4B	2.03	1.47	1.42
22	4	310	CLA	CHC-C1C	2.03	1.42	1.38
22	A	813	CLA	CHC-C1C	2.03	1.42	1.38
30	2	316	XAT	O4-C5	-2.03	1.43	1.46
22	K	101	CLA	CHC-C1C	2.03	1.42	1.38
22	4	313	CLA	C1B-C2B	2.03	1.48	1.43
22	8	309	CLA	CMC-C2C	-2.03	1.46	1.50
22	2	308	CLA	C1B-C2B	2.03	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	306	CHL	C1B-C2B	2.03	1.48	1.43
22	9	308	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	809	CLA	C1B-C2B	2.03	1.48	1.43
22	4	313	CLA	MG-ND	-2.03	2.01	2.05
25	B	848	8CT	C33-C32	-2.03	1.44	1.50
22	4	312	CLA	C1B-NB	-2.03	1.35	1.37
22	7	313	CLA	MG-ND	-2.02	2.01	2.05
22	7	315	CLA	CHC-C1C	2.02	1.42	1.38
22	9	305	CLA	CHC-C1C	2.02	1.42	1.38
22	0	305	CLA	MG-ND	-2.02	2.01	2.05
25	A	850	8CT	C33-C32	-2.02	1.44	1.50
22	2	304	CLA	MG-ND	-2.02	2.01	2.05
22	1	301	CLA	MG-ND	-2.02	2.01	2.05
22	H	201	CLA	CHC-C1C	2.02	1.42	1.38
22	2	319	CLA	CHC-C1C	2.02	1.42	1.38
29	2	305	CHL	C1C-NC	-2.02	1.34	1.37
22	L	203	CLA	CHC-C1C	2.02	1.42	1.38
22	2	309	CLA	CAC-C3C	-2.02	1.45	1.51
22	A	838	CLA	C1B-NB	-2.02	1.35	1.37
22	6	309	CLA	C1B-NB	-2.02	1.35	1.37
22	G	103	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	810	CLA	C1B-NB	-2.02	1.35	1.37
22	B	824	CLA	C1B-NB	-2.02	1.35	1.37
22	M	101	CLA	MG-ND	-2.02	2.01	2.05
22	6	304	CLA	C1B-C2B	2.02	1.48	1.43
30	8	316	XAT	O4-C5	-2.02	1.43	1.46
22	8	313	CLA	CMC-C2C	-2.02	1.46	1.50
22	1	312	CLA	MG-ND	-2.02	2.01	2.05
22	6	305	CLA	MG-ND	-2.02	2.01	2.05
22	7	312	CLA	CMC-C2C	-2.02	1.46	1.50
22	8	302	CLA	C1B-NB	-2.02	1.35	1.37
22	A	815	CLA	CHC-C1C	2.01	1.42	1.38
22	8	313	CLA	CHC-C1C	2.01	1.42	1.38
22	B	816	CLA	MG-ND	-2.01	2.01	2.05
22	3	303	CLA	CHC-C1C	2.01	1.42	1.38
25	B	843	8CT	C24-C23	2.01	1.39	1.34
31	5	319	LMG	O6-C5	-2.01	1.39	1.44
22	2	302	CLA	CMD-C2D	-2.01	1.46	1.50
22	7	310	CLA	C1B-NB	-2.01	1.35	1.37
22	A	839	CLA	CMC-C2C	-2.01	1.46	1.50
22	A	834	CLA	C1B-C2B	2.01	1.48	1.43
22	0	303	CLA	MG-ND	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	321	8CT	C33-C32	-2.01	1.44	1.50
22	B	832	CLA	MG-ND	-2.01	2.01	2.05
22	9	309	CLA	CMC-C2C	-2.01	1.46	1.50
22	A	843	CLA	C1B-NB	-2.01	1.35	1.37
29	9	302	CHL	CHB-C4A	-2.01	1.32	1.37
22	G	102	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	834	CLA	CHC-C1C	2.01	1.42	1.38
22	0	307	CLA	CMC-C2C	-2.00	1.46	1.50
22	8	312	CLA	MG-ND	-2.00	2.01	2.05
30	3	314	XAT	C22-C21	-2.00	1.51	1.54
29	0	301	CHL	C4C-C3C	2.00	1.48	1.45
29	8	307	CHL	C1B-C2B	2.00	1.48	1.43
22	L	204	CLA	CMC-C2C	-2.00	1.46	1.50
22	3	310	CLA	C1B-NB	-2.00	1.35	1.37
25	B	847	8CT	C33-C32	-2.00	1.44	1.50
22	7	302	CLA	CMC-C2C	-2.00	1.46	1.50
22	A	806	CLA	CHC-C1C	2.00	1.42	1.38
22	1	301	CLA	C1B-C2B	2.00	1.48	1.43
22	B	811	CLA	CAC-C3C	-2.00	1.46	1.51
29	2	301	CHL	CHB-C4A	-2.00	1.32	1.37
22	A	841	CLA	C1B-NB	-2.00	1.35	1.37
22	A	801	CLA	MG-ND	-2.00	2.01	2.05
22	A	833	CLA	CMC-C2C	-2.00	1.46	1.50
22	9	313	CLA	CMC-C2C	-2.00	1.46	1.50
22	2	314	CLA	C1B-NB	-2.00	1.35	1.37
22	3	309	CLA	C1B-NB	-2.00	1.35	1.37
22	7	316	CLA	MG-ND	-2.00	2.01	2.05

All (3387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	315	XAT	O4-C5-C4	-26.68	93.34	113.38
30	0	313	XAT	O24-C25-C24	-23.72	95.57	113.38
30	5	315	XAT	O24-C25-C38	-20.89	90.03	115.06
30	5	315	XAT	O24-C25-C24	-18.04	99.83	113.38
30	2	315	XAT	O4-C5-C18	-18.03	93.46	115.06
30	0	313	XAT	O24-C25-C38	-17.92	93.58	115.06
30	6	320	XAT	C17-C1-C16	-17.70	81.27	107.37
30	2	315	XAT	C37-C21-C36	-16.56	82.94	107.37
30	1	314	XAT	C17-C1-C16	-16.28	83.35	107.37
30	9	314	XAT	C37-C21-C36	-16.15	83.54	107.37
30	3	314	XAT	C17-C1-C16	-16.01	83.75	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	314	XAT	C17-C1-C2	-15.50	82.05	108.98
30	6	320	XAT	C17-C1-C2	-14.32	84.10	108.98
30	9	314	XAT	C37-C21-C22	-13.49	85.55	108.98
30	3	314	XAT	C17-C1-C2	-13.33	85.82	108.98
30	2	315	XAT	C37-C21-C22	-12.85	86.65	108.98
25	3	318	8CT	C24-C25-C26	-11.71	110.60	127.31
25	I	101	8CT	C33-C32-C31	-11.51	113.81	124.85
25	J	101	8CT	C33-C32-C31	-11.40	113.92	124.85
30	9	314	XAT	O4-C5-C4	11.36	121.92	113.38
25	B	844	8CT	C33-C32-C31	-11.24	114.07	124.85
25	3	318	8CT	C18-C17-C16	-11.07	111.50	127.31
25	7	321	8CT	C18-C17-C16	-10.93	111.71	127.31
25	A	846	8CT	C33-C32-C31	-10.92	114.38	124.85
30	7	319	XAT	O24-C25-C24	10.83	121.52	113.38
25	L	205	8CT	C18-C17-C16	-10.82	111.87	127.31
30	1	315	XAT	O24-C25-C24	10.69	121.41	113.38
29	8	307	CHL	C2B-C1B-NB	10.65	117.37	110.23
25	5	317	8CT	C33-C32-C31	-10.53	114.76	124.85
25	A	848	8CT	C33-C32-C31	-10.51	114.77	124.85
30	9	315	XAT	O24-C25-C24	10.19	121.04	113.38
29	7	308	CHL	C2B-C1B-NB	10.15	117.04	110.23
25	7	321	8CT	C19-C20-C21	-10.06	112.95	127.31
29	6	308	CHL	C2B-C1B-NB	10.00	116.94	110.23
25	B	845	8CT	C33-C32-C31	-9.96	115.30	124.85
29	2	301	CHL	C2B-C1B-NB	9.94	116.90	110.23
30	2	316	XAT	C18-C5-C6	-9.93	105.62	122.26
25	B	846	8CT	C33-C32-C31	-9.91	115.34	124.85
25	2	317	8CT	C33-C32-C31	-9.88	115.38	124.85
25	A	847	8CT	C33-C32-C31	-9.86	115.40	124.85
25	8	318	8CT	C33-C32-C31	-9.84	115.42	124.85
29	2	307	CHL	C2B-C1B-NB	9.84	116.83	110.23
29	5	301	CHL	C2B-C1B-NB	9.77	116.78	110.23
25	3	316	8CT	C33-C32-C31	-9.77	115.48	124.85
29	4	301	CHL	C2B-C1B-NB	9.75	116.77	110.23
30	2	316	XAT	O24-C25-C24	9.71	120.68	113.38
29	6	316	CHL	C2B-C1B-NB	9.67	116.72	110.23
30	5	316	XAT	O24-C25-C24	9.67	120.64	113.38
30	8	317	XAT	O24-C25-C24	9.67	120.64	113.38
30	3	314	XAT	O24-C25-C24	9.62	120.61	113.38
29	8	306	CHL	C2B-C1B-NB	9.56	116.64	110.23
30	8	316	XAT	C15-C14-C13	-9.55	113.67	127.31
30	6	320	XAT	O24-C25-C24	9.50	120.52	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	317	8CT	C19-C20-C21	-9.49	113.77	127.31
25	L	206	8CT	C33-C32-C31	-9.41	115.83	124.85
30	7	320	XAT	O24-C25-C24	9.41	120.45	113.38
25	3	318	8CT	C19-C20-C21	-9.40	113.89	127.31
29	4	305	CHL	C2B-C1B-NB	9.38	116.52	110.23
25	F	302	8CT	C33-C32-C31	-9.38	115.86	124.85
30	2	316	XAT	O4-C5-C18	9.33	126.23	115.06
29	1	305	CHL	C2B-C1B-NB	9.30	116.47	110.23
25	A	854	8CT	C33-C32-C31	-9.28	115.95	124.85
29	6	306	CHL	C2B-C1B-NB	9.25	116.43	110.23
29	9	302	CHL	C2B-C1B-NB	9.23	116.42	110.23
30	0	313	XAT	O4-C5-C4	9.23	120.31	113.38
25	B	847	8CT	C33-C32-C31	-9.17	116.06	124.85
25	F	302	8CT	C14-C13-C12	-9.14	114.26	127.31
29	2	305	CHL	C2B-C1B-NB	9.14	116.36	110.23
25	B	804	8CT	C33-C32-C31	-9.11	116.11	124.85
25	7	321	8CT	C33-C32-C31	-9.09	116.14	124.85
29	9	307	CHL	C2B-C1B-NB	9.08	116.32	110.23
29	2	301	CHL	CMD-C2D-C1D	9.00	140.58	124.71
29	7	308	CHL	CMD-C2D-C1D	8.99	140.56	124.71
29	4	307	CHL	C2B-C1B-NB	8.96	116.24	110.23
29	8	305	CHL	C2B-C1B-NB	8.95	116.23	110.23
30	1	314	XAT	C7-C8-C9	-8.86	111.78	125.53
29	3	306	CHL	CMD-C2D-C1D	8.80	140.22	124.71
25	6	321	8CT	C18-C17-C16	-8.80	114.76	127.31
29	6	307	CHL	C2B-C1B-NB	8.74	116.09	110.23
30	3	314	XAT	C15-C14-C13	-8.70	114.89	127.31
30	0	314	XAT	O4-C5-C4	8.70	119.92	113.38
25	7	301	8CT	C33-C32-C31	-8.69	116.52	124.85
29	3	306	CHL	C2B-C1B-NB	8.64	116.02	110.23
30	3	314	XAT	C35-C34-C33	-8.60	115.03	127.31
29	4	307	CHL	CMD-C2D-C1D	8.57	139.81	124.71
25	8	301	8CT	C33-C32-C31	-8.57	116.64	124.85
29	2	306	CHL	C2B-C1B-NB	8.55	115.97	110.23
29	2	305	CHL	CMD-C2D-C1D	8.54	139.77	124.71
29	4	306	CHL	C2B-C1B-NB	8.49	115.92	110.23
29	6	302	CHL	C2B-C1B-NB	8.44	115.89	110.23
30	8	316	XAT	C11-C10-C9	-8.40	115.32	127.31
29	5	306	CHL	C2B-C1B-NB	8.39	115.86	110.23
25	G	104	8CT	C33-C32-C31	-8.35	116.85	124.85
29	2	307	CHL	CMD-C2D-C1D	8.34	139.41	124.71
25	B	848	8CT	C33-C32-C31	-8.33	116.87	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	305	CHL	C2C-C3C-C4C	-8.32	100.56	106.49
25	L	206	8CT	C24-C25-C26	-8.32	115.43	127.31
25	A	849	8CT	C33-C32-C31	-8.31	116.88	124.85
29	8	305	CHL	CMD-C2D-C1D	8.29	139.33	124.71
25	B	845	8CT	C24-C25-C26	-8.26	115.52	127.31
22	7	310	CLA	C4A-NA-C1A	8.26	110.42	106.71
29	5	301	CHL	C2C-C3C-C4C	-8.24	100.61	106.49
29	6	316	CHL	CMD-C2D-C1D	8.24	139.23	124.71
29	4	301	CHL	C2C-C3C-C4C	-8.24	100.62	106.49
25	J	104	8CT	C33-C32-C31	-8.23	116.95	124.85
30	6	320	XAT	C18-C5-C6	-8.23	108.47	122.26
29	9	302	CHL	C2C-C3C-C4C	-8.21	100.64	106.49
29	9	307	CHL	CMD-C2D-C1D	8.20	139.16	124.71
29	6	308	CHL	CMD-C2D-C1D	8.19	139.15	124.71
29	2	301	CHL	C2C-C3C-C4C	-8.17	100.66	106.49
25	5	317	8CT	C24-C25-C26	-8.16	115.67	127.31
29	1	305	CHL	CMD-C2D-C1D	8.15	139.07	124.71
25	A	850	8CT	C33-C32-C31	-8.13	117.05	124.85
25	7	321	8CT	C24-C25-C26	-8.13	115.71	127.31
25	1	316	8CT	C33-C32-C31	-8.12	117.07	124.85
25	6	321	8CT	C33-C32-C31	-8.09	117.10	124.85
25	6	321	8CT	C14-C13-C12	-8.06	115.80	127.31
29	4	301	CHL	CMD-C2D-C1D	8.06	138.92	124.71
29	9	302	CHL	CMD-C2D-C1D	8.06	138.91	124.71
30	6	319	XAT	C15-C14-C13	-8.05	115.83	127.31
29	0	306	CHL	C2B-C1B-NB	8.04	115.62	110.23
25	B	846	8CT	C24-C25-C26	-8.04	115.84	127.31
29	4	305	CHL	CMD-C2D-C1D	8.03	138.86	124.71
29	5	301	CHL	CMD-C2D-C1D	8.01	138.84	124.71
29	8	314	CHL	CMD-C2D-C1D	8.01	138.83	124.71
29	0	306	CHL	CMD-C2D-C1D	8.00	138.81	124.71
29	8	306	CHL	CMD-C2D-C1D	7.98	138.78	124.71
29	6	306	CHL	CMD-C2D-C1D	7.98	138.77	124.71
29	2	306	CHL	CMD-C2D-C1D	7.96	138.75	124.71
25	6	321	8CT	C24-C25-C26	-7.96	115.95	127.31
29	8	307	CHL	CMD-C2D-C1D	7.95	138.72	124.71
25	3	318	8CT	C33-C32-C31	-7.93	117.25	124.85
29	0	301	CHL	C2B-C1B-NB	7.90	115.53	110.23
25	B	804	8CT	C14-C13-C12	-7.89	116.05	127.31
29	8	305	CHL	C2C-C3C-C4C	-7.87	100.88	106.49
25	7	301	8CT	C24-C25-C26	-7.86	116.09	127.31
30	8	316	XAT	C38-C25-C26	-7.86	109.09	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	314	XAT	C31-C30-C29	-7.85	116.11	127.31
25	5	317	8CT	C30-C31-C32	-7.83	111.83	121.47
29	4	306	CHL	CMD-C2D-C1D	7.81	138.48	124.71
25	L	205	8CT	C33-C32-C31	-7.80	117.37	124.85
25	B	843	8CT	C33-C32-C31	-7.77	117.40	124.85
29	5	306	CHL	CMD-C2D-C1D	7.77	138.41	124.71
29	0	301	CHL	CMD-C2D-C1D	7.75	138.38	124.71
22	7	317	CLA	C4A-NA-C1A	7.75	110.19	106.71
25	7	323	8CT	C33-C32-C31	-7.74	117.42	124.85
30	0	314	XAT	C38-C25-C26	-7.74	109.30	122.26
29	2	306	CHL	C2C-C3C-C4C	-7.72	100.98	106.49
22	B	806	CLA	C4A-NA-C1A	7.72	110.18	106.71
30	4	316	XAT	O24-C25-C24	7.71	119.17	113.38
30	4	315	XAT	C35-C34-C33	-7.70	116.32	127.31
30	1	314	XAT	C17-C1-C6	-7.70	89.27	110.05
29	6	302	CHL	C2C-C3C-C4C	-7.68	101.01	106.49
25	B	851	8CT	C33-C32-C31	-7.66	117.51	124.85
29	4	306	CHL	C2C-C3C-C4C	-7.65	101.03	106.49
22	K	105	CLA	C4A-NA-C1A	7.65	110.15	106.71
22	9	305	CLA	C4A-NA-C1A	7.64	110.14	106.71
22	B	818	CLA	C4A-NA-C1A	7.60	110.12	106.71
29	6	307	CHL	C2C-C3C-C4C	-7.60	101.07	106.49
22	B	833	CLA	C4A-NA-C1A	7.60	110.12	106.71
30	2	315	XAT	C26-C27-C28	-7.58	109.97	125.99
30	0	313	XAT	C18-C5-C6	-7.58	109.56	122.26
25	4	317	8CT	C33-C32-C31	-7.57	117.59	124.85
25	A	850	8CT	C19-C20-C21	-7.57	116.51	127.31
29	8	314	CHL	C2C-C3C-C4C	-7.54	101.11	106.49
25	I	101	8CT	C18-C17-C16	-7.53	116.56	127.31
22	A	804	CLA	C4A-NA-C1A	7.52	110.09	106.71
29	8	314	CHL	C2B-C1B-NB	7.52	115.28	110.23
29	4	306	CHL	CHD-C1D-ND	-7.51	117.56	124.45
22	9	303	CLA	C4A-NA-C1A	7.51	110.08	106.71
30	6	320	XAT	C17-C1-C6	-7.48	89.84	110.05
30	2	315	XAT	C37-C21-C26	-7.48	89.86	110.05
30	5	315	XAT	C31-C30-C29	-7.47	116.65	127.31
29	4	305	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
29	7	308	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
25	F	302	8CT	C19-C20-C21	-7.46	116.66	127.31
30	3	314	XAT	C17-C1-C6	-7.45	89.93	110.05
25	K	103	8CT	C33-C32-C31	-7.45	117.71	124.85
29	6	302	CHL	CMD-C2D-C1D	7.45	137.84	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	307	CHL	CMD-C2D-C1D	7.45	137.84	124.71
22	5	308	CLA	C4A-NA-C1A	7.44	110.05	106.71
22	B	815	CLA	C4A-NA-C1A	7.44	110.05	106.71
22	7	318	CLA	C4A-NA-C1A	7.42	110.04	106.71
30	4	315	XAT	O24-C25-C24	7.40	118.94	113.38
22	8	310	CLA	C4A-NA-C1A	7.38	110.02	106.71
30	7	319	XAT	C11-C10-C9	-7.37	116.80	127.31
29	3	306	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
25	J	104	8CT	C24-C25-C26	-7.34	116.83	127.31
22	L	202	CLA	C4A-NA-C1A	7.32	110.00	106.71
29	4	307	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
30	5	316	XAT	C35-C34-C33	-7.31	116.87	127.31
25	B	843	8CT	C19-C20-C21	-7.31	116.88	127.31
29	8	307	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
29	2	307	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
22	B	807	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	B	840	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	A	822	CLA	C4A-NA-C1A	7.27	109.97	106.71
30	3	314	XAT	C6-C7-C8	-7.24	110.69	125.99
22	A	832	CLA	C4A-NA-C1A	7.23	109.95	106.71
22	7	313	CLA	C4A-NA-C1A	7.22	109.95	106.71
22	3	311	CLA	C4A-NA-C1A	7.22	109.95	106.71
25	A	846	8CT	C30-C31-C32	-7.22	112.59	121.47
22	B	829	CLA	C4A-NA-C1A	7.22	109.95	106.71
22	5	312	CLA	C4A-NA-C1A	7.21	109.95	106.71
29	9	307	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
22	A	820	CLA	C4A-NA-C1A	7.20	109.94	106.71
30	1	315	XAT	C26-C27-C28	-7.19	110.79	125.99
29	5	306	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
30	0	314	XAT	O24-C25-C24	7.17	118.77	113.38
30	9	314	XAT	C37-C21-C26	-7.17	90.69	110.05
22	3	308	CLA	C4A-NA-C1A	7.16	109.92	106.71
22	3	319	CLA	C4A-NA-C1A	7.15	109.92	106.71
25	8	301	8CT	C24-C25-C26	-7.14	117.12	127.31
22	6	318	CLA	C4A-NA-C1A	7.12	109.91	106.71
30	5	316	XAT	C18-C5-C6	-7.12	110.33	122.26
25	B	843	8CT	C18-C17-C16	-7.12	117.15	127.31
22	B	824	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	A	808	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	B	808	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	A	805	CLA	C4A-NA-C1A	7.09	109.89	106.71
30	8	316	XAT	O4-C5-C4	7.09	118.71	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	305	CHL	C2C-C3C-C4C	-7.09	101.44	106.49
25	F	302	8CT	C24-C25-C26	-7.08	117.20	127.31
25	F	302	8CT	C18-C17-C16	-7.07	117.21	127.31
30	8	316	XAT	C18-C5-C6	-7.07	110.41	122.26
30	2	315	XAT	C36-C21-C22	7.06	121.25	108.98
30	8	317	XAT	C18-C5-C6	-7.06	110.43	122.26
22	7	307	CLA	C4A-NA-C1A	7.06	109.88	106.71
30	6	320	XAT	O4-C5-C4	7.06	118.68	113.38
22	4	308	CLA	C4A-NA-C1A	7.04	109.87	106.71
30	5	316	XAT	C26-C27-C28	-7.03	111.12	125.99
22	B	820	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	9	309	CLA	C4A-NA-C1A	7.03	109.87	106.71
30	4	316	XAT	C27-C28-C29	-7.02	114.63	125.53
22	A	817	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	9	311	CLA	C4A-NA-C1A	7.02	109.86	106.71
29	6	316	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
30	4	316	XAT	C18-C5-C6	-7.00	110.53	122.26
22	4	311	CLA	C4A-NA-C1A	7.00	109.85	106.71
22	6	313	CLA	C4A-NA-C1A	7.00	109.85	106.71
29	0	301	CHL	C2C-C3C-C4C	-6.99	101.50	106.49
30	1	314	XAT	O4-C5-C18	6.98	123.42	115.06
22	B	801	CLA	C4A-NA-C1A	6.98	109.84	106.71
22	A	826	CLA	C4A-NA-C1A	6.97	109.84	106.71
25	I	101	8CT	C10-C11-C12	-6.97	115.70	126.23
29	6	306	CHL	C2C-C3C-C4C	-6.96	101.53	106.49
29	1	305	CHL	CHD-C1D-ND	-6.96	118.06	124.45
22	4	312	CLA	C4A-NA-C1A	6.95	109.83	106.71
30	9	314	XAT	C36-C21-C22	6.95	121.06	108.98
25	A	847	8CT	C30-C31-C32	-6.95	112.92	121.47
22	J	103	CLA	C4A-NA-C1A	6.94	109.82	106.71
30	1	314	XAT	C38-C25-C26	-6.93	110.64	122.26
29	0	306	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
30	3	315	XAT	C38-C25-C26	-6.93	110.65	122.26
29	2	306	CHL	CHD-C1D-ND	-6.92	118.10	124.45
29	8	305	CHL	CHD-C1D-ND	-6.92	118.10	124.45
25	J	104	8CT	C10-C11-C12	-6.91	115.79	126.23
30	5	316	XAT	O4-C5-C4	6.90	118.57	113.38
22	A	812	CLA	C4A-NA-C1A	6.90	109.81	106.71
25	7	321	8CT	C10-C11-C12	-6.90	115.81	126.23
22	1	310	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	B	835	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	A	837	CLA	C4A-NA-C1A	6.88	109.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	5	315	XAT	O4-C5-C4	6.87	118.54	113.38
22	L	203	CLA	C4A-NA-C1A	6.86	109.79	106.71
30	4	315	XAT	C38-C25-C26	-6.86	110.76	122.26
22	4	310	CLA	C4A-NA-C1A	6.86	109.79	106.71
29	6	308	CHL	C2C-C3C-C4C	-6.85	101.60	106.49
22	6	309	CLA	C4A-NA-C1A	6.85	109.79	106.71
22	A	807	CLA	C4A-NA-C1A	6.85	109.78	106.71
22	3	307	CLA	C4A-NA-C1A	6.85	109.78	106.71
29	9	307	CHL	CHD-C1D-ND	-6.84	118.17	124.45
25	B	804	8CT	C10-C11-C12	-6.84	115.90	126.23
22	A	816	CLA	C4A-NA-C1A	6.84	109.78	106.71
29	8	314	CHL	CHD-C1D-ND	-6.83	118.18	124.45
22	A	810	CLA	C4A-NA-C1A	6.82	109.77	106.71
30	6	319	XAT	C18-C5-C6	-6.82	110.83	122.26
22	L	201	CLA	C4A-NA-C1A	6.82	109.77	106.71
25	J	101	8CT	C30-C31-C32	-6.82	113.08	121.47
30	9	314	XAT	C38-C25-C26	-6.82	110.84	122.26
29	8	306	CHL	C2C-C3C-C4C	-6.81	101.63	106.49
22	4	303	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	A	824	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	8	312	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	6	314	CLA	C4A-NA-C1A	6.79	109.76	106.71
30	9	315	XAT	C18-C5-C6	-6.78	110.89	122.26
25	L	205	8CT	C19-C20-C21	-6.78	117.63	127.31
22	6	311	CLA	C4A-NA-C1A	6.78	109.75	106.71
25	B	844	8CT	C35-C30-C29	-6.78	104.14	112.70
22	1	311	CLA	C4A-NA-C1A	6.78	109.75	106.71
22	6	304	CLA	C4A-NA-C1A	6.77	109.75	106.71
22	B	816	CLA	C4A-NA-C1A	6.76	109.75	106.71
29	0	301	CHL	CHD-C1D-ND	-6.76	118.24	124.45
30	6	320	XAT	C38-C25-C26	-6.76	110.93	122.26
22	A	823	CLA	C4A-NA-C1A	6.75	109.74	106.71
30	0	313	XAT	C15-C14-C13	-6.75	117.68	127.31
22	5	311	CLA	C4A-NA-C1A	6.75	109.74	106.71
29	6	316	CHL	CHD-C1D-ND	-6.75	118.25	124.45
30	6	320	XAT	C16-C1-C2	6.75	120.70	108.98
22	G	103	CLA	C4A-NA-C1A	6.74	109.73	106.71
22	2	308	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	811	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	5	309	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	1	301	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	1	307	CLA	C4A-NA-C1A	6.72	109.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	0	308	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	2	303	CLA	C4A-NA-C1A	6.72	109.73	106.71
30	3	314	XAT	C16-C1-C2	6.72	120.66	108.98
30	7	320	XAT	C18-C5-C6	-6.72	111.00	122.26
22	A	843	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	A	830	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	5	303	CLA	C4A-NA-C1A	6.72	109.72	106.71
22	1	303	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	5	316	XAT	C38-C25-C26	-6.71	111.01	122.26
22	3	312	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	B	810	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	B	836	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	7	316	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	K	102	CLA	C4A-NA-C1A	6.70	109.72	106.71
25	3	318	8CT	C14-C13-C12	-6.70	117.75	127.31
22	2	313	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	B	845	8CT	C19-C20-C21	-6.69	117.76	127.31
22	2	311	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	6	312	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	8	304	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	3	313	CLA	C4A-NA-C1A	6.67	109.71	106.71
22	6	310	CLA	C4A-NA-C1A	6.67	109.70	106.71
30	9	315	XAT	C38-C25-C26	-6.67	111.08	122.26
22	0	305	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	0	304	CLA	C4A-NA-C1A	6.64	109.69	106.71
30	8	317	XAT	C38-C25-C26	-6.64	111.14	122.26
22	2	304	CLA	C4A-NA-C1A	6.64	109.69	106.71
30	2	315	XAT	C38-C25-C26	-6.63	111.14	122.26
30	7	319	XAT	C38-C25-C26	-6.63	111.14	122.26
22	1	308	CLA	C4A-NA-C1A	6.63	109.69	106.71
25	A	848	8CT	C04-C03-C02	-6.62	113.28	122.61
22	K	104	CLA	C4A-NA-C1A	6.62	109.68	106.71
30	6	319	XAT	C38-C25-C26	-6.61	111.17	122.26
22	6	303	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	8	313	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	B	825	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	2	312	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	5	304	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	6	307	CHL	CHD-C1D-ND	-6.60	118.39	124.45
25	A	848	8CT	C30-C31-C32	-6.60	113.35	121.47
22	6	317	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	B	837	CLA	C4A-NA-C1A	6.59	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	313	CLA	C4A-NA-C1A	6.58	109.66	106.71
25	L	206	8CT	C10-C11-C12	-6.57	116.30	126.23
22	8	315	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	9	306	CLA	C4A-NA-C1A	6.55	109.65	106.71
25	A	846	8CT	C18-C17-C16	-6.54	117.98	127.31
25	J	101	8CT	C14-C13-C12	-6.53	117.99	127.31
22	B	813	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	A	831	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	3	301	CLA	C4A-NA-C1A	6.51	109.64	106.71
22	G	102	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	0	310	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	0	312	CLA	C4A-NA-C1A	6.50	109.63	106.71
30	3	315	XAT	C18-C5-C6	-6.50	111.36	122.26
30	3	314	XAT	C18-C5-C6	-6.50	111.37	122.26
29	6	308	CHL	CHD-C1D-ND	-6.49	118.49	124.45
25	7	323	8CT	C14-C13-C12	-6.49	118.05	127.31
22	A	815	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	3	305	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	8	306	CHL	CHD-C1D-ND	-6.48	118.50	124.45
22	A	838	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	1	302	CLA	C4A-NA-C1A	6.47	109.61	106.71
29	5	301	CHL	CHD-C1D-ND	-6.46	118.52	124.45
22	4	314	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	4	316	XAT	O4-C5-C4	6.45	118.23	113.38
22	A	825	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	B	834	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	G	101	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	B	817	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	7	304	CLA	C4A-NA-C1A	6.43	109.60	106.71
30	5	315	XAT	C18-C5-C6	-6.43	111.49	122.26
22	8	303	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	B	821	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	9	308	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	A	852	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	7	302	CLA	C4A-NA-C1A	6.41	109.59	106.71
30	3	314	XAT	C38-C25-C26	-6.41	111.52	122.26
30	3	314	XAT	O4-C5-C4	6.41	118.19	113.38
22	B	822	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	A	811	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	3	310	CLA	C4A-NA-C1A	6.40	109.58	106.71
30	0	314	XAT	C18-C5-C6	-6.39	111.55	122.26
22	A	840	CLA	C4A-NA-C1A	6.39	109.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	315	XAT	C18-C5-C6	-6.39	111.56	122.26
30	7	319	XAT	C31-C30-C29	-6.38	118.21	127.31
22	0	307	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	A	828	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	B	814	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	B	832	CLA	C4A-NA-C1A	6.37	109.57	106.71
30	1	315	XAT	C35-C34-C33	-6.37	118.22	127.31
22	A	833	CLA	C4A-NA-C1A	6.36	109.57	106.71
22	5	302	CLA	C4A-NA-C1A	6.36	109.56	106.71
29	2	301	CHL	CHD-C1D-ND	-6.35	118.62	124.45
30	8	316	XAT	O24-C25-C38	6.35	122.66	115.06
25	B	847	8CT	C30-C31-C32	-6.35	113.66	121.47
22	1	306	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	1	309	CLA	C4A-NA-C1A	6.35	109.56	106.71
29	9	302	CHL	CHD-C1D-ND	-6.34	118.63	124.45
22	4	302	CLA	C4A-NA-C1A	6.33	109.55	106.71
25	6	321	8CT	C10-C11-C12	-6.32	116.68	126.23
22	L	204	CLA	C4A-NA-C1A	6.32	109.55	106.71
29	0	306	CHL	CHB-C1B-NB	-6.32	117.57	124.26
29	4	307	CHL	CHD-C1D-ND	-6.31	118.65	124.45
22	A	802	CLA	C4A-NA-C1A	6.31	109.54	106.71
30	5	315	XAT	C27-C28-C29	-6.31	115.74	125.53
22	A	841	CLA	C4A-NA-C1A	6.30	109.54	106.71
30	7	319	XAT	C18-C5-C6	-6.30	111.70	122.26
22	A	821	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	B	823	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	A	829	CLA	C4A-NA-C1A	6.29	109.53	106.71
30	9	314	XAT	C31-C30-C29	-6.28	118.35	127.31
22	3	303	CLA	C4A-NA-C1A	6.28	109.53	106.71
29	2	307	CHL	CHD-C1D-ND	-6.28	118.68	124.45
25	L	206	8CT	C18-C17-C16	-6.27	118.36	127.31
22	5	310	CLA	C4A-NA-C1A	6.27	109.53	106.71
22	2	310	CLA	C4A-NA-C1A	6.27	109.52	106.71
30	1	314	XAT	O24-C25-C24	6.25	118.08	113.38
29	0	306	CHL	CHD-C1D-ND	-6.25	118.71	124.45
30	0	313	XAT	C35-C34-C33	-6.25	118.39	127.31
22	8	309	CLA	C4A-NA-C1A	6.25	109.51	106.71
29	5	306	CHL	CHD-C1D-ND	-6.24	118.72	124.45
22	6	301	CLA	C4A-NA-C1A	6.24	109.51	106.71
22	8	308	CLA	C4A-NA-C1A	6.23	109.51	106.71
25	B	851	8CT	C18-C17-C16	-6.22	118.43	127.31
29	4	301	CHL	O2D-CGD-CBD	6.22	122.33	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	836	CLA	C4A-NA-C1A	6.22	109.50	106.71
22	B	819	CLA	C4A-NA-C1A	6.22	109.50	106.71
22	3	309	CLA	C4A-NA-C1A	6.21	109.50	106.71
25	L	205	8CT	C10-C11-C12	-6.21	116.85	126.23
30	1	315	XAT	C18-C5-C6	-6.20	111.87	122.26
22	7	309	CLA	C4A-NA-C1A	6.18	109.48	106.71
22	A	803	CLA	C4A-NA-C1A	6.17	109.48	106.71
30	4	315	XAT	O4-C5-C4	6.17	118.02	113.38
22	2	302	CLA	C4A-NA-C1A	6.16	109.48	106.71
30	6	319	XAT	O24-C25-C24	6.16	118.01	113.38
25	3	316	8CT	C10-C11-C12	-6.15	116.94	126.23
25	A	847	8CT	C14-C13-C12	-6.14	118.54	127.31
22	5	314	CLA	C4A-NA-C1A	6.14	109.47	106.71
22	1	312	CLA	C4A-NA-C1A	6.13	109.46	106.71
22	7	314	CLA	C4A-NA-C1A	6.13	109.46	106.71
22	B	827	CLA	C4A-NA-C1A	6.12	109.46	106.71
25	7	323	8CT	C19-C20-C21	-6.12	118.57	127.31
22	A	814	CLA	C4A-NA-C1A	6.12	109.46	106.71
22	4	304	CLA	C4A-NA-C1A	6.11	109.45	106.71
22	B	809	CLA	C4A-NA-C1A	6.11	109.45	106.71
22	7	315	CLA	C4A-NA-C1A	6.11	109.45	106.71
25	3	316	8CT	C24-C25-C26	-6.11	118.60	127.31
30	1	315	XAT	C6-C7-C8	-6.10	113.09	125.99
22	B	828	CLA	C4A-NA-C1A	6.10	109.45	106.71
22	B	830	CLA	C4A-NA-C1A	6.10	109.45	106.71
25	K	103	8CT	C18-C17-C16	-6.10	118.61	127.31
22	A	839	CLA	C4A-NA-C1A	6.09	109.44	106.71
22	2	314	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	5	317	8CT	C14-C13-C12	-6.09	118.62	127.31
22	A	813	CLA	C4A-NA-C1A	6.08	109.44	106.71
25	3	316	8CT	C18-C17-C16	-6.08	118.64	127.31
29	4	305	CHL	CHD-C1D-ND	-6.07	118.87	124.45
25	J	101	8CT	C10-C11-C12	-6.07	117.06	126.23
29	4	306	CHL	O2D-CGD-CBD	6.07	122.05	111.27
22	9	313	CLA	C4A-NA-C1A	6.07	109.43	106.71
30	1	314	XAT	C18-C5-C6	-6.07	112.09	122.26
25	A	847	8CT	C19-C20-C21	-6.06	118.66	127.31
30	3	315	XAT	C6-C7-C8	-6.06	113.18	125.99
30	6	320	XAT	C15-C14-C13	-6.06	118.66	127.31
22	A	809	CLA	C4A-NA-C1A	6.06	109.43	106.71
29	8	307	CHL	CHD-C1D-ND	-6.05	118.89	124.45
22	9	310	CLA	C4A-NA-C1A	6.05	109.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	103	8CT	C19-C20-C21	-6.05	118.68	127.31
22	7	305	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	9	301	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	4	309	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	1	316	8CT	C14-C13-C12	-6.03	118.70	127.31
22	0	309	CLA	C4A-NA-C1A	6.03	109.42	106.71
29	9	302	CHL	O2D-CGD-CBD	6.03	121.98	111.27
29	7	308	CHL	CHD-C1D-ND	-6.02	118.92	124.45
25	B	846	8CT	C10-C11-C12	-6.02	117.14	126.23
30	1	315	XAT	C38-C25-C26	-6.02	112.17	122.26
30	9	314	XAT	C18-C5-C6	-6.02	112.18	122.26
29	8	314	CHL	CHB-C1B-NB	-6.00	117.90	124.26
22	6	305	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	2	317	8CT	C18-C17-C16	-5.99	118.77	127.31
29	6	302	CHL	CHD-C1D-ND	-5.99	118.95	124.45
22	A	827	CLA	C4A-NA-C1A	5.99	109.40	106.71
29	3	306	CHL	CHD-C1D-ND	-5.98	118.96	124.45
22	2	309	CLA	C4A-NA-C1A	5.98	109.39	106.71
22	4	313	CLA	C4A-NA-C1A	5.97	109.39	106.71
22	B	841	CLA	C4A-NA-C1A	5.95	109.38	106.71
22	7	311	CLA	C4A-NA-C1A	5.95	109.38	106.71
30	7	320	XAT	C38-C25-C26	-5.95	112.29	122.26
30	9	314	XAT	O24-C25-C38	5.95	122.18	115.06
25	B	848	8CT	C10-C11-C12	-5.95	117.25	126.23
22	A	834	CLA	C4A-NA-C1A	5.95	109.38	106.71
29	7	308	CHL	C3B-C2B-C1B	-5.94	99.99	107.16
25	2	317	8CT	C24-C25-C26	-5.94	118.83	127.31
25	7	323	8CT	C04-C03-C02	-5.93	114.25	122.61
30	0	313	XAT	C31-C30-C29	-5.93	118.84	127.31
22	B	839	CLA	C4A-NA-C1A	5.93	109.37	106.71
22	A	819	CLA	C4A-NA-C1A	5.92	109.37	106.71
22	F	301	CLA	C4A-NA-C1A	5.92	109.37	106.71
22	0	303	CLA	C4A-NA-C1A	5.91	109.36	106.71
30	1	314	XAT	C10-C11-C12	5.89	141.61	123.22
22	B	838	CLA	C4A-NA-C1A	5.88	109.35	106.71
22	B	812	CLA	C4A-NA-C1A	5.87	109.34	106.71
22	0	302	CLA	C4A-NA-C1A	5.87	109.34	106.71
22	5	307	CLA	C4A-NA-C1A	5.86	109.34	106.71
22	9	312	CLA	C4A-NA-C1A	5.86	109.34	106.71
22	0	311	CLA	C4A-NA-C1A	5.85	109.34	106.71
25	L	205	8CT	C14-C13-C12	-5.85	118.96	127.31
22	A	818	CLA	C4A-NA-C1A	5.85	109.34	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	304	CLA	C4A-NA-C1A	5.85	109.34	106.71
30	2	316	XAT	C38-C25-C26	-5.85	112.46	122.26
22	7	303	CLA	C4A-NA-C1A	5.83	109.33	106.71
25	I	101	8CT	C24-C25-C26	-5.82	119.00	127.31
30	0	313	XAT	C7-C8-C9	-5.82	116.50	125.53
25	B	847	8CT	C18-C17-C16	-5.81	119.02	127.31
25	B	845	8CT	C14-C13-C12	-5.80	119.03	127.31
22	2	319	CLA	C4A-NA-C1A	5.80	109.31	106.71
25	B	844	8CT	C30-C31-C32	-5.80	114.33	121.47
22	B	803	CLA	C4A-NA-C1A	5.80	109.31	106.71
22	B	850	CLA	C4A-NA-C1A	5.80	109.31	106.71
29	6	306	CHL	CHD-C1D-ND	-5.79	119.13	124.45
29	8	307	CHL	C3B-C2B-C1B	-5.78	100.18	107.16
22	A	835	CLA	C4A-NA-C1A	5.76	109.30	106.71
22	5	313	CLA	C4A-NA-C1A	5.76	109.30	106.71
30	8	316	XAT	C31-C30-C29	-5.75	119.10	127.31
22	K	101	CLA	C4A-NA-C1A	5.75	109.29	106.71
22	6	323	CLA	C4A-NA-C1A	5.74	109.29	106.71
29	2	305	CHL	C3C-C4C-NC	5.73	117.00	110.57
29	2	305	CHL	CHD-C1D-ND	-5.73	119.19	124.45
22	B	826	CLA	C4A-NA-C1A	5.73	109.28	106.71
22	3	302	CLA	C4A-NA-C1A	5.72	109.28	106.71
25	B	843	8CT	C14-C13-C12	-5.72	119.15	127.31
29	4	305	CHL	C3B-C2B-C1B	-5.72	100.26	107.16
25	J	104	8CT	C18-C17-C16	-5.69	119.19	127.31
29	8	306	CHL	O2D-CGD-CBD	5.69	121.38	111.27
29	6	316	CHL	O2D-CGD-CBD	5.69	121.37	111.27
22	9	304	CLA	C4A-NA-C1A	5.68	109.26	106.71
25	3	316	8CT	C19-C20-C21	-5.68	119.20	127.31
25	A	849	8CT	C24-C25-C26	-5.68	119.21	127.31
25	2	317	8CT	C14-C13-C12	-5.67	119.21	127.31
25	B	844	8CT	C01-C02-C03	-5.67	118.16	124.53
25	A	854	8CT	C18-C17-C16	-5.67	119.22	127.31
25	I	101	8CT	C35-C30-C29	-5.66	105.55	112.70
22	5	305	CLA	C4A-NA-C1A	5.65	109.24	106.71
30	9	314	XAT	C7-C8-C9	5.64	134.28	125.53
29	4	301	CHL	C3C-C4C-NC	5.64	116.90	110.57
29	0	301	CHL	CHB-C1B-NB	-5.64	118.29	124.26
25	A	850	8CT	C10-C11-C12	-5.63	117.73	126.23
29	9	307	CHL	O2D-CGD-CBD	5.59	121.20	111.27
25	K	103	8CT	C04-C03-C02	-5.59	114.74	122.61
29	8	314	CHL	O2D-CGD-CBD	5.58	121.18	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	308	CHL	C3B-C2B-C1B	-5.58	100.43	107.16
22	H	201	CLA	C4A-NA-C1A	5.57	109.21	106.71
25	I	101	8CT	C01-C02-C03	-5.56	118.28	124.53
30	8	317	XAT	C6-C7-C8	-5.56	114.24	125.99
29	1	305	CHL	C3B-C2B-C1B	-5.54	100.47	107.16
22	A	801	CLA	C4A-NA-C1A	5.54	109.19	106.71
22	8	311	CLA	C4A-NA-C1A	5.53	109.19	106.71
29	6	316	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
25	7	321	8CT	C04-C03-C02	-5.51	114.85	122.61
22	1	304	CLA	C4A-NA-C1A	5.51	109.18	106.71
25	A	850	8CT	C07-C02-C03	-5.50	114.75	122.73
29	6	307	CHL	CHB-C1B-NB	-5.50	118.44	124.26
25	4	317	8CT	C14-C13-C12	-5.48	119.49	127.31
22	8	302	CLA	C4A-NA-C1A	5.47	109.17	106.71
30	2	316	XAT	C26-C27-C28	-5.47	114.44	125.99
25	B	848	8CT	C04-C03-C02	-5.46	114.93	122.61
29	7	308	CHL	C3C-C4C-NC	5.46	116.69	110.57
25	7	301	8CT	C30-C31-C32	-5.45	114.76	121.47
22	6	315	CLA	C4A-NA-C1A	5.45	109.16	106.71
30	6	320	XAT	C26-C27-C28	-5.45	114.47	125.99
22	A	853	CLA	C4A-NA-C1A	5.45	109.16	106.71
30	9	315	XAT	O4-C5-C4	5.44	117.47	113.38
29	7	308	CHL	CHD-C4C-C3C	-5.44	116.85	124.84
25	A	847	8CT	C24-C25-C26	-5.43	119.57	127.31
30	3	315	XAT	O4-C5-C18	5.42	121.55	115.06
30	7	320	XAT	O4-C5-C4	5.41	117.44	113.38
29	6	307	CHL	C3B-C2B-C1B	-5.41	100.63	107.16
29	5	301	CHL	C3B-C2B-C1B	-5.39	100.65	107.16
30	8	317	XAT	O4-C5-C4	5.39	117.43	113.38
29	3	306	CHL	C3D-C2D-C1D	-5.39	98.47	105.83
25	B	846	8CT	C30-C31-C32	-5.39	114.84	121.47
22	B	805	CLA	C4A-NA-C1A	5.39	109.13	106.71
25	A	854	8CT	C14-C13-C12	-5.38	119.62	127.31
25	B	804	8CT	C24-C25-C26	-5.38	119.63	127.31
22	B	831	CLA	C4A-NA-C1A	5.37	109.12	106.71
25	A	850	8CT	C30-C31-C32	-5.36	114.88	121.47
30	7	319	XAT	C27-C28-C29	-5.36	117.22	125.53
29	8	305	CHL	C3C-C4C-NC	5.34	116.56	110.57
29	8	306	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
30	6	319	XAT	O4-C5-C4	5.34	117.39	113.38
25	B	804	8CT	C01-C02-C03	-5.34	118.54	124.53
25	A	846	8CT	C19-C18-C17	-5.33	112.55	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	8	307	CHL	O2D-CGD-CBD	5.33	120.73	111.27
30	8	316	XAT	C7-C8-C9	-5.32	117.27	125.53
25	G	104	8CT	C18-C17-C16	-5.32	119.71	127.31
25	B	846	8CT	C04-C03-C02	-5.32	115.13	122.61
30	1	314	XAT	O24-C25-C38	5.31	121.42	115.06
30	0	314	XAT	C27-C28-C29	-5.30	117.30	125.53
29	0	306	CHL	O2D-CGD-CBD	5.29	120.66	111.27
25	2	317	8CT	C30-C31-C32	-5.29	114.97	121.47
29	2	307	CHL	C3B-C2B-C1B	-5.28	100.78	107.16
30	6	319	XAT	C11-C10-C9	-5.28	119.78	127.31
30	3	315	XAT	O24-C25-C24	5.28	117.34	113.38
29	9	302	CHL	C3C-C4C-NC	5.26	116.47	110.57
30	7	319	XAT	O4-C5-C4	5.26	117.33	113.38
30	1	314	XAT	C11-C10-C9	-5.25	119.81	127.31
25	7	301	8CT	C10-C11-C12	-5.25	118.30	126.23
30	6	320	XAT	O4-C5-C18	5.25	121.34	115.06
25	J	101	8CT	C19-C20-C21	-5.25	119.82	127.31
22	M	101	CLA	C4A-NA-C1A	5.25	109.06	106.71
22	A	806	CLA	C4A-NA-C1A	5.24	109.06	106.71
25	A	849	8CT	C10-C11-C12	-5.24	118.32	126.23
25	1	316	8CT	C19-C20-C21	-5.23	119.84	127.31
29	1	305	CHL	CHB-C1B-NB	-5.23	118.72	124.26
30	8	316	XAT	C32-C33-C34	5.22	126.95	118.94
29	9	307	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
29	4	301	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
29	5	306	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
25	F	302	8CT	C04-C03-C02	-5.21	115.27	122.61
29	9	302	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
29	6	302	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
30	8	317	XAT	C26-C27-C28	-5.19	115.03	125.99
30	7	320	XAT	C6-C7-C8	-5.18	115.03	125.99
30	2	315	XAT	O24-C25-C24	5.18	117.27	113.38
29	6	306	CHL	C3C-C4C-NC	5.18	116.38	110.57
30	7	319	XAT	C35-C34-C33	-5.18	119.92	127.31
25	B	847	8CT	C14-C13-C12	-5.17	119.93	127.31
30	6	319	XAT	C31-C32-C33	-5.17	111.90	126.42
25	1	316	8CT	C10-C11-C12	-5.17	118.43	126.23
29	0	301	CHL	C3B-C2B-C1B	-5.16	100.93	107.16
25	7	321	8CT	C30-C31-C32	-5.16	115.12	121.47
30	8	316	XAT	O4-C5-C18	5.15	121.23	115.06
30	9	315	XAT	C6-C7-C8	-5.15	115.10	125.99
29	3	306	CHL	C3C-C4C-NC	5.15	116.35	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	301	CHL	C3B-C4B-NB	5.14	115.28	110.52
25	8	318	8CT	C19-C20-C21	-5.14	119.98	127.31
30	4	315	XAT	C7-C8-C9	-5.14	117.56	125.53
22	7	306	CLA	C4A-NA-C1A	5.13	109.01	106.71
30	9	315	XAT	O4-C5-C18	5.12	121.19	115.06
25	A	850	8CT	C24-C25-C26	-5.12	120.00	127.31
25	B	845	8CT	C30-C31-C32	-5.11	115.18	121.47
30	8	316	XAT	C15-C35-C34	-5.11	113.01	123.47
25	2	317	8CT	C04-C03-C02	-5.10	115.43	122.61
25	7	321	8CT	C14-C15-C16	-5.10	112.08	126.42
22	7	312	CLA	C4A-NA-C1A	5.10	109.00	106.71
29	2	306	CHL	C3B-C2B-C1B	-5.10	101.01	107.16
29	4	307	CHL	C3D-C2D-C1D	-5.09	98.89	105.83
25	A	847	8CT	C10-C11-C12	-5.09	118.55	126.23
25	2	317	8CT	C10-C11-C12	-5.09	118.55	126.23
25	A	849	8CT	C18-C17-C16	-5.06	120.09	127.31
29	2	305	CHL	C3B-C2B-C1B	-5.06	101.06	107.16
25	B	844	8CT	C10-C11-C12	-5.06	118.60	126.23
25	7	321	8CT	C07-C02-C03	-5.05	115.40	122.73
29	6	306	CHL	O2D-CGD-CBD	5.05	120.24	111.27
30	9	314	XAT	O24-C25-C24	5.05	117.17	113.38
25	A	846	8CT	C04-C03-C02	-5.05	115.50	122.61
29	2	305	CHL	CHD-C4C-C3C	-5.05	117.42	124.84
29	0	306	CHL	C3B-C2B-C1B	-5.05	101.07	107.16
30	8	317	XAT	C35-C34-C33	-5.04	120.11	127.31
25	5	317	8CT	C10-C11-C12	-5.04	118.62	126.23
30	2	315	XAT	O24-C25-C38	5.04	121.09	115.06
29	4	307	CHL	C3C-C4C-NC	5.04	116.22	110.57
29	4	301	CHL	CHD-C1D-ND	-5.04	119.83	124.45
25	8	318	8CT	C14-C13-C12	-5.04	120.12	127.31
29	3	306	CHL	CHD-C4C-C3C	-5.04	117.44	124.84
25	J	104	8CT	C01-C02-C03	-5.03	118.88	124.53
25	J	104	8CT	C30-C31-C32	-5.02	115.29	121.47
29	5	306	CHL	CHB-C1B-NB	-5.02	118.94	124.26
29	4	307	CHL	CHD-C4C-C3C	-5.02	117.47	124.84
30	8	316	XAT	C40-C33-C34	-5.00	115.92	122.92
25	A	846	8CT	C24-C25-C26	-5.00	120.18	127.31
29	8	305	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
29	8	305	CHL	C3B-C2B-C1B	-4.97	101.16	107.16
29	8	305	CHL	O2D-CGD-CBD	4.97	120.09	111.27
29	6	306	CHL	C3B-C2B-C1B	-4.96	101.17	107.16
29	6	307	CHL	O2D-CGD-CBD	4.96	120.08	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	318	8CT	C18-C17-C16	-4.96	120.23	127.31
30	6	319	XAT	C15-C35-C34	-4.96	113.31	123.47
30	0	314	XAT	C15-C14-C13	-4.95	120.25	127.31
29	2	301	CHL	OMC-CMC-C2C	-4.95	114.50	125.69
30	1	314	XAT	C16-C1-C2	4.94	117.57	108.98
25	A	849	8CT	C19-C20-C21	-4.94	120.26	127.31
25	6	321	8CT	C04-C03-C02	-4.94	115.66	122.61
30	9	315	XAT	C26-C27-C28	-4.93	115.56	125.99
29	8	307	CHL	C3C-C4C-NC	4.93	116.10	110.57
29	8	314	CHL	C3B-C2B-C1B	-4.92	101.22	107.16
29	4	306	CHL	C3B-C2B-C1B	-4.92	101.23	107.16
25	B	804	8CT	C18-C17-C16	-4.89	120.34	127.31
30	7	319	XAT	O4-C5-C18	4.88	120.91	115.06
29	2	306	CHL	C3C-C4C-NC	4.88	116.05	110.57
25	7	301	8CT	C01-C02-C03	-4.88	119.05	124.53
30	4	316	XAT	O4-C5-C18	4.88	120.90	115.06
29	5	301	CHL	C3C-C4C-NC	4.87	116.04	110.57
25	B	843	8CT	C24-C25-C26	-4.87	120.35	127.31
29	6	302	CHL	C3C-C4C-NC	4.87	116.04	110.57
25	A	847	8CT	C01-C02-C03	-4.87	119.06	124.53
25	B	845	8CT	C10-C11-C12	-4.87	118.88	126.23
30	6	319	XAT	C32-C33-C34	4.86	126.40	118.94
30	4	315	XAT	C20-C13-C14	-4.86	116.12	122.92
25	A	848	8CT	C18-C17-C16	-4.86	120.38	127.31
25	J	101	8CT	C18-C17-C16	-4.86	120.38	127.31
25	3	318	8CT	C10-C11-C12	-4.86	118.90	126.23
25	L	206	8CT	C19-C20-C21	-4.85	120.38	127.31
29	4	307	CHL	C2D-C1D-ND	4.85	113.68	110.10
25	7	323	8CT	C07-C02-C03	-4.85	115.69	122.73
25	2	317	8CT	C35-C30-C29	-4.85	106.57	112.70
29	6	302	CHL	O2D-CGD-CBD	4.85	119.89	111.27
29	2	307	CHL	C3C-C4C-NC	4.85	116.01	110.57
29	2	301	CHL	C3C-C4C-NC	4.84	116.00	110.57
25	J	104	8CT	C04-C03-C02	-4.83	115.80	122.61
25	K	103	8CT	C07-C02-C03	-4.83	115.71	122.73
25	B	848	8CT	C30-C31-C32	-4.82	115.53	121.47
25	L	206	8CT	C30-C31-C32	-4.82	115.53	121.47
29	9	302	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
25	A	854	8CT	C19-C20-C21	-4.82	120.43	127.31
25	6	321	8CT	C01-C02-C03	-4.82	119.12	124.53
25	B	847	8CT	C19-C20-C21	-4.81	120.45	127.31
29	2	301	CHL	C3B-C2B-C1B	-4.80	101.36	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	316	8CT	C04-C03-C02	-4.80	115.86	122.61
29	4	305	CHL	C3C-C4C-NC	4.79	115.94	110.57
29	2	306	CHL	O2D-CGD-CBD	4.78	119.76	111.27
29	2	301	CHL	O2D-CGD-CBD	4.78	119.76	111.27
25	2	317	8CT	C07-C02-C03	-4.78	115.80	122.73
30	4	315	XAT	O4-C5-C18	4.77	120.77	115.06
30	5	315	XAT	O4-C5-C18	4.77	120.77	115.06
25	G	104	8CT	C19-C20-C21	-4.77	120.51	127.31
29	3	306	CHL	C3B-C2B-C1B	-4.77	101.41	107.16
25	L	205	8CT	C01-C02-C03	-4.76	119.18	124.53
29	6	302	CHL	C3D-C2D-C1D	-4.76	99.33	105.83
30	0	314	XAT	C11-C10-C9	-4.76	120.52	127.31
25	1	316	8CT	C18-C17-C16	-4.75	120.53	127.31
30	5	316	XAT	C35-C15-C14	-4.75	113.75	123.47
30	3	315	XAT	O24-C25-C38	4.75	120.74	115.06
25	L	205	8CT	C14-C15-C16	-4.74	113.10	126.42
29	1	305	CHL	O2D-CGD-CBD	4.73	119.67	111.27
25	B	848	8CT	C18-C19-C20	-4.73	113.79	123.47
29	4	307	CHL	C3B-C2B-C1B	-4.72	101.46	107.16
29	6	308	CHL	C3C-C4C-NC	4.71	115.86	110.57
29	8	306	CHL	C3C-C4C-NC	4.71	115.86	110.57
25	G	104	8CT	C07-C02-C03	-4.71	115.89	122.73
25	A	850	8CT	C14-C13-C12	-4.71	120.59	127.31
30	8	316	XAT	C11-C12-C13	-4.71	113.19	126.42
29	2	307	CHL	CHD-C4C-C3C	-4.71	117.92	124.84
30	6	319	XAT	C31-C30-C29	-4.71	120.59	127.31
30	2	315	XAT	C15-C14-C13	-4.70	120.60	127.31
30	3	314	XAT	C40-C33-C34	-4.70	116.34	122.92
29	3	306	CHL	C2D-C1D-ND	4.69	113.56	110.10
29	5	301	CHL	O2D-CGD-CBD	4.69	119.60	111.27
29	2	301	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
25	A	848	8CT	C07-C02-C03	-4.69	115.93	122.73
29	5	301	CHL	C3D-C2D-C1D	-4.69	99.44	105.83
29	2	307	CHL	C3D-C2D-C1D	-4.68	99.44	105.83
25	B	847	8CT	C07-C02-C03	-4.68	115.93	122.73
30	4	315	XAT	C15-C14-C13	-4.68	120.63	127.31
25	K	103	8CT	C10-C11-C12	-4.67	119.17	126.23
29	7	308	CHL	O2D-CGD-CBD	4.67	119.57	111.27
25	B	844	8CT	C39-C16-C17	-4.66	116.39	122.92
25	A	850	8CT	C04-C03-C02	-4.66	116.05	122.61
29	6	307	CHL	C3C-C4C-NC	4.66	115.80	110.57
25	B	846	8CT	C07-C02-C03	-4.66	115.97	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	316	CHL	C3D-C2D-C1D	-4.65	99.49	105.83
30	0	313	XAT	O4-C5-C18	4.65	120.62	115.06
29	6	316	CHL	C3C-C4C-NC	4.65	115.78	110.57
25	L	206	8CT	C01-C02-C03	-4.65	119.31	124.53
25	A	849	8CT	C04-C03-C02	-4.64	116.07	122.61
25	A	848	8CT	C19-C20-C21	-4.64	120.69	127.31
25	B	845	8CT	C18-C17-C16	-4.64	120.69	127.31
25	3	316	8CT	C04-C03-C02	-4.64	116.08	122.61
30	4	316	XAT	C35-C34-C33	-4.63	120.70	127.31
25	A	847	8CT	C18-C17-C16	-4.63	120.70	127.31
25	B	848	8CT	C07-C02-C03	-4.63	116.02	122.73
25	5	317	8CT	C04-C03-C02	-4.62	116.10	122.61
29	4	306	CHL	C3C-C4C-NC	4.62	115.75	110.57
30	1	315	XAT	O4-C5-C4	4.62	116.85	113.38
29	8	306	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
29	6	308	CHL	CHD-C4C-C3C	-4.62	118.06	124.84
30	1	315	XAT	O4-C5-C18	4.60	120.57	115.06
25	7	323	8CT	C01-C02-C03	-4.60	119.36	124.53
29	4	301	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
29	8	314	CHL	C3C-C4C-NC	4.60	115.73	110.57
29	8	314	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
29	2	306	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
25	B	843	8CT	C01-C02-C03	-4.58	119.38	124.53
29	4	301	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
29	0	301	CHL	O2D-CGD-CBD	4.58	119.41	111.27
25	8	301	8CT	C14-C13-C12	-4.58	120.78	127.31
29	7	308	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
29	6	308	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
25	1	316	8CT	C24-C25-C26	-4.56	120.81	127.31
30	5	315	XAT	C20-C13-C14	-4.56	116.54	122.92
29	5	306	CHL	O2D-CGD-CBD	4.54	119.34	111.27
30	9	315	XAT	C15-C14-C13	-4.54	120.83	127.31
29	2	307	CHL	C1-C2-C3	-4.53	119.42	126.75
29	4	305	CHL	C3D-C2D-C1D	-4.53	99.65	105.83
25	8	301	8CT	C30-C31-C32	-4.53	115.90	121.47
25	A	854	8CT	C24-C25-C26	-4.53	120.85	127.31
25	8	301	8CT	C10-C11-C12	-4.52	119.41	126.23
29	8	305	CHL	CHD-C4C-C3C	-4.52	118.20	124.84
30	5	316	XAT	C6-C7-C8	-4.51	116.45	125.99
30	1	314	XAT	C28-C29-C30	4.51	125.86	118.94
25	B	804	8CT	C30-C31-C32	-4.50	115.93	121.47
29	2	305	CHL	C3D-C2D-C1D	-4.50	99.70	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	843	8CT	C10-C11-C12	-4.49	119.44	126.23
29	4	306	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
30	4	315	XAT	O24-C25-C38	4.49	120.44	115.06
30	6	319	XAT	O4-C5-C18	4.49	120.44	115.06
30	8	317	XAT	C18-C5-C4	4.49	119.33	114.28
29	4	305	CHL	O2D-CGD-CBD	4.49	119.24	111.27
30	6	319	XAT	C26-C27-C28	-4.48	116.52	125.99
25	6	321	8CT	C07-C02-C03	-4.48	116.23	122.73
29	0	301	CHL	C3D-C2D-C1D	-4.48	99.72	105.83
25	7	321	8CT	C24-C23-C21	-4.48	113.84	126.42
25	K	103	8CT	C01-C02-C03	-4.47	119.51	124.53
25	6	321	8CT	C30-C31-C32	-4.47	115.97	121.47
29	5	306	CHL	C3C-C4C-NC	4.47	115.58	110.57
25	5	317	8CT	C24-C23-C21	-4.45	113.91	126.42
25	8	318	8CT	C30-C31-C32	-4.45	115.99	121.47
30	6	319	XAT	C20-C13-C14	-4.44	116.70	122.92
25	G	104	8CT	C24-C25-C26	-4.43	120.98	127.31
25	A	850	8CT	C01-C02-C03	-4.43	119.55	124.53
29	4	307	CHL	C1D-ND-C4D	-4.43	103.19	106.33
29	6	306	CHL	C3D-C2D-C1D	-4.43	99.78	105.83
30	3	314	XAT	C31-C30-C29	-4.43	120.99	127.31
29	1	305	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
24	1	317	LHG	O4-P-O5	4.42	134.09	112.24
30	9	315	XAT	C35-C34-C33	-4.42	121.00	127.31
25	G	104	8CT	C14-C13-C12	-4.41	121.01	127.31
25	2	317	8CT	C01-C02-C03	-4.41	119.57	124.53
25	B	846	8CT	C19-C20-C21	-4.41	121.01	127.31
25	K	103	8CT	C14-C13-C12	-4.41	121.01	127.31
30	5	315	XAT	C12-C13-C14	4.41	125.70	118.94
29	1	305	CHL	C3C-C4C-NC	4.41	115.51	110.57
30	3	315	XAT	C26-C27-C28	-4.41	116.68	125.99
30	3	314	XAT	O4-C5-C18	4.40	120.33	115.06
25	G	104	8CT	C01-C02-C03	-4.40	119.59	124.53
30	8	316	XAT	C12-C13-C14	4.40	125.69	118.94
29	3	306	CHL	O2D-CGD-CBD	4.40	119.08	111.27
25	3	316	8CT	C07-C02-C03	-4.39	116.35	122.73
25	B	851	8CT	C19-C20-C21	-4.39	121.04	127.31
29	2	307	CHL	O2D-CGD-CBD	4.39	119.06	111.27
29	8	307	CHL	C3D-C2D-C1D	-4.38	99.85	105.83
30	0	314	XAT	O24-C25-C38	4.38	120.30	115.06
29	8	306	CHL	CHD-C4C-C3C	-4.38	118.41	124.84
30	4	316	XAT	C6-C7-C8	-4.37	116.74	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	318	LHG	O4-P-O5	4.37	133.85	112.24
25	B	846	8CT	C01-C02-C03	-4.37	119.62	124.53
30	7	319	XAT	C6-C7-C8	-4.37	116.76	125.99
30	7	320	XAT	O4-C5-C18	4.37	120.29	115.06
24	5	318	LHG	O4-P-O5	4.36	133.80	112.24
29	9	307	CHL	C3D-C2D-C1D	-4.36	99.88	105.83
29	9	302	CHL	CHD-C4C-C3C	-4.36	118.44	124.84
29	4	305	CHL	CHB-C1B-NB	-4.35	119.65	124.26
24	B	852	LHG	O4-P-O5	4.35	133.76	112.24
30	3	315	XAT	C18-C5-C4	4.35	119.17	114.28
30	6	319	XAT	C40-C33-C34	-4.34	116.84	122.92
24	3	317	LHG	O4-P-O5	4.34	133.71	112.24
25	A	849	8CT	C07-C02-C03	-4.34	116.43	122.73
30	9	314	XAT	C27-C28-C29	-4.33	118.81	125.53
29	2	307	CHL	C1D-ND-C4D	-4.33	103.26	106.33
30	6	319	XAT	O24-C25-C38	4.32	120.24	115.06
29	9	307	CHL	C3C-C4C-NC	4.32	115.42	110.57
25	A	854	8CT	C30-C31-C32	-4.32	116.15	121.47
29	2	307	CHL	C2D-C1D-ND	4.32	113.29	110.10
25	B	847	8CT	C10-C11-C12	-4.32	119.71	126.23
25	G	104	8CT	C04-C03-C02	-4.31	116.54	122.61
30	1	314	XAT	C32-C33-C34	4.31	125.56	118.94
29	0	306	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
25	B	845	8CT	C39-C16-C15	4.30	124.85	118.08
25	A	854	8CT	C10-C11-C12	-4.30	119.74	126.23
29	5	306	CHL	C3D-C2D-C1D	-4.29	99.97	105.83
25	B	848	8CT	C01-C02-C03	-4.29	119.71	124.53
25	7	321	8CT	C35-C30-C29	-4.29	107.28	112.70
25	8	301	8CT	C07-C02-C03	-4.28	116.51	122.73
30	0	314	XAT	C31-C30-C29	-4.27	121.21	127.31
25	3	318	8CT	C24-C23-C21	-4.26	114.45	126.42
25	2	317	8CT	C19-C20-C21	-4.26	121.23	127.31
24	A	844	LHG	O4-P-O5	4.26	133.30	112.24
25	B	848	8CT	C35-C30-C29	-4.26	107.32	112.70
25	J	101	8CT	C01-C02-C03	-4.25	119.75	124.53
25	B	851	8CT	C30-C31-C32	-4.25	116.24	121.47
25	8	318	8CT	C07-C02-C03	-4.25	116.56	122.73
25	I	101	8CT	C19-C20-C21	-4.25	121.25	127.31
24	9	316	LHG	O4-P-O5	4.24	133.22	112.24
25	7	323	8CT	C35-C30-C29	-4.24	107.34	112.70
25	I	101	8CT	C30-C31-C32	-4.24	116.25	121.47
29	9	302	CHL	C2D-C1D-ND	4.23	113.22	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	318	8CT	C10-C11-C12	-4.21	119.87	126.23
29	6	302	CHL	CHB-C1B-NB	-4.21	119.80	124.26
25	A	854	8CT	C07-C02-C03	-4.21	116.62	122.73
24	A	845	LHG	O4-P-O5	4.21	133.05	112.24
25	5	317	8CT	C01-C02-C03	-4.21	119.81	124.53
29	5	301	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
30	8	316	XAT	C31-C32-C33	-4.20	114.61	126.42
25	3	318	8CT	C14-C15-C16	-4.20	114.61	126.42
25	B	851	8CT	C10-C11-C12	-4.19	119.90	126.23
29	6	306	CHL	CHD-C4C-C3C	-4.19	118.68	124.84
25	B	847	8CT	C01-C02-C03	-4.19	119.82	124.53
25	L	206	8CT	C04-C03-C02	-4.19	116.71	122.61
25	G	104	8CT	C30-C31-C32	-4.19	116.31	121.47
25	6	321	8CT	C35-C30-C29	-4.18	107.41	112.70
25	A	854	8CT	C01-C02-C03	-4.18	119.83	124.53
25	B	845	8CT	C01-C02-C03	-4.17	119.84	124.53
24	0	315	LHG	O4-P-O5	4.17	132.87	112.24
29	2	301	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
25	7	323	8CT	C30-C31-C32	-4.17	116.34	121.47
30	9	314	XAT	C19-C9-C8	4.16	124.64	118.08
24	6	322	LHG	O4-P-O5	4.16	132.79	112.24
29	8	305	CHL	C2D-C1D-ND	4.15	113.16	110.10
29	6	307	CHL	C3D-C2D-C1D	-4.15	100.17	105.83
30	7	319	XAT	C15-C14-C13	-4.14	121.40	127.31
25	B	843	8CT	C04-C03-C02	-4.14	116.78	122.61
29	4	307	CHL	O2D-CGD-CBD	4.14	118.62	111.27
29	6	306	CHL	CAC-C3C-C4C	4.14	130.18	124.81
29	2	301	CHL	C2D-C1D-ND	4.13	113.15	110.10
22	B	816	CLA	O2D-CGD-O1D	-4.13	115.76	123.84
25	5	317	8CT	C19-C18-C17	-4.13	115.02	123.47
30	0	313	XAT	C20-C13-C14	-4.13	117.14	122.92
29	0	301	CHL	C3C-C4C-NC	4.12	115.20	110.57
30	8	316	XAT	O24-C25-C24	4.12	116.48	113.38
25	B	844	8CT	C14-C13-C12	-4.12	121.43	127.31
29	8	314	CHL	CMB-C2B-C1B	4.12	131.65	125.37
25	4	317	8CT	C35-C30-C29	-4.11	107.51	112.70
30	8	316	XAT	C20-C13-C14	-4.11	117.17	122.92
30	5	315	XAT	C11-C10-C9	-4.10	121.46	127.31
25	4	317	8CT	C18-C19-C20	-4.10	115.08	123.47
28	B	849	DGD	O3G-C3G-C2G	-4.09	101.02	110.90
29	6	308	CHL	O2D-CGD-CBD	4.09	118.54	111.27
29	0	306	CHL	CAC-C3C-C4C	4.09	130.12	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	316	XAT	C35-C34-C33	-4.09	121.47	127.31
29	2	301	CHL	CAC-C3C-C4C	4.08	130.11	124.81
25	8	318	8CT	C01-C02-C03	-4.07	119.96	124.53
25	G	104	8CT	C10-C11-C12	-4.05	120.12	126.23
25	7	323	8CT	C18-C17-C16	-4.04	121.54	127.31
25	B	851	8CT	C39-C16-C17	-4.04	117.26	122.92
25	7	301	8CT	C07-C02-C03	-4.04	116.86	122.73
30	3	315	XAT	C15-C14-C13	-4.04	121.55	127.31
30	8	317	XAT	O4-C5-C18	4.04	119.89	115.06
25	3	318	8CT	C28-C26-C25	4.04	125.13	118.94
30	7	320	XAT	C26-C27-C28	-4.03	117.47	125.99
25	L	205	8CT	C24-C23-C21	-4.03	115.10	126.42
25	A	849	8CT	C01-C02-C03	-4.03	120.00	124.53
24	7	322	LHG	O4-P-O5	4.02	132.13	112.24
29	2	301	CHL	C1D-ND-C4D	-4.02	103.48	106.33
25	8	318	8CT	C04-C03-C02	-4.02	116.95	122.61
25	8	301	8CT	C01-C02-C03	-4.02	120.02	124.53
25	4	317	8CT	C04-C03-C02	-4.02	116.96	122.61
30	9	314	XAT	C26-C27-C28	-4.01	117.51	125.99
25	A	854	8CT	C04-C03-C02	-4.01	116.97	122.61
29	0	306	CHL	C3B-C4B-NB	3.99	114.21	110.52
29	4	301	CHL	C2D-C1D-ND	3.98	113.04	110.10
25	B	844	8CT	C24-C25-C26	-3.97	121.64	127.31
25	B	843	8CT	C22-C21-C20	-3.97	117.36	122.92
30	6	319	XAT	C6-C7-C8	-3.97	117.59	125.99
30	0	314	XAT	C20-C13-C14	-3.97	117.36	122.92
25	J	104	8CT	C07-C02-C03	-3.97	116.97	122.73
30	7	320	XAT	C24-C23-C22	-3.97	103.11	110.77
30	8	316	XAT	C24-C23-C22	-3.97	103.11	110.77
29	8	307	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
30	7	319	XAT	C8-C9-C10	3.96	125.02	118.94
25	7	321	8CT	C15-C16-C17	3.96	125.02	118.94
25	F	302	8CT	C10-C11-C12	-3.96	120.25	126.23
29	6	308	CHL	C2D-C1D-ND	3.96	113.02	110.10
25	L	206	8CT	C14-C13-C12	-3.95	121.67	127.31
25	B	843	8CT	C35-C30-C29	-3.95	107.71	112.70
25	4	317	8CT	C10-C11-C12	-3.95	120.27	126.23
29	6	302	CHL	CHD-C4C-C3C	-3.94	119.04	124.84
30	5	316	XAT	O4-C5-C18	3.94	119.78	115.06
30	0	313	XAT	C27-C28-C29	-3.94	119.42	125.53
29	2	301	CHL	CHB-C1B-NB	-3.94	120.09	124.26
25	B	804	8CT	C19-C20-C21	-3.93	121.70	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	313	XAT	C20-C13-C12	3.93	124.27	118.08
30	3	315	XAT	C5-C4-C3	-3.93	104.97	112.75
29	7	308	CHL	C1D-ND-C4D	-3.93	103.54	106.33
25	A	846	8CT	C01-C02-C03	-3.92	120.12	124.53
25	J	101	8CT	C24-C25-C26	-3.92	121.72	127.31
22	B	803	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
22	7	303	CLA	C1-C2-C3	-3.92	119.27	126.04
22	B	850	CLA	CAA-CBA-CGA	-3.91	101.81	113.25
25	5	317	8CT	C07-C02-C03	-3.91	117.05	122.73
29	6	308	CHL	C1D-ND-C4D	-3.91	103.56	106.33
25	8	301	8CT	C35-C30-C29	-3.90	107.77	112.70
22	A	803	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
25	B	848	8CT	C14-C15-C16	-3.89	115.50	126.42
29	4	307	CHL	C1-C2-C3	-3.88	120.47	126.75
25	L	205	8CT	C19-C18-C17	3.88	131.43	123.47
22	B	822	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
22	B	828	CLA	C1-C2-C3	-3.88	119.33	126.04
25	J	101	8CT	C04-C03-C02	-3.88	117.15	122.61
25	6	321	8CT	C18-C19-C20	-3.88	115.54	123.47
22	A	828	CLA	C1-C2-C3	-3.88	119.34	126.04
25	1	316	8CT	C07-C02-C03	-3.87	117.11	122.73
30	7	320	XAT	C18-C5-C4	3.87	118.64	114.28
29	2	307	CHL	C3B-C4B-NB	3.87	114.11	110.52
30	4	316	XAT	C24-C23-C22	-3.87	103.30	110.77
30	5	315	XAT	C40-C33-C34	-3.87	117.50	122.92
29	4	306	CHL	CHB-C1B-NB	-3.86	120.17	124.26
29	6	316	CHL	CAC-C3C-C4C	3.85	129.81	124.81
30	2	316	XAT	C7-C8-C9	-3.85	119.55	125.53
29	2	305	CHL	C2D-C1D-ND	3.85	112.94	110.10
30	4	315	XAT	C24-C23-C22	-3.85	103.34	110.77
29	4	305	CHL	CAC-C3C-C4C	3.85	129.80	124.81
29	8	307	CHL	C1-C2-C3	-3.85	120.53	126.75
25	6	321	8CT	C14-C15-C16	-3.84	115.62	126.42
25	B	851	8CT	C04-C03-C02	-3.84	117.20	122.61
30	2	316	XAT	C18-C5-C4	3.84	118.60	114.28
29	8	306	CHL	C2D-C1D-ND	3.83	112.93	110.10
30	1	315	XAT	C5-C4-C3	-3.83	105.17	112.75
29	6	316	CHL	CHB-C1B-NB	-3.83	120.21	124.26
29	2	306	CHL	CHD-C4C-C3C	-3.82	119.22	124.84
25	A	850	8CT	C14-C15-C16	-3.82	115.68	126.42
30	0	314	XAT	O4-C5-C18	3.82	119.63	115.06
29	2	305	CHL	C1D-ND-C4D	-3.81	103.62	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	316	8CT	C30-C31-C32	-3.81	116.78	121.47
25	B	845	8CT	C19-C18-C17	-3.81	115.67	123.47
29	9	302	CHL	C1D-ND-C4D	-3.81	103.63	106.33
30	9	314	XAT	C6-C7-C8	3.80	134.03	125.99
25	3	316	8CT	C01-C02-C03	-3.80	120.26	124.53
29	4	301	CHL	C4-C3-C5	3.80	121.66	115.27
30	5	315	XAT	C31-C32-C33	-3.79	115.77	126.42
30	3	315	XAT	C24-C23-C22	-3.79	103.46	110.77
30	1	315	XAT	C18-C5-C4	3.79	118.54	114.28
29	4	306	CHL	C1-C2-C3	-3.78	120.63	126.75
30	4	316	XAT	C31-C30-C29	-3.78	121.91	127.31
22	A	807	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
22	B	850	CLA	CAA-C2A-C1A	-3.78	99.60	111.97
22	4	312	CLA	O2D-CGD-O1D	-3.78	116.46	123.84
25	A	846	8CT	C07-C02-C03	-3.77	117.25	122.73
22	9	312	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
29	3	306	CHL	C1D-ND-C4D	-3.77	103.66	106.33
30	4	315	XAT	C32-C33-C34	3.77	124.72	118.94
30	1	314	XAT	C31-C32-C33	-3.76	115.84	126.42
29	9	302	CHL	CAC-C3C-C4C	3.76	129.69	124.81
29	9	302	CHL	C3B-C4B-NB	3.76	114.00	110.52
25	B	851	8CT	C01-C02-C03	-3.75	120.31	124.53
30	3	315	XAT	C38-C25-C24	3.75	118.50	114.28
30	8	316	XAT	C38-C25-C24	3.75	118.50	114.28
30	4	315	XAT	C31-C30-C29	-3.75	121.96	127.31
25	I	101	8CT	C14-C13-C12	-3.74	121.97	127.31
29	7	308	CHL	C2D-C1D-ND	3.74	112.86	110.10
25	4	317	8CT	C01-C02-C07	3.74	120.81	113.62
25	L	206	8CT	C35-C30-C29	-3.74	107.97	112.70
25	3	318	8CT	C01-C02-C03	-3.74	120.33	124.53
25	7	321	8CT	C39-C16-C17	-3.74	117.69	122.92
29	4	306	CHL	CAC-C3C-C4C	3.73	129.65	124.81
30	5	316	XAT	C28-C29-C30	-3.73	113.22	118.94
22	8	309	CLA	C1-C2-C3	-3.73	119.59	126.04
25	A	849	8CT	C35-C30-C29	-3.73	107.99	112.70
25	8	318	8CT	C24-C25-C26	-3.73	121.99	127.31
25	7	301	8CT	C05-C04-C03	3.72	116.20	110.48
29	2	307	CHL	CAC-C3C-C4C	3.70	129.61	124.81
29	6	308	CHL	C3D-C4D-ND	3.70	116.22	110.24
29	8	307	CHL	C3B-C4B-NB	3.70	113.94	110.52
25	A	849	8CT	C30-C31-C32	-3.70	116.92	121.47
25	5	317	8CT	C14-C15-C16	-3.69	116.05	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	9	314	XAT	C40-C33-C32	3.69	123.89	118.08
29	0	301	CHL	CHC-C4B-NB	-3.69	120.35	124.26
29	6	307	CHL	CAC-C3C-C4C	3.69	129.59	124.81
25	7	321	8CT	C01-C02-C07	3.69	120.70	113.62
25	B	851	8CT	C07-C02-C03	-3.68	117.39	122.73
29	6	302	CHL	C2D-C1D-ND	3.68	112.82	110.10
25	L	205	8CT	C18-C19-C20	3.68	131.01	123.47
25	3	318	8CT	C35-C30-C29	-3.68	108.05	112.70
29	4	301	CHL	C3B-C4B-NB	3.68	113.93	110.52
25	5	317	8CT	C27-C26-C25	-3.68	117.77	122.92
25	B	851	8CT	C27-C26-C25	-3.67	117.78	122.92
25	5	317	8CT	C28-C26-C25	3.67	124.58	118.94
25	8	301	8CT	C18-C17-C16	-3.66	122.08	127.31
29	0	301	CHL	C4A-NA-C1A	3.66	108.35	106.71
30	0	314	XAT	C20-C13-C12	3.66	123.84	118.08
29	9	307	CHL	CHB-C1B-NB	-3.66	120.38	124.26
29	0	306	CHL	C3C-C4C-NC	3.65	114.67	110.57
25	B	845	8CT	C05-C04-C03	3.64	116.09	110.48
29	9	307	CHL	CHD-C4C-C3C	-3.64	119.49	124.84
29	2	306	CHL	CAC-C3C-C4C	3.64	129.53	124.81
22	2	302	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
23	A	842	PQN	C11-C12-C13	-3.63	120.75	126.79
22	B	807	CLA	CHB-C4A-NA	3.63	129.53	124.51
22	A	827	CLA	C3B-C4B-NB	-3.63	107.15	110.52
29	5	301	CHL	C2D-C1D-ND	3.63	112.78	110.10
22	A	813	CLA	C3B-C4B-NB	-3.62	107.15	110.52
30	5	315	XAT	C11-C12-C13	-3.62	116.24	126.42
30	1	315	XAT	C28-C29-C30	-3.62	113.39	118.94
22	B	832	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
30	5	315	XAT	C39-C29-C30	-3.62	117.86	122.92
25	4	317	8CT	C30-C31-C32	-3.61	117.03	121.47
29	6	316	CHL	CHD-C4C-C3C	-3.61	119.53	124.84
25	F	302	8CT	C01-C02-C03	-3.61	120.48	124.53
22	3	308	CLA	C3B-C4B-NB	-3.60	107.17	110.52
25	L	206	8CT	C14-C15-C16	-3.60	116.29	126.42
29	6	306	CHL	C2D-C1D-ND	3.60	112.76	110.10
22	A	821	CLA	C1-C2-C3	-3.59	119.83	126.04
22	B	809	CLA	C3B-C4B-NB	-3.59	107.18	110.52
30	2	316	XAT	C5-C4-C3	-3.59	105.65	112.75
25	I	101	8CT	C07-C02-C03	-3.59	117.52	122.73
29	6	316	CHL	C2D-C1D-ND	3.59	112.75	110.10
29	2	307	CHL	C3D-C4D-ND	3.58	116.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	847	8CT	C07-C02-C03	-3.58	117.53	122.73
29	9	302	CHL	C3D-C4D-ND	3.58	116.03	110.24
30	5	315	XAT	O24-C25-C26	-3.58	56.00	58.96
22	7	314	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
29	6	306	CHL	C3B-C4B-NB	3.57	113.83	110.52
25	3	318	8CT	C15-C16-C17	3.57	124.42	118.94
30	8	317	XAT	C10-C11-C12	-3.57	112.07	123.22
30	4	316	XAT	C35-C15-C14	-3.57	116.16	123.47
30	0	313	XAT	O24-C25-C26	-3.57	56.01	58.96
22	2	319	CLA	C3B-C4B-NB	-3.57	107.21	110.52
25	B	851	8CT	C28-C26-C25	3.57	124.41	118.94
25	B	845	8CT	C07-C02-C03	-3.56	117.56	122.73
30	5	315	XAT	C32-C33-C34	3.56	124.41	118.94
29	9	307	CHL	C3D-C4D-ND	3.56	116.00	110.24
29	1	305	CHL	CAC-C3C-C4C	3.56	129.43	124.81
25	B	844	8CT	C22-C21-C20	-3.56	117.93	122.92
25	7	321	8CT	C01-C02-C03	-3.56	120.53	124.53
22	6	318	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
30	2	316	XAT	C4-C3-C2	-3.55	103.91	110.77
25	1	316	8CT	C01-C02-C07	3.55	120.44	113.62
22	3	309	CLA	CAA-C2A-C3A	-3.55	107.81	116.10
22	5	308	CLA	CHB-C4A-NA	3.55	129.42	124.51
29	8	306	CHL	C3D-C4D-ND	3.54	115.97	110.24
24	A	845	LHG	O8-C23-C24	3.54	120.67	111.38
29	7	308	CHL	C3D-C4D-ND	3.54	115.96	110.24
30	1	314	XAT	C11-C12-C13	3.54	136.36	126.42
25	B	845	8CT	C22-C21-C20	-3.54	117.97	122.92
29	0	301	CHL	CAC-C3C-C4C	3.54	129.40	124.81
30	4	315	XAT	C20-C13-C12	3.53	123.64	118.08
22	2	302	CLA	C3B-C4B-NB	-3.53	107.24	110.52
29	5	301	CHL	C1-C2-C3	-3.53	119.94	126.04
30	4	315	XAT	C4-C3-C2	-3.53	103.96	110.77
25	6	321	8CT	C19-C20-C21	-3.53	122.28	127.31
25	4	317	8CT	C01-C02-C03	-3.52	120.58	124.53
29	4	301	CHL	C1D-ND-C4D	-3.51	103.84	106.33
22	F	301	CLA	C3B-C4B-NB	-3.51	107.26	110.52
22	2	312	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
29	5	301	CHL	CAC-C3C-C4C	3.51	129.36	124.81
29	2	301	CHL	CHB-C4A-NA	3.51	129.37	124.51
25	B	844	8CT	C07-C02-C03	-3.51	117.64	122.73
22	9	301	CLA	C3B-C4B-NB	-3.51	107.88	110.23
22	A	806	CLA	C3B-C4B-NB	-3.51	107.26	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	9	302	CHL	CHB-C1B-NB	-3.51	120.55	124.26
30	4	316	XAT	C38-C25-C26	-3.51	116.39	122.26
25	B	845	8CT	C39-C16-C17	-3.50	118.02	122.92
25	8	301	8CT	C04-C03-C02	-3.50	117.69	122.61
22	B	812	CLA	C3B-C4B-NB	-3.50	107.27	110.52
29	4	307	CHL	C3B-C4B-NB	3.49	113.76	110.52
25	3	316	8CT	C01-C02-C07	3.49	120.33	113.62
25	B	845	8CT	C22-C21-C23	3.49	123.58	118.08
29	2	306	CHL	CHB-C1B-NB	-3.49	120.56	124.26
29	8	314	CHL	CAC-C3C-C4C	3.49	129.34	124.81
30	1	314	XAT	C8-C9-C10	3.49	124.30	118.94
25	7	301	8CT	C14-C15-C16	-3.48	116.64	126.42
25	J	101	8CT	C01-C02-C07	3.48	120.30	113.62
25	3	316	8CT	C35-C30-C29	-3.48	108.30	112.70
22	L	202	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
30	9	314	XAT	O4-C5-C18	3.48	119.22	115.06
22	A	819	CLA	O2D-CGD-O1D	-3.47	117.04	123.84
30	1	315	XAT	C38-C25-C24	3.47	118.19	114.28
29	5	301	CHL	C4-C3-C5	3.47	121.11	115.27
22	B	825	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
29	6	308	CHL	C3B-C4B-NB	3.47	113.73	110.52
29	8	306	CHL	C3B-C4B-NB	3.46	113.73	110.52
25	A	848	8CT	C11-C10-C03	-3.46	117.48	127.20
25	A	850	8CT	C19-C18-C17	-3.46	116.38	123.47
25	I	101	8CT	C18-C19-C20	-3.46	116.39	123.47
31	8	319	LMG	O6-C1-O1	-3.46	101.78	109.97
30	2	316	XAT	C30-C31-C32	-3.46	112.42	123.22
29	5	306	CHL	CAC-C3C-C4C	3.46	129.30	124.81
29	8	305	CHL	C1D-ND-C4D	-3.46	103.88	106.33
29	5	301	CHL	C3D-C4D-ND	3.46	115.83	110.24
25	L	205	8CT	C01-C02-C07	3.45	120.25	113.62
30	6	319	XAT	C4-C3-C2	-3.45	104.12	110.77
29	0	306	CHL	CMB-C2B-C1B	3.44	130.62	125.37
22	9	303	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
29	8	307	CHL	CAC-C3C-C4C	3.44	129.28	124.81
29	8	306	CHL	C1D-ND-C4D	-3.44	103.89	106.33
22	A	822	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
25	A	854	8CT	C01-C02-C07	3.43	120.21	113.62
29	0	301	CHL	C1-C2-C3	-3.43	120.11	126.04
29	2	301	CHL	C1-C2-C3	-3.43	120.11	126.04
29	8	307	CHL	C2D-C1D-ND	3.43	112.63	110.10
29	4	305	CHL	CHD-C4C-C3C	-3.43	119.80	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	305	CHL	C3D-C4D-ND	3.43	115.78	110.24
29	1	305	CHL	CHD-C4C-C3C	-3.43	119.80	124.84
29	8	307	CHL	C3D-C4D-ND	3.42	115.78	110.24
22	3	301	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
30	2	315	XAT	C36-C21-C26	3.42	119.28	110.05
22	8	308	CLA	CBC-CAC-C3C	-3.42	103.00	112.43
25	5	317	8CT	C22-C21-C20	-3.42	118.13	122.92
22	7	310	CLA	C1-C2-C3	-3.42	121.22	126.75
25	B	846	8CT	C39-C16-C17	-3.42	118.14	122.92
25	8	301	8CT	C19-C20-C21	-3.42	122.43	127.31
22	9	305	CLA	O2D-CGD-CBD	3.42	117.34	111.27
30	5	316	XAT	C30-C31-C32	-3.41	112.56	123.22
25	A	847	8CT	C04-C03-C02	-3.41	117.80	122.61
22	1	312	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
30	7	320	XAT	C15-C14-C13	-3.41	122.44	127.31
30	8	316	XAT	C8-C9-C10	3.41	124.18	118.94
30	2	315	XAT	O4-C5-C6	-3.41	56.14	58.96
30	3	314	XAT	C16-C1-C6	3.41	119.25	110.05
29	4	307	CHL	C3D-C4D-ND	3.40	115.75	110.24
29	2	301	CHL	C3D-C4D-ND	3.40	115.74	110.24
22	1	301	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
25	8	318	8CT	C01-C02-C07	3.40	120.15	113.62
30	1	314	XAT	C26-C27-C28	-3.40	118.80	125.99
22	9	305	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
24	3	317	LHG	O8-C23-C24	3.40	120.29	111.38
25	7	323	8CT	C10-C11-C12	-3.40	121.10	126.23
25	G	104	8CT	C35-C30-C29	-3.40	108.41	112.70
25	4	317	8CT	C27-C26-C25	-3.39	118.17	122.92
30	1	315	XAT	C10-C11-C12	-3.39	112.62	123.22
29	4	305	CHL	OMC-CMC-C2C	-3.39	118.01	125.69
25	A	846	8CT	C01-C02-C07	3.39	120.13	113.62
22	4	313	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
29	7	308	CHL	CMD-C2D-C3D	-3.39	119.83	127.61
29	8	314	CHL	CHD-C4C-C3C	-3.38	119.88	124.84
29	6	306	CHL	C3D-C4D-ND	3.37	115.70	110.24
25	A	849	8CT	C01-C02-C07	3.37	120.09	113.62
30	1	314	XAT	C40-C33-C34	-3.37	118.20	122.92
22	B	815	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
22	A	840	CLA	C3B-C4B-NB	-3.37	107.39	110.52
25	F	302	8CT	C11-C10-C03	-3.37	117.75	127.20
25	B	845	8CT	C01-C02-C07	3.36	120.08	113.62
30	2	316	XAT	C11-C10-C9	-3.36	122.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	317	8CT	C39-C16-C17	-3.36	118.21	122.92
29	8	306	CHL	C1-C2-C3	-3.36	121.31	126.75
25	1	316	8CT	C01-C02-C03	-3.36	120.75	124.53
22	4	302	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
22	A	830	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
25	7	321	8CT	C22-C21-C20	-3.36	118.22	122.92
25	A	850	8CT	C01-C02-C07	3.36	120.06	113.62
22	1	301	CLA	C3B-C4B-NB	-3.36	107.40	110.52
29	8	305	CHL	C3D-C4D-ND	3.35	115.66	110.24
22	3	311	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
29	9	307	CHL	CAC-C3C-C4C	3.35	129.15	124.81
22	B	830	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
30	8	316	XAT	C19-C9-C10	-3.34	118.24	122.92
25	1	316	8CT	C30-C31-C32	-3.34	117.36	121.47
22	B	831	CLA	CMB-C2B-C1B	-3.34	120.28	125.37
29	6	306	CHL	C1D-ND-C4D	-3.34	103.96	106.33
25	4	317	8CT	C07-C02-C03	-3.33	117.89	122.73
30	0	314	XAT	C38-C25-C24	3.33	118.03	114.28
30	0	313	XAT	C38-C25-C24	-3.33	110.53	114.28
25	A	848	8CT	C01-C02-C07	3.33	120.01	113.62
22	6	303	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
25	7	323	8CT	C24-C25-C26	-3.32	122.57	127.31
30	3	314	XAT	C27-C28-C29	-3.32	120.37	125.53
29	5	301	CHL	CHB-C1B-NB	-3.32	120.74	124.26
22	A	834	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
22	A	812	CLA	C3B-C4B-NB	-3.32	107.44	110.52
25	B	847	8CT	C04-C03-C02	-3.32	117.94	122.61
25	B	843	8CT	C07-C02-C03	-3.32	117.92	122.73
29	2	301	CHL	CMD-C2D-C3D	-3.32	119.99	127.61
22	1	313	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
30	3	314	XAT	O24-C25-C38	3.31	119.02	115.06
30	7	320	XAT	C4-C3-C2	-3.31	104.39	110.77
22	B	826	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
25	5	317	8CT	C01-C02-C07	3.30	119.96	113.62
22	3	302	CLA	C3B-C4B-NB	-3.30	107.45	110.52
22	2	313	CLA	C3B-C4B-NB	-3.30	107.46	110.52
22	3	303	CLA	C3B-C4B-NB	-3.30	107.46	110.52
29	6	308	CHL	CHB-C1B-NB	-3.29	120.77	124.26
22	7	313	CLA	C1-C2-C3	-3.29	120.35	126.04
30	6	319	XAT	C20-C13-C12	3.29	123.26	118.08
25	8	301	8CT	C01-C02-C07	3.29	119.94	113.62
25	B	804	8CT	C18-C19-C20	-3.29	116.74	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	843	8CT	C01-C02-C07	3.29	119.93	113.62
22	A	808	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
29	3	306	CHL	CAC-C3C-C4C	3.28	129.07	124.81
22	8	308	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
29	5	301	CHL	C1D-ND-C4D	-3.28	104.00	106.33
22	B	820	CLA	C3B-C4B-NB	-3.28	107.47	110.52
30	1	314	XAT	C39-C29-C30	-3.28	118.33	122.92
30	6	319	XAT	C18-C5-C4	3.28	117.97	114.28
29	8	314	CHL	C2D-C1D-ND	3.27	112.52	110.10
22	5	305	CLA	C3B-C4B-NB	-3.27	107.48	110.52
29	6	302	CHL	CMB-C2B-C1B	3.27	130.35	125.37
22	A	836	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
22	K	102	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
25	K	103	8CT	C30-C31-C32	-3.27	117.45	121.47
29	2	307	CHL	OMC-CMC-C2C	-3.27	118.30	125.69
22	3	313	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
29	4	307	CHL	CAA-CBA-CGA	-3.26	103.72	113.25
24	7	322	LHG	O8-C23-C24	3.26	119.94	111.38
30	9	314	XAT	C10-C11-C12	-3.26	113.03	123.22
31	5	319	LMG	O6-C1-O1	-3.26	102.25	109.97
22	3	312	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
22	A	811	CLA	C3B-C4B-NB	-3.26	107.49	110.52
22	B	826	CLA	CAA-CBA-CGA	-3.26	103.73	113.25
30	0	313	XAT	C11-C10-C9	-3.26	122.66	127.31
25	B	847	8CT	C01-C02-C07	3.26	119.88	113.62
29	9	307	CHL	C3B-C4B-NB	3.26	113.54	110.52
25	6	321	8CT	C39-C16-C17	-3.26	118.36	122.92
22	B	836	CLA	C3B-C4B-NB	-3.25	107.50	110.52
25	7	301	8CT	C14-C13-C12	-3.25	122.67	127.31
22	B	827	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
29	6	316	CHL	C3D-C4D-ND	3.25	115.49	110.24
30	0	313	XAT	C40-C33-C32	3.25	123.19	118.08
22	A	835	CLA	CMB-C2B-C1B	-3.24	120.43	125.37
30	8	317	XAT	C4-C3-C2	-3.24	104.53	110.77
22	2	310	CLA	C3B-C4B-NB	-3.23	107.52	110.52
25	B	804	8CT	C07-C02-C03	-3.23	118.04	122.73
29	2	305	CHL	O2D-CGD-CBD	3.23	117.01	111.27
22	7	310	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
22	B	824	CLA	C3B-C4B-NB	-3.23	107.52	110.52
22	B	814	CLA	C3B-C4B-NB	-3.23	107.52	110.52
22	A	828	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
22	B	831	CLA	CHB-C1B-NB	3.23	127.67	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	302	CHL	O2A-CGA-CBA	3.23	122.03	111.91
25	B	847	8CT	C24-C23-C21	-3.22	117.36	126.42
25	B	848	8CT	C14-C13-C12	-3.22	122.71	127.31
30	0	313	XAT	C40-C33-C34	-3.22	118.41	122.92
29	6	302	CHL	C3D-C4D-ND	3.22	115.45	110.24
22	B	801	CLA	C3B-C4B-NB	-3.22	107.53	110.52
25	A	846	8CT	C10-C11-C12	-3.22	121.37	126.23
29	2	306	CHL	C3D-C4D-ND	3.22	115.44	110.24
30	5	315	XAT	C28-C29-C30	3.22	123.88	118.94
22	6	304	CLA	C3B-C4B-NB	-3.22	107.53	110.52
25	B	846	8CT	C27-C26-C25	-3.22	118.42	122.92
22	B	807	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
22	3	302	CLA	CHB-C1B-NB	3.21	127.66	124.26
22	A	831	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
29	6	307	CHL	CMB-C2B-C1B	3.21	130.26	125.37
29	6	302	CHL	CAC-C3C-C4C	3.21	128.97	124.81
30	2	315	XAT	C10-C11-C12	-3.21	113.20	123.22
22	2	319	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
30	6	319	XAT	C38-C25-C24	3.21	117.89	114.28
22	7	304	CLA	C3B-C4B-NB	-3.21	107.54	110.52
30	9	314	XAT	C8-C9-C10	-3.20	114.03	118.94
25	B	848	8CT	C01-C02-C07	3.20	119.77	113.62
25	L	206	8CT	C24-C23-C21	-3.20	117.43	126.42
30	9	315	XAT	C4-C3-C2	-3.20	104.59	110.77
30	6	320	XAT	C35-C34-C33	-3.20	122.74	127.31
25	L	206	8CT	C07-C02-C03	-3.20	118.08	122.73
30	8	316	XAT	C37-C21-C36	3.20	112.08	107.37
22	B	805	CLA	C3B-C4B-NB	-3.19	107.55	110.52
30	5	316	XAT	C38-C25-C24	3.19	117.87	114.28
22	1	303	CLA	C3B-C4B-NB	-3.19	107.55	110.52
22	2	308	CLA	C3B-C4B-NB	-3.19	107.55	110.52
30	1	315	XAT	C35-C15-C14	-3.19	116.93	123.47
22	A	803	CLA	C3B-C4B-NB	-3.19	107.55	110.52
30	7	319	XAT	O24-C25-C38	3.19	118.88	115.06
29	4	306	CHL	O2D-CGD-O1D	-3.19	117.60	123.84
22	A	818	CLA	C3B-C4B-NB	-3.19	107.56	110.52
22	7	303	CLA	C3B-C4B-NB	-3.19	107.56	110.52
22	8	309	CLA	C3B-C4B-NB	-3.19	107.56	110.52
30	9	314	XAT	C36-C21-C26	3.19	118.65	110.05
25	8	318	8CT	C35-C30-C29	-3.19	108.67	112.70
25	7	323	8CT	C11-C10-C03	-3.18	118.26	127.20
22	B	816	CLA	C3B-C4B-NB	-3.18	107.56	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	831	CLA	C1-C2-C3	-3.18	121.60	126.75
30	1	315	XAT	C4-C3-C2	-3.18	104.63	110.77
22	B	824	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
22	A	808	CLA	C3B-C4B-NB	-3.18	107.57	110.52
29	4	301	CHL	C3D-C4D-ND	3.18	115.38	110.24
29	8	314	CHL	C3D-C4D-ND	3.17	115.37	110.24
30	0	314	XAT	C6-C7-C8	-3.17	119.29	125.99
29	6	316	CHL	C3B-C4B-NB	3.17	113.46	110.52
22	7	312	CLA	C3B-C4B-NB	-3.17	107.58	110.52
25	3	318	8CT	C27-C26-C25	-3.16	118.49	122.92
29	8	307	CHL	C1D-ND-C4D	-3.16	104.09	106.33
22	6	317	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	B	801	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	0	304	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
30	2	315	XAT	C6-C7-C8	-3.16	119.31	125.99
29	4	307	CHL	O2A-CGA-CBA	3.16	121.81	111.91
29	5	301	CHL	CHC-C4B-NB	-3.16	120.92	124.26
30	5	316	XAT	C18-C5-C4	3.16	117.83	114.28
25	A	848	8CT	C14-C13-C12	-3.16	122.81	127.31
22	9	304	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
22	B	808	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	B	851	8CT	C01-C02-C07	3.15	119.67	113.62
22	A	830	CLA	CMB-C2B-C1B	-3.15	120.57	125.37
30	5	316	XAT	C4-C3-C2	-3.15	104.69	110.77
25	K	103	8CT	C01-C02-C07	3.15	119.67	113.62
28	B	849	DGD	O3G-C1D-C2D	-3.15	103.39	108.30
22	A	804	CLA	CHB-C4A-NA	3.15	128.87	124.51
22	A	852	CLA	C3B-C4B-NB	-3.14	107.60	110.52
30	6	319	XAT	C7-C8-C9	-3.14	120.66	125.53
30	5	315	XAT	C35-C15-C14	-3.14	117.05	123.47
29	8	314	CHL	C4A-NA-C1A	3.13	108.11	106.71
22	B	833	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
25	J	104	8CT	C40-C12-C13	-3.13	118.53	122.92
22	5	309	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
29	8	306	CHL	C2A-C3A-C4A	-3.13	96.81	101.87
30	6	319	XAT	C24-C23-C22	-3.13	104.72	110.77
22	A	819	CLA	CMB-C2B-C1B	-3.13	120.60	125.37
25	L	205	8CT	C15-C16-C17	3.13	123.74	118.94
29	8	306	CHL	CHB-C1B-NB	-3.13	120.94	124.26
22	A	840	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
29	2	306	CHL	C2D-C1D-ND	3.13	112.41	110.10
25	7	323	8CT	C18-C19-C20	-3.13	117.07	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	825	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
29	2	307	CHL	CHB-C1B-NB	-3.12	120.95	124.26
22	A	804	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
25	A	850	8CT	C35-C30-C29	-3.12	108.75	112.70
30	2	315	XAT	C15-C35-C34	-3.12	117.08	123.47
29	3	306	CHL	C3B-C4B-NB	3.12	113.41	110.52
25	G	104	8CT	C01-C02-C07	3.12	119.61	113.62
29	4	301	CHL	CAC-C3C-C4C	3.12	128.86	124.81
30	4	315	XAT	C8-C9-C10	3.12	123.72	118.94
22	5	307	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	6	313	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	4	311	CLA	C3B-C4B-NB	-3.11	107.63	110.52
22	3	305	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	1	304	CLA	C3B-C4B-NB	-3.11	107.63	110.52
22	B	827	CLA	C3B-C4B-NB	-3.11	107.63	110.52
31	4	318	LMG	C1-O6-C5	-3.10	107.60	113.69
22	A	827	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
30	1	314	XAT	C18-C5-C4	3.10	117.77	114.28
29	4	301	CHL	O2D-CGD-O1D	-3.10	117.78	123.84
29	6	308	CHL	O2A-CGA-CBA	3.10	121.63	111.91
22	B	821	CLA	C3B-C4B-NB	-3.10	107.64	110.52
29	1	305	CHL	C3B-C4B-NB	3.10	113.39	110.52
22	B	834	CLA	C3B-C4B-NB	-3.09	107.64	110.52
22	3	305	CLA	C3B-C4B-NB	-3.09	107.64	110.52
22	K	105	CLA	CHB-C4A-NA	3.09	128.79	124.51
22	A	841	CLA	C2D-C1D-ND	-3.09	107.83	110.10
29	9	307	CHL	C2D-C1D-ND	3.09	112.38	110.10
25	B	846	8CT	C01-C02-C07	3.09	119.55	113.62
22	4	310	CLA	C3B-C4B-NB	-3.09	107.65	110.52
22	6	323	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
29	0	306	CHL	C3D-C4D-ND	3.09	115.23	110.24
22	2	309	CLA	O2A-CGA-O1A	-3.09	115.80	123.59
30	3	315	XAT	C4-C3-C2	-3.09	104.81	110.77
29	5	306	CHL	CHD-C4C-C3C	-3.09	120.30	124.84
30	0	313	XAT	C35-C15-C14	3.09	129.80	123.47
22	B	841	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
29	7	308	CHL	C2A-C1A-CHA	-3.08	118.47	123.86
22	A	819	CLA	C3B-C4B-NB	-3.08	107.66	110.52
29	2	305	CHL	CAC-C3C-C4C	3.08	128.81	124.81
30	7	319	XAT	C39-C29-C30	-3.08	118.61	122.92
29	2	305	CHL	CMD-C2D-C3D	-3.08	120.53	127.61
22	A	815	CLA	C3B-C4B-NB	-3.08	107.66	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	0	303	CLA	C3B-C4B-NB	-3.08	107.66	110.52
22	A	814	CLA	C3B-C4B-NB	-3.07	107.66	110.52
22	A	824	CLA	C3B-C4B-NB	-3.07	107.66	110.52
29	6	308	CHL	CMB-C2B-C1B	3.07	130.05	125.37
22	B	831	CLA	C3B-C4B-NB	-3.07	107.67	110.52
30	8	316	XAT	C4-C3-C2	-3.07	104.84	110.77
30	3	315	XAT	O4-C5-C4	3.07	115.69	113.38
30	4	315	XAT	C26-C27-C28	-3.07	119.50	125.99
29	6	307	CHL	CHD-C4C-C3C	-3.07	120.33	124.84
22	B	811	CLA	C3B-C4B-NB	-3.06	107.67	110.52
22	5	304	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
22	A	834	CLA	CHB-C1B-NB	3.06	127.50	124.26
22	B	818	CLA	CHB-C4A-NA	3.06	128.75	124.51
30	3	314	XAT	C40-C33-C32	3.06	122.90	118.08
30	0	313	XAT	C19-C9-C10	-3.06	118.64	122.92
22	4	304	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
22	0	310	CLA	C3B-C4B-NB	-3.06	107.68	110.52
25	B	851	8CT	C22-C21-C20	-3.06	118.64	122.92
30	4	316	XAT	O24-C25-C38	3.06	118.72	115.06
25	7	321	8CT	C23-C21-C20	3.06	123.63	118.94
22	B	807	CLA	C3B-C4B-NB	-3.06	107.68	110.52
25	B	851	8CT	C05-C04-C03	3.05	115.18	110.48
22	6	318	CLA	C3B-C4B-NB	-3.05	107.68	110.52
29	8	314	CHL	C3B-C4B-NB	3.05	113.35	110.52
22	3	319	CLA	C3B-C4B-NB	-3.05	107.69	110.52
25	A	849	8CT	C14-C13-C12	-3.05	122.96	127.31
25	5	317	8CT	C23-C21-C20	3.05	123.62	118.94
25	3	316	8CT	C40-C12-C13	-3.05	118.65	122.92
22	B	830	CLA	CMB-C2B-C1B	-3.05	120.73	125.37
29	6	307	CHL	C3D-C4D-ND	3.05	115.17	110.24
25	J	104	8CT	C01-C02-C07	3.05	119.47	113.62
25	F	302	8CT	C14-C15-C16	-3.04	117.86	126.42
22	A	829	CLA	C3B-C4B-NB	-3.04	107.69	110.52
22	A	835	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	6	305	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	A	850	8CT	C24-C23-C21	-3.04	117.87	126.42
22	7	312	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	0	311	CLA	C1-C2-C3	-3.04	120.79	126.04
25	F	302	8CT	C40-C12-C13	-3.04	118.67	122.92
29	8	305	CHL	CAC-C3C-C4C	3.04	128.75	124.81
22	6	311	CLA	CHB-C4A-NA	3.04	128.71	124.51
22	L	204	CLA	O2D-CGD-O1D	-3.03	117.91	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	815	CLA	C1-C2-C3	-3.03	120.80	126.04
22	L	204	CLA	C3B-C4B-NB	-3.03	107.70	110.52
25	B	848	8CT	C27-C26-C25	-3.03	118.67	122.92
29	1	305	CHL	C3D-C4D-ND	3.03	115.14	110.24
22	B	806	CLA	CHB-C4A-NA	3.03	128.70	124.51
29	2	307	CHL	CMB-C2B-C1B	3.02	129.97	125.37
22	B	813	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
29	2	306	CHL	CMB-C2B-C1B	3.02	129.97	125.37
25	K	103	8CT	C24-C25-C26	-3.02	123.00	127.31
29	8	305	CHL	OMC-CMC-C2C	-3.02	118.85	125.69
22	0	310	CLA	CHB-C4A-NA	3.02	128.69	124.51
22	A	826	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	3	307	CLA	C3B-C4B-NB	-3.02	107.71	110.52
25	J	104	8CT	C35-C30-C29	-3.02	108.88	112.70
25	4	317	8CT	C28-C26-C25	3.02	123.57	118.94
25	6	321	8CT	C01-C02-C07	3.02	119.41	113.62
22	A	836	CLA	C3B-C4B-NB	-3.02	107.72	110.52
22	A	838	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
23	A	842	PQN	C14-C13-C15	3.02	120.34	115.27
29	2	305	CHL	C3B-C4B-NB	3.02	113.31	110.52
22	7	318	CLA	CHB-C4A-NA	3.01	128.68	124.51
29	4	301	CHL	CHB-C1B-NB	-3.01	121.07	124.26
30	7	319	XAT	C19-C9-C10	-3.01	118.70	122.92
22	A	809	CLA	CAA-CBA-CGA	-3.01	104.46	113.25
22	A	821	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	7	306	CLA	CMB-C2B-C1B	-3.01	120.79	125.37
22	6	310	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	L	201	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	B	806	CLA	C3B-C4B-NB	-3.01	107.72	110.52
25	1	316	8CT	C35-C30-C29	-3.01	108.90	112.70
22	7	318	CLA	C2A-C1A-CHA	3.00	129.11	123.86
25	B	845	8CT	C11-C10-C03	-3.00	118.76	127.20
30	1	315	XAT	C30-C31-C32	-3.00	113.84	123.22
25	B	847	8CT	C35-C30-C29	-3.00	108.91	112.70
22	8	311	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
30	5	316	XAT	C39-C29-C28	3.00	122.81	118.08
31	4	318	LMG	O1-C7-C8	-3.00	103.66	110.90
25	2	317	8CT	C01-C02-C07	3.00	119.38	113.62
22	B	828	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
29	7	308	CHL	CHB-C4A-NA	3.00	128.66	124.51
28	B	849	DGD	O6D-C1D-O3G	-2.99	102.89	109.97
22	5	313	CLA	O2D-CGD-O1D	-2.99	117.99	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	319	XAT	C18-C5-C4	2.99	117.65	114.28
22	3	310	CLA	C3B-C4B-NB	-2.99	107.74	110.52
22	B	808	CLA	C3B-C4B-NB	-2.99	107.74	110.52
22	5	302	CLA	C3B-C4B-NB	-2.99	107.74	110.52
22	A	839	CLA	C3B-C4B-NB	-2.98	107.75	110.52
29	4	305	CHL	C2D-C1D-ND	2.98	112.30	110.10
22	0	312	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	A	849	8CT	C14-C15-C16	-2.98	118.04	126.42
22	G	102	CLA	C3B-C4B-NB	-2.98	107.75	110.52
30	2	316	XAT	C15-C14-C13	-2.98	123.06	127.31
25	B	804	8CT	C14-C15-C16	-2.98	118.05	126.42
22	L	202	CLA	CHB-C4A-NA	2.98	128.63	124.51
29	0	306	CHL	CHC-C4B-NB	-2.98	121.11	124.26
29	4	305	CHL	C4-C3-C5	2.97	120.27	115.27
29	6	307	CHL	CHC-C4B-NB	-2.97	121.11	124.26
30	6	320	XAT	C30-C31-C32	-2.97	113.94	123.22
29	4	307	CHL	OMC-CMC-C2C	-2.97	118.97	125.69
22	0	302	CLA	C3B-C4B-NB	-2.97	107.76	110.52
22	B	828	CLA	CMB-C2B-C1B	-2.97	120.84	125.37
22	B	834	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
30	0	314	XAT	C31-C32-C33	-2.97	118.07	126.42
22	7	306	CLA	C3B-C4B-NB	-2.97	107.76	110.52
22	0	303	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	G	101	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
29	4	305	CHL	C3B-C4B-NB	2.97	113.27	110.52
22	A	832	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	B	823	CLA	C1-C2-C3	-2.96	120.92	126.04
22	K	104	CLA	C3B-C4B-NB	-2.96	107.77	110.52
22	K	101	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	A	817	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	G	102	CLA	CHB-C4A-NA	2.96	128.60	124.51
22	B	801	CLA	C1-C2-C3	-2.96	120.92	126.04
29	4	305	CHL	C3D-C4D-ND	2.96	115.02	110.24
30	9	315	XAT	C10-C11-C12	-2.96	113.99	123.22
30	4	315	XAT	C31-C32-C33	-2.95	118.12	126.42
22	F	301	CLA	CHB-C1B-NB	2.95	127.38	124.26
22	B	822	CLA	C3B-C4B-NB	-2.95	107.78	110.52
22	5	310	CLA	C3B-C4B-NB	-2.95	107.78	110.52
25	7	301	8CT	C24-C23-C21	-2.95	118.13	126.42
22	A	853	CLA	C3B-C4B-NB	-2.95	107.78	110.52
22	7	305	CLA	C3B-C4B-NB	-2.95	107.78	110.52
25	A	846	8CT	C18-C19-C20	2.95	129.52	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	206	8CT	C27-C26-C25	-2.95	118.79	122.92
29	9	307	CHL	C1D-ND-C4D	-2.95	104.24	106.33
22	5	309	CLA	C3B-C4B-NB	-2.95	107.78	110.52
22	J	103	CLA	CHB-C4A-NA	2.95	128.59	124.51
30	7	320	XAT	C10-C11-C12	-2.95	114.02	123.22
30	2	315	XAT	C30-C31-C32	-2.95	114.03	123.22
22	A	813	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	2	317	8CT	C14-C15-C16	-2.94	118.14	126.42
25	7	301	8CT	C35-C30-C29	-2.94	108.98	112.70
29	4	306	CHL	C3D-C4D-ND	2.94	115.00	110.24
25	7	301	8CT	C27-C26-C25	-2.94	118.80	122.92
22	6	303	CLA	C3B-C4B-NB	-2.94	107.79	110.52
29	5	306	CHL	CMB-C2B-C1B	2.94	129.84	125.37
22	B	813	CLA	C3B-C4B-NB	-2.94	107.79	110.52
22	6	318	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	7	323	8CT	C01-C02-C07	2.94	119.26	113.62
22	A	830	CLA	CHB-C1B-NB	2.93	127.36	124.26
22	A	835	CLA	CHB-C1B-NB	2.93	127.36	124.26
22	4	302	CLA	C3B-C4B-NB	-2.93	107.79	110.52
25	F	302	8CT	C24-C23-C21	-2.93	118.18	126.42
22	A	804	CLA	C3B-C4B-NB	-2.93	107.80	110.52
22	2	314	CLA	C3B-C4B-NB	-2.93	107.80	110.52
25	B	845	8CT	C35-C30-C29	-2.93	109.00	112.70
25	3	318	8CT	C19-C18-C17	2.93	129.47	123.47
22	2	310	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
30	8	316	XAT	C26-C27-C28	-2.92	119.81	125.99
25	A	850	8CT	C18-C17-C16	-2.92	123.14	127.31
29	3	306	CHL	C3D-C4D-ND	2.92	114.96	110.24
29	2	305	CHL	CMB-C2B-C1B	2.92	129.82	125.37
29	8	314	CHL	CHC-C4B-NB	-2.92	121.17	124.26
22	A	801	CLA	C3B-C4B-NB	-2.92	107.81	110.52
22	B	803	CLA	C3B-C4B-NB	-2.92	107.81	110.52
29	5	306	CHL	C3B-C4B-NB	2.92	113.22	110.52
29	2	307	CHL	C2A-C1A-CHA	-2.92	118.75	123.86
22	6	311	CLA	C3B-C4B-NB	-2.92	107.81	110.52
22	8	302	CLA	C3B-C4B-NB	-2.92	107.81	110.52
25	B	804	8CT	C04-C03-C02	-2.92	118.51	122.61
22	8	308	CLA	C3B-C4B-NB	-2.91	107.81	110.52
25	B	843	8CT	C22-C21-C23	2.91	122.67	118.08
22	5	314	CLA	C3B-C4B-NB	-2.91	107.81	110.52
22	B	850	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	1	309	CLA	C3B-C4B-NB	-2.91	107.81	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	315	CLA	C3B-C4B-NB	-2.91	107.81	110.52
22	B	805	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	9	310	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	9	301	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	9	302	CHL	O2D-CGD-O1D	-2.91	118.15	123.84
25	B	846	8CT	C40-C12-C13	-2.91	118.85	122.92
25	7	301	8CT	C04-C03-C02	-2.91	118.52	122.61
22	B	812	CLA	CHB-C1B-NB	2.91	127.33	124.26
29	1	305	CHL	C2D-C1D-ND	2.91	112.25	110.10
22	4	312	CLA	C3B-C4B-NB	-2.91	107.82	110.52
30	7	320	XAT	C30-C31-C32	-2.91	114.15	123.22
29	0	301	CHL	O2A-CGA-CBA	2.90	121.02	111.91
25	7	323	8CT	C14-C15-C16	-2.90	118.26	126.42
22	B	837	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	J	104	8CT	C19-C20-C21	-2.90	123.17	127.31
22	4	314	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	B	823	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	8	312	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
30	4	316	XAT	C4-C3-C2	-2.90	105.18	110.77
22	A	820	CLA	CHB-C4A-NA	2.90	128.52	124.51
29	6	306	CHL	C1C-C2C-C3C	-2.90	104.81	107.11
22	1	306	CLA	CHB-C1B-NB	2.90	127.32	124.26
22	9	306	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
29	0	301	CHL	C2D-C1D-ND	2.89	112.24	110.10
25	5	317	8CT	C15-C16-C17	2.89	123.38	118.94
22	A	815	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	5	312	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
29	6	316	CHL	C1D-ND-C4D	-2.89	104.28	106.33
30	8	317	XAT	C15-C14-C13	-2.89	123.18	127.31
22	B	827	CLA	C1-C2-C3	-2.89	121.04	126.04
29	9	307	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
22	7	313	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	3	313	CLA	CHB-C4A-NA	2.89	128.51	124.51
30	7	319	XAT	C4-C3-C2	-2.89	105.19	110.77
28	B	849	DGD	C3G-C2G-C1G	-2.89	104.96	111.79
22	A	816	CLA	C3B-C4B-NB	-2.88	107.84	110.52
22	7	313	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	6	321	8CT	C40-C12-C13	-2.88	118.89	122.92
29	4	306	CHL	CHD-C4C-C3C	-2.88	120.60	124.84
22	B	821	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	B	806	CLA	CAC-C3C-C4C	2.88	128.54	124.81
22	2	311	CLA	O2D-CGD-O1D	-2.88	118.21	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	M	101	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	7	302	CLA	CAA-CBA-CGA	-2.87	104.85	113.25
22	3	303	CLA	CHB-C1B-NB	2.87	127.30	124.26
22	3	310	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	B	810	CLA	C3B-C4B-NB	-2.87	107.85	110.52
29	0	306	CHL	C4A-NA-C1A	2.87	108.00	106.71
22	4	304	CLA	C3B-C4B-NB	-2.87	107.85	110.52
22	7	309	CLA	C3B-C4B-NB	-2.87	107.85	110.52
22	K	104	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	6	320	XAT	O24-C25-C38	2.87	118.49	115.06
29	2	307	CHL	CHB-C4A-NA	2.87	128.48	124.51
25	3	318	8CT	C07-C02-C03	-2.87	118.57	122.73
22	1	310	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	0	310	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
22	4	313	CLA	C3B-C4B-NB	-2.87	107.86	110.52
22	8	311	CLA	C3B-C4B-NB	-2.87	107.86	110.52
25	B	846	8CT	C28-C26-C25	2.86	123.34	118.94
22	1	301	CLA	CHB-C1B-NB	2.86	127.29	124.26
22	A	822	CLA	CHB-C4A-NA	2.86	128.47	124.51
22	6	314	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	8	309	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	B	830	CLA	CHB-C1B-NB	2.86	127.29	124.26
22	A	805	CLA	C3B-C4B-NB	-2.86	107.86	110.52
22	2	310	CLA	CAA-C2A-C3A	-2.86	109.43	116.10
30	2	316	XAT	C35-C15-C14	-2.86	117.62	123.47
30	8	317	XAT	C24-C23-C22	-2.86	105.25	110.77
22	8	303	CLA	C3B-C4B-NB	-2.86	107.86	110.52
25	J	101	8CT	C07-C02-C03	-2.86	118.58	122.73
29	1	305	CHL	CMB-C2B-C1B	2.86	129.72	125.37
30	2	316	XAT	C6-C7-C8	-2.85	119.96	125.99
25	A	846	8CT	C39-C16-C17	-2.85	118.92	122.92
22	7	310	CLA	C3B-C4B-NB	-2.85	107.87	110.52
22	A	810	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	0	301	CHL	C3D-C4D-ND	2.85	114.85	110.24
22	A	818	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	G	103	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	B	831	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	8	312	CLA	C3B-C4B-NB	-2.85	107.87	110.52
29	7	308	CHL	CMB-C2B-C1B	2.85	129.70	125.37
29	6	306	CHL	C2A-C1A-CHA	-2.85	118.88	123.86
22	8	304	CLA	C3B-C4B-NB	-2.85	107.88	110.52
29	4	305	CHL	CMB-C2B-C1B	2.85	129.70	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	829	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
22	B	841	CLA	C3B-C4B-NB	-2.84	107.88	110.52
30	0	314	XAT	C24-C23-C22	-2.84	105.28	110.77
25	A	846	8CT	C28-C26-C25	2.84	123.30	118.94
22	A	826	CLA	C3B-C4B-NB	-2.84	107.88	110.52
22	5	310	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	B	810	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	B	818	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	1	311	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	B	832	CLA	C3B-C4B-NB	-2.84	107.88	110.52
29	5	306	CHL	C3D-C4D-ND	2.84	114.83	110.24
22	B	839	CLA	C3B-C4B-NB	-2.84	107.88	110.52
30	7	320	XAT	O24-C25-C38	2.84	118.45	115.06
30	6	320	XAT	C16-C1-C6	2.84	117.70	110.05
22	B	815	CLA	O2D-CGD-CBD	2.84	116.31	111.27
22	A	841	CLA	C3B-C4B-NB	-2.83	107.89	110.52
30	5	315	XAT	C6-C7-C8	-2.83	120.00	125.99
30	2	315	XAT	C18-C5-C4	-2.83	111.09	114.28
22	5	312	CLA	CHB-C4A-NA	2.83	128.43	124.51
22	9	312	CLA	C3B-C4B-NB	-2.83	107.89	110.52
22	4	304	CLA	CMB-C2B-C1B	-2.83	121.06	125.37
29	6	307	CHL	C4A-NA-C1A	2.83	107.98	106.71
29	3	306	CHL	OMC-CMC-C2C	-2.83	119.28	125.69
30	6	320	XAT	C20-C13-C14	-2.83	118.96	122.92
22	B	811	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	2	307	CHL	O2A-CGA-CBA	2.83	120.79	111.91
22	A	829	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	A	812	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	0	305	CLA	CBC-CAC-C3C	2.82	120.22	112.43
25	F	302	8CT	C07-C02-C03	-2.82	118.63	122.73
22	1	302	CLA	C3B-C4B-NB	-2.82	107.90	110.52
22	6	323	CLA	C3B-C4B-NB	-2.82	107.90	110.52
22	B	830	CLA	C2D-C1D-ND	-2.82	108.03	110.10
22	2	311	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	3	318	8CT	C18-C19-C20	2.82	129.25	123.47
29	1	305	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
25	A	846	8CT	C11-C10-C03	-2.82	119.28	127.20
22	7	315	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	B	809	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	B	814	CLA	CMB-C2B-C1B	-2.82	121.08	125.37
22	A	809	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	A	814	CLA	O2D-CGD-O1D	-2.81	118.34	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	307	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
22	7	313	CLA	C3B-C4B-NB	-2.81	107.91	110.52
22	A	824	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	7	317	CLA	C3B-C4B-NB	-2.81	107.91	110.52
22	B	837	CLA	C3B-C4B-NB	-2.81	107.91	110.52
29	6	307	CHL	OMC-CMC-C2C	-2.81	119.34	125.69
30	4	315	XAT	C19-C9-C10	-2.81	118.99	122.92
22	2	303	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
22	2	304	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	1	308	CLA	C3B-C4B-NB	-2.80	107.92	110.52
22	6	313	CLA	C3B-C4B-NB	-2.80	107.92	110.52
22	9	313	CLA	C3B-C4B-NB	-2.80	107.92	110.52
25	7	321	8CT	C27-C26-C25	-2.80	119.00	122.92
24	A	844	LHG	O8-C23-C24	2.80	120.70	111.91
29	5	306	CHL	C2D-C1D-ND	2.80	112.17	110.10
25	L	205	8CT	C35-C30-C31	2.80	116.43	111.42
22	1	302	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
29	8	307	CHL	CHB-C4A-NA	2.80	128.38	124.51
22	8	313	CLA	C3B-C4B-NB	-2.80	107.92	110.52
25	F	302	8CT	C30-C31-C32	-2.80	118.03	121.47
22	1	306	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
22	A	810	CLA	C3B-C4B-NB	-2.79	107.92	110.52
22	B	826	CLA	CMB-C2B-C1B	-2.79	121.11	125.37
22	J	103	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	B	820	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
30	1	314	XAT	C24-C23-C22	-2.79	105.38	110.77
22	6	301	CLA	C3B-C4B-NB	-2.79	107.92	110.52
25	8	301	8CT	C19-C18-C17	-2.79	117.76	123.47
22	A	840	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
25	7	301	8CT	C18-C17-C16	-2.79	123.33	127.31
22	B	825	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
25	L	206	8CT	C28-C26-C25	2.79	123.22	118.94
29	8	306	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
25	8	301	8CT	C14-C15-C16	-2.79	118.59	126.42
22	4	310	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	A	850	8CT	C22-C21-C20	-2.79	119.02	122.92
29	9	302	CHL	CMB-C2B-C1B	2.78	129.61	125.37
22	B	826	CLA	C3B-C4B-NB	-2.78	107.93	110.52
22	6	314	CLA	C3B-C4B-NB	-2.78	107.93	110.52
22	6	309	CLA	CHB-C4A-NA	2.78	128.36	124.51
22	6	312	CLA	CHB-C4A-NA	2.78	128.36	124.51
22	9	311	CLA	C1-C2-C3	-2.78	121.23	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	846	8CT	C18-C17-C16	-2.78	123.34	127.31
25	8	318	8CT	C11-C10-C03	-2.78	119.39	127.20
30	1	315	XAT	C15-C14-C13	-2.78	123.34	127.31
29	4	306	CHL	CMB-C2B-C1B	2.78	129.60	125.37
22	A	813	CLA	CMB-C2B-C1B	-2.78	121.14	125.37
22	2	314	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	K	103	8CT	C39-C16-C17	-2.78	119.03	122.92
22	9	309	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	5	314	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	A	827	CLA	C1-C2-C3	-2.78	121.24	126.04
22	9	304	CLA	C3B-C4B-NB	-2.77	107.94	110.52
29	6	308	CHL	CAC-C3C-C4C	2.77	128.41	124.81
30	3	314	XAT	C8-C9-C10	-2.77	114.69	118.94
22	B	816	CLA	O2D-CGD-CBD	2.77	116.19	111.27
25	6	321	8CT	C27-C26-C25	-2.77	119.04	122.92
29	6	308	CHL	C1-C2-C3	-2.77	122.27	126.75
29	6	308	CHL	CMD-C2D-C3D	-2.77	121.24	127.61
29	0	306	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
22	L	202	CLA	C3B-C4B-NB	-2.77	107.95	110.52
29	8	307	CHL	CHB-C1B-NB	-2.77	121.33	124.26
22	0	305	CLA	CHC-C4B-NB	2.77	127.19	124.26
22	7	304	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
25	A	854	8CT	C11-C10-C03	-2.77	119.44	127.20
25	I	101	8CT	C35-C30-C31	2.76	116.37	111.42
22	7	311	CLA	C3B-C4B-NB	-2.76	107.95	110.52
22	8	315	CLA	C3B-C4B-NB	-2.76	107.95	110.52
22	A	843	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
22	A	812	CLA	CHB-C4A-NA	2.76	128.33	124.51
30	7	320	XAT	C27-C28-C29	-2.76	121.24	125.53
22	B	817	CLA	C3B-C4B-NB	-2.76	107.95	110.52
22	A	806	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	3	318	8CT	C39-C16-C17	-2.76	119.06	122.92
22	7	302	CLA	C3B-C4B-NB	-2.76	107.95	110.52
22	7	302	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	4	307	CHL	CHB-C1B-NB	-2.76	121.33	124.26
29	4	307	CHL	CMB-C2B-C1B	2.76	129.57	125.37
29	0	301	CHL	CMB-C2B-C1B	2.76	129.57	125.37
22	B	822	CLA	O2D-CGD-CBD	2.76	116.17	111.27
25	4	317	8CT	C11-C10-C03	-2.76	119.46	127.20
22	1	304	CLA	O2A-CGA-O1A	-2.76	116.64	123.59
22	1	304	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	A	832	CLA	CHB-C4A-NA	2.76	128.32	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	310	CLA	C3B-C4B-NB	-2.76	107.96	110.52
25	A	854	8CT	C35-C30-C29	-2.75	109.22	112.70
22	1	312	CLA	C3B-C4B-NB	-2.75	107.96	110.52
24	A	844	LHG	C11-C10-C9	-2.75	100.45	114.42
22	9	303	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	0	302	CLA	C1-C2-C3	-2.75	121.28	126.04
22	A	806	CLA	CHB-C1B-NB	2.75	127.17	124.26
22	B	830	CLA	C1-C2-C3	-2.75	121.28	126.04
25	L	206	8CT	C01-C02-C07	2.75	118.90	113.62
22	1	303	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	6	316	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
29	8	305	CHL	C1-C2-C3	-2.75	121.28	126.04
22	A	821	CLA	C3B-C4B-NB	-2.75	107.96	110.52
22	1	313	CLA	C3B-C4B-NB	-2.75	107.96	110.52
25	B	844	8CT	C39-C16-C15	2.75	122.41	118.08
25	K	103	8CT	C27-C26-C25	-2.75	119.07	122.92
22	7	317	CLA	CHB-C4A-NA	2.75	128.31	124.51
25	B	843	8CT	C39-C16-C15	2.75	122.41	118.08
30	0	314	XAT	C40-C33-C34	-2.75	119.07	122.92
22	A	835	CLA	C3B-C4B-NB	-2.75	107.96	110.52
22	B	815	CLA	CHB-C4A-NA	2.75	128.31	124.51
24	0	315	LHG	O8-C23-C24	2.75	120.53	111.91
30	7	319	XAT	C11-C12-C13	-2.75	118.70	126.42
25	A	848	8CT	C01-C02-C03	-2.75	121.44	124.53
29	8	307	CHL	CAA-CBA-CGA	-2.75	105.22	113.25
29	8	307	CHL	CMB-C2B-C1B	2.75	129.55	125.37
22	K	101	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	4	308	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	1	309	CLA	CAA-C2A-C3A	-2.74	109.69	116.10
29	3	306	CHL	CMD-C2D-C3D	-2.74	121.30	127.61
25	2	317	8CT	C22-C21-C20	-2.74	119.08	122.92
22	A	813	CLA	C1-C2-C3	-2.74	121.30	126.04
22	A	813	CLA	CHB-C1B-NB	2.74	127.16	124.26
29	4	307	CHL	CMD-C2D-C3D	-2.74	121.30	127.61
29	8	306	CHL	CAC-C3C-C4C	2.74	128.37	124.81
22	9	305	CLA	C3B-C4B-NB	-2.74	107.97	110.52
23	B	842	PQN	C14-C13-C15	2.74	119.88	115.27
25	B	843	8CT	C27-C26-C25	-2.74	119.08	122.92
22	A	827	CLA	CHB-C1B-NB	2.74	127.16	124.26
25	F	302	8CT	C27-C26-C25	-2.74	119.09	122.92
29	8	305	CHL	O2A-CGA-CBA	2.74	120.50	111.91
30	5	316	XAT	C15-C14-C13	-2.74	123.40	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	315	XAT	C15-C35-C34	2.74	129.08	123.47
30	0	313	XAT	C39-C29-C30	-2.74	119.09	122.92
29	4	306	CHL	CHC-C4B-NB	-2.74	121.36	124.26
29	2	301	CHL	O2A-CGA-CBA	2.74	120.50	111.91
29	5	301	CHL	O2A-CGA-CBA	2.74	120.49	111.91
25	B	804	8CT	C27-C26-C28	2.73	122.39	118.08
25	7	301	8CT	C01-C02-C07	2.73	118.87	113.62
22	B	811	CLA	C1-C2-C3	-2.73	121.31	126.04
22	A	832	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	2	311	CLA	CHB-C4A-NA	2.73	128.29	124.51
22	6	315	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
22	3	313	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	3	311	CLA	CHB-C4A-NA	2.73	128.29	124.51
22	A	819	CLA	CHB-C1B-NB	2.73	127.15	124.26
25	A	847	8CT	C24-C23-C21	-2.73	118.74	126.42
25	J	104	8CT	C11-C12-C13	2.73	123.13	118.94
22	9	309	CLA	C1-C2-C3	-2.73	121.32	126.04
25	B	851	8CT	C11-C10-C03	-2.73	119.54	127.20
22	7	311	CLA	CHC-C4B-NB	2.73	127.15	124.26
22	M	101	CLA	CHB-C1B-NB	2.73	127.15	124.26
22	G	102	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	4	311	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	B	825	CLA	CHB-C4A-NA	2.73	128.28	124.51
30	5	315	XAT	C4-C3-C2	-2.73	105.51	110.77
22	6	312	CLA	C3B-C4B-NB	-2.73	107.98	110.52
29	6	302	CHL	C1D-ND-C4D	-2.73	104.40	106.33
29	4	305	CHL	O2A-CGA-CBA	2.73	120.46	111.91
25	B	804	8CT	C25-C24-C23	-2.73	114.71	123.22
22	1	312	CLA	CHB-C1B-NB	2.73	127.14	124.26
22	7	307	CLA	CHB-C4A-NA	2.72	128.28	124.51
22	F	301	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	A	806	CLA	C1-C2-C3	-2.72	121.33	126.04
25	B	851	8CT	C14-C13-C12	-2.72	123.42	127.31
22	A	802	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	B	850	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	8	301	8CT	C27-C26-C25	-2.72	119.12	122.92
29	8	306	CHL	O2A-CGA-CBA	2.72	120.43	111.91
29	6	302	CHL	C3B-C4B-NB	2.72	113.03	110.52
22	9	309	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	0	312	CLA	CHB-C1B-NB	2.71	127.13	124.26
30	6	320	XAT	C6-C7-C8	-2.71	120.26	125.99
22	K	105	CLA	O2D-CGD-O1D	-2.71	118.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	803	CLA	O2D-CGD-CBD	2.71	116.09	111.27
22	B	840	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	A	810	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	5	303	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	1	309	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	5	310	CLA	CAA-C2A-C3A	-2.71	109.78	116.10
22	A	852	CLA	CHB-C4A-NA	2.71	128.26	124.51
29	4	307	CHL	CHB-C4A-NA	2.71	128.25	124.51
22	A	823	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	B	806	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
30	8	317	XAT	O24-C25-C38	2.71	118.30	115.06
29	1	305	CHL	O2A-CGA-CBA	2.71	120.40	111.91
30	3	315	XAT	C30-C31-C32	-2.71	114.77	123.22
22	1	306	CLA	C1-C2-C3	-2.71	121.36	126.04
22	A	843	CLA	CHB-C4A-NA	2.71	128.25	124.51
22	7	304	CLA	O2A-CGA-O1A	-2.71	116.77	123.59
22	9	309	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
22	A	831	CLA	C3B-C4B-NB	-2.70	108.01	110.52
22	B	817	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
22	A	839	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	A	833	CLA	C3B-C4B-NB	-2.70	108.01	110.52
22	3	310	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	B	842	PQN	C11-C12-C13	-2.70	122.30	126.79
31	8	319	LMG	O1-C1-C2	-2.70	104.09	108.30
25	F	302	8CT	C01-C02-C07	2.70	118.80	113.62
22	3	319	CLA	O1D-CGD-CBD	2.69	130.00	124.48
30	3	314	XAT	C11-C12-C13	-2.69	118.85	126.42
25	L	205	8CT	C35-C30-C29	-2.69	109.30	112.70
30	9	315	XAT	C18-C5-C4	2.69	117.31	114.28
22	B	814	CLA	CHB-C1B-NB	2.69	127.11	124.26
22	7	306	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
22	L	201	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	A	853	CLA	C1-C2-C3	-2.69	121.39	126.04
29	0	306	CHL	O2A-CGA-CBA	2.69	120.35	111.91
29	9	302	CHL	O2A-CGA-CBA	2.69	120.35	111.91
22	A	841	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
29	8	307	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
22	A	822	CLA	O2D-CGD-CBD	2.69	116.05	111.27
25	I	101	8CT	C01-C02-C07	2.69	118.78	113.62
22	6	314	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	B	835	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	0	314	XAT	C35-C34-C33	-2.69	123.48	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	841	CLA	CHB-C1B-NB	2.69	127.10	124.26
22	1	302	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
29	8	307	CHL	O2A-CGA-CBA	2.68	120.33	111.91
22	1	307	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
29	4	306	CHL	C2D-C1D-ND	2.68	112.08	110.10
22	1	313	CLA	O2D-CGD-CBD	2.68	116.03	111.27
29	6	306	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
29	6	306	CHL	CMB-C2B-C1B	2.68	129.45	125.37
28	B	849	DGD	CDB-CCB-CBB	-2.68	100.83	114.42
25	3	318	8CT	C11-C10-C03	-2.68	119.69	127.20
22	A	823	CLA	CHB-C4A-NA	2.68	128.21	124.51
22	A	843	CLA	C3B-C4B-NB	-2.68	108.03	110.52
22	B	825	CLA	C3B-C4B-NB	-2.67	108.03	110.52
22	B	819	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	B	804	8CT	C01-C02-C07	2.67	118.75	113.62
22	B	833	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	3	318	8CT	C05-C04-C03	2.67	114.60	110.48
25	B	848	8CT	C28-C26-C25	2.67	123.04	118.94
22	A	809	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
22	0	304	CLA	C1-C2-C3	-2.67	121.42	126.04
22	A	807	CLA	C3B-C4B-NB	-2.67	108.04	110.52
30	3	315	XAT	C19-C9-C8	2.67	122.28	118.08
25	L	205	8CT	C10-C03-C02	-2.67	115.00	121.46
25	B	844	8CT	C04-C03-C02	-2.67	118.85	122.61
22	6	318	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
30	8	317	XAT	C38-C25-C24	2.67	117.28	114.28
30	8	316	XAT	C27-C28-C29	-2.66	121.39	125.53
30	3	314	XAT	C39-C29-C30	-2.66	119.19	122.92
29	0	301	CHL	CHD-C4C-C3C	-2.66	120.92	124.84
22	B	833	CLA	CAA-CBA-CGA	-2.66	105.47	113.25
22	9	305	CLA	CHB-C4A-NA	2.66	128.20	124.51
22	8	310	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
22	B	815	CLA	C3B-C4B-NB	-2.66	108.04	110.52
22	B	811	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	1	308	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
29	2	305	CHL	C2A-C1A-CHA	-2.66	119.20	123.86
22	B	829	CLA	C3B-C4B-NB	-2.66	108.05	110.52
22	5	307	CLA	C3B-C4B-NB	-2.66	108.05	110.52
30	5	315	XAT	C7-C8-C9	-2.66	121.40	125.53
22	2	309	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
29	4	305	CHL	CMD-C2D-C3D	-2.66	121.49	127.61
29	4	301	CHL	CMD-C2D-C3D	-2.66	121.49	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	312	CLA	C3B-C4B-NB	-2.66	108.05	110.52
22	8	308	CLA	C3C-C4C-NC	-2.66	107.59	110.57
22	6	303	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	7	316	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
31	8	319	LMG	O3-C3-C2	-2.65	104.21	110.35
22	0	311	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
30	6	320	XAT	C28-C29-C30	-2.65	114.87	118.94
22	A	837	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
29	6	306	CHL	CHB-C1B-NB	-2.65	121.45	124.26
29	5	306	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
22	B	814	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	A	847	8CT	C35-C30-C29	-2.65	109.35	112.70
22	6	304	CLA	CHB-C1B-NB	2.65	127.06	124.26
22	H	201	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
22	2	313	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
29	6	316	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
22	A	834	CLA	C3B-C4B-NB	-2.65	108.06	110.52
29	2	306	CHL	O2A-CGA-CBA	2.65	120.22	111.91
25	3	316	8CT	C11-C12-C13	2.65	123.01	118.94
22	B	818	CLA	CHD-C1D-ND	-2.65	122.02	124.45
22	B	836	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	4	310	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	7	310	CLA	CHB-C4A-NA	2.65	128.18	124.51
29	2	306	CHL	OMC-CMC-C2C	-2.65	119.70	125.69
29	6	302	CHL	CHC-C4B-NB	-2.65	121.45	124.26
22	4	302	CLA	CHB-C4A-NA	2.65	128.17	124.51
30	4	316	XAT	C15-C14-C13	-2.65	123.53	127.31
29	1	305	CHL	CHC-C4B-NB	-2.65	121.46	124.26
22	9	304	CLA	C2D-C1D-ND	-2.64	108.16	110.10
22	B	836	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	A	807	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	4	311	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	3	303	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
24	6	322	LHG	O8-C23-C24	2.64	120.19	111.91
22	8	312	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	A	818	CLA	CHB-C1B-NB	2.64	127.05	124.26
22	0	309	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
29	8	314	CHL	O2D-CGD-O1D	-2.64	118.69	123.84
22	2	302	CLA	CHB-C1B-NB	2.63	127.05	124.26
22	7	314	CLA	C3B-C4B-NB	-2.63	108.07	110.52
29	8	306	CHL	CMB-C2B-C1B	2.63	129.38	125.37
22	4	309	CLA	C1-C2-C3	-2.63	121.49	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	101	8CT	C40-C12-C13	-2.63	119.23	122.92
22	A	811	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
31	5	319	LMG	C7-O1-C1	2.63	118.87	113.74
29	9	302	CHL	C2A-C1A-CHA	-2.63	119.27	123.86
22	B	801	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	8	309	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
22	J	103	CLA	C3B-C4B-NB	-2.63	108.08	110.52
22	1	312	CLA	CMB-C2B-C1B	-2.63	121.37	125.37
25	B	843	8CT	C35-C30-C31	2.62	116.12	111.42
22	A	841	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	4	304	CLA	CHB-C1B-NB	2.62	127.03	124.26
22	9	311	CLA	CHB-C4A-NA	2.62	128.14	124.51
30	1	314	XAT	C15-C14-C13	-2.62	123.57	127.31
22	4	309	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	A	820	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	A	833	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	8	302	CLA	CHB-C1B-NB	2.62	127.03	124.26
22	4	309	CLA	C3B-C4B-NB	-2.62	108.08	110.52
25	B	843	8CT	C11-C10-C03	-2.62	119.84	127.20
22	H	201	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
22	A	816	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	B	848	8CT	C25-C24-C23	-2.62	115.05	123.22
22	0	308	CLA	C3B-C4B-NB	-2.62	108.09	110.52
25	A	846	8CT	C19-C20-C21	-2.62	123.58	127.31
31	4	318	LMG	O2-C2-C1	-2.62	103.69	110.05
22	G	103	CLA	C3B-C4B-NB	-2.62	108.09	110.52
22	3	308	CLA	CHB-C4A-NA	2.61	128.13	124.51
29	9	307	CHL	CMB-C2B-C1B	2.61	129.35	125.37
22	A	823	CLA	C3B-C4B-NB	-2.61	108.09	110.52
25	F	302	8CT	C11-C12-C13	2.61	122.95	118.94
29	8	314	CHL	CMD-C2D-C3D	-2.61	121.60	127.61
22	0	307	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	B	827	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
22	A	830	CLA	O2D-CGD-CBD	2.61	115.91	111.27
22	A	829	CLA	C1-C2-C3	-2.61	121.53	126.04
22	A	853	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	B	816	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	9	301	CLA	CMB-C2B-C3B	2.61	130.35	123.59
22	7	302	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	B	846	8CT	C14-C13-C12	-2.61	123.59	127.31
22	9	308	CLA	C3B-C4B-NB	-2.61	108.10	110.52
22	F	301	CLA	CHB-C4A-NA	2.61	128.12	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	306	CHL	CMD-C2D-C3D	-2.61	121.62	127.61
22	A	802	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
30	7	319	XAT	C28-C29-C30	2.61	122.94	118.94
22	B	816	CLA	CHB-C1B-NB	2.61	127.02	124.26
22	A	825	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	B	838	CLA	CMB-C2B-C1B	-2.60	121.40	125.37
22	B	810	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	8	313	CLA	CHD-C1D-ND	-2.60	122.06	124.45
22	B	818	CLA	CHB-C1B-NB	2.60	127.01	124.26
24	5	318	LHG	O8-C23-C24	2.60	120.07	111.91
22	1	311	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	3	304	CLA	C3B-C4B-NB	-2.60	108.10	110.52
29	5	306	CHL	CHC-C4B-NB	-2.60	121.50	124.26
22	4	308	CLA	C1-C2-C3	-2.60	122.54	126.75
22	1	302	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	7	306	CLA	CHB-C1B-NB	2.60	127.01	124.26
22	A	818	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	2	312	CLA	C3B-C4B-NB	-2.60	108.10	110.52
29	6	307	CHL	C2D-C1D-ND	2.60	112.02	110.10
22	K	102	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	5	312	CLA	C3B-C4B-NB	-2.60	108.11	110.52
22	A	807	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
29	4	301	CHL	CHB-C4A-NA	2.60	128.10	124.51
29	8	305	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
22	A	815	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	0	308	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	4	308	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	0	307	CLA	C3B-C4B-NB	-2.59	108.11	110.52
25	2	317	8CT	C27-C26-C25	-2.59	119.29	122.92
22	7	311	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	3	304	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
30	2	316	XAT	O24-C25-C38	2.59	118.16	115.06
22	A	843	CLA	CHB-C1B-NB	2.59	127.00	124.26
30	0	314	XAT	C39-C29-C30	-2.59	119.29	122.92
25	A	847	8CT	C18-C19-C20	-2.59	118.17	123.47
22	6	301	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	8	308	CLA	CHB-C1B-NB	2.59	127.00	124.26
22	A	817	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	A	818	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
22	0	307	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	5	306	CHL	C4A-NA-C1A	2.59	107.87	106.71
22	A	836	CLA	CHB-C4A-NA	2.59	128.09	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	301	CHL	O2A-CGA-CBA	2.59	120.03	111.91
23	A	842	PQN	C21-C20-C18	-2.59	107.56	115.92
24	2	318	LHG	C11-C10-C9	-2.59	101.30	114.42
30	9	315	XAT	C24-C23-C22	-2.59	105.78	110.77
22	4	303	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	5	305	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	B	823	CLA	CHB-C1B-NB	2.59	126.99	124.26
22	7	305	CLA	CHB-C1B-NB	2.59	126.99	124.26
29	4	301	CHL	C1-C2-C3	-2.59	121.57	126.04
30	2	315	XAT	C38-C25-C24	2.58	117.19	114.28
29	4	306	CHL	C3B-C4B-NB	2.58	112.91	110.52
28	B	849	DGD	O5D-C6D-C5D	-2.58	104.26	109.05
29	2	301	CHL	CMB-C2B-C1B	2.58	129.30	125.37
22	H	201	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	B	840	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	8	302	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	6	321	8CT	C15-C16-C17	2.58	122.90	118.94
22	7	315	CLA	CHB-C1B-NB	2.58	126.99	124.26
22	6	317	CLA	C3B-C4B-NB	-2.58	108.12	110.52
29	8	306	CHL	CMD-C2D-C3D	-2.58	121.68	127.61
22	B	814	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
30	3	315	XAT	C31-C30-C29	-2.58	123.63	127.31
22	B	828	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	3	301	CLA	C3B-C4B-NB	-2.58	108.13	110.52
22	A	824	CLA	CHB-C4A-NA	2.58	128.07	124.51
25	J	104	8CT	C18-C19-C20	-2.58	118.20	123.47
22	A	839	CLA	CHB-C1B-NB	2.57	126.98	124.26
29	2	306	CHL	CMD-C2D-C3D	-2.57	121.69	127.61
22	4	312	CLA	CHB-C4A-NA	2.57	128.07	124.51
25	B	804	8CT	C40-C12-C13	-2.57	119.32	122.92
25	A	846	8CT	C35-C30-C29	2.57	115.95	112.70
30	2	316	XAT	C20-C13-C12	2.57	122.13	118.08
22	B	832	CLA	O2D-CGD-CBD	2.57	115.84	111.27
30	9	315	XAT	C30-C31-C32	-2.57	115.19	123.22
22	1	310	CLA	C3B-C4B-NB	-2.57	108.13	110.52
30	9	315	XAT	C38-C25-C24	2.57	117.17	114.28
22	9	304	CLA	CHB-C1B-NB	2.57	126.98	124.26
22	1	307	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	2	309	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	5	303	CLA	C3B-C4B-NB	-2.57	108.13	110.52
25	A	846	8CT	C15-C16-C17	2.57	122.88	118.94
22	5	304	CLA	CHB-C4A-NA	2.57	128.06	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	303	CLA	CHB-C1B-NB	2.57	126.98	124.26
22	8	310	CLA	C3B-C4B-NB	-2.57	108.13	110.52
25	3	316	8CT	C24-C23-C21	-2.57	119.20	126.42
22	B	832	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	9	313	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	B	826	CLA	CHB-C1B-NB	2.57	126.98	124.26
25	B	847	8CT	C14-C15-C16	-2.57	119.20	126.42
29	6	302	CHL	C4-C3-C5	2.57	119.59	115.27
25	G	104	8CT	C11-C10-C03	-2.57	119.99	127.20
22	A	829	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	1	307	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	8	308	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	4	313	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	9	316	LHG	C11-C10-C9	-2.56	101.41	114.42
25	A	854	8CT	C14-C15-C16	-2.56	119.21	126.42
22	3	307	CLA	CHB-C1B-NB	2.56	126.97	124.26
22	3	312	CLA	CHB-C4A-NA	2.56	128.06	124.51
22	7	303	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	B	829	CLA	CHB-C1B-NB	2.56	126.97	124.26
22	B	819	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
22	9	303	CLA	CHC-C4B-NB	2.56	126.97	124.26
29	5	301	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
22	B	822	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	9	308	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	A	808	CLA	O2D-CGD-CBD	2.56	115.81	111.27
22	A	827	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
22	B	841	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	A	838	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	1	306	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	3	319	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	A	819	CLA	CMB-C2B-C3B	2.56	132.78	126.59
22	B	821	CLA	CHB-C1B-NB	2.56	126.96	124.26
29	9	307	CHL	O2A-CGA-CBA	2.56	119.93	111.91
22	6	310	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	0	312	CLA	C3B-C4B-NB	-2.56	108.14	110.52
29	8	307	CHL	C1C-C2C-C3C	-2.56	105.09	107.11
29	2	306	CHL	C3B-C4B-NB	2.55	112.89	110.52
29	8	305	CHL	C4-C3-C5	2.55	119.57	115.27
22	2	314	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	2	316	XAT	C39-C29-C28	2.55	122.10	118.08
30	3	314	XAT	C18-C5-C4	2.55	117.15	114.28
29	8	306	CHL	O2D-CGD-O1D	-2.55	118.84	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	315	XAT	C39-C29-C28	2.55	122.10	118.08
22	B	836	CLA	CHB-C1B-NB	2.55	126.96	124.26
22	8	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	835	CLA	C3B-C4B-NB	-2.55	108.15	110.52
22	6	312	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
29	8	307	CHL	C2A-C1A-CHA	-2.55	119.40	123.86
22	3	311	CLA	C3B-C4B-NB	-2.55	108.15	110.52
25	J	104	8CT	C27-C26-C25	-2.55	119.35	122.92
24	2	318	LHG	O8-C23-C24	2.55	119.91	111.91
22	A	840	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	809	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	A	837	CLA	C3B-C4B-NB	-2.55	108.15	110.52
30	5	316	XAT	C24-C23-C22	-2.55	105.85	110.77
22	8	310	CLA	CHB-C4A-NA	2.55	128.03	124.51
29	0	306	CHL	C2D-C1D-ND	2.55	111.98	110.10
29	4	301	CHL	CMB-C2B-C1B	2.55	129.25	125.37
22	1	309	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	3	316	8CT	C13-C14-C15	-2.55	115.27	123.22
29	2	305	CHL	OMC-CMC-C2C	-2.55	119.93	125.69
29	5	301	CHL	CMB-C2B-C1B	2.55	129.25	125.37
22	A	839	CLA	CAC-C3C-C2C	2.54	131.88	127.53
22	L	203	CLA	C3B-C4B-NB	-2.54	108.15	110.52
30	2	315	XAT	C24-C23-C22	-2.54	105.86	110.77
22	B	839	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
22	6	301	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	B	832	CLA	CHB-C1B-NB	2.54	126.95	124.26
22	K	104	CLA	CHB-C1B-NB	2.54	126.95	124.26
22	4	309	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
22	9	313	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
22	4	308	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
22	B	812	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
22	B	839	CLA	CHB-C1B-NB	2.54	126.95	124.26
22	B	814	CLA	C1-C2-C3	-2.54	121.65	126.04
22	6	318	CLA	O2D-CGD-CBD	2.54	115.78	111.27
22	A	825	CLA	C1-C2-C3	-2.54	121.65	126.04
25	A	847	8CT	C11-C10-C03	-2.54	120.08	127.20
22	5	311	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	B	819	CLA	C3B-C4B-NB	-2.53	108.16	110.52
22	A	816	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	A	828	CLA	C3B-C4B-NB	-2.53	108.17	110.52
25	B	846	8CT	C19-C18-C17	-2.53	118.28	123.47
30	4	316	XAT	C10-C11-C12	-2.53	115.31	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	306	CHL	O2A-CGA-CBA	2.53	119.85	111.91
22	A	853	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
22	B	831	CLA	C2D-C1D-ND	-2.53	108.24	110.10
25	A	847	8CT	C40-C12-C13	-2.53	119.38	122.92
29	0	306	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
22	5	304	CLA	C3B-C4B-NB	-2.53	108.17	110.52
22	9	313	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
22	A	820	CLA	C3B-C4B-NB	-2.53	108.17	110.52
24	A	845	LHG	C11-C10-C9	-2.53	101.61	114.42
22	A	852	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
22	9	311	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
29	1	305	CHL	OMC-CMC-C2C	-2.52	119.98	125.69
30	0	314	XAT	C19-C9-C10	-2.52	119.39	122.92
22	B	818	CLA	C3B-C4B-NB	-2.52	108.17	110.52
25	2	317	8CT	C24-C23-C21	-2.52	119.33	126.42
29	4	306	CHL	CMD-C2D-C3D	-2.52	121.81	127.61
22	3	309	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
22	A	805	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	A	804	CLA	CAA-CBA-CGA	-2.52	105.89	113.25
22	1	303	CLA	CHB-C4A-NA	2.52	128.00	124.51
30	2	315	XAT	C35-C34-C33	-2.52	123.71	127.31
25	1	316	8CT	C40-C12-C13	-2.52	119.39	122.92
22	6	312	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
22	1	304	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	B	820	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	B	812	CLA	C1-C2-C3	-2.52	121.69	126.04
22	9	301	CLA	CAB-C3B-C2B	2.52	130.11	123.59
22	8	309	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	3	314	XAT	C15-C35-C34	2.52	128.63	123.47
29	9	307	CHL	CHC-C4B-NB	-2.51	121.59	124.26
22	9	308	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
22	0	312	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
22	6	315	CLA	C3B-C4B-NB	-2.51	108.18	110.52
22	6	304	CLA	CHB-C4A-NA	2.51	127.99	124.51
29	9	302	CHL	CMD-C2D-C3D	-2.51	121.83	127.61
30	5	316	XAT	C10-C11-C12	-2.51	115.38	123.22
22	4	304	CLA	C1-C2-C3	-2.51	122.69	126.75
22	B	813	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	9	306	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	3	308	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
22	B	810	CLA	C1-C2-C3	-2.51	121.70	126.04
22	8	312	CLA	CHB-C1B-NB	2.51	126.91	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	203	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
22	5	303	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	6	315	CLA	CHB-C1B-NB	2.51	126.91	124.26
22	8	311	CLA	CHB-C1B-NB	2.51	126.91	124.26
25	F	302	8CT	C22-C21-C20	-2.51	119.41	122.92
30	5	316	XAT	C19-C9-C8	2.50	122.02	118.08
30	3	314	XAT	C19-C9-C8	2.50	122.02	118.08
22	7	307	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	A	811	CLA	CHB-C1B-NB	2.50	126.90	124.26
30	4	315	XAT	C40-C33-C34	-2.50	119.42	122.92
22	3	303	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	4	303	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	B	847	8CT	C11-C10-C03	-2.50	120.19	127.20
22	B	817	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	B	829	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	2	308	CLA	CHB-C1B-NB	2.49	126.90	124.26
22	3	301	CLA	O2D-CGD-CBD	2.49	115.70	111.27
22	4	304	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	2	303	CLA	C3B-C4B-NB	-2.49	108.20	110.52
30	9	314	XAT	C20-C13-C12	2.49	122.00	118.08
22	B	807	CLA	O2D-CGD-CBD	2.49	115.70	111.27
25	7	301	8CT	C39-C16-C15	2.49	122.00	118.08
29	2	305	CHL	CHB-C4A-NA	2.49	127.95	124.51
22	1	304	CLA	CHB-C1B-NB	2.49	126.89	124.26
22	A	803	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	3	307	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
30	9	315	XAT	C39-C29-C28	2.49	121.99	118.08
22	A	803	CLA	CHB-C1B-NB	2.49	126.89	124.26
22	0	310	CLA	CHB-C1B-NB	2.49	126.89	124.26
22	A	838	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	L	204	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	A	813	CLA	CMB-C2B-C3B	2.48	132.61	126.59
22	A	833	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	7	304	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	0	307	CLA	CBC-CAC-C3C	2.48	119.28	112.43
22	A	803	CLA	C1-C2-C3	-2.48	121.75	126.04
22	B	840	CLA	C3B-C4B-NB	-2.48	108.21	110.52
29	0	301	CHL	CMD-C2D-C3D	-2.48	121.90	127.61
22	2	313	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	8	308	CLA	CHD-C1D-ND	-2.48	122.17	124.45
22	H	201	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	6	309	CLA	C3B-C4B-NB	-2.48	108.22	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	315	XAT	C35-C34-C33	-2.48	123.77	127.31
29	6	316	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
22	B	834	CLA	C2D-C1D-ND	-2.48	108.28	110.10
22	B	834	CLA	CHB-C1B-NB	2.48	126.88	124.26
22	B	836	CLA	C1-C2-C3	-2.48	121.76	126.04
22	G	103	CLA	CHB-C1B-NB	2.48	126.88	124.26
29	6	306	CHL	CHB-C4A-NA	2.47	127.93	124.51
29	8	305	CHL	C3B-C4B-NB	2.47	112.81	110.52
22	B	837	CLA	CHB-C4A-NA	2.47	127.93	124.51
29	2	306	CHL	C1D-ND-C4D	-2.47	104.58	106.33
29	4	307	CHL	C2A-C1A-CHA	-2.47	119.54	123.86
29	8	306	CHL	OMC-CMC-C2C	-2.47	120.10	125.69
24	6	322	LHG	C11-C10-C9	-2.47	101.89	114.42
22	3	308	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
30	2	316	XAT	C24-C23-C22	-2.47	106.00	110.77
24	0	315	LHG	C11-C10-C9	-2.47	101.89	114.42
22	4	314	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	K	101	CLA	CHB-C1B-NB	2.47	126.87	124.26
25	3	316	8CT	C39-C16-C17	-2.47	119.47	122.92
22	A	801	CLA	C1-C2-C3	-2.47	121.78	126.04
22	B	823	CLA	C3B-C4B-NB	-2.47	108.23	110.52
29	6	308	CHL	C1C-C2C-C3C	-2.47	105.16	107.11
29	6	316	CHL	OMC-CMC-C2C	-2.47	120.11	125.69
22	H	201	CLA	C1-C2-C3	-2.47	121.78	126.04
25	L	206	8CT	C39-C16-C17	-2.47	119.47	122.92
25	A	849	8CT	C19-C18-C17	-2.47	118.42	123.47
22	0	305	CLA	C3B-C4B-NB	-2.47	108.23	110.52
22	B	827	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	B	841	CLA	C1-C2-C3	-2.46	121.78	126.04
24	1	317	LHG	O8-C23-C24	2.46	119.63	111.91
25	3	316	8CT	C19-C18-C17	-2.46	118.43	123.47
22	B	819	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	3	311	CLA	C1-C2-C3	-2.46	121.79	126.04
22	5	307	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	A	821	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	A	840	CLA	CHB-C1B-NB	2.46	126.86	124.26
22	4	314	CLA	C3B-C4B-NB	-2.46	108.23	110.52
22	0	304	CLA	CHB-C4A-NA	2.46	127.91	124.51
29	9	302	CHL	CHB-C4A-NA	2.46	127.91	124.51
29	8	307	CHL	C5-C3-C4	2.46	120.03	114.60
22	A	815	CLA	CHB-C1B-NB	2.46	126.86	124.26
22	1	306	CLA	CHB-C4A-NA	2.46	127.91	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	303	CLA	CMB-C2B-C1B	-2.46	121.63	125.37
24	5	318	LHG	C11-C10-C9	-2.46	101.96	114.42
22	B	812	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
22	B	805	CLA	O2A-CGA-O1A	-2.46	117.40	123.59
22	A	822	CLA	C3B-C4B-NB	-2.45	108.24	110.52
22	A	835	CLA	CMB-C2B-C3B	2.45	132.53	126.59
22	B	827	CLA	CHB-C1B-NB	2.45	126.85	124.26
22	4	312	CLA	CHB-C1B-NB	2.45	126.85	124.26
22	5	309	CLA	C1-C2-C3	-2.45	121.80	126.04
25	7	323	8CT	C40-C12-C13	-2.45	119.49	122.92
22	1	309	CLA	CHB-C1B-NB	2.45	126.85	124.26
29	7	308	CHL	C3B-C4B-NB	2.45	112.79	110.52
24	1	317	LHG	C11-C10-C9	-2.45	101.98	114.42
22	7	304	CLA	CHB-C1B-NB	2.45	126.85	124.26
22	0	312	CLA	O2D-CGD-CBD	2.45	115.62	111.27
29	6	307	CHL	CMD-C2D-C3D	-2.45	121.98	127.61
22	L	203	CLA	CHD-C1D-ND	-2.45	122.20	124.45
29	6	308	CHL	C2A-C1A-CHA	-2.45	119.58	123.86
22	1	307	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
30	7	320	XAT	C35-C15-C14	-2.45	118.46	123.47
22	5	310	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	5	308	CLA	C2A-C1A-CHA	2.45	128.13	123.86
22	A	837	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
22	7	310	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
22	B	838	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	7	312	CLA	CHB-C1B-NB	2.44	126.84	124.26
25	7	323	8CT	C22-C21-C20	-2.44	119.50	122.92
22	6	310	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
22	8	315	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	0	313	XAT	C5-C4-C3	2.44	117.58	112.75
22	L	201	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	A	838	CLA	CHB-C1B-NB	2.44	126.84	124.26
29	8	314	CHL	C1D-ND-C4D	-2.44	104.60	106.33
22	7	314	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	7	305	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
30	4	315	XAT	C18-C5-C4	2.44	117.02	114.28
22	1	310	CLA	CHB-C4A-NA	2.44	127.88	124.51
30	9	315	XAT	O24-C25-C38	2.44	117.98	115.06
22	0	305	CLA	CBA-CAA-C2A	-2.44	106.67	113.86
22	A	804	CLA	C1-C2-C3	-2.44	121.83	126.04
24	9	316	LHG	O8-C23-C24	2.43	119.55	111.91
22	A	839	CLA	CHB-C4A-NA	2.43	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	315	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
22	2	302	CLA	O2D-CGD-CBD	2.43	115.59	111.27
22	B	808	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
29	9	307	CHL	O1D-CGD-CBD	-2.43	119.50	124.48
25	5	317	8CT	C40-C12-C13	-2.43	119.51	122.92
22	4	304	CLA	CMB-C2B-C3B	2.43	132.48	126.59
29	6	307	CHL	C3B-C4B-NB	2.43	112.77	110.52
25	4	317	8CT	C40-C12-C13	-2.43	119.52	122.92
25	A	849	8CT	C11-C10-C03	-2.43	120.37	127.20
25	B	846	8CT	C11-C12-C13	2.43	122.67	118.94
22	6	310	CLA	C1-C2-C3	-2.43	121.84	126.04
22	2	313	CLA	CHC-C4B-NB	2.43	126.83	124.26
22	2	304	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	1	308	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
22	G	101	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	A	848	8CT	C24-C25-C26	-2.43	123.84	127.31
22	B	835	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	5	303	CLA	CHD-C1D-ND	-2.43	122.22	124.45
22	G	103	CLA	CHB-C4A-NA	2.43	127.87	124.51
30	8	317	XAT	C30-C31-C32	-2.43	115.65	123.22
22	8	313	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
22	6	305	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
22	2	309	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
29	8	305	CHL	CHB-C1B-NB	-2.42	121.69	124.26
29	1	305	CHL	CED-O2D-CGD	2.42	121.42	115.94
22	5	314	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	A	808	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	J	101	8CT	C05-C04-C03	2.42	114.21	110.48
29	1	305	CHL	C4A-NA-C1A	2.42	107.80	106.71
22	2	304	CLA	C3B-C4B-NB	-2.42	108.27	110.52
22	1	312	CLA	CHB-C4A-NA	2.42	127.86	124.51
29	5	301	CHL	O2D-CGD-O1D	-2.42	119.11	123.84
22	B	811	CLA	CHB-C1B-NB	2.42	126.82	124.26
22	9	303	CLA	O2D-CGD-CBD	2.42	115.57	111.27
24	9	316	LHG	C5-O7-C7	-2.42	111.84	117.79
31	4	318	LMG	O1-C1-C2	-2.42	104.53	108.30
22	2	302	CLA	CAC-C3C-C4C	2.42	127.95	124.81
25	J	104	8CT	C14-C13-C12	-2.42	123.86	127.31
22	8	302	CLA	C2D-C1D-ND	-2.42	108.32	110.10
22	2	309	CLA	CHB-C4A-NA	2.42	127.85	124.51
30	0	314	XAT	C4-C3-C2	-2.42	106.11	110.77
22	B	806	CLA	O2A-CGA-O1A	-2.41	117.50	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	202	CLA	CMB-C2B-C1B	-2.41	121.69	125.37
22	8	304	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	0	311	CLA	C3B-C4B-NB	-2.41	108.28	110.52
22	A	825	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
22	6	310	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	H	201	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
29	3	306	CHL	CHB-C1B-NB	-2.41	121.71	124.26
25	K	103	8CT	C11-C10-C03	-2.41	120.44	127.20
25	B	844	8CT	C28-C26-C25	2.41	122.64	118.94
22	5	304	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	7	303	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
30	1	314	XAT	C19-C9-C10	-2.41	119.55	122.92
25	2	317	8CT	C39-C16-C17	-2.41	119.55	122.92
25	I	101	8CT	C24-C23-C21	-2.41	119.66	126.42
22	2	312	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	2	312	CLA	CHB-C1B-NB	2.41	126.80	124.26
25	K	103	8CT	C22-C21-C20	-2.41	119.55	122.92
25	L	205	8CT	C27-C26-C25	-2.41	119.55	122.92
22	6	304	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
22	A	835	CLA	CHB-C4A-NA	2.40	127.84	124.51
22	3	301	CLA	CHB-C4A-NA	2.40	127.84	124.51
22	A	824	CLA	CHB-C1B-NB	2.40	126.80	124.26
22	2	310	CLA	CMA-C3A-C2A	-2.40	110.49	116.10
29	2	306	CHL	O1D-CGD-CBD	-2.40	119.57	124.48
30	1	315	XAT	C39-C29-C28	2.40	121.86	118.08
22	6	317	CLA	CHB-C4A-NA	2.40	127.83	124.51
29	5	306	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
22	7	310	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
22	A	836	CLA	C1-C2-C3	-2.40	121.89	126.04
22	B	829	CLA	C2D-C1D-ND	-2.40	108.34	110.10
22	0	303	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	K	102	CLA	O2D-CGD-CBD	2.40	115.53	111.27
22	B	809	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
22	H	201	CLA	CHB-C1B-NB	2.40	126.79	124.26
22	5	305	CLA	CHB-C1B-NB	2.40	126.79	124.26
22	8	302	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
22	B	830	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	1	311	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	1	317	LHG	C20-C19-C18	-2.39	102.28	114.42
22	5	307	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
28	B	849	DGD	O3E-C3E-C2E	-2.39	104.82	110.35
22	B	837	CLA	CMB-C2B-C1B	-2.39	121.73	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	313	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	2	316	XAT	C28-C29-C30	-2.39	115.27	118.94
29	5	301	CHL	C3B-C4B-NB	2.39	112.73	110.52
22	2	311	CLA	CHB-C1B-NB	2.39	126.78	124.26
22	7	309	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
22	L	203	CLA	CHB-C4A-NA	2.39	127.81	124.51
29	2	305	CHL	CHB-C1B-NB	-2.39	121.73	124.26
22	6	318	CLA	CHB-C1B-NB	2.39	126.78	124.26
22	2	308	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	8	304	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	A	814	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	A	819	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	9	310	CLA	CHB-C4A-NA	2.38	127.81	124.51
29	6	307	CHL	O1D-CGD-CBD	-2.38	119.61	124.48
22	B	837	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
24	A	844	LHG	C18-C17-C16	-2.38	102.33	114.42
22	5	308	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
25	B	804	8CT	C11-C10-C03	-2.38	120.52	127.20
22	M	101	CLA	C3B-C4B-NB	-2.38	108.31	110.52
22	4	310	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
31	4	318	LMG	C6-C5-C4	-2.38	107.44	113.00
22	A	801	CLA	C1D-ND-C4D	-2.38	104.65	106.33
30	1	314	XAT	C16-C1-C6	2.38	116.46	110.05
29	7	308	CHL	O2A-CGA-CBA	2.38	121.63	112.23
29	6	316	CHL	CMB-C2B-C1B	2.38	128.99	125.37
24	A	844	LHG	C20-C19-C18	-2.38	102.37	114.42
25	G	104	8CT	C14-C15-C16	-2.37	119.75	126.42
22	A	836	CLA	CHD-C1D-ND	-2.37	122.27	124.45
22	B	811	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
22	5	302	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
22	B	839	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	6	316	CHL	O1D-CGD-CBD	-2.37	119.63	124.48
22	B	850	CLA	O2D-CGD-CBD	2.37	115.48	111.27
29	4	306	CHL	O2A-CGA-CBA	2.37	119.34	111.91
30	8	317	XAT	C39-C29-C28	2.37	121.81	118.08
29	8	305	CHL	C2A-C1A-CHA	-2.37	119.72	123.86
22	A	803	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
25	1	316	8CT	C24-C23-C21	-2.37	119.77	126.42
22	2	304	CLA	CHB-C1B-NB	2.37	126.76	124.26
30	7	320	XAT	C35-C34-C33	-2.37	123.93	127.31
22	6	311	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
29	7	308	CHL	C1C-C2C-C3C	-2.37	105.24	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	813	CLA	O1D-CGD-CBD	2.36	129.32	124.48
22	0	311	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	L	205	8CT	C05-C04-C03	2.36	114.12	110.48
22	K	104	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	1	304	CLA	C2D-C1D-ND	-2.36	108.36	110.10
30	3	314	XAT	O4-C5-C6	-2.36	57.00	58.96
22	A	817	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
22	B	808	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	6	303	CLA	CHB-C1B-NB	2.36	126.75	124.26
30	7	320	XAT	C5-C4-C3	-2.36	108.08	112.75
29	4	306	CHL	OMC-CMC-C2C	-2.36	120.35	125.69
29	2	306	CHL	CHC-C4B-NB	-2.36	121.76	124.26
22	5	311	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	0	307	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
25	A	854	8CT	C39-C16-C17	-2.36	119.62	122.92
22	1	304	CLA	CHC-C4B-NB	2.36	126.75	124.26
30	4	316	XAT	C18-C5-C4	2.36	116.93	114.28
25	A	849	8CT	C24-C23-C21	-2.36	119.80	126.42
29	6	308	CHL	CHB-C4A-NA	2.36	127.77	124.51
22	A	802	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
22	9	312	CLA	O2D-CGD-CBD	2.35	115.45	111.27
22	7	309	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	B	838	CLA	CMB-C2B-C3B	2.35	132.29	126.59
22	B	833	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
22	3	302	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	A	813	CLA	CHD-C1D-ND	-2.35	122.29	124.45
30	7	320	XAT	C19-C9-C8	2.35	121.78	118.08
22	0	305	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	2	319	CLA	O2D-CGD-CBD	2.35	115.44	111.27
25	3	316	8CT	C22-C21-C20	-2.35	119.63	122.92
22	A	805	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	A	806	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	1	301	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
22	6	303	CLA	CHC-C4B-NB	2.35	126.74	124.26
29	2	301	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
22	A	834	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	2	310	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	B	807	CLA	CHB-C1B-NB	2.35	126.74	124.26
22	4	304	CLA	CAA-CBA-CGA	-2.35	106.40	113.25
22	4	303	CLA	C3B-C4B-NB	-2.34	108.34	110.52
29	7	308	CHL	CHB-C1B-NB	-2.34	121.78	124.26
22	8	304	CLA	CHB-C1B-NB	2.34	126.74	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	316	XAT	C30-C31-C32	-2.34	115.91	123.22
22	7	307	CLA	C3B-C4B-NB	-2.34	108.34	110.52
22	B	839	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
29	2	307	CHL	CAA-CBA-CGA	-2.34	106.41	113.25
22	0	309	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	A	821	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
29	9	302	CHL	C4-C3-C5	2.34	119.21	115.27
22	A	807	CLA	CHD-C1D-ND	-2.34	122.31	124.45
25	B	847	8CT	C24-C25-C26	-2.34	123.97	127.31
22	5	311	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
22	3	301	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
25	B	843	8CT	C30-C31-C32	-2.34	118.59	121.47
22	0	308	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
31	4	318	LMG	O3-C3-C2	-2.33	104.95	110.35
22	A	831	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	A	809	CLA	C3B-C4B-NB	-2.33	108.35	110.52
22	0	309	CLA	C3B-C4B-NB	-2.33	108.35	110.52
25	4	317	8CT	C25-C24-C23	-2.33	115.94	123.22
22	3	304	CLA	CHC-C4B-NB	2.33	126.72	124.26
22	0	308	CLA	CHB-C1B-NB	2.33	126.72	124.26
25	K	103	8CT	C40-C12-C13	-2.33	119.66	122.92
30	9	314	XAT	C5-C4-C3	2.33	117.36	112.75
22	A	821	CLA	CHB-C1B-NB	2.33	126.72	124.26
22	2	310	CLA	CHB-C1B-NB	2.33	126.72	124.26
22	A	826	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	2	302	CLA	CHD-C1D-ND	-2.33	122.31	124.45
22	9	311	CLA	C3B-C4B-NB	-2.33	108.35	110.52
22	B	817	CLA	CHB-C1B-NB	2.33	126.72	124.26
30	3	314	XAT	C24-C23-C22	-2.33	106.28	110.77
22	6	310	CLA	CHB-C1B-NB	2.33	126.72	124.26
22	3	304	CLA	C2D-C1D-ND	-2.33	108.39	110.10
22	4	302	CLA	CHB-C1B-NB	2.33	126.72	124.26
22	7	314	CLA	O2D-CGD-CBD	2.33	115.40	111.27
22	3	305	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	1	308	CLA	CHB-C4A-NA	2.33	127.73	124.51
29	9	307	CHL	O2D-CGD-O1D	-2.32	119.29	123.84
22	7	316	CLA	CHB-C4A-NA	2.32	127.73	124.51
22	3	308	CLA	C1-C2-C3	-2.32	122.99	126.75
22	1	306	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
23	A	842	PQN	C2M-C2-C3	-2.32	120.61	124.40
22	5	305	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
22	A	827	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	841	CLA	CHC-C4B-NB	2.32	126.72	124.26
22	A	825	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	3	308	CLA	CMB-C2B-C3B	2.32	132.21	126.59
22	A	805	CLA	CHB-C1B-NB	2.32	126.72	124.26
25	B	843	8CT	C40-C12-C13	-2.32	119.67	122.92
22	B	807	CLA	CMA-C3A-C4A	-2.32	105.53	111.77
25	I	101	8CT	C14-C15-C16	-2.32	119.90	126.42
22	6	313	CLA	CMD-C2D-C1D	-2.32	120.62	124.71
22	8	311	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	B	807	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
29	8	305	CHL	O1D-CGD-CBD	-2.32	119.74	124.48
22	3	302	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	B	822	CLA	CHB-C1B-NB	2.32	126.71	124.26
22	5	307	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	8	309	CLA	CHD-C1D-ND	-2.32	122.32	124.45
29	0	301	CHL	C1C-C2C-C3C	-2.32	105.28	107.11
22	B	833	CLA	C1-C2-C3	-2.32	122.03	126.04
22	B	829	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
30	7	319	XAT	C5-C4-C3	-2.32	108.17	112.75
22	B	832	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
22	B	831	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	1	313	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	B	829	CLA	CMC-C2C-C1C	-2.32	121.51	125.04
22	A	806	CLA	CHC-C4B-NB	2.32	126.71	124.26
25	I	101	8CT	C11-C10-C03	-2.31	120.70	127.20
29	8	306	CHL	C5-C3-C4	2.31	119.71	114.60
30	2	315	XAT	C28-C29-C30	-2.31	115.39	118.94
22	5	309	CLA	CHB-C1B-NB	2.31	126.71	124.26
29	3	306	CHL	O2A-CGA-CBA	2.31	121.37	112.23
22	4	309	CLA	CHB-C1B-NB	2.31	126.70	124.26
22	B	831	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
29	8	305	CHL	CMB-C2B-C1B	2.31	128.89	125.37
22	1	301	CLA	C1-C2-C3	-2.31	122.05	126.04
30	8	317	XAT	C40-C33-C34	-2.31	119.69	122.92
30	9	314	XAT	C31-C32-C33	2.31	132.91	126.42
22	B	830	CLA	C3B-C4B-NB	-2.31	108.37	110.52
29	4	306	CHL	CHD-C1D-C2D	2.31	130.32	125.48
24	1	317	LHG	C27-C26-C25	-2.31	102.70	114.42
29	0	306	CHL	OMC-CMC-C2C	-2.31	120.47	125.69
22	M	101	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
22	B	818	CLA	C1-C2-C3	-2.31	122.05	126.04
22	5	310	CLA	CHB-C1B-NB	2.31	126.70	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	309	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	A	809	CLA	C2D-C1D-ND	-2.31	108.40	110.10
30	8	316	XAT	C35-C15-C14	2.31	128.20	123.47
23	A	842	PQN	C21-C22-C23	-2.31	108.46	115.92
22	A	808	CLA	CHB-C1B-NB	2.31	126.70	124.26
22	3	313	CLA	CHB-C1B-NB	2.31	126.70	124.26
22	0	303	CLA	CHB-C1B-NB	2.31	126.70	124.26
22	A	807	CLA	O2D-CGD-CBD	2.31	115.37	111.27
25	F	302	8CT	C10-C03-C02	-2.31	115.87	121.46
22	B	820	CLA	CHB-C1B-NB	2.31	126.70	124.26
25	7	321	8CT	C19-C18-C17	2.31	128.20	123.47
22	7	303	CLA	CHB-C1B-NB	2.31	126.70	124.26
22	A	817	CLA	C3B-C4B-NB	-2.31	108.38	110.52
22	5	309	CLA	CHB-C4A-NA	2.30	127.70	124.51
29	6	302	CHL	OMC-CMC-C2C	-2.30	120.48	125.69
25	G	104	8CT	C39-C16-C17	-2.30	119.69	122.92
29	3	306	CHL	C2A-C1A-CHA	-2.30	119.83	123.86
29	3	306	CHL	OBD-CAD-C3D	-2.30	122.98	128.52
22	3	304	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	1	302	CLA	CHC-C4B-NB	2.30	126.69	124.26
22	A	825	CLA	O2D-CGD-CBD	2.30	115.36	111.27
29	8	306	CHL	O1D-CGD-CBD	-2.30	119.77	124.48
22	9	304	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	A	831	CLA	CHB-C1B-NB	2.30	126.69	124.26
22	B	809	CLA	CHB-C1B-NB	2.30	126.69	124.26
30	0	313	XAT	C8-C9-C10	2.30	122.47	118.94
22	9	303	CLA	C3B-C4B-NB	-2.30	108.38	110.52
22	B	841	CLA	C16-C15-C13	-2.30	108.48	115.92
25	7	321	8CT	C40-C12-C11	2.30	121.70	118.08
22	A	830	CLA	C3B-C4B-NB	-2.30	108.38	110.52
22	B	821	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	8	301	8CT	C11-C10-C03	-2.30	120.75	127.20
22	1	301	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	K	101	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	9	312	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	B	828	CLA	CMB-C2B-C3B	2.30	132.15	126.59
24	5	318	LHG	C20-C19-C18	-2.30	102.77	114.42
29	4	305	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
22	7	306	CLA	CMB-C2B-C3B	2.30	132.15	126.59
22	7	309	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	8	303	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	1	315	XAT	C24-C23-C22	-2.30	106.34	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	305	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	B	823	CLA	C2D-C1D-ND	-2.29	108.41	110.10
25	A	847	8CT	C38-C31-C32	-2.29	114.17	122.33
31	4	318	LMG	O6-C1-O1	-2.29	104.54	109.97
22	1	302	CLA	CHB-C1B-NB	2.29	126.69	124.26
22	2	308	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
22	8	303	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
22	B	814	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
22	A	853	CLA	CHB-C1B-NB	2.29	126.68	124.26
22	5	314	CLA	CHC-C4B-NB	2.29	126.68	124.26
30	3	315	XAT	C25-C24-C23	-2.29	108.22	112.75
22	7	305	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	2	317	8CT	C40-C12-C13	-2.29	119.71	122.92
30	4	315	XAT	C38-C25-C24	2.29	116.86	114.28
22	4	311	CLA	CHB-C1B-NB	2.29	126.68	124.26
22	9	304	CLA	CHC-C4B-NB	2.29	126.68	124.26
22	A	837	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	3	306	CHL	CHB-C4A-NA	2.29	127.68	124.51
25	B	851	8CT	C40-C12-C13	-2.29	119.72	122.92
25	I	101	8CT	C04-C03-C02	-2.29	119.39	122.61
22	2	314	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
22	6	303	CLA	O1D-CGD-CBD	2.29	129.17	124.48
22	8	309	CLA	CHB-C1B-NB	2.29	126.68	124.26
22	5	311	CLA	C3B-C4B-NB	-2.29	108.39	110.52
29	9	302	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
22	B	850	CLA	C1-C2-C3	-2.29	122.09	126.04
30	3	314	XAT	C35-C15-C14	2.29	128.16	123.47
29	8	307	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
22	B	817	CLA	C1-C2-C3	-2.29	122.09	126.04
22	B	850	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	A	812	CLA	CHB-C1B-NB	2.28	126.68	124.26
22	B	809	CLA	C1-C2-C3	-2.28	122.09	126.04
22	3	319	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
22	B	831	CLA	CMB-C2B-C3B	2.28	132.12	126.59
22	B	801	CLA	CHB-C1B-NB	2.28	126.67	124.26
22	4	309	CLA	C2D-C1D-ND	-2.28	108.42	110.10
22	8	308	CLA	O2D-CGD-CBD	2.28	115.32	111.27
22	A	837	CLA	CHB-C1B-NB	2.28	126.67	124.26
22	7	318	CLA	C3B-C4B-NB	-2.28	108.40	110.52
22	B	836	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
22	A	801	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
22	0	310	CLA	O2A-CGA-O1A	-2.28	117.84	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	308	CLA	C3A-C2A-C1A	2.28	104.75	101.34
22	3	319	CLA	CHB-C1B-NB	2.27	126.67	124.26
22	0	311	CLA	CHB-C1B-NB	2.27	126.67	124.26
31	4	318	LMG	C1-C2-C3	-2.27	105.26	110.00
22	A	807	CLA	CHB-C1B-NB	2.27	126.66	124.26
22	6	309	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
22	0	312	CLA	CHD-C1D-ND	-2.27	122.37	124.45
24	0	315	LHG	C20-C19-C18	-2.27	102.90	114.42
30	8	316	XAT	C25-C24-C23	-2.27	108.26	112.75
22	B	840	CLA	CHB-C1B-NB	2.27	126.66	124.26
22	0	311	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
22	K	102	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
22	B	830	CLA	CMB-C2B-C3B	2.27	132.08	126.59
22	3	307	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	1	311	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	B	840	CLA	C1-C2-C3	-2.27	122.12	126.04
22	B	811	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	5	313	CLA	CHD-C1D-ND	-2.27	122.37	124.45
29	3	306	CHL	CMB-C2B-C1B	2.26	128.82	125.37
22	A	829	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	8	318	8CT	C19-C18-C17	-2.26	118.84	123.47
22	4	314	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
28	B	849	DGD	O2E-C2E-C1E	-2.26	104.55	110.05
22	B	814	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	A	818	CLA	C2D-C1D-ND	-2.26	108.44	110.10
22	A	833	CLA	CHB-C1B-NB	2.26	126.65	124.26
29	4	301	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
22	G	102	CLA	CHB-C1B-NB	2.26	126.65	124.26
22	9	312	CLA	CHB-C1B-NB	2.26	126.65	124.26
29	8	314	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
25	B	804	8CT	C05-C04-C03	2.26	113.96	110.48
30	8	317	XAT	C19-C9-C8	2.26	121.64	118.08
29	6	308	CHL	C5-C3-C4	2.26	119.60	114.60
22	B	810	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
22	B	833	CLA	C3B-C4B-NB	-2.26	108.42	110.52
22	A	840	CLA	C11-C12-C13	-2.26	108.61	115.92
25	L	205	8CT	C04-C03-C02	-2.26	119.43	122.61
29	0	306	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
30	0	314	XAT	C32-C33-C34	2.26	122.41	118.94
29	6	302	CHL	O2A-CGA-O1A	-2.26	117.89	123.59
29	9	302	CHL	O1D-CGD-CBD	-2.26	119.87	124.48
22	B	810	CLA	CHD-C1D-ND	-2.26	122.38	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	316	LHG	C20-C19-C18	-2.26	102.97	114.42
25	A	850	8CT	C11-C10-C03	-2.26	120.87	127.20
25	B	847	8CT	C40-C12-C13	-2.26	119.76	122.92
22	A	838	CLA	CAA-CBA-CGA	-2.26	106.66	113.25
22	0	304	CLA	C3B-C4B-NB	-2.26	108.42	110.52
30	4	316	XAT	C20-C13-C12	2.26	121.63	118.08
24	5	318	LHG	C27-C26-C25	-2.25	102.98	114.42
22	B	818	CLA	CHC-C1C-NC	2.25	127.62	124.20
22	A	813	CLA	CHB-C4A-NA	2.25	127.63	124.51
22	0	302	CLA	O1D-CGD-CBD	2.25	129.10	124.48
29	2	306	CHL	CAA-C2A-C3A	-2.25	106.61	112.78
25	B	844	8CT	C19-C20-C21	-2.25	124.09	127.31
22	G	101	CLA	O2A-CGA-O1A	-2.25	117.69	123.30
22	4	314	CLA	O2D-CGD-CBD	2.25	115.27	111.27
22	B	823	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	A	818	CLA	CHD-C1D-ND	-2.25	122.39	124.45
22	A	836	CLA	CAC-C3C-C4C	2.25	127.73	124.81
29	4	305	CHL	CHC-C4B-NB	-2.25	121.88	124.26
29	8	307	CHL	O1D-CGD-CBD	-2.25	119.89	124.48
22	A	822	CLA	CHD-C1D-ND	-2.25	122.39	124.45
29	2	305	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
29	6	308	CHL	OMC-CMC-C2C	-2.25	120.61	125.69
22	B	825	CLA	C2D-C1D-ND	-2.25	108.45	110.10
22	B	835	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	B	814	CLA	CMB-C2B-C3B	2.24	132.03	126.59
22	A	811	CLA	CHB-C4A-NA	2.24	127.62	124.51
29	8	314	CHL	OMC-CMC-C2C	-2.24	120.61	125.69
29	4	307	CHL	C1C-C2C-C3C	-2.24	105.33	107.11
30	9	314	XAT	C30-C31-C32	2.24	130.22	123.22
22	5	314	CLA	CHB-C1B-NB	2.24	126.63	124.26
29	2	305	CHL	CGD-CBD-CAD	-2.24	103.47	110.73
22	6	311	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
22	3	312	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
22	A	831	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
25	7	301	8CT	C06-C07-C02	-2.24	110.08	114.08
22	6	323	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	A	823	CLA	CHB-C1B-NB	2.24	126.63	124.26
22	2	302	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
29	5	301	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
22	8	315	CLA	CHB-C1B-NB	2.24	126.63	124.26
22	5	312	CLA	C1-C2-C3	-2.24	122.17	126.04
30	9	315	XAT	C20-C13-C12	2.24	121.60	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	308	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
22	A	803	CLA	O2D-CGD-CBD	2.24	115.24	111.27
22	0	305	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	A	804	CLA	O2D-CGD-CBD	2.24	115.24	111.27
22	A	815	CLA	CAA-CBA-CGA	-2.24	106.72	113.25
30	9	314	XAT	C35-C34-C33	-2.24	124.12	127.31
25	A	849	8CT	C27-C26-C25	-2.24	119.79	122.92
30	9	315	XAT	C19-C9-C8	2.23	121.60	118.08
29	0	306	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
30	4	315	XAT	C11-C12-C13	2.23	132.69	126.42
22	0	302	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
22	A	822	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
25	L	205	8CT	C39-C16-C17	-2.23	119.80	122.92
22	7	315	CLA	CHD-C1D-ND	-2.23	122.40	124.45
25	F	302	8CT	C35-C30-C29	-2.23	109.88	112.70
22	B	815	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
30	5	316	XAT	C11-C10-C9	-2.23	124.13	127.31
22	A	829	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
22	A	822	CLA	C3A-C2A-C1A	2.23	104.68	101.34
22	B	803	CLA	CHB-C4A-NA	2.23	127.59	124.51
22	7	313	CLA	CHB-C1B-NB	2.23	126.62	124.26
22	9	308	CLA	CHB-C1B-NB	2.23	126.62	124.26
24	1	317	LHG	C18-C17-C16	-2.23	103.12	114.42
22	9	306	CLA	CHB-C1B-NB	2.22	126.61	124.26
30	6	319	XAT	C27-C28-C29	-2.22	122.08	125.53
22	B	836	CLA	CBA-CAA-C2A	-2.22	107.30	113.86
22	6	315	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
22	6	313	CLA	CHC-C4B-NB	2.22	126.61	124.26
29	6	308	CHL	CBC-CAC-C3C	-2.22	106.31	112.43
22	7	318	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
22	A	839	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
29	4	307	CHL	C5-C3-C4	2.22	119.51	114.60
30	4	316	XAT	C19-C9-C8	2.22	121.58	118.08
22	2	304	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
22	0	302	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	3	319	CLA	C1-C2-C3	2.22	129.88	126.04
22	A	823	CLA	C2D-C1D-ND	-2.22	108.47	110.10
22	0	307	CLA	CMC-C2C-C1C	-2.22	121.66	125.04
22	L	203	CLA	CHB-C1B-NB	2.22	126.61	124.26
22	2	309	CLA	CHB-C1B-NB	2.22	126.60	124.26
22	6	301	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
22	5	308	CLA	C3B-C4B-NB	-2.22	108.46	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	302	CHL	CAA-CBA-CGA	-2.22	106.78	113.25
28	B	849	DGD	CBB-CAB-C9B	-2.21	103.18	114.42
22	1	313	CLA	CHB-C1B-NB	2.21	126.60	124.26
22	B	827	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
22	K	105	CLA	C3B-C4B-NB	-2.21	108.46	110.52
22	7	311	CLA	CAA-C2A-C3A	-2.21	110.93	116.10
22	B	826	CLA	O2D-CGD-CBD	2.21	115.20	111.27
25	A	848	8CT	C14-C15-C16	-2.21	120.20	126.42
22	A	828	CLA	CAA-CBA-CGA	-2.21	106.79	113.25
22	B	837	CLA	CHD-C1D-ND	-2.21	122.42	124.45
22	K	102	CLA	C3B-C4B-NB	-2.21	108.46	110.52
29	4	301	CHL	CGD-CBD-CAD	-2.21	103.57	110.73
29	6	308	CHL	CAA-CBA-CGA	-2.21	106.79	113.25
22	B	803	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	9	305	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	A	839	CLA	CAC-C3C-C4C	-2.21	121.94	124.81
22	7	304	CLA	CHC-C4B-NB	2.21	126.60	124.26
22	A	823	CLA	C1-C2-C3	-2.21	122.22	126.04
22	A	813	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
29	6	306	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
22	A	809	CLA	CHC-C4B-NB	2.21	126.59	124.26
22	2	319	CLA	CHB-C4A-NA	2.21	127.56	124.51
25	A	854	8CT	C24-C23-C21	-2.21	120.22	126.42
22	5	302	CLA	CHB-C4A-NA	2.20	127.56	124.51
22	A	828	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
22	B	837	CLA	C1-C2-C3	-2.20	122.23	126.04
22	B	838	CLA	CHC-C4B-NB	2.20	126.59	124.26
29	0	306	CHL	CHD-C4C-C3C	-2.20	121.60	124.84
22	8	312	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
22	B	801	CLA	O2D-CGD-CBD	2.20	115.18	111.27
22	B	835	CLA	CHC-C4B-NB	2.20	126.59	124.26
30	5	316	XAT	O24-C25-C38	2.20	117.69	115.06
22	B	828	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
29	7	308	CHL	CAC-C3C-C4C	2.20	127.67	124.81
22	9	305	CLA	CHD-C1D-ND	-2.20	122.43	124.45
22	B	826	CLA	CMB-C2B-C3B	2.20	131.92	126.59
22	4	312	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
22	A	819	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
25	B	848	8CT	C22-C21-C23	2.20	121.54	118.08
22	9	311	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
22	7	317	CLA	C2A-C1A-CHA	2.20	127.70	123.86
29	8	307	CHL	OMC-CMC-C2C	-2.20	120.72	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	301	8CT	C40-C12-C13	-2.20	119.84	122.92
22	9	309	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
30	6	320	XAT	C38-C25-C24	2.20	116.75	114.28
22	A	812	CLA	C1-C2-C3	-2.20	122.24	126.04
22	7	313	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
22	A	814	CLA	O2A-CGA-O1A	-2.20	117.83	123.30
22	G	103	CLA	CMB-C2B-C1B	-2.20	122.03	125.37
22	9	304	CLA	CMB-C2B-C1B	-2.20	122.03	125.37
29	4	301	CHL	C2A-C1A-CHA	-2.20	120.02	123.86
30	4	316	XAT	O24-C25-C26	-2.19	57.14	58.96
30	2	315	XAT	C19-C9-C8	2.19	121.53	118.08
22	4	308	CLA	C2D-C1D-ND	-2.19	108.49	110.10
25	A	847	8CT	C27-C26-C28	2.19	121.53	118.08
22	A	826	CLA	C1-C2-C3	-2.19	122.25	126.04
22	J	103	CLA	CHB-C1B-NB	2.19	126.58	124.26
30	7	320	XAT	C38-C25-C24	2.19	116.74	114.28
22	A	802	CLA	CHB-C4A-NA	2.19	127.54	124.51
22	6	315	CLA	CHB-C4A-NA	2.19	127.54	124.51
22	A	839	CLA	CBC-CAC-C3C	2.19	118.46	112.43
25	3	318	8CT	C01-C02-C07	2.19	117.82	113.62
22	6	313	CLA	CMD-C2D-C3D	2.19	132.64	127.61
25	B	847	8CT	C39-C16-C17	-2.19	119.86	122.92
22	1	303	CLA	C1-C2-C3	-2.19	122.26	126.04
22	A	843	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
22	2	312	CLA	CMB-C2B-C1B	-2.18	122.04	125.37
22	B	834	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
30	2	315	XAT	O24-C25-C26	-2.18	57.15	58.96
25	L	205	8CT	C24-C25-C26	-2.18	124.20	127.31
30	3	314	XAT	C20-C13-C14	-2.18	119.87	122.92
22	7	310	CLA	CMB-C2B-C3B	2.18	131.87	126.59
22	A	821	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	A	801	CLA	O1D-CGD-CBD	2.18	128.94	124.48
22	4	314	CLA	CHB-C1B-NB	2.18	126.56	124.26
22	A	801	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
22	L	202	CLA	C1-C2-C3	-2.18	122.28	126.04
30	6	320	XAT	C12-C13-C14	2.18	122.28	118.94
31	8	319	LMG	C3-C4-C5	-2.18	106.35	110.24
22	B	837	CLA	CHB-C1B-NB	2.18	126.56	124.26
30	4	316	XAT	O4-C5-C6	-2.18	57.16	58.96
30	6	319	XAT	O4-C5-C6	-2.18	57.16	58.96
25	7	321	8CT	C14-C13-C12	-2.18	124.20	127.31
22	B	832	CLA	CHD-C1D-ND	-2.18	122.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	847	8CT	C35-C30-C31	2.18	115.32	111.42
22	B	828	CLA	CHB-C4A-NA	2.18	127.52	124.51
22	9	301	CLA	CHB-C4A-NA	2.18	127.52	124.51
22	A	852	CLA	CHB-C1B-NB	2.18	126.56	124.26
29	0	301	CHL	C3B-C4B-NB	2.18	112.53	110.52
22	9	305	CLA	CGD-CBD-CAD	-2.18	103.69	110.73
22	A	817	CLA	O2D-CGD-CBD	2.18	115.13	111.27
22	4	303	CLA	CHB-C1B-NB	2.18	126.56	124.26
22	5	305	CLA	CHC-C4B-NB	2.18	126.56	124.26
22	9	301	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	G	104	8CT	C22-C21-C20	-2.17	119.88	122.92
22	G	102	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	A	830	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	6	313	CLA	CHB-C1B-NB	2.17	126.56	124.26
24	9	316	LHG	C27-C26-C25	-2.17	103.39	114.42
22	7	318	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
22	5	307	CLA	CHB-C1B-NB	2.17	126.56	124.26
22	7	312	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	3	308	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	B	805	CLA	C16-C15-C13	-2.17	108.90	115.92
22	6	304	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
29	0	301	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
25	A	854	8CT	C40-C12-C13	-2.17	119.88	122.92
22	B	841	CLA	O1D-CGD-CBD	2.17	128.92	124.48
22	A	833	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	A	806	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	B	828	CLA	O2D-CGD-CBD	2.17	115.12	111.27
22	B	819	CLA	CMB-C2B-C3B	2.17	131.83	126.59
22	B	827	CLA	CMB-C2B-C3B	2.17	131.83	126.59
22	9	306	CLA	C3B-C4B-NB	-2.17	108.51	110.52
22	B	816	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	4	311	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
29	4	305	CHL	C1D-ND-C4D	-2.17	104.80	106.33
22	0	309	CLA	CAA-C2A-C3A	-2.16	111.05	116.10
25	1	316	8CT	C19-C18-C17	-2.16	119.04	123.47
22	7	313	CLA	CHD-C1D-ND	-2.16	122.47	124.45
22	6	318	CLA	C1-C2-C3	-2.16	122.30	126.04
22	A	838	CLA	C1-C2-C3	-2.16	122.30	126.04
29	2	301	CHL	C6-C5-C3	-2.16	107.78	113.45
22	B	834	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	B	841	CLA	C2D-C1D-ND	-2.16	108.51	110.10
22	B	812	CLA	CHB-C4A-NA	2.16	127.50	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	303	CLA	C6-C5-C3	-2.16	111.08	114.62
30	7	319	XAT	C35-C15-C14	-2.16	119.05	123.47
22	A	805	CLA	CHD-C1D-ND	-2.16	122.47	124.45
29	6	302	CHL	C4-C3-C2	-2.16	118.14	123.68
22	2	312	CLA	C1-C2-C3	-2.16	122.31	126.04
29	2	301	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
22	A	828	CLA	C16-C15-C13	-2.16	108.94	115.92
29	4	306	CHL	C5-C3-C4	2.16	119.37	114.60
22	5	302	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	7	306	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	0	303	CLA	CHC-C4B-NB	2.16	126.54	124.26
28	B	849	DGD	CFB-CEB-CDB	-2.16	103.47	114.42
29	2	307	CHL	O2D-CGD-O1D	-2.16	119.62	123.84
29	8	314	CHL	C4D-CHA-C1A	-2.16	118.62	121.25
22	A	816	CLA	CHB-C1B-NB	2.16	126.54	124.26
29	2	307	CHL	C5-C3-C4	2.16	119.37	114.60
22	2	304	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
25	5	317	8CT	C11-C10-C03	-2.16	121.14	127.20
24	A	844	LHG	C27-C26-C25	-2.16	103.48	114.42
22	2	302	CLA	CHB-C4A-NA	2.16	127.49	124.51
22	8	308	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
25	K	103	8CT	C34-C33-C32	-2.16	108.42	112.00
22	G	101	CLA	C3B-C4B-NB	-2.16	108.52	110.52
30	8	317	XAT	C5-C4-C3	-2.16	108.48	112.75
22	A	837	CLA	O1D-CGD-CBD	2.16	128.90	124.48
22	K	105	CLA	CMA-C3A-C4A	-2.16	105.98	111.77
22	4	303	CLA	C2D-C1D-ND	-2.15	108.52	110.10
25	B	845	8CT	C08-C04-C03	-2.15	106.80	110.30
22	3	305	CLA	CHB-C1B-NB	2.15	126.54	124.26
22	4	312	CLA	O1D-CGD-CBD	2.15	128.89	124.48
22	L	202	CLA	O2D-CGD-CBD	2.15	115.09	111.27
22	8	313	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
25	B	848	8CT	C39-C16-C15	2.15	121.47	118.08
22	B	808	CLA	C11-C10-C8	-2.15	108.97	115.92
22	F	301	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
25	B	843	8CT	C39-C16-C17	-2.15	119.91	122.92
25	3	318	8CT	C35-C30-C31	2.15	115.27	111.42
22	A	806	CLA	C2D-C1D-ND	-2.15	108.52	110.10
24	5	318	LHG	C18-C17-C16	-2.15	103.51	114.42
22	B	824	CLA	CHB-C4A-NA	2.15	127.48	124.51
22	L	202	CLA	CMB-C2B-C3B	2.15	131.79	126.59
22	A	843	CLA	C2D-C1D-ND	-2.15	108.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	318	8CT	C40-C12-C13	-2.15	119.92	122.92
30	3	315	XAT	C10-C11-C12	-2.15	116.52	123.22
22	7	315	CLA	CMB-C2B-C1B	-2.15	122.10	125.37
22	L	204	CLA	CHB-C1B-NB	2.15	126.53	124.26
22	9	310	CLA	CAA-C2A-C3A	-2.15	111.09	116.10
22	L	204	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
30	8	316	XAT	C36-C21-C26	-2.15	104.25	110.05
28	B	849	DGD	CAB-C9B-C8B	-2.15	103.53	114.42
29	5	301	CHL	CAA-CBA-CGA	-2.15	106.98	113.25
22	4	308	CLA	CMB-C2B-C1B	-2.15	122.10	125.37
22	B	819	CLA	CHD-C1D-ND	-2.14	122.48	124.45
22	B	838	CLA	CHD-C1D-ND	-2.14	122.48	124.45
30	8	316	XAT	O24-C25-C26	-2.14	57.18	58.96
29	7	308	CHL	CHB-C1B-C2B	-2.14	121.18	127.24
22	A	843	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
29	2	301	CHL	C4A-NA-C1A	2.14	107.67	106.71
30	8	317	XAT	C28-C29-C30	-2.14	115.66	118.94
22	6	303	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
29	4	305	CHL	C1-C2-C3	-2.14	122.34	126.04
22	6	312	CLA	CHB-C1B-NB	2.14	126.52	124.26
22	A	818	CLA	CMB-C2B-C3B	2.14	131.77	126.59
25	A	849	8CT	C22-C21-C20	-2.14	119.92	122.92
22	7	311	CLA	C2D-C1D-ND	-2.14	108.53	110.10
22	5	312	CLA	CHB-C1B-NB	2.14	126.52	124.26
22	B	818	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
22	A	836	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
25	B	804	8CT	C27-C26-C25	-2.14	119.93	122.92
22	B	824	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
22	A	805	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
25	8	301	8CT	C40-C12-C13	-2.13	119.94	122.92
22	1	309	CLA	CMA-C3A-C2A	-2.13	111.12	116.10
29	2	306	CHL	CED-O2D-CGD	2.13	120.76	115.94
22	K	101	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	1	316	8CT	C22-C21-C20	-2.13	119.94	122.92
22	1	312	CLA	CMB-C2B-C3B	2.13	131.75	126.59
29	8	305	CHL	CHB-C4A-NA	2.13	127.46	124.51
29	8	314	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
22	1	311	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	3	316	8CT	C27-C26-C25	-2.13	119.94	122.92
29	9	307	CHL	C2A-C1A-CHA	-2.13	120.14	123.86
30	4	315	XAT	C37-C21-C36	2.13	110.51	107.37
22	3	311	CLA	CHB-C1B-NB	2.13	126.51	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	306	CLA	CHC-C4B-NB	2.13	126.51	124.26
24	0	315	LHG	C27-C26-C25	-2.13	103.63	114.42
22	1	310	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
30	2	315	XAT	C7-C8-C9	-2.13	122.23	125.53
22	B	850	CLA	C4-C3-C5	2.13	118.85	115.27
29	9	307	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
22	B	818	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
22	B	850	CLA	CAC-C3C-C4C	2.12	127.57	124.81
22	6	310	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
22	3	307	CLA	C1-C2-C3	-2.12	123.32	126.75
22	A	825	CLA	CHC-C4B-NB	2.12	126.50	124.26
25	B	804	8CT	C11-C12-C13	2.12	122.20	118.94
22	0	312	CLA	CHB-C4A-NA	2.12	127.45	124.51
22	B	819	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
22	2	313	CLA	CHB-C1B-NB	2.12	126.50	124.26
29	1	305	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
22	1	301	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
29	4	301	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
22	0	307	CLA	C2D-C1D-ND	-2.12	108.54	110.10
25	8	318	8CT	C39-C16-C17	-2.12	119.95	122.92
29	5	301	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
22	3	310	CLA	C1-C2-C3	-2.12	122.38	126.04
22	1	309	CLA	O2D-CGD-CBD	2.12	115.03	111.27
22	9	301	CLA	CHB-C1B-NB	2.12	126.50	124.26
25	3	316	8CT	C11-C10-C03	-2.12	121.25	127.20
29	0	301	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
22	6	313	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
29	9	307	CHL	C1C-C2C-C3C	-2.12	105.44	107.11
25	A	846	8CT	C14-C13-C12	-2.12	124.29	127.31
22	3	309	CLA	CMB-C2B-C3B	2.12	131.71	126.59
22	B	850	CLA	CHD-C1D-ND	-2.11	122.51	124.45
25	B	844	8CT	C19-C18-C17	-2.11	119.15	123.47
22	8	303	CLA	O1D-CGD-CBD	2.11	128.81	124.48
22	K	104	CLA	CHC-C4B-NB	2.11	126.49	124.26
29	5	306	CHL	O1D-CGD-CBD	-2.11	120.16	124.48
30	5	315	XAT	C18-C5-C4	2.11	116.65	114.28
22	B	821	CLA	C1-C2-C3	-2.11	123.34	126.75
22	B	821	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
22	A	817	CLA	CHC-C4B-NB	2.11	126.49	124.26
22	G	101	CLA	CHB-C4A-NA	2.11	127.42	124.51
22	A	819	CLA	CHD-C1D-ND	-2.11	122.52	124.45
22	0	311	CLA	CHD-C1D-ND	-2.11	122.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	314	CLA	CHC-C4B-NB	2.11	126.49	124.26
22	2	302	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
22	1	302	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
22	9	308	CLA	C2D-C1D-ND	-2.10	108.55	110.10
22	4	309	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	7	317	CLA	C1-C2-C3	-2.10	122.41	126.04
22	B	824	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
25	J	104	8CT	C39-C16-C17	-2.10	119.98	122.92
22	7	315	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	6	305	CLA	CHB-C1B-NB	2.10	126.48	124.26
29	8	307	CHL	CHB-C1B-C2B	-2.10	121.30	127.24
25	J	101	8CT	C22-C21-C20	-2.10	119.98	122.92
25	8	318	8CT	C14-C15-C16	-2.10	120.52	126.42
22	2	312	CLA	CHC-C4B-NB	2.10	126.48	124.26
22	1	307	CLA	O2D-CGD-CBD	2.10	114.99	111.27
22	A	812	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
29	3	306	CHL	C1C-C2C-C3C	-2.10	105.45	107.11
30	2	315	XAT	C11-C10-C9	-2.10	124.32	127.31
22	1	302	CLA	C2D-C1D-ND	-2.10	108.56	110.10
22	A	808	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	B	824	CLA	C1-C2-C3	-2.09	122.42	126.04
22	3	310	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	B	819	CLA	C2D-C1D-ND	-2.09	108.56	110.10
22	3	312	CLA	O2D-CGD-CBD	2.09	114.99	111.27
22	H	201	CLA	CMB-C2B-C3B	2.09	131.65	126.59
25	A	848	8CT	C25-C24-C23	-2.09	116.69	123.22
22	B	803	CLA	C2D-C1D-ND	-2.09	108.56	110.10
22	2	302	CLA	C11-C10-C8	-2.09	109.16	115.92
25	8	318	8CT	C22-C21-C20	-2.09	119.99	122.92
22	8	313	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	A	834	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	2	311	CLA	C1-C2-C3	-2.09	122.43	126.04
22	6	301	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	5	304	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	5	307	CLA	O1D-CGD-CBD	2.09	128.76	124.48
22	2	304	CLA	CHD-C1D-ND	-2.09	122.53	124.45
31	5	319	LMG	O2-C2-C1	-2.09	104.97	110.05
22	7	303	CLA	CHB-C4A-NA	2.09	127.40	124.51
22	1	311	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	A	820	CLA	C2D-C1D-ND	-2.09	108.57	110.10
22	B	839	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
22	A	817	CLA	CMB-C2B-C3B	2.09	131.64	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	302	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
22	A	853	CLA	O2D-CGD-CBD	2.08	114.97	111.27
22	8	308	CLA	C2D-C1D-ND	-2.08	108.57	110.10
22	3	311	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	A	837	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	8	303	CLA	CHB-C1B-NB	2.08	126.46	124.26
22	4	302	CLA	O2D-CGD-CBD	2.08	114.97	111.27
29	6	302	CHL	CMD-C2D-C3D	-2.08	122.83	127.61
25	B	851	8CT	C39-C16-C15	2.08	121.36	118.08
30	2	315	XAT	C31-C30-C29	-2.08	124.34	127.31
22	4	313	CLA	CHB-C1B-NB	2.08	126.46	124.26
22	5	302	CLA	CHB-C1B-NB	2.08	126.46	124.26
30	7	319	XAT	C20-C13-C14	-2.08	120.01	122.92
25	A	848	8CT	C10-C11-C12	-2.08	123.09	126.23
29	8	305	CHL	C1C-C2C-C3C	-2.08	105.46	107.11
30	9	314	XAT	O24-C25-C26	-2.08	57.24	58.96
22	A	840	CLA	C11-C10-C8	-2.08	109.20	115.92
22	B	841	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
22	A	835	CLA	CHD-C1D-ND	-2.08	122.54	124.45
25	7	301	8CT	C28-C26-C25	2.08	122.13	118.94
22	2	314	CLA	O2D-CGD-CBD	2.08	114.96	111.27
22	L	204	CLA	C1-C2-C3	-2.08	123.39	126.75
29	5	306	CHL	C2A-C3A-C4A	-2.08	98.51	101.87
22	6	314	CLA	CHB-C1B-NB	2.08	126.46	124.26
31	4	318	LMG	C4-C3-C2	-2.08	107.20	110.82
22	A	836	CLA	CHB-C1B-NB	2.08	126.45	124.26
29	6	306	CHL	O2D-CGD-O1D	-2.08	119.78	123.84
22	B	837	CLA	CMB-C2B-C3B	2.08	131.62	126.59
25	G	104	8CT	C18-C19-C20	-2.08	119.22	123.47
25	2	317	8CT	C11-C10-C03	-2.08	121.37	127.20
22	A	833	CLA	C2D-C1D-ND	-2.07	108.58	110.10
25	L	205	8CT	C07-C02-C03	-2.07	119.72	122.73
22	3	312	CLA	CHD-C1D-ND	-2.07	122.55	124.45
22	4	310	CLA	CHB-C1B-NB	2.07	126.45	124.26
22	6	311	CLA	CHB-C1B-NB	2.07	126.45	124.26
22	0	303	CLA	C2D-C1D-ND	-2.07	108.58	110.10
30	7	319	XAT	C40-C33-C34	-2.07	120.02	122.92
22	6	309	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
25	K	103	8CT	C28-C26-C25	2.07	122.12	118.94
22	1	303	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
22	B	829	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	1	305	CHL	C1D-ND-C4D	-2.07	104.87	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	104	8CT	C24-C23-C21	-2.07	120.61	126.42
22	6	301	CLA	C1-C2-C3	-2.07	122.47	126.04
25	J	104	8CT	C22-C21-C23	2.07	121.33	118.08
22	9	303	CLA	C1-C2-C3	-2.07	122.47	126.04
22	7	304	CLA	CHD-C1D-ND	-2.07	122.56	124.45
30	9	314	XAT	C40-C33-C34	-2.07	120.03	122.92
22	3	312	CLA	CHB-C1B-NB	2.07	126.44	124.26
22	9	305	CLA	CHB-C1B-NB	2.07	126.44	124.26
22	1	307	CLA	CHC-C4B-NB	2.06	126.44	124.26
22	0	302	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	3	319	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
29	4	301	CHL	OMC-CMC-C2C	-2.06	121.02	125.69
22	6	323	CLA	CHB-C1B-NB	2.06	126.44	124.26
30	6	320	XAT	C24-C23-C22	-2.06	106.79	110.77
25	1	316	8CT	C11-C10-C03	-2.06	121.41	127.20
22	3	309	CLA	C3B-C4B-NB	-2.06	108.60	110.52
30	7	319	XAT	C31-C32-C33	-2.06	120.63	126.42
22	7	318	CLA	CHA-C1A-NA	-2.06	121.68	126.40
25	A	850	8CT	C39-C16-C15	2.06	121.32	118.08
25	J	101	8CT	C18-C19-C20	-2.06	119.26	123.47
25	7	321	8CT	C18-C19-C20	2.06	127.69	123.47
22	5	311	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
22	A	827	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	5	309	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	6	317	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
22	4	313	CLA	CHD-C1D-ND	-2.06	122.56	124.45
30	2	315	XAT	C40-C33-C32	2.06	121.32	118.08
22	A	810	CLA	CHB-C1B-NB	2.06	126.44	124.26
22	2	302	CLA	CMB-C2B-C3B	2.06	131.57	126.59
25	J	101	8CT	C35-C30-C29	-2.06	110.10	112.70
22	K	102	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	8	302	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
22	7	307	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	A	827	CLA	CMB-C2B-C3B	2.06	131.57	126.59
22	K	101	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
23	A	842	PQN	C16-C17-C18	-2.05	109.28	115.92
22	8	310	CLA	CHB-C1B-NB	2.05	126.43	124.26
22	H	201	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	9	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	B	847	8CT	C18-C19-C20	-2.05	119.27	123.47
29	4	307	CHL	CBC-CAC-C3C	-2.05	106.77	112.43
30	4	315	XAT	O4-C5-C6	-2.05	57.26	58.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	314	CLA	CHB-C1B-NB	2.05	126.43	124.26
22	B	820	CLA	O2D-CGD-CBD	2.05	114.91	111.27
25	I	101	8CT	C39-C16-C17	-2.05	120.05	122.92
22	A	824	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	B	836	CLA	CMB-C2B-C3B	2.05	131.56	126.59
22	9	312	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	8	305	CHL	CHC-C4B-NB	-2.05	122.09	124.26
22	4	308	CLA	CHB-C1B-NB	2.05	126.43	124.26
25	A	847	8CT	C01-C02-C07	2.05	117.55	113.62
22	A	804	CLA	CHC-C4B-NB	2.05	126.43	124.26
22	A	839	CLA	CHC-C4B-NB	2.05	126.43	124.26
22	A	831	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	3	303	CLA	O1A-CGA-CBA	2.05	129.66	123.08
22	B	810	CLA	CHB-C1B-NB	2.05	126.43	124.26
22	A	817	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	A	853	CLA	CHB-C4A-NA	2.05	127.34	124.51
29	6	302	CHL	C1C-C2C-C3C	-2.05	105.49	107.11
22	B	829	CLA	CHC-C1C-NC	2.05	127.31	124.20
22	5	308	CLA	CHB-C1B-NB	2.05	126.42	124.26
22	1	307	CLA	C2D-C1D-ND	-2.05	108.59	110.10
22	B	829	CLA	CMC-C2C-C3C	2.05	131.67	126.12
22	A	814	CLA	CHB-C1B-NB	2.05	126.42	124.26
22	B	835	CLA	CHB-C1B-NB	2.05	126.42	124.26
22	9	301	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
22	A	836	CLA	CHC-C4B-NB	2.05	126.42	124.26
22	5	302	CLA	C1-C2-C3	-2.05	122.50	126.04
22	3	312	CLA	O2A-CGA-O1A	-2.04	118.20	123.30
22	6	303	CLA	C7-C6-C5	-2.04	107.81	113.36
22	6	310	CLA	O1D-CGD-CBD	2.04	128.67	124.48
22	B	840	CLA	CHC-C4B-NB	2.04	126.42	124.26
25	A	847	8CT	C14-C15-C16	-2.04	120.68	126.42
25	7	323	8CT	C25-C24-C23	-2.04	116.84	123.22
22	7	306	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	6	317	CLA	CHC-C4B-NB	2.04	126.42	124.26
22	7	303	CLA	CHC-C4B-NB	2.04	126.42	124.26
28	B	849	DGD	C3D-C4D-C5D	-2.04	106.60	110.24
25	B	851	8CT	C22-C21-C23	2.04	121.29	118.08
22	B	823	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
22	A	827	CLA	CHD-C1D-ND	-2.04	122.58	124.45
30	2	316	XAT	C10-C11-C12	-2.04	116.85	123.22
25	8	301	8CT	C04-C03-C10	2.04	121.55	115.78
22	A	828	CLA	CMB-C2B-C3B	2.04	131.53	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	302	CLA	C6-C5-C3	-2.04	108.11	113.45
31	8	319	LMG	O1-C7-C8	-2.04	105.98	110.90
28	B	849	DGD	O2D-C2D-C1D	-2.04	105.09	110.05
22	G	102	CLA	C1-C2-C3	-2.04	123.45	126.75
29	1	305	CHL	O1D-CGD-CBD	-2.04	120.32	124.48
22	A	805	CLA	CAA-CBA-CGA	-2.04	107.31	113.25
22	0	305	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
22	1	307	CLA	CHB-C1B-NB	2.03	126.41	124.26
22	2	312	CLA	CHD-C1D-ND	-2.03	122.58	124.45
22	0	304	CLA	CHB-C1B-NB	2.03	126.41	124.26
22	A	809	CLA	CHB-C4A-NA	2.03	127.32	124.51
29	6	308	CHL	O2A-CGA-O1A	-2.03	118.46	123.59
22	A	824	CLA	CHD-C1D-ND	-2.03	122.59	124.45
31	5	319	LMG	O3-C3-C2	-2.03	105.65	110.35
22	9	306	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	2	308	CLA	C1-C2-C3	-2.03	123.47	126.75
22	A	821	CLA	C2D-C1D-ND	-2.03	108.61	110.10
25	A	854	8CT	C22-C21-C20	-2.03	120.08	122.92
25	G	104	8CT	C27-C26-C25	-2.03	120.08	122.92
31	5	319	LMG	O7-C10-O9	-2.03	118.79	123.70
31	5	319	LMG	O1-C1-C2	2.03	111.47	108.30
29	4	306	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
29	8	314	CHL	CMA-C3A-C2A	-2.03	105.64	113.83
25	B	845	8CT	C25-C24-C23	2.03	129.55	123.22
22	5	302	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
22	5	312	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	A	802	CLA	CMB-C2B-C3B	2.03	131.50	126.59
22	A	820	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	2	319	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	L	202	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
29	6	302	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
25	A	848	8CT	C18-C19-C20	-2.03	119.33	123.47
30	1	315	XAT	C19-C9-C8	2.03	121.27	118.08
29	6	308	CHL	CBB-CAB-C3B	-2.02	117.55	127.62
25	8	318	8CT	C40-C12-C13	-2.02	120.09	122.92
22	A	840	CLA	CHC-C4B-NB	2.02	126.40	124.26
22	1	308	CLA	C1-C2-C3	-2.02	122.54	126.04
25	I	101	8CT	C40-C12-C11	2.02	121.27	118.08
22	B	817	CLA	C2D-C1D-ND	-2.02	108.61	110.10
30	9	315	XAT	O4-C5-C6	-2.02	57.28	58.96
25	B	844	8CT	C11-C10-C03	-2.02	121.52	127.20
22	B	808	CLA	C16-C15-C13	-2.02	109.38	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	311	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	6	317	CLA	O2D-CGD-CBD	2.02	114.86	111.27
22	3	305	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
29	0	301	CHL	OMC-CMC-C2C	-2.02	121.12	125.69
22	B	832	CLA	C3C-C4C-NC	-2.02	108.31	110.57
22	6	313	CLA	C1-C2-C3	-2.02	122.55	126.04
22	1	308	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
25	A	846	8CT	C04-C03-C10	2.02	121.49	115.78
25	L	206	8CT	C22-C21-C20	-2.02	120.09	122.92
22	9	305	CLA	CHC-C4B-NB	2.02	126.39	124.26
22	3	309	CLA	CMA-C3A-C2A	-2.02	111.39	116.10
22	B	803	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
22	8	312	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	4	304	CLA	C2D-C1D-ND	-2.02	108.62	110.10
22	K	102	CLA	CHB-C1B-NB	2.01	126.39	124.26
22	1	308	CLA	CHB-C1B-NB	2.01	126.39	124.26
29	3	306	CHL	CAA-CBA-CGA	-2.01	107.37	113.25
30	5	315	XAT	C35-C34-C33	-2.01	124.44	127.31
22	B	806	CLA	O1D-CGD-CBD	2.01	128.60	124.48
22	9	309	CLA	CHD-C1D-ND	-2.01	122.60	124.45
22	A	821	CLA	CMB-C2B-C3B	2.01	131.46	126.59
22	B	807	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
22	6	304	CLA	CHD-C1D-ND	-2.01	122.61	124.45
25	1	316	8CT	C39-C16-C17	-2.01	120.11	122.92
22	1	311	CLA	C3C-C4C-NC	-2.01	108.32	110.57
25	L	206	8CT	C11-C10-C03	-2.01	121.56	127.20
29	4	305	CHL	O2D-CGD-O1D	-2.01	119.91	123.84
24	1	317	LHG	O8-C23-O10	-2.01	118.52	123.59
22	B	813	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	5	311	CLA	CMB-C2B-C3B	2.01	131.45	126.59
25	J	101	8CT	C24-C23-C21	-2.01	120.77	126.42
22	5	303	CLA	CHC-C4B-NB	2.01	126.38	124.26
30	2	316	XAT	C20-C13-C14	-2.01	120.11	122.92
30	1	315	XAT	O24-C25-C26	-2.01	57.30	58.96
22	A	830	CLA	CMB-C2B-C3B	2.01	131.45	126.59
22	0	309	CLA	CHD-C1D-ND	-2.01	122.61	124.45
29	7	308	CHL	O2D-CGD-O1D	-2.01	119.92	123.84
22	4	311	CLA	CHC-C4B-NB	2.01	126.38	124.26
22	M	101	CLA	O2D-CGD-CBD	2.01	114.83	111.27
22	A	843	CLA	CAC-C3C-C4C	2.01	127.41	124.81
22	1	303	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	A	803	CLA	CAA-CBA-CGA	-2.00	107.39	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	322	LHG	C27-C26-C25	-2.00	104.25	114.42
30	2	316	XAT	C38-C25-C24	2.00	116.53	114.28
25	J	101	8CT	C39-C16-C17	-2.00	120.12	122.92
22	B	807	CLA	CMB-C2B-C3B	2.00	131.44	126.59
22	1	306	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	A	809	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	A	838	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	6	305	CLA	C3B-C4B-NB	-2.00	108.66	110.52
22	A	839	CLA	CMC-C2C-C1C	-2.00	121.99	125.04
29	1	305	CHL	CHD-C1D-C2D	2.00	129.68	125.48
22	5	313	CLA	O2D-CGD-CBD	2.00	114.83	111.27
22	0	307	CLA	CHB-C1B-NB	2.00	126.38	124.26
22	7	305	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
22	A	801	CLA	CAC-C3C-C4C	2.00	127.41	124.81
22	A	825	CLA	CHB-C1B-NB	2.00	126.38	124.26
22	A	815	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	2	301	CHL	C8
29	4	301	CHL	C8
29	4	305	CHL	C8
29	6	302	CHL	C8
29	5	301	CHL	C8
29	8	305	CHL	C8
29	9	302	CHL	C8
29	0	301	CHL	C8

All (3507) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	803	CLA	CAD-CBD-CGD-O1D
22	A	803	CLA	CAD-CBD-CGD-O2D
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	805	CLA	C14-C13-C15-C16
22	A	806	CLA	O1A-CGA-O2A-C1
22	A	808	CLA	C1A-C2A-CAA-CBA
22	A	808	CLA	C3A-C2A-CAA-CBA
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	809	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	811	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	O1D-CGD-O2D-CED
22	A	811	CLA	C14-C13-C15-C16
22	A	813	CLA	CHA-CBD-CGD-O1D
22	A	813	CLA	CHA-CBD-CGD-O2D
22	A	813	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CHA-CBD-CGD-O1D
22	A	814	CLA	CHA-CBD-CGD-O2D
22	A	814	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CAD-CBD-CGD-O2D
22	A	815	CLA	CBD-CGD-O2D-CED
22	A	816	CLA	CAD-CBD-CGD-O1D
22	A	816	CLA	CAD-CBD-CGD-O2D
22	A	818	CLA	C3A-C2A-CAA-CBA
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	822	CLA	C2B-C3B-CAB-CBB
22	A	822	CLA	C4B-C3B-CAB-CBB
22	A	823	CLA	C1A-C2A-CAA-CBA
22	A	823	CLA	C3A-C2A-CAA-CBA
22	A	824	CLA	CHA-CBD-CGD-O1D
22	A	824	CLA	CHA-CBD-CGD-O2D
22	A	826	CLA	C3A-C2A-CAA-CBA
22	A	828	CLA	C1A-C2A-CAA-CBA
22	A	832	CLA	C1A-C2A-CAA-CBA
22	A	832	CLA	C4B-C3B-CAB-CBB
22	A	833	CLA	C3A-C2A-CAA-CBA
22	A	836	CLA	C1A-C2A-CAA-CBA
22	A	836	CLA	C3A-C2A-CAA-CBA
22	A	836	CLA	CHA-CBD-CGD-O1D
22	A	839	CLA	C2B-C3B-CAB-CBB
22	A	839	CLA	C4B-C3B-CAB-CBB
22	A	839	CLA	C11-C12-C13-C14
22	A	840	CLA	C2B-C3B-CAB-CBB
22	A	840	CLA	C4B-C3B-CAB-CBB
22	A	840	CLA	C4-C3-C5-C6
22	A	843	CLA	CHA-CBD-CGD-O1D
22	A	843	CLA	CHA-CBD-CGD-O2D
22	A	853	CLA	CBD-CGD-O2D-CED
22	B	801	CLA	C2-C3-C5-C6
22	B	801	CLA	C4-C3-C5-C6
22	B	803	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	803	CLA	CAD-CBD-CGD-O2D
22	B	803	CLA	O2A-C1-C2-C3
22	B	806	CLA	CBD-CGD-O2D-CED
22	B	807	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	C1A-C2A-CAA-CBA
22	B	808	CLA	C3A-C2A-CAA-CBA
22	B	812	CLA	CBD-CGD-O2D-CED
22	B	814	CLA	CHA-CBD-CGD-O1D
22	B	814	CLA	CHA-CBD-CGD-O2D
22	B	814	CLA	C11-C12-C13-C14
22	B	815	CLA	CBD-CGD-O2D-CED
22	B	816	CLA	CAD-CBD-CGD-O1D
22	B	816	CLA	CAD-CBD-CGD-O2D
22	B	817	CLA	CBD-CGD-O2D-CED
22	B	817	CLA	O1D-CGD-O2D-CED
22	B	818	CLA	C3A-C2A-CAA-CBA
22	B	819	CLA	C1A-C2A-CAA-CBA
22	B	819	CLA	C3A-C2A-CAA-CBA
22	B	820	CLA	CBD-CGD-O2D-CED
22	B	821	CLA	CHA-CBD-CGD-O1D
22	B	821	CLA	CHA-CBD-CGD-O2D
22	B	821	CLA	CAD-CBD-CGD-O1D
22	B	821	CLA	CAD-CBD-CGD-O2D
22	B	822	CLA	CBA-CGA-O2A-C1
22	B	822	CLA	C4B-C3B-CAB-CBB
22	B	823	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	CHA-CBD-CGD-O1D
22	B	825	CLA	CHA-CBD-CGD-O2D
22	B	825	CLA	CAD-CBD-CGD-O1D
22	B	825	CLA	CAD-CBD-CGD-O2D
22	B	826	CLA	C1A-C2A-CAA-CBA
22	B	826	CLA	C3A-C2A-CAA-CBA
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C3A-C2A-CAA-CBA
22	B	827	CLA	CAD-CBD-CGD-O1D
22	B	827	CLA	CAD-CBD-CGD-O2D
22	B	828	CLA	C1A-C2A-CAA-CBA
22	B	828	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	CBD-CGD-O2D-CED
22	B	829	CLA	C1A-C2A-CAA-CBA
22	B	829	CLA	CHA-CBD-CGD-O1D
22	B	829	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	829	CLA	CBD-CGD-O2D-CED
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	C3A-C2A-CAA-CBA
22	B	832	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C3A-C2A-CAA-CBA
22	B	835	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	C2-C3-C5-C6
22	B	836	CLA	C4-C3-C5-C6
22	B	837	CLA	C11-C12-C13-C14
22	B	841	CLA	C1A-C2A-CAA-CBA
22	B	850	CLA	CHA-CBD-CGD-O1D
22	B	850	CLA	CHA-CBD-CGD-O2D
22	G	102	CLA	C2B-C3B-CAB-CBB
22	G	102	CLA	C4B-C3B-CAB-CBB
22	G	102	CLA	CHA-CBD-CGD-O1D
22	G	102	CLA	CHA-CBD-CGD-O2D
22	G	103	CLA	C1A-C2A-CAA-CBA
22	G	103	CLA	C3A-C2A-CAA-CBA
22	H	201	CLA	C1A-C2A-CAA-CBA
22	J	103	CLA	C1A-C2A-CAA-CBA
22	J	103	CLA	CHA-CBD-CGD-O1D
22	J	103	CLA	CHA-CBD-CGD-O2D
22	J	103	CLA	CAD-CBD-CGD-O1D
22	J	103	CLA	CAD-CBD-CGD-O2D
22	J	103	CLA	CBD-CGD-O2D-CED
22	K	102	CLA	C1A-C2A-CAA-CBA
22	K	102	CLA	C3A-C2A-CAA-CBA
22	K	102	CLA	CHA-CBD-CGD-O2D
22	K	104	CLA	CHA-CBD-CGD-O1D
22	K	104	CLA	CHA-CBD-CGD-O2D
22	K	105	CLA	CBD-CGD-O2D-CED
22	L	201	CLA	C2B-C3B-CAB-CBB
22	L	201	CLA	C4B-C3B-CAB-CBB
22	L	201	CLA	C4-C3-C5-C6
22	L	201	CLA	C6-C7-C8-C9
22	L	202	CLA	C3A-C2A-CAA-CBA
22	L	204	CLA	C3A-C2A-CAA-CBA
22	L	204	CLA	O1A-CGA-O2A-C1
22	L	204	CLA	C2B-C3B-CAB-CBB
22	L	204	CLA	C4B-C3B-CAB-CBB
22	L	204	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	1	302	CLA	CBD-CGD-O2D-CED
22	1	302	CLA	C2-C3-C5-C6
22	1	302	CLA	C4-C3-C5-C6
22	1	303	CLA	CBD-CGD-O2D-CED
22	1	304	CLA	C2B-C3B-CAB-CBB
22	1	304	CLA	C4B-C3B-CAB-CBB
22	1	306	CLA	C2B-C3B-CAB-CBB
22	1	306	CLA	C4B-C3B-CAB-CBB
22	1	307	CLA	C1A-C2A-CAA-CBA
22	1	307	CLA	C3A-C2A-CAA-CBA
22	1	308	CLA	CHA-CBD-CGD-O1D
22	1	308	CLA	CHA-CBD-CGD-O2D
22	1	310	CLA	C1A-C2A-CAA-CBA
22	1	312	CLA	C1A-C2A-CAA-CBA
22	1	312	CLA	C3A-C2A-CAA-CBA
22	1	313	CLA	C4B-C3B-CAB-CBB
22	2	302	CLA	C4-C3-C5-C6
22	2	304	CLA	CBD-CGD-O2D-CED
22	2	304	CLA	C2-C3-C5-C6
22	2	304	CLA	C4-C3-C5-C6
22	2	308	CLA	CBD-CGD-O2D-CED
22	2	310	CLA	CBD-CGD-O2D-CED
22	2	314	CLA	C2B-C3B-CAB-CBB
22	2	314	CLA	C4B-C3B-CAB-CBB
22	2	314	CLA	CHA-CBD-CGD-O1D
22	2	314	CLA	CHA-CBD-CGD-O2D
22	2	319	CLA	C3A-C2A-CAA-CBA
22	2	319	CLA	CHA-CBD-CGD-O1D
22	3	301	CLA	CHA-CBD-CGD-O1D
22	3	301	CLA	CHA-CBD-CGD-O2D
22	3	305	CLA	C1A-C2A-CAA-CBA
22	3	305	CLA	C3A-C2A-CAA-CBA
22	3	305	CLA	C2B-C3B-CAB-CBB
22	3	305	CLA	C4B-C3B-CAB-CBB
22	3	311	CLA	C1A-C2A-CAA-CBA
22	3	313	CLA	C1A-C2A-CAA-CBA
22	3	313	CLA	C3A-C2A-CAA-CBA
22	3	313	CLA	CBA-CGA-O2A-C1
22	3	313	CLA	C2B-C3B-CAB-CBB
22	3	313	CLA	C4B-C3B-CAB-CBB
22	3	319	CLA	CHA-CBD-CGD-O1D
22	3	319	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	3	319	CLA	CBD-CGD-O2D-CED
22	3	319	CLA	O2A-C1-C2-C3
22	4	302	CLA	CHA-CBD-CGD-O1D
22	4	302	CLA	CHA-CBD-CGD-O2D
22	4	302	CLA	CBD-CGD-O2D-CED
22	4	309	CLA	C4-C3-C5-C6
22	4	311	CLA	CBD-CGD-O2D-CED
22	4	313	CLA	C2B-C3B-CAB-CBB
22	4	313	CLA	C4B-C3B-CAB-CBB
22	4	313	CLA	CAD-CBD-CGD-O1D
22	4	313	CLA	CAD-CBD-CGD-O2D
22	6	301	CLA	C1A-C2A-CAA-CBA
22	6	301	CLA	C3A-C2A-CAA-CBA
22	6	301	CLA	CBD-CGD-O2D-CED
22	6	304	CLA	C2-C3-C5-C6
22	6	304	CLA	C4-C3-C5-C6
22	6	304	CLA	C6-C7-C8-C9
22	6	309	CLA	CBD-CGD-O2D-CED
22	6	310	CLA	CBD-CGD-O2D-CED
22	6	312	CLA	CBD-CGD-O2D-CED
22	6	312	CLA	C2-C3-C5-C6
22	6	312	CLA	C4-C3-C5-C6
22	6	314	CLA	CHA-CBD-CGD-O1D
22	6	314	CLA	CHA-CBD-CGD-O2D
22	6	314	CLA	CAD-CBD-CGD-O1D
22	6	314	CLA	CAD-CBD-CGD-O2D
22	6	314	CLA	CBD-CGD-O2D-CED
22	6	315	CLA	CBD-CGD-O2D-CED
22	6	318	CLA	C1A-C2A-CAA-CBA
22	6	318	CLA	C3A-C2A-CAA-CBA
22	6	323	CLA	C1A-C2A-CAA-CBA
22	6	323	CLA	C2B-C3B-CAB-CBB
22	6	323	CLA	C4B-C3B-CAB-CBB
22	5	302	CLA	CBD-CGD-O2D-CED
22	5	303	CLA	CBD-CGD-O2D-CED
22	5	304	CLA	CBD-CGD-O2D-CED
22	5	307	CLA	CAD-CBD-CGD-O1D
22	5	308	CLA	CBD-CGD-O2D-CED
22	5	312	CLA	CBD-CGD-O2D-CED
22	5	312	CLA	C6-C7-C8-C9
22	5	313	CLA	C4B-C3B-CAB-CBB
22	5	314	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	5	314	CLA	C4B-C3B-CAB-CBB
22	5	314	CLA	CHA-CBD-CGD-O1D
22	5	314	CLA	CHA-CBD-CGD-O2D
22	5	314	CLA	CBD-CGD-O2D-CED
22	7	303	CLA	CHA-CBD-CGD-O1D
22	7	303	CLA	CHA-CBD-CGD-O2D
22	7	303	CLA	CAD-CBD-CGD-O1D
22	7	303	CLA	C4-C3-C5-C6
22	7	304	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	C1A-C2A-CAA-CBA
22	7	306	CLA	C3A-C2A-CAA-CBA
22	7	309	CLA	C4B-C3B-CAB-CBB
22	7	310	CLA	CHA-CBD-CGD-O1D
22	7	310	CLA	CHA-CBD-CGD-O2D
22	7	313	CLA	C1A-C2A-CAA-CBA
22	7	313	CLA	C3A-C2A-CAA-CBA
22	7	315	CLA	CBA-CGA-O2A-C1
22	7	316	CLA	C2B-C3B-CAB-CBB
22	7	316	CLA	C4B-C3B-CAB-CBB
22	7	317	CLA	C1A-C2A-CAA-CBA
22	7	317	CLA	C3A-C2A-CAA-CBA
22	7	317	CLA	CBD-CGD-O2D-CED
22	7	318	CLA	C1A-C2A-CAA-CBA
22	8	302	CLA	CBD-CGD-O2D-CED
22	8	304	CLA	CBD-CGD-O2D-CED
22	8	308	CLA	C3A-C2A-CAA-CBA
22	8	310	CLA	CBD-CGD-O2D-CED
22	8	311	CLA	C3-C5-C6-C7
22	8	315	CLA	CHA-CBD-CGD-O1D
22	8	315	CLA	CHA-CBD-CGD-O2D
22	8	315	CLA	CBD-CGD-O2D-CED
22	8	315	CLA	C11-C12-C13-C14
22	9	306	CLA	CBD-CGD-O2D-CED
22	9	309	CLA	CHA-CBD-CGD-O1D
22	9	309	CLA	CHA-CBD-CGD-O2D
22	9	311	CLA	CBD-CGD-O2D-CED
22	9	312	CLA	CHA-CBD-CGD-O1D
22	9	312	CLA	CHA-CBD-CGD-O2D
22	9	312	CLA	CAD-CBD-CGD-O1D
22	9	312	CLA	CAD-CBD-CGD-O2D
22	9	313	CLA	C3A-C2A-CAA-CBA
22	9	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	9	313	CLA	C2-C3-C5-C6
22	9	313	CLA	C4-C3-C5-C6
22	0	303	CLA	C2B-C3B-CAB-CBB
22	0	303	CLA	C4B-C3B-CAB-CBB
22	0	303	CLA	C2-C3-C5-C6
22	0	303	CLA	C4-C3-C5-C6
22	0	304	CLA	C1A-C2A-CAA-CBA
22	0	304	CLA	C3A-C2A-CAA-CBA
22	0	304	CLA	C2-C3-C5-C6
22	0	304	CLA	C4-C3-C5-C6
22	0	305	CLA	C1A-C2A-CAA-CBA
22	0	307	CLA	CBD-CGD-O2D-CED
22	0	308	CLA	CBD-CGD-O2D-CED
22	0	309	CLA	CBD-CGD-O2D-CED
22	0	310	CLA	C1A-C2A-CAA-CBA
22	0	310	CLA	C3A-C2A-CAA-CBA
22	0	311	CLA	CBD-CGD-O2D-CED
22	M	101	CLA	CHA-CBD-CGD-O1D
22	M	101	CLA	CHA-CBD-CGD-O2D
24	A	844	LHG	C1-C2-C3-O3
24	A	844	LHG	C3-O3-P-O6
24	A	845	LHG	O2-C2-C3-O3
24	A	845	LHG	C3-O3-P-O4
24	A	845	LHG	C3-O3-P-O5
24	A	845	LHG	C4-O6-P-O4
24	A	845	LHG	C4-O6-P-O5
24	A	845	LHG	O6-C4-C5-O7
24	A	845	LHG	C8-C7-O7-C5
24	B	852	LHG	C3-O3-P-O5
24	B	852	LHG	C6-C5-O7-C7
24	B	852	LHG	O9-C7-O7-C5
24	B	852	LHG	C8-C7-O7-C5
24	1	317	LHG	O2-C2-C3-O3
24	1	317	LHG	C4-O6-P-O5
24	2	318	LHG	C1-C2-C3-O3
24	2	318	LHG	C3-O3-P-O4
24	2	318	LHG	C4-O6-P-O4
24	3	317	LHG	O1-C1-C2-C3
24	3	317	LHG	C3-O3-P-O5
24	3	317	LHG	C4-C5-O7-C7
24	6	322	LHG	O1-C1-C2-C3
24	6	322	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	6	322	LHG	C3-O3-P-O4
24	5	318	LHG	C1-C2-C3-O3
24	5	318	LHG	O2-C2-C3-O3
24	5	318	LHG	C4-O6-P-O5
24	7	322	LHG	O1-C1-C2-C3
24	7	322	LHG	C4-O6-P-O5
24	7	322	LHG	C6-C5-O7-C7
24	9	316	LHG	C3-O3-P-O4
24	9	316	LHG	C3-O3-P-O6
24	9	316	LHG	O7-C5-C6-O8
24	0	315	LHG	C1-C2-C3-O3
24	0	315	LHG	C3-O3-P-O4
24	0	315	LHG	C4-O6-P-O3
24	0	315	LHG	C4-O6-P-O4
25	A	846	8CT	C02-C03-C10-C11
25	A	846	8CT	C04-C03-C10-C11
25	A	846	8CT	C18-C19-C20-C21
25	A	846	8CT	C23-C24-C25-C26
25	A	846	8CT	C28-C29-C30-C35
25	A	847	8CT	C10-C11-C12-C13
25	A	847	8CT	C10-C11-C12-C40
25	A	848	8CT	C12-C13-C14-C15
25	A	849	8CT	C04-C03-C10-C11
25	A	849	8CT	C10-C11-C12-C13
25	A	849	8CT	C10-C11-C12-C40
25	A	849	8CT	C14-C15-C16-C17
25	A	849	8CT	C14-C15-C16-C39
25	A	850	8CT	C02-C03-C10-C11
25	A	850	8CT	C10-C11-C12-C13
25	A	850	8CT	C10-C11-C12-C40
25	A	850	8CT	C12-C13-C14-C15
25	A	850	8CT	C28-C29-C30-C35
25	A	854	8CT	C04-C03-C10-C11
25	A	854	8CT	C12-C13-C14-C15
25	A	854	8CT	C14-C15-C16-C17
25	A	854	8CT	C14-C15-C16-C39
25	A	854	8CT	C20-C21-C23-C24
25	A	854	8CT	C22-C21-C23-C24
25	A	854	8CT	C28-C29-C30-C31
25	A	854	8CT	C28-C29-C30-C35
25	B	804	8CT	C25-C26-C28-C29
25	B	804	8CT	C27-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
25	B	804	8CT	C28-C29-C30-C35
25	B	843	8CT	C10-C11-C12-C13
25	B	843	8CT	C10-C11-C12-C40
25	B	843	8CT	C14-C15-C16-C17
25	B	843	8CT	C14-C15-C16-C39
25	B	843	8CT	C20-C21-C23-C24
25	B	843	8CT	C22-C21-C23-C24
25	B	843	8CT	C28-C29-C30-C35
25	B	844	8CT	C10-C11-C12-C13
25	B	844	8CT	C10-C11-C12-C40
25	B	844	8CT	C18-C19-C20-C21
25	B	844	8CT	C20-C21-C23-C24
25	B	844	8CT	C22-C21-C23-C24
25	B	845	8CT	C25-C26-C28-C29
25	B	845	8CT	C27-C26-C28-C29
25	B	846	8CT	C14-C15-C16-C17
25	B	846	8CT	C14-C15-C16-C39
25	B	846	8CT	C27-C26-C28-C29
25	B	846	8CT	C28-C29-C30-C35
25	B	847	8CT	C10-C11-C12-C13
25	B	847	8CT	C10-C11-C12-C40
25	B	847	8CT	C20-C21-C23-C24
25	B	847	8CT	C22-C21-C23-C24
25	B	847	8CT	C23-C24-C25-C26
25	B	851	8CT	C10-C11-C12-C13
25	B	851	8CT	C10-C11-C12-C40
25	B	851	8CT	C12-C13-C14-C15
25	B	851	8CT	C14-C15-C16-C17
25	B	851	8CT	C14-C15-C16-C39
25	B	851	8CT	C20-C21-C23-C24
25	B	851	8CT	C22-C21-C23-C24
25	F	302	8CT	C28-C29-C30-C31
25	F	302	8CT	C28-C29-C30-C35
25	G	104	8CT	C02-C03-C10-C11
25	G	104	8CT	C10-C11-C12-C13
25	G	104	8CT	C10-C11-C12-C40
25	G	104	8CT	C18-C19-C20-C21
25	G	104	8CT	C25-C26-C28-C29
25	G	104	8CT	C27-C26-C28-C29
25	G	104	8CT	C28-C29-C30-C35
25	I	101	8CT	C10-C11-C12-C13
25	I	101	8CT	C10-C11-C12-C40

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Mol	Chain	Res	Type	Atoms
25	I	101	8CT	C25-C26-C28-C29
25	I	101	8CT	C27-C26-C28-C29
25	I	101	8CT	C28-C29-C30-C31
25	I	101	8CT	C28-C29-C30-C35
25	J	101	8CT	C28-C29-C30-C35
25	J	104	8CT	C04-C03-C10-C11
25	J	104	8CT	C28-C29-C30-C31
25	J	104	8CT	C28-C29-C30-C35
25	K	103	8CT	C14-C15-C16-C17
25	K	103	8CT	C14-C15-C16-C39
25	L	205	8CT	C02-C03-C10-C11
25	L	205	8CT	C10-C11-C12-C13
25	L	205	8CT	C10-C11-C12-C40
25	L	205	8CT	C20-C21-C23-C24
25	L	205	8CT	C22-C21-C23-C24
25	L	206	8CT	C20-C21-C23-C24
25	L	206	8CT	C22-C21-C23-C24
25	L	206	8CT	C28-C29-C30-C35
25	1	316	8CT	C02-C03-C10-C11
25	1	316	8CT	C04-C03-C10-C11
25	1	316	8CT	C20-C21-C23-C24
25	1	316	8CT	C22-C21-C23-C24
25	1	316	8CT	C25-C26-C28-C29
25	1	316	8CT	C27-C26-C28-C29
25	1	316	8CT	C28-C29-C30-C35
25	2	317	8CT	C10-C11-C12-C13
25	2	317	8CT	C10-C11-C12-C40
25	2	317	8CT	C28-C29-C30-C35
25	3	316	8CT	C23-C24-C25-C26
25	3	316	8CT	C25-C26-C28-C29
25	3	316	8CT	C27-C26-C28-C29
25	3	318	8CT	C10-C11-C12-C13
25	3	318	8CT	C10-C11-C12-C40
25	3	318	8CT	C20-C21-C23-C24
25	3	318	8CT	C22-C21-C23-C24
25	3	318	8CT	C23-C24-C25-C26
25	6	321	8CT	C10-C11-C12-C13
25	6	321	8CT	C10-C11-C12-C40
25	5	317	8CT	C04-C03-C10-C11
25	5	317	8CT	C28-C29-C30-C31
25	5	317	8CT	C28-C29-C30-C35
25	7	301	8CT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	7	321	8CT	C22-C21-C23-C24
25	7	321	8CT	C25-C26-C28-C29
25	7	321	8CT	C27-C26-C28-C29
25	7	321	8CT	C28-C29-C30-C31
25	7	321	8CT	C28-C29-C30-C35
25	7	323	8CT	C04-C03-C10-C11
25	7	323	8CT	C23-C24-C25-C26
25	7	323	8CT	C25-C26-C28-C29
25	7	323	8CT	C27-C26-C28-C29
25	8	301	8CT	C18-C19-C20-C21
25	8	301	8CT	C20-C21-C23-C24
25	8	301	8CT	C22-C21-C23-C24
25	8	301	8CT	C23-C24-C25-C26
25	8	301	8CT	C28-C29-C30-C35
25	8	318	8CT	C04-C03-C10-C11
25	8	318	8CT	C27-C26-C28-C29
25	8	318	8CT	C28-C29-C30-C35
26	A	851	HTG	O5-C1-S1-C1'
29	2	301	CHL	C1C-C2C-CMC-OMC
29	2	301	CHL	CHA-CBD-CGD-O1D
29	2	301	CHL	CHA-CBD-CGD-O2D
29	2	301	CHL	CAD-CBD-CGD-O1D
29	2	305	CHL	C3C-C2C-CMC-OMC
29	2	307	CHL	C4B-C3B-CAB-CBB
29	2	307	CHL	C3C-C2C-CMC-OMC
29	2	307	CHL	CBD-CGD-O2D-CED
29	4	305	CHL	C1C-C2C-CMC-OMC
29	4	305	CHL	C3C-C2C-CMC-OMC
29	4	305	CHL	C2-C3-C5-C6
29	4	305	CHL	C4-C3-C5-C6
29	4	306	CHL	C1A-C2A-CAA-CBA
29	4	306	CHL	C3A-C2A-CAA-CBA
29	4	307	CHL	C1C-C2C-CMC-OMC
29	4	307	CHL	C3C-C2C-CMC-OMC
29	6	306	CHL	C1A-C2A-CAA-CBA
29	6	307	CHL	C1A-C2A-CAA-CBA
29	6	307	CHL	C3A-C2A-CAA-CBA
29	6	307	CHL	C1C-C2C-CMC-OMC
29	6	307	CHL	C3C-C2C-CMC-OMC
29	6	308	CHL	C1A-C2A-CAA-CBA
29	6	308	CHL	C3A-C2A-CAA-CBA
29	6	308	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	6	308	CHL	C4B-C3B-CAB-CBB
29	6	308	CHL	CBD-CGD-O2D-CED
29	6	316	CHL	C3C-C2C-CMC-OMC
29	5	306	CHL	C3C-C2C-CMC-OMC
29	8	305	CHL	C1C-C2C-CMC-OMC
29	8	306	CHL	C1A-C2A-CAA-CBA
29	8	306	CHL	CHA-CBD-CGD-O1D
29	8	306	CHL	CHA-CBD-CGD-O2D
29	8	307	CHL	C2B-C3B-CAB-CBB
29	8	307	CHL	C4B-C3B-CAB-CBB
29	0	301	CHL	C1A-C2A-CAA-CBA
29	0	301	CHL	C3A-C2A-CAA-CBA
29	0	301	CHL	C11-C10-C8-C9
30	1	314	XAT	C1-C6-C7-C8
30	1	314	XAT	C7-C8-C9-C10
30	1	314	XAT	C7-C8-C9-C19
30	1	314	XAT	C11-C12-C13-C14
30	1	314	XAT	C11-C12-C13-C20
30	2	315	XAT	C1-C6-C7-C8
30	2	316	XAT	O4-C6-C7-C8
30	3	314	XAT	C31-C32-C33-C40
30	4	315	XAT	O24-C26-C27-C28
30	6	320	XAT	C7-C8-C9-C10
30	6	320	XAT	C7-C8-C9-C19
30	6	320	XAT	C9-C10-C11-C12
30	5	315	XAT	O4-C6-C7-C8
30	5	315	XAT	C25-C26-C27-C28
30	7	319	XAT	C7-C8-C9-C10
30	7	319	XAT	C7-C8-C9-C19
30	7	319	XAT	C11-C12-C13-C14
30	7	319	XAT	C11-C12-C13-C20
30	7	319	XAT	O24-C26-C27-C28
30	8	316	XAT	C25-C26-C27-C28
30	8	316	XAT	O24-C26-C27-C28
30	0	313	XAT	O4-C6-C7-C8
30	0	313	XAT	C7-C8-C9-C19
30	0	313	XAT	C13-C14-C15-C35
30	0	313	XAT	C21-C26-C27-C28
30	0	313	XAT	C25-C26-C27-C28
30	0	313	XAT	O24-C26-C27-C28
30	0	313	XAT	C31-C32-C33-C34
30	0	313	XAT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
30	0	314	XAT	O4-C6-C7-C8
30	0	314	XAT	O24-C26-C27-C28
31	4	318	LMG	O6-C1-O1-C7
31	5	319	LMG	C2-C1-O1-C7
31	5	319	LMG	O6-C1-O1-C7
31	8	319	LMG	C2-C1-O1-C7
31	8	319	LMG	O6-C1-O1-C7
22	A	816	CLA	O1D-CGD-O2D-CED
22	A	853	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	O1D-CGD-O2D-CED
22	K	105	CLA	O1D-CGD-O2D-CED
22	2	310	CLA	O1D-CGD-O2D-CED
22	3	303	CLA	O1D-CGD-O2D-CED
22	4	313	CLA	O1D-CGD-O2D-CED
22	5	303	CLA	O1D-CGD-O2D-CED
22	5	307	CLA	O1D-CGD-O2D-CED
22	7	302	CLA	O1D-CGD-O2D-CED
22	7	303	CLA	O1D-CGD-O2D-CED
22	7	306	CLA	O1D-CGD-O2D-CED
22	8	315	CLA	O1D-CGD-O2D-CED
22	9	306	CLA	O1D-CGD-O2D-CED
22	9	311	CLA	O1D-CGD-O2D-CED
22	A	839	CLA	C2C-C3C-CAC-CBC
22	A	839	CLA	C4C-C3C-CAC-CBC
22	A	815	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	O1D-CGD-O2D-CED
22	B	823	CLA	O1D-CGD-O2D-CED
22	G	103	CLA	O1D-CGD-O2D-CED
22	L	204	CLA	O1D-CGD-O2D-CED
22	2	304	CLA	O1D-CGD-O2D-CED
22	3	302	CLA	O1D-CGD-O2D-CED
22	3	319	CLA	O1D-CGD-O2D-CED
22	6	304	CLA	O1D-CGD-O2D-CED
22	6	315	CLA	O1D-CGD-O2D-CED
22	5	308	CLA	O1D-CGD-O2D-CED
22	7	304	CLA	O1D-CGD-O2D-CED
22	7	317	CLA	O1D-CGD-O2D-CED
22	9	313	CLA	O1D-CGD-O2D-CED
22	0	308	CLA	O1D-CGD-O2D-CED
29	7	308	CHL	O1D-CGD-O2D-CED
22	A	814	CLA	CBD-CGD-O2D-CED
22	A	816	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	829	CLA	CBD-CGD-O2D-CED
22	A	832	CLA	CBD-CGD-O2D-CED
22	A	837	CLA	CBD-CGD-O2D-CED
22	A	839	CLA	CBD-CGD-O2D-CED
22	A	841	CLA	CBD-CGD-O2D-CED
22	B	805	CLA	CBD-CGD-O2D-CED
22	B	814	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	CBD-CGD-O2D-CED
22	F	301	CLA	CBD-CGD-O2D-CED
22	G	101	CLA	CBD-CGD-O2D-CED
22	G	103	CLA	CBD-CGD-O2D-CED
22	H	201	CLA	CBD-CGD-O2D-CED
22	K	101	CLA	CBD-CGD-O2D-CED
22	1	308	CLA	CBD-CGD-O2D-CED
22	2	302	CLA	CBD-CGD-O2D-CED
22	3	302	CLA	CBD-CGD-O2D-CED
22	3	303	CLA	CBD-CGD-O2D-CED
22	3	305	CLA	CBD-CGD-O2D-CED
22	4	310	CLA	CBD-CGD-O2D-CED
22	4	313	CLA	CBD-CGD-O2D-CED
22	4	314	CLA	CBD-CGD-O2D-CED
22	6	303	CLA	CBD-CGD-O2D-CED
22	6	304	CLA	CBD-CGD-O2D-CED
22	6	305	CLA	CBD-CGD-O2D-CED
22	6	311	CLA	CBD-CGD-O2D-CED
22	5	307	CLA	CBD-CGD-O2D-CED
22	5	310	CLA	CBD-CGD-O2D-CED
22	7	302	CLA	CBD-CGD-O2D-CED
22	7	303	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CBD-CGD-O2D-CED
22	7	316	CLA	CBD-CGD-O2D-CED
22	9	303	CLA	CBD-CGD-O2D-CED
22	9	310	CLA	CBD-CGD-O2D-CED
22	0	302	CLA	CBD-CGD-O2D-CED
22	M	101	CLA	CBD-CGD-O2D-CED
29	4	305	CHL	CBD-CGD-O2D-CED
29	6	307	CHL	CBD-CGD-O2D-CED
29	7	308	CHL	CBD-CGD-O2D-CED
29	8	314	CHL	CBD-CGD-O2D-CED
22	A	808	CLA	O1A-CGA-O2A-C1
22	A	819	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	852	CLA	O1A-CGA-O2A-C1
22	7	317	CLA	O1A-CGA-O2A-C1
22	0	305	CLA	O1A-CGA-O2A-C1
24	7	322	LHG	O10-C23-O8-C6
22	A	832	CLA	O1D-CGD-O2D-CED
22	B	829	CLA	O1D-CGD-O2D-CED
22	G	101	CLA	O1D-CGD-O2D-CED
22	1	302	CLA	O1D-CGD-O2D-CED
22	4	310	CLA	O1D-CGD-O2D-CED
22	6	301	CLA	O1D-CGD-O2D-CED
22	0	302	CLA	O1D-CGD-O2D-CED
22	K	104	CLA	CBA-CGA-O2A-C1
22	4	303	CLA	CBA-CGA-O2A-C1
22	0	307	CLA	C4C-C3C-CAC-CBC
22	A	837	CLA	O1D-CGD-O2D-CED
22	B	814	CLA	O1D-CGD-O2D-CED
22	B	815	CLA	O1D-CGD-O2D-CED
22	B	828	CLA	O1D-CGD-O2D-CED
22	J	103	CLA	O1D-CGD-O2D-CED
22	1	303	CLA	O1D-CGD-O2D-CED
22	2	308	CLA	O1D-CGD-O2D-CED
22	6	309	CLA	O1D-CGD-O2D-CED
22	6	311	CLA	O1D-CGD-O2D-CED
22	6	312	CLA	O1D-CGD-O2D-CED
22	5	302	CLA	O1D-CGD-O2D-CED
22	5	312	CLA	O1D-CGD-O2D-CED
22	8	310	CLA	O1D-CGD-O2D-CED
22	0	307	CLA	O1D-CGD-O2D-CED
22	0	311	CLA	O1D-CGD-O2D-CED
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	808	CLA	CBA-CGA-O2A-C1
22	7	317	CLA	CBA-CGA-O2A-C1
22	9	301	CLA	CBA-CGA-O2A-C1
24	1	317	LHG	C24-C23-O8-C6
22	A	804	CLA	CBD-CGD-O2D-CED
22	A	817	CLA	CBD-CGD-O2D-CED
22	A	819	CLA	CBD-CGD-O2D-CED
22	A	833	CLA	CBD-CGD-O2D-CED
22	B	810	CLA	CBD-CGD-O2D-CED
22	G	102	CLA	CBD-CGD-O2D-CED
22	L	203	CLA	CBD-CGD-O2D-CED
22	1	301	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	2	303	CLA	CBD-CGD-O2D-CED
22	3	301	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CBD-CGD-O2D-CED
22	4	304	CLA	CBD-CGD-O2D-CED
22	6	323	CLA	CBD-CGD-O2D-CED
22	7	314	CLA	CBD-CGD-O2D-CED
22	7	315	CLA	CBD-CGD-O2D-CED
22	0	304	CLA	CBD-CGD-O2D-CED
29	1	305	CHL	CBD-CGD-O2D-CED
29	2	306	CHL	CBD-CGD-O2D-CED
29	4	307	CHL	CBD-CGD-O2D-CED
29	8	305	CHL	CBD-CGD-O2D-CED
29	0	301	CHL	CBD-CGD-O2D-CED
22	A	805	CLA	O1A-CGA-O2A-C1
22	A	810	CLA	O1A-CGA-O2A-C1
22	A	811	CLA	O1A-CGA-O2A-C1
22	B	823	CLA	O1A-CGA-O2A-C1
22	B	850	CLA	O1A-CGA-O2A-C1
22	L	202	CLA	O1A-CGA-O2A-C1
22	1	302	CLA	O1A-CGA-O2A-C1
22	4	314	CLA	O1A-CGA-O2A-C1
22	7	316	CLA	O1A-CGA-O2A-C1
22	9	301	CLA	O1A-CGA-O2A-C1
22	9	304	CLA	O1A-CGA-O2A-C1
24	1	317	LHG	O10-C23-O8-C6
24	3	317	LHG	O10-C23-O8-C6
24	5	318	LHG	O10-C23-O8-C6
29	2	307	CHL	O1A-CGA-O2A-C1
29	8	307	CHL	O1A-CGA-O2A-C1
22	B	822	CLA	O1A-CGA-O2A-C1
22	K	104	CLA	O1A-CGA-O2A-C1
22	3	313	CLA	O1A-CGA-O2A-C1
22	7	315	CLA	O1A-CGA-O2A-C1
22	B	807	CLA	O1D-CGD-O2D-CED
22	B	835	CLA	O1D-CGD-O2D-CED
22	5	304	CLA	O1D-CGD-O2D-CED
29	2	307	CHL	O1D-CGD-O2D-CED
29	6	308	CHL	O1D-CGD-O2D-CED
22	2	304	CLA	C8-C10-C11-C12
22	4	302	CLA	O1D-CGD-O2D-CED
22	4	311	CLA	O1D-CGD-O2D-CED
22	6	310	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	5	314	CLA	O1D-CGD-O2D-CED
22	8	302	CLA	O1D-CGD-O2D-CED
22	8	304	CLA	O1D-CGD-O2D-CED
22	0	309	CLA	O1D-CGD-O2D-CED
22	6	317	CLA	C4C-C3C-CAC-CBC
22	A	810	CLA	CBD-CGD-O2D-CED
22	A	820	CLA	CBD-CGD-O2D-CED
22	B	819	CLA	CBD-CGD-O2D-CED
22	B	837	CLA	CBD-CGD-O2D-CED
22	5	309	CLA	CBD-CGD-O2D-CED
22	7	313	CLA	CBD-CGD-O2D-CED
22	B	820	CLA	O1D-CGD-O2D-CED
22	H	201	CLA	O1D-CGD-O2D-CED
22	6	314	CLA	O1D-CGD-O2D-CED
24	A	844	LHG	O9-C7-O7-C5
31	5	319	LMG	O9-C10-O7-C8
22	2	319	CLA	CBA-CGA-O2A-C1
22	5	314	CLA	O1A-CGA-O2A-C1
22	A	817	CLA	C3-C5-C6-C7
22	A	828	CLA	C3-C5-C6-C7
22	A	832	CLA	C3-C5-C6-C7
22	A	833	CLA	C3-C5-C6-C7
22	A	838	CLA	C3-C5-C6-C7
22	A	841	CLA	C3-C5-C6-C7
22	B	816	CLA	C3-C5-C6-C7
22	B	817	CLA	C3-C5-C6-C7
22	B	833	CLA	C3-C5-C6-C7
22	B	834	CLA	C3-C5-C6-C7
22	2	309	CLA	C3-C5-C6-C7
22	7	303	CLA	C3-C5-C6-C7
22	9	313	CLA	C3-C5-C6-C7
22	0	308	CLA	C3-C5-C6-C7
29	4	301	CHL	C3-C5-C6-C7
29	0	301	CHL	C3-C5-C6-C7
22	A	806	CLA	CBA-CGA-O2A-C1
22	A	819	CLA	CBA-CGA-O2A-C1
22	A	822	CLA	CBA-CGA-O2A-C1
22	A	852	CLA	CBA-CGA-O2A-C1
22	B	823	CLA	CBA-CGA-O2A-C1
22	B	850	CLA	CBA-CGA-O2A-C1
22	L	204	CLA	CBA-CGA-O2A-C1
22	5	313	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	7	304	CLA	CBA-CGA-O2A-C1
22	7	316	CLA	CBA-CGA-O2A-C1
22	9	304	CLA	CBA-CGA-O2A-C1
22	9	308	CLA	CBA-CGA-O2A-C1
22	0	305	CLA	CBA-CGA-O2A-C1
24	7	322	LHG	C24-C23-O8-C6
29	8	307	CHL	CBA-CGA-O2A-C1
31	5	319	LMG	C11-C10-O7-C8
22	A	841	CLA	O1D-CGD-O2D-CED
22	B	805	CLA	O1D-CGD-O2D-CED
22	7	316	CLA	O1D-CGD-O2D-CED
22	B	841	CLA	CBD-CGD-O2D-CED
22	9	304	CLA	CBD-CGD-O2D-CED
22	6	317	CLA	C2C-C3C-CAC-CBC
22	0	307	CLA	C2C-C3C-CAC-CBC
22	2	319	CLA	O1A-CGA-O2A-C1
22	4	303	CLA	O1A-CGA-O2A-C1
22	6	323	CLA	CBA-CGA-O2A-C1
22	5	314	CLA	CBA-CGA-O2A-C1
22	3	310	CLA	C3-C5-C6-C7
22	B	840	CLA	C4-C3-C5-C6
22	5	303	CLA	C4-C3-C5-C6
22	9	309	CLA	C4-C3-C5-C6
28	B	849	DGD	C4E-C5E-C6E-O5E
31	5	319	LMG	C4-C5-C6-O5
22	A	840	CLA	C2-C3-C5-C6
22	L	201	CLA	C2-C3-C5-C6
22	2	302	CLA	C2-C3-C5-C6
22	4	309	CLA	C2-C3-C5-C6
22	7	303	CLA	C2-C3-C5-C6
22	9	309	CLA	C2-C3-C5-C6
22	1	312	CLA	CBD-CGD-O2D-CED
29	6	316	CHL	CBD-CGD-O2D-CED
22	A	819	CLA	C2A-CAA-CBA-CGA
22	B	823	CLA	C2A-CAA-CBA-CGA
22	B	829	CLA	C2A-CAA-CBA-CGA
22	K	105	CLA	C2A-CAA-CBA-CGA
22	L	201	CLA	C2A-CAA-CBA-CGA
22	3	307	CLA	C2A-CAA-CBA-CGA
22	4	303	CLA	C2A-CAA-CBA-CGA
22	6	301	CLA	C2A-CAA-CBA-CGA
22	6	303	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	6	305	CLA	C2A-CAA-CBA-CGA
22	5	303	CLA	C2A-CAA-CBA-CGA
22	5	304	CLA	C2A-CAA-CBA-CGA
22	5	305	CLA	C2A-CAA-CBA-CGA
22	5	313	CLA	C2A-CAA-CBA-CGA
22	5	314	CLA	C2A-CAA-CBA-CGA
22	7	318	CLA	C2A-CAA-CBA-CGA
22	8	308	CLA	C2A-CAA-CBA-CGA
22	8	310	CLA	C2A-CAA-CBA-CGA
22	8	311	CLA	C2A-CAA-CBA-CGA
22	8	315	CLA	C2A-CAA-CBA-CGA
22	9	301	CLA	C2A-CAA-CBA-CGA
29	2	307	CHL	C2A-CAA-CBA-CGA
22	F	301	CLA	O1D-CGD-O2D-CED
22	K	101	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	C3-C5-C6-C7
22	2	302	CLA	C3-C5-C6-C7
22	5	303	CLA	C3-C5-C6-C7
22	7	316	CLA	C3-C5-C6-C7
23	A	842	PQN	C13-C15-C16-C17
22	A	810	CLA	CBA-CGA-O2A-C1
22	A	811	CLA	CBA-CGA-O2A-C1
22	A	817	CLA	CBA-CGA-O2A-C1
22	A	821	CLA	CBA-CGA-O2A-C1
22	A	837	CLA	CBA-CGA-O2A-C1
22	A	843	CLA	CBA-CGA-O2A-C1
22	B	817	CLA	CBA-CGA-O2A-C1
22	B	819	CLA	CBA-CGA-O2A-C1
22	L	202	CLA	CBA-CGA-O2A-C1
22	1	302	CLA	CBA-CGA-O2A-C1
22	2	304	CLA	CBA-CGA-O2A-C1
22	4	314	CLA	CBA-CGA-O2A-C1
22	6	303	CLA	CBA-CGA-O2A-C1
22	0	308	CLA	CBA-CGA-O2A-C1
29	2	301	CHL	CBA-CGA-O2A-C1
29	2	307	CHL	CBA-CGA-O2A-C1
29	4	306	CHL	CBA-CGA-O2A-C1
31	8	319	LMG	C29-C28-O8-C9
22	A	814	CLA	O1D-CGD-O2D-CED
22	4	314	CLA	O1D-CGD-O2D-CED
22	9	303	CLA	O1D-CGD-O2D-CED
29	6	307	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	0	312	CLA	CBD-CGD-O2D-CED
29	8	307	CHL	CBD-CGD-O2D-CED
26	A	851	HTG	S1-C1'-C2'-C3'
22	A	829	CLA	O1D-CGD-O2D-CED
22	6	303	CLA	O1D-CGD-O2D-CED
22	6	305	CLA	O1D-CGD-O2D-CED
22	9	310	CLA	O1D-CGD-O2D-CED
22	M	101	CLA	O1D-CGD-O2D-CED
24	A	845	LHG	O9-C7-O7-C5
28	B	849	DGD	O1B-C1B-O2G-C2G
22	A	843	CLA	O1A-CGA-O2A-C1
22	B	817	CLA	O1A-CGA-O2A-C1
22	B	819	CLA	O1A-CGA-O2A-C1
22	B	824	CLA	O1A-CGA-O2A-C1
22	B	833	CLA	O1A-CGA-O2A-C1
22	B	834	CLA	O1A-CGA-O2A-C1
22	K	105	CLA	O1A-CGA-O2A-C1
22	2	304	CLA	O1A-CGA-O2A-C1
22	6	301	CLA	O1A-CGA-O2A-C1
22	6	303	CLA	O1A-CGA-O2A-C1
22	9	308	CLA	O1A-CGA-O2A-C1
31	8	319	LMG	O10-C28-O8-C9
22	7	310	CLA	O1D-CGD-O2D-CED
25	B	847	8CT	C18-C19-C20-C21
25	J	101	8CT	C12-C13-C14-C15
25	J	101	8CT	C18-C19-C20-C21
25	L	205	8CT	C18-C19-C20-C21
25	L	206	8CT	C23-C24-C25-C26
25	3	316	8CT	C16-C17-C18-C19
25	4	317	8CT	C16-C17-C18-C19
25	6	321	8CT	C12-C13-C14-C15
25	7	301	8CT	C16-C17-C18-C19
25	7	301	8CT	C18-C19-C20-C21
25	7	321	8CT	C12-C13-C14-C15
25	7	323	8CT	C18-C19-C20-C21
25	8	301	8CT	C16-C17-C18-C19
22	B	805	CLA	C5-C6-C7-C8
22	A	809	CLA	CBD-CGD-O2D-CED
22	B	850	CLA	CBD-CGD-O2D-CED
22	2	313	CLA	CBD-CGD-O2D-CED
22	8	309	CLA	CBD-CGD-O2D-CED
22	9	301	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	8	306	CHL	CBD-CGD-O2D-CED
22	2	302	CLA	O1D-CGD-O2D-CED
24	A	844	LHG	O2-C2-C3-O3
24	2	318	LHG	O2-C2-C3-O3
24	6	322	LHG	O2-C2-C3-O3
24	9	316	LHG	O2-C2-C3-O3
24	0	315	LHG	O2-C2-C3-O3
22	A	813	CLA	C3-C5-C6-C7
22	6	315	CLA	C3-C5-C6-C7
22	B	831	CLA	CBA-CGA-O2A-C1
22	B	833	CLA	CBA-CGA-O2A-C1
22	B	834	CLA	CBA-CGA-O2A-C1
22	K	105	CLA	CBA-CGA-O2A-C1
22	6	301	CLA	CBA-CGA-O2A-C1
22	5	307	CLA	CBA-CGA-O2A-C1
22	9	313	CLA	CBA-CGA-O2A-C1
24	3	317	LHG	C24-C23-O8-C6
24	5	318	LHG	C24-C23-O8-C6
29	4	301	CHL	CBA-CGA-O2A-C1
22	A	817	CLA	O1A-CGA-O2A-C1
22	A	822	CLA	O1A-CGA-O2A-C1
22	3	305	CLA	O1A-CGA-O2A-C1
22	5	313	CLA	O1A-CGA-O2A-C1
22	7	304	CLA	O1A-CGA-O2A-C1
22	9	313	CLA	O1A-CGA-O2A-C1
29	2	301	CHL	O1A-CGA-O2A-C1
29	4	306	CHL	O1A-CGA-O2A-C1
28	B	849	DGD	C2B-C1B-O2G-C2G
31	8	319	LMG	C11-C10-O7-C8
22	7	302	CLA	CBA-CGA-O2A-C1
22	A	835	CLA	CBD-CGD-O2D-CED
22	B	818	CLA	CBD-CGD-O2D-CED
22	2	311	CLA	CBD-CGD-O2D-CED
22	4	309	CLA	CBD-CGD-O2D-CED
29	3	306	CHL	CBD-CGD-O2D-CED
22	1	309	CLA	C2C-C3C-CAC-CBC
22	A	837	CLA	O1A-CGA-O2A-C1
22	A	813	CLA	CBD-CGD-O2D-CED
22	B	824	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	C3-C5-C6-C7
22	4	312	CLA	C3-C5-C6-C7
22	B	816	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	824	CLA	CBA-CGA-O2A-C1
22	3	305	CLA	CBA-CGA-O2A-C1
29	5	301	CHL	CBA-CGA-O2A-C1
22	3	305	CLA	O1D-CGD-O2D-CED
29	4	305	CHL	O1D-CGD-O2D-CED
31	8	319	LMG	O6-C5-C6-O5
22	A	821	CLA	O1A-CGA-O2A-C1
22	6	312	CLA	C3-C5-C6-C7
31	5	319	LMG	O6-C5-C6-O5
22	B	830	CLA	C4-C3-C5-C6
22	B	837	CLA	C4-C3-C5-C6
22	1	311	CLA	C4-C3-C5-C6
29	4	301	CHL	C4-C3-C5-C6
22	B	830	CLA	C2-C3-C5-C6
22	B	837	CLA	C2-C3-C5-C6
22	1	311	CLA	C2-C3-C5-C6
29	4	301	CHL	C2-C3-C5-C6
22	A	836	CLA	CBD-CGD-O2D-CED
22	A	839	CLA	C2A-CAA-CBA-CGA
22	A	841	CLA	C2A-CAA-CBA-CGA
22	B	817	CLA	C2A-CAA-CBA-CGA
22	B	832	CLA	C2A-CAA-CBA-CGA
22	K	104	CLA	C2A-CAA-CBA-CGA
22	8	313	CLA	C2A-CAA-CBA-CGA
22	B	806	CLA	C2C-C3C-CAC-CBC
22	B	816	CLA	O1A-CGA-O2A-C1
22	B	831	CLA	O1A-CGA-O2A-C1
22	0	308	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	O1D-CGD-O2D-CED
22	1	309	CLA	C4C-C3C-CAC-CBC
22	6	323	CLA	O1A-CGA-O2A-C1
22	A	840	CLA	CBA-CGA-O2A-C1
22	1	312	CLA	CBA-CGA-O2A-C1
22	4	310	CLA	CBA-CGA-O2A-C1
22	9	303	CLA	CBA-CGA-O2A-C1
29	0	301	CHL	O1D-CGD-O2D-CED
28	B	849	DGD	O6E-C5E-C6E-O5E
22	A	839	CLA	O1D-CGD-O2D-CED
22	1	308	CLA	O1D-CGD-O2D-CED
22	5	310	CLA	O1D-CGD-O2D-CED
29	8	314	CHL	O1D-CGD-O2D-CED
22	5	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	4	301	CHL	O1A-CGA-O2A-C1
29	5	301	CHL	O1A-CGA-O2A-C1
22	3	301	CLA	O1D-CGD-O2D-CED
22	1	312	CLA	O1A-CGA-O2A-C1
22	4	310	CLA	O1A-CGA-O2A-C1
22	0	305	CLA	C2C-C3C-CAC-CBC
22	B	832	CLA	C3-C5-C6-C7
22	B	810	CLA	O1D-CGD-O2D-CED
29	4	307	CHL	O1D-CGD-O2D-CED
22	A	823	CLA	CBA-CGA-O2A-C1
22	A	841	CLA	CBA-CGA-O2A-C1
22	1	304	CLA	CBA-CGA-O2A-C1
22	1	311	CLA	CBA-CGA-O2A-C1
22	5	303	CLA	CBA-CGA-O2A-C1
22	7	312	CLA	CBA-CGA-O2A-C1
22	8	310	CLA	CBA-CGA-O2A-C1
22	0	304	CLA	CBA-CGA-O2A-C1
29	0	301	CHL	CBA-CGA-O2A-C1
29	4	301	CHL	C5-C6-C7-C8
22	B	821	CLA	CBD-CGD-O2D-CED
22	9	305	CLA	CBD-CGD-O2D-CED
25	A	847	8CT	C23-C24-C25-C26
25	A	849	8CT	C16-C17-C18-C19
25	B	804	8CT	C12-C13-C14-C15
25	B	804	8CT	C23-C24-C25-C26
25	B	848	8CT	C16-C17-C18-C19
25	1	316	8CT	C12-C13-C14-C15
25	7	323	8CT	C12-C13-C14-C15
30	1	314	XAT	C9-C10-C11-C12
24	1	317	LHG	C23-C24-C25-C26
22	H	201	CLA	C5-C6-C7-C8
22	5	312	CLA	C10-C11-C12-C13
22	9	303	CLA	O1A-CGA-O2A-C1
31	8	319	LMG	C4-C5-C6-O5
22	A	809	CLA	C8-C10-C11-C12
22	B	819	CLA	C10-C11-C12-C13
22	B	834	CLA	C8-C10-C11-C12
22	B	840	CLA	C5-C6-C7-C8
22	G	103	CLA	CBA-CGA-O2A-C1
31	5	319	LMG	C28-C29-C30-C31
22	1	303	CLA	C3-C5-C6-C7
22	6	301	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	0	304	CLA	C3-C5-C6-C7
22	3	308	CLA	O1D-CGD-O2D-CED
22	7	314	CLA	O1D-CGD-O2D-CED
24	A	844	LHG	O7-C5-C6-O8
22	8	310	CLA	O1A-CGA-O2A-C1
22	6	310	CLA	C4-C3-C5-C6
23	A	842	PQN	C14-C13-C15-C16
22	B	840	CLA	C2-C3-C5-C6
22	A	825	CLA	C6-C7-C8-C9
22	A	826	CLA	C14-C13-C15-C16
22	A	838	CLA	C11-C10-C8-C9
22	A	839	CLA	C6-C7-C8-C9
22	A	853	CLA	C6-C7-C8-C9
22	B	801	CLA	C6-C7-C8-C9
22	B	806	CLA	C6-C7-C8-C9
22	B	806	CLA	C14-C13-C15-C16
22	B	808	CLA	C11-C12-C13-C14
22	B	811	CLA	C6-C7-C8-C9
22	B	811	CLA	C14-C13-C15-C16
22	B	819	CLA	C6-C7-C8-C9
22	B	839	CLA	C11-C12-C13-C14
22	L	203	CLA	C11-C10-C8-C9
22	1	301	CLA	C11-C12-C13-C14
22	1	306	CLA	C6-C7-C8-C9
22	1	306	CLA	C14-C13-C15-C16
22	1	307	CLA	C6-C7-C8-C9
22	1	307	CLA	C11-C12-C13-C14
22	1	307	CLA	C14-C13-C15-C16
22	2	309	CLA	C11-C10-C8-C9
22	3	301	CLA	C11-C10-C8-C9
22	3	319	CLA	C11-C12-C13-C14
22	5	303	CLA	C11-C12-C13-C14
22	5	309	CLA	C6-C7-C8-C9
22	7	317	CLA	C11-C10-C8-C9
22	9	309	CLA	C6-C7-C8-C9
22	9	312	CLA	C11-C10-C8-C9
22	0	307	CLA	C6-C7-C8-C9
29	9	302	CHL	C6-C7-C8-C9
22	A	817	CLA	O1D-CGD-O2D-CED
22	A	833	CLA	O1D-CGD-O2D-CED
22	4	304	CLA	O1D-CGD-O2D-CED
22	6	323	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	1	305	CHL	O1D-CGD-O2D-CED
22	1	311	CLA	CBD-CGD-O2D-CED
22	1	302	CLA	C15-C16-C17-C18
22	5	311	CLA	C2A-CAA-CBA-CGA
29	8	307	CHL	C2A-CAA-CBA-CGA
25	A	846	8CT	C10-C11-C12-C40
25	A	846	8CT	C14-C15-C16-C39
25	A	846	8CT	C22-C21-C23-C24
25	A	847	8CT	C27-C26-C28-C29
25	A	848	8CT	C10-C11-C12-C40
25	A	850	8CT	C14-C15-C16-C39
25	A	850	8CT	C27-C26-C28-C29
25	B	804	8CT	C10-C11-C12-C40
25	B	804	8CT	C22-C21-C23-C24
25	B	845	8CT	C10-C11-C12-C40
25	B	847	8CT	C27-C26-C28-C29
25	B	848	8CT	C14-C15-C16-C39
25	G	104	8CT	C14-C15-C16-C39
25	L	206	8CT	C14-C15-C16-C39
25	2	317	8CT	C27-C26-C28-C29
25	3	316	8CT	C14-C15-C16-C39
25	4	317	8CT	C14-C15-C16-C39
25	5	317	8CT	C10-C11-C12-C40
25	7	301	8CT	C14-C15-C16-C39
25	7	323	8CT	C10-C11-C12-C40
25	7	323	8CT	C14-C15-C16-C39
25	8	301	8CT	C10-C11-C12-C40
25	8	301	8CT	C14-C15-C16-C39
25	8	318	8CT	C10-C11-C12-C40
25	8	318	8CT	C22-C21-C23-C24
30	1	314	XAT	C27-C28-C29-C39
30	2	316	XAT	C7-C8-C9-C19
30	4	315	XAT	C27-C28-C29-C39
30	7	319	XAT	C31-C32-C33-C40
30	8	316	XAT	C27-C28-C29-C39
25	A	846	8CT	C10-C11-C12-C13
25	A	846	8CT	C14-C15-C16-C17
25	A	847	8CT	C25-C26-C28-C29
25	A	848	8CT	C10-C11-C12-C13
25	A	849	8CT	C25-C26-C28-C29
25	A	850	8CT	C14-C15-C16-C17
25	A	850	8CT	C25-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
25	B	804	8CT	C10-C11-C12-C13
25	B	804	8CT	C20-C21-C23-C24
25	B	845	8CT	C10-C11-C12-C13
25	B	847	8CT	C25-C26-C28-C29
25	B	848	8CT	C14-C15-C16-C17
25	G	104	8CT	C14-C15-C16-C17
25	L	206	8CT	C14-C15-C16-C17
25	2	317	8CT	C25-C26-C28-C29
25	5	317	8CT	C10-C11-C12-C13
25	7	301	8CT	C14-C15-C16-C17
25	7	321	8CT	C10-C11-C12-C13
25	7	323	8CT	C10-C11-C12-C13
25	7	323	8CT	C14-C15-C16-C17
25	8	301	8CT	C10-C11-C12-C13
25	8	301	8CT	C14-C15-C16-C17
25	8	318	8CT	C10-C11-C12-C13
30	1	314	XAT	C27-C28-C29-C30
30	2	316	XAT	C7-C8-C9-C10
30	4	315	XAT	C27-C28-C29-C30
30	4	316	XAT	C27-C28-C29-C30
30	7	319	XAT	C31-C32-C33-C34
30	8	316	XAT	C27-C28-C29-C30
22	A	841	CLA	O1A-CGA-O2A-C1
22	5	303	CLA	O1A-CGA-O2A-C1
29	0	301	CHL	O1A-CGA-O2A-C1
22	A	811	CLA	C13-C15-C16-C17
22	A	818	CLA	C15-C16-C17-C18
22	A	829	CLA	C13-C15-C16-C17
22	6	313	CLA	C13-C15-C16-C17
29	2	301	CHL	C10-C11-C12-C13
29	4	305	CHL	C5-C6-C7-C8
22	G	102	CLA	O1D-CGD-O2D-CED
22	L	203	CLA	O1D-CGD-O2D-CED
26	A	851	HTG	O5-C5-C6-O6
22	2	303	CLA	O1D-CGD-O2D-CED
22	B	813	CLA	C3-C5-C6-C7
22	A	807	CLA	CBA-CGA-O2A-C1
22	8	315	CLA	CBA-CGA-O2A-C1
22	A	825	CLA	C13-C15-C16-C17
22	A	827	CLA	C8-C10-C11-C12
22	B	801	CLA	C5-C6-C7-C8
22	B	812	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	820	CLA	C8-C10-C11-C12
22	B	832	CLA	C8-C10-C11-C12
22	B	836	CLA	C5-C6-C7-C8
22	1	306	CLA	C10-C11-C12-C13
22	0	311	CLA	C15-C16-C17-C18
29	5	301	CHL	C5-C6-C7-C8
24	6	322	LHG	C23-C24-C25-C26
29	2	306	CHL	O1D-CGD-O2D-CED
22	1	307	CLA	CBD-CGD-O2D-CED
22	8	312	CLA	CBD-CGD-O2D-CED
29	0	306	CHL	C2C-C3C-CAC-CBC
22	A	828	CLA	C10-C11-C12-C13
22	A	828	CLA	C15-C16-C17-C18
22	A	840	CLA	C13-C15-C16-C17
22	B	808	CLA	C15-C16-C17-C18
22	B	809	CLA	C5-C6-C7-C8
22	B	809	CLA	C15-C16-C17-C18
22	B	810	CLA	C13-C15-C16-C17
22	B	811	CLA	C8-C10-C11-C12
22	B	817	CLA	C5-C6-C7-C8
22	B	830	CLA	C5-C6-C7-C8
22	B	832	CLA	C15-C16-C17-C18
22	2	303	CLA	C8-C10-C11-C12
22	6	303	CLA	C10-C11-C12-C13
22	6	304	CLA	C5-C6-C7-C8
22	6	304	CLA	C15-C16-C17-C18
22	6	310	CLA	C8-C10-C11-C12
22	6	311	CLA	C15-C16-C17-C18
22	8	309	CLA	C10-C11-C12-C13
22	9	308	CLA	C5-C6-C7-C8
23	A	842	PQN	C15-C16-C17-C18
29	6	302	CHL	C10-C11-C12-C13
29	0	301	CHL	C8-C10-C11-C12
22	7	302	CLA	O1A-CGA-O2A-C1
24	3	317	LHG	O1-C1-C2-O2
24	A	844	LHG	C23-C24-C25-C26
24	6	322	LHG	C7-C8-C9-C10
22	1	313	CLA	CBD-CGD-O2D-CED
22	A	838	CLA	C5-C6-C7-C8
22	B	834	CLA	C5-C6-C7-C8
22	2	309	CLA	C8-C10-C11-C12
22	7	318	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	A	805	CLA	C2-C1-O2A-CGA
22	A	841	CLA	C2-C1-O2A-CGA
22	B	834	CLA	C2-C1-O2A-CGA
22	5	303	CLA	C2-C1-O2A-CGA
22	8	315	CLA	C2-C1-O2A-CGA
24	5	318	LHG	C32-C33-C34-C35
22	B	816	CLA	C5-C6-C7-C8
22	6	311	CLA	C5-C6-C7-C8
22	5	307	CLA	C10-C11-C12-C13
22	0	302	CLA	C5-C6-C7-C8
24	9	316	LHG	C23-C24-C25-C26
22	7	318	CLA	CBD-CGD-O2D-CED
22	3	319	CLA	C5-C6-C7-C8
22	6	313	CLA	C15-C16-C17-C18
22	1	301	CLA	O1D-CGD-O2D-CED
22	0	304	CLA	O1D-CGD-O2D-CED
22	A	809	CLA	C6-C7-C8-C10
22	A	827	CLA	C6-C7-C8-C10
22	A	828	CLA	C11-C10-C8-C7
22	A	838	CLA	C11-C12-C13-C15
22	A	840	CLA	C6-C7-C8-C10
22	B	803	CLA	C6-C7-C8-C10
22	B	809	CLA	C11-C10-C8-C7
22	B	833	CLA	C6-C7-C8-C10
22	B	837	CLA	C6-C7-C8-C10
22	H	201	CLA	C11-C12-C13-C15
22	3	301	CLA	C11-C10-C8-C7
22	5	307	CLA	C12-C13-C15-C16
22	7	316	CLA	C12-C13-C15-C16
22	8	315	CLA	C12-C13-C15-C16
22	9	308	CLA	C12-C13-C15-C16
22	A	821	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	6	304	CLA	C3-C5-C6-C7
23	B	842	PQN	C13-C15-C16-C17
22	1	311	CLA	O1A-CGA-O2A-C1
22	7	312	CLA	O1A-CGA-O2A-C1
25	A	846	8CT	C12-C13-C14-C15
25	A	854	8CT	C23-C24-C25-C26
25	B	847	8CT	C12-C13-C14-C15
25	B	851	8CT	C18-C19-C20-C21
25	G	104	8CT	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	I	101	8CT	C18-C19-C20-C21
25	J	101	8CT	C23-C24-C25-C26
25	3	316	8CT	C18-C19-C20-C21
25	6	321	8CT	C18-C19-C20-C21
25	8	301	8CT	C12-C13-C14-C15
25	8	318	8CT	C16-C17-C18-C19
30	0	313	XAT	C33-C34-C35-C15
22	9	312	CLA	CBA-CGA-O2A-C1
22	A	808	CLA	C2A-CAA-CBA-CGA
22	A	840	CLA	C2A-CAA-CBA-CGA
22	B	803	CLA	C2A-CAA-CBA-CGA
22	B	822	CLA	C2A-CAA-CBA-CGA
22	K	102	CLA	C2A-CAA-CBA-CGA
22	4	310	CLA	C2A-CAA-CBA-CGA
22	6	317	CLA	C2A-CAA-CBA-CGA
22	7	305	CLA	C2A-CAA-CBA-CGA
22	8	304	CLA	C2A-CAA-CBA-CGA
29	5	306	CHL	C2A-CAA-CBA-CGA
22	A	804	CLA	O1D-CGD-O2D-CED
22	A	819	CLA	O1D-CGD-O2D-CED
22	A	820	CLA	O1D-CGD-O2D-CED
22	B	819	CLA	O1D-CGD-O2D-CED
22	B	837	CLA	O1D-CGD-O2D-CED
22	7	313	CLA	O1D-CGD-O2D-CED
22	7	315	CLA	O1D-CGD-O2D-CED
29	8	305	CHL	O1D-CGD-O2D-CED
22	A	826	CLA	C13-C15-C16-C17
22	A	832	CLA	C10-C11-C12-C13
22	B	809	CLA	C10-C11-C12-C13
22	B	818	CLA	C5-C6-C7-C8
22	2	302	CLA	C5-C6-C7-C8
22	2	302	CLA	C13-C15-C16-C17
22	2	309	CLA	C10-C11-C12-C13
22	4	309	CLA	C10-C11-C12-C13
22	9	309	CLA	C5-C6-C7-C8
23	B	842	PQN	C18-C20-C21-C22
22	0	304	CLA	O1A-CGA-O2A-C1
22	B	809	CLA	CBD-CGD-O2D-CED
29	2	301	CHL	CBD-CGD-O2D-CED
22	A	836	CLA	C2C-C3C-CAC-CBC
24	7	322	LHG	O2-C2-C3-O3
31	8	319	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
22	A	827	CLA	C3-C5-C6-C7
29	6	302	CHL	C3-C5-C6-C7
22	B	803	CLA	C13-C15-C16-C17
22	B	810	CLA	C10-C11-C12-C13
22	B	811	CLA	C13-C15-C16-C17
22	B	828	CLA	C8-C10-C11-C12
22	B	836	CLA	C8-C10-C11-C12
22	1	306	CLA	C8-C10-C11-C12
22	5	307	CLA	C5-C6-C7-C8
22	8	309	CLA	C5-C6-C7-C8
22	0	307	CLA	C10-C11-C12-C13
22	A	823	CLA	O1A-CGA-O2A-C1
22	A	840	CLA	O1A-CGA-O2A-C1
22	1	304	CLA	O1A-CGA-O2A-C1
22	1	313	CLA	CBA-CGA-O2A-C1
22	A	810	CLA	O1D-CGD-O2D-CED
22	A	821	CLA	C15-C16-C17-C18
22	A	826	CLA	C15-C16-C17-C18
22	B	808	CLA	C8-C10-C11-C12
22	B	820	CLA	C10-C11-C12-C13
22	B	824	CLA	C5-C6-C7-C8
22	B	825	CLA	C13-C15-C16-C17
22	B	841	CLA	C10-C11-C12-C13
22	L	202	CLA	C13-C15-C16-C17
22	1	302	CLA	C5-C6-C7-C8
22	1	311	CLA	C13-C15-C16-C17
22	4	314	CLA	C8-C10-C11-C12
22	7	318	CLA	C5-C6-C7-C8
22	0	303	CLA	C5-C6-C7-C8
29	4	301	CHL	C10-C11-C12-C13
22	B	841	CLA	O1D-CGD-O2D-CED
22	5	309	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	O1A-CGA-O2A-C1
22	8	315	CLA	O1A-CGA-O2A-C1
22	0	305	CLA	C4C-C3C-CAC-CBC
22	A	828	CLA	C13-C15-C16-C17
22	A	839	CLA	C8-C10-C11-C12
22	A	841	CLA	C15-C16-C17-C18
22	B	806	CLA	C8-C10-C11-C12
22	B	814	CLA	C10-C11-C12-C13
22	2	304	CLA	C10-C11-C12-C13
22	3	319	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	6	305	CLA	C10-C11-C12-C13
22	8	315	CLA	C13-C15-C16-C17
22	0	308	CLA	C10-C11-C12-C13
23	B	842	PQN	C20-C21-C22-C23
24	A	845	LHG	C3-O3-P-O6
24	A	845	LHG	C4-O6-P-O3
24	2	318	LHG	C3-O3-P-O6
24	2	318	LHG	C4-O6-P-O3
24	5	318	LHG	C4-O6-P-O3
24	7	322	LHG	C3-O3-P-O6
24	7	322	LHG	C4-O6-P-O3
24	0	315	LHG	C3-O3-P-O6
24	5	318	LHG	C7-C8-C9-C10
22	9	308	CLA	C3-C5-C6-C7
22	3	307	CLA	CBA-CGA-O2A-C1
22	4	304	CLA	CBA-CGA-O2A-C1
22	6	313	CLA	CBA-CGA-O2A-C1
29	5	306	CHL	CBA-CGA-O2A-C1
29	9	302	CHL	CBA-CGA-O2A-C1
22	A	806	CLA	C8-C10-C11-C12
22	B	832	CLA	C10-C11-C12-C13
22	9	304	CLA	O1D-CGD-O2D-CED
24	A	845	LHG	C1-C2-C3-O3
24	1	317	LHG	C1-C2-C3-O3
24	7	322	LHG	C1-C2-C3-O3
22	A	828	CLA	C4-C3-C5-C6
22	A	832	CLA	C4-C3-C5-C6
22	9	308	CLA	C4-C3-C5-C6
22	5	303	CLA	C2-C3-C5-C6
22	A	825	CLA	C10-C11-C12-C13
22	1	302	CLA	C10-C11-C12-C13
22	7	303	CLA	C5-C6-C7-C8
22	B	815	CLA	C2A-CAA-CBA-CGA
22	7	313	CLA	C2A-CAA-CBA-CGA
22	9	306	CLA	C2A-CAA-CBA-CGA
22	0	308	CLA	C2A-CAA-CBA-CGA
22	M	101	CLA	C2A-CAA-CBA-CGA
22	B	803	CLA	C16-C17-C18-C19
22	L	203	CLA	C16-C17-C18-C19
22	2	304	CLA	C11-C12-C13-C15
22	3	319	CLA	C16-C17-C18-C19
22	7	303	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	A	808	CLA	C3-C5-C6-C7
22	A	809	CLA	C3-C5-C6-C7
22	1	302	CLA	C3-C5-C6-C7
22	A	824	CLA	CBA-CGA-O2A-C1
22	2	314	CLA	CBA-CGA-O2A-C1
22	0	311	CLA	CBA-CGA-O2A-C1
29	6	316	CHL	O1D-CGD-O2D-CED
25	A	846	8CT	C16-C17-C18-C19
25	F	302	8CT	C12-C13-C14-C15
25	I	101	8CT	C16-C17-C18-C19
25	L	206	8CT	C12-C13-C14-C15
25	L	206	8CT	C16-C17-C18-C19
25	L	206	8CT	C18-C19-C20-C21
25	1	316	8CT	C23-C24-C25-C26
24	5	318	LHG	C11-C10-C9-C8
31	5	319	LMG	C17-C18-C19-C20
22	6	318	CLA	CBD-CGD-O2D-CED
24	A	844	LHG	C8-C7-O7-C5
24	0	315	LHG	C8-C7-O7-C5
22	A	830	CLA	C13-C15-C16-C17
22	B	830	CLA	C10-C11-C12-C13
22	5	312	CLA	C13-C15-C16-C17
22	0	312	CLA	C5-C6-C7-C8
22	B	809	CLA	C3-C5-C6-C7
22	B	812	CLA	C3-C5-C6-C7
22	B	841	CLA	C3-C5-C6-C7
22	0	307	CLA	C3-C5-C6-C7
24	A	844	LHG	C27-C28-C29-C30
24	A	845	LHG	C9-C10-C11-C12
24	1	317	LHG	C13-C14-C15-C16
24	1	317	LHG	C14-C15-C16-C17
22	A	827	CLA	C16-C17-C18-C19
22	B	813	CLA	C6-C7-C8-C10
22	L	201	CLA	C16-C17-C18-C19
22	6	305	CLA	C11-C12-C13-C14
22	6	311	CLA	C16-C17-C18-C19
22	8	302	CLA	C11-C12-C13-C15
22	9	309	CLA	C11-C12-C13-C14
29	4	305	CHL	C6-C7-C8-C9
22	A	801	CLA	CBA-CGA-O2A-C1
22	B	826	CLA	CBA-CGA-O2A-C1
22	9	306	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	6	322	LHG	C26-C27-C28-C29
24	5	318	LHG	C13-C14-C15-C16
22	A	807	CLA	C13-C15-C16-C17
22	2	302	CLA	C15-C16-C17-C18
31	8	319	LMG	C10-C11-C12-C13
22	A	828	CLA	CBD-CGD-O2D-CED
31	4	318	LMG	C21-C22-C23-C24
22	A	809	CLA	O1D-CGD-O2D-CED
22	1	312	CLA	O1D-CGD-O2D-CED
22	5	305	CLA	C3-C5-C6-C7
28	B	849	DGD	C2E-C1E-O5D-C6D
22	2	312	CLA	CBA-CGA-O2A-C1
29	8	305	CHL	CBA-CGA-O2A-C1
24	0	315	LHG	C34-C35-C36-C37
22	1	301	CLA	C16-C17-C18-C19
22	7	317	CLA	C16-C17-C18-C19
22	0	307	CLA	C16-C17-C18-C19
29	6	302	CHL	C11-C12-C13-C15
22	A	801	CLA	C4-C3-C5-C6
22	A	808	CLA	C4-C3-C5-C6
22	B	805	CLA	C4-C3-C5-C6
22	2	312	CLA	C4-C3-C5-C6
22	5	305	CLA	C4-C3-C5-C6
22	0	307	CLA	C4-C3-C5-C6
24	A	844	LHG	C10-C11-C12-C13
24	1	317	LHG	C9-C10-C11-C12
24	6	322	LHG	C24-C25-C26-C27
24	0	315	LHG	C9-C10-C11-C12
24	0	315	LHG	C12-C13-C14-C15
22	A	808	CLA	C2-C3-C5-C6
22	9	308	CLA	C2-C3-C5-C6
22	A	805	CLA	C11-C12-C13-C14
22	A	808	CLA	C11-C12-C13-C14
22	A	826	CLA	C11-C12-C13-C14
22	A	827	CLA	C6-C7-C8-C9
22	A	837	CLA	C6-C7-C8-C9
22	A	838	CLA	C6-C7-C8-C9
22	B	806	CLA	C11-C10-C8-C9
22	B	827	CLA	C11-C10-C8-C9
22	3	319	CLA	C11-C10-C8-C9
22	0	308	CLA	C6-C7-C8-C9
22	9	301	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	8	307	CHL	O1D-CGD-O2D-CED
31	4	318	LMG	C28-C29-C30-C31
24	1	317	LHG	C15-C16-C17-C18
24	1	317	LHG	C32-C33-C34-C35
22	A	826	CLA	C8-C10-C11-C12
22	3	311	CLA	C5-C6-C7-C8
29	5	301	CHL	C8-C10-C11-C12
22	A	829	CLA	C2A-CAA-CBA-CGA
22	A	843	CLA	C2A-CAA-CBA-CGA
22	3	312	CLA	C2A-CAA-CBA-CGA
22	6	313	CLA	C2A-CAA-CBA-CGA
22	7	303	CLA	C2A-CAA-CBA-CGA
22	9	312	CLA	O1A-CGA-O2A-C1
25	A	849	8CT	C27-C26-C28-C29
25	B	804	8CT	C14-C15-C16-C39
25	F	302	8CT	C10-C11-C12-C40
25	L	206	8CT	C10-C11-C12-C40
25	2	317	8CT	C22-C21-C23-C24
25	6	321	8CT	C22-C21-C23-C24
25	7	301	8CT	C22-C21-C23-C24
25	7	321	8CT	C10-C11-C12-C40
25	7	323	8CT	C22-C21-C23-C24
30	4	316	XAT	C27-C28-C29-C39
24	B	852	LHG	O1-C1-C2-C3
24	1	317	LHG	O1-C1-C2-C3
24	2	318	LHG	O1-C1-C2-C3
24	5	318	LHG	O1-C1-C2-C3
24	9	316	LHG	O1-C1-C2-C3
25	B	804	8CT	C14-C15-C16-C17
25	B	846	8CT	C25-C26-C28-C29
25	B	848	8CT	C10-C11-C12-C13
25	F	302	8CT	C10-C11-C12-C13
25	L	206	8CT	C10-C11-C12-C13
25	2	317	8CT	C20-C21-C23-C24
25	3	316	8CT	C14-C15-C16-C17
25	6	321	8CT	C20-C21-C23-C24
25	7	301	8CT	C20-C21-C23-C24
25	7	321	8CT	C20-C21-C23-C24
25	7	323	8CT	C20-C21-C23-C24
30	0	313	XAT	C7-C8-C9-C10
22	B	834	CLA	C10-C11-C12-C13
22	6	310	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	5	318	LHG	C27-C28-C29-C30
28	B	849	DGD	C8A-C9A-CAA-CBA
28	B	849	DGD	CAA-CBA-CCA-CDA
22	3	312	CLA	CBD-CGD-O2D-CED
24	2	318	LHG	C23-C24-C25-C26
24	9	316	LHG	C16-C17-C18-C19
22	A	818	CLA	C4B-C3B-CAB-CBB
22	A	833	CLA	C4B-C3B-CAB-CBB
22	B	817	CLA	C4B-C3B-CAB-CBB
22	B	824	CLA	C4B-C3B-CAB-CBB
22	B	833	CLA	C4B-C3B-CAB-CBB
22	G	101	CLA	C4B-C3B-CAB-CBB
22	L	203	CLA	C4B-C3B-CAB-CBB
22	1	302	CLA	C4B-C3B-CAB-CBB
22	1	309	CLA	C4B-C3B-CAB-CBB
22	3	304	CLA	C4B-C3B-CAB-CBB
22	3	307	CLA	C4B-C3B-CAB-CBB
22	6	301	CLA	C4B-C3B-CAB-CBB
22	6	311	CLA	C4B-C3B-CAB-CBB
22	6	317	CLA	C4B-C3B-CAB-CBB
22	5	303	CLA	C4B-C3B-CAB-CBB
22	5	305	CLA	C4B-C3B-CAB-CBB
22	5	310	CLA	C4B-C3B-CAB-CBB
22	7	311	CLA	C4B-C3B-CAB-CBB
22	8	312	CLA	C4B-C3B-CAB-CBB
22	9	310	CLA	C4B-C3B-CAB-CBB
22	9	311	CLA	C4B-C3B-CAB-CBB
22	0	305	CLA	C4B-C3B-CAB-CBB
22	0	310	CLA	C4B-C3B-CAB-CBB
22	A	824	CLA	C6-C7-C8-C10
22	B	803	CLA	C16-C17-C18-C20
22	B	815	CLA	C16-C17-C18-C19
22	B	825	CLA	C16-C17-C18-C19
22	B	825	CLA	C16-C17-C18-C20
22	L	201	CLA	C16-C17-C18-C20
22	L	203	CLA	C16-C17-C18-C20
22	2	304	CLA	C11-C12-C13-C14
22	2	312	CLA	C16-C17-C18-C20
22	7	303	CLA	C11-C12-C13-C14
22	8	302	CLA	C11-C12-C13-C14
29	4	305	CHL	C6-C7-C8-C10
28	B	849	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
22	A	853	CLA	C15-C16-C17-C18
22	1	308	CLA	C8-C10-C11-C12
22	0	302	CLA	C15-C16-C17-C18
28	B	849	DGD	C9B-CAB-CBB-CCB
22	3	304	CLA	CBD-CGD-O2D-CED
22	2	313	CLA	O1D-CGD-O2D-CED
31	4	318	LMG	C17-C18-C19-C20
24	A	844	LHG	C7-C8-C9-C10
24	5	318	LHG	C23-C24-C25-C26
22	0	307	CLA	C8-C10-C11-C12
29	9	302	CHL	C5-C6-C7-C8
22	2	314	CLA	O1A-CGA-O2A-C1
22	4	304	CLA	O1A-CGA-O2A-C1
29	5	306	CHL	O1A-CGA-O2A-C1
24	1	317	LHG	C27-C28-C29-C30
22	A	818	CLA	C3-C5-C6-C7
22	0	302	CLA	C3-C5-C6-C7
22	2	308	CLA	CBA-CGA-O2A-C1
22	2	311	CLA	CBA-CGA-O2A-C1
24	A	844	LHG	C9-C10-C11-C12
31	4	318	LMG	C18-C19-C20-C21
22	0	312	CLA	O1D-CGD-O2D-CED
29	8	306	CHL	O1D-CGD-O2D-CED
22	A	803	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	C3A-C2A-CAA-CBA
22	A	813	CLA	C3A-C2A-CAA-CBA
22	A	853	CLA	C3A-C2A-CAA-CBA
22	B	829	CLA	C3A-C2A-CAA-CBA
22	B	832	CLA	C3A-C2A-CAA-CBA
22	B	850	CLA	C3A-C2A-CAA-CBA
22	H	201	CLA	C3A-C2A-CAA-CBA
22	1	302	CLA	C3A-C2A-CAA-CBA
22	1	304	CLA	C3A-C2A-CAA-CBA
22	1	310	CLA	C3A-C2A-CAA-CBA
22	3	311	CLA	C3A-C2A-CAA-CBA
22	7	318	CLA	C3A-C2A-CAA-CBA
22	9	311	CLA	C3A-C2A-CAA-CBA
22	0	312	CLA	C3A-C2A-CAA-CBA
22	5	303	CLA	C15-C16-C17-C18
22	A	835	CLA	O1D-CGD-O2D-CED
22	8	309	CLA	O1D-CGD-O2D-CED
22	3	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	6	313	CLA	O1A-CGA-O2A-C1
22	B	815	CLA	C16-C17-C18-C20
22	B	836	CLA	C11-C12-C13-C14
22	1	301	CLA	C16-C17-C18-C20
22	2	312	CLA	C16-C17-C18-C19
22	3	301	CLA	C11-C12-C13-C14
22	9	309	CLA	C11-C12-C13-C15
29	6	302	CHL	C11-C12-C13-C14
29	0	301	CHL	C11-C12-C13-C15
24	A	844	LHG	C12-C13-C14-C15
29	5	301	CHL	CBD-CGD-O2D-CED
22	L	202	CLA	C3-C5-C6-C7
22	7	316	CLA	C10-C11-C12-C13
22	9	308	CLA	C15-C16-C17-C18
22	0	307	CLA	C15-C16-C17-C18
22	A	817	CLA	C4-C3-C5-C6
22	A	825	CLA	C4-C3-C5-C6
22	B	808	CLA	C4-C3-C5-C6
22	1	306	CLA	C4-C3-C5-C6
22	1	307	CLA	C4-C3-C5-C6
22	3	311	CLA	C4-C3-C5-C6
22	A	801	CLA	C2-C3-C5-C6
22	A	825	CLA	C2-C3-C5-C6
22	B	808	CLA	C2-C3-C5-C6
22	1	306	CLA	C2-C3-C5-C6
22	3	311	CLA	C2-C3-C5-C6
22	5	305	CLA	C2-C3-C5-C6
24	6	322	LHG	C8-C7-O7-C5
24	1	317	LHG	O1-C1-C2-O2
24	6	322	LHG	O1-C1-C2-O2
24	7	322	LHG	O1-C1-C2-O2
24	6	322	LHG	C25-C26-C27-C28
31	5	319	LMG	C18-C19-C20-C21
31	8	319	LMG	C16-C17-C18-C19
24	B	852	LHG	C7-C8-C9-C10
22	A	824	CLA	O1A-CGA-O2A-C1
29	9	302	CHL	O1A-CGA-O2A-C1
22	B	813	CLA	C6-C7-C8-C9
22	B	819	CLA	C11-C12-C13-C14
22	1	302	CLA	C16-C17-C18-C19
22	6	311	CLA	C16-C17-C18-C20
22	B	806	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	G	103	CLA	O1A-CGA-O2A-C1
22	A	818	CLA	C2B-C3B-CAB-CBB
22	A	826	CLA	C2B-C3B-CAB-CBB
22	A	832	CLA	C2B-C3B-CAB-CBB
22	A	833	CLA	C2B-C3B-CAB-CBB
22	B	817	CLA	C2B-C3B-CAB-CBB
22	B	822	CLA	C2B-C3B-CAB-CBB
22	B	833	CLA	C2B-C3B-CAB-CBB
22	B	839	CLA	C2B-C3B-CAB-CBB
22	L	203	CLA	C2B-C3B-CAB-CBB
22	1	302	CLA	C2B-C3B-CAB-CBB
22	1	309	CLA	C2B-C3B-CAB-CBB
22	1	313	CLA	C2B-C3B-CAB-CBB
22	2	319	CLA	C2B-C3B-CAB-CBB
22	3	304	CLA	C2B-C3B-CAB-CBB
22	6	301	CLA	C2B-C3B-CAB-CBB
22	6	311	CLA	C2B-C3B-CAB-CBB
22	6	317	CLA	C2B-C3B-CAB-CBB
22	5	303	CLA	C2B-C3B-CAB-CBB
22	5	305	CLA	C2B-C3B-CAB-CBB
22	5	310	CLA	C2B-C3B-CAB-CBB
22	5	313	CLA	C2B-C3B-CAB-CBB
22	7	309	CLA	C2B-C3B-CAB-CBB
22	7	311	CLA	C2B-C3B-CAB-CBB
22	7	314	CLA	C2B-C3B-CAB-CBB
22	7	318	CLA	C2B-C3B-CAB-CBB
22	8	312	CLA	C2B-C3B-CAB-CBB
22	9	310	CLA	C2B-C3B-CAB-CBB
22	9	311	CLA	C2B-C3B-CAB-CBB
22	0	305	CLA	C2B-C3B-CAB-CBB
22	0	310	CLA	C2B-C3B-CAB-CBB
29	2	307	CHL	C2B-C3B-CAB-CBB
22	0	311	CLA	O1A-CGA-O2A-C1
22	A	825	CLA	C15-C16-C17-C18
22	B	814	CLA	C13-C15-C16-C17
22	6	303	CLA	C13-C15-C16-C17
24	A	844	LHG	C11-C10-C9-C8
24	1	317	LHG	C11-C10-C9-C8
28	B	849	DGD	C7B-C8B-C9B-CAB
22	A	843	CLA	C2-C1-O2A-CGA
22	4	314	CLA	C2-C1-O2A-CGA
22	B	801	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	B	803	CLA	C8-C10-C11-C12
22	L	201	CLA	C15-C16-C17-C18
22	L	203	CLA	C5-C6-C7-C8
22	B	826	CLA	O1A-CGA-O2A-C1
22	2	312	CLA	O1A-CGA-O2A-C1
22	9	306	CLA	O1A-CGA-O2A-C1
29	8	305	CHL	O1A-CGA-O2A-C1
22	6	305	CLA	C11-C12-C13-C15
22	0	307	CLA	C16-C17-C18-C20
22	B	811	CLA	C3-C5-C6-C7
25	A	848	8CT	C04-C03-C10-C11
25	B	804	8CT	C02-C03-C10-C11
25	B	843	8CT	C02-C03-C10-C11
25	B	843	8CT	C04-C03-C10-C11
25	B	851	8CT	C02-C03-C10-C11
25	F	302	8CT	C04-C03-C10-C11
25	G	104	8CT	C04-C03-C10-C11
25	I	101	8CT	C02-C03-C10-C11
25	I	101	8CT	C04-C03-C10-C11
25	J	101	8CT	C02-C03-C10-C11
25	J	101	8CT	C04-C03-C10-C11
25	K	103	8CT	C02-C03-C10-C11
25	L	205	8CT	C04-C03-C10-C11
25	L	206	8CT	C02-C03-C10-C11
25	3	316	8CT	C02-C03-C10-C11
25	6	321	8CT	C02-C03-C10-C11
25	5	317	8CT	C02-C03-C10-C11
25	7	321	8CT	C02-C03-C10-C11
25	8	318	8CT	C02-C03-C10-C11
24	0	315	LHG	C33-C34-C35-C36
22	A	807	CLA	C8-C10-C11-C12
22	A	807	CLA	C15-C16-C17-C18
22	A	833	CLA	C8-C10-C11-C12
22	B	806	CLA	C10-C11-C12-C13
22	B	814	CLA	C8-C10-C11-C12
22	0	303	CLA	C15-C16-C17-C18
22	0	311	CLA	C5-C6-C7-C8
22	4	309	CLA	O1D-CGD-O2D-CED
22	A	801	CLA	O1A-CGA-O2A-C1
31	4	318	LMG	C10-C11-C12-C13
24	5	318	LHG	C30-C31-C32-C33
31	8	319	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	A	838	CLA	C4-C3-C5-C6
22	B	850	CLA	O1D-CGD-O2D-CED
22	2	311	CLA	O1D-CGD-O2D-CED
22	A	803	CLA	C12-C13-C15-C16
22	A	805	CLA	C11-C12-C13-C15
22	A	806	CLA	C11-C12-C13-C15
22	A	807	CLA	C11-C12-C13-C15
22	A	811	CLA	C12-C13-C15-C16
22	A	818	CLA	C11-C12-C13-C15
22	A	825	CLA	C11-C10-C8-C7
22	A	826	CLA	C11-C12-C13-C15
22	A	837	CLA	C6-C7-C8-C10
22	A	837	CLA	C12-C13-C15-C16
22	A	838	CLA	C2-C3-C5-C6
22	A	838	CLA	C6-C7-C8-C10
22	A	838	CLA	C11-C10-C8-C7
22	A	838	CLA	C12-C13-C15-C16
22	A	839	CLA	C6-C7-C8-C10
22	B	805	CLA	C2-C3-C5-C6
22	B	806	CLA	C11-C10-C8-C7
22	B	811	CLA	C6-C7-C8-C10
22	B	827	CLA	C11-C10-C8-C7
22	B	832	CLA	C2-C3-C5-C6
22	1	306	CLA	C6-C7-C8-C10
22	1	307	CLA	C2-C3-C5-C6
22	2	304	CLA	C11-C10-C8-C7
22	2	312	CLA	C2-C3-C5-C6
22	3	319	CLA	C11-C10-C8-C7
22	5	303	CLA	C6-C7-C8-C10
22	7	316	CLA	C11-C12-C13-C15
22	7	317	CLA	C11-C10-C8-C7
22	7	318	CLA	C11-C12-C13-C15
22	0	303	CLA	C11-C12-C13-C15
22	0	307	CLA	C11-C12-C13-C15
22	0	308	CLA	C6-C7-C8-C10
22	2	308	CLA	O1A-CGA-O2A-C1
22	2	311	CLA	O1A-CGA-O2A-C1
24	2	318	LHG	O10-C23-O8-C6
22	2	309	CLA	C5-C6-C7-C8
22	2	312	CLA	C13-C15-C16-C17
25	B	845	8CT	C12-C13-C14-C15
22	6	303	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	7	317	CLA	C16-C17-C18-C20
24	0	315	LHG	O9-C7-O7-C5
22	A	804	CLA	CBA-CGA-O2A-C1
22	A	830	CLA	CBA-CGA-O2A-C1
22	B	813	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	CBA-CGA-O2A-C1
22	B	839	CLA	CBA-CGA-O2A-C1
22	8	304	CLA	CBA-CGA-O2A-C1
22	9	305	CLA	CBA-CGA-O2A-C1
22	9	309	CLA	CBA-CGA-O2A-C1
26	A	851	HTG	C4-C5-C6-O6
22	A	817	CLA	C2A-CAA-CBA-CGA
22	B	807	CLA	C2A-CAA-CBA-CGA
22	G	101	CLA	C2A-CAA-CBA-CGA
22	1	307	CLA	C2A-CAA-CBA-CGA
29	8	306	CHL	C2A-CAA-CBA-CGA
22	1	306	CLA	C13-C15-C16-C17
22	5	307	CLA	C13-C15-C16-C17
22	0	307	CLA	C5-C6-C7-C8
31	4	318	LMG	O6-C5-C6-O5
24	2	318	LHG	C7-C8-C9-C10
22	A	811	CLA	C8-C10-C11-C12
22	B	806	CLA	C5-C6-C7-C8
22	A	853	CLA	C3-C5-C6-C7
29	6	316	CHL	C2C-C3C-CAC-CBC
31	5	319	LMG	C16-C17-C18-C19
22	7	318	CLA	O1D-CGD-O2D-CED
29	3	306	CHL	O1D-CGD-O2D-CED
24	9	316	LHG	C8-C7-O7-C5
22	A	803	CLA	C5-C6-C7-C8
22	A	808	CLA	C15-C16-C17-C18
22	0	311	CLA	C10-C11-C12-C13
24	0	315	LHG	C27-C28-C29-C30
22	A	819	CLA	C3-C5-C6-C7
28	B	849	DGD	C1B-C2B-C3B-C4B
24	5	318	LHG	O7-C5-C6-O8
26	J	102	HTG	O5-C5-C6-O6
28	B	849	DGD	C4B-C5B-C6B-C7B
22	A	827	CLA	C16-C17-C18-C20
22	3	319	CLA	C16-C17-C18-C20
22	5	303	CLA	C16-C17-C18-C19
24	A	844	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
22	6	315	CLA	C5-C6-C7-C8
22	B	818	CLA	O1D-CGD-O2D-CED
22	A	829	CLA	C4-C3-C5-C6
22	B	832	CLA	C4-C3-C5-C6
22	0	302	CLA	C4-C3-C5-C6
22	A	828	CLA	C2-C3-C5-C6
22	A	832	CLA	C2-C3-C5-C6
22	6	310	CLA	C2-C3-C5-C6
22	0	307	CLA	C2-C3-C5-C6
23	A	842	PQN	C12-C13-C15-C16
26	J	102	HTG	C3'-C4'-C5'-C6'
22	A	803	CLA	C14-C13-C15-C16
22	A	806	CLA	C11-C12-C13-C14
22	A	807	CLA	C6-C7-C8-C9
22	A	817	CLA	C11-C10-C8-C9
22	A	817	CLA	C11-C12-C13-C14
22	A	818	CLA	C11-C12-C13-C14
22	A	826	CLA	C11-C10-C8-C9
22	A	828	CLA	C11-C10-C8-C9
22	A	838	CLA	C11-C12-C13-C14
22	B	809	CLA	C14-C13-C15-C16
22	B	832	CLA	C6-C7-C8-C9
22	B	833	CLA	C6-C7-C8-C9
22	B	836	CLA	C6-C7-C8-C9
22	B	837	CLA	C6-C7-C8-C9
22	B	839	CLA	C14-C13-C15-C16
22	H	201	CLA	C11-C12-C13-C14
22	2	304	CLA	C11-C10-C8-C9
22	4	314	CLA	C14-C13-C15-C16
22	6	315	CLA	C14-C13-C15-C16
22	7	303	CLA	C6-C7-C8-C9
22	7	316	CLA	C11-C12-C13-C14
22	7	318	CLA	C11-C12-C13-C14
22	9	308	CLA	C14-C13-C15-C16
22	0	303	CLA	C11-C12-C13-C14
29	2	301	CHL	C6-C7-C8-C9
22	A	838	CLA	CBD-CGD-O2D-CED
22	B	831	CLA	CBD-CGD-O2D-CED
22	2	309	CLA	CBD-CGD-O2D-CED
29	5	301	CHL	C3-C5-C6-C7
22	A	806	CLA	C2A-CAA-CBA-CGA
22	A	828	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	852	CLA	C2A-CAA-CBA-CGA
22	B	828	CLA	C2A-CAA-CBA-CGA
22	1	303	CLA	C2A-CAA-CBA-CGA
22	3	311	CLA	C2A-CAA-CBA-CGA
22	9	303	CLA	C2A-CAA-CBA-CGA
24	1	317	LHG	C12-C13-C14-C15
25	B	848	8CT	C10-C11-C12-C40
25	4	317	8CT	C10-C11-C12-C40
22	1	311	CLA	O1D-CGD-O2D-CED
22	B	837	CLA	C15-C16-C17-C18
24	A	844	LHG	C24-C25-C26-C27
24	1	317	LHG	C30-C31-C32-C33
24	9	316	LHG	C24-C25-C26-C27
22	A	830	CLA	O1A-CGA-O2A-C1
22	B	813	CLA	O1A-CGA-O2A-C1
22	B	829	CLA	O1A-CGA-O2A-C1
22	B	839	CLA	O1A-CGA-O2A-C1
22	A	803	CLA	C1A-C2A-CAA-CBA
22	A	806	CLA	C1A-C2A-CAA-CBA
22	A	813	CLA	C1A-C2A-CAA-CBA
22	A	818	CLA	C1A-C2A-CAA-CBA
22	A	826	CLA	C1A-C2A-CAA-CBA
22	A	829	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C1A-C2A-CAA-CBA
22	A	841	CLA	C1A-C2A-CAA-CBA
22	A	843	CLA	C1A-C2A-CAA-CBA
22	A	853	CLA	C1A-C2A-CAA-CBA
22	B	816	CLA	C1A-C2A-CAA-CBA
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	C1A-C2A-CAA-CBA
22	B	839	CLA	C1A-C2A-CAA-CBA
22	K	101	CLA	C1A-C2A-CAA-CBA
22	K	105	CLA	C1A-C2A-CAA-CBA
22	L	202	CLA	C1A-C2A-CAA-CBA
22	L	204	CLA	C1A-C2A-CAA-CBA
22	1	304	CLA	C1A-C2A-CAA-CBA
22	1	306	CLA	C1A-C2A-CAA-CBA
22	1	308	CLA	C1A-C2A-CAA-CBA
22	1	313	CLA	C1A-C2A-CAA-CBA
22	2	319	CLA	C1A-C2A-CAA-CBA
22	4	309	CLA	C1A-C2A-CAA-CBA
22	6	305	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	5	309	CLA	C1A-C2A-CAA-CBA
22	5	313	CLA	C1A-C2A-CAA-CBA
22	7	305	CLA	C1A-C2A-CAA-CBA
22	8	308	CLA	C1A-C2A-CAA-CBA
22	8	309	CLA	C1A-C2A-CAA-CBA
22	9	309	CLA	C1A-C2A-CAA-CBA
22	9	311	CLA	C1A-C2A-CAA-CBA
22	9	313	CLA	C1A-C2A-CAA-CBA
22	0	312	CLA	C1A-C2A-CAA-CBA
29	4	307	CHL	C1A-C2A-CAA-CBA
29	8	307	CHL	C1A-C2A-CAA-CBA
22	B	836	CLA	C11-C12-C13-C15
22	1	302	CLA	C16-C17-C18-C20
22	6	303	CLA	C16-C17-C18-C20
24	1	317	LHG	O9-C7-O7-C5
25	1	316	8CT	C16-C17-C18-C19
25	8	318	8CT	C23-C24-C25-C26
22	L	201	CLA	C13-C15-C16-C17
22	L	203	CLA	C13-C15-C16-C17
24	6	322	LHG	C4-O6-P-O3
22	9	312	CLA	C11-C12-C13-C14
22	A	839	CLA	C3-C5-C6-C7
22	B	823	CLA	C3-C5-C6-C7
22	B	805	CLA	C8-C10-C11-C12
24	0	315	LHG	C28-C29-C30-C31
22	A	853	CLA	C10-C11-C12-C13
22	B	812	CLA	C15-C16-C17-C18
22	A	824	CLA	C6-C7-C8-C9
22	1	308	CLA	C11-C12-C13-C15
22	7	313	CLA	C3-C5-C6-C7
22	A	807	CLA	C10-C11-C12-C13
28	B	849	DGD	C2A-C1A-O1G-C1G
29	6	306	CHL	C3A-C2A-CAA-CBA
22	A	804	CLA	O1A-CGA-O2A-C1
22	9	305	CLA	O1A-CGA-O2A-C1
28	B	849	DGD	C8B-C9B-CAB-CBB
22	A	840	CLA	C5-C6-C7-C8
22	B	827	CLA	C10-C11-C12-C13
22	1	304	CLA	C2A-CAA-CBA-CGA
29	4	305	CHL	C2A-CAA-CBA-CGA
22	A	810	CLA	C16-C17-C18-C19
22	A	825	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	3	301	CLA	C11-C12-C13-C15
22	B	824	CLA	O1D-CGD-O2D-CED
22	L	203	CLA	C3-C5-C6-C7
31	4	318	LMG	C7-C8-C9-O8
31	8	319	LMG	O1-C7-C8-C9
26	J	102	HTG	C1'-C2'-C3'-C4'
22	L	203	CLA	CBA-CGA-O2A-C1
22	8	304	CLA	O1A-CGA-O2A-C1
22	9	309	CLA	O1A-CGA-O2A-C1
28	B	849	DGD	C5D-C6D-O5D-C1E
22	A	813	CLA	O1D-CGD-O2D-CED
22	2	302	CLA	C10-C11-C12-C13
22	B	805	CLA	CAA-CBA-CGA-O2A
22	M	101	CLA	CBA-CGA-O2A-C1
24	2	318	LHG	O1-C1-C2-O2
24	5	318	LHG	O1-C1-C2-O2
22	A	801	CLA	C5-C6-C7-C8
22	A	841	CLA	C13-C15-C16-C17
22	A	853	CLA	C8-C10-C11-C12
22	B	837	CLA	C8-C10-C11-C12
22	2	303	CLA	C10-C11-C12-C13
22	6	311	CLA	C8-C10-C11-C12
22	1	313	CLA	O1A-CGA-O2A-C1
22	B	828	CLA	C4-C3-C5-C6
22	B	833	CLA	C4-C3-C5-C6
22	7	318	CLA	C16-C17-C18-C20
29	4	301	CHL	C11-C12-C13-C15
29	0	301	CHL	C11-C12-C13-C14
22	6	315	CLA	CBA-CGA-O2A-C1
22	B	806	CLA	C13-C15-C16-C17
22	7	317	CLA	C8-C10-C11-C12
29	8	305	CHL	C5-C6-C7-C8
24	9	316	LHG	C28-C29-C30-C31
22	B	821	CLA	O1D-CGD-O2D-CED
22	A	813	CLA	C2A-CAA-CBA-CGA
22	A	808	CLA	C5-C6-C7-C8
22	B	837	CLA	C3-C5-C6-C7
22	B	839	CLA	C3-C5-C6-C7
29	0	306	CHL	C4C-C3C-CAC-CBC
22	A	836	CLA	O1D-CGD-O2D-CED
22	B	832	CLA	C5-C6-C7-C8
24	0	315	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	4	318	LMG	C31-C32-C33-C34
22	1	307	CLA	CBA-CGA-O2A-C1
31	4	318	LMG	C29-C28-O8-C9
22	3	307	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	C5-C6-C7-C8
22	B	809	CLA	O1D-CGD-O2D-CED
22	1	313	CLA	O1D-CGD-O2D-CED
22	6	318	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	C13-C15-C16-C17
22	B	834	CLA	C13-C15-C16-C17
29	2	306	CHL	CAA-CBA-CGA-O2A
31	4	318	LMG	O7-C8-C9-O8
24	6	322	LHG	C27-C28-C29-C30
22	A	821	CLA	C13-C15-C16-C17
22	A	818	CLA	C16-C17-C18-C19
22	9	303	CLA	C16-C17-C18-C20
24	0	315	LHG	C11-C10-C9-C8
22	B	823	CLA	C4-C3-C5-C6
22	L	203	CLA	C4-C3-C5-C6
22	4	311	CLA	C4-C3-C5-C6
22	B	806	CLA	C15-C16-C17-C18
22	A	803	CLA	C6-C7-C8-C10
22	A	806	CLA	C12-C13-C15-C16
22	A	807	CLA	C6-C7-C8-C10
22	A	808	CLA	C11-C10-C8-C7
22	A	810	CLA	C12-C13-C15-C16
22	A	817	CLA	C11-C10-C8-C7
22	A	817	CLA	C12-C13-C15-C16
22	A	827	CLA	C11-C12-C13-C15
22	A	829	CLA	C2-C3-C5-C6
22	A	830	CLA	C11-C10-C8-C7
22	A	830	CLA	C12-C13-C15-C16
22	B	803	CLA	C12-C13-C15-C16
22	B	809	CLA	C12-C13-C15-C16
22	B	814	CLA	C11-C12-C13-C15
22	B	825	CLA	C6-C7-C8-C10
22	B	825	CLA	C11-C10-C8-C7
22	B	825	CLA	C11-C12-C13-C15
22	B	827	CLA	C6-C7-C8-C10
22	B	827	CLA	C12-C13-C15-C16
22	B	828	CLA	C2-C3-C5-C6
22	B	829	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	832	CLA	C6-C7-C8-C10
22	B	836	CLA	C6-C7-C8-C10
22	B	839	CLA	C12-C13-C15-C16
22	B	840	CLA	C12-C13-C15-C16
22	L	201	CLA	C6-C7-C8-C10
22	L	201	CLA	C11-C12-C13-C15
22	1	311	CLA	C11-C12-C13-C15
22	2	302	CLA	C11-C12-C13-C15
22	2	303	CLA	C11-C12-C13-C15
22	2	309	CLA	C11-C10-C8-C7
22	4	314	CLA	C12-C13-C15-C16
22	6	315	CLA	C12-C13-C15-C16
22	5	302	CLA	C11-C10-C8-C7
22	5	309	CLA	C6-C7-C8-C10
22	5	312	CLA	C6-C7-C8-C10
22	8	315	CLA	C6-C7-C8-C10
22	9	303	CLA	C12-C13-C15-C16
22	9	309	CLA	C11-C10-C8-C7
22	0	307	CLA	C12-C13-C15-C16
29	9	302	CHL	C6-C7-C8-C10
29	9	302	CHL	C11-C10-C8-C7
22	A	803	CLA	C6-C7-C8-C9
22	A	803	CLA	C11-C12-C13-C14
22	A	806	CLA	C14-C13-C15-C16
22	A	809	CLA	C6-C7-C8-C9
22	A	817	CLA	C14-C13-C15-C16
22	A	818	CLA	C14-C13-C15-C16
22	A	825	CLA	C11-C10-C8-C9
22	A	827	CLA	C14-C13-C15-C16
22	A	830	CLA	C11-C10-C8-C9
22	A	830	CLA	C14-C13-C15-C16
22	A	838	CLA	C14-C13-C15-C16
22	B	803	CLA	C6-C7-C8-C9
22	B	805	CLA	C6-C7-C8-C9
22	B	809	CLA	C11-C10-C8-C9
22	B	814	CLA	C14-C13-C15-C16
22	B	819	CLA	C11-C10-C8-C9
22	B	825	CLA	C11-C12-C13-C14
22	B	827	CLA	C11-C12-C13-C14
22	B	827	CLA	C14-C13-C15-C16
22	B	839	CLA	C6-C7-C8-C9
22	H	201	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	L	201	CLA	C11-C12-C13-C14
22	2	303	CLA	C11-C12-C13-C14
22	4	314	CLA	C6-C7-C8-C9
22	6	303	CLA	C11-C10-C8-C9
22	6	305	CLA	C6-C7-C8-C9
22	6	315	CLA	C11-C10-C8-C9
22	5	302	CLA	C11-C10-C8-C9
22	5	307	CLA	C11-C12-C13-C14
22	8	315	CLA	C6-C7-C8-C9
22	8	315	CLA	C14-C13-C15-C16
22	9	303	CLA	C14-C13-C15-C16
22	9	309	CLA	C11-C10-C8-C9
22	0	302	CLA	C14-C13-C15-C16
22	0	308	CLA	C11-C10-C8-C9
23	A	842	PQN	C16-C17-C18-C19
29	5	301	CHL	C11-C10-C8-C9
25	A	849	8CT	C12-C13-C14-C15
31	4	318	LMG	C30-C31-C32-C33
22	0	312	CLA	CBA-CGA-O2A-C1
22	5	303	CLA	C2C-C3C-CAC-CBC
25	J	101	8CT	C27-C26-C28-C29
25	3	316	8CT	C22-C21-C23-C24
25	7	301	8CT	C10-C11-C12-C40
22	L	202	CLA	C15-C16-C17-C18
22	A	810	CLA	C16-C17-C18-C20
22	B	824	CLA	C11-C12-C13-C15
22	4	310	CLA	C6-C7-C8-C10
29	8	305	CHL	C6-C7-C8-C9
29	7	308	CHL	C2C-C3C-CAC-CBC
22	9	305	CLA	O1D-CGD-O2D-CED
25	J	101	8CT	C25-C26-C28-C29
25	4	317	8CT	C10-C11-C12-C13
25	7	301	8CT	C10-C11-C12-C13
25	8	318	8CT	C25-C26-C28-C29
22	1	311	CLA	C3-C5-C6-C7
29	2	301	CHL	O1D-CGD-O2D-CED
22	A	810	CLA	C13-C15-C16-C17
22	6	309	CLA	CBA-CGA-O2A-C1
22	6	311	CLA	CBA-CGA-O2A-C1
22	B	815	CLA	C13-C15-C16-C17
22	B	819	CLA	C5-C6-C7-C8
24	9	316	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
28	B	849	DGD	CFB-CGB-CHB-CIB
22	A	806	CLA	C4B-C3B-CAB-CBB
22	A	809	CLA	C4B-C3B-CAB-CBB
22	A	811	CLA	C4B-C3B-CAB-CBB
22	A	812	CLA	C4B-C3B-CAB-CBB
22	A	814	CLA	C4B-C3B-CAB-CBB
22	A	826	CLA	C4B-C3B-CAB-CBB
22	A	836	CLA	C4B-C3B-CAB-CBB
22	A	841	CLA	C4B-C3B-CAB-CBB
22	B	810	CLA	C4B-C3B-CAB-CBB
22	B	835	CLA	C4B-C3B-CAB-CBB
22	B	839	CLA	C4B-C3B-CAB-CBB
22	F	301	CLA	C4B-C3B-CAB-CBB
22	K	101	CLA	C4B-C3B-CAB-CBB
22	2	313	CLA	C4B-C3B-CAB-CBB
22	2	319	CLA	C4B-C3B-CAB-CBB
22	3	310	CLA	C4B-C3B-CAB-CBB
22	4	302	CLA	C4B-C3B-CAB-CBB
22	4	312	CLA	C4B-C3B-CAB-CBB
22	6	313	CLA	C4B-C3B-CAB-CBB
22	5	307	CLA	C4B-C3B-CAB-CBB
22	5	308	CLA	C4B-C3B-CAB-CBB
22	7	302	CLA	C4B-C3B-CAB-CBB
22	7	304	CLA	C4B-C3B-CAB-CBB
22	7	313	CLA	C4B-C3B-CAB-CBB
22	7	314	CLA	C4B-C3B-CAB-CBB
22	7	318	CLA	C4B-C3B-CAB-CBB
22	9	313	CLA	C4B-C3B-CAB-CBB
22	0	307	CLA	C4B-C3B-CAB-CBB
22	0	309	CLA	C4B-C3B-CAB-CBB
22	1	308	CLA	C11-C12-C13-C14
24	A	845	LHG	O6-C4-C5-C6
24	0	315	LHG	O6-C4-C5-C6
22	B	814	CLA	CBA-CGA-O2A-C1
22	5	313	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	O1D-CGD-O2D-CED
22	3	319	CLA	C4-C3-C5-C6
22	A	817	CLA	C2-C3-C5-C6
22	B	823	CLA	C2-C3-C5-C6
22	L	203	CLA	C2-C3-C5-C6
22	L	203	CLA	C8-C10-C11-C12
22	4	302	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	L	203	CLA	O1A-CGA-O2A-C1
22	8	312	CLA	O1D-CGD-O2D-CED
22	5	302	CLA	C16-C17-C18-C20
22	B	809	CLA	CBA-CGA-O2A-C1
22	0	303	CLA	CBA-CGA-O2A-C1
24	7	322	LHG	C2-C3-O3-P
22	A	828	CLA	C3A-C2A-CAA-CBA
22	A	832	CLA	C3A-C2A-CAA-CBA
22	A	841	CLA	C3A-C2A-CAA-CBA
22	B	841	CLA	C3A-C2A-CAA-CBA
22	K	105	CLA	C3A-C2A-CAA-CBA
22	L	201	CLA	C3A-C2A-CAA-CBA
22	1	303	CLA	C3A-C2A-CAA-CBA
22	1	313	CLA	C3A-C2A-CAA-CBA
22	4	314	CLA	C3A-C2A-CAA-CBA
22	6	309	CLA	C3A-C2A-CAA-CBA
22	6	311	CLA	C3A-C2A-CAA-CBA
22	6	323	CLA	C3A-C2A-CAA-CBA
22	7	305	CLA	C3A-C2A-CAA-CBA
22	8	304	CLA	C3A-C2A-CAA-CBA
22	8	315	CLA	C3A-C2A-CAA-CBA
22	0	305	CLA	C3A-C2A-CAA-CBA
25	A	849	8CT	C18-C19-C20-C21
30	0	314	XAT	C33-C34-C35-C15
22	4	309	CLA	C3-C5-C6-C7
22	A	803	CLA	C13-C15-C16-C17
22	4	310	CLA	C6-C7-C8-C9
22	0	307	CLA	CBA-CGA-O2A-C1
29	9	302	CHL	C8-C10-C11-C12
24	B	852	LHG	C4-C5-C6-O8
24	2	318	LHG	C4-C5-C6-O8
24	5	318	LHG	C4-C5-C6-O8
28	B	849	DGD	O1G-C1G-C2G-C3G
28	B	849	DGD	C1G-C2G-C3G-O3G
22	2	304	CLA	C3-C5-C6-C7
22	B	819	CLA	C4-C3-C5-C6
22	A	825	CLA	C16-C17-C18-C20
22	5	302	CLA	C16-C17-C18-C19
22	5	307	CLA	C16-C17-C18-C19
29	4	301	CHL	C11-C12-C13-C14
22	3	304	CLA	O1D-CGD-O2D-CED
29	2	301	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
29	6	302	CHL	C3C-C2C-CMC-OMC
29	8	305	CHL	C3C-C2C-CMC-OMC
29	9	307	CHL	C3C-C2C-CMC-OMC
22	1	307	CLA	O1A-CGA-O2A-C1
31	4	318	LMG	C4-C5-C6-O5
22	B	816	CLA	C2A-CAA-CBA-CGA
24	B	852	LHG	O1-C1-C2-O2
24	3	317	LHG	O6-C4-C5-O7
24	0	315	LHG	O6-C4-C5-O7
22	B	812	CLA	CBA-CGA-O2A-C1
22	1	310	CLA	CBA-CGA-O2A-C1
22	5	312	CLA	CBA-CGA-O2A-C1
22	6	315	CLA	O1A-CGA-O2A-C1
22	B	809	CLA	C16-C17-C18-C19
22	B	824	CLA	C11-C12-C13-C14
29	8	305	CHL	C6-C7-C8-C10
22	B	818	CLA	C8-C10-C11-C12
31	8	319	LMG	C31-C32-C33-C34
29	7	308	CHL	CBA-CGA-O2A-C1
22	A	809	CLA	C2B-C3B-CAB-CBB
22	A	811	CLA	C2B-C3B-CAB-CBB
22	A	812	CLA	C2B-C3B-CAB-CBB
22	A	814	CLA	C2B-C3B-CAB-CBB
22	A	836	CLA	C2B-C3B-CAB-CBB
22	B	824	CLA	C2B-C3B-CAB-CBB
22	G	101	CLA	C2B-C3B-CAB-CBB
22	3	307	CLA	C2B-C3B-CAB-CBB
22	4	312	CLA	C2B-C3B-CAB-CBB
22	5	304	CLA	C2B-C3B-CAB-CBB
22	0	309	CLA	C2B-C3B-CAB-CBB
22	8	310	CLA	C2C-C3C-CAC-CBC
28	B	849	DGD	CFA-CGA-CHA-CIA
22	0	312	CLA	O1A-CGA-O2A-C1
28	B	849	DGD	O2G-C2G-C3G-O3G
22	A	827	CLA	CBA-CGA-O2A-C1
22	3	312	CLA	O1D-CGD-O2D-CED
25	B	845	8CT	C18-C19-C20-C21
25	B	848	8CT	C12-C13-C14-C15
25	7	323	8CT	C16-C17-C18-C19
22	A	818	CLA	C16-C17-C18-C20
22	B	805	CLA	C16-C17-C18-C20
24	9	316	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
22	A	817	CLA	C2-C1-O2A-CGA
22	A	824	CLA	C2-C1-O2A-CGA
22	B	808	CLA	C2-C1-O2A-CGA
22	2	314	CLA	C2-C1-O2A-CGA
22	6	303	CLA	C2-C1-O2A-CGA
22	9	303	CLA	C2-C1-O2A-CGA
29	8	307	CHL	C2-C1-O2A-CGA
24	9	316	LHG	C29-C30-C31-C32
24	0	315	LHG	C32-C33-C34-C35
31	5	319	LMG	C23-C24-C25-C26
22	A	802	CLA	C14-C13-C15-C16
22	A	808	CLA	C11-C10-C8-C9
22	A	809	CLA	C11-C12-C13-C14
22	A	810	CLA	C14-C13-C15-C16
22	A	833	CLA	C6-C7-C8-C9
22	A	837	CLA	C11-C10-C8-C9
22	B	803	CLA	C14-C13-C15-C16
22	B	818	CLA	C6-C7-C8-C9
22	B	820	CLA	C11-C10-C8-C9
22	B	826	CLA	C11-C12-C13-C14
22	B	828	CLA	C11-C12-C13-C14
22	B	837	CLA	C14-C13-C15-C16
22	B	841	CLA	C6-C7-C8-C9
22	1	301	CLA	C14-C13-C15-C16
22	1	311	CLA	C11-C12-C13-C14
22	2	302	CLA	C6-C7-C8-C9
22	3	301	CLA	C6-C7-C8-C9
22	3	319	CLA	C14-C13-C15-C16
22	6	303	CLA	C14-C13-C15-C16
22	5	307	CLA	C14-C13-C15-C16
22	7	317	CLA	C11-C12-C13-C14
22	7	310	CLA	CBA-CGA-O2A-C1
24	9	316	LHG	C33-C34-C35-C36
22	B	825	CLA	C8-C10-C11-C12
22	B	839	CLA	C13-C15-C16-C17
22	1	301	CLA	C8-C10-C11-C12
24	2	318	LHG	C2-C3-O3-P
24	5	318	LHG	C2-C3-O3-P
24	5	318	LHG	C25-C26-C27-C28
22	G	103	CLA	C2A-CAA-CBA-CGA
22	6	313	CLA	C16-C17-C18-C20
22	5	303	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	A	849	8CT	C02-C03-C10-C11
25	B	844	8CT	C02-C03-C10-C11
25	B	844	8CT	C04-C03-C10-C11
25	B	848	8CT	C02-C03-C10-C11
25	7	301	8CT	C02-C03-C10-C11
22	A	827	CLA	C10-C11-C12-C13
22	5	303	CLA	C5-C6-C7-C8
25	L	205	8CT	C14-C15-C16-C39
25	A	846	8CT	C20-C21-C23-C24
25	4	317	8CT	C14-C15-C16-C17
25	8	318	8CT	C20-C21-C23-C24
30	3	314	XAT	C31-C32-C33-C34
22	2	312	CLA	C5-C6-C7-C8
22	6	304	CLA	C10-C11-C12-C13
24	5	318	LHG	C11-C12-C13-C14
24	9	316	LHG	C27-C28-C29-C30
22	9	304	CLA	O2A-C1-C2-C3
22	A	804	CLA	C6-C7-C8-C10
22	B	819	CLA	C11-C12-C13-C15
22	9	303	CLA	C16-C17-C18-C19
22	A	801	CLA	C3-C5-C6-C7
29	9	307	CHL	CBD-CGD-O2D-CED
22	6	309	CLA	O1A-CGA-O2A-C1
22	A	828	CLA	O1D-CGD-O2D-CED
24	2	318	LHG	O6-C4-C5-C6
24	3	317	LHG	O6-C4-C5-C6
24	6	322	LHG	O6-C4-C5-C6
22	A	838	CLA	O1D-CGD-O2D-CED
24	0	315	LHG	C14-C15-C16-C17
22	A	802	CLA	C12-C13-C15-C16
22	A	803	CLA	C11-C12-C13-C15
22	A	805	CLA	C12-C13-C15-C16
22	A	811	CLA	C11-C12-C13-C15
22	A	826	CLA	C12-C13-C15-C16
22	A	837	CLA	C11-C10-C8-C7
22	B	803	CLA	C11-C12-C13-C15
22	B	805	CLA	C6-C7-C8-C10
22	B	805	CLA	C11-C10-C8-C7
22	B	811	CLA	C12-C13-C15-C16
22	B	814	CLA	C12-C13-C15-C16
22	B	819	CLA	C11-C10-C8-C7
22	B	827	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	828	CLA	C11-C12-C13-C15
22	B	837	CLA	C11-C12-C13-C15
22	B	837	CLA	C12-C13-C15-C16
22	B	839	CLA	C6-C7-C8-C10
22	H	201	CLA	C11-C10-C8-C7
22	L	203	CLA	C11-C10-C8-C7
22	1	301	CLA	C12-C13-C15-C16
22	1	306	CLA	C11-C12-C13-C15
22	1	308	CLA	C6-C7-C8-C10
22	2	312	CLA	C11-C12-C13-C15
22	3	301	CLA	C6-C7-C8-C10
22	3	319	CLA	C12-C13-C15-C16
22	4	314	CLA	C6-C7-C8-C10
22	6	303	CLA	C11-C10-C8-C7
22	6	303	CLA	C12-C13-C15-C16
22	6	305	CLA	C6-C7-C8-C10
22	6	311	CLA	C11-C10-C8-C7
22	6	315	CLA	C11-C10-C8-C7
22	5	307	CLA	C11-C12-C13-C15
22	7	316	CLA	C6-C7-C8-C10
22	7	317	CLA	C12-C13-C15-C16
22	8	315	CLA	C11-C12-C13-C15
22	9	309	CLA	C6-C7-C8-C10
22	9	312	CLA	C11-C10-C8-C7
22	0	302	CLA	C11-C10-C8-C7
22	0	302	CLA	C12-C13-C15-C16
22	0	308	CLA	C11-C10-C8-C7
23	A	842	PQN	C16-C17-C18-C20
29	0	301	CHL	C6-C7-C8-C10
31	8	319	LMG	C11-C12-C13-C14
22	A	829	CLA	C5-C6-C7-C8
25	A	847	8CT	C18-C19-C20-C21
25	A	854	8CT	C16-C17-C18-C19
25	B	804	8CT	C16-C17-C18-C19
25	B	848	8CT	C18-C19-C20-C21
25	G	104	8CT	C12-C13-C14-C15
25	5	317	8CT	C18-C19-C20-C21
25	7	301	8CT	C23-C24-C25-C26
25	8	318	8CT	C18-C19-C20-C21
22	A	808	CLA	C16-C17-C18-C19
22	A	808	CLA	C16-C17-C18-C20
22	H	201	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
28	B	849	DGD	C2A-C3A-C4A-C5A
22	A	824	CLA	C2A-CAA-CBA-CGA
22	1	306	CLA	C2A-CAA-CBA-CGA
29	1	305	CHL	C2A-CAA-CBA-CGA
29	2	306	CHL	C2A-CAA-CBA-CGA
22	9	308	CLA	C13-C15-C16-C17
22	B	805	CLA	C16-C17-C18-C19
22	5	307	CLA	C16-C17-C18-C20
22	B	809	CLA	C8-C10-C11-C12
22	B	815	CLA	CBA-CGA-O2A-C1
22	4	311	CLA	CBA-CGA-O2A-C1
22	8	311	CLA	CBA-CGA-O2A-C1
22	4	311	CLA	C3-C5-C6-C7
24	1	317	LHG	C28-C29-C30-C31
22	B	826	CLA	C13-C15-C16-C17
31	4	318	LMG	C16-C17-C18-C19
22	A	806	CLA	CAD-CBD-CGD-O2D
22	A	807	CLA	CAD-CBD-CGD-O2D
22	A	811	CLA	CAD-CBD-CGD-O2D
22	A	820	CLA	CAD-CBD-CGD-O2D
22	A	835	CLA	CAD-CBD-CGD-O2D
22	A	852	CLA	CAD-CBD-CGD-O2D
22	B	805	CLA	CAD-CBD-CGD-O2D
22	B	811	CLA	CAD-CBD-CGD-O2D
22	B	819	CLA	CAD-CBD-CGD-O2D
22	B	826	CLA	CAD-CBD-CGD-O2D
22	B	835	CLA	CAD-CBD-CGD-O2D
22	B	838	CLA	CAD-CBD-CGD-O2D
22	2	308	CLA	CAD-CBD-CGD-O2D
22	3	311	CLA	CAD-CBD-CGD-O2D
22	4	308	CLA	CAD-CBD-CGD-O2D
22	4	309	CLA	CAD-CBD-CGD-O2D
22	6	301	CLA	CAD-CBD-CGD-O2D
22	6	311	CLA	CAD-CBD-CGD-O2D
22	6	312	CLA	CAD-CBD-CGD-O2D
22	5	309	CLA	CAD-CBD-CGD-O2D
22	7	303	CLA	CAD-CBD-CGD-O2D
22	8	308	CLA	CAD-CBD-CGD-O2D
22	8	309	CLA	CAD-CBD-CGD-O2D
22	9	303	CLA	CAD-CBD-CGD-O2D
22	9	304	CLA	CAD-CBD-CGD-O2D
29	1	305	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	2	301	CHL	CAD-CBD-CGD-O2D
29	4	306	CHL	CAD-CBD-CGD-O2D
22	2	309	CLA	O1D-CGD-O2D-CED
24	A	844	LHG	C32-C33-C34-C35
24	A	844	LHG	C34-C35-C36-C37
22	7	309	CLA	CBA-CGA-O2A-C1
29	9	307	CHL	CBA-CGA-O2A-C1
22	A	803	CLA	C4-C3-C5-C6
22	A	837	CLA	C4-C3-C5-C6
22	7	318	CLA	C16-C17-C18-C19
22	0	312	CLA	C6-C7-C8-C9
24	5	318	LHG	C16-C17-C18-C19
24	A	844	LHG	C4-C5-C6-O8
31	4	318	LMG	O1-C7-C8-C9
31	5	319	LMG	O1-C7-C8-C9
22	A	827	CLA	O1A-CGA-O2A-C1
22	6	311	CLA	O1A-CGA-O2A-C1
22	8	311	CLA	O1A-CGA-O2A-C1
24	6	322	LHG	O6-C4-C5-O7
22	A	832	CLA	C5-C6-C7-C8
22	B	823	CLA	C5-C6-C7-C8
22	B	808	CLA	CAA-CBA-CGA-O2A
28	B	849	DGD	C2B-C3B-C4B-C5B
22	B	812	CLA	O1A-CGA-O2A-C1
22	5	312	CLA	O1A-CGA-O2A-C1
22	B	801	CLA	C16-C17-C18-C19
22	A	808	CLA	CHA-CBD-CGD-O1D
22	A	808	CLA	CHA-CBD-CGD-O2D
22	A	817	CLA	CHA-CBD-CGD-O1D
22	A	817	CLA	CHA-CBD-CGD-O2D
22	A	833	CLA	CHA-CBD-CGD-O1D
22	A	836	CLA	CHA-CBD-CGD-O2D
22	A	838	CLA	CHA-CBD-CGD-O1D
22	A	838	CLA	CHA-CBD-CGD-O2D
22	B	801	CLA	CHA-CBD-CGD-O1D
22	B	801	CLA	CHA-CBD-CGD-O2D
22	B	808	CLA	CHA-CBD-CGD-O1D
22	B	833	CLA	CHA-CBD-CGD-O1D
22	F	301	CLA	CHA-CBD-CGD-O1D
22	F	301	CLA	CHA-CBD-CGD-O2D
22	K	102	CLA	CHA-CBD-CGD-O1D
22	1	301	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	1	301	CLA	CHA-CBD-CGD-O2D
22	1	303	CLA	CHA-CBD-CGD-O1D
22	2	319	CLA	CHA-CBD-CGD-O2D
22	3	303	CLA	CHA-CBD-CGD-O1D
22	3	303	CLA	CHA-CBD-CGD-O2D
22	3	312	CLA	CHA-CBD-CGD-O1D
22	4	314	CLA	CHA-CBD-CGD-O1D
22	6	323	CLA	CHA-CBD-CGD-O1D
22	6	323	CLA	CHA-CBD-CGD-O2D
22	7	302	CLA	CHA-CBD-CGD-O1D
22	7	302	CLA	CHA-CBD-CGD-O2D
22	7	305	CLA	CHA-CBD-CGD-O1D
22	7	305	CLA	CHA-CBD-CGD-O2D
22	8	304	CLA	CHA-CBD-CGD-O1D
22	9	305	CLA	CHA-CBD-CGD-O1D
22	9	305	CLA	CHA-CBD-CGD-O2D
22	0	302	CLA	CHA-CBD-CGD-O1D
22	0	303	CLA	CHA-CBD-CGD-O1D
22	0	303	CLA	CHA-CBD-CGD-O2D
29	6	302	CHL	CHA-CBD-CGD-O1D
29	6	302	CHL	CHA-CBD-CGD-O2D
29	6	316	CHL	CHA-CBD-CGD-O1D
29	6	316	CHL	CHA-CBD-CGD-O2D
22	A	837	CLA	C3-C5-C6-C7
22	B	809	CLA	O1A-CGA-O2A-C1
22	B	814	CLA	O1A-CGA-O2A-C1
22	0	303	CLA	O1A-CGA-O2A-C1
22	0	307	CLA	O1A-CGA-O2A-C1
28	B	849	DGD	CBA-CCA-CDA-CEA
24	B	852	LHG	O7-C5-C6-O8
24	2	318	LHG	O7-C5-C6-O8
28	B	849	DGD	O1G-C1G-C2G-O2G
31	4	318	LMG	O1-C7-C8-O7
22	A	822	CLA	CBD-CGD-O2D-CED
22	2	312	CLA	C8-C10-C11-C12
22	1	310	CLA	O1A-CGA-O2A-C1
22	7	310	CLA	O1A-CGA-O2A-C1
22	B	826	CLA	C16-C17-C18-C19
22	B	834	CLA	C16-C17-C18-C19
22	K	101	CLA	C2C-C3C-CAC-CBC
22	B	814	CLA	C4-C3-C5-C6
22	A	812	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	850	CLA	C2C-C3C-CAC-CBC
24	A	845	LHG	C10-C11-C12-C13
24	6	322	LHG	O9-C7-O7-C5
22	B	812	CLA	C5-C6-C7-C8
22	A	811	CLA	C11-C12-C13-C14
22	A	840	CLA	C14-C13-C15-C16
22	A	853	CLA	C11-C12-C13-C14
22	B	826	CLA	C6-C7-C8-C9
22	B	828	CLA	C6-C7-C8-C9
22	2	312	CLA	C11-C12-C13-C14
22	0	302	CLA	C11-C10-C8-C9
23	B	842	PQN	C21-C22-C23-C24
24	0	315	LHG	C30-C31-C32-C33
22	A	806	CLA	C15-C16-C17-C18
22	B	837	CLA	C13-C15-C16-C17
22	8	310	CLA	C4C-C3C-CAC-CBC
22	B	814	CLA	C2A-CAA-CBA-CGA
22	5	312	CLA	C2A-CAA-CBA-CGA
25	A	854	8CT	C10-C11-C12-C40
24	A	844	LHG	C28-C29-C30-C31
25	A	854	8CT	C10-C11-C12-C13
25	3	316	8CT	C20-C21-C23-C24
22	A	811	CLA	C1A-C2A-CAA-CBA
22	1	302	CLA	C1A-C2A-CAA-CBA
22	4	314	CLA	C1A-C2A-CAA-CBA
22	6	310	CLA	C1A-C2A-CAA-CBA
22	6	311	CLA	C1A-C2A-CAA-CBA
22	7	310	CLA	C1A-C2A-CAA-CBA
22	8	315	CLA	C1A-C2A-CAA-CBA
29	2	307	CHL	C1A-C2A-CAA-CBA
29	3	306	CHL	C1A-C2A-CAA-CBA
22	A	806	CLA	C16-C17-C18-C19
22	A	809	CLA	C16-C17-C18-C19
22	B	817	CLA	C6-C7-C8-C9
22	1	312	CLA	C6-C7-C8-C9
22	8	315	CLA	C16-C17-C18-C20
22	A	808	CLA	C13-C15-C16-C17
24	0	315	LHG	C24-C25-C26-C27
24	B	852	LHG	C3-O3-P-O6
24	5	318	LHG	C3-O3-P-O6
24	5	318	LHG	C28-C29-C30-C31
22	6	305	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	0	302	CLA	C2-C3-C5-C6
22	7	309	CLA	O1A-CGA-O2A-C1
29	9	307	CHL	O1A-CGA-O2A-C1
22	A	801	CLA	C4B-C3B-CAB-CBB
22	A	805	CLA	C4B-C3B-CAB-CBB
22	A	824	CLA	C4B-C3B-CAB-CBB
22	A	834	CLA	C4B-C3B-CAB-CBB
22	B	805	CLA	C4B-C3B-CAB-CBB
22	B	808	CLA	C4B-C3B-CAB-CBB
22	B	816	CLA	C4B-C3B-CAB-CBB
22	B	820	CLA	C4B-C3B-CAB-CBB
22	B	834	CLA	C4B-C3B-CAB-CBB
22	K	104	CLA	C4B-C3B-CAB-CBB
22	K	105	CLA	C4B-C3B-CAB-CBB
22	1	301	CLA	C4B-C3B-CAB-CBB
22	1	303	CLA	C4B-C3B-CAB-CBB
22	1	307	CLA	C4B-C3B-CAB-CBB
22	1	310	CLA	C4B-C3B-CAB-CBB
22	3	303	CLA	C4B-C3B-CAB-CBB
22	3	311	CLA	C4B-C3B-CAB-CBB
22	3	319	CLA	C4B-C3B-CAB-CBB
22	4	310	CLA	C4B-C3B-CAB-CBB
22	4	311	CLA	C4B-C3B-CAB-CBB
22	4	314	CLA	C4B-C3B-CAB-CBB
22	6	315	CLA	C4B-C3B-CAB-CBB
22	6	318	CLA	C4B-C3B-CAB-CBB
22	5	304	CLA	C4B-C3B-CAB-CBB
22	5	309	CLA	C4B-C3B-CAB-CBB
22	7	312	CLA	C4B-C3B-CAB-CBB
22	7	317	CLA	C4B-C3B-CAB-CBB
22	8	303	CLA	C4B-C3B-CAB-CBB
22	8	311	CLA	C4B-C3B-CAB-CBB
22	9	308	CLA	C4B-C3B-CAB-CBB
22	0	302	CLA	C4B-C3B-CAB-CBB
22	0	304	CLA	C4B-C3B-CAB-CBB
22	0	311	CLA	C4B-C3B-CAB-CBB
24	A	844	LHG	C3-O3-P-O4
24	2	318	LHG	C4-O6-P-O5
24	6	322	LHG	C4-O6-P-O4
24	5	318	LHG	C3-O3-P-O4
24	5	318	LHG	C4-O6-P-O4
24	7	322	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
24	7	322	LHG	C4-O6-P-O4
22	A	821	CLA	C16-C17-C18-C20
22	B	809	CLA	C16-C17-C18-C20
22	4	309	CLA	C11-C12-C13-C15
22	6	304	CLA	C16-C17-C18-C20
22	3	311	CLA	CBA-CGA-O2A-C1
24	2	318	LHG	C24-C23-O8-C6
22	A	801	CLA	CAA-CBA-CGA-O2A
22	G	102	CLA	C2A-CAA-CBA-CGA
22	1	311	CLA	C2A-CAA-CBA-CGA
22	9	312	CLA	C3-C5-C6-C7
22	4	311	CLA	O1A-CGA-O2A-C1
22	A	823	CLA	C2-C3-C5-C6
22	A	832	CLA	CAD-CBD-CGD-O1D
22	A	836	CLA	CAD-CBD-CGD-O1D
22	B	808	CLA	CAD-CBD-CGD-O1D
22	B	814	CLA	CAD-CBD-CGD-O1D
22	2	319	CLA	CAD-CBD-CGD-O1D
22	3	303	CLA	CAD-CBD-CGD-O1D
22	6	303	CLA	CAD-CBD-CGD-O1D
22	6	323	CLA	CAD-CBD-CGD-O1D
22	5	304	CLA	CAD-CBD-CGD-O1D
22	5	312	CLA	CAD-CBD-CGD-O1D
22	7	305	CLA	CAD-CBD-CGD-O1D
22	7	314	CLA	CAD-CBD-CGD-O1D
22	8	304	CLA	CAD-CBD-CGD-O1D
22	8	311	CLA	CAD-CBD-CGD-O1D
22	0	302	CLA	CAD-CBD-CGD-O1D
22	0	303	CLA	CAD-CBD-CGD-O1D
29	2	305	CHL	CAD-CBD-CGD-O1D
29	6	302	CHL	CAD-CBD-CGD-O1D
22	B	837	CLA	C10-C11-C12-C13
22	B	815	CLA	O1A-CGA-O2A-C1
22	2	303	CLA	C15-C16-C17-C18
24	9	316	LHG	C9-C10-C11-C12
22	B	836	CLA	CBA-CGA-O2A-C1
29	4	305	CHL	CBA-CGA-O2A-C1
22	4	309	CLA	O1A-CGA-O2A-C1
22	L	202	CLA	CBD-CGD-O2D-CED
22	A	833	CLA	C4-C3-C5-C6
22	A	819	CLA	C11-C12-C13-C15
22	A	819	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	A	828	CLA	C11-C12-C13-C15
22	A	833	CLA	C6-C7-C8-C10
22	A	840	CLA	C12-C13-C15-C16
22	A	841	CLA	C6-C7-C8-C10
22	B	806	CLA	C6-C7-C8-C10
22	B	808	CLA	C11-C10-C8-C7
22	B	808	CLA	C11-C12-C13-C15
22	B	809	CLA	C11-C12-C13-C15
22	B	826	CLA	C6-C7-C8-C10
22	B	828	CLA	C6-C7-C8-C10
22	B	830	CLA	C11-C12-C13-C15
22	B	834	CLA	C11-C10-C8-C7
22	J	103	CLA	C3A-C2A-CAA-CBA
22	2	302	CLA	C12-C13-C15-C16
22	2	303	CLA	C6-C7-C8-C10
22	3	319	CLA	C6-C7-C8-C10
22	0	307	CLA	C6-C7-C8-C10
25	B	843	8CT	C28-C29-C30-C31
25	B	846	8CT	C28-C29-C30-C31
25	L	206	8CT	C28-C29-C30-C31
25	1	316	8CT	C28-C29-C30-C31
25	2	317	8CT	C28-C29-C30-C31
25	8	301	8CT	C28-C29-C30-C31
25	8	318	8CT	C28-C29-C30-C31
29	0	301	CHL	C11-C10-C8-C7
25	4	317	8CT	C12-C13-C14-C15
22	7	307	CLA	CBD-CGD-O2D-CED
22	9	312	CLA	C8-C10-C11-C12
22	B	803	CLA	C2C-C3C-CAC-CBC
29	6	316	CHL	C4C-C3C-CAC-CBC
22	A	832	CLA	C2A-CAA-CBA-CGA
22	A	836	CLA	C2A-CAA-CBA-CGA
22	9	305	CLA	C2A-CAA-CBA-CGA
22	B	814	CLA	C16-C17-C18-C19
22	B	828	CLA	C16-C17-C18-C19
24	7	322	LHG	C4-C5-C6-O8
24	9	316	LHG	C4-C5-C6-O8
29	2	305	CHL	C1C-C2C-CMC-OMC
29	2	307	CHL	C1C-C2C-CMC-OMC
29	6	302	CHL	C1C-C2C-CMC-OMC
29	6	316	CHL	C1C-C2C-CMC-OMC
29	5	306	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
29	9	307	CHL	C1C-C2C-CMC-OMC
31	5	319	LMG	O1-C7-C8-O7
31	8	319	LMG	O1-C7-C8-O7
31	5	319	LMG	C29-C30-C31-C32
22	1	312	CLA	C6-C7-C8-C10
22	B	827	CLA	C13-C15-C16-C17
22	6	310	CLA	C10-C11-C12-C13
22	0	311	CLA	C13-C15-C16-C17
22	A	826	CLA	C2C-C3C-CAC-CBC
22	K	102	CLA	C2C-C3C-CAC-CBC
22	B	836	CLA	O1A-CGA-O2A-C1
22	3	311	CLA	O1A-CGA-O2A-C1
22	4	314	CLA	C5-C6-C7-C8
22	8	315	CLA	C4-C3-C5-C6
22	5	304	CLA	CBA-CGA-O2A-C1
22	A	803	CLA	C2-C3-C5-C6
22	B	828	CLA	CAA-CBA-CGA-O2A
22	1	312	CLA	CAA-CBA-CGA-O2A
22	B	813	CLA	C5-C6-C7-C8
22	L	201	CLA	C8-C10-C11-C12
22	A	811	CLA	C6-C7-C8-C9
22	A	840	CLA	C6-C7-C8-C9
22	A	841	CLA	C6-C7-C8-C9
22	B	803	CLA	C11-C12-C13-C14
22	B	805	CLA	C11-C10-C8-C9
22	B	809	CLA	C11-C12-C13-C14
22	B	825	CLA	C6-C7-C8-C9
22	B	827	CLA	C6-C7-C8-C9
22	B	829	CLA	C14-C13-C15-C16
22	B	840	CLA	C14-C13-C15-C16
22	1	306	CLA	C11-C12-C13-C14
22	1	308	CLA	C6-C7-C8-C9
22	2	303	CLA	C11-C10-C8-C9
22	4	312	CLA	C6-C7-C8-C9
22	6	311	CLA	C11-C10-C8-C9
22	7	316	CLA	C6-C7-C8-C9
22	7	317	CLA	C14-C13-C15-C16
22	8	302	CLA	C11-C10-C8-C9
22	0	311	CLA	C6-C7-C8-C9
29	9	302	CHL	C11-C10-C8-C9
29	0	301	CHL	C6-C7-C8-C9
22	B	834	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	4	309	CLA	C11-C12-C13-C14
29	4	305	CHL	O1A-CGA-O2A-C1
22	7	316	CLA	C2A-CAA-CBA-CGA
22	3	319	CLA	C15-C16-C17-C18
25	B	843	8CT	C13-C14-C15-C16
25	B	843	8CT	C21-C23-C24-C25
25	B	844	8CT	C13-C14-C15-C16
25	B	844	8CT	C21-C23-C24-C25
25	B	845	8CT	C13-C14-C15-C16
25	B	845	8CT	C21-C23-C24-C25
25	B	846	8CT	C13-C14-C15-C16
25	B	846	8CT	C21-C23-C24-C25
25	B	851	8CT	C13-C14-C15-C16
25	B	851	8CT	C21-C23-C24-C25
25	J	104	8CT	C21-C23-C24-C25
25	K	103	8CT	C13-C14-C15-C16
25	K	103	8CT	C21-C23-C24-C25
25	L	205	8CT	C21-C23-C24-C25
25	6	321	8CT	C21-C23-C24-C25
30	1	314	XAT	C10-C11-C12-C13
30	3	314	XAT	C30-C31-C32-C33
30	4	315	XAT	C10-C11-C12-C13
30	6	319	XAT	C10-C11-C12-C13
30	9	314	XAT	C30-C31-C32-C33
30	0	313	XAT	C10-C11-C12-C13
30	0	313	XAT	C30-C31-C32-C33
30	0	314	XAT	C10-C11-C12-C13
25	A	847	8CT	C16-C17-C18-C19
22	A	821	CLA	C16-C17-C18-C19
22	8	315	CLA	C16-C17-C18-C19
22	8	315	CLA	C4C-C3C-CAC-CBC
25	L	205	8CT	C14-C15-C16-C17
22	1	308	CLA	C5-C6-C7-C8
22	A	801	CLA	C2B-C3B-CAB-CBB
22	A	806	CLA	C2B-C3B-CAB-CBB
22	A	841	CLA	C2B-C3B-CAB-CBB
22	B	805	CLA	C2B-C3B-CAB-CBB
22	B	810	CLA	C2B-C3B-CAB-CBB
22	B	818	CLA	C2B-C3B-CAB-CBB
22	B	820	CLA	C2B-C3B-CAB-CBB
22	B	835	CLA	C2B-C3B-CAB-CBB
22	B	841	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	F	301	CLA	C2B-C3B-CAB-CBB
22	K	101	CLA	C2B-C3B-CAB-CBB
22	K	104	CLA	C2B-C3B-CAB-CBB
22	K	105	CLA	C2B-C3B-CAB-CBB
22	1	303	CLA	C2B-C3B-CAB-CBB
22	2	313	CLA	C2B-C3B-CAB-CBB
22	3	310	CLA	C2B-C3B-CAB-CBB
22	4	302	CLA	C2B-C3B-CAB-CBB
22	4	310	CLA	C2B-C3B-CAB-CBB
22	6	313	CLA	C2B-C3B-CAB-CBB
22	6	314	CLA	C2B-C3B-CAB-CBB
22	5	307	CLA	C2B-C3B-CAB-CBB
22	5	308	CLA	C2B-C3B-CAB-CBB
22	7	302	CLA	C2B-C3B-CAB-CBB
22	7	304	CLA	C2B-C3B-CAB-CBB
22	7	307	CLA	C2B-C3B-CAB-CBB
22	7	313	CLA	C2B-C3B-CAB-CBB
22	9	309	CLA	C2B-C3B-CAB-CBB
22	9	313	CLA	C2B-C3B-CAB-CBB
22	0	307	CLA	C2B-C3B-CAB-CBB
22	5	304	CLA	O1A-CGA-O2A-C1
22	B	814	CLA	C2-C3-C5-C6
22	B	833	CLA	C2-C3-C5-C6
22	4	311	CLA	C2-C3-C5-C6
22	B	831	CLA	O1D-CGD-O2D-CED
22	A	806	CLA	C10-C11-C12-C13
22	B	840	CLA	C16-C17-C18-C19
22	B	850	CLA	C6-C7-C8-C9
22	9	313	CLA	C6-C7-C8-C10
22	A	822	CLA	C1-C2-C3-C4
22	A	852	CLA	C1-C2-C3-C4
22	2	314	CLA	C1-C2-C3-C4
22	A	813	CLA	C13-C15-C16-C17
22	L	202	CLA	C2A-CAA-CBA-CGA
22	2	314	CLA	C2A-CAA-CBA-CGA
22	5	302	CLA	C2A-CAA-CBA-CGA
22	0	311	CLA	C2A-CAA-CBA-CGA
22	B	810	CLA	C5-C6-C7-C8
22	B	814	CLA	C2-C1-O2A-CGA
22	B	819	CLA	C2-C1-O2A-CGA
22	B	820	CLA	C2-C1-O2A-CGA
22	B	821	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	H	201	CLA	C2-C1-O2A-CGA
22	2	309	CLA	C2-C1-O2A-CGA
22	6	305	CLA	C2-C1-O2A-CGA
29	4	301	CHL	C2-C1-O2A-CGA
29	9	302	CHL	C2-C1-O2A-CGA
29	7	308	CHL	C4C-C3C-CAC-CBC
29	9	307	CHL	O1D-CGD-O2D-CED
22	L	201	CLA	C3-C5-C6-C7
24	1	317	LHG	C24-C25-C26-C27
22	M	101	CLA	O1A-CGA-O2A-C1
24	1	317	LHG	C2-C3-O3-P
25	J	101	8CT	C16-C17-C18-C19
24	2	318	LHG	O6-C4-C5-O7
22	6	311	CLA	C4-C3-C5-C6
25	A	847	8CT	C04-C03-C10-C11
22	4	309	CLA	CBA-CGA-O2A-C1
22	A	833	CLA	C13-C15-C16-C17
22	B	821	CLA	C2C-C3C-CAC-CBC
22	5	303	CLA	C4C-C3C-CAC-CBC
22	5	309	CLA	C11-C12-C13-C14
22	3	319	CLA	C2A-CAA-CBA-CGA
22	5	313	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	O1A-CGA-O2A-C1
24	1	317	LHG	C3-O3-P-O6
24	1	317	LHG	C4-O6-P-O3
24	3	317	LHG	C3-O3-P-O6
22	A	811	CLA	C16-C17-C18-C20
22	B	817	CLA	C6-C7-C8-C10
22	B	824	CLA	C10-C11-C12-C13
22	B	815	CLA	C4C-C3C-CAC-CBC
22	A	805	CLA	C4-C3-C5-C6
22	B	827	CLA	C4-C3-C5-C6
22	A	808	CLA	C11-C12-C13-C15
22	A	811	CLA	C6-C7-C8-C10
22	A	818	CLA	C12-C13-C15-C16
22	A	827	CLA	C12-C13-C15-C16
22	A	853	CLA	C6-C7-C8-C10
22	B	816	CLA	C11-C10-C8-C7
22	6	315	CLA	C6-C7-C8-C10
23	B	842	PQN	C21-C22-C23-C25
29	2	301	CHL	C6-C7-C8-C10
22	6	309	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	A	807	CLA	C11-C12-C13-C14
22	A	819	CLA	C11-C12-C13-C14
22	A	819	CLA	C14-C13-C15-C16
22	A	828	CLA	C11-C12-C13-C14
22	A	837	CLA	C14-C13-C15-C16
22	B	808	CLA	C11-C10-C8-C9
22	B	830	CLA	C11-C12-C13-C14
22	2	302	CLA	C11-C12-C13-C14
22	2	302	CLA	C14-C13-C15-C16
22	2	303	CLA	C6-C7-C8-C9
22	7	316	CLA	C14-C13-C15-C16
22	0	307	CLA	C14-C13-C15-C16
22	H	201	CLA	C13-C15-C16-C17
22	7	307	CLA	O1D-CGD-O2D-CED
25	A	848	8CT	C16-C17-C18-C19
25	B	846	8CT	C12-C13-C14-C15
25	J	104	8CT	C16-C17-C18-C19
25	K	103	8CT	C12-C13-C14-C15
25	3	318	8CT	C18-C19-C20-C21
22	9	308	CLA	C16-C17-C18-C19
22	B	830	CLA	C15-C16-C17-C18
24	5	318	LHG	C9-C10-C11-C12
22	B	805	CLA	CAA-CBA-CGA-O1A
22	B	825	CLA	C2A-CAA-CBA-CGA
22	B	834	CLA	C2A-CAA-CBA-CGA
22	6	311	CLA	C3-C5-C6-C7
22	6	313	CLA	C16-C17-C18-C19
31	8	319	LMG	C30-C31-C32-C33
22	L	201	CLA	C5-C6-C7-C8
29	9	307	CHL	C2C-C3C-CAC-CBC
22	B	819	CLA	C2-C3-C5-C6
22	8	315	CLA	C2-C3-C5-C6
22	A	807	CLA	C16-C17-C18-C20
22	6	304	CLA	C16-C17-C18-C19
22	B	806	CLA	CBA-CGA-O2A-C1
22	4	309	CLA	C8-C10-C11-C12
28	B	849	DGD	O1A-C1A-O1G-C1G
22	A	828	CLA	CAA-CBA-CGA-O2A
22	B	826	CLA	C2C-C3C-CAC-CBC
24	0	315	LHG	C16-C17-C18-C19
22	K	102	CLA	CBA-CGA-O2A-C1
22	B	818	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	B	821	CLA	C4B-C3B-CAB-CBB
22	B	841	CLA	C4B-C3B-CAB-CBB
22	6	304	CLA	C4B-C3B-CAB-CBB
22	6	314	CLA	C4B-C3B-CAB-CBB
22	8	304	CLA	C4B-C3B-CAB-CBB
22	9	305	CLA	C4B-C3B-CAB-CBB
22	9	309	CLA	C4B-C3B-CAB-CBB
25	B	843	8CT	C18-C19-C20-C21
25	L	205	8CT	C12-C13-C14-C15
22	A	840	CLA	C3-C5-C6-C7
22	9	310	CLA	C2C-C3C-CAC-CBC
28	B	849	DGD	O6D-C5D-C6D-O5D
22	7	303	CLA	C10-C11-C12-C13
22	7	305	CLA	CAA-CBA-CGA-O1A
22	H	201	CLA	C16-C17-C18-C19
22	0	308	CLA	C11-C12-C13-C15
22	L	202	CLA	O1D-CGD-O2D-CED
22	A	802	CLA	C4-C3-C5-C6
22	B	839	CLA	C4-C3-C5-C6
22	F	301	CLA	CAA-CBA-CGA-O1A
22	7	317	CLA	C10-C11-C12-C13
22	B	839	CLA	C2-C3-C5-C6
22	A	803	CLA	O1A-CGA-O2A-C1
22	A	839	CLA	C10-C11-C12-C13
23	A	842	PQN	C23-C25-C26-C27
28	B	849	DGD	CAB-CBB-CCB-CDB
31	4	318	LMG	C22-C23-C24-C25
22	A	832	CLA	C2-C1-O2A-CGA
22	B	841	CLA	C2-C1-O2A-CGA
22	1	302	CLA	C2-C1-O2A-CGA
22	6	313	CLA	C2-C1-O2A-CGA
29	0	301	CHL	C2-C1-O2A-CGA
22	8	315	CLA	C2C-C3C-CAC-CBC
22	3	319	CLA	C8-C10-C11-C12
22	A	818	CLA	C2A-CAA-CBA-CGA
22	A	837	CLA	C2A-CAA-CBA-CGA
22	A	853	CLA	C2A-CAA-CBA-CGA
22	B	809	CLA	C2A-CAA-CBA-CGA
22	B	810	CLA	C2A-CAA-CBA-CGA
22	4	302	CLA	C2A-CAA-CBA-CGA
22	4	312	CLA	C2A-CAA-CBA-CGA
22	7	304	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	9	304	CLA	C2A-CAA-CBA-CGA
24	9	316	LHG	C31-C32-C33-C34
22	B	809	CLA	C3A-C2A-CAA-CBA
22	3	307	CLA	C3A-C2A-CAA-CBA
29	2	306	CHL	C3A-C2A-CAA-CBA
29	8	306	CHL	C3A-C2A-CAA-CBA
22	B	815	CLA	C2C-C3C-CAC-CBC
22	A	822	CLA	O2A-C1-C2-C3
24	A	844	LHG	C13-C14-C15-C16
30	3	314	XAT	C33-C34-C35-C15
22	A	813	CLA	C11-C10-C8-C9
22	A	837	CLA	C11-C12-C13-C14
22	B	841	CLA	C11-C10-C8-C9
22	2	312	CLA	C11-C10-C8-C9
22	5	302	CLA	C11-C12-C13-C14
22	5	312	CLA	C14-C13-C15-C16
29	6	302	CHL	C11-C10-C8-C9
22	A	817	CLA	C16-C17-C18-C20
24	A	845	LHG	C4-C5-C6-O8
25	B	843	8CT	C39-C16-C17-C18
25	B	844	8CT	C39-C16-C17-C18
25	B	844	8CT	C19-C20-C21-C22
25	B	844	8CT	C24-C25-C26-C27
25	B	845	8CT	C39-C16-C17-C18
25	B	845	8CT	C24-C25-C26-C27
25	B	846	8CT	C40-C12-C13-C14
25	B	846	8CT	C39-C16-C17-C18
25	B	848	8CT	C24-C25-C26-C27
25	B	851	8CT	C40-C12-C13-C14
25	B	851	8CT	C24-C25-C26-C27
25	J	104	8CT	C40-C12-C13-C14
25	K	103	8CT	C40-C12-C13-C14
25	K	103	8CT	C19-C20-C21-C22
25	K	103	8CT	C24-C25-C26-C27
25	L	205	8CT	C24-C25-C26-C27
25	2	317	8CT	C19-C20-C21-C22
25	3	316	8CT	C40-C12-C13-C14
25	4	317	8CT	C24-C25-C26-C27
25	5	317	8CT	C39-C16-C17-C18
30	1	314	XAT	C40-C33-C34-C35
30	4	315	XAT	C11-C10-C9-C19
30	4	315	XAT	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	6	319	XAT	C40-C33-C34-C35
30	5	315	XAT	C20-C13-C14-C15
30	5	315	XAT	C40-C33-C34-C35
30	8	316	XAT	C40-C33-C34-C35
30	9	314	XAT	C39-C29-C30-C31
30	0	313	XAT	C11-C10-C9-C19
30	0	313	XAT	C40-C33-C34-C35
30	0	314	XAT	C39-C29-C30-C31
30	0	314	XAT	C40-C33-C34-C35
22	5	309	CLA	C11-C12-C13-C15
22	9	308	CLA	C16-C17-C18-C20
22	A	803	CLA	CBA-CGA-O2A-C1
22	2	310	CLA	C4C-C3C-CAC-CBC
22	F	301	CLA	CAA-CBA-CGA-O2A
25	L	206	8CT	C27-C26-C28-C29
29	5	301	CHL	O1D-CGD-O2D-CED
22	A	843	CLA	C2C-C3C-CAC-CBC
22	0	308	CLA	C8-C10-C11-C12
22	A	853	CLA	C4-C3-C5-C6
22	A	802	CLA	C1A-C2A-CAA-CBA
22	A	831	CLA	C1A-C2A-CAA-CBA
22	B	809	CLA	C1A-C2A-CAA-CBA
22	B	830	CLA	C1A-C2A-CAA-CBA
22	B	838	CLA	C1A-C2A-CAA-CBA
22	B	840	CLA	C1A-C2A-CAA-CBA
22	B	850	CLA	C1A-C2A-CAA-CBA
22	L	201	CLA	C1A-C2A-CAA-CBA
22	2	309	CLA	C1A-C2A-CAA-CBA
22	3	307	CLA	C1A-C2A-CAA-CBA
22	6	309	CLA	C1A-C2A-CAA-CBA
22	8	304	CLA	C1A-C2A-CAA-CBA
29	5	301	CHL	C1A-C2A-CAA-CBA
22	A	817	CLA	C11-C12-C13-C15
22	A	825	CLA	C6-C7-C8-C10
22	A	853	CLA	C2-C3-C5-C6
22	B	812	CLA	C11-C12-C13-C15
22	B	824	CLA	C6-C7-C8-C10
22	B	840	CLA	C11-C12-C13-C15
22	1	302	CLA	C6-C7-C8-C10
22	3	319	CLA	C2-C3-C5-C6
22	5	303	CLA	C11-C10-C8-C7
22	8	302	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	6	321	8CT	C16-C17-C18-C19
22	A	835	CLA	CAA-CBA-CGA-O1A
22	A	835	CLA	CAA-CBA-CGA-O2A
22	A	804	CLA	C6-C7-C8-C9
22	B	823	CLA	C6-C7-C8-C9
24	0	315	LHG	C13-C14-C15-C16
22	B	824	CLA	C2A-CAA-CBA-CGA
22	2	304	CLA	C2A-CAA-CBA-CGA
22	2	312	CLA	C2A-CAA-CBA-CGA
22	3	305	CLA	C2A-CAA-CBA-CGA
22	6	318	CLA	C2A-CAA-CBA-CGA
22	A	826	CLA	C5-C6-C7-C8
22	1	307	CLA	C10-C11-C12-C13
22	5	302	CLA	C13-C15-C16-C17
22	5	303	CLA	C13-C15-C16-C17
22	9	309	CLA	C8-C10-C11-C12
24	6	322	LHG	C12-C13-C14-C15
22	B	807	CLA	CAA-CBA-CGA-O2A
22	B	811	CLA	C4-C3-C5-C6
22	4	312	CLA	C4-C3-C5-C6
22	9	306	CLA	C4-C3-C5-C6
22	8	315	CLA	C10-C11-C12-C13
29	6	302	CHL	C5-C6-C7-C8
22	A	802	CLA	C2-C3-C5-C6
22	A	805	CLA	C2B-C3B-CAB-CBB
22	A	824	CLA	C2B-C3B-CAB-CBB
22	A	834	CLA	C2B-C3B-CAB-CBB
22	B	808	CLA	C2B-C3B-CAB-CBB
22	B	816	CLA	C2B-C3B-CAB-CBB
22	B	834	CLA	C2B-C3B-CAB-CBB
22	1	301	CLA	C2B-C3B-CAB-CBB
22	1	307	CLA	C2B-C3B-CAB-CBB
22	1	310	CLA	C2B-C3B-CAB-CBB
22	3	303	CLA	C2B-C3B-CAB-CBB
22	3	311	CLA	C2B-C3B-CAB-CBB
22	3	319	CLA	C2B-C3B-CAB-CBB
22	4	311	CLA	C2B-C3B-CAB-CBB
22	4	314	CLA	C2B-C3B-CAB-CBB
22	6	304	CLA	C2B-C3B-CAB-CBB
22	6	315	CLA	C2B-C3B-CAB-CBB
22	5	309	CLA	C2B-C3B-CAB-CBB
22	7	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	7	312	CLA	C2B-C3B-CAB-CBB
22	7	317	CLA	C2B-C3B-CAB-CBB
22	8	303	CLA	C2B-C3B-CAB-CBB
22	8	304	CLA	C2B-C3B-CAB-CBB
22	8	311	CLA	C2B-C3B-CAB-CBB
22	9	303	CLA	C2B-C3B-CAB-CBB
22	9	308	CLA	C2B-C3B-CAB-CBB
22	0	302	CLA	C2B-C3B-CAB-CBB
22	0	304	CLA	C2B-C3B-CAB-CBB
22	0	311	CLA	C2B-C3B-CAB-CBB
29	6	316	CHL	C2B-C3B-CAB-CBB
29	7	308	CHL	C2B-C3B-CAB-CBB
31	4	318	LMG	C19-C20-C21-C22
22	7	305	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	C16-C17-C18-C19
25	B	843	8CT	C15-C16-C17-C18
25	B	844	8CT	C15-C16-C17-C18
25	B	844	8CT	C19-C20-C21-C23
25	B	844	8CT	C24-C25-C26-C28
25	B	845	8CT	C15-C16-C17-C18
25	B	845	8CT	C24-C25-C26-C28
25	B	846	8CT	C11-C12-C13-C14
25	B	846	8CT	C15-C16-C17-C18
25	B	848	8CT	C24-C25-C26-C28
25	B	851	8CT	C11-C12-C13-C14
25	B	851	8CT	C24-C25-C26-C28
25	J	104	8CT	C11-C12-C13-C14
25	K	103	8CT	C11-C12-C13-C14
25	K	103	8CT	C19-C20-C21-C23
25	K	103	8CT	C24-C25-C26-C28
25	L	205	8CT	C24-C25-C26-C28
25	2	317	8CT	C19-C20-C21-C23
25	3	316	8CT	C11-C12-C13-C14
25	4	317	8CT	C24-C25-C26-C28
25	5	317	8CT	C15-C16-C17-C18
30	1	314	XAT	C32-C33-C34-C35
30	4	315	XAT	C11-C10-C9-C8
30	4	315	XAT	C12-C13-C14-C15
30	6	319	XAT	C32-C33-C34-C35
30	5	315	XAT	C12-C13-C14-C15
30	5	315	XAT	C32-C33-C34-C35
30	8	316	XAT	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	9	314	XAT	C28-C29-C30-C31
30	0	313	XAT	C11-C10-C9-C8
30	0	313	XAT	C32-C33-C34-C35
30	0	314	XAT	C28-C29-C30-C31
30	0	314	XAT	C32-C33-C34-C35
24	0	315	LHG	O7-C5-C6-O8
22	3	307	CLA	CAA-CBA-CGA-O1A
22	3	313	CLA	C2A-CAA-CBA-CGA
25	B	804	8CT	C18-C19-C20-C21
25	F	302	8CT	C16-C17-C18-C19
25	F	302	8CT	C18-C19-C20-C21
30	1	315	XAT	C29-C30-C31-C32
30	5	316	XAT	C29-C30-C31-C32
22	4	313	CLA	CAA-CBA-CGA-O2A
22	B	816	CLA	C10-C11-C12-C13
22	B	820	CLA	C16-C17-C18-C19
22	8	309	CLA	C11-C12-C13-C14
22	7	318	CLA	C15-C16-C17-C18
24	3	317	LHG	C1-C2-C3-O3
22	B	807	CLA	CAA-CBA-CGA-O1A
22	8	313	CLA	CAA-CBA-CGA-O2A
22	B	836	CLA	C4C-C3C-CAC-CBC
29	0	306	CHL	C2-C1-O2A-CGA
22	A	843	CLA	C4-C3-C5-C6
22	0	305	CLA	C4-C3-C5-C6
22	A	819	CLA	C2-C1-O2A-CGA
22	A	837	CLA	C2-C1-O2A-CGA
22	2	302	CLA	C2-C1-O2A-CGA
29	7	308	CHL	O1A-CGA-O2A-C1
22	A	805	CLA	C2-C3-C5-C6
22	B	840	CLA	C16-C17-C18-C20
22	A	807	CLA	C14-C13-C15-C16
22	B	812	CLA	C6-C7-C8-C9
22	9	303	CLA	C6-C7-C8-C9
22	9	308	CLA	C11-C10-C8-C9
22	B	808	CLA	C3-C5-C6-C7
22	7	316	CLA	C5-C6-C7-C8
29	6	302	CHL	C2A-CAA-CBA-CGA
22	A	832	CLA	O1A-CGA-O2A-C1
25	8	301	8CT	C02-C03-C10-C11
22	A	837	CLA	C10-C11-C12-C13
22	A	836	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	1	311	CLA	C10-C11-C12-C13
28	B	849	DGD	C3A-C4A-C5A-C6A
25	A	848	8CT	C18-C19-C20-C21
31	5	319	LMG	C30-C31-C32-C33
22	7	318	CLA	C4-C3-C5-C6
22	A	811	CLA	C15-C16-C17-C18
24	5	318	LHG	C17-C18-C19-C20
22	A	833	CLA	C2-C3-C5-C6
22	6	311	CLA	C2-C3-C5-C6
22	B	850	CLA	C3-C5-C6-C7
22	8	313	CLA	CAA-CBA-CGA-O1A
29	2	306	CHL	CAA-CBA-CGA-O1A
29	1	305	CHL	C2-C1-O2A-CGA
29	4	301	CHL	C8-C10-C11-C12
22	A	811	CLA	C16-C17-C18-C19
22	8	310	CLA	C6-C7-C8-C10
29	5	301	CHL	C11-C12-C13-C15
22	4	313	CLA	CAA-CBA-CGA-O1A
22	A	807	CLA	C4B-C3B-CAB-CBB
22	6	312	CLA	C4B-C3B-CAB-CBB
22	8	309	CLA	C4B-C3B-CAB-CBB
22	9	303	CLA	C4B-C3B-CAB-CBB
22	A	810	CLA	C15-C16-C17-C18
29	9	302	CHL	C4-C3-C5-C6
22	A	801	CLA	C12-C13-C15-C16
22	A	806	CLA	C6-C7-C8-C10
22	A	843	CLA	C2-C3-C5-C6
22	B	819	CLA	C6-C7-C8-C10
22	B	839	CLA	C11-C12-C13-C15
22	1	311	CLA	C12-C13-C15-C16
22	6	304	CLA	C6-C7-C8-C10
22	7	318	CLA	C2-C3-C5-C6
22	9	308	CLA	C11-C10-C8-C7
22	0	311	CLA	C11-C12-C13-C15
22	6	309	CLA	C4C-C3C-CAC-CBC
24	3	317	LHG	O8-C23-C24-C25
24	7	322	LHG	O8-C23-C24-C25
22	5	314	CLA	CAA-CBA-CGA-O2A
22	A	839	CLA	C16-C17-C18-C20
22	A	825	CLA	O1A-CGA-O2A-C1
22	A	832	CLA	CBA-CGA-O2A-C1
24	1	317	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
22	A	852	CLA	O2A-C1-C2-C3
22	B	820	CLA	C15-C16-C17-C18
22	6	311	CLA	C10-C11-C12-C13
22	A	853	CLA	C16-C17-C18-C19
22	B	801	CLA	C16-C17-C18-C20
22	0	308	CLA	C11-C12-C13-C14
22	A	825	CLA	CBA-CGA-O2A-C1
24	0	315	LHG	C24-C23-O8-C6
22	B	832	CLA	CAA-CBA-CGA-O2A
22	1	307	CLA	CAA-CBA-CGA-O2A
22	0	312	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	C4-C3-C5-C6
22	L	202	CLA	C4-C3-C5-C6
22	9	312	CLA	C4-C3-C5-C6
22	A	837	CLA	C2-C3-C5-C6
22	B	834	CLA	CAA-CBA-CGA-O2A
22	7	318	CLA	CAA-CBA-CGA-O2A
22	A	802	CLA	C6-C7-C8-C9
22	A	818	CLA	C11-C10-C8-C9
22	A	826	CLA	C6-C7-C8-C9
22	B	803	CLA	C11-C10-C8-C9
22	B	816	CLA	C11-C10-C8-C9
22	B	824	CLA	C6-C7-C8-C9
22	B	824	CLA	C11-C10-C8-C9
22	B	825	CLA	C14-C13-C15-C16
22	B	834	CLA	C11-C10-C8-C9
22	B	840	CLA	C11-C12-C13-C14
22	1	302	CLA	C6-C7-C8-C9
22	5	303	CLA	C6-C7-C8-C9
22	5	303	CLA	C11-C10-C8-C9
22	7	317	CLA	C6-C7-C8-C9
22	0	307	CLA	C11-C12-C13-C14
22	6	317	CLA	CAA-CBA-CGA-O1A
22	A	814	CLA	C3A-C2A-CAA-CBA
22	B	822	CLA	C3A-C2A-CAA-CBA
22	B	837	CLA	C3A-C2A-CAA-CBA
22	F	301	CLA	C3A-C2A-CAA-CBA
22	5	304	CLA	C3A-C2A-CAA-CBA
22	7	316	CLA	C3A-C2A-CAA-CBA
22	9	306	CLA	C3A-C2A-CAA-CBA
29	5	306	CHL	C3A-C2A-CAA-CBA
24	A	844	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
22	B	838	CLA	CAA-CBA-CGA-O2A
22	H	201	CLA	CAA-CBA-CGA-O2A
22	A	813	CLA	CAD-CBD-CGD-O2D
22	A	823	CLA	CAD-CBD-CGD-O2D
22	A	827	CLA	CAD-CBD-CGD-O2D
22	A	828	CLA	CAD-CBD-CGD-O2D
22	A	833	CLA	CAD-CBD-CGD-O2D
22	A	840	CLA	CAD-CBD-CGD-O2D
22	B	818	CLA	CAD-CBD-CGD-O2D
22	B	820	CLA	CAD-CBD-CGD-O2D
22	B	822	CLA	CAD-CBD-CGD-O2D
22	B	830	CLA	CAD-CBD-CGD-O2D
22	B	831	CLA	CAD-CBD-CGD-O2D
22	1	313	CLA	CAD-CBD-CGD-O2D
22	2	311	CLA	CAD-CBD-CGD-O2D
22	3	304	CLA	CAD-CBD-CGD-O2D
22	3	305	CLA	CAD-CBD-CGD-O2D
22	3	307	CLA	CAD-CBD-CGD-O2D
22	3	308	CLA	CAD-CBD-CGD-O2D
22	4	312	CLA	CAD-CBD-CGD-O2D
22	4	314	CLA	CAD-CBD-CGD-O2D
22	6	310	CLA	CAD-CBD-CGD-O2D
22	6	318	CLA	CAD-CBD-CGD-O2D
22	5	310	CLA	CAD-CBD-CGD-O2D
22	5	313	CLA	CAD-CBD-CGD-O2D
22	7	304	CLA	CAD-CBD-CGD-O2D
22	7	307	CLA	CAD-CBD-CGD-O2D
22	7	312	CLA	CAD-CBD-CGD-O2D
22	7	313	CLA	CAD-CBD-CGD-O2D
22	7	316	CLA	CAD-CBD-CGD-O2D
22	8	303	CLA	CAD-CBD-CGD-O2D
22	0	304	CLA	CAD-CBD-CGD-O2D
22	0	305	CLA	CAD-CBD-CGD-O2D
22	0	307	CLA	CAD-CBD-CGD-O2D
22	0	311	CLA	CAD-CBD-CGD-O2D
29	5	301	CHL	CAD-CBD-CGD-O2D
24	5	318	LHG	C19-C20-C21-C22
22	B	811	CLA	C10-C11-C12-C13
22	4	314	CLA	C10-C11-C12-C13
22	A	809	CLA	C10-C11-C12-C13
22	6	309	CLA	C2-C1-O2A-CGA
22	G	101	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	A	822	CLA	CAA-CBA-CGA-O2A
22	2	319	CLA	CAA-CBA-CGA-O2A
31	5	319	LMG	O7-C10-C11-C12
22	2	310	CLA	C2C-C3C-CAC-CBC
22	B	818	CLA	C4-C3-C5-C6
22	7	313	CLA	C4-C3-C5-C6
22	7	313	CLA	C6-C7-C8-C10
22	A	815	CLA	C2-C1-O2A-CGA
22	B	818	CLA	C11-C12-C13-C14
22	B	811	CLA	C2-C3-C5-C6
22	L	202	CLA	C2-C3-C5-C6
22	4	312	CLA	C2-C3-C5-C6
22	A	806	CLA	CAA-CBA-CGA-O2A
22	1	302	CLA	CAA-CBA-CGA-O2A
22	3	311	CLA	CAA-CBA-CGA-O2A
22	6	301	CLA	CAA-CBA-CGA-O2A
29	0	301	CHL	CAA-CBA-CGA-O2A
24	9	316	LHG	C18-C19-C20-C21
25	B	843	8CT	C25-C26-C28-C29
25	L	206	8CT	C25-C26-C28-C29
22	1	310	CLA	C3-C5-C6-C7
30	2	315	XAT	O4-C6-C7-C8
30	4	316	XAT	O24-C26-C27-C28
30	6	320	XAT	O4-C6-C7-C8
30	5	316	XAT	O24-C26-C27-C28
30	8	316	XAT	O4-C6-C7-C8
22	A	822	CLA	O1D-CGD-O2D-CED
22	6	304	CLA	CAA-CBA-CGA-O2A
29	5	301	CHL	CAA-CBA-CGA-O2A
24	6	322	LHG	C10-C11-C12-C13
22	K	101	CLA	CAA-CBA-CGA-O2A
22	A	805	CLA	O2A-C1-C2-C3
22	A	808	CLA	O2A-C1-C2-C3
22	A	810	CLA	O2A-C1-C2-C3
22	A	840	CLA	O2A-C1-C2-C3
22	B	834	CLA	O2A-C1-C2-C3
22	L	204	CLA	O2A-C1-C2-C3
22	8	315	CLA	O2A-C1-C2-C3
22	9	313	CLA	O2A-C1-C2-C3
29	6	308	CHL	O2A-C1-C2-C3
29	9	302	CHL	O2A-C1-C2-C3
22	B	836	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
28	B	849	DGD	C6A-C7A-C8A-C9A
29	5	301	CHL	C2A-CAA-CBA-CGA
22	A	829	CLA	CAA-CBA-CGA-O2A
22	1	310	CLA	CAA-CBA-CGA-O2A
22	3	312	CLA	CAA-CBA-CGA-O2A
22	H	201	CLA	C15-C16-C17-C18
22	9	313	CLA	C6-C7-C8-C9
22	6	309	CLA	C2C-C3C-CAC-CBC
22	A	809	CLA	CHA-CBD-CGD-O1D
22	A	809	CLA	CHA-CBD-CGD-O2D
22	A	822	CLA	CHA-CBD-CGD-O1D
22	A	822	CLA	CHA-CBD-CGD-O2D
22	A	830	CLA	CHA-CBD-CGD-O1D
22	A	830	CLA	CHA-CBD-CGD-O2D
22	A	833	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O1D
22	A	837	CLA	CHA-CBD-CGD-O2D
22	B	803	CLA	CHA-CBD-CGD-O1D
22	B	803	CLA	CHA-CBD-CGD-O2D
22	B	816	CLA	CHA-CBD-CGD-O1D
22	B	816	CLA	CHA-CBD-CGD-O2D
22	B	824	CLA	CHA-CBD-CGD-O2D
22	B	827	CLA	CHA-CBD-CGD-O1D
22	B	827	CLA	CHA-CBD-CGD-O2D
22	B	833	CLA	CHA-CBD-CGD-O2D
22	G	103	CLA	CHA-CBD-CGD-O1D
22	1	302	CLA	CHA-CBD-CGD-O1D
22	1	302	CLA	CHA-CBD-CGD-O2D
22	1	303	CLA	CHA-CBD-CGD-O2D
22	2	302	CLA	CHA-CBD-CGD-O1D
22	3	312	CLA	CHA-CBD-CGD-O2D
22	4	314	CLA	CHA-CBD-CGD-O2D
22	6	303	CLA	CHA-CBD-CGD-O1D
22	6	305	CLA	CHA-CBD-CGD-O2D
22	6	315	CLA	CHA-CBD-CGD-O1D
22	6	315	CLA	CHA-CBD-CGD-O2D
22	5	303	CLA	CHA-CBD-CGD-O1D
22	5	303	CLA	CHA-CBD-CGD-O2D
22	5	305	CLA	CHA-CBD-CGD-O1D
22	5	305	CLA	CHA-CBD-CGD-O2D
22	7	318	CLA	CHA-CBD-CGD-O1D
22	8	304	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	8	312	CLA	CHA-CBD-CGD-O1D
22	8	312	CLA	CHA-CBD-CGD-O2D
22	9	304	CLA	CHA-CBD-CGD-O2D
22	0	302	CLA	CHA-CBD-CGD-O2D
29	2	306	CHL	CHA-CBD-CGD-O1D
29	2	306	CHL	CHA-CBD-CGD-O2D
22	G	101	CLA	CAA-CBA-CGA-O1A
22	K	101	CLA	CAA-CBA-CGA-O1A
22	3	312	CLA	CAA-CBA-CGA-O1A
22	B	812	CLA	C4-C3-C5-C6
29	6	302	CHL	C8-C10-C11-C12
22	A	819	CLA	C16-C17-C18-C20
22	B	833	CLA	CAA-CBA-CGA-O2A
22	7	313	CLA	CAA-CBA-CGA-O2A
29	7	308	CHL	CAA-CBA-CGA-O2A
24	7	322	LHG	O7-C5-C6-O8
22	8	308	CLA	O1A-CGA-O2A-C1
22	B	818	CLA	C3-C5-C6-C7
22	A	839	CLA	CAA-CBA-CGA-O2A
22	3	313	CLA	CAA-CBA-CGA-O2A
22	6	312	CLA	CAA-CBA-CGA-O2A
22	0	308	CLA	CAA-CBA-CGA-O2A
29	4	306	CHL	CAA-CBA-CGA-O2A
22	B	831	CLA	C2A-CAA-CBA-CGA
22	6	317	CLA	CAA-CBA-CGA-O2A
24	2	318	LHG	C24-C25-C26-C27
22	A	813	CLA	C11-C12-C13-C15
22	A	839	CLA	C11-C10-C8-C7
22	A	839	CLA	C11-C12-C13-C15
22	B	805	CLA	C12-C13-C15-C16
22	B	826	CLA	C11-C12-C13-C15
22	7	313	CLA	C2-C3-C5-C6
22	7	317	CLA	C11-C12-C13-C15
22	0	303	CLA	C6-C7-C8-C10
22	0	307	CLA	C11-C10-C8-C7
22	A	806	CLA	C16-C17-C18-C20
22	8	308	CLA	CBA-CGA-O2A-C1
22	A	805	CLA	CAA-CBA-CGA-O2A
22	A	821	CLA	CAA-CBA-CGA-O2A
22	K	105	CLA	CAA-CBA-CGA-O2A
22	A	806	CLA	C11-C10-C8-C9
22	B	841	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	2	304	CLA	C6-C7-C8-C9
22	6	315	CLA	C6-C7-C8-C9
22	8	309	CLA	C6-C7-C8-C9
25	5	317	8CT	C16-C17-C18-C19
24	3	317	LHG	O2-C2-C3-O3
22	7	317	CLA	CAA-CBA-CGA-O2A
22	B	834	CLA	CAA-CBA-CGA-O1A
22	0	311	CLA	C3-C5-C6-C7
22	B	815	CLA	C15-C16-C17-C18
22	A	802	CLA	C2A-CAA-CBA-CGA
22	8	302	CLA	C2A-CAA-CBA-CGA
22	8	312	CLA	C2A-CAA-CBA-CGA
24	A	844	LHG	O10-C23-C24-C25
29	0	301	CHL	CAA-CBA-CGA-O1A
29	9	307	CHL	C4C-C3C-CAC-CBC
22	B	838	CLA	CAA-CBA-CGA-O1A
22	A	813	CLA	C15-C16-C17-C18
22	6	305	CLA	C5-C6-C7-C8
22	9	310	CLA	C4C-C3C-CAC-CBC
24	0	315	LHG	O1-C1-C2-C3
22	A	843	CLA	C3-C5-C6-C7
22	A	806	CLA	CAA-CBA-CGA-O1A
22	0	312	CLA	CAA-CBA-CGA-O1A
22	0	302	CLA	C13-C15-C16-C17
22	A	814	CLA	C1A-C2A-CAA-CBA
22	A	852	CLA	C1A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	F	301	CLA	C1A-C2A-CAA-CBA
22	1	303	CLA	C1A-C2A-CAA-CBA
22	2	303	CLA	C1A-C2A-CAA-CBA
22	6	312	CLA	C1A-C2A-CAA-CBA
22	7	316	CLA	C1A-C2A-CAA-CBA
22	9	301	CLA	C1A-C2A-CAA-CBA
22	9	306	CLA	C1A-C2A-CAA-CBA
22	0	307	CLA	C1A-C2A-CAA-CBA
29	5	306	CHL	C1A-C2A-CAA-CBA
22	B	832	CLA	CAA-CBA-CGA-O1A
22	1	310	CLA	CAA-CBA-CGA-O1A
22	2	319	CLA	CAA-CBA-CGA-O1A
22	6	323	CLA	CAA-CBA-CGA-O2A
22	A	805	CLA	C8-C10-C11-C12
24	6	322	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	A	825	CLA	O1D-CGD-O2D-CED
22	1	304	CLA	C2-C1-O2A-CGA
28	B	849	DGD	C6B-C7B-C8B-C9B
22	A	804	CLA	C5-C6-C7-C8
22	9	308	CLA	C8-C10-C11-C12
22	1	302	CLA	CAA-CBA-CGA-O1A
22	1	307	CLA	CAA-CBA-CGA-O1A
24	5	318	LHG	O10-C23-C24-C25
22	0	307	CLA	C13-C15-C16-C17
22	9	312	CLA	C2A-CAA-CBA-CGA
22	0	304	CLA	C2A-CAA-CBA-CGA
22	K	102	CLA	CBD-CGD-O2D-CED
22	A	813	CLA	C16-C17-C18-C20
22	5	314	CLA	CAA-CBA-CGA-O1A
22	7	318	CLA	CAA-CBA-CGA-O1A
31	5	319	LMG	O10-C28-C29-C30
31	4	318	LMG	C11-C12-C13-C14
29	8	306	CHL	O1A-CGA-O2A-C1
22	7	303	CLA	CAA-CBA-CGA-O2A
22	8	303	CLA	CAA-CBA-CGA-O2A
24	A	844	LHG	O8-C23-C24-C25
24	6	322	LHG	C5-C4-O6-P
22	H	201	CLA	CAA-CBA-CGA-O1A
22	K	105	CLA	CAA-CBA-CGA-O1A
22	3	311	CLA	CAA-CBA-CGA-O1A
22	B	827	CLA	C2-C3-C5-C6
29	9	307	CHL	C2-C1-O2A-CGA
22	A	823	CLA	C4B-C3B-CAB-CBB
22	A	853	CLA	C4B-C3B-CAB-CBB
22	B	840	CLA	C4B-C3B-CAB-CBB
22	2	310	CLA	C4B-C3B-CAB-CBB
22	4	303	CLA	C4B-C3B-CAB-CBB
22	7	305	CLA	C4B-C3B-CAB-CBB
22	7	307	CLA	C4B-C3B-CAB-CBB
22	8	315	CLA	C4B-C3B-CAB-CBB
24	1	317	LHG	C3-O3-P-O5
24	6	322	LHG	C4-O6-P-O5
24	9	316	LHG	C4-O6-P-O5
29	4	305	CHL	C4B-C3B-CAB-CBB
29	6	316	CHL	C4B-C3B-CAB-CBB
29	7	308	CHL	C4B-C3B-CAB-CBB
24	A	845	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
22	A	821	CLA	CAA-CBA-CGA-O1A
22	7	317	CLA	CAA-CBA-CGA-O1A
29	7	308	CHL	CAA-CBA-CGA-O1A
22	L	204	CLA	CAA-CBA-CGA-O2A
22	5	307	CLA	CAA-CBA-CGA-O2A
22	7	302	CLA	CAA-CBA-CGA-O2A
22	A	827	CLA	C15-C16-C17-C18
22	B	803	CLA	C4C-C3C-CAC-CBC
22	A	814	CLA	CAA-CBA-CGA-O2A
25	A	850	8CT	C04-C03-C10-C11
25	F	302	8CT	C02-C03-C10-C11
25	7	323	8CT	C02-C03-C10-C11
22	6	304	CLA	C13-C15-C16-C17
30	9	314	XAT	C6-C7-C8-C9
22	A	805	CLA	CAA-CBA-CGA-O1A
22	A	829	CLA	CAA-CBA-CGA-O1A
22	6	301	CLA	CAA-CBA-CGA-O1A
22	0	308	CLA	CAA-CBA-CGA-O1A
22	6	311	CLA	CAA-CBA-CGA-O2A
22	L	202	CLA	C16-C17-C18-C20
22	7	313	CLA	C6-C7-C8-C9
22	0	303	CLA	C2A-CAA-CBA-CGA
22	7	316	CLA	CAA-CBA-CGA-O2A
22	9	313	CLA	CAA-CBA-CGA-O2A
22	A	822	CLA	CAA-CBA-CGA-O1A
22	6	304	CLA	CAA-CBA-CGA-O1A
22	A	828	CLA	C16-C17-C18-C20
22	A	805	CLA	CAD-CBD-CGD-O1D
22	A	817	CLA	CAD-CBD-CGD-O1D
22	A	827	CLA	CAD-CBD-CGD-O1D
22	A	836	CLA	C2-C3-C5-C6
22	B	836	CLA	CAD-CBD-CGD-O1D
22	B	840	CLA	CAD-CBD-CGD-O1D
22	B	841	CLA	CAD-CBD-CGD-O1D
22	G	103	CLA	CAD-CBD-CGD-O1D
22	K	101	CLA	CAD-CBD-CGD-O1D
22	2	302	CLA	CAD-CBD-CGD-O1D
22	3	310	CLA	CAD-CBD-CGD-O1D
22	4	303	CLA	CAD-CBD-CGD-O1D
22	4	311	CLA	CAD-CBD-CGD-O1D
22	7	318	CLA	CAD-CBD-CGD-O1D
29	8	314	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	833	CLA	CAA-CBA-CGA-O1A
22	7	303	CLA	CAA-CBA-CGA-O1A
29	5	301	CHL	CAA-CBA-CGA-O1A
22	B	840	CLA	CAA-CBA-CGA-O2A
22	A	802	CLA	C11-C12-C13-C14
22	A	813	CLA	C11-C12-C13-C14
22	A	839	CLA	C11-C10-C8-C9
22	B	828	CLA	C14-C13-C15-C16
22	L	202	CLA	C6-C7-C8-C9
22	1	311	CLA	C6-C7-C8-C9
22	6	313	CLA	C11-C10-C8-C9
22	9	308	CLA	C6-C7-C8-C9
22	0	303	CLA	C6-C7-C8-C9
22	0	307	CLA	C11-C10-C8-C9
22	0	311	CLA	C11-C12-C13-C14
22	2	312	CLA	C15-C16-C17-C18
29	4	306	CHL	CAA-CBA-CGA-O1A
29	8	306	CHL	CBA-CGA-O2A-C1
22	1	312	CLA	C3-C5-C6-C7
22	B	814	CLA	CAA-CBA-CGA-O2A
22	B	841	CLA	CAA-CBA-CGA-O2A
22	4	302	CLA	CAA-CBA-CGA-O2A
31	5	319	LMG	O8-C28-C29-C30
22	6	310	CLA	O1A-CGA-O2A-C1
22	3	313	CLA	CAA-CBA-CGA-O1A
22	6	312	CLA	CAA-CBA-CGA-O1A
22	4	309	CLA	C5-C6-C7-C8
22	B	837	CLA	C2A-CAA-CBA-CGA
22	3	301	CLA	C2A-CAA-CBA-CGA
22	0	302	CLA	C2A-CAA-CBA-CGA
22	B	801	CLA	CAA-CBA-CGA-O2A
22	2	311	CLA	CAA-CBA-CGA-O2A
22	4	303	CLA	CAA-CBA-CGA-O2A
22	M	101	CLA	CAA-CBA-CGA-O2A
29	1	305	CHL	CAA-CBA-CGA-O2A
29	2	307	CHL	CAA-CBA-CGA-O2A
29	9	307	CHL	CAA-CBA-CGA-O2A
31	8	319	LMG	O7-C10-C11-C12
22	A	839	CLA	CAA-CBA-CGA-O1A
22	A	806	CLA	C11-C10-C8-C7
22	B	812	CLA	C11-C10-C8-C7
22	B	814	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	818	CLA	C6-C7-C8-C10
22	B	826	CLA	C12-C13-C15-C16
22	B	828	CLA	C12-C13-C15-C16
22	B	841	CLA	C11-C12-C13-C15
22	L	201	CLA	C11-C10-C8-C7
22	L	202	CLA	C6-C7-C8-C10
22	1	307	CLA	C6-C7-C8-C10
22	1	311	CLA	C6-C7-C8-C10
22	2	304	CLA	C6-C7-C8-C10
22	2	312	CLA	C6-C7-C8-C10
22	3	319	CLA	C11-C12-C13-C15
22	5	312	CLA	C12-C13-C15-C16
25	A	847	8CT	C28-C29-C30-C31
25	B	804	8CT	C28-C29-C30-C31
25	B	847	8CT	C28-C29-C30-C31
25	G	104	8CT	C28-C29-C30-C31
22	L	204	CLA	CAA-CBA-CGA-O1A
22	A	820	CLA	CAA-CBA-CGA-O2A
28	B	849	DGD	C5B-C6B-C7B-C8B
22	A	832	CLA	CAA-CBA-CGA-O2A
22	B	813	CLA	CAA-CBA-CGA-O2A
22	6	313	CLA	CAA-CBA-CGA-O2A
22	7	309	CLA	CAA-CBA-CGA-O2A
24	9	316	LHG	O7-C7-C8-C9
29	6	302	CHL	CAA-CBA-CGA-O2A
29	0	306	CHL	CAA-CBA-CGA-O2A
22	A	803	CLA	C3-C5-C6-C7
25	A	850	8CT	C20-C21-C23-C24
22	A	832	CLA	CAA-CBA-CGA-O1A
22	6	311	CLA	CAA-CBA-CGA-O1A
22	7	314	CLA	CAA-CBA-CGA-O1A
24	A	844	LHG	C15-C16-C17-C18
22	5	304	CLA	CAA-CBA-CGA-O2A
22	B	840	CLA	C15-C16-C17-C18
22	4	314	CLA	C15-C16-C17-C18
22	A	834	CLA	O1A-CGA-O2A-C1
22	B	840	CLA	CAA-CBA-CGA-O1A
22	2	311	CLA	CAA-CBA-CGA-O1A
22	4	302	CLA	CAA-CBA-CGA-O1A
22	5	307	CLA	CAA-CBA-CGA-O1A
22	7	313	CLA	CAA-CBA-CGA-O1A
29	1	305	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	0	306	CHL	CAA-CBA-CGA-O1A
22	B	808	CLA	CAA-CBA-CGA-O1A
22	6	323	CLA	CAA-CBA-CGA-O1A
22	7	309	CLA	CAA-CBA-CGA-O1A
22	8	303	CLA	CAA-CBA-CGA-O1A
29	6	308	CHL	C2A-CAA-CBA-CGA
24	9	316	LHG	C17-C18-C19-C20
22	B	817	CLA	C4-C3-C5-C6
22	K	102	CLA	O1A-CGA-O2A-C1
22	A	825	CLA	CAA-CBA-CGA-O2A
22	A	814	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

295 monomers are involved in 1342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	7	322	LHG	2	0
30	6	319	XAT	7	0
25	B	847	8CT	13	0
29	5	301	CHL	12	0
25	A	847	8CT	1	0
22	6	312	CLA	1	0
22	B	831	CLA	1	0
22	1	310	CLA	4	0
22	8	312	CLA	2	0
22	6	314	CLA	5	0
29	5	306	CHL	4	0
22	B	805	CLA	7	0
22	2	319	CLA	1	0
22	3	310	CLA	1	0
22	B	839	CLA	2	0
31	8	319	LMG	6	0
22	9	312	CLA	9	0
22	H	201	CLA	16	0
27	C	101	SF4	1	0
22	A	836	CLA	3	0
31	5	319	LMG	6	0
22	A	803	CLA	5	0
22	6	305	CLA	11	0
30	7	319	XAT	6	0
22	A	831	CLA	4	0
22	B	823	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	803	CLA	16	0
22	1	301	CLA	6	0
22	5	303	CLA	11	0
22	B	810	CLA	7	0
22	4	314	CLA	4	0
22	2	309	CLA	4	0
22	4	303	CLA	1	0
22	L	201	CLA	4	0
22	A	804	CLA	3	0
30	8	317	XAT	9	0
22	6	313	CLA	5	0
22	6	301	CLA	4	0
23	A	842	PQN	3	0
22	G	101	CLA	1	0
22	B	814	CLA	8	0
22	9	309	CLA	9	0
30	1	314	XAT	9	0
24	A	845	LHG	1	0
22	B	824	CLA	7	0
22	9	313	CLA	2	0
22	B	837	CLA	5	0
25	8	318	8CT	2	0
22	B	826	CLA	9	0
22	1	308	CLA	6	0
22	A	816	CLA	2	0
22	8	304	CLA	3	0
26	J	102	HTG	1	0
29	8	314	CHL	11	0
22	4	313	CLA	4	0
22	G	102	CLA	7	0
25	2	317	8CT	13	0
22	B	816	CLA	5	0
22	5	302	CLA	7	0
22	B	829	CLA	9	0
22	B	815	CLA	6	0
22	2	303	CLA	2	0
25	6	321	8CT	14	0
22	3	308	CLA	4	0
22	7	318	CLA	4	0
30	5	316	XAT	6	0
22	A	810	CLA	4	0
25	A	850	8CT	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	820	CLA	4	0
22	6	318	CLA	6	0
22	5	313	CLA	6	0
22	0	302	CLA	12	0
22	6	310	CLA	9	0
22	K	101	CLA	2	0
24	2	318	LHG	3	0
24	1	317	LHG	3	0
22	1	304	CLA	13	0
22	7	303	CLA	9	0
22	0	309	CLA	2	0
29	2	301	CHL	5	0
22	8	315	CLA	3	0
22	K	104	CLA	6	0
22	3	302	CLA	1	0
22	8	308	CLA	9	0
30	9	314	XAT	5	0
22	7	314	CLA	2	0
22	A	817	CLA	6	0
22	J	103	CLA	1	0
29	1	305	CHL	3	0
22	7	302	CLA	1	0
22	A	835	CLA	1	0
22	3	313	CLA	4	0
24	B	852	LHG	1	0
22	A	827	CLA	8	0
22	3	301	CLA	4	0
22	A	808	CLA	9	0
24	9	316	LHG	8	0
22	L	203	CLA	5	0
22	A	833	CLA	5	0
22	A	825	CLA	9	0
22	0	303	CLA	1	0
22	A	818	CLA	2	0
22	B	825	CLA	4	0
29	6	316	CHL	3	0
22	A	805	CLA	7	0
29	6	302	CHL	7	0
22	B	813	CLA	9	0
22	B	807	CLA	5	0
22	8	311	CLA	6	0
22	9	306	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	7	307	CLA	12	0
25	1	316	8CT	13	0
22	7	316	CLA	6	0
22	A	801	CLA	6	0
22	1	313	CLA	1	0
25	3	316	8CT	11	0
22	A	814	CLA	5	0
22	B	801	CLA	3	0
22	A	813	CLA	12	0
22	7	306	CLA	5	0
22	5	314	CLA	1	0
25	A	854	8CT	3	0
22	7	309	CLA	4	0
31	4	318	LMG	1	0
22	2	311	CLA	1	0
29	9	302	CHL	2	0
22	B	828	CLA	5	0
29	6	307	CHL	9	0
22	2	312	CLA	3	0
22	4	302	CLA	3	0
22	8	313	CLA	1	0
29	2	306	CHL	2	0
22	A	819	CLA	5	0
22	4	311	CLA	4	0
22	A	830	CLA	2	0
22	0	307	CLA	5	0
22	8	310	CLA	8	0
25	B	843	8CT	3	0
30	9	315	XAT	7	0
29	2	307	CHL	3	0
29	7	308	CHL	8	0
27	B	802	SF4	1	0
29	4	305	CHL	9	0
22	A	843	CLA	1	0
25	G	104	8CT	19	0
25	7	321	8CT	13	0
22	3	319	CLA	8	0
29	8	307	CHL	6	0
22	6	303	CLA	4	0
22	3	307	CLA	5	0
22	5	308	CLA	6	0
22	A	840	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	806	CLA	4	0
22	0	312	CLA	5	0
22	B	840	CLA	14	0
22	A	828	CLA	9	0
22	B	806	CLA	10	0
22	3	309	CLA	1	0
22	M	101	CLA	4	0
29	0	306	CHL	2	0
22	9	303	CLA	5	0
22	A	838	CLA	2	0
30	8	316	XAT	11	0
22	0	305	CLA	4	0
25	J	104	8CT	16	0
22	1	306	CLA	4	0
25	7	323	8CT	22	0
22	5	304	CLA	8	0
22	B	820	CLA	3	0
22	9	311	CLA	2	0
29	6	308	CHL	4	0
22	6	304	CLA	4	0
29	4	307	CHL	10	0
22	8	309	CLA	11	0
22	1	312	CLA	8	0
25	B	848	8CT	13	0
30	5	315	XAT	7	0
22	A	824	CLA	2	0
22	7	310	CLA	5	0
22	K	105	CLA	15	0
22	B	850	CLA	16	0
22	7	315	CLA	1	0
22	B	836	CLA	2	0
22	A	826	CLA	9	0
30	3	314	XAT	8	0
24	A	844	LHG	3	0
22	2	308	CLA	6	0
22	A	841	CLA	4	0
22	K	102	CLA	5	0
22	L	202	CLA	10	0
30	7	320	XAT	8	0
22	5	311	CLA	4	0
22	9	308	CLA	3	0
22	A	829	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	841	CLA	5	0
22	B	817	CLA	5	0
25	A	849	8CT	7	0
22	A	809	CLA	11	0
22	5	305	CLA	2	0
22	5	307	CLA	2	0
22	5	312	CLA	5	0
29	8	305	CHL	7	0
22	A	832	CLA	4	0
22	B	835	CLA	1	0
22	A	811	CLA	4	0
22	B	827	CLA	8	0
29	0	301	CHL	15	0
22	1	309	CLA	2	0
22	4	312	CLA	5	0
29	4	306	CHL	2	0
29	6	306	CHL	2	0
22	B	818	CLA	4	0
22	A	839	CLA	8	0
22	A	823	CLA	1	0
22	9	304	CLA	2	0
22	L	204	CLA	4	0
22	A	853	CLA	5	0
25	4	317	8CT	12	0
25	5	317	8CT	5	0
22	6	309	CLA	5	0
22	B	833	CLA	8	0
22	7	304	CLA	3	0
22	7	305	CLA	3	0
22	1	303	CLA	11	0
30	2	316	XAT	6	0
22	0	308	CLA	3	0
22	0	310	CLA	2	0
22	3	303	CLA	1	0
22	B	819	CLA	3	0
23	B	842	PQN	3	0
22	A	834	CLA	1	0
22	B	830	CLA	6	0
22	1	311	CLA	12	0
29	2	305	CHL	9	0
22	B	834	CLA	6	0
30	4	316	XAT	6	0

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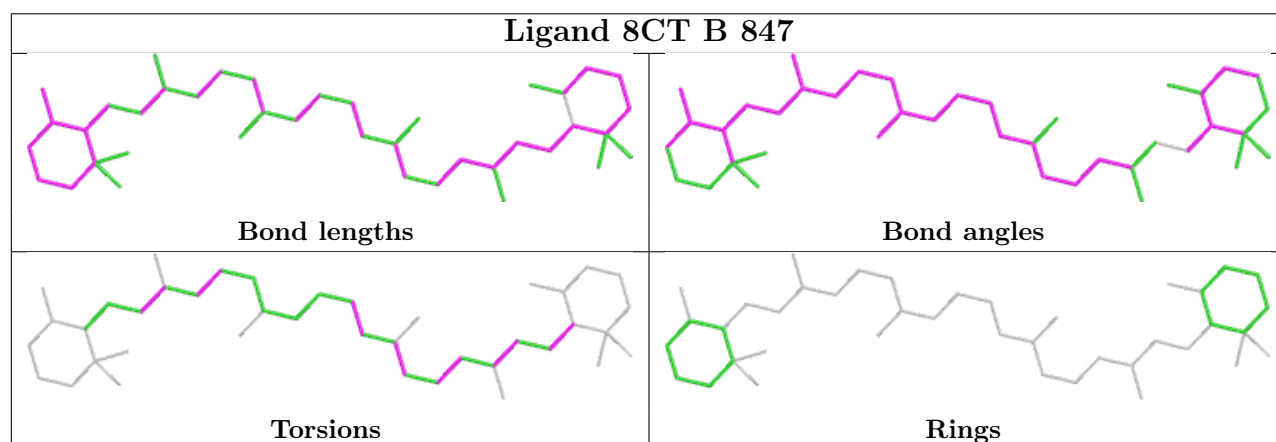
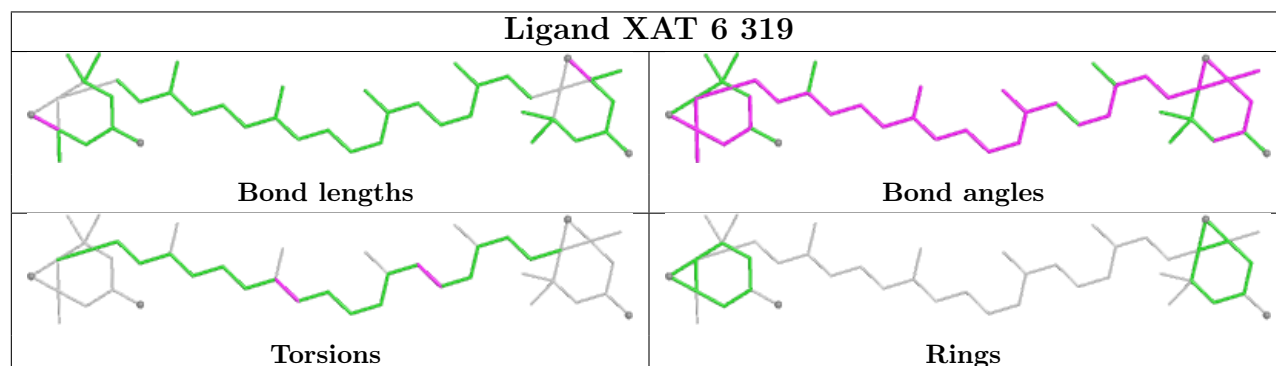
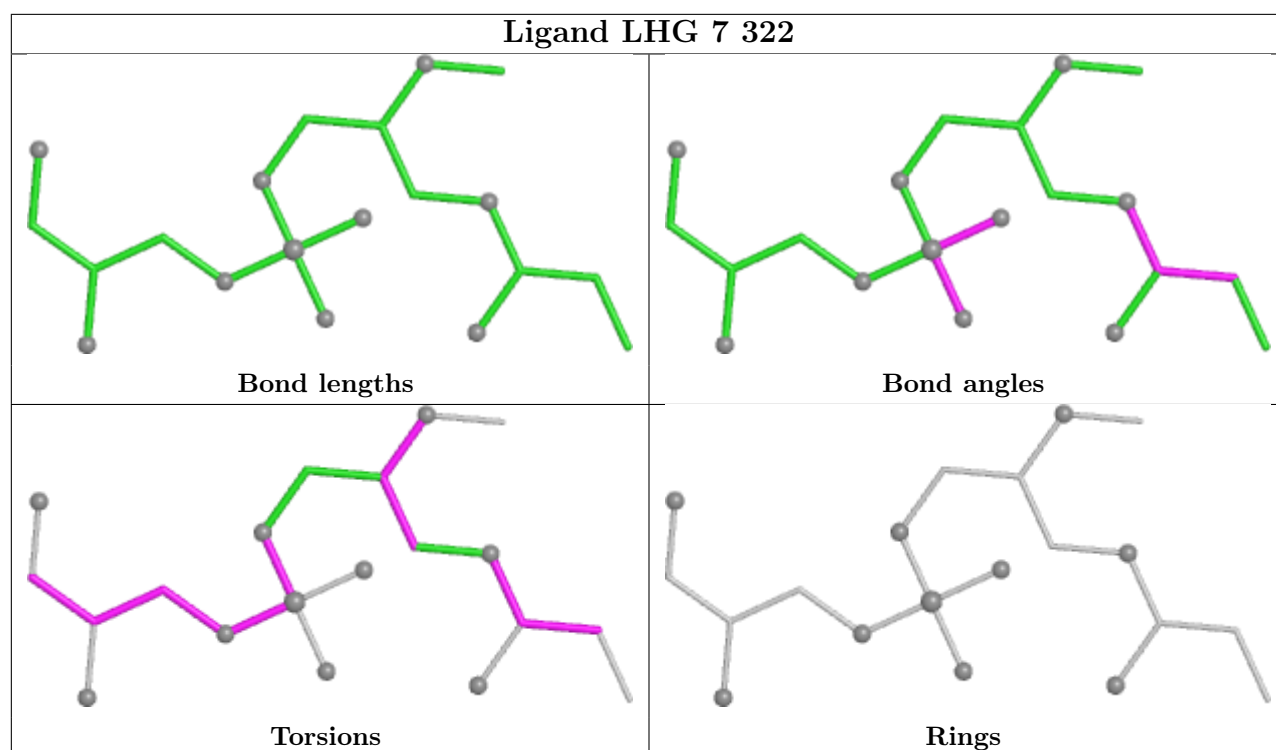
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	G	103	CLA	7	0
22	3	311	CLA	7	0
30	0	313	XAT	8	0
25	J	101	8CT	10	0
30	3	315	XAT	9	0
29	4	301	CHL	8	0
30	4	315	XAT	8	0
22	6	315	CLA	4	0
22	0	311	CLA	7	0
24	5	318	LHG	8	0
25	A	846	8CT	1	0
22	9	310	CLA	2	0
22	A	815	CLA	2	0
25	B	846	8CT	11	0
22	6	317	CLA	3	0
22	0	304	CLA	3	0
22	A	812	CLA	3	0
29	9	307	CHL	1	0
22	B	832	CLA	8	0
22	B	812	CLA	3	0
22	3	312	CLA	2	0
22	B	811	CLA	3	0
29	3	306	CHL	4	0
22	9	301	CLA	5	0
24	0	315	LHG	11	0
22	F	301	CLA	5	0
22	1	302	CLA	4	0
22	7	312	CLA	3	0
22	5	310	CLA	1	0
22	A	822	CLA	4	0
22	7	317	CLA	11	0
25	8	301	8CT	11	0
30	0	314	XAT	8	0
22	7	313	CLA	7	0
25	B	851	8CT	1	0
30	6	320	XAT	7	0
22	4	310	CLA	1	0
22	A	837	CLA	5	0
22	4	309	CLA	6	0
22	A	802	CLA	4	0
22	A	821	CLA	2	0

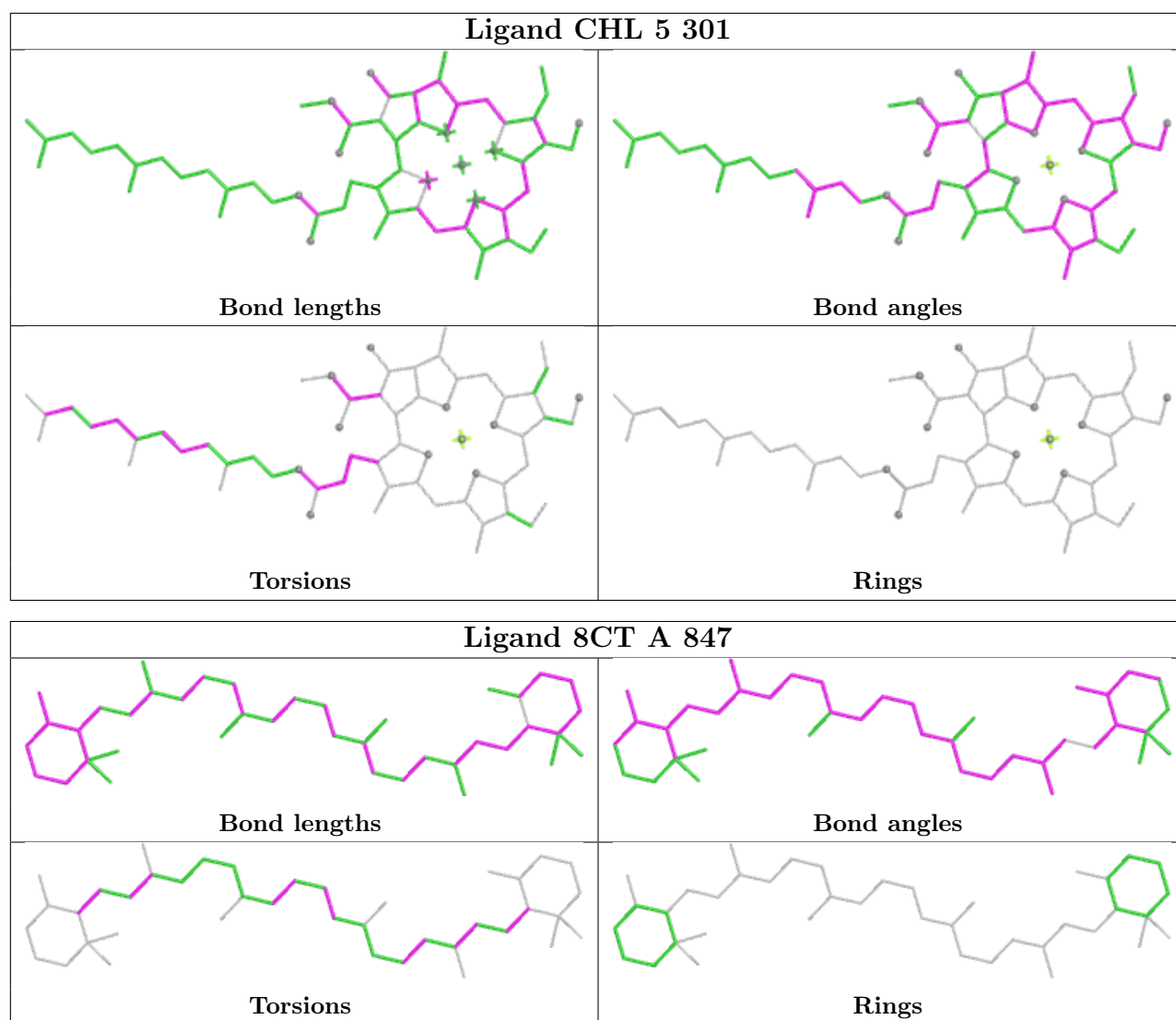
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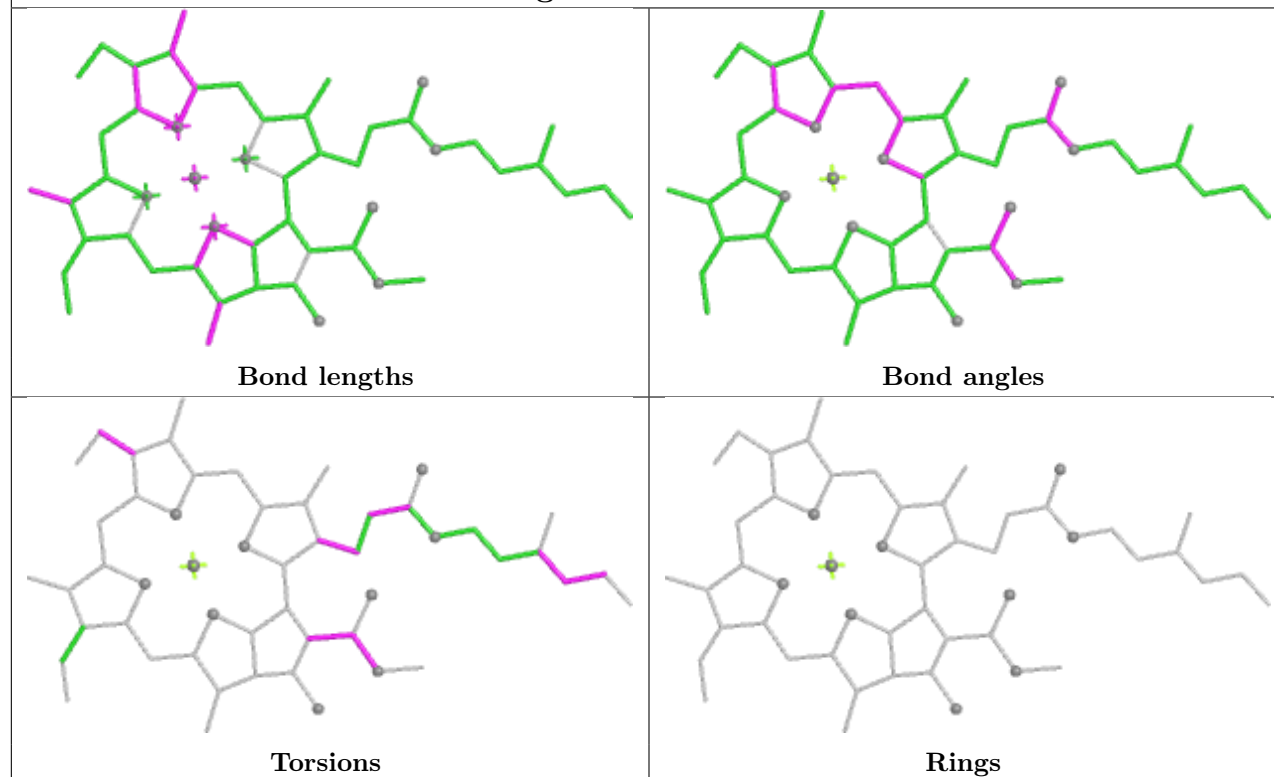
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	4	308	CLA	2	0
30	1	315	XAT	5	0
24	6	322	LHG	4	0
22	6	311	CLA	3	0
22	6	323	CLA	4	0
22	8	302	CLA	2	0
22	B	808	CLA	7	0
28	B	849	DGD	11	0
22	5	309	CLA	9	0
24	3	317	LHG	4	0
22	2	304	CLA	4	0
25	K	103	8CT	13	0
22	B	809	CLA	6	0
22	1	307	CLA	4	0
30	2	315	XAT	6	0
22	2	302	CLA	7	0

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

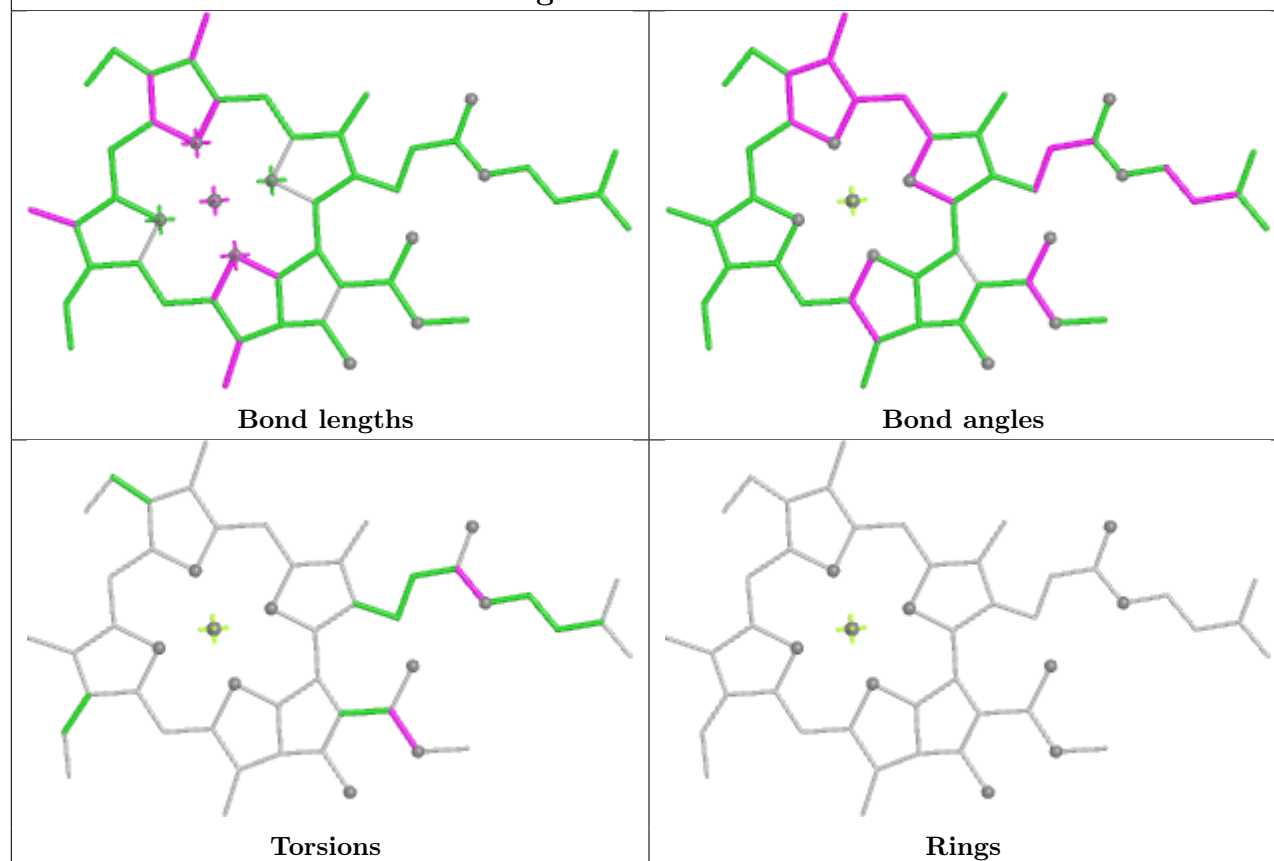




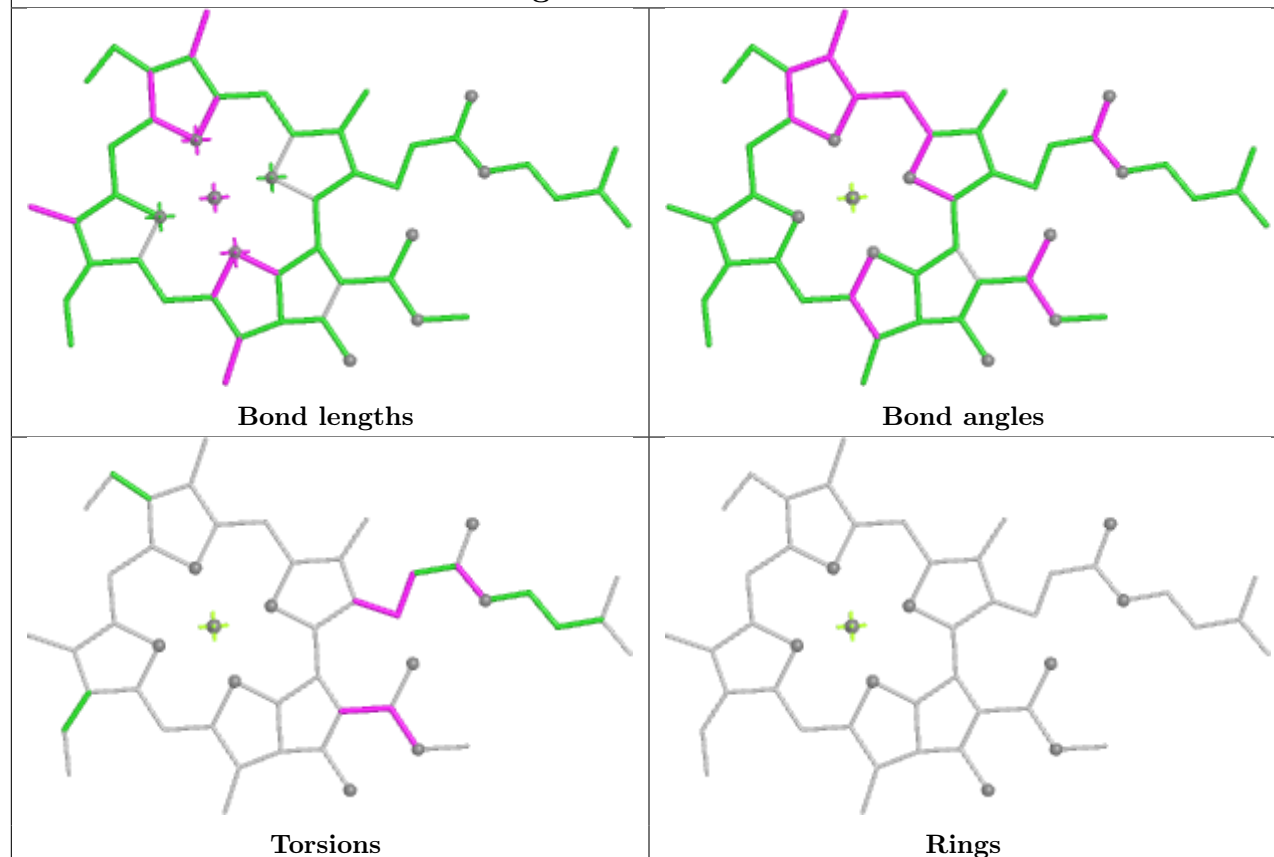
Ligand CLA 6 312



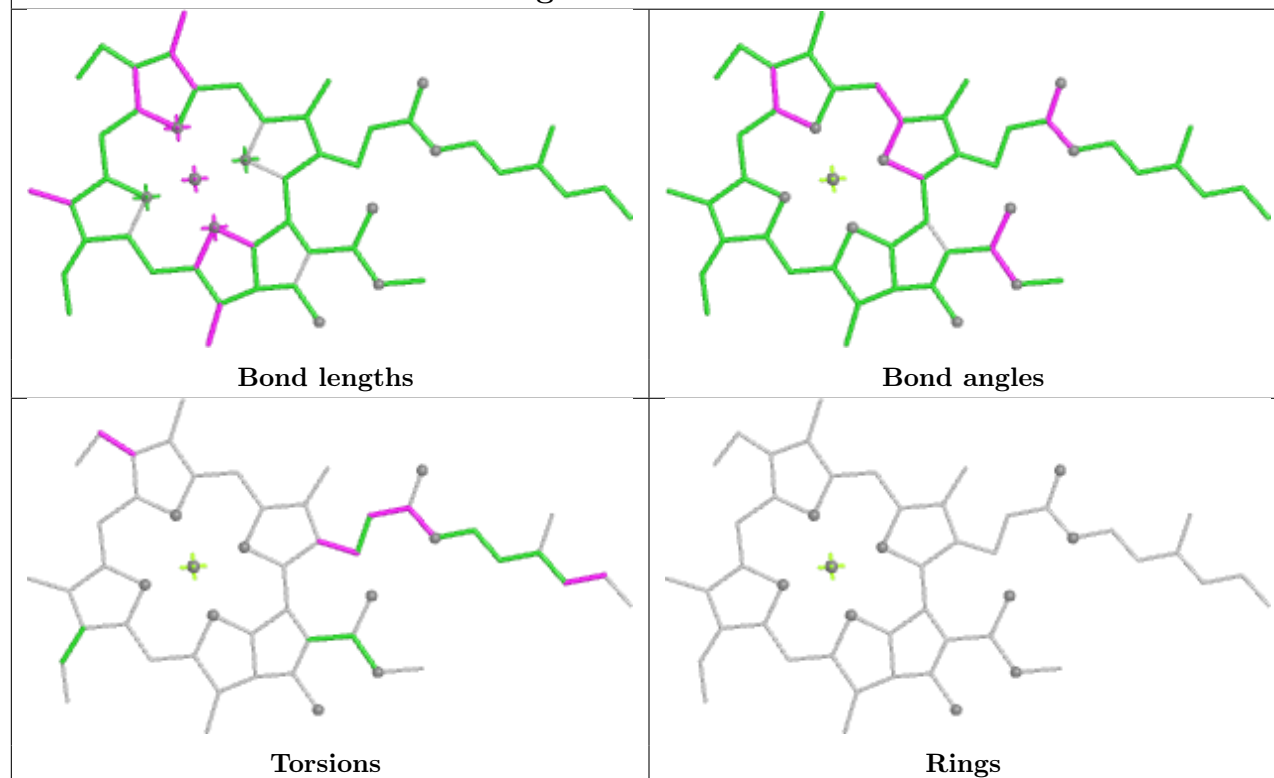
Ligand CLA 4 304

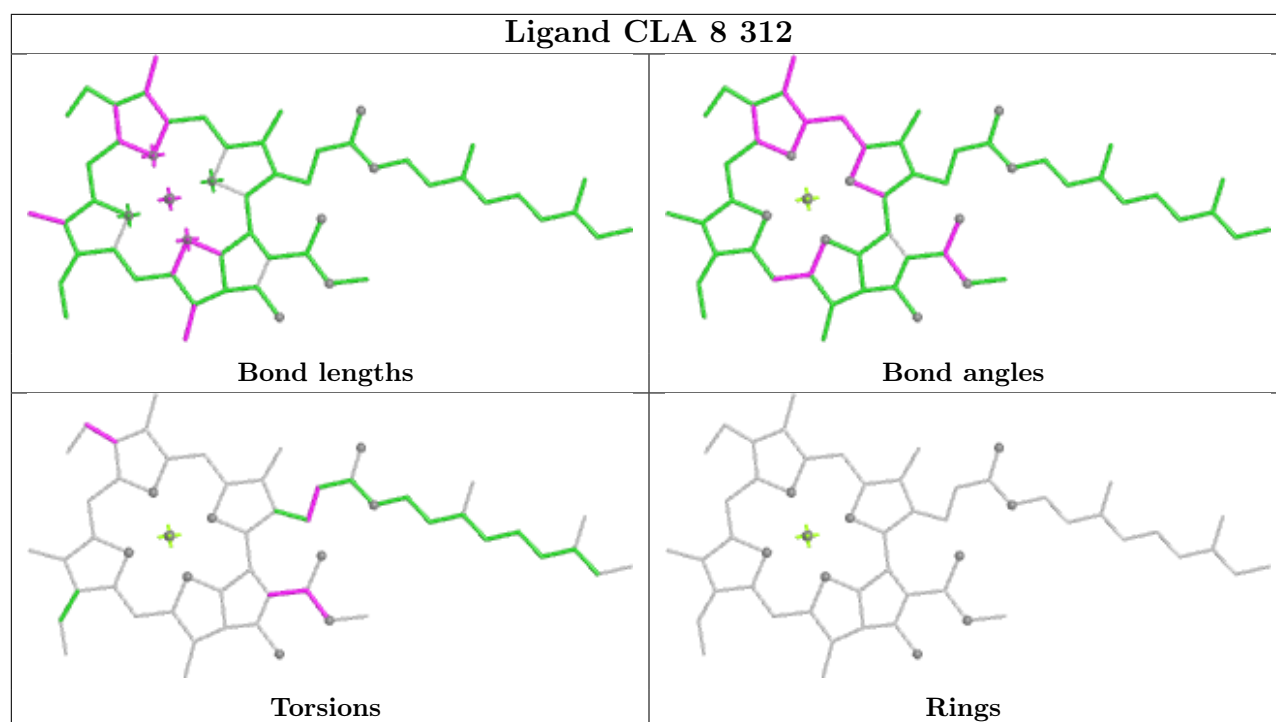


Ligand CLA B 831

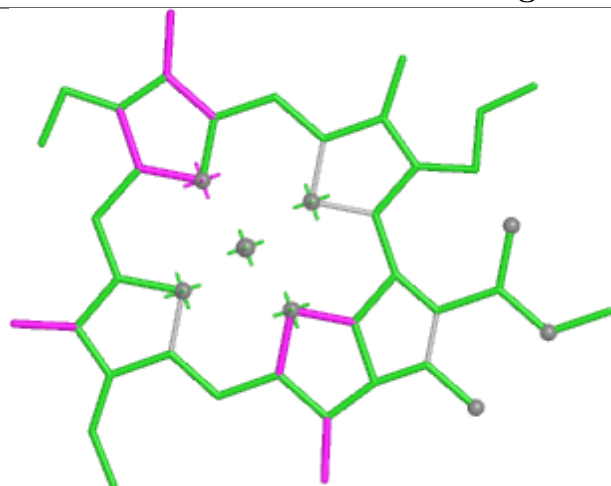


Ligand CLA 1 310

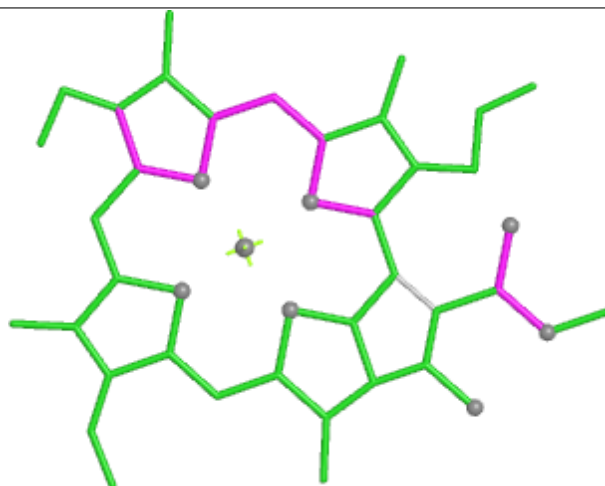




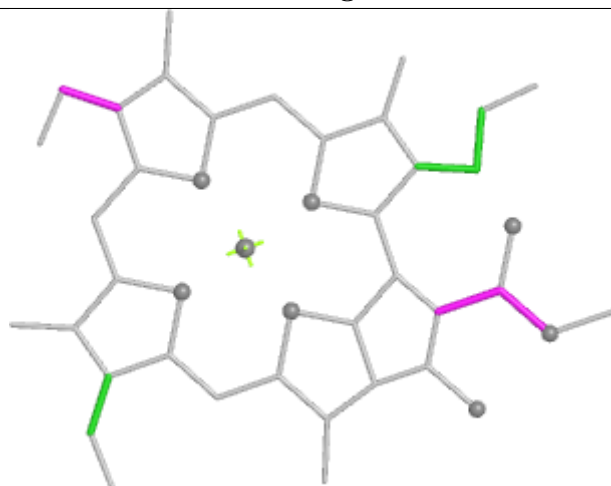
Ligand CLA 6 314



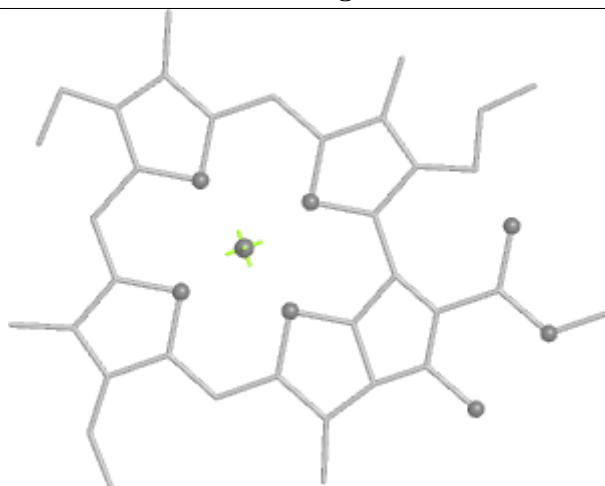
Bond lengths



Bond angles

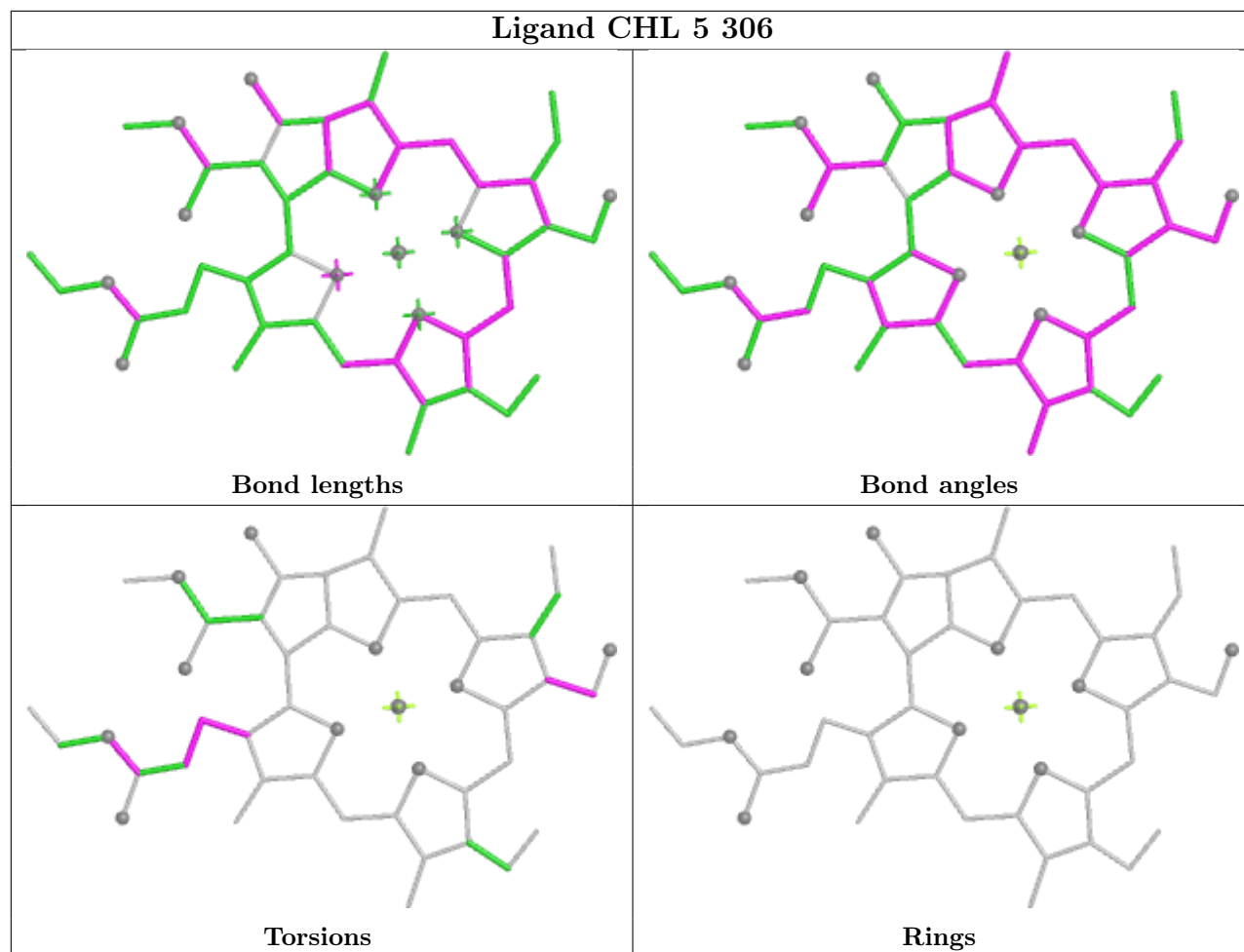


Torsions

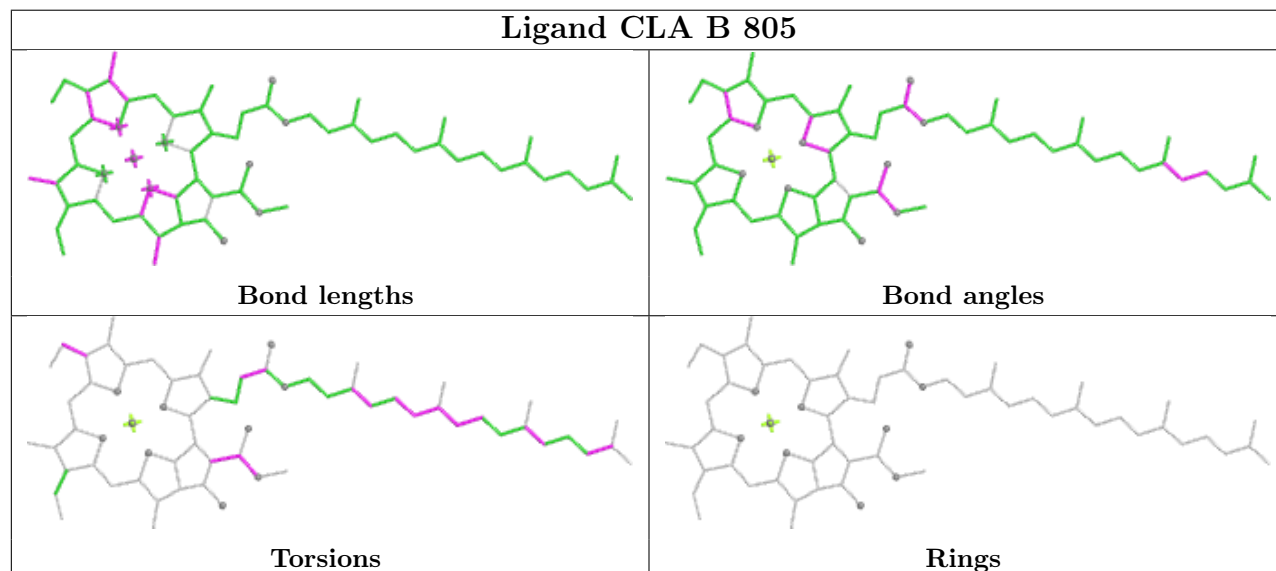


Rings

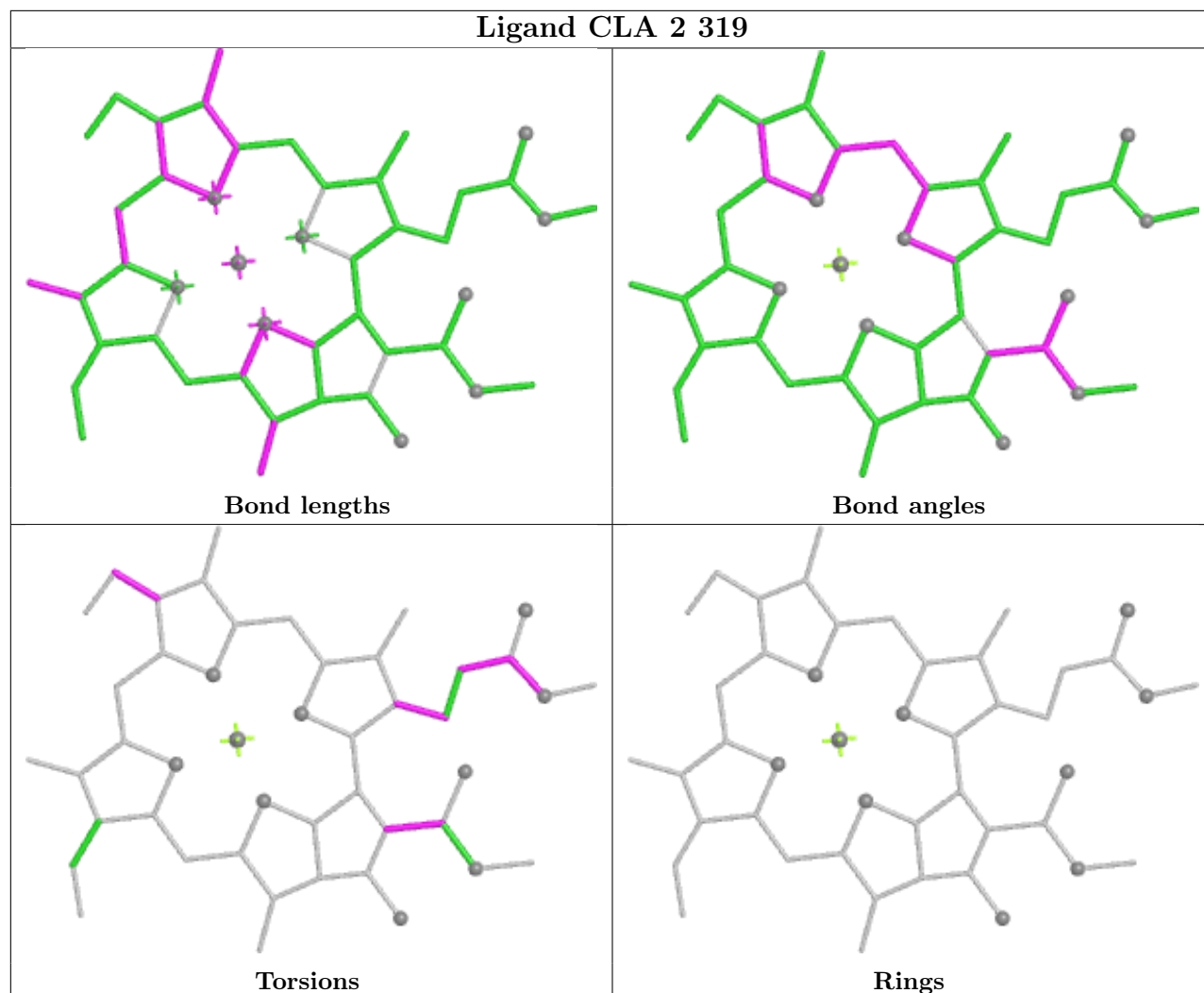
Ligand CHL 5 306



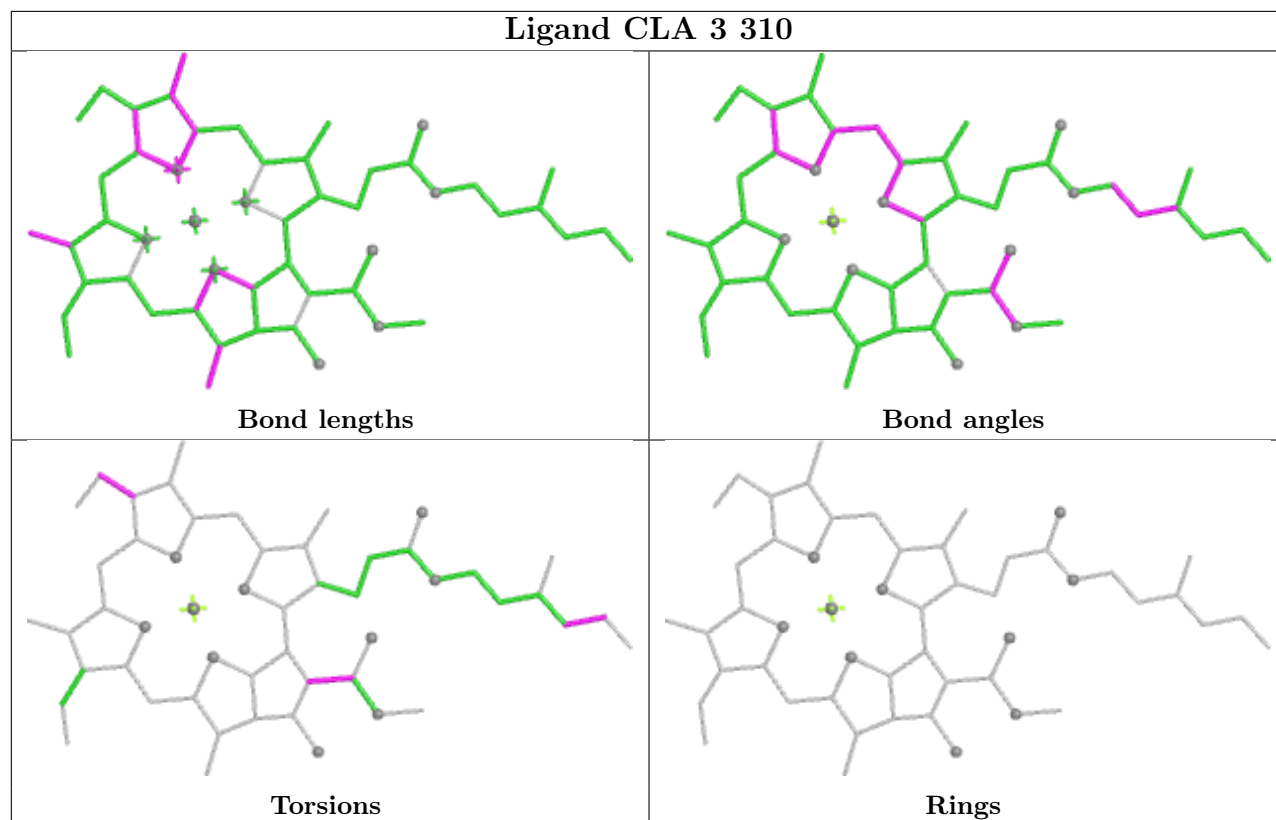
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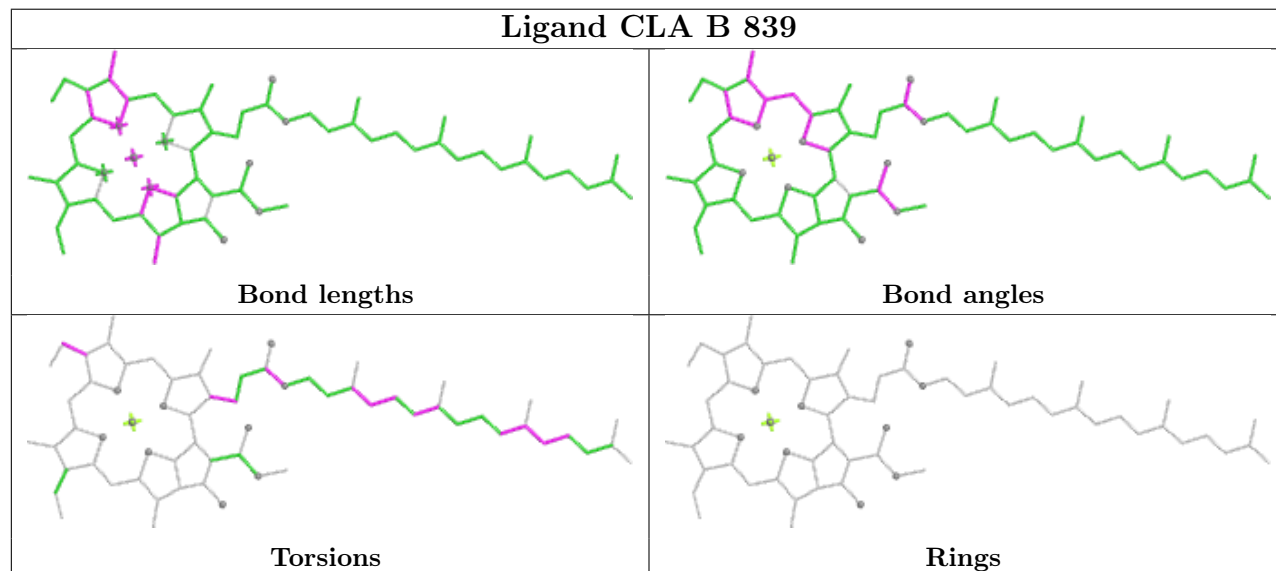
Ligand CLA 2 319

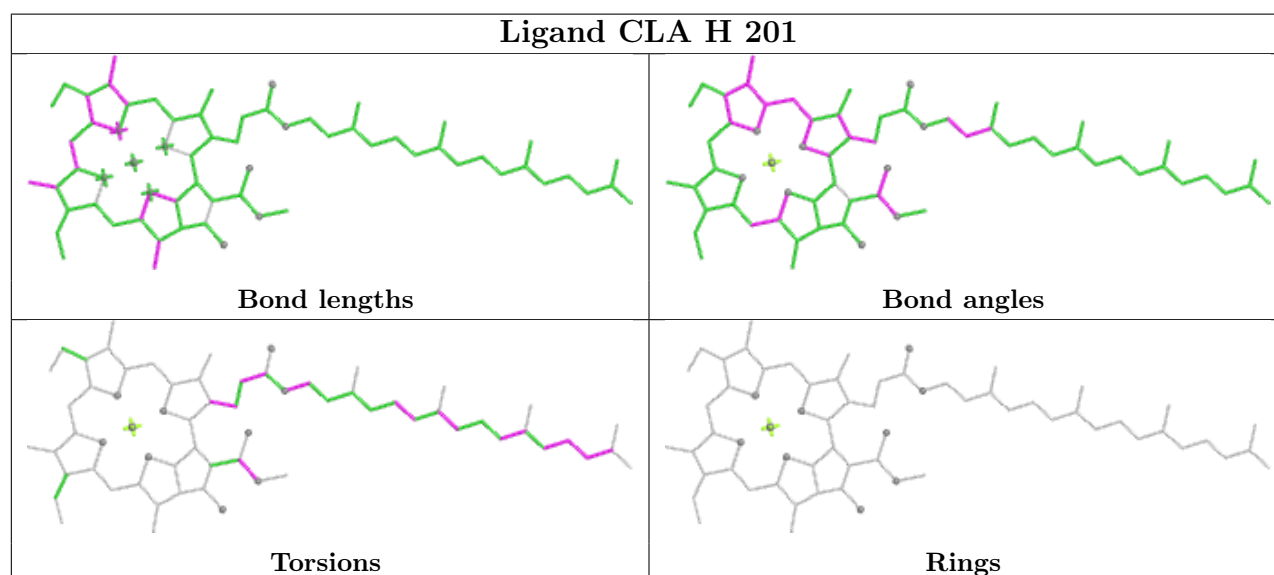
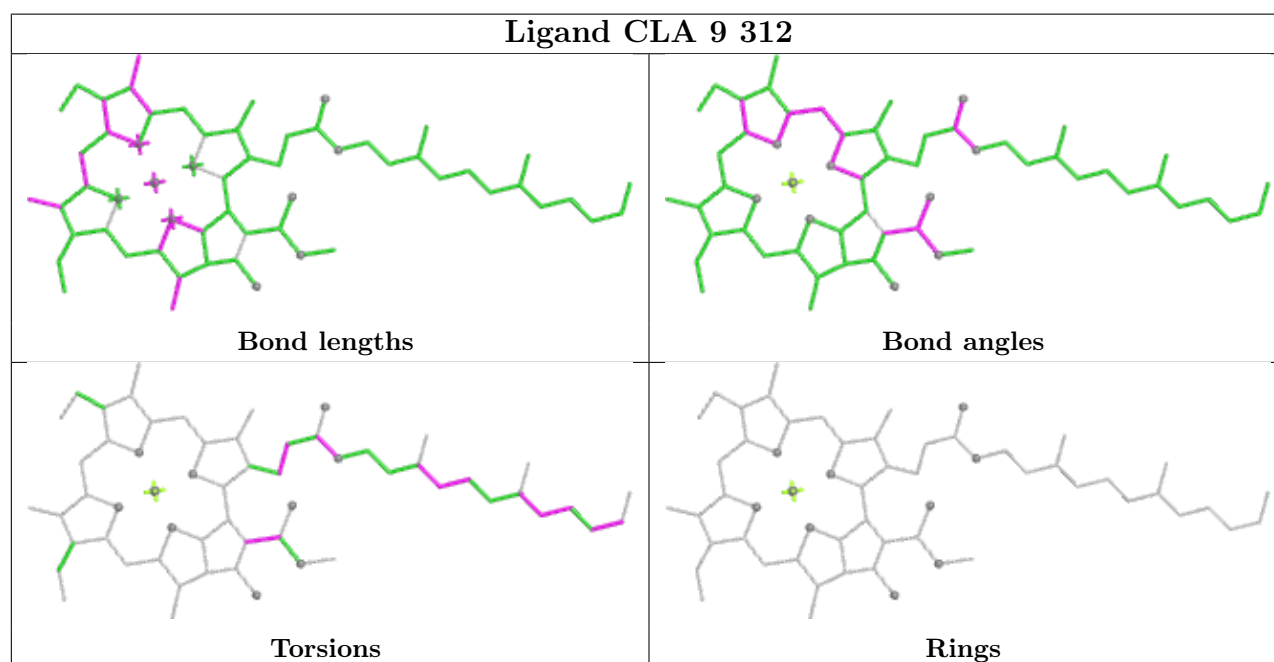
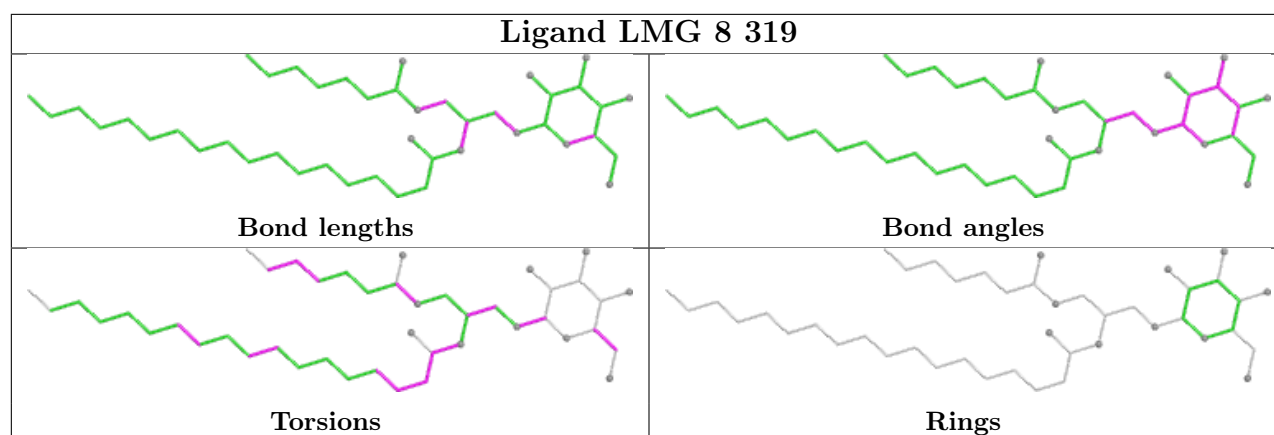


Ligand CLA 3 310

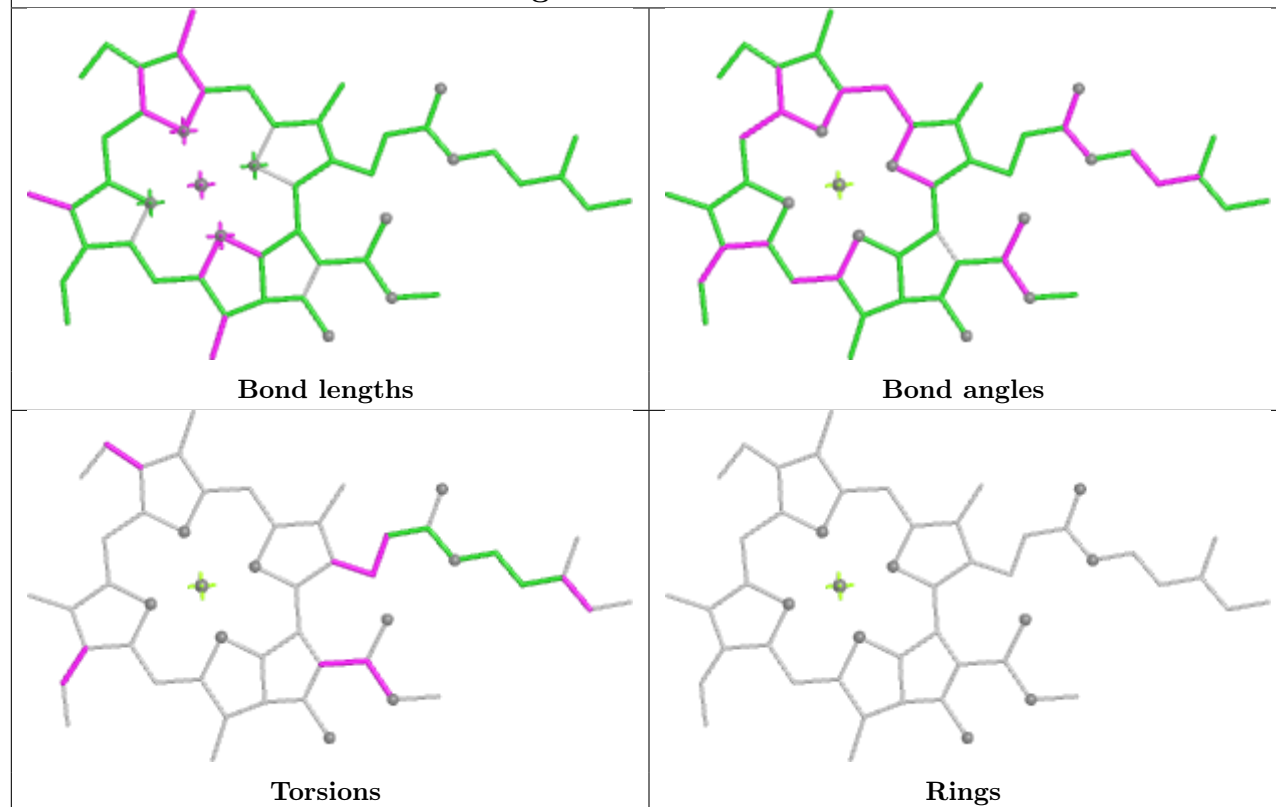


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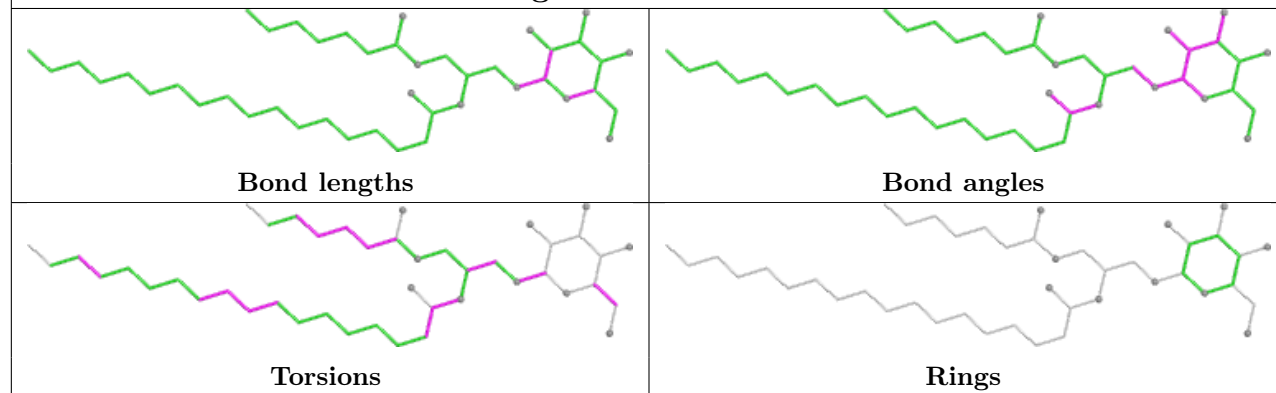




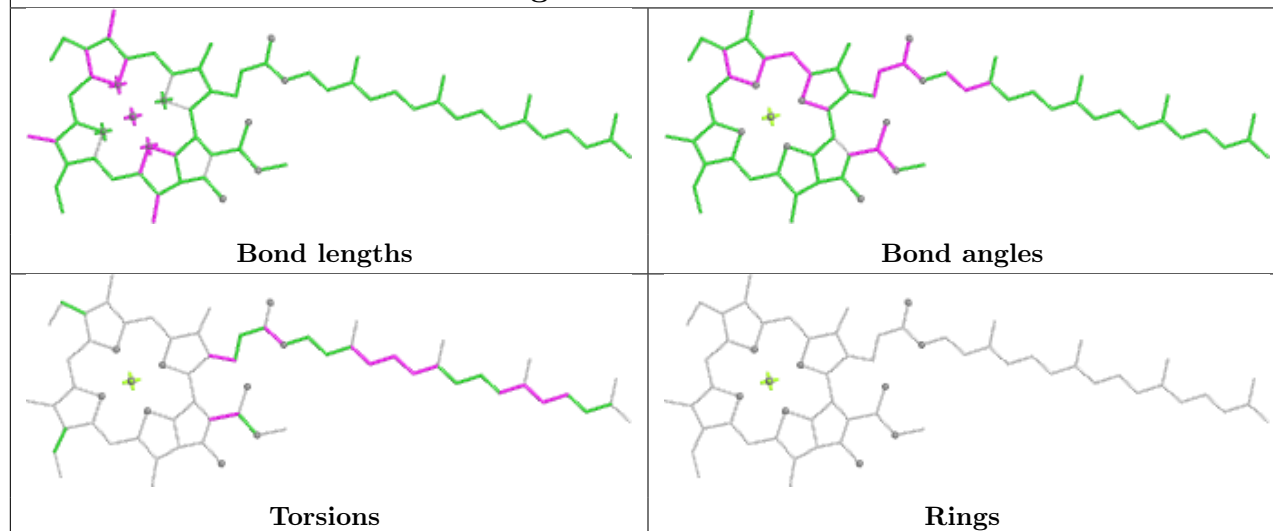
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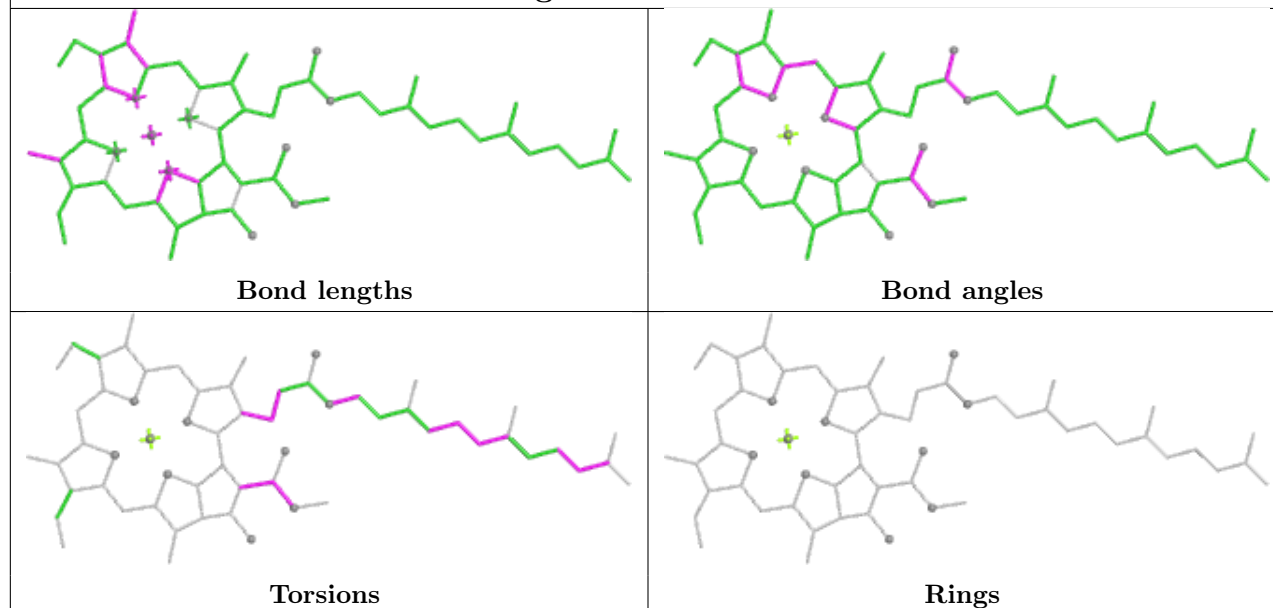
Ligand LMG 5 319



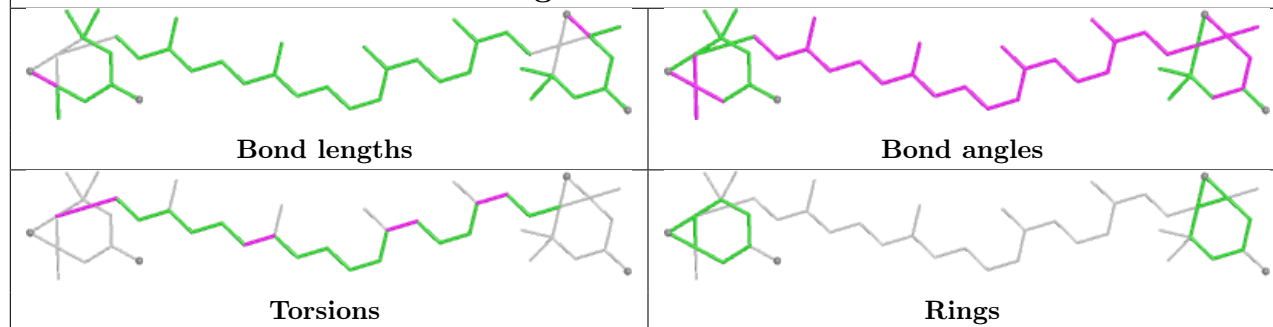
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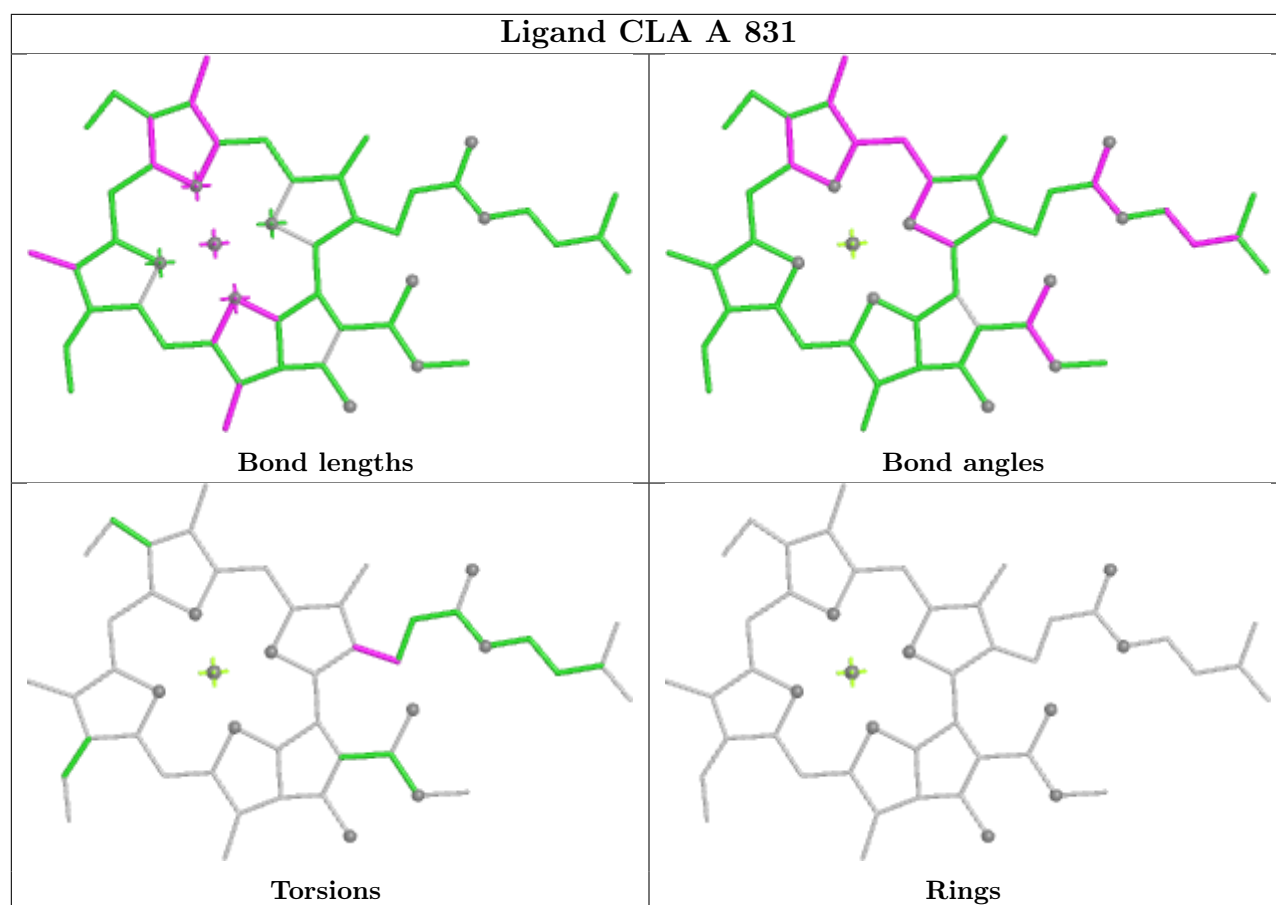


Ligand CLA 6 305

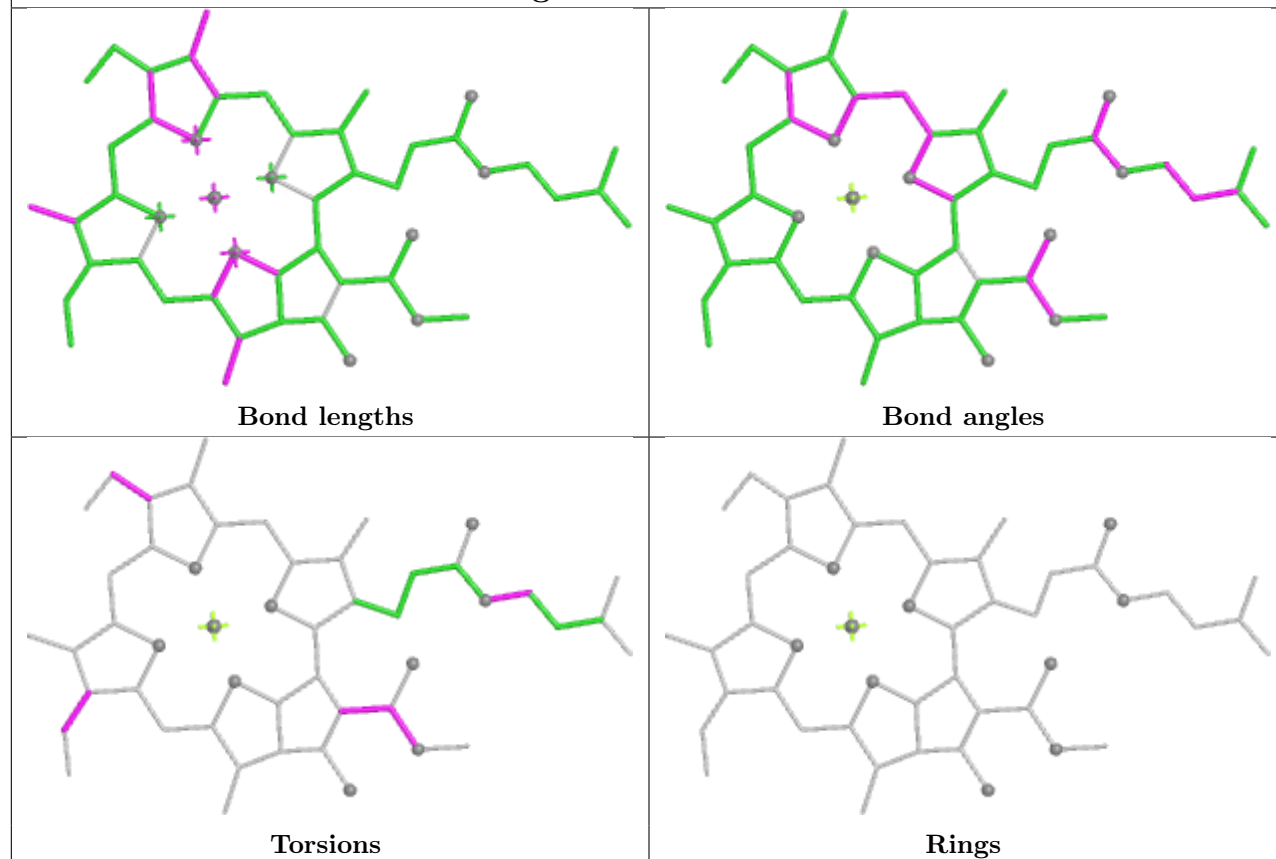


Ligand XAT 7 319

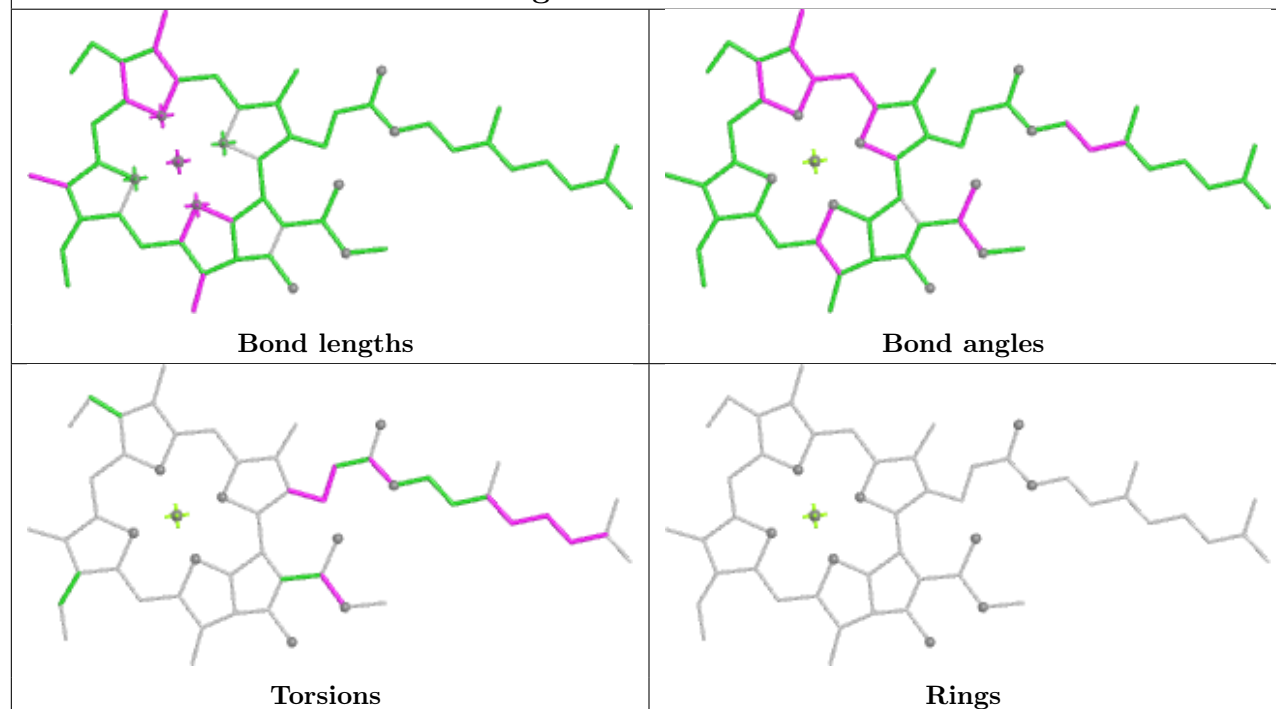


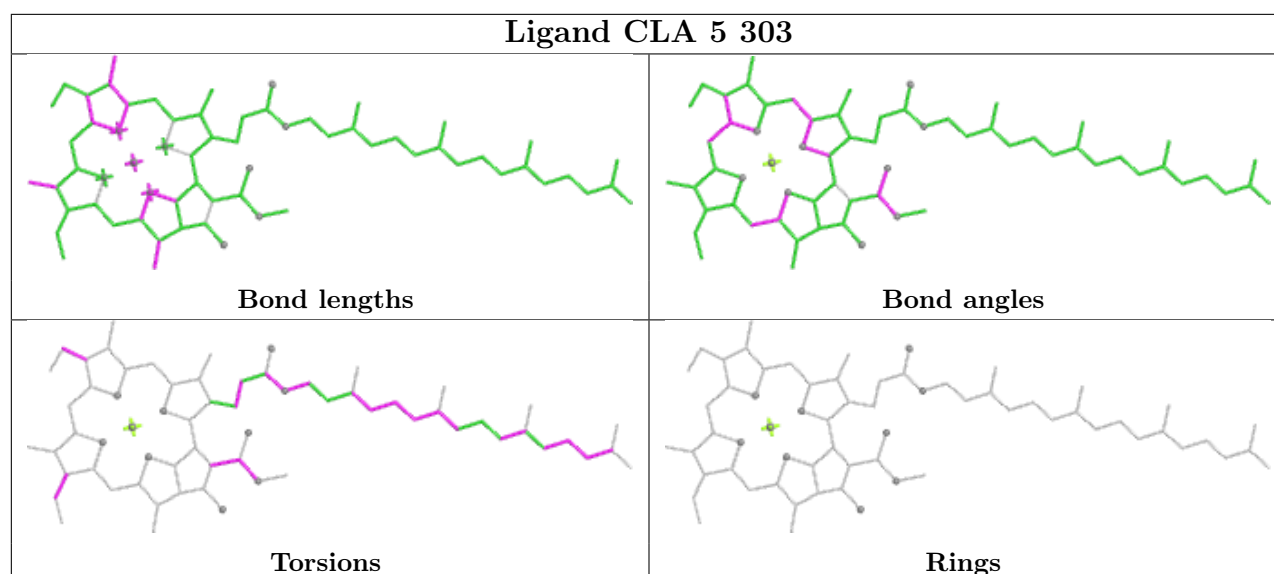
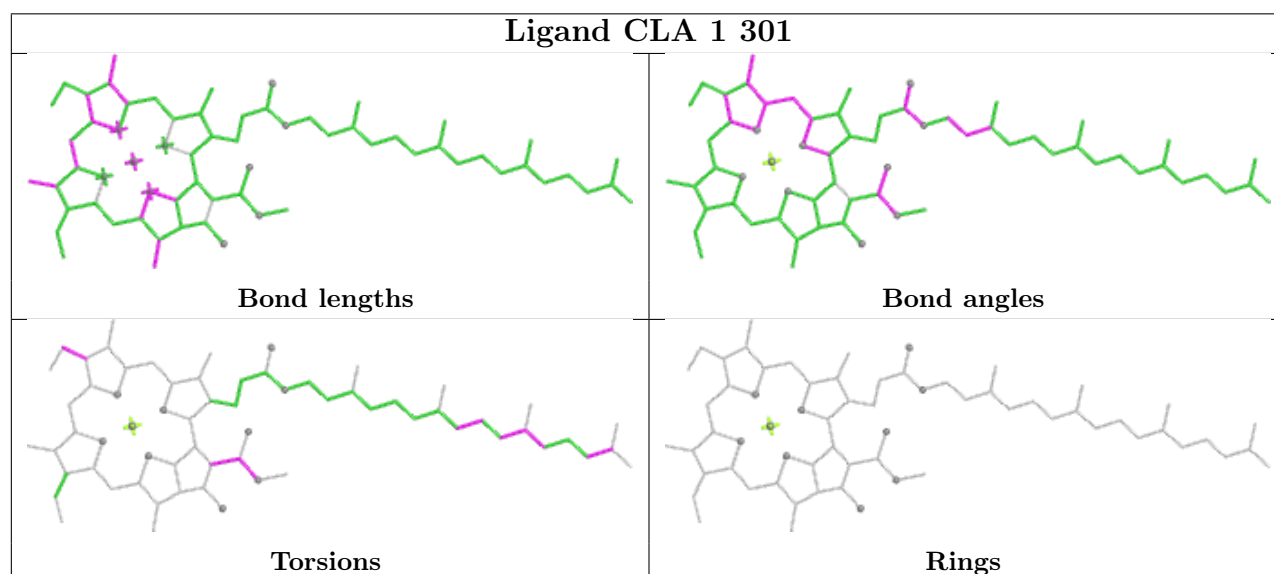
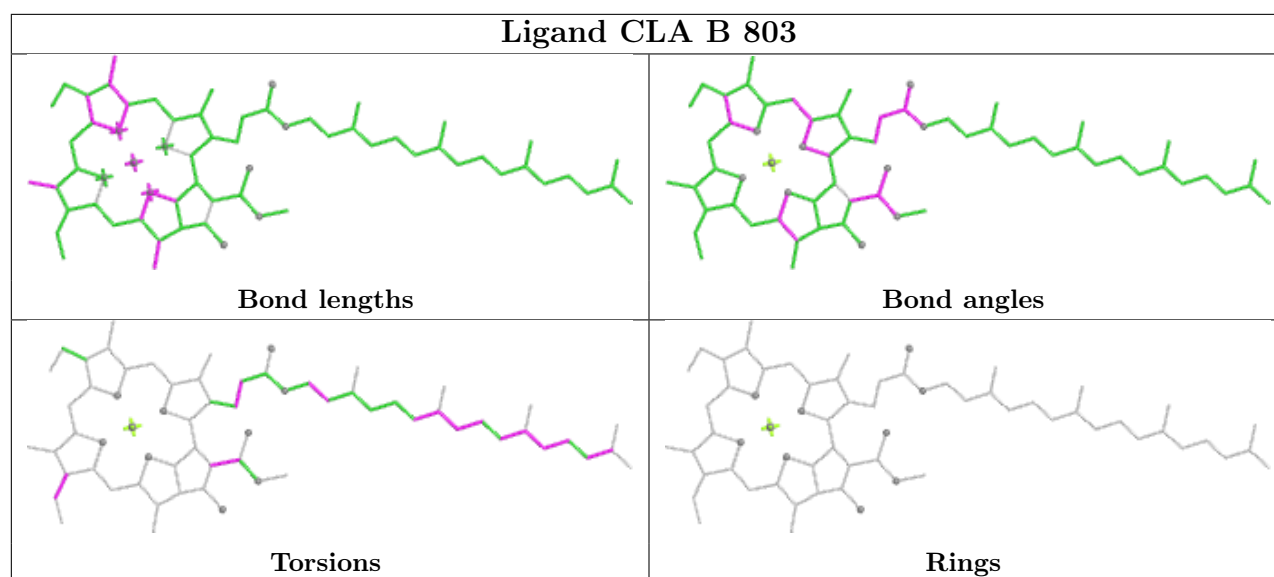


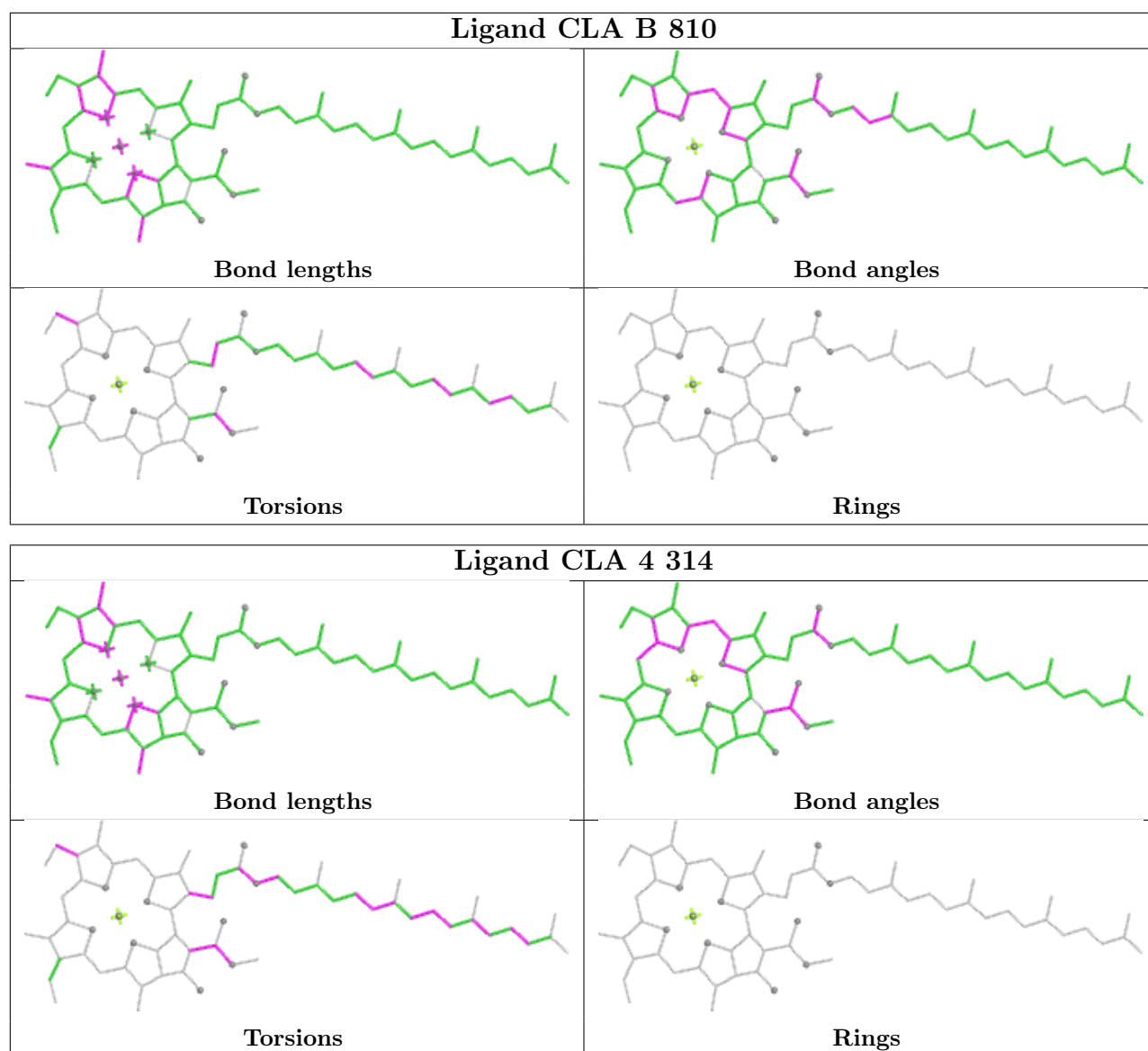
Ligand CLA B 821



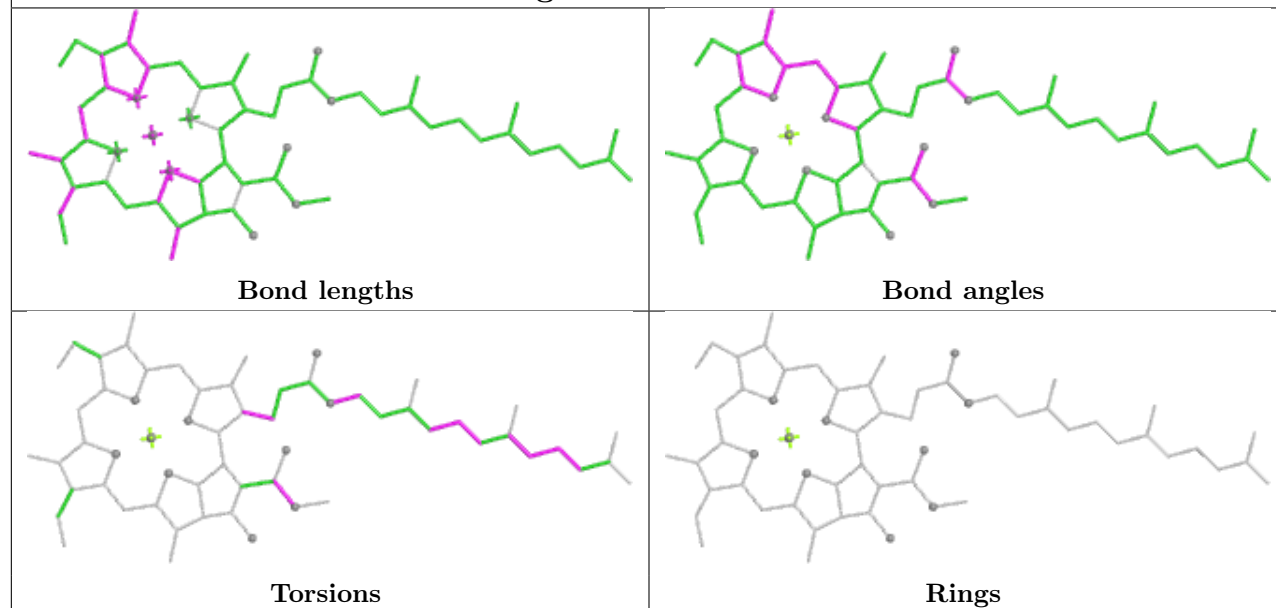
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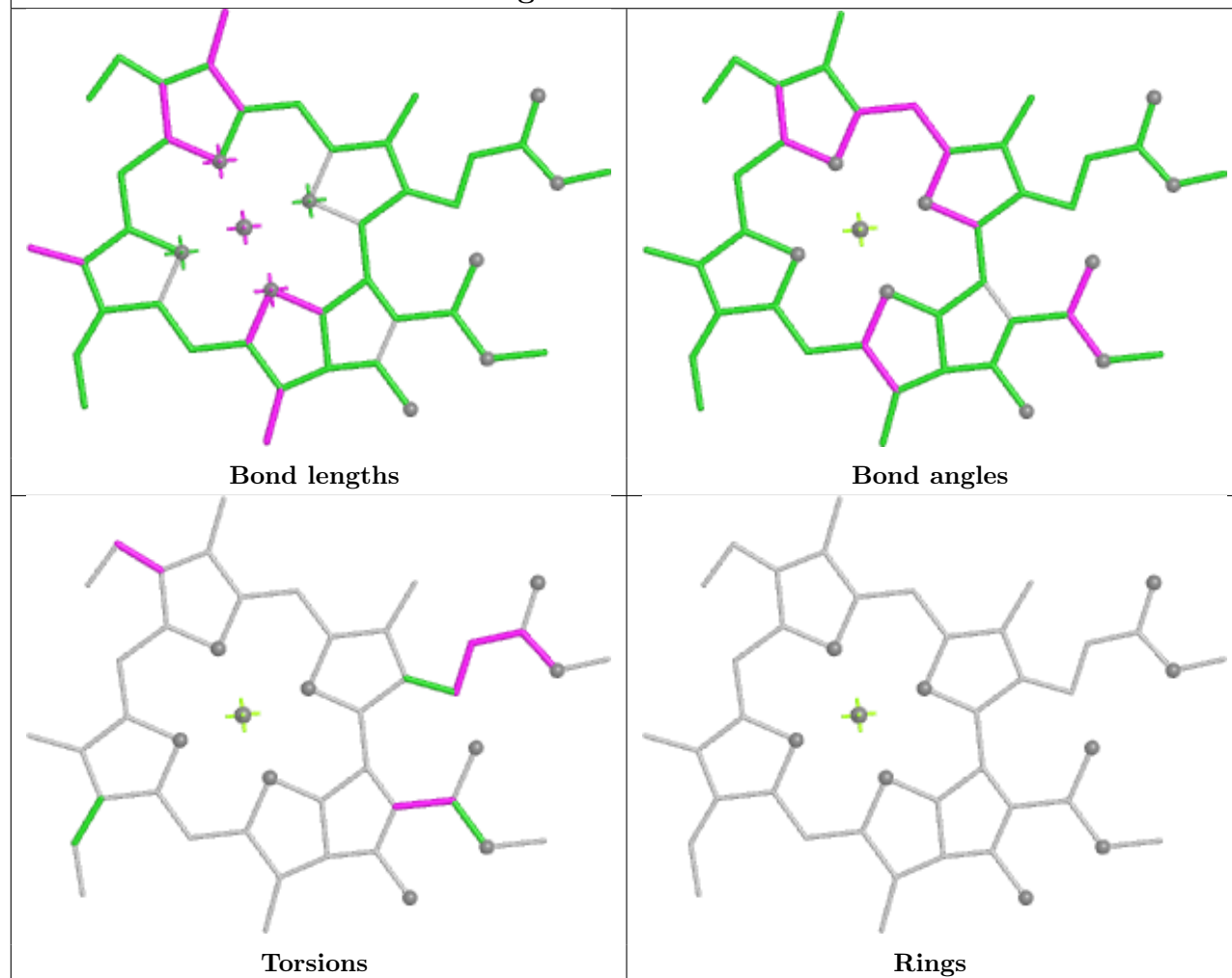




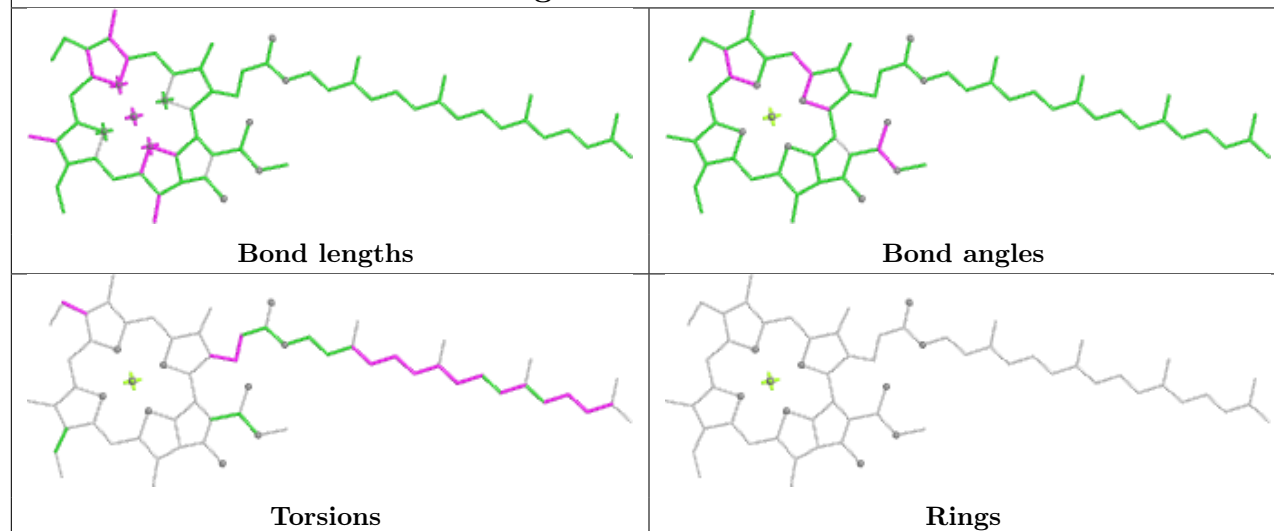
Ligand CLA 2 309



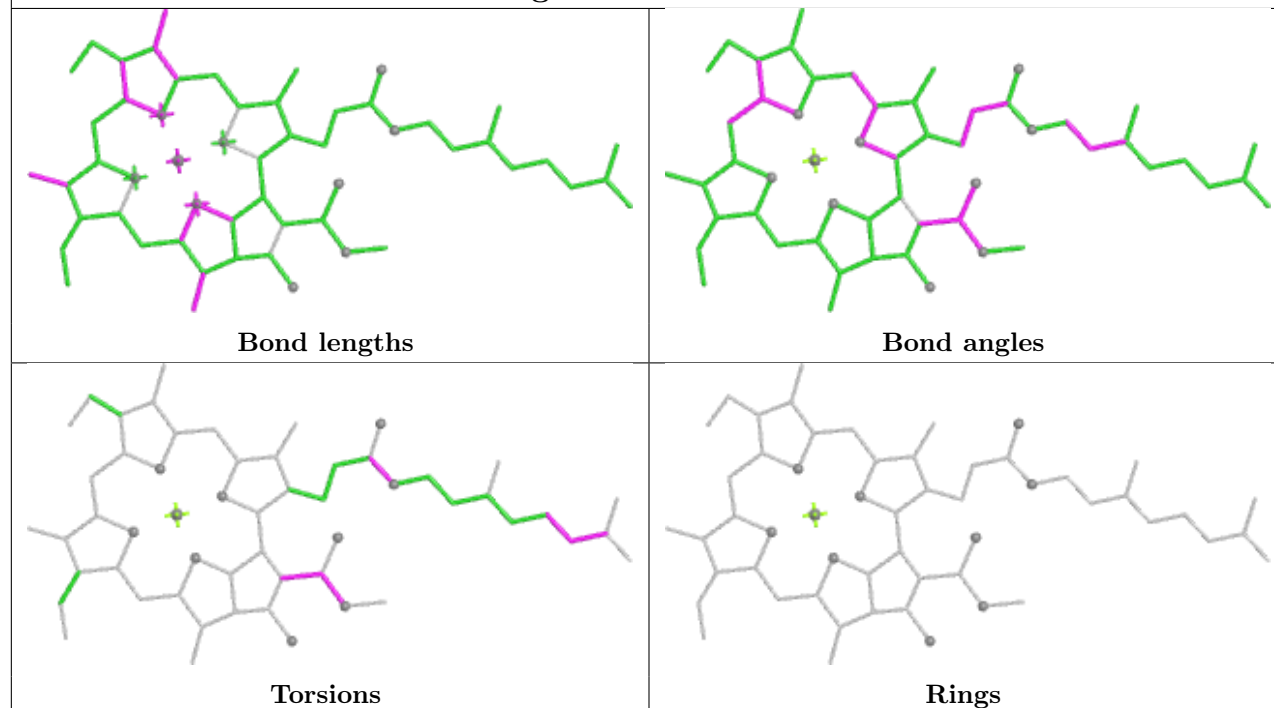
Ligand CLA 4 303



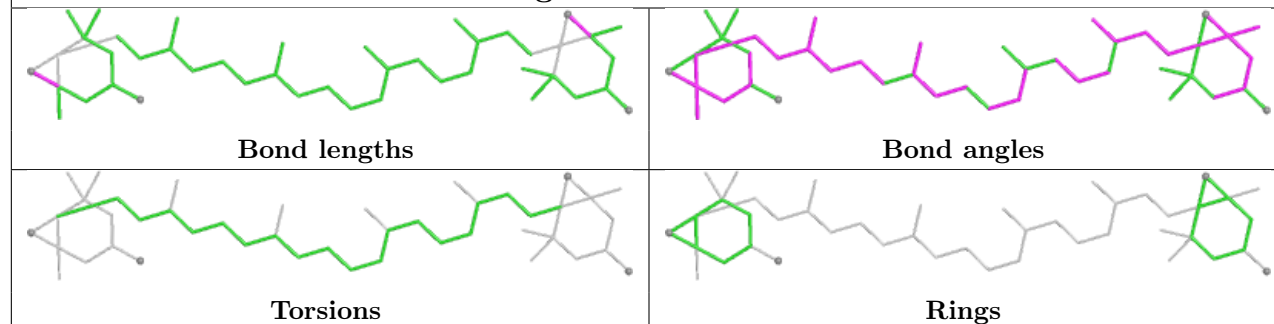
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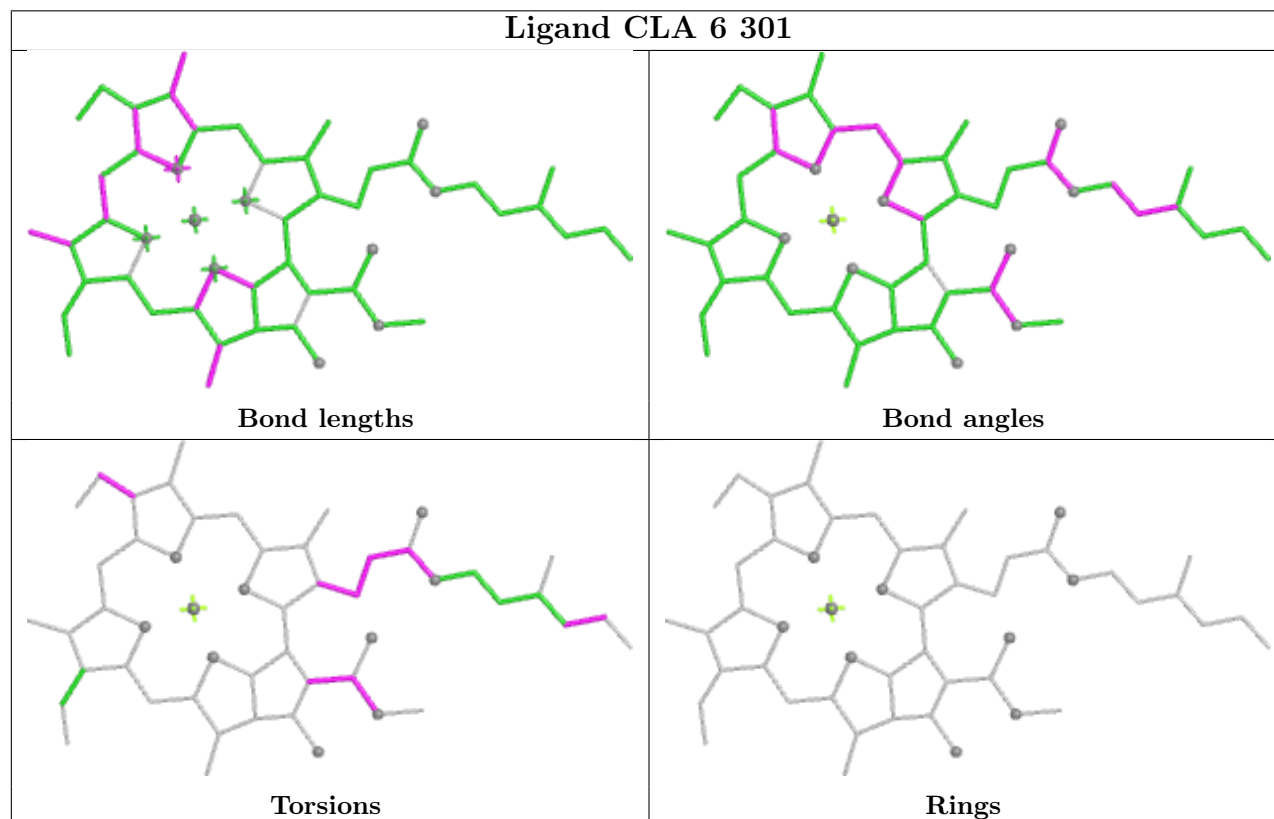
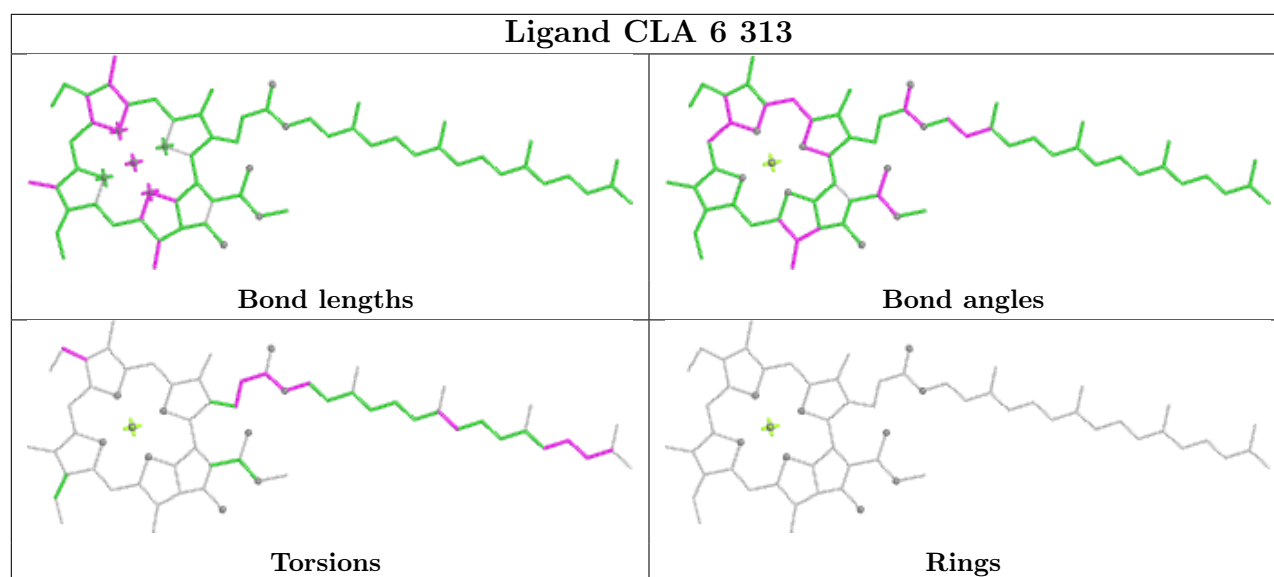


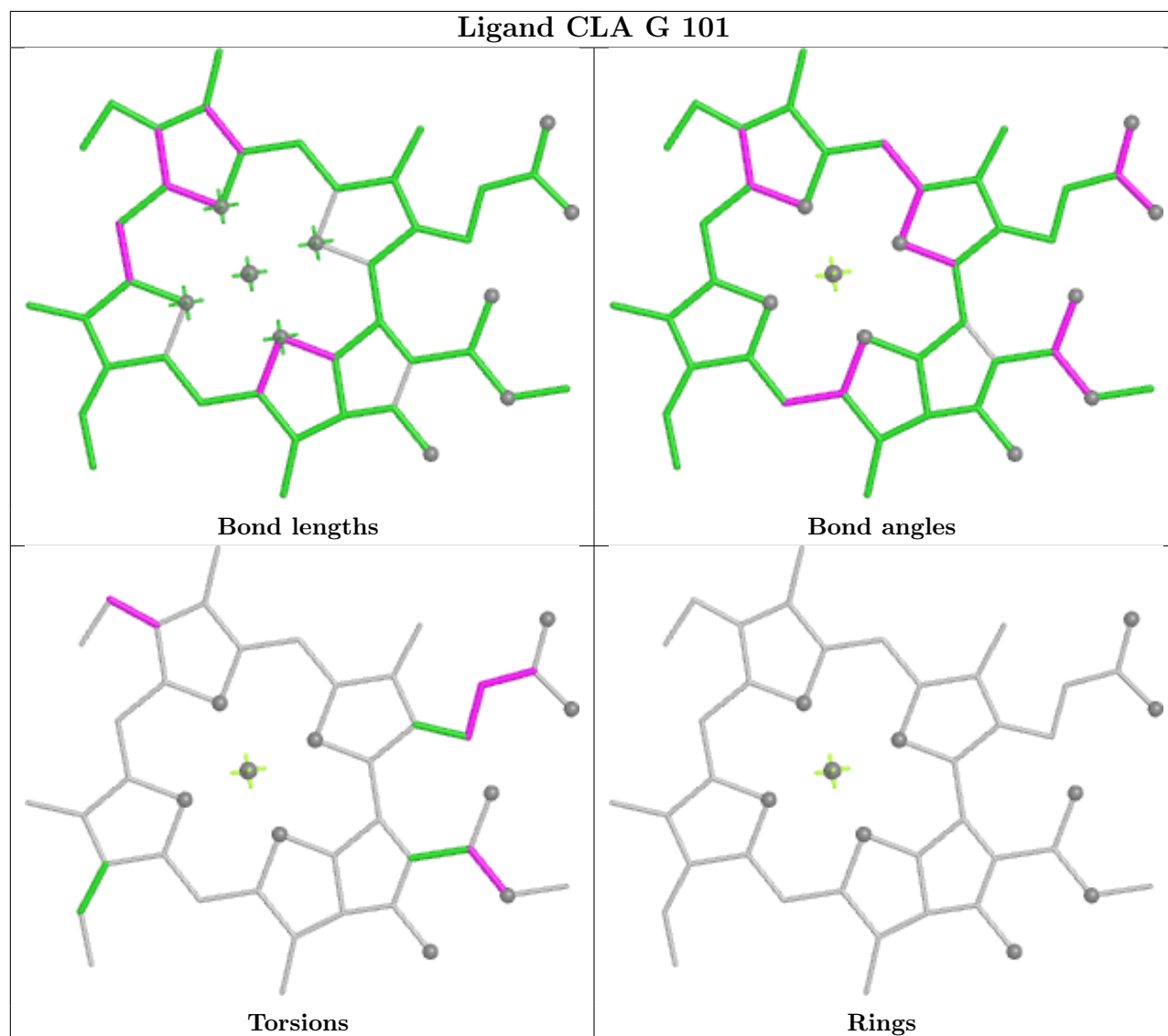
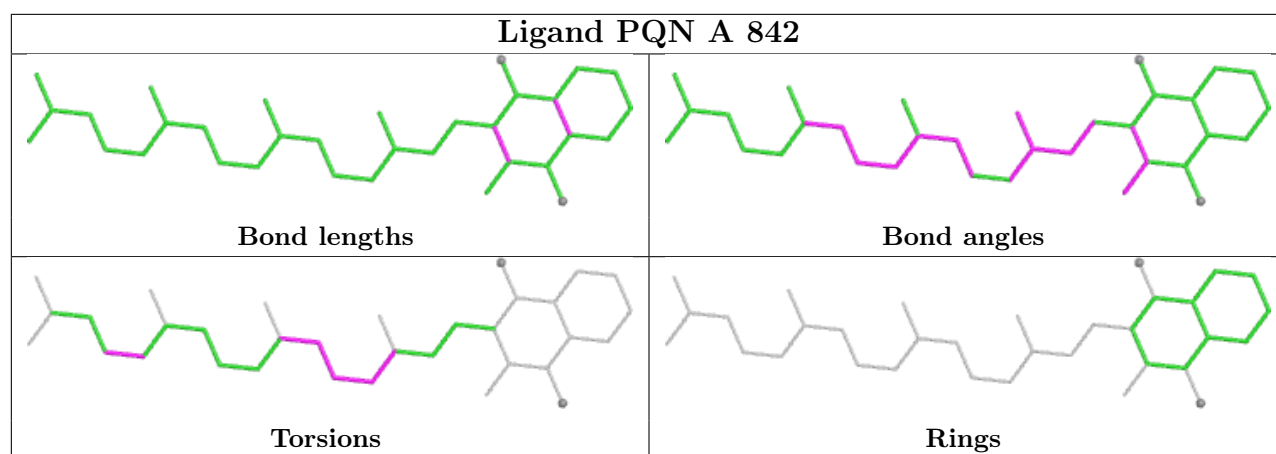
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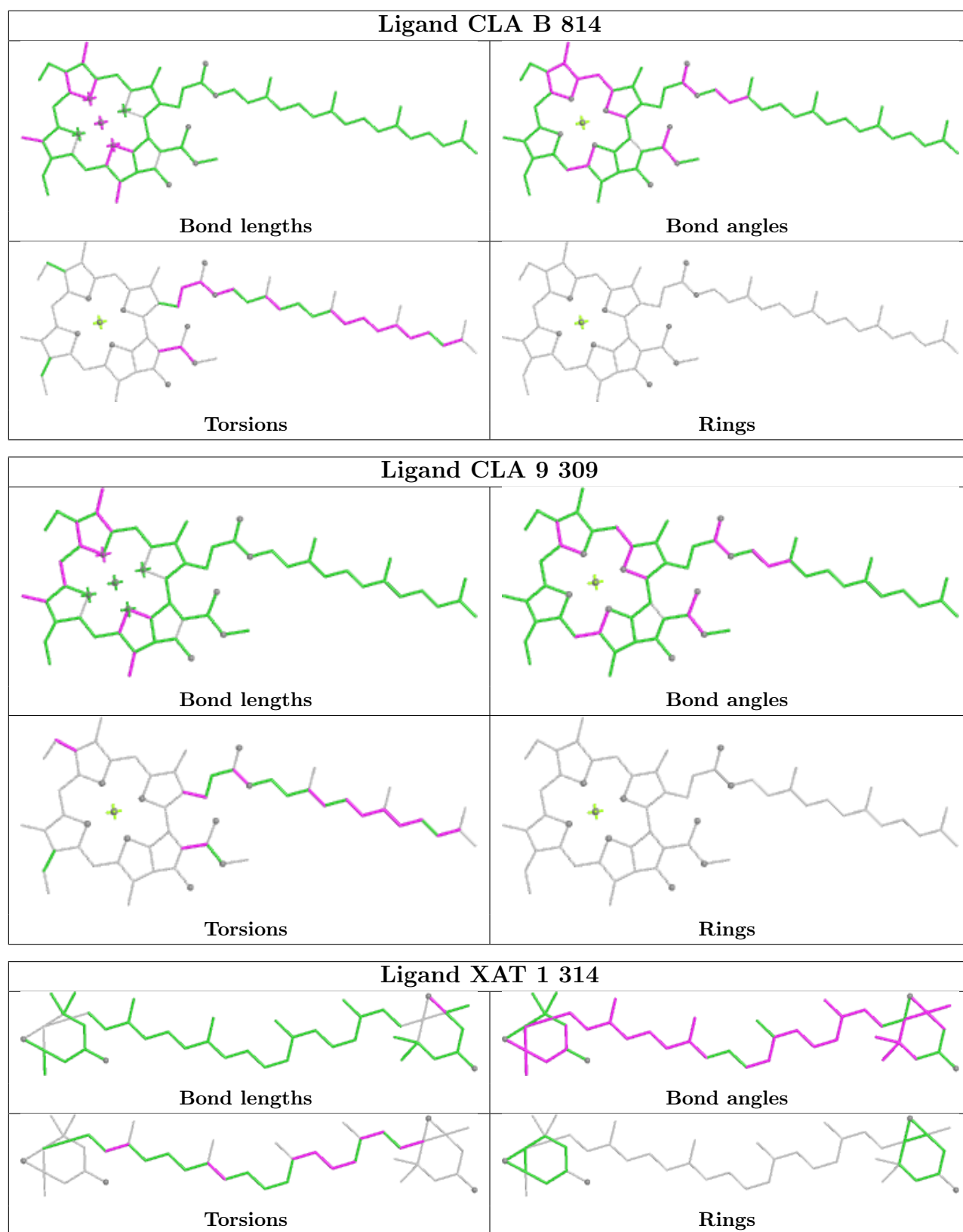


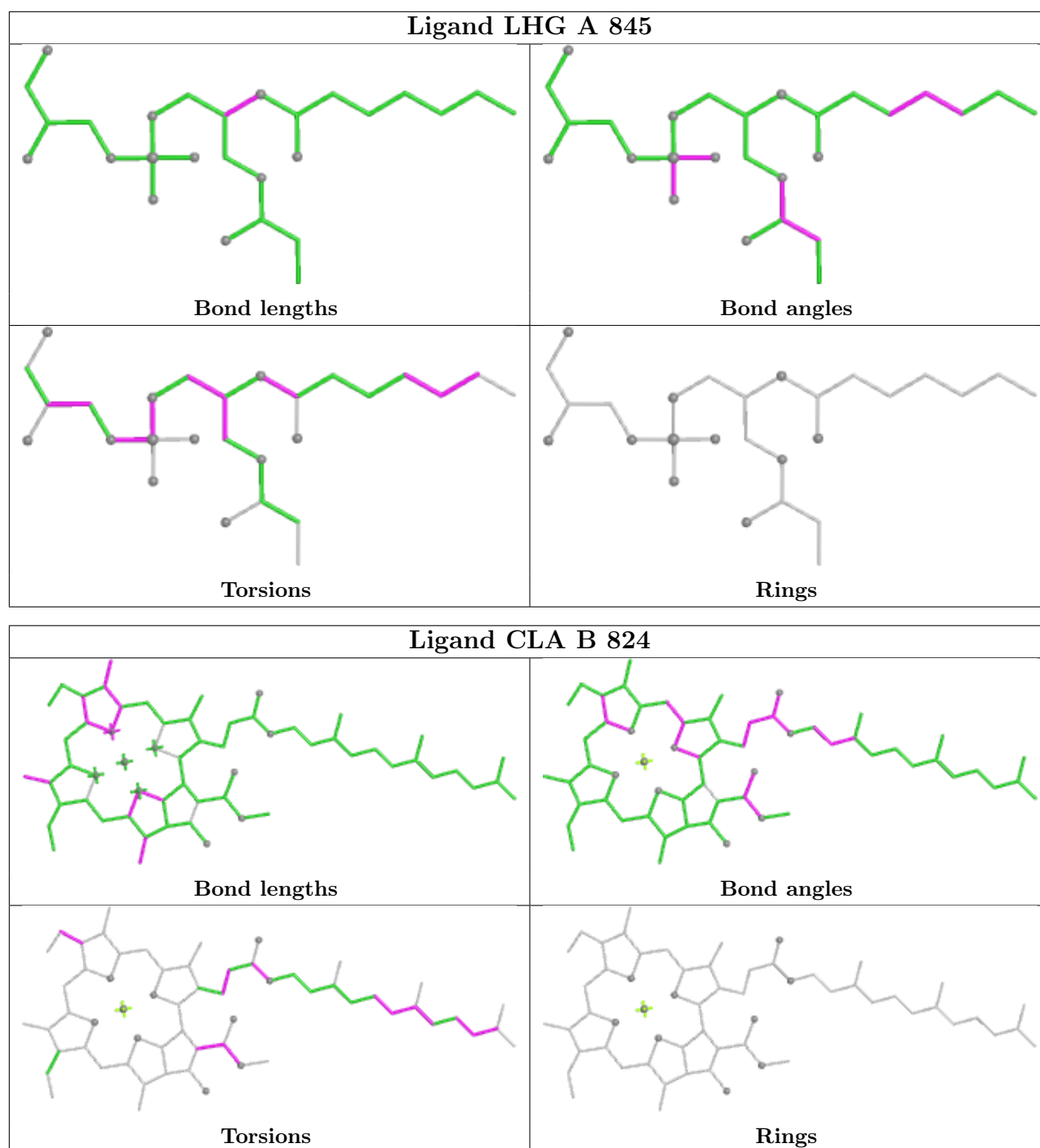
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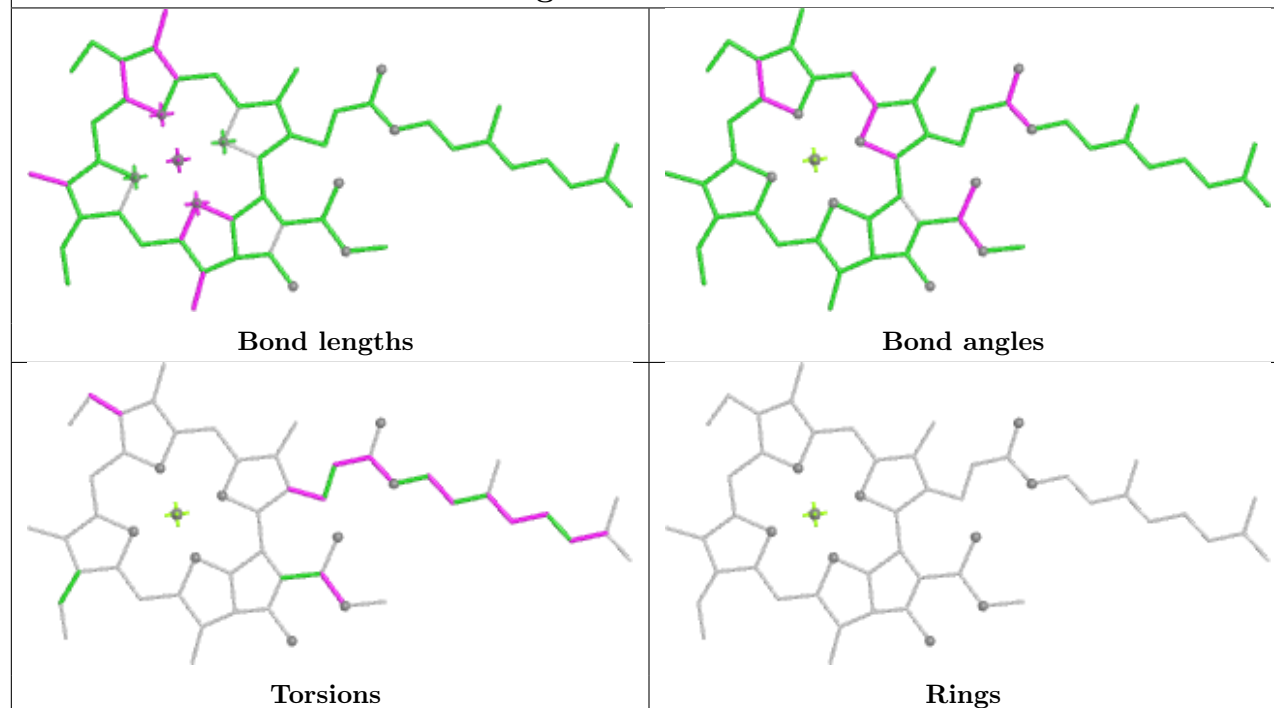




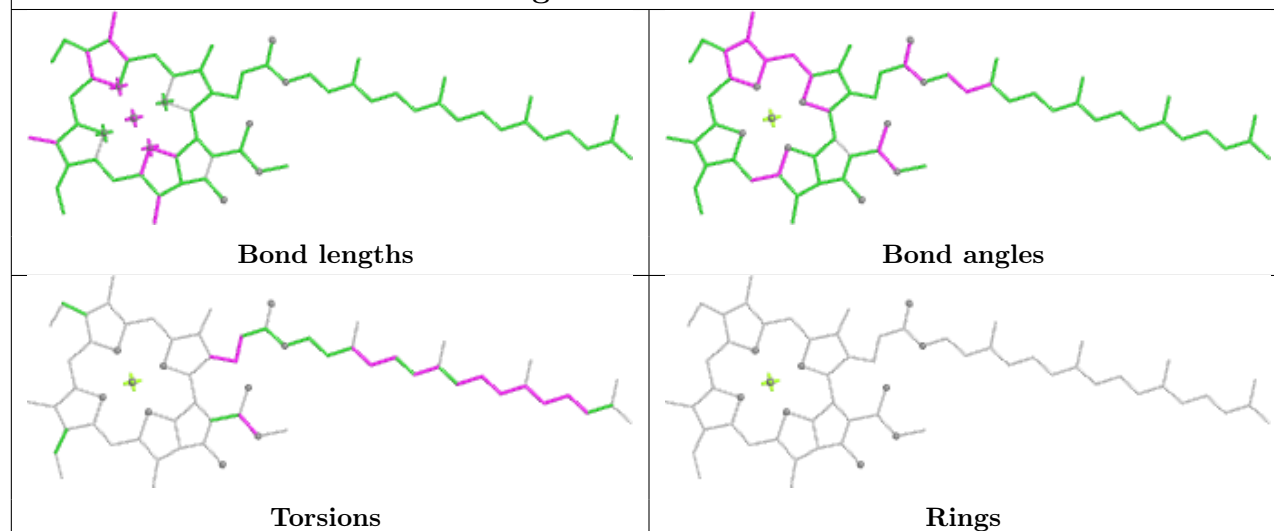




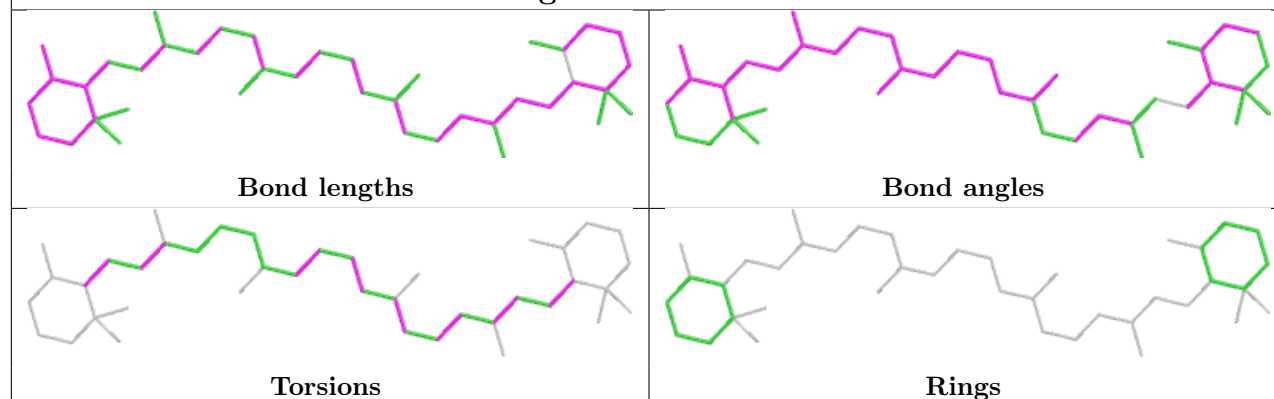
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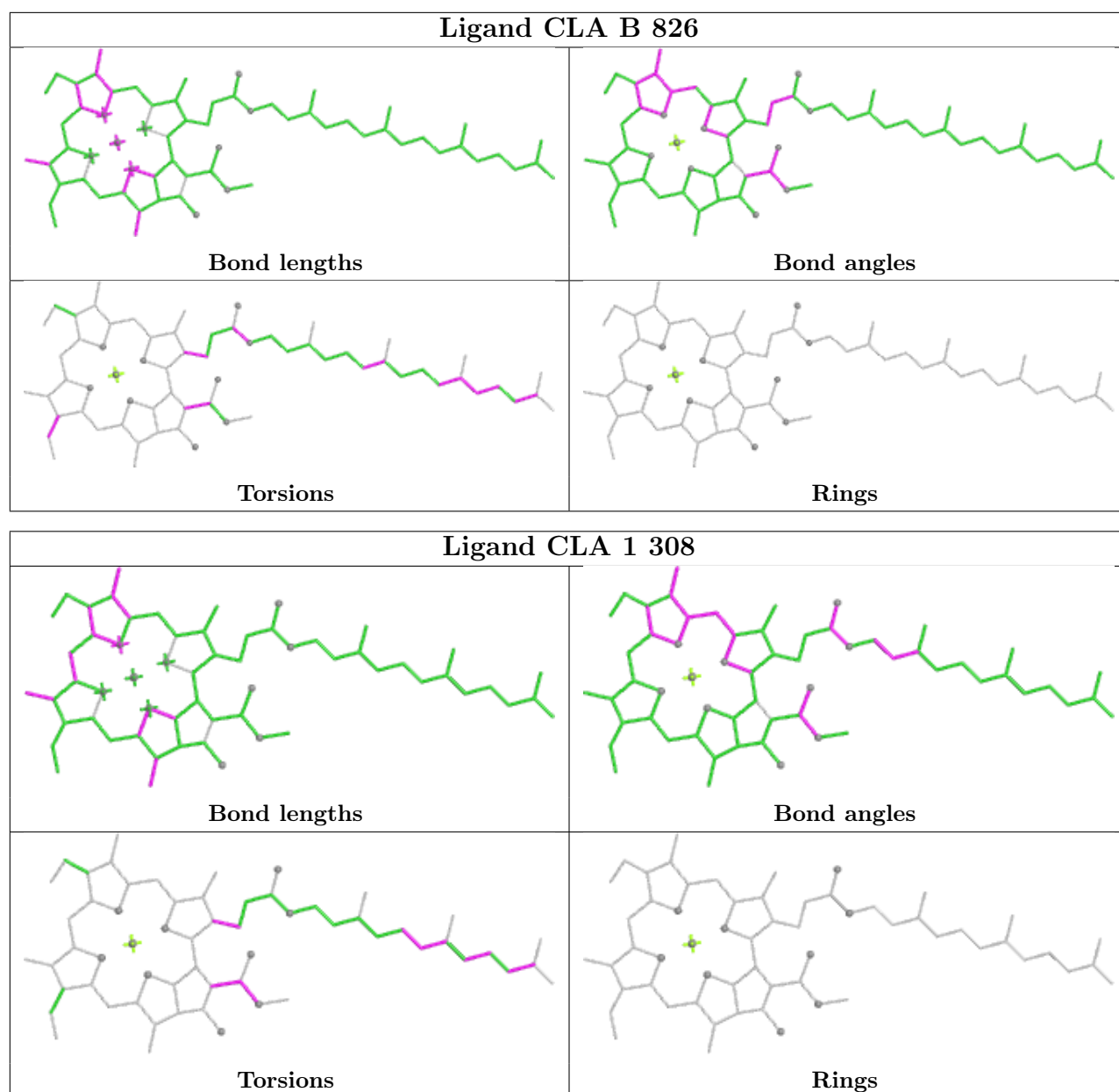


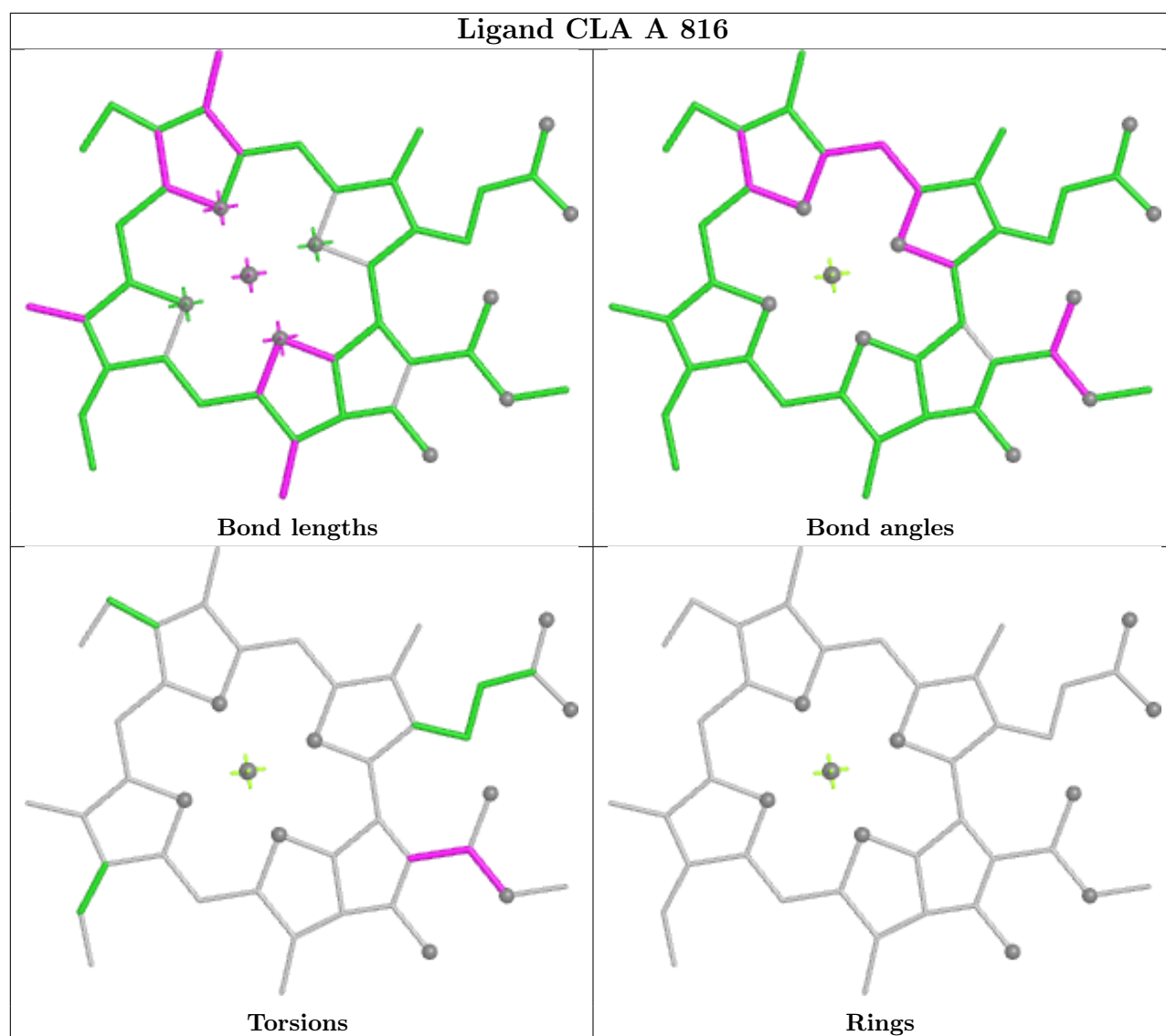
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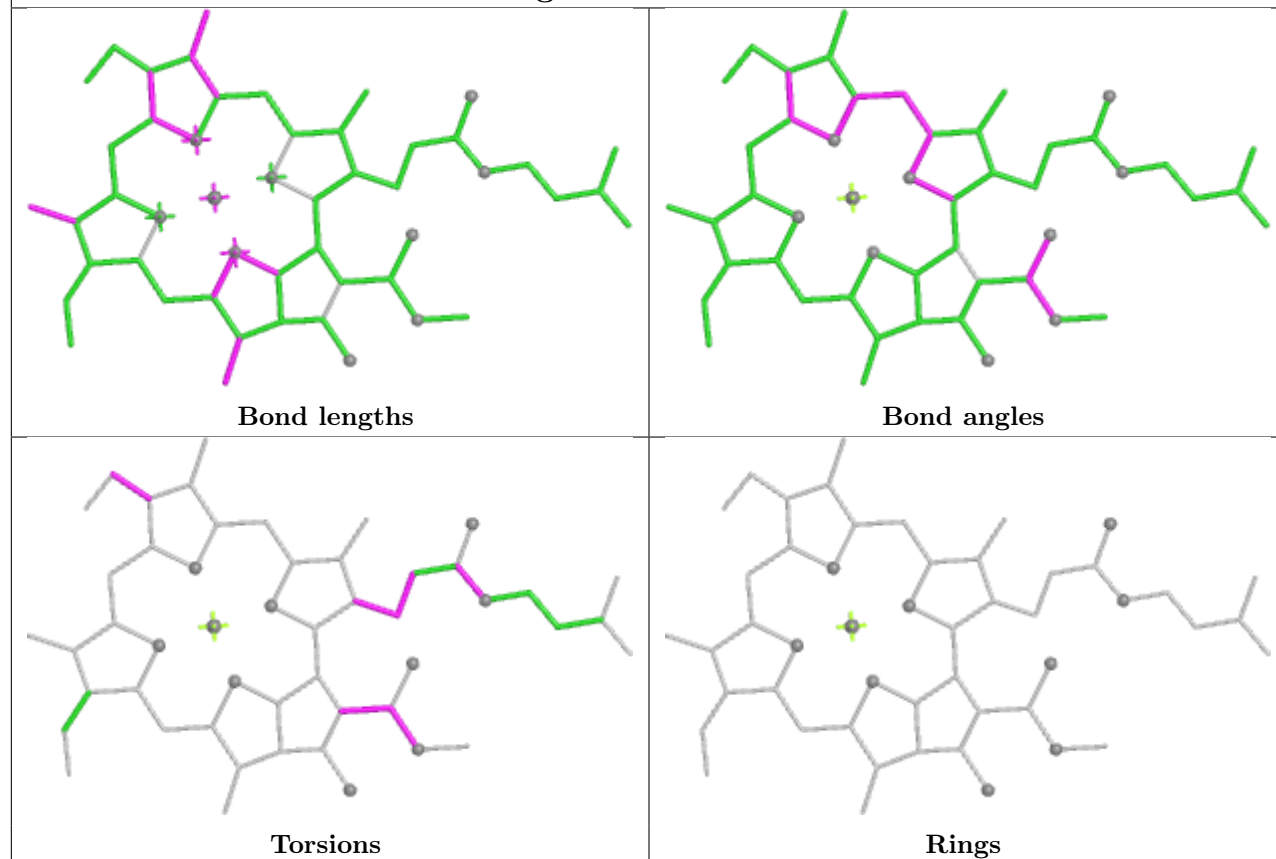
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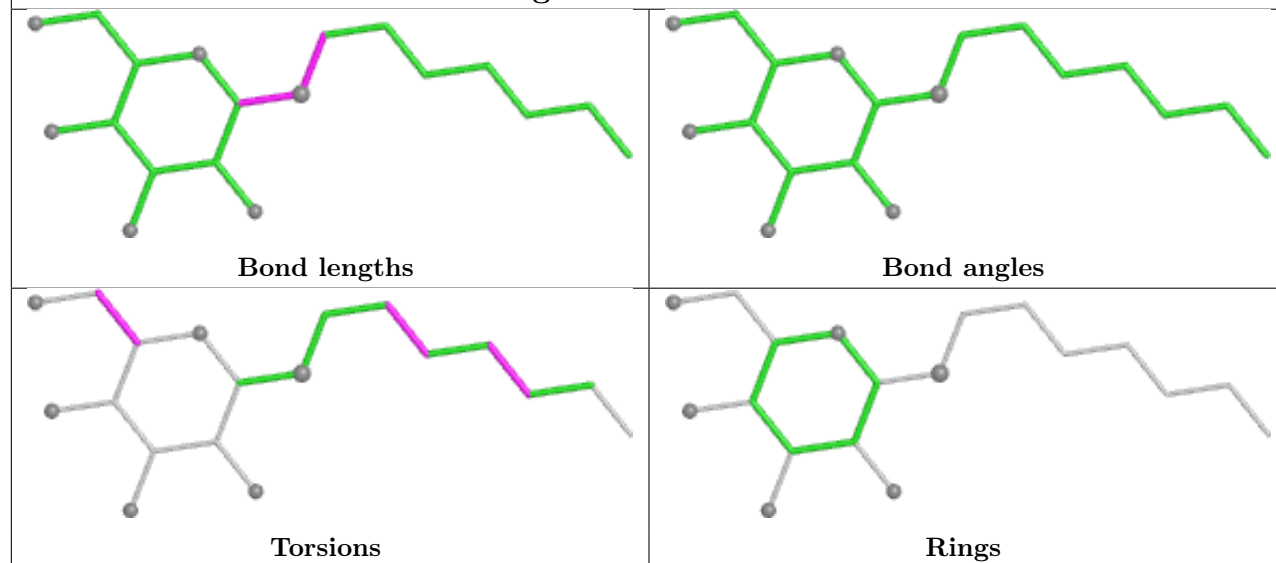




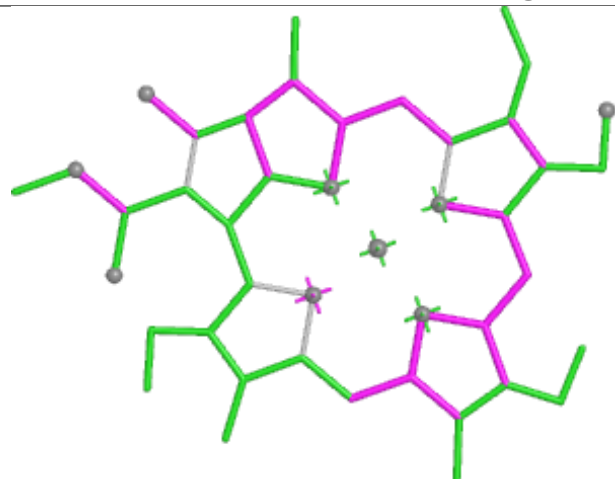
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Ligand HTG J 102



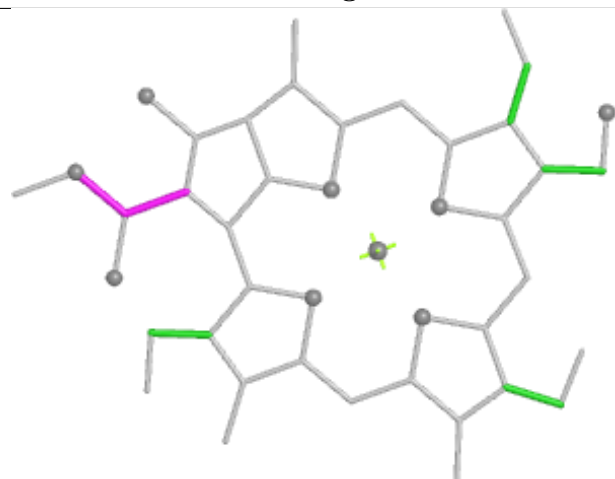
Ligand CHL 8 314



Bond lengths



Bond angles

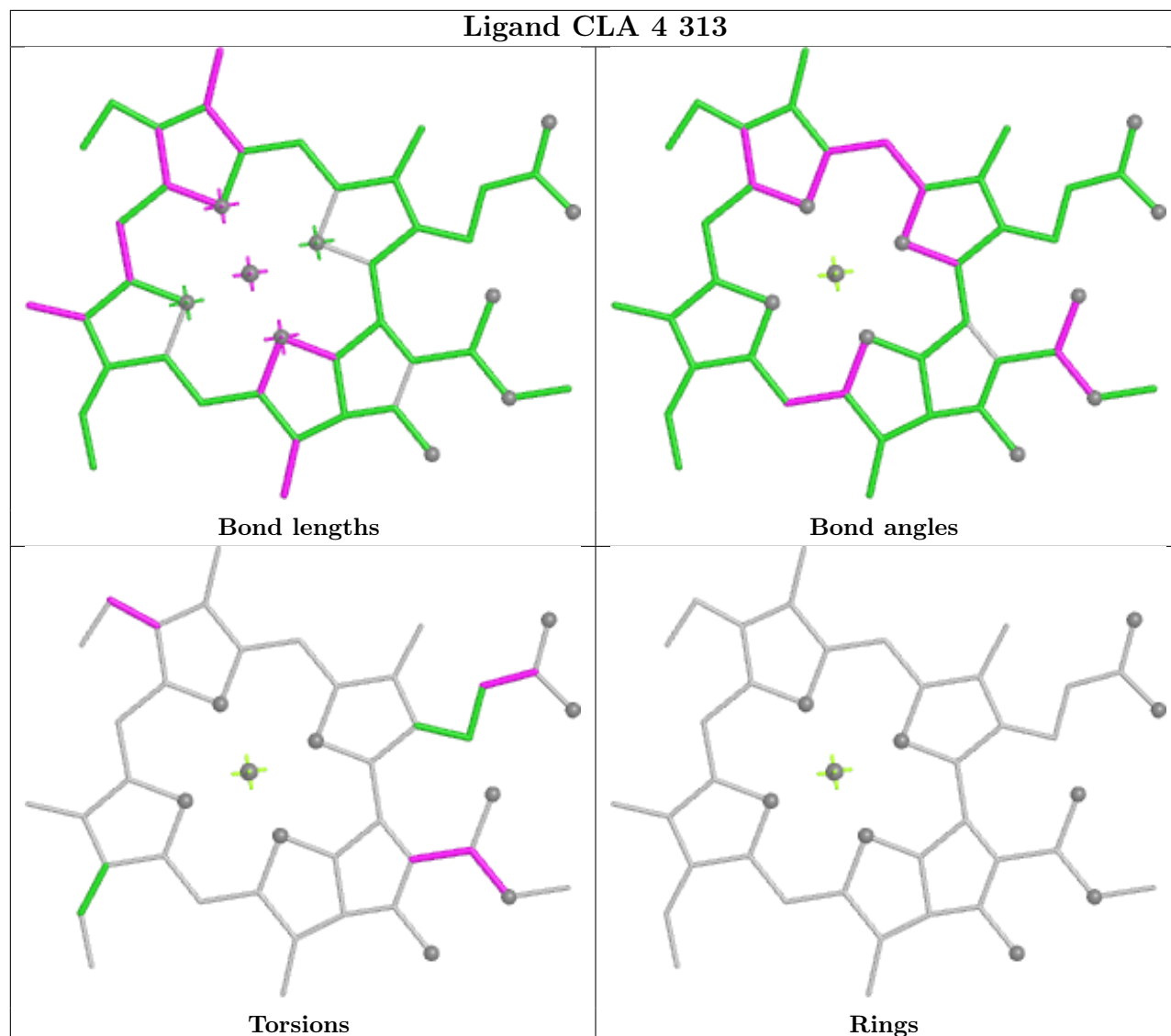


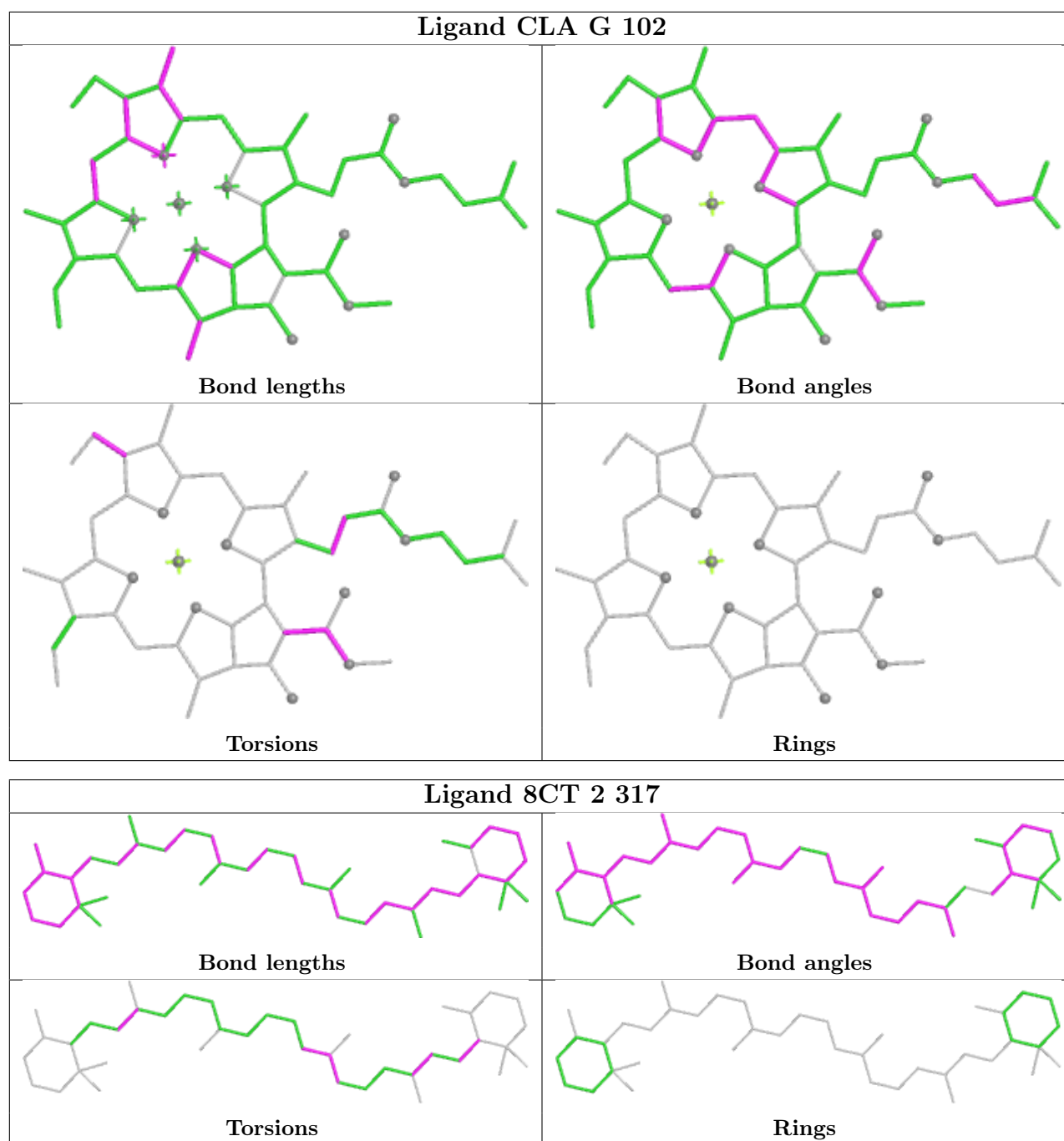
Torsions

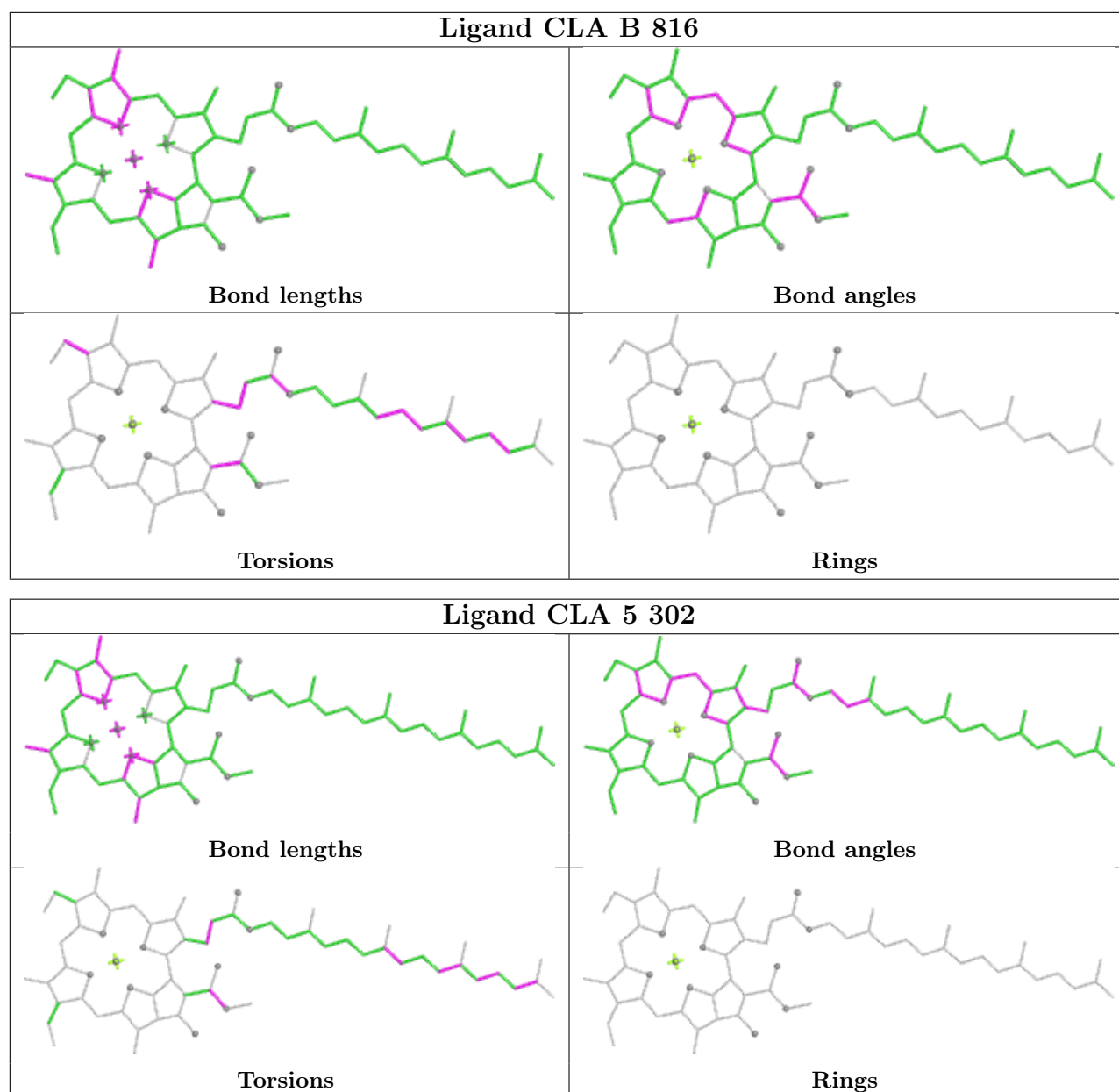


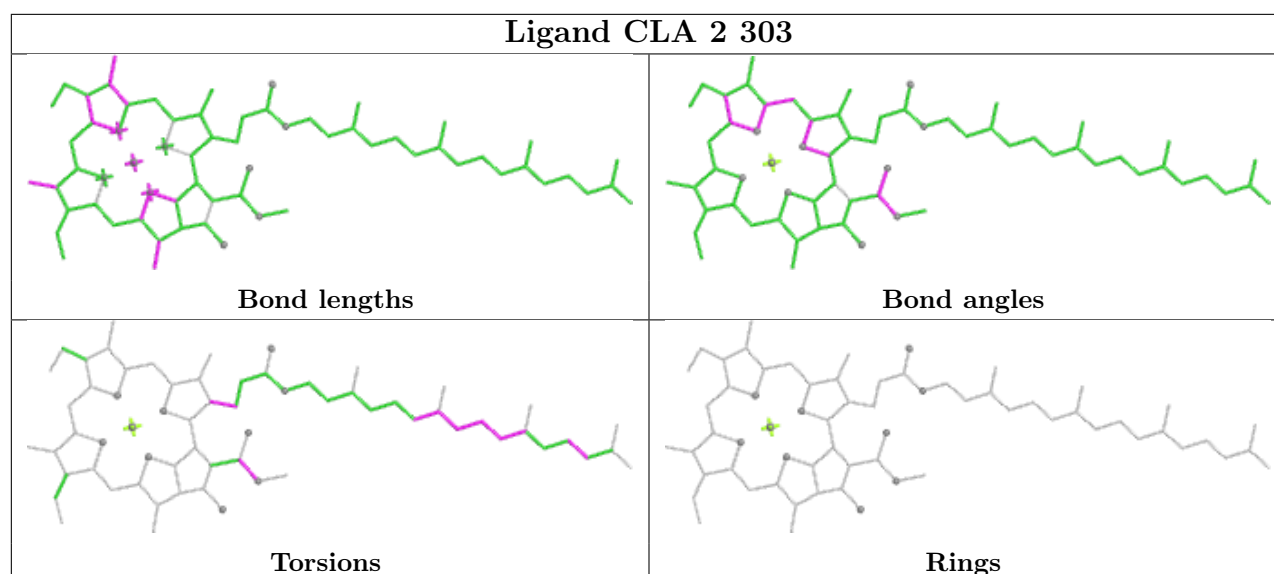
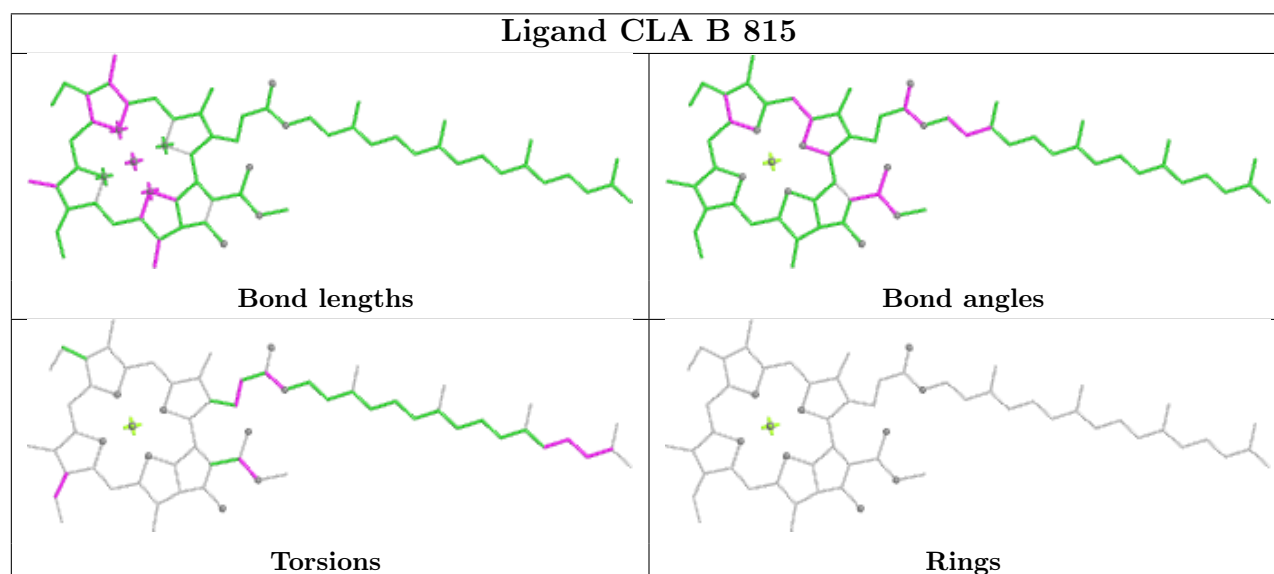
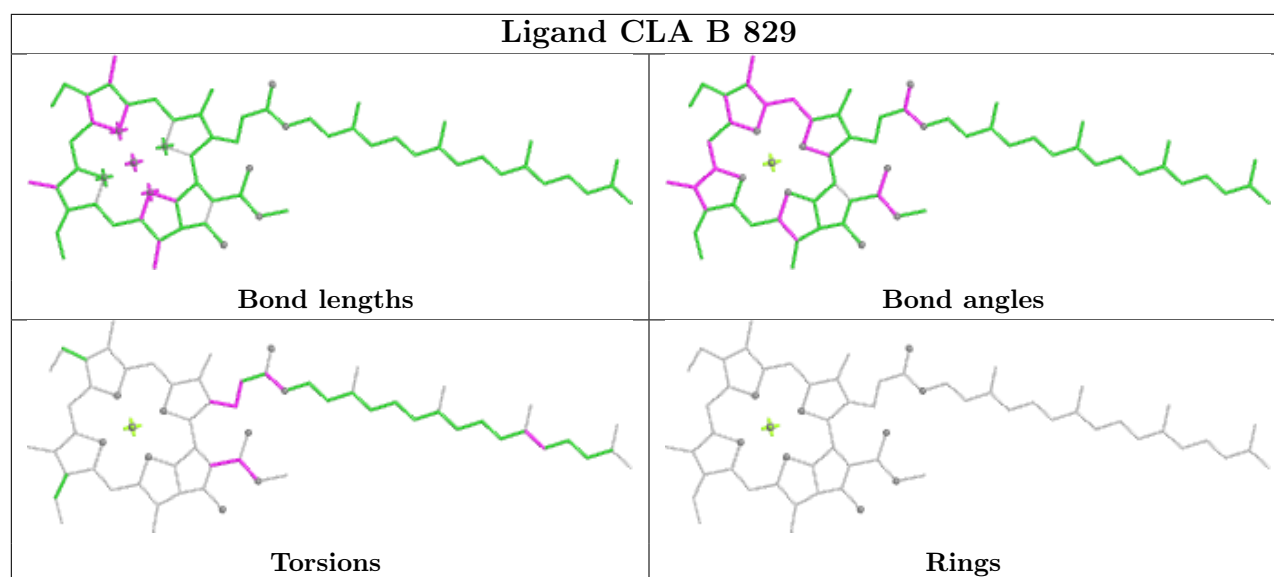
Rings

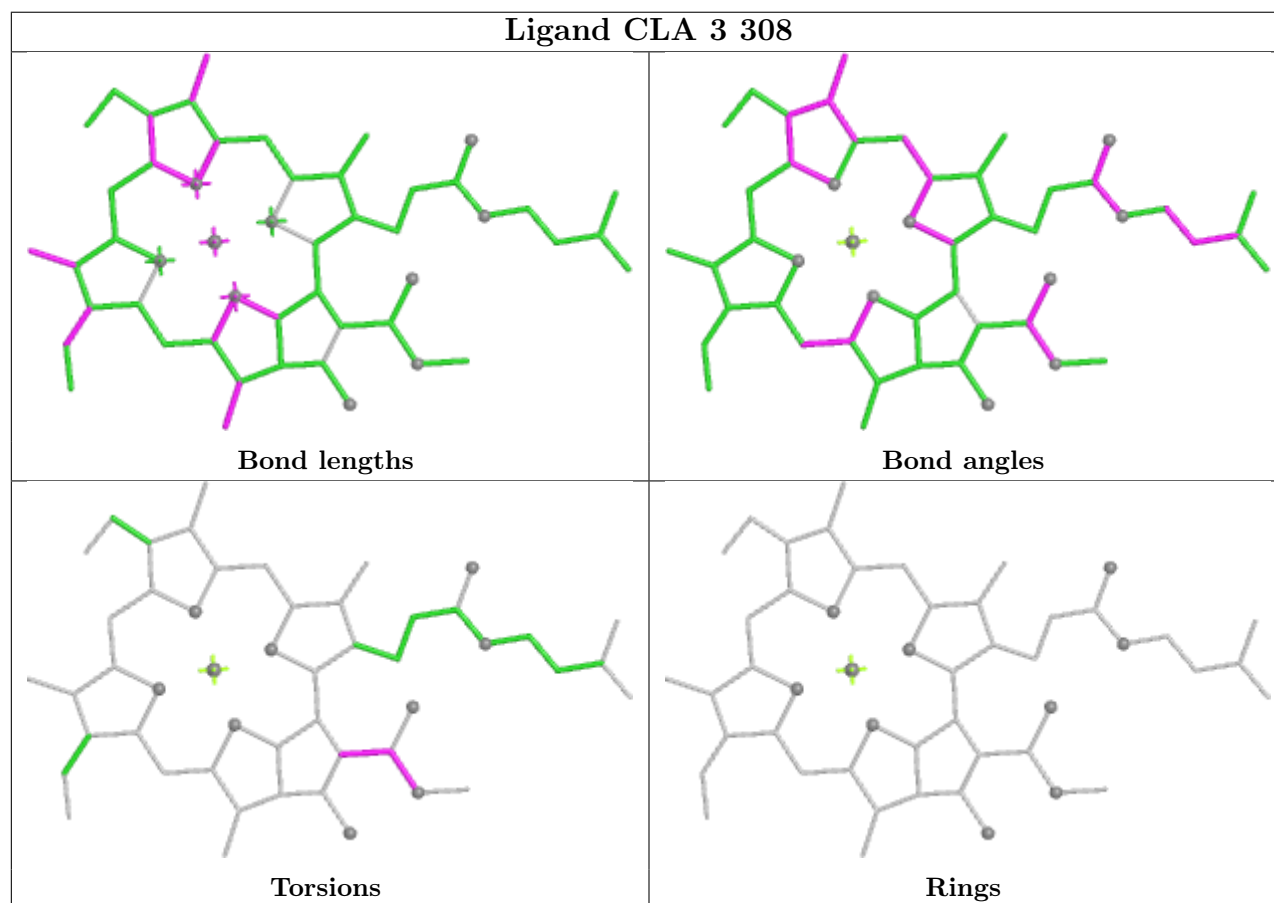
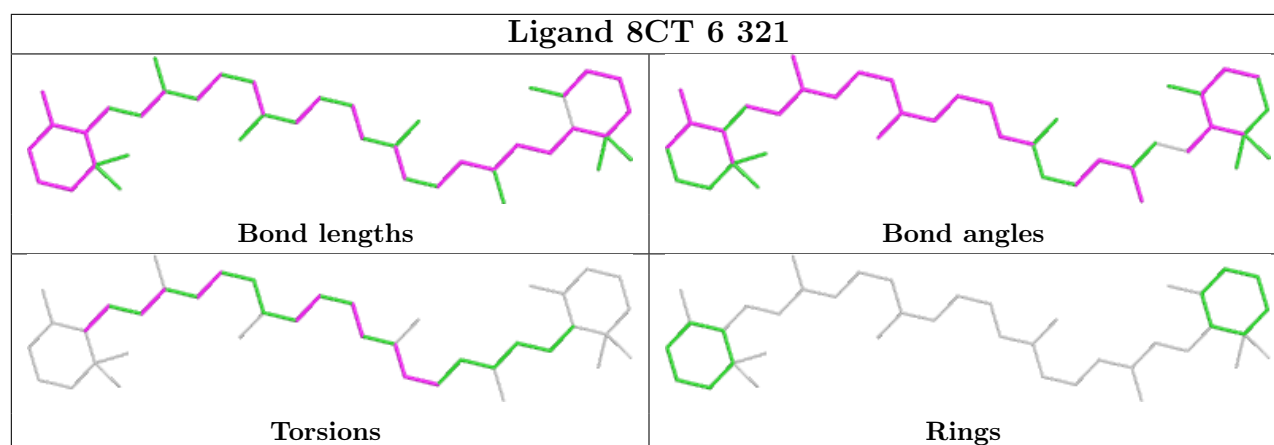
Ligand CLA 4 313



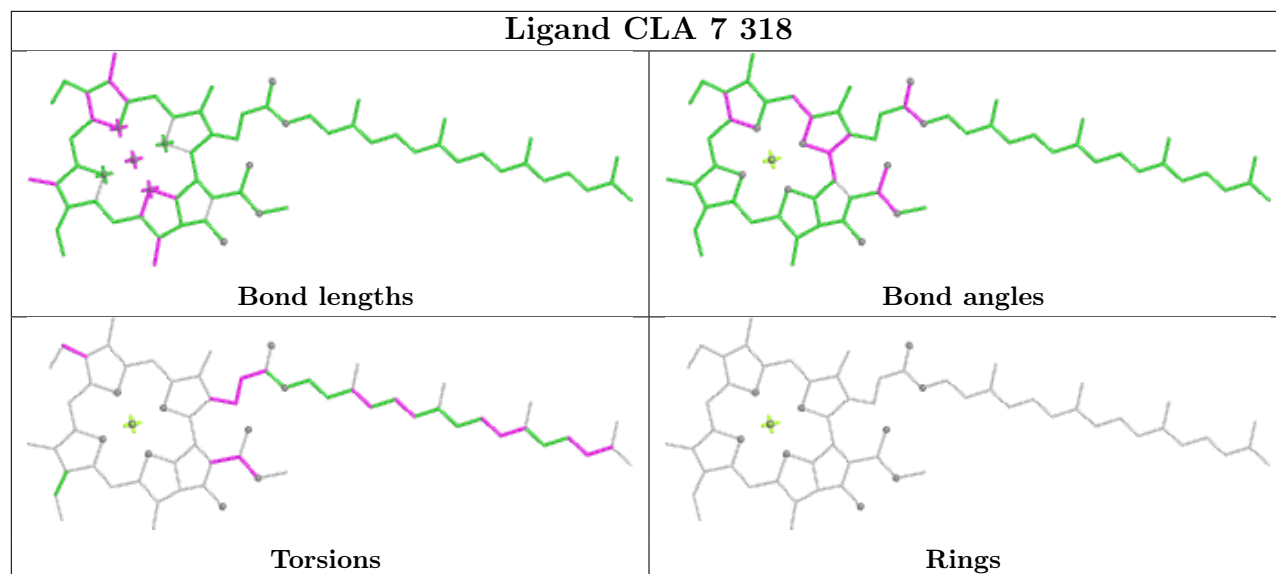




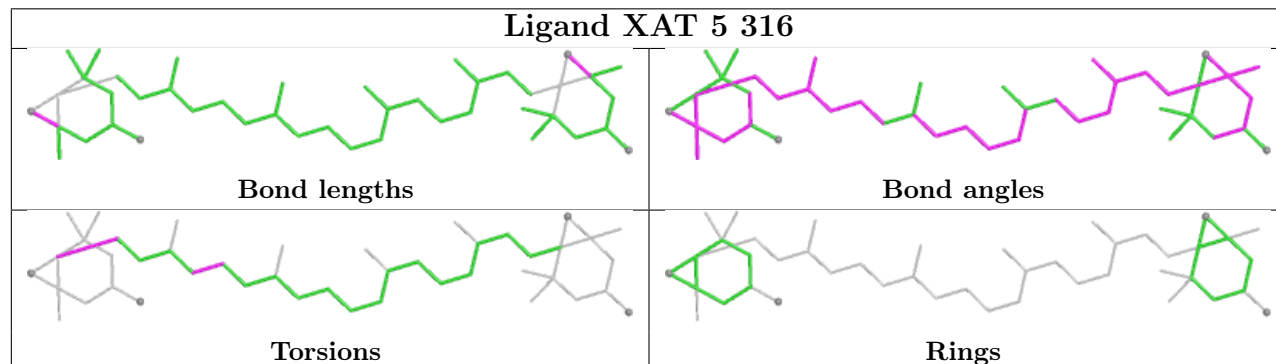




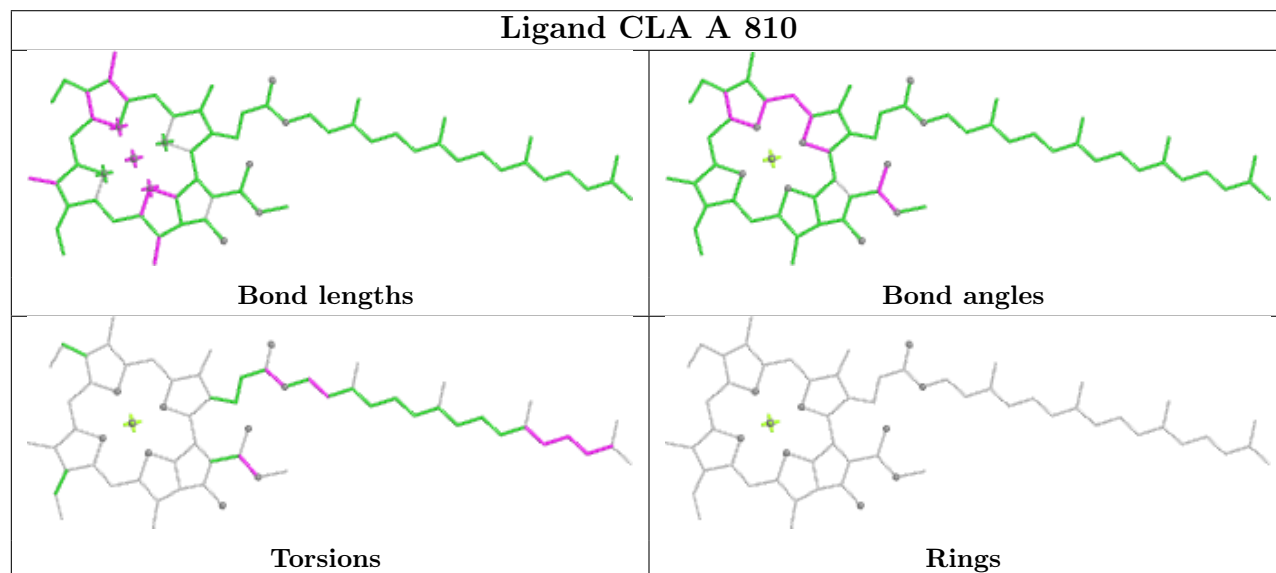
Ligand CLA 7 318

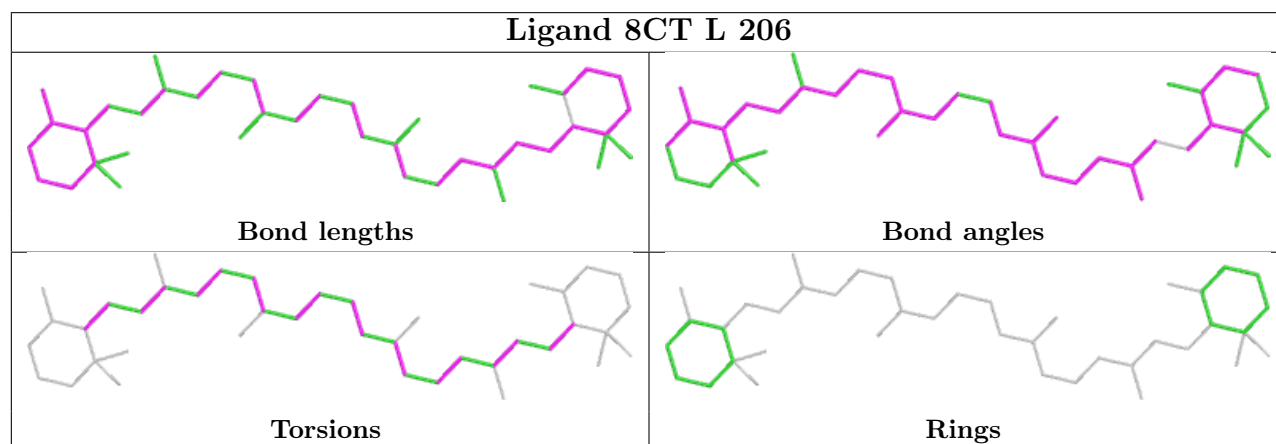
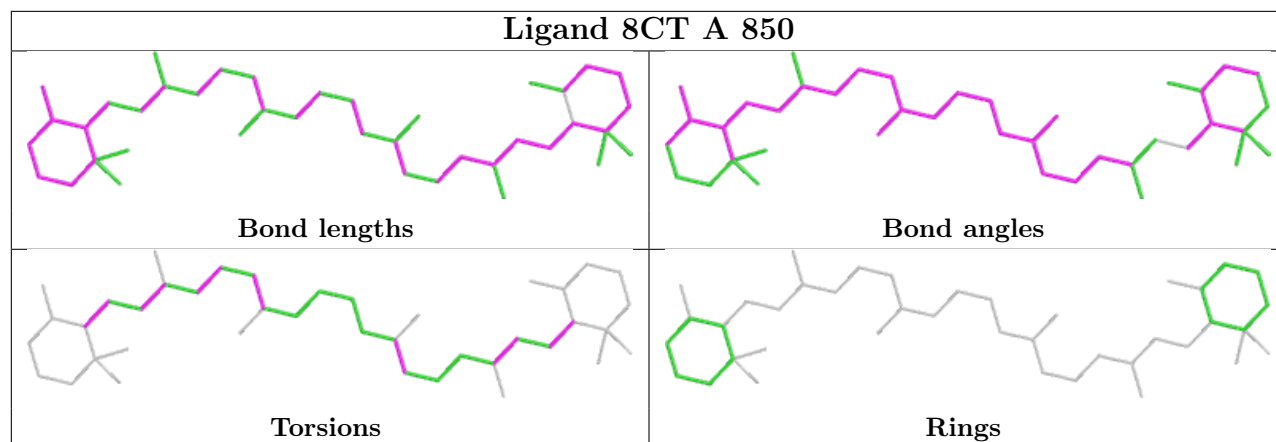


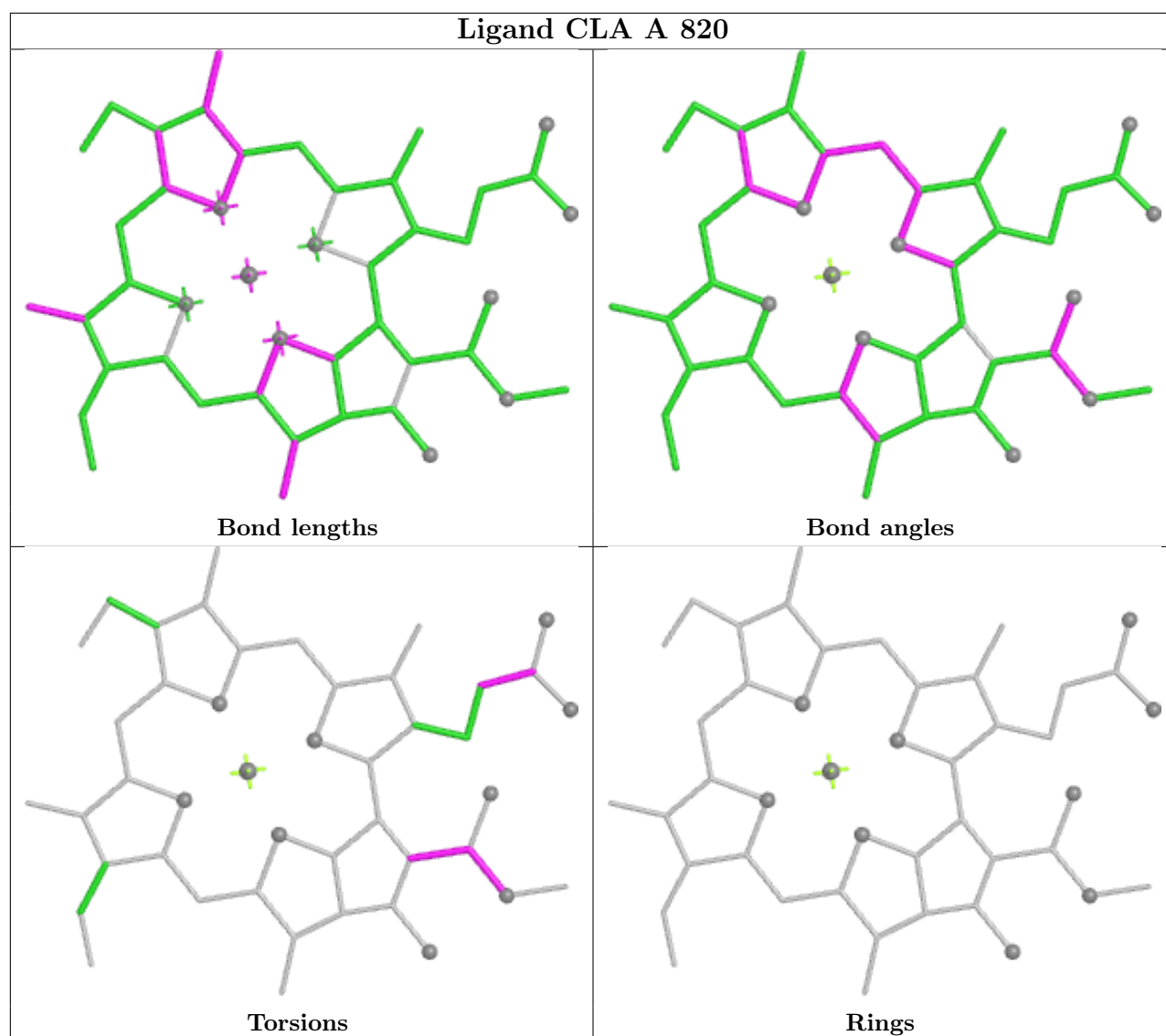
Ligand XAT 5 316



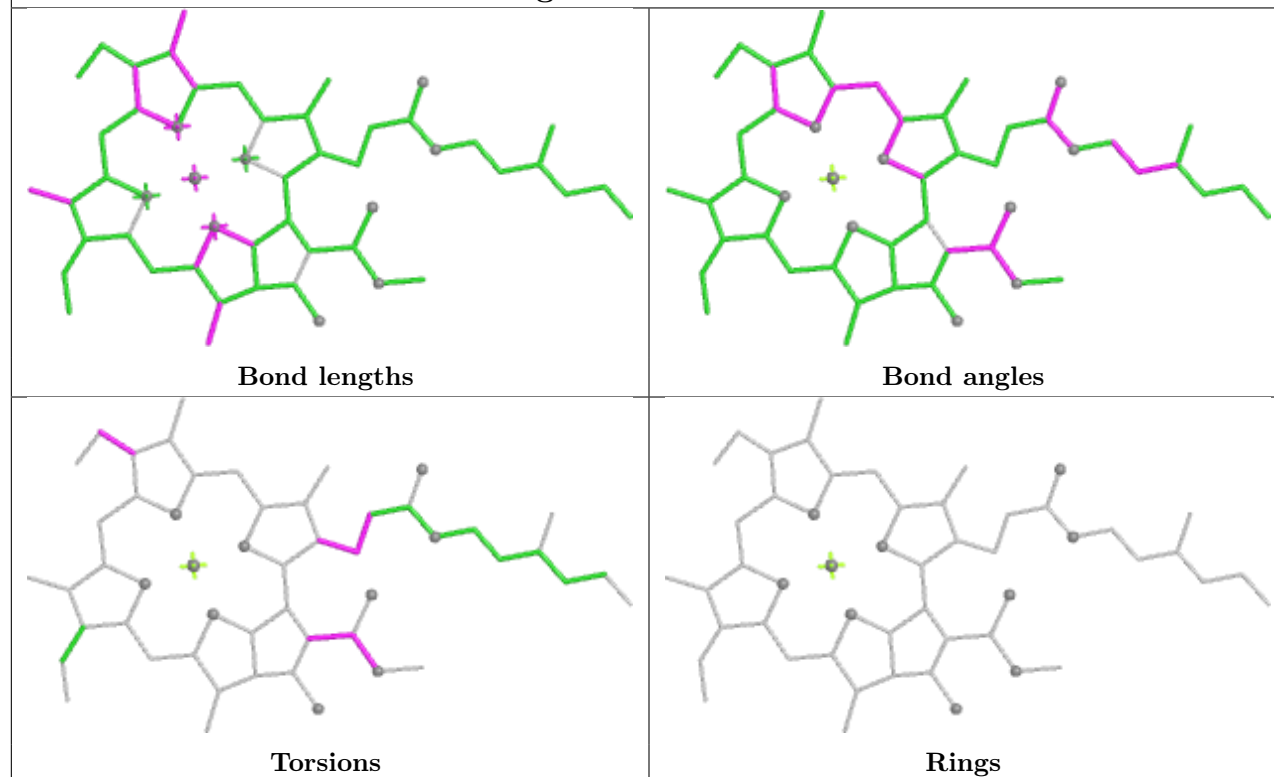
Ligand CLA A 810



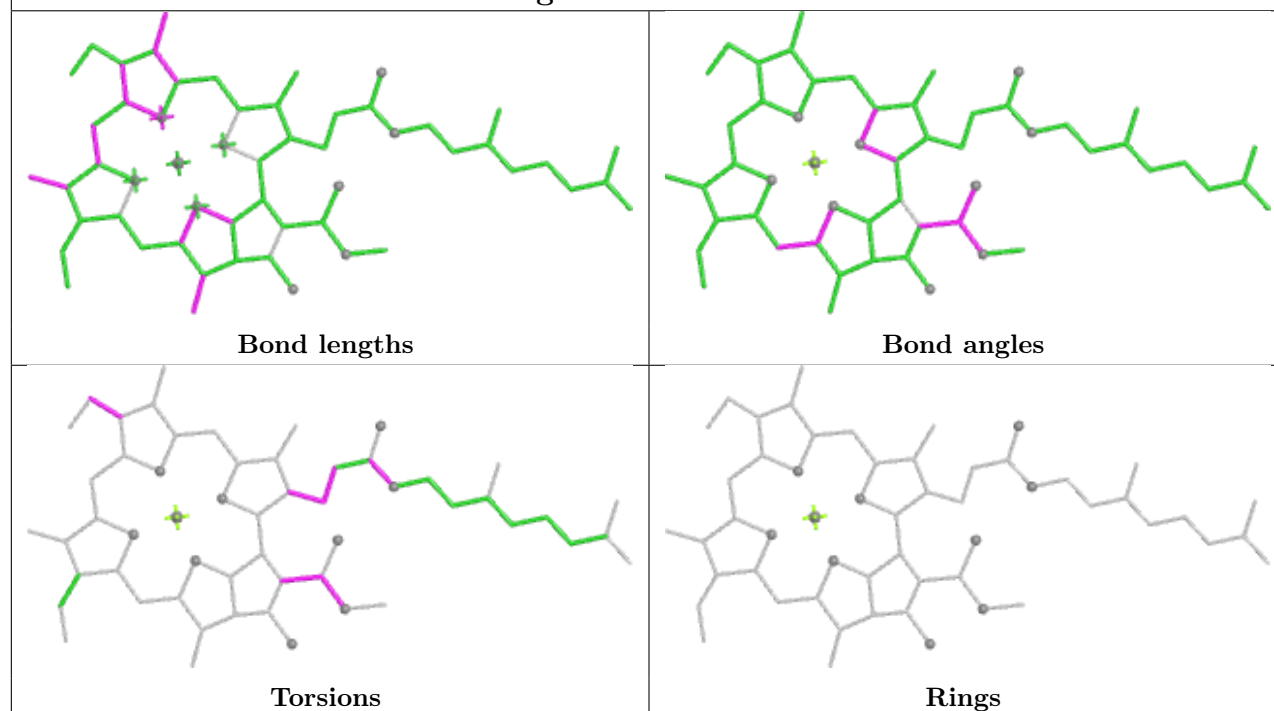


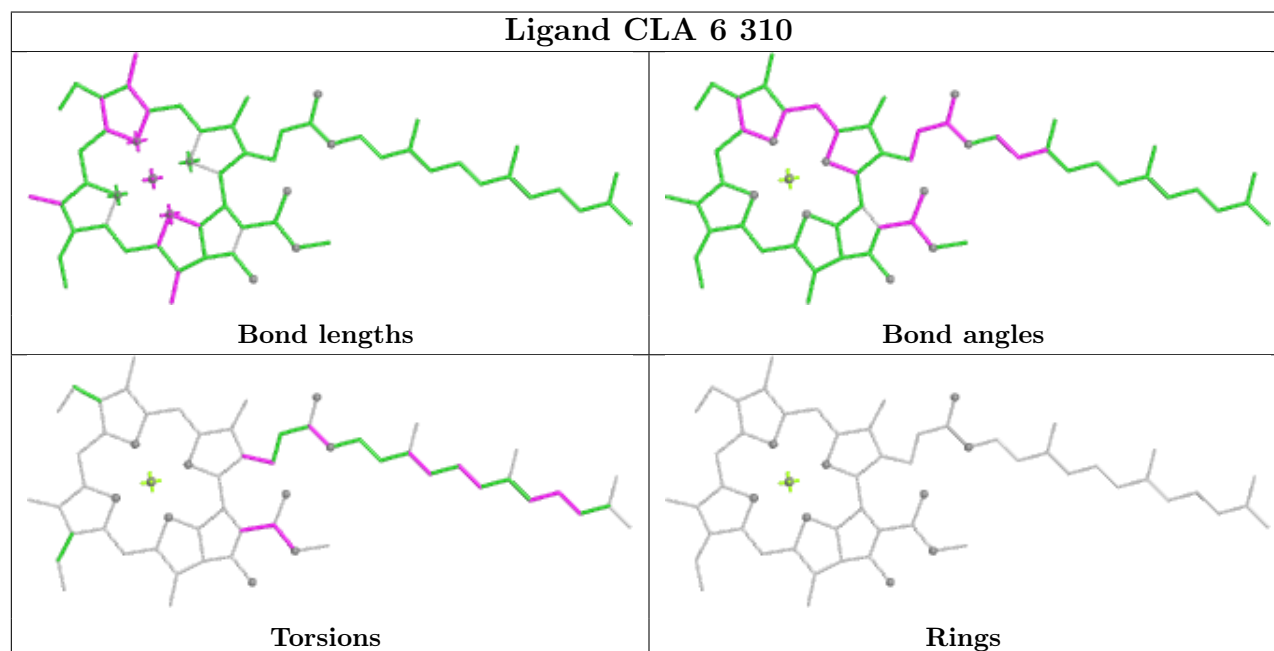
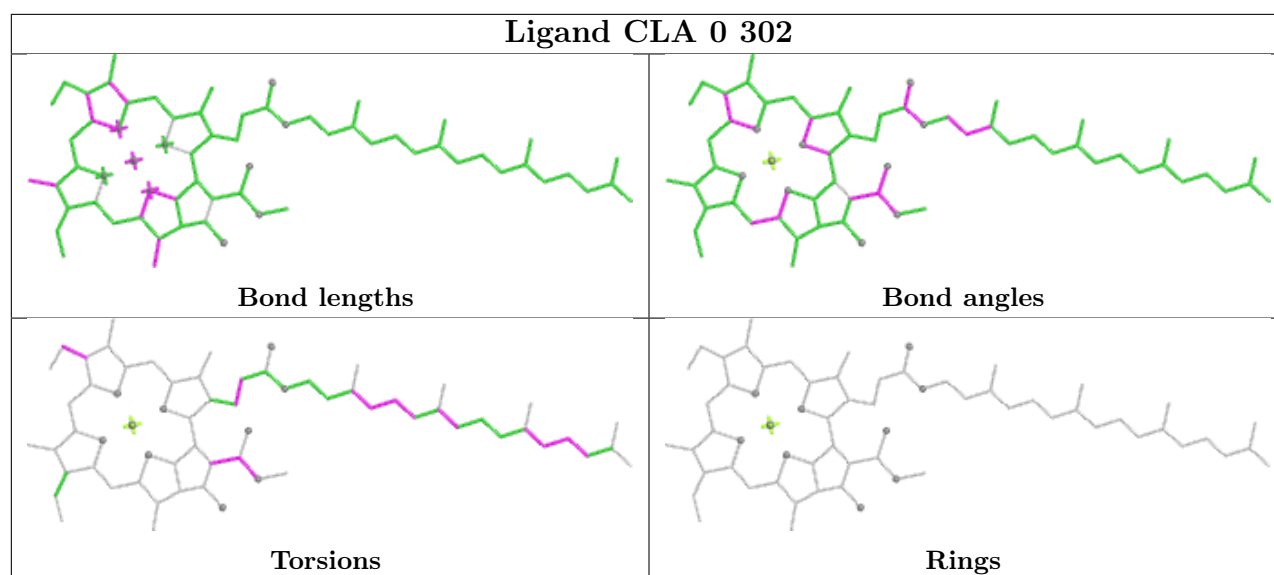


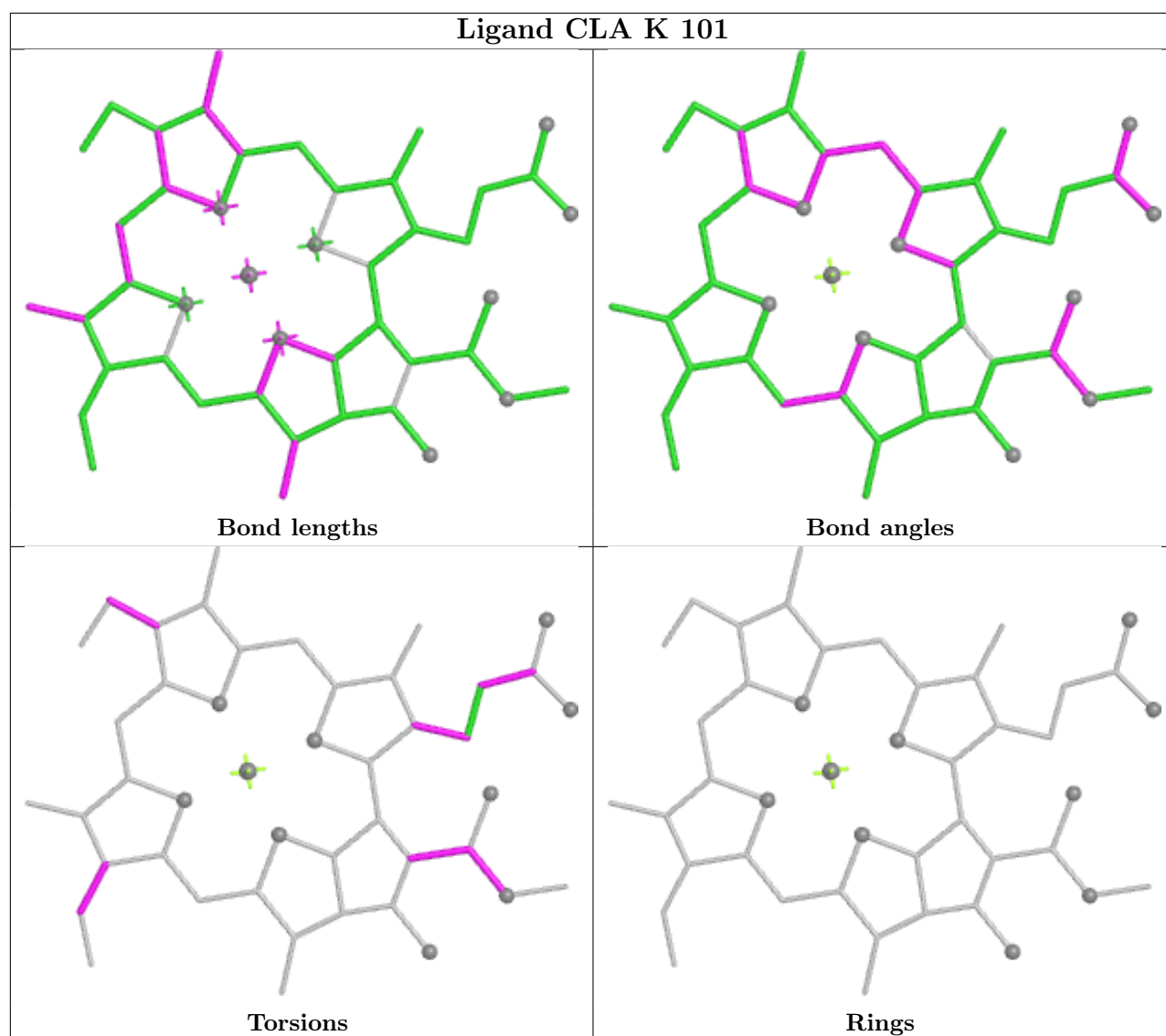
Ligand CLA 6 318

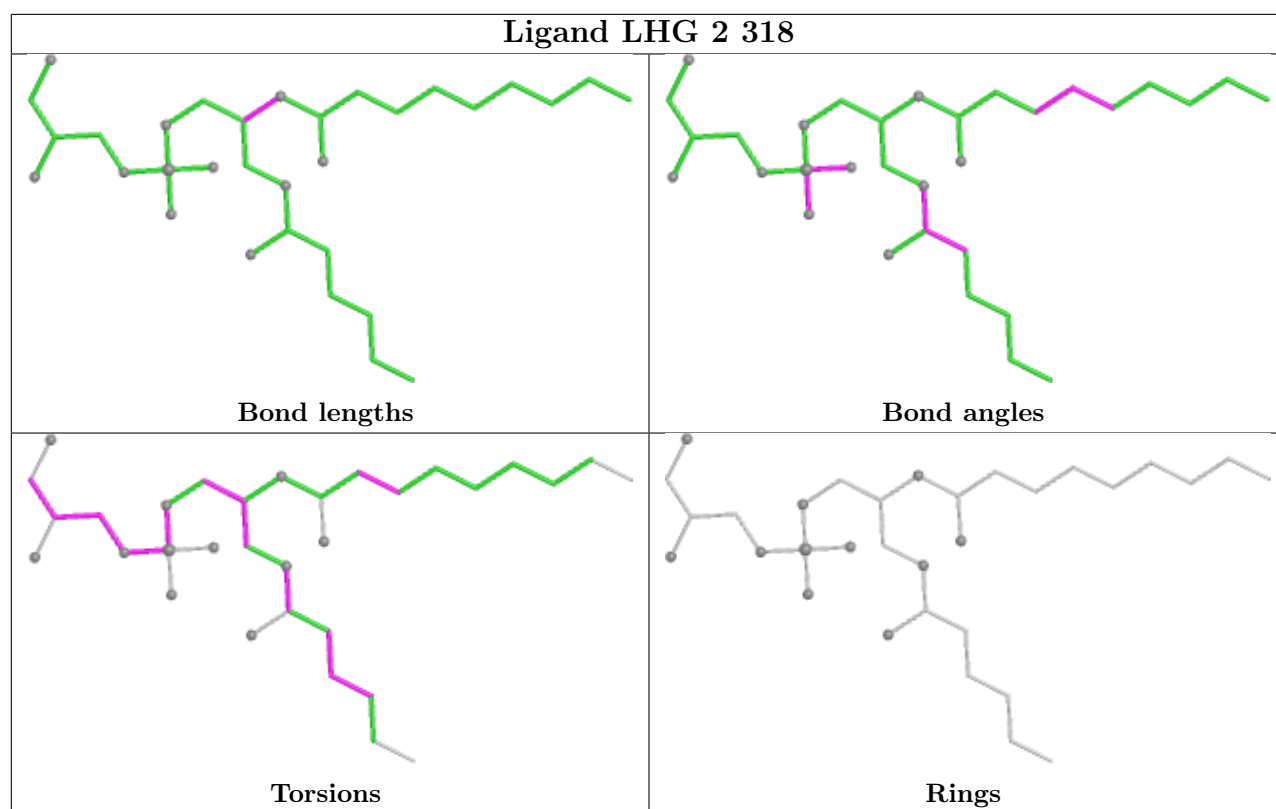


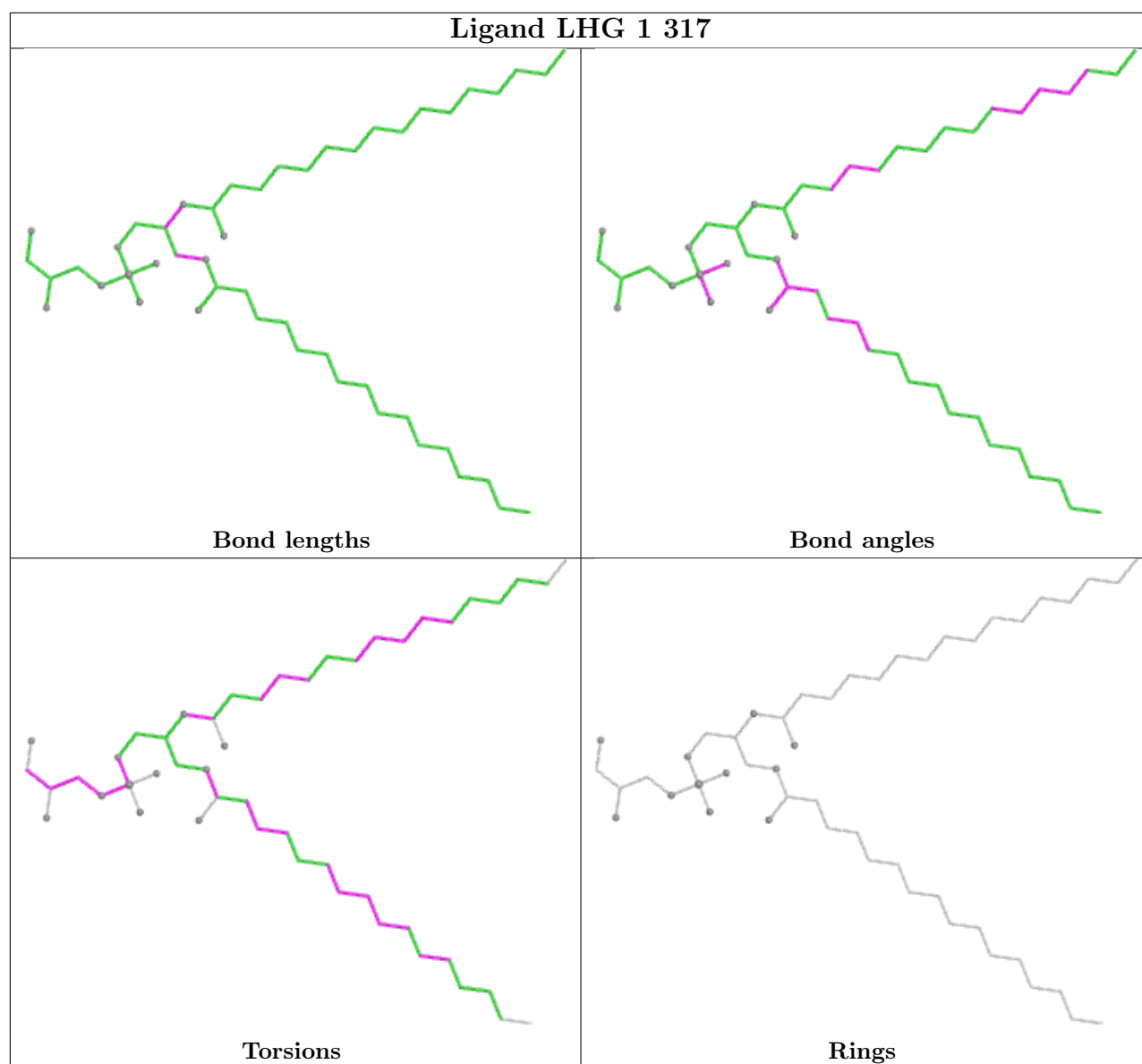
Ligand CLA 5 313



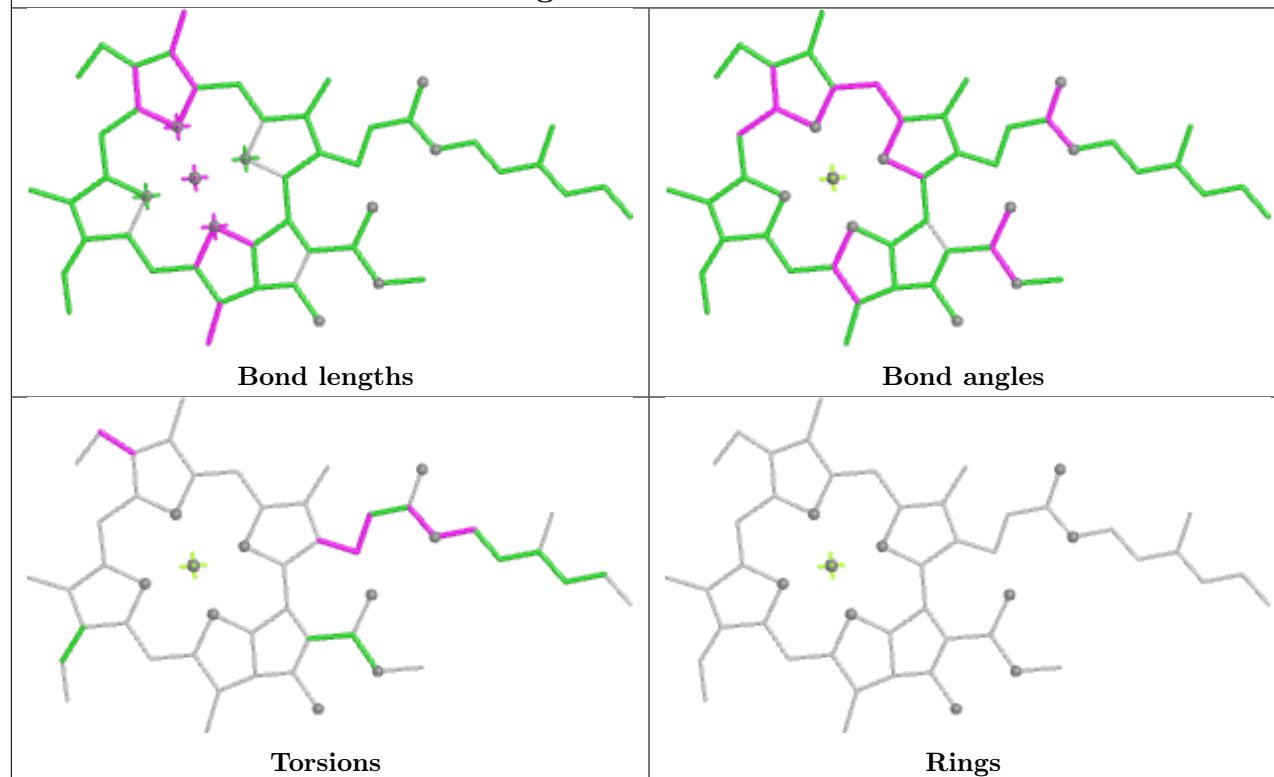




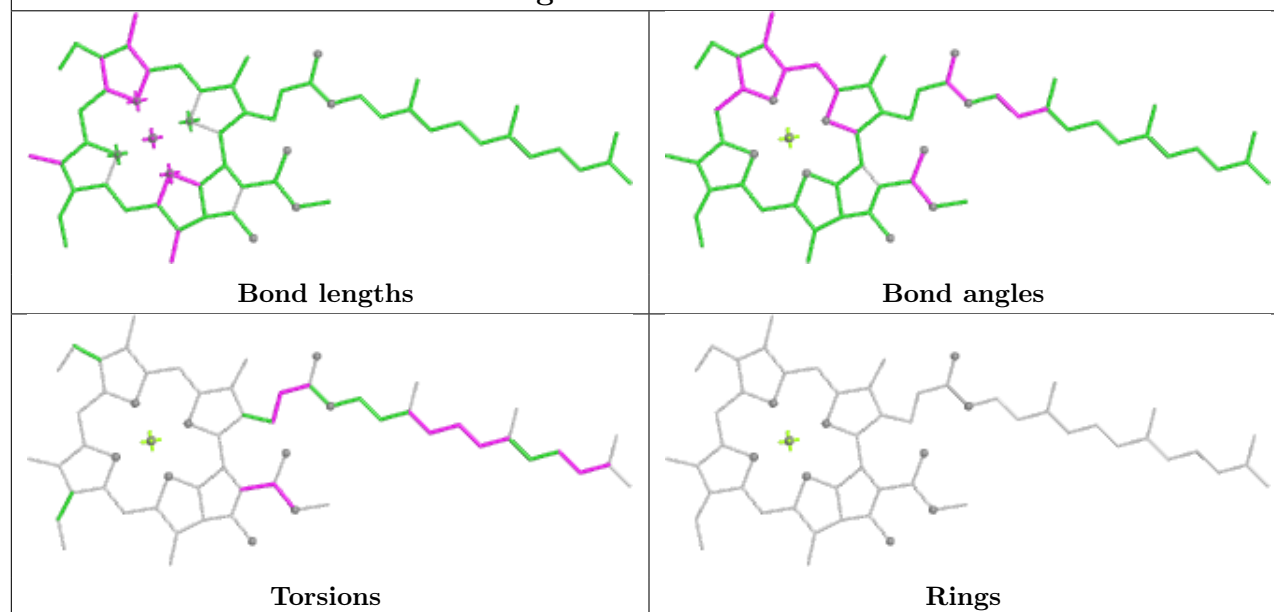




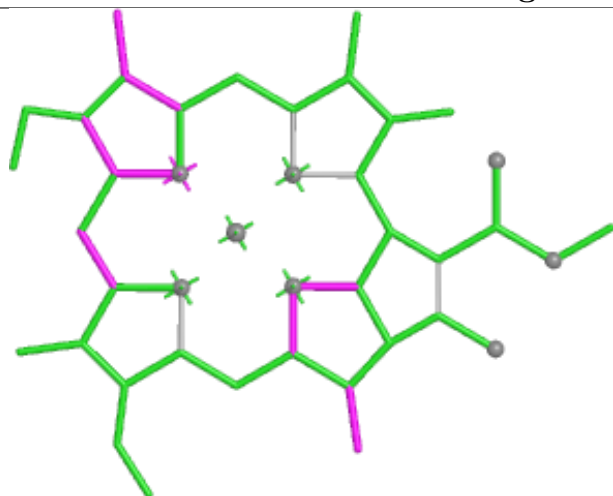
Ligand CLA 1 304



Ligand CLA 7 303



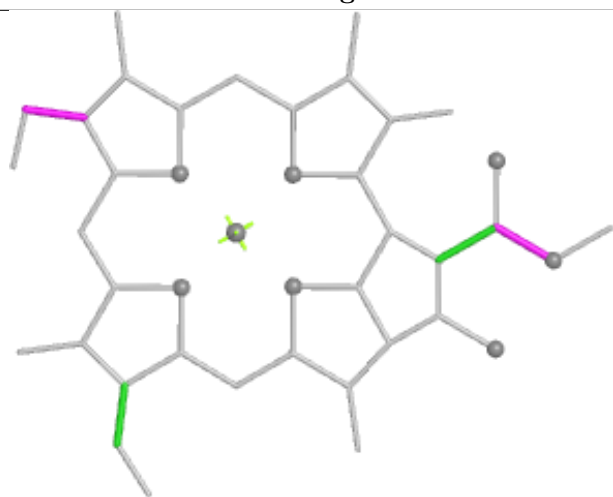
Ligand CLA 0 309



Bond lengths



Bond angles

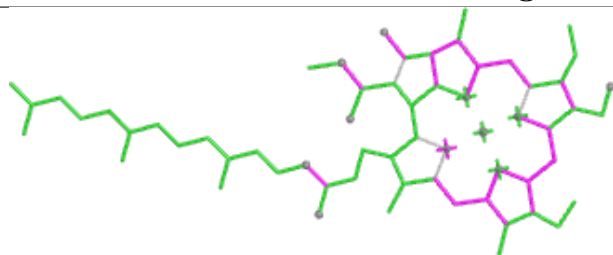


Torsions

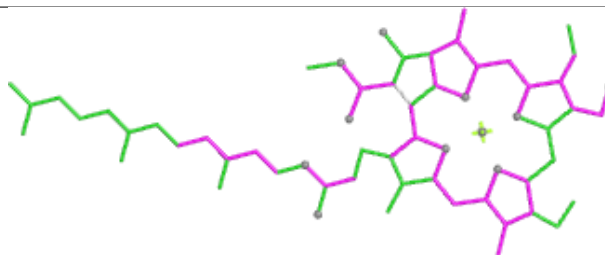


Rings

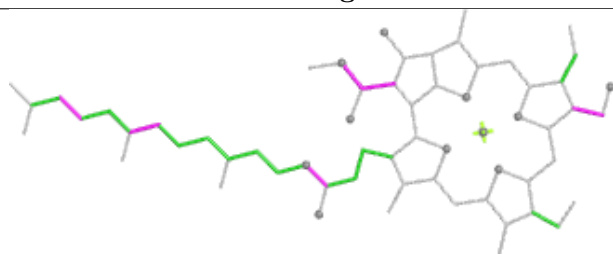
Ligand CHL 2 301



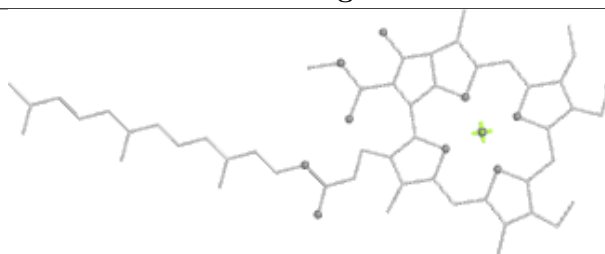
Bond lengths



Bond angles

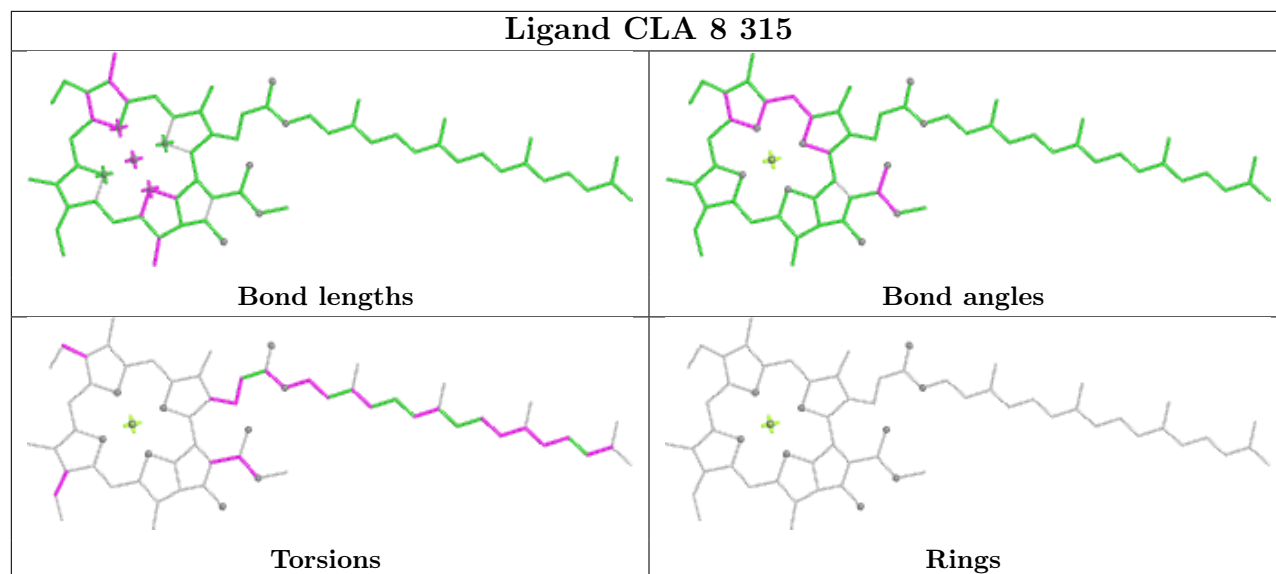


Torsions

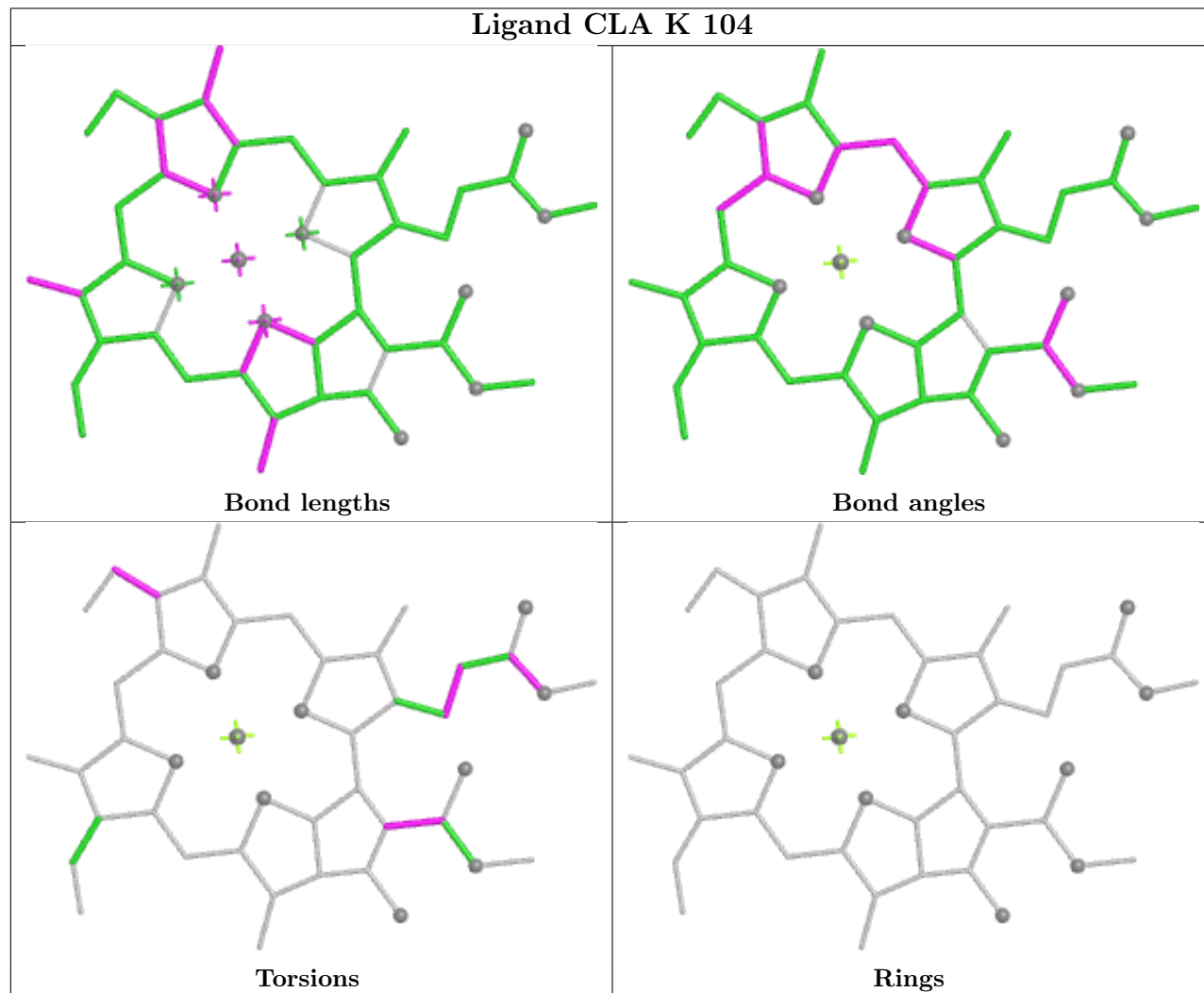


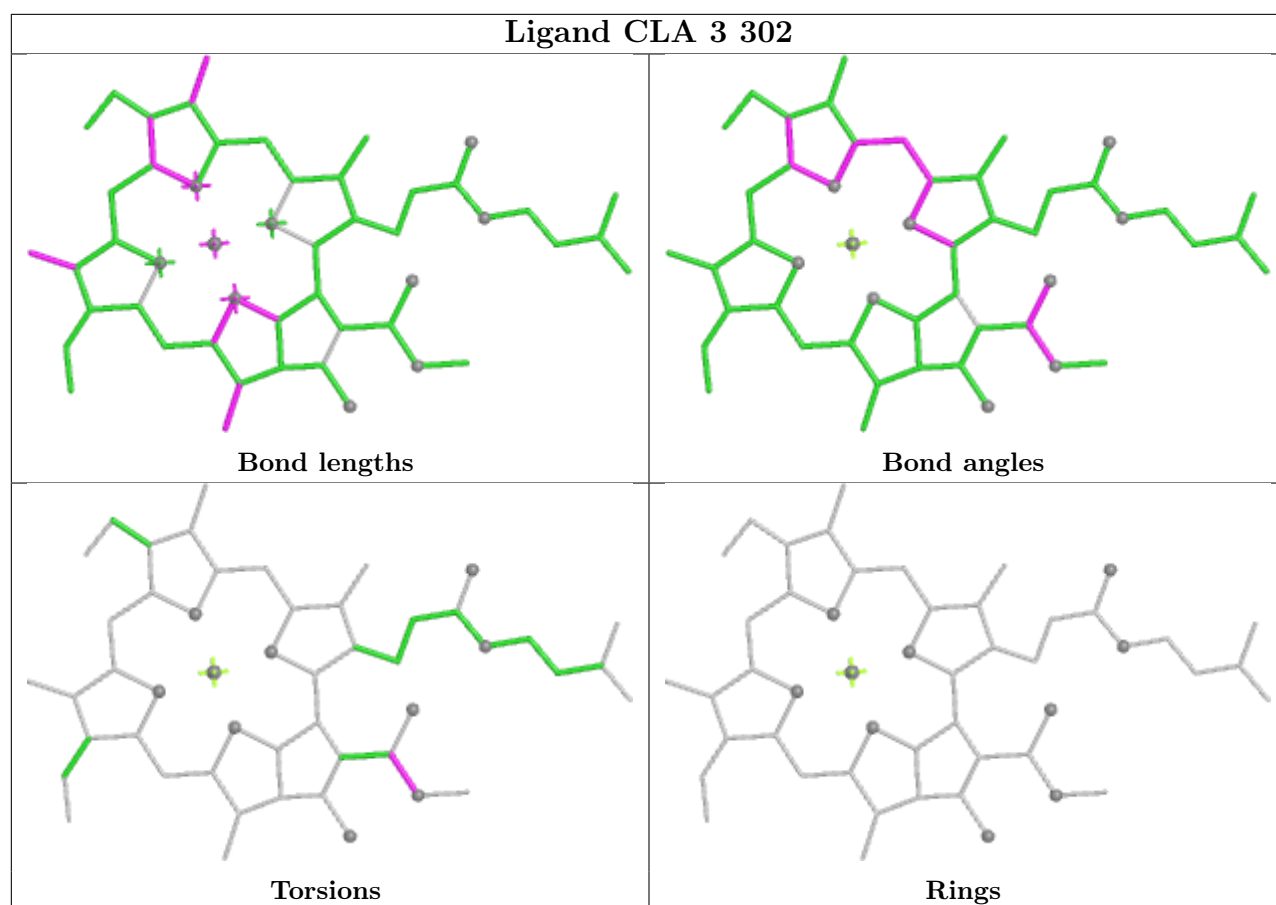
Rings

Ligand CLA 8 315

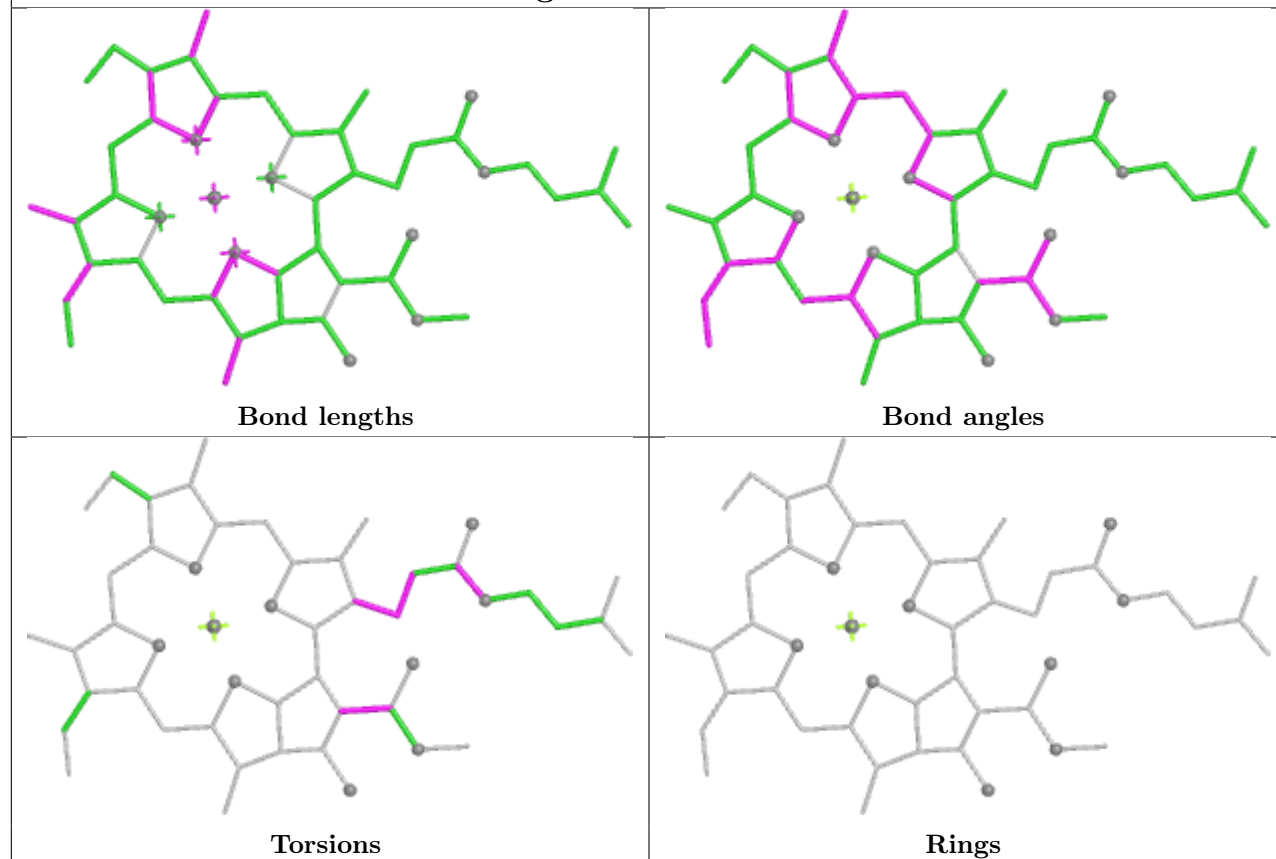


Ligand CLA K 104

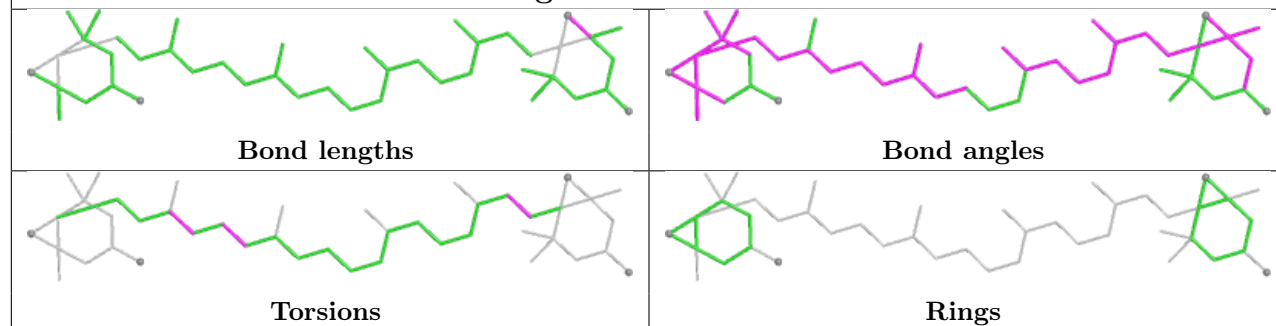




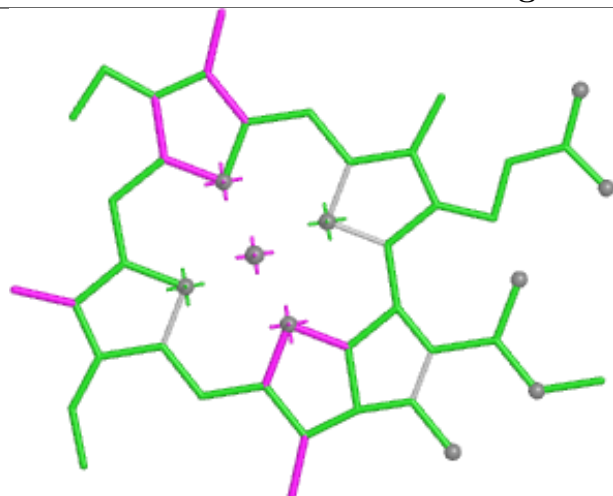
Ligand CLA 8 308



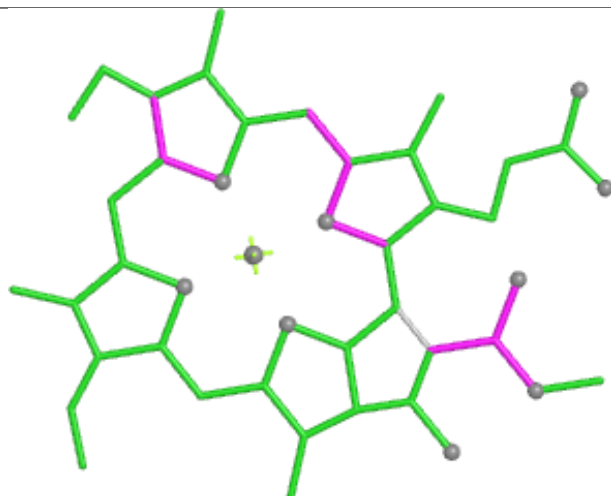
Ligand XAT 9 314



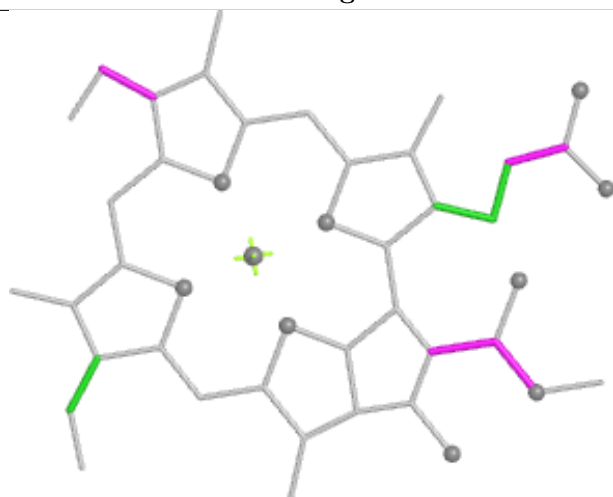
Ligand CLA 7 314



Bond lengths



Bond angles

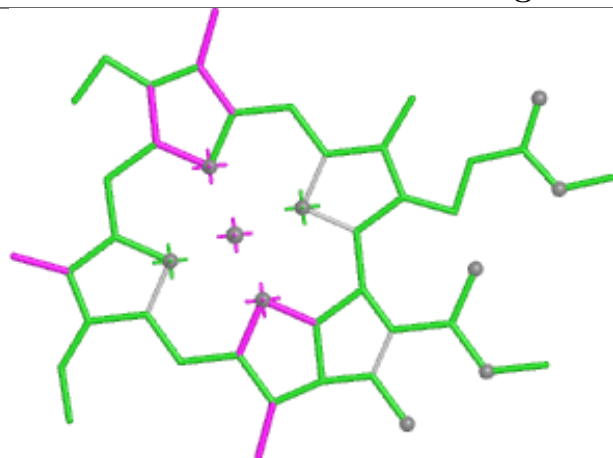


Torsions

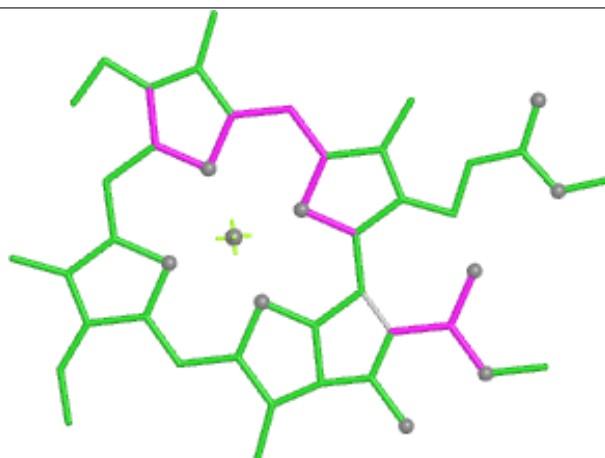


Rings

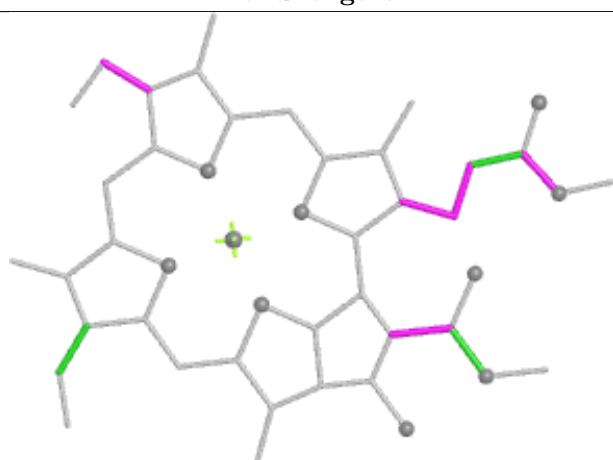
Ligand CLA B 822



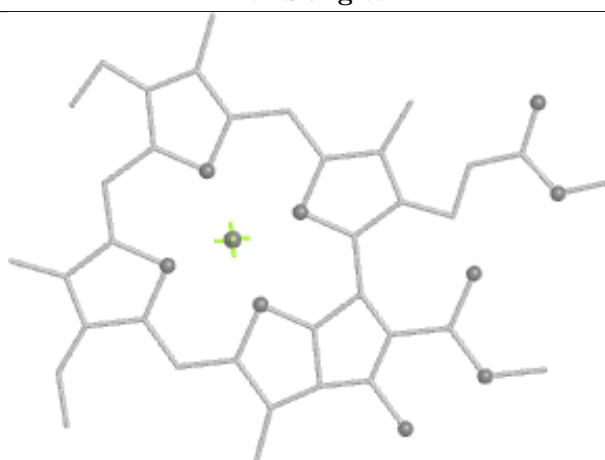
Bond lengths



Bond angles

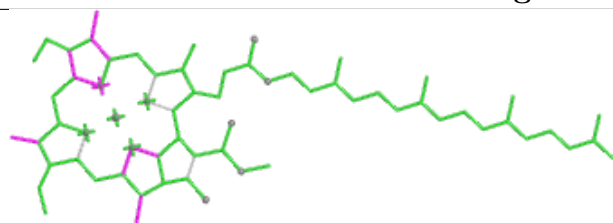


Torsions

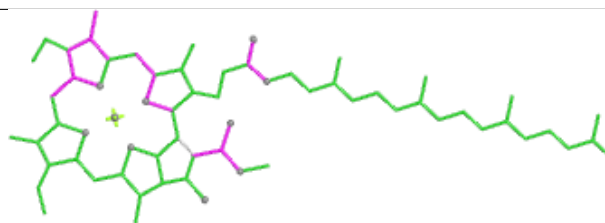


Rings

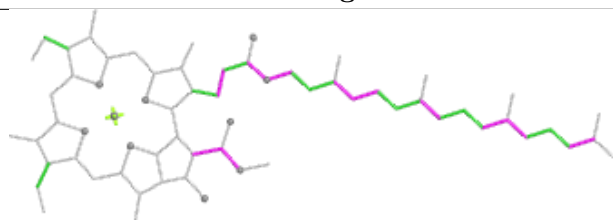
Ligand CLA A 817



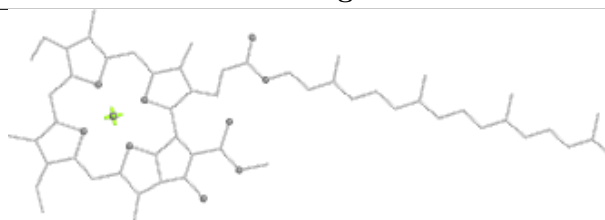
Bond lengths



Bond angles

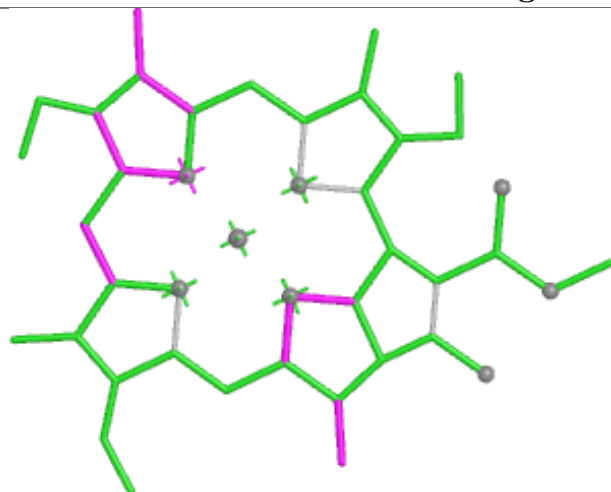


Torsions

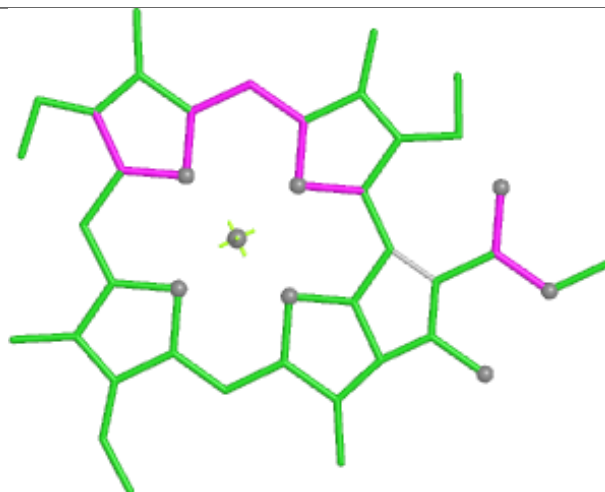


Rings

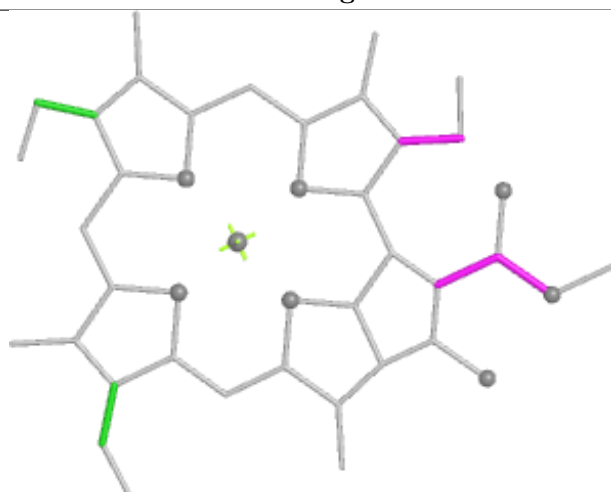
Ligand CLA J 103



Bond lengths



Bond angles

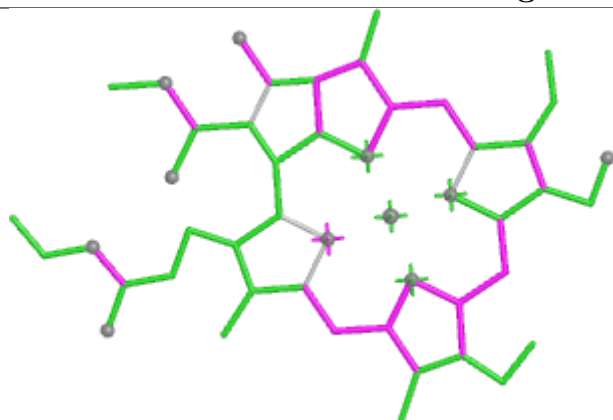


Torsions

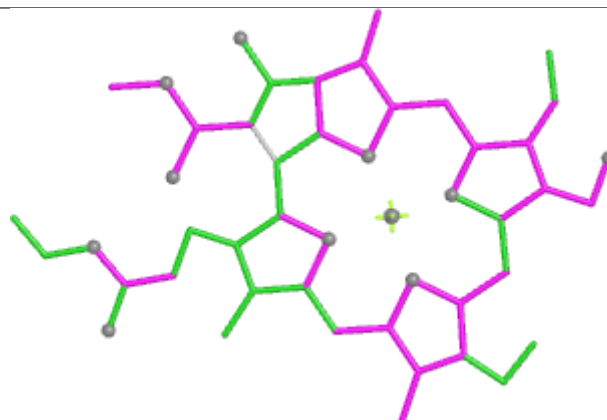


Rings

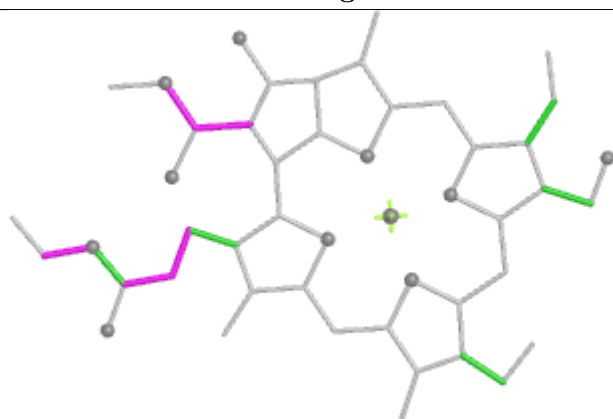
Ligand CHL 1 305



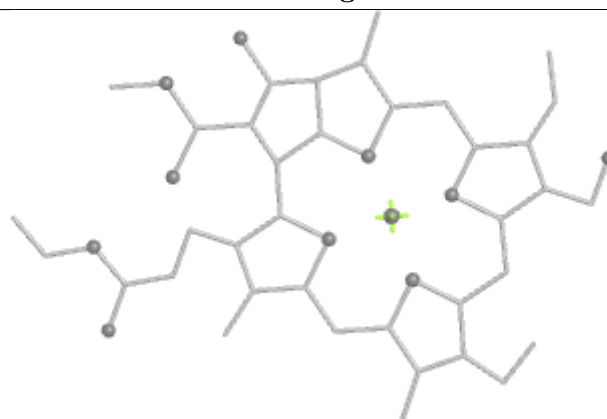
Bond lengths



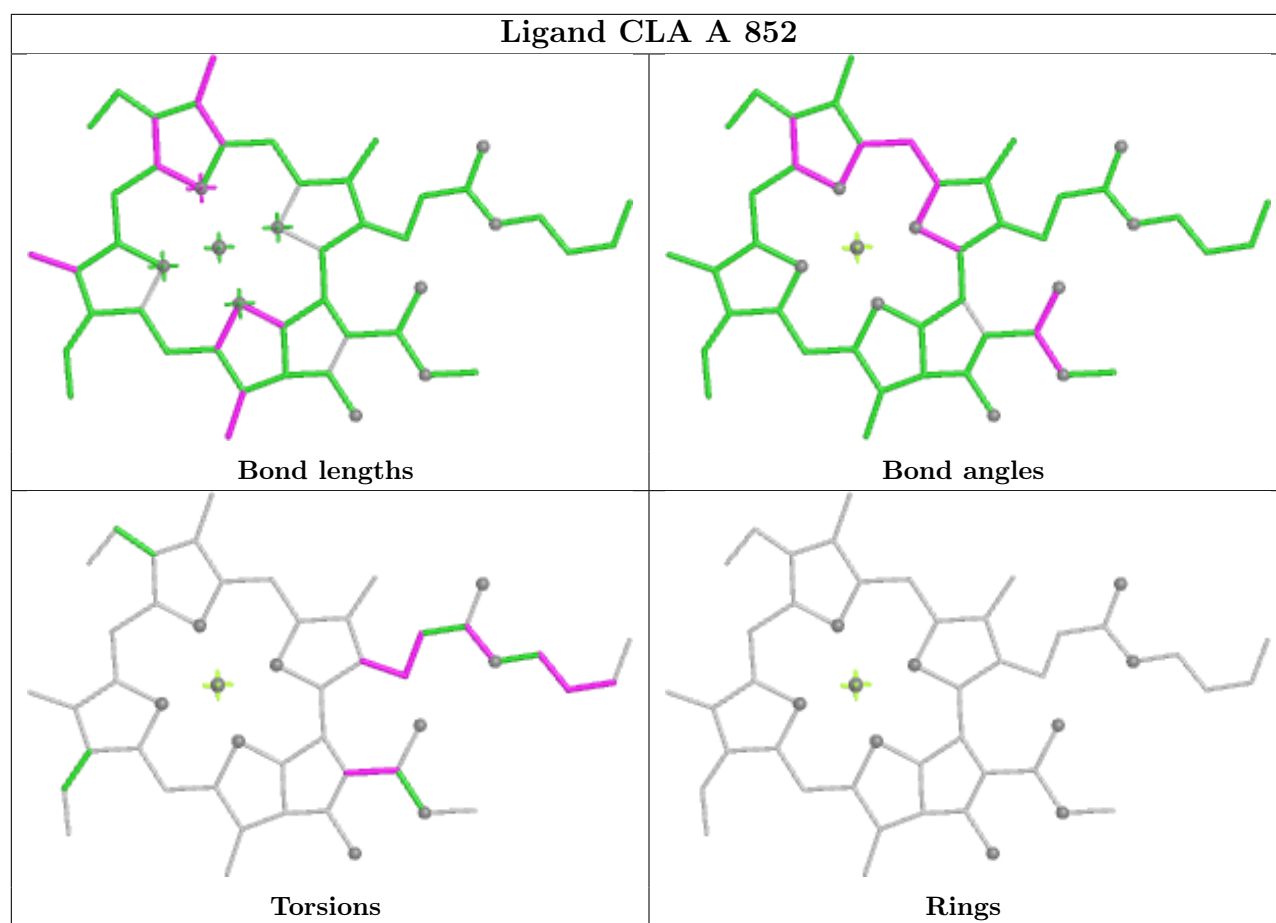
Bond angles



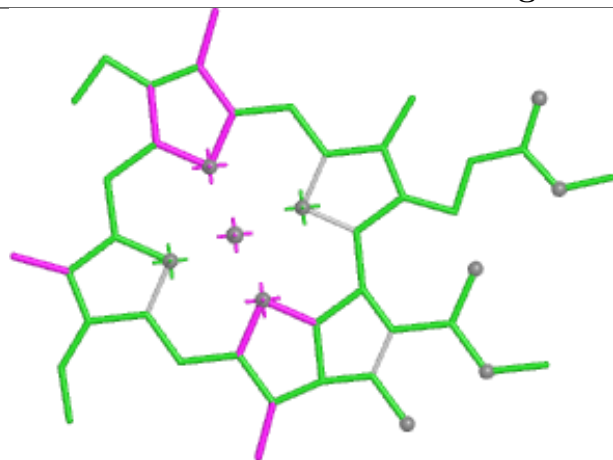
Torsions



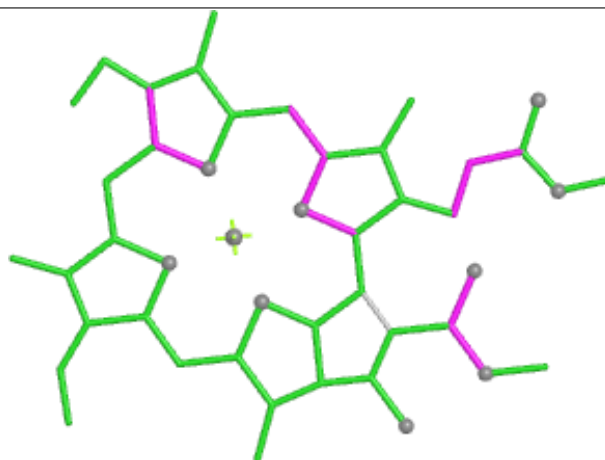
Rings



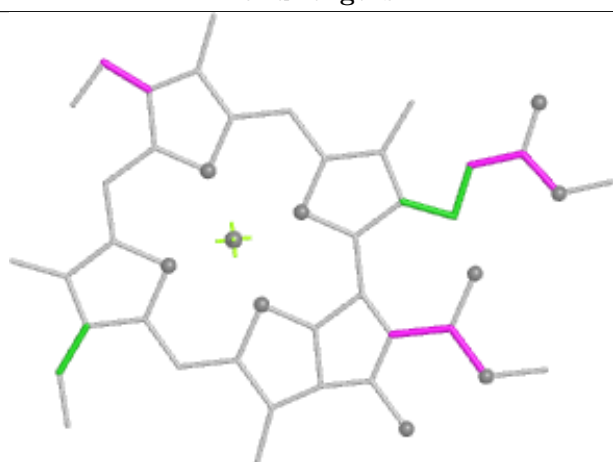
Ligand CLA 7 302



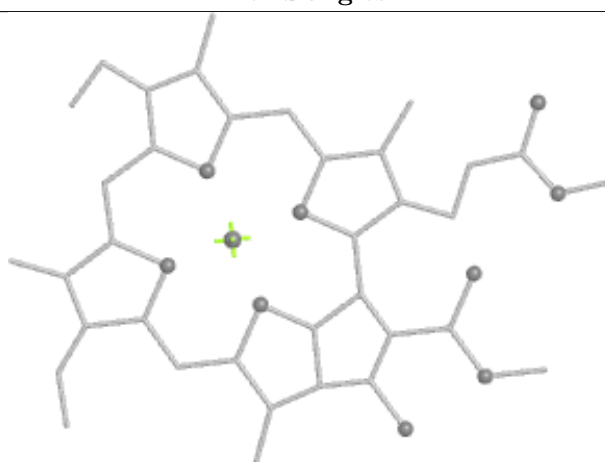
Bond lengths



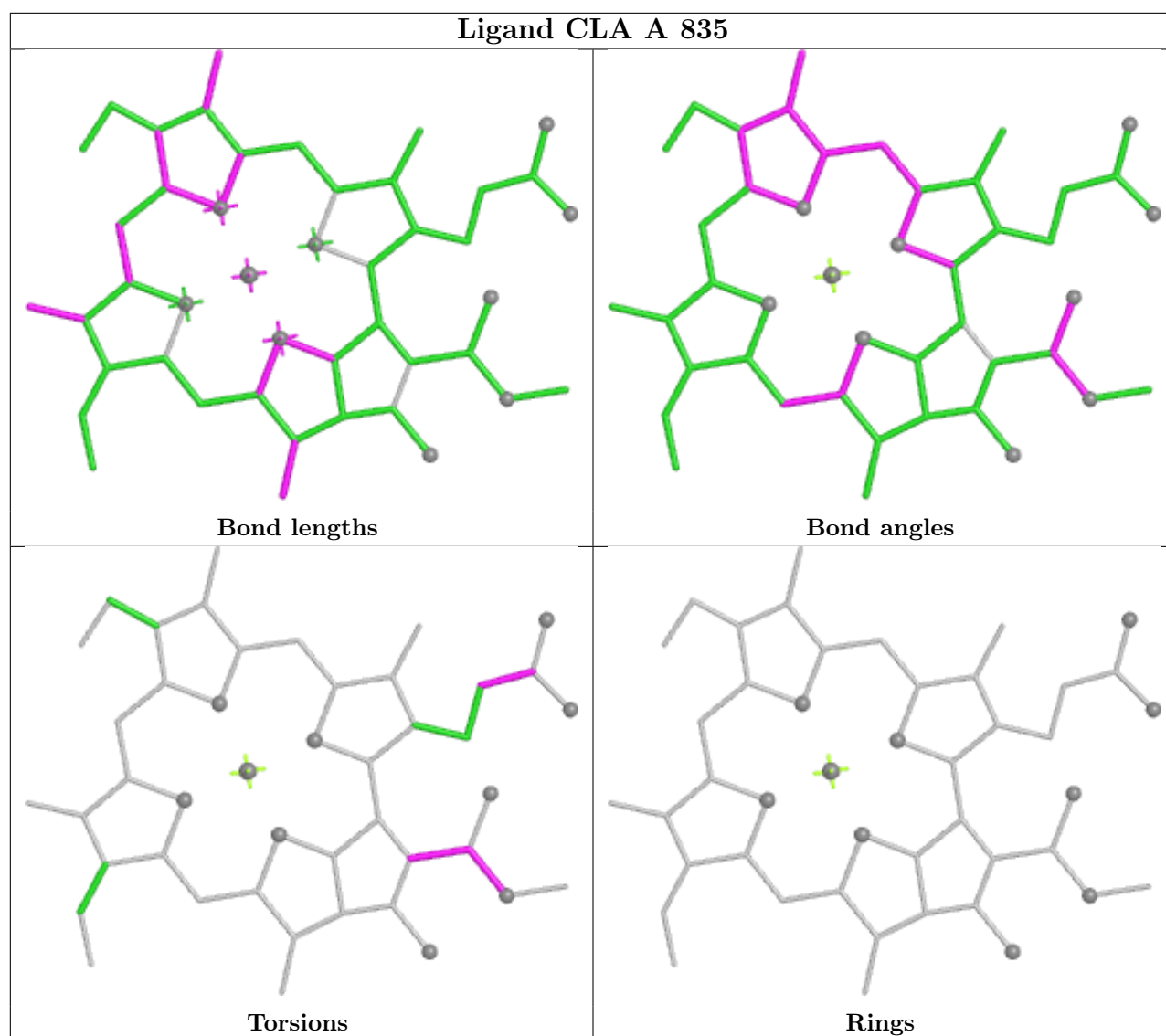
Bond angles



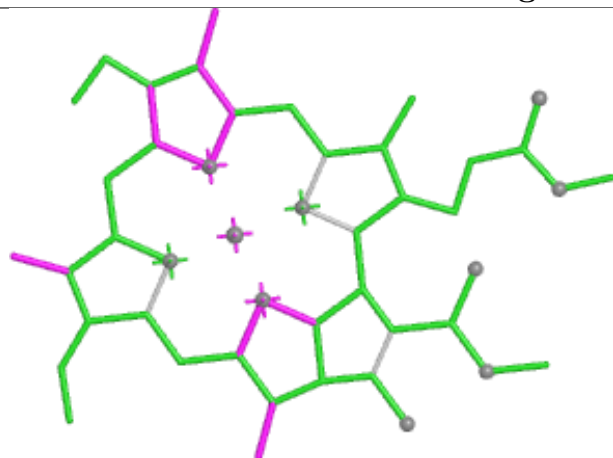
Torsions



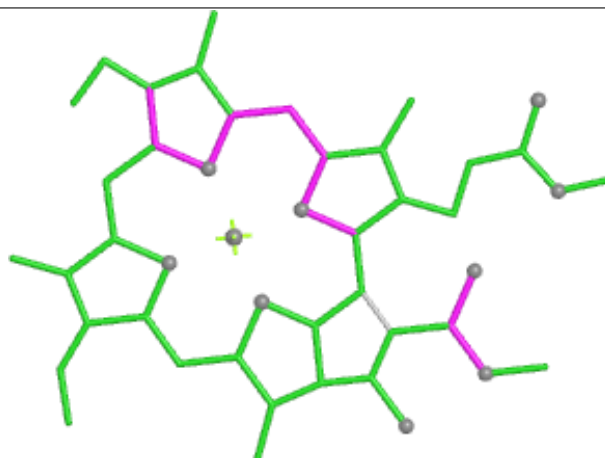
Rings



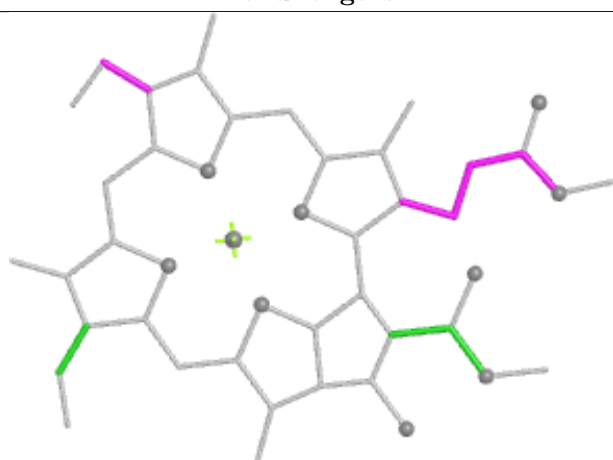
Ligand CLA 3 313



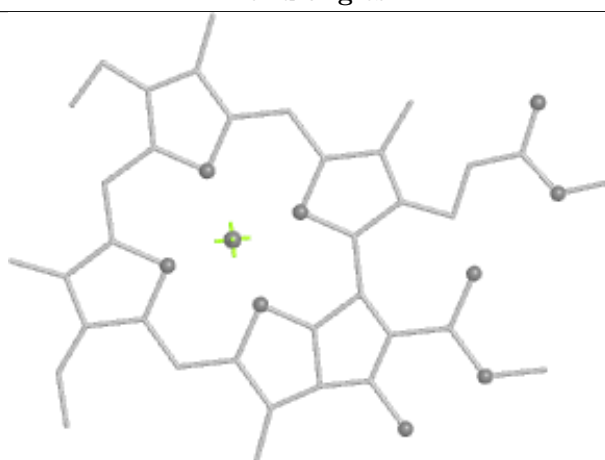
Bond lengths



Bond angles

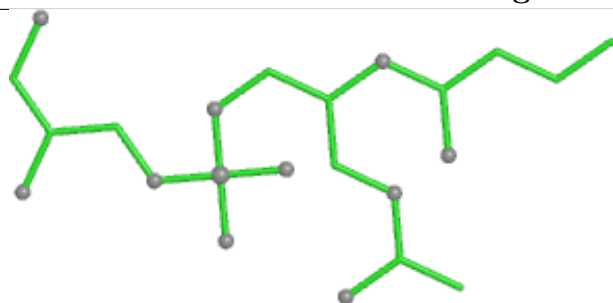


Torsions

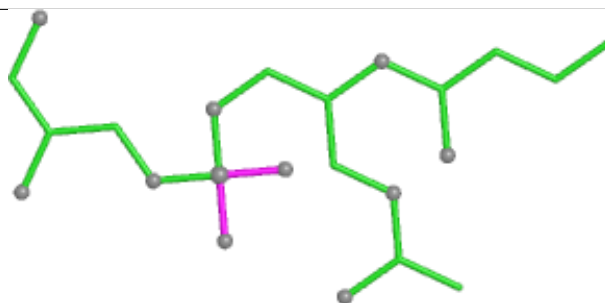


Rings

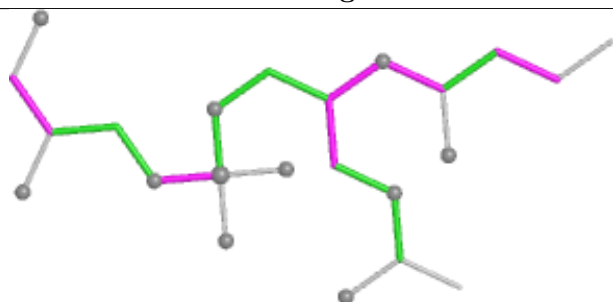
Ligand LHG B 852



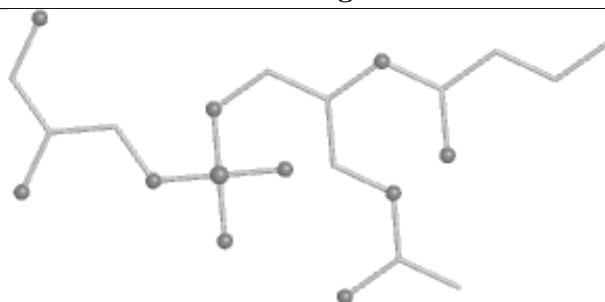
Bond lengths



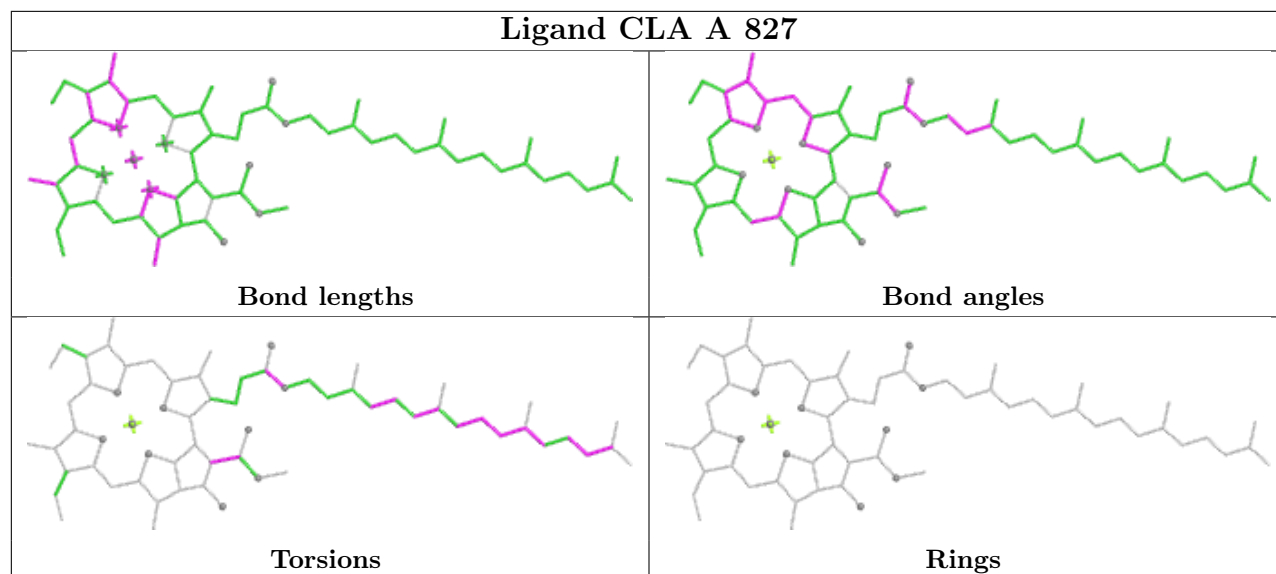
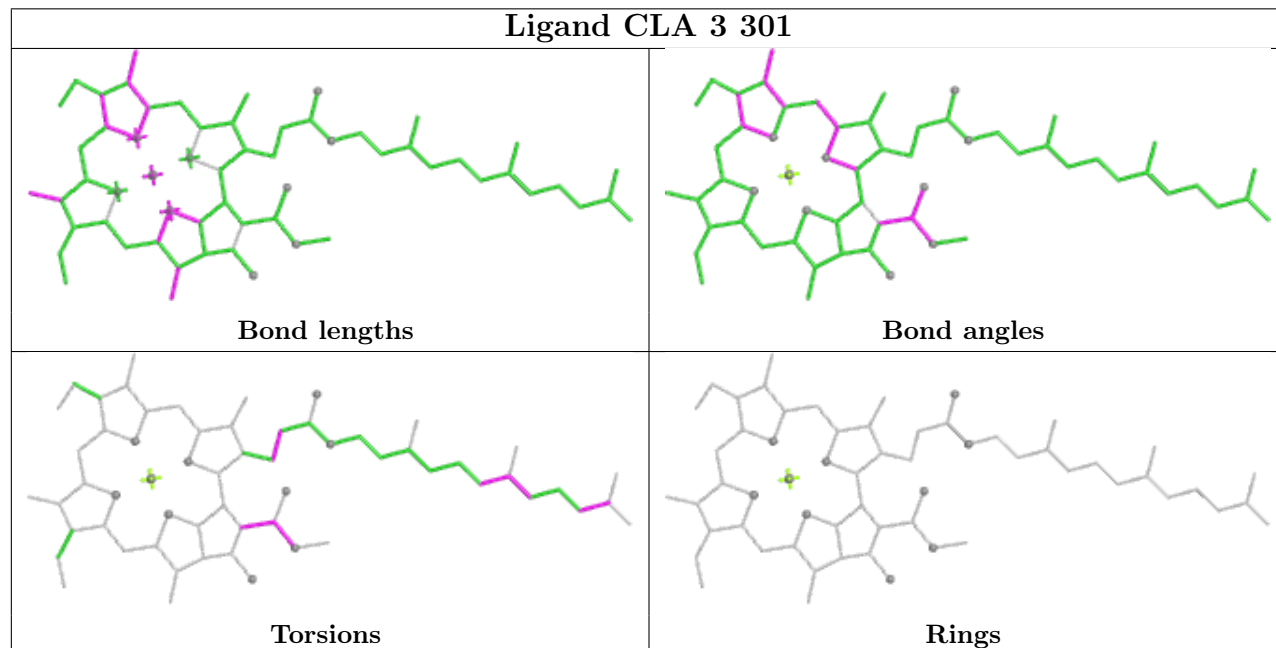
Bond angles

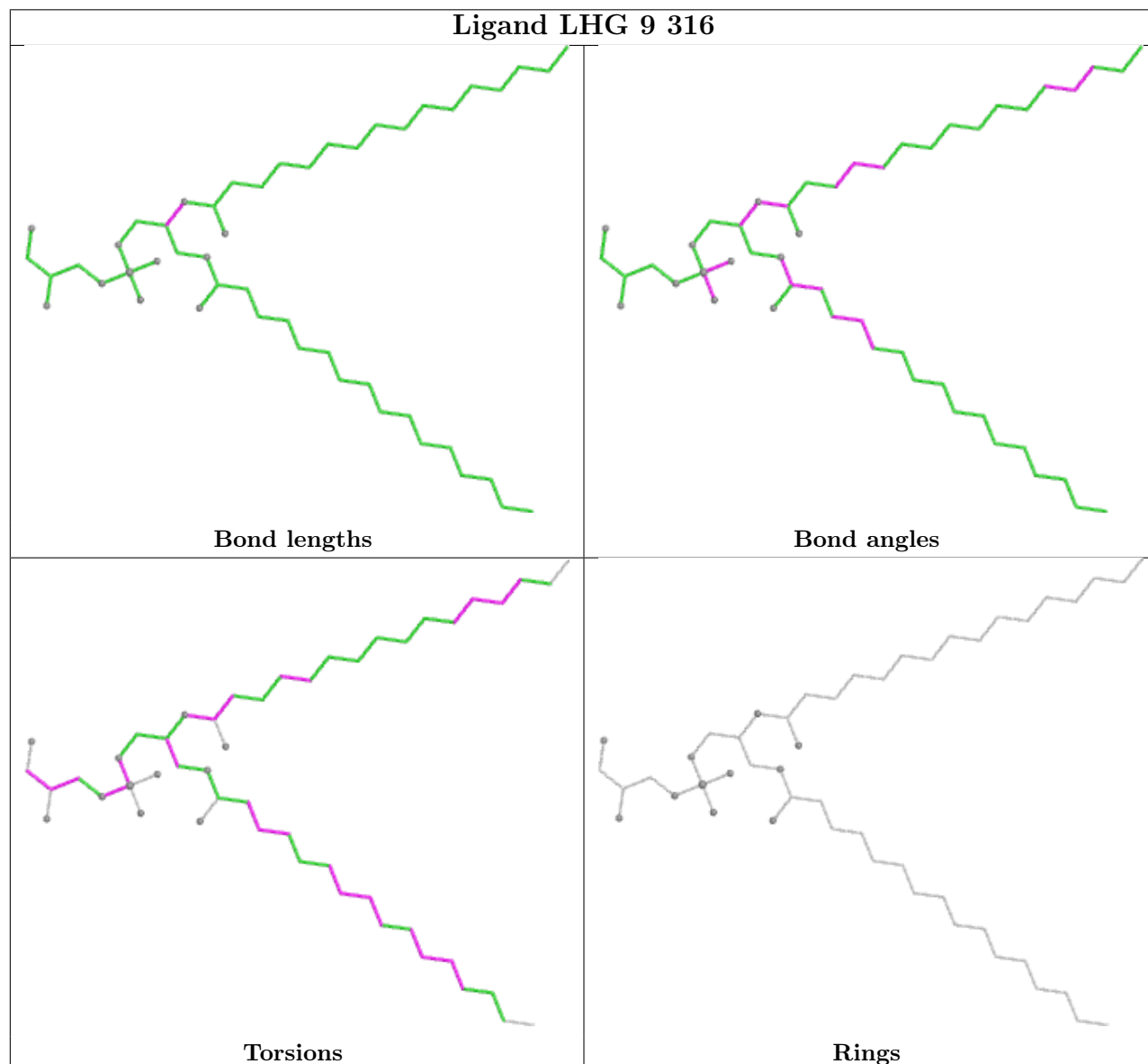
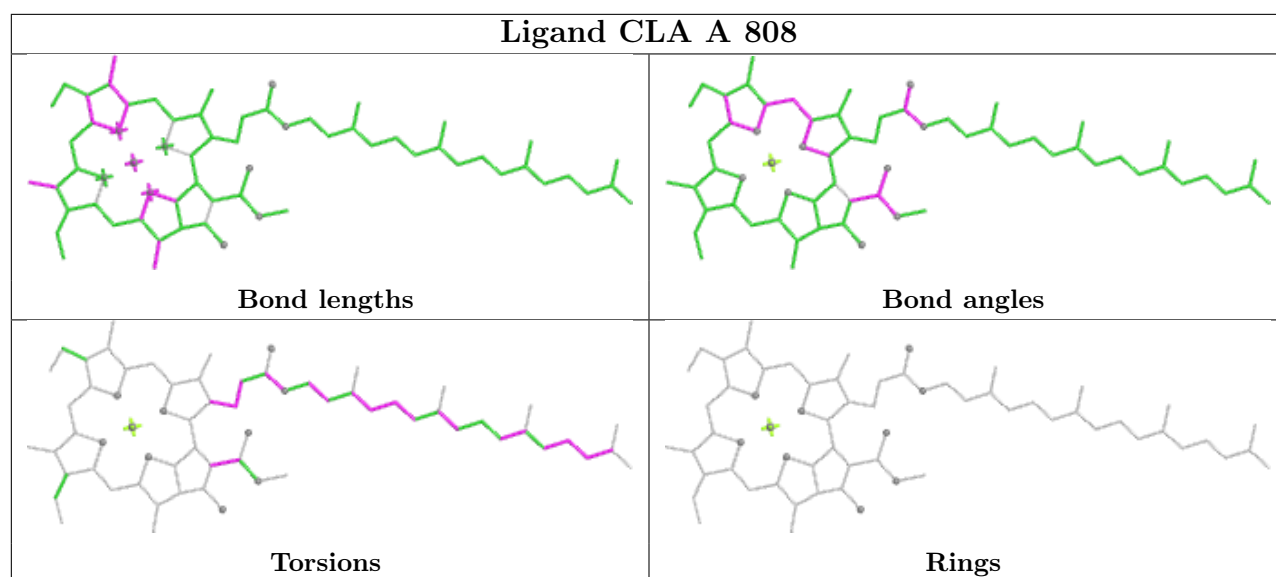


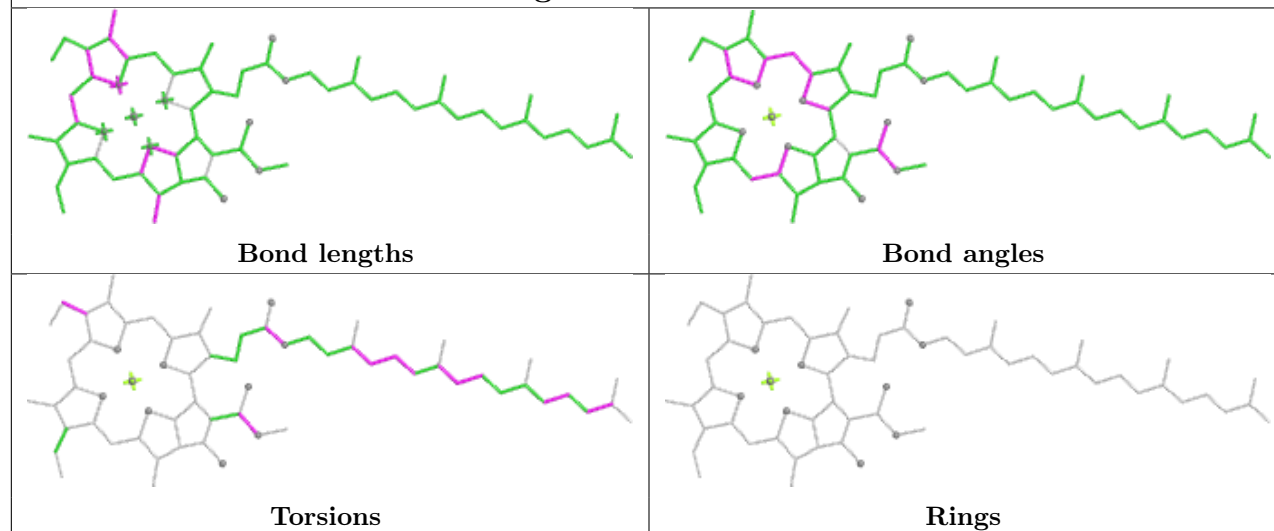
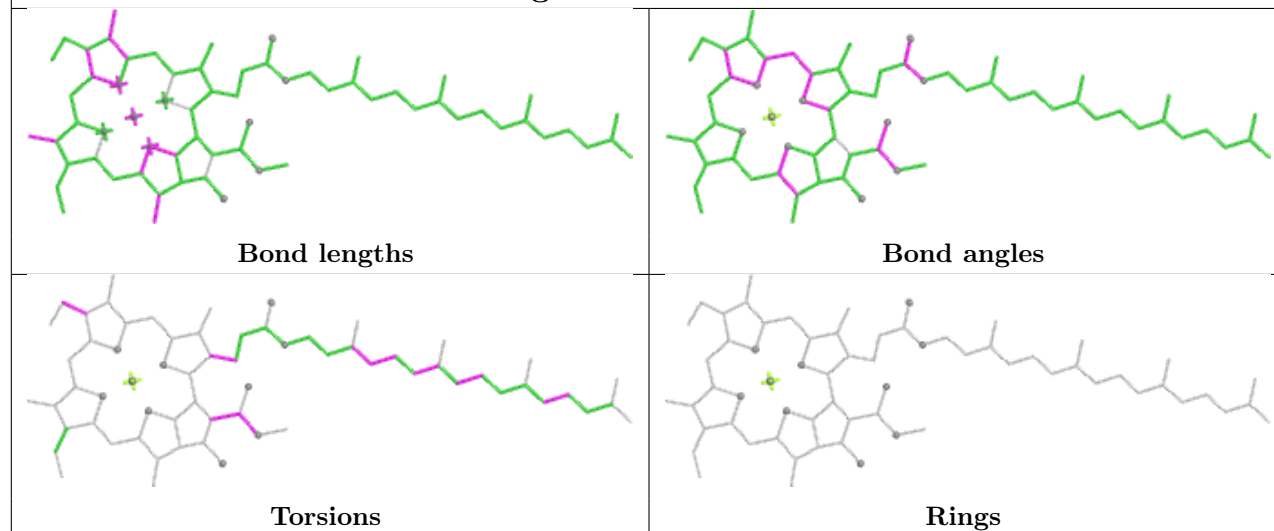
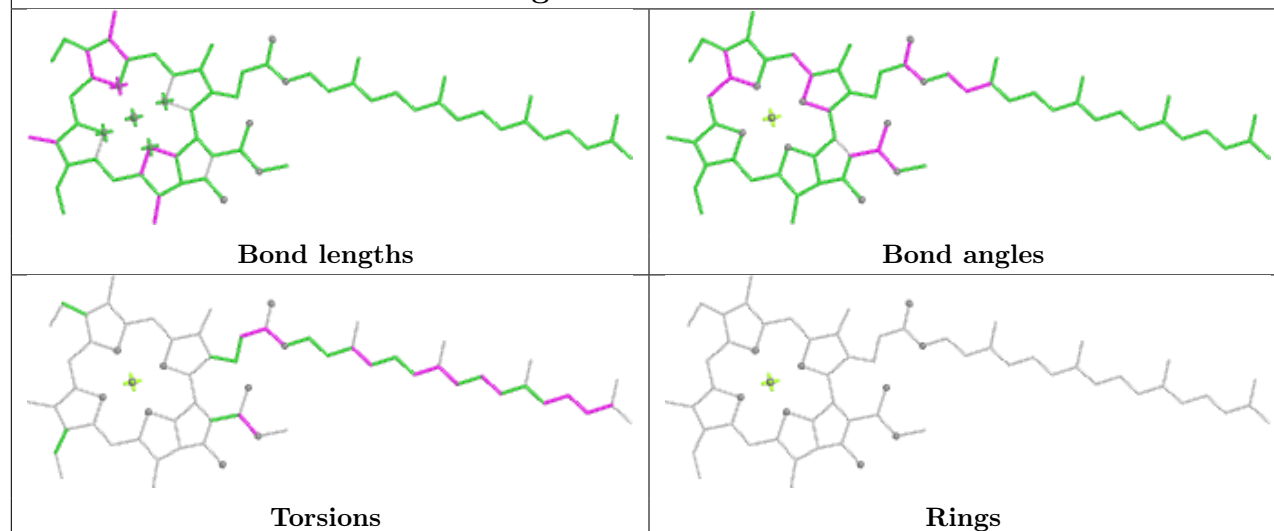
Torsions

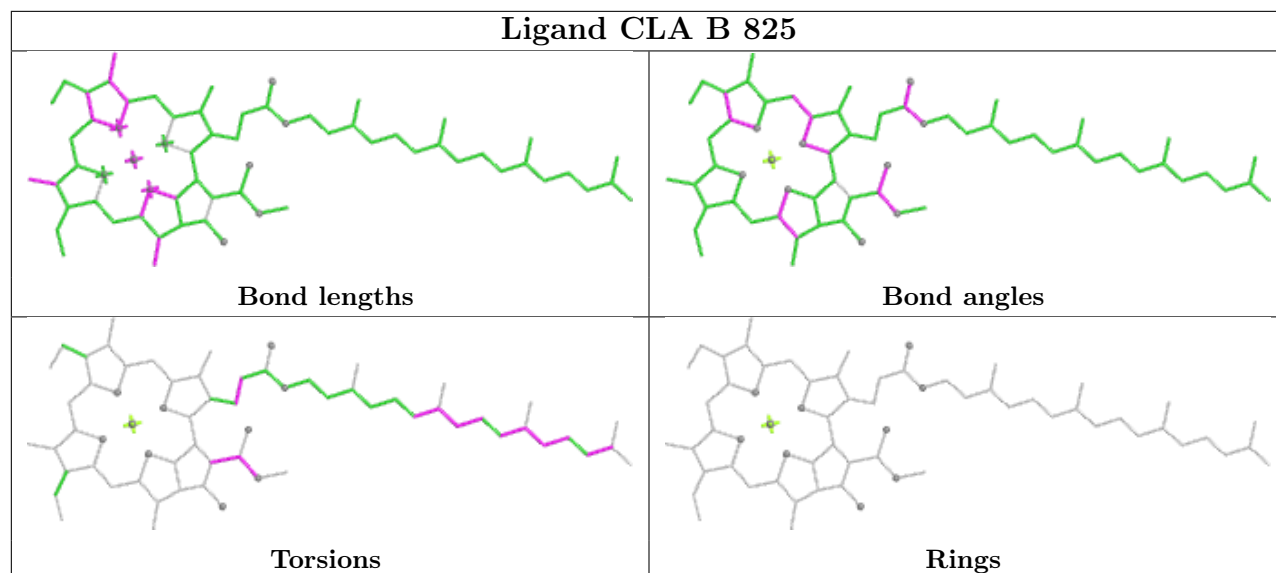
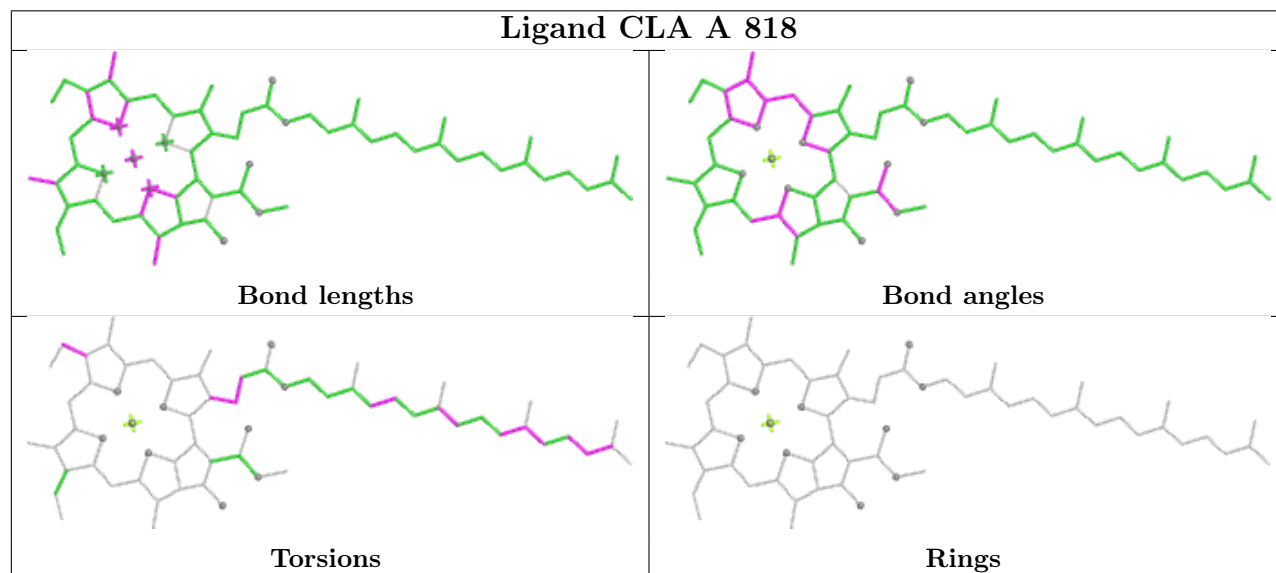
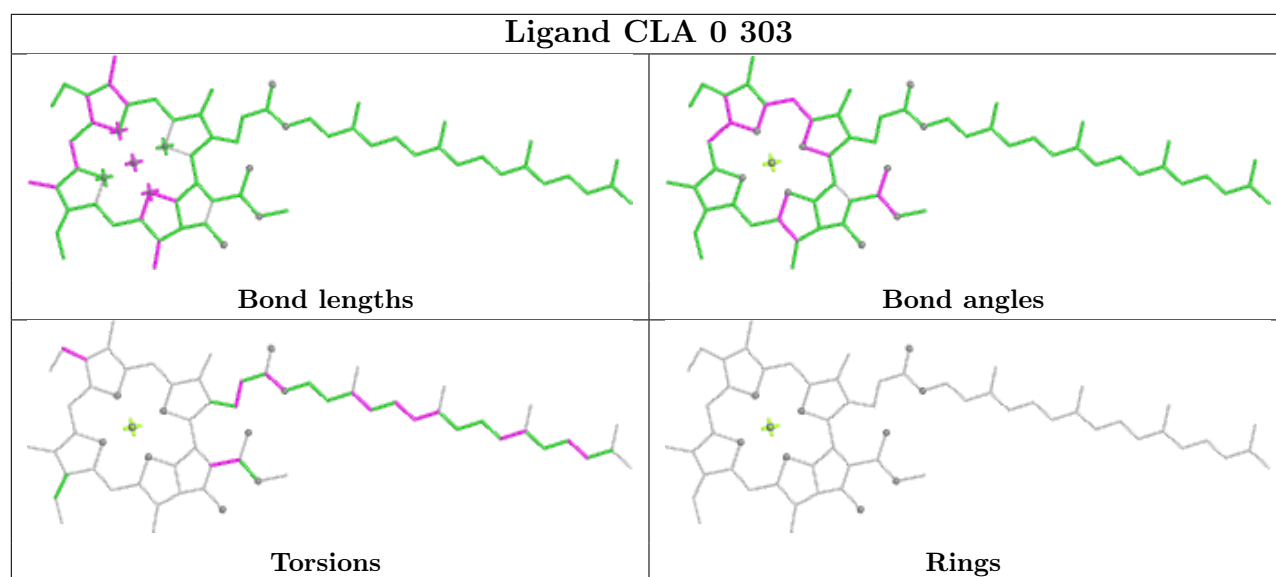


Rings

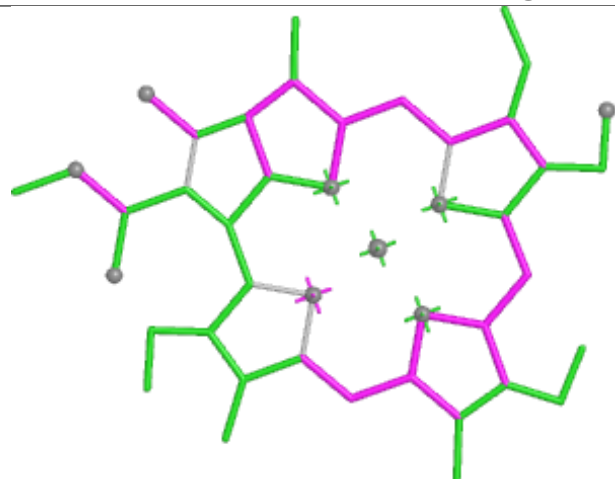
Ligand CLA A 827**Ligand CLA 3 301**



Ligand CLA L 203**Ligand CLA A 833****Ligand CLA A 825**



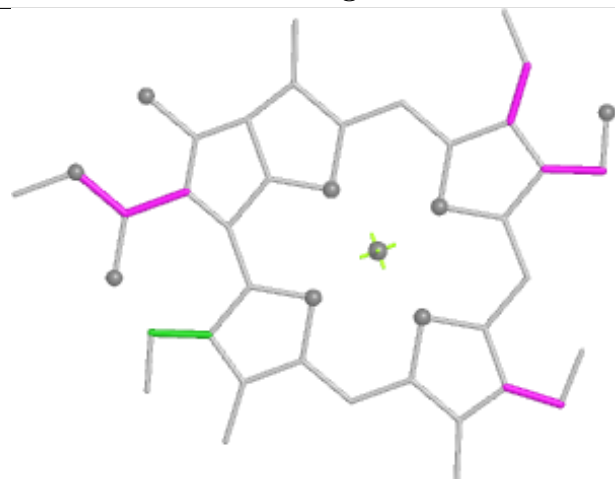
Ligand CHL 6 316



Bond lengths



Bond angles

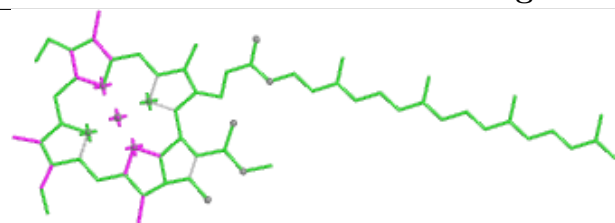


Torsions

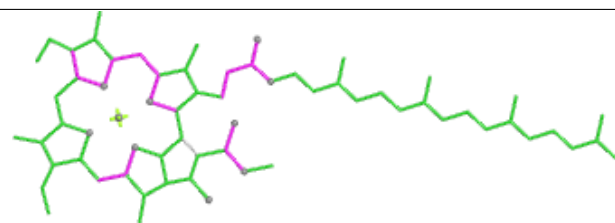


Rings

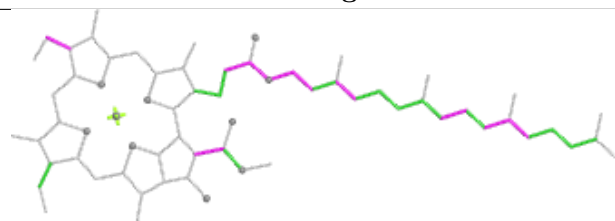
Ligand CLA A 805



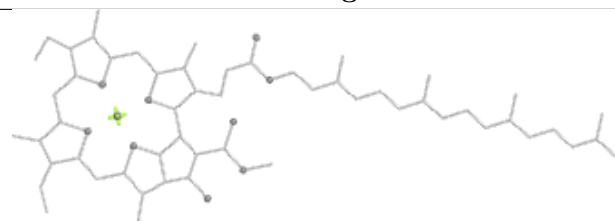
Bond lengths



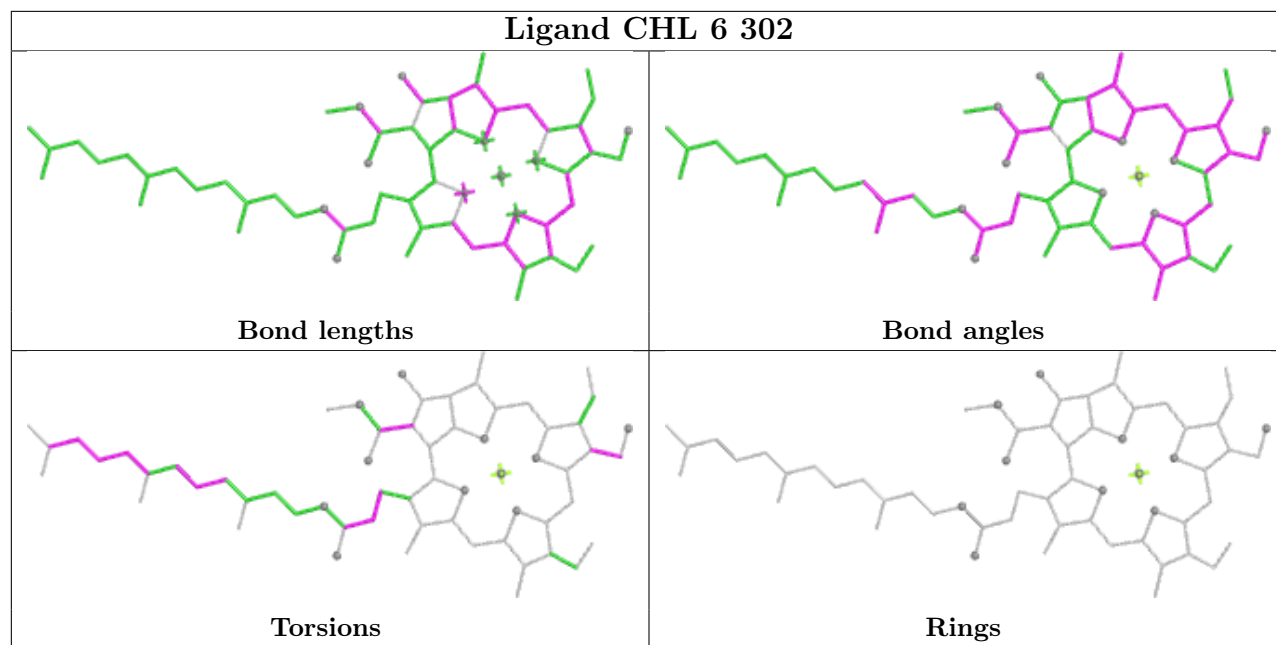
Bond angles



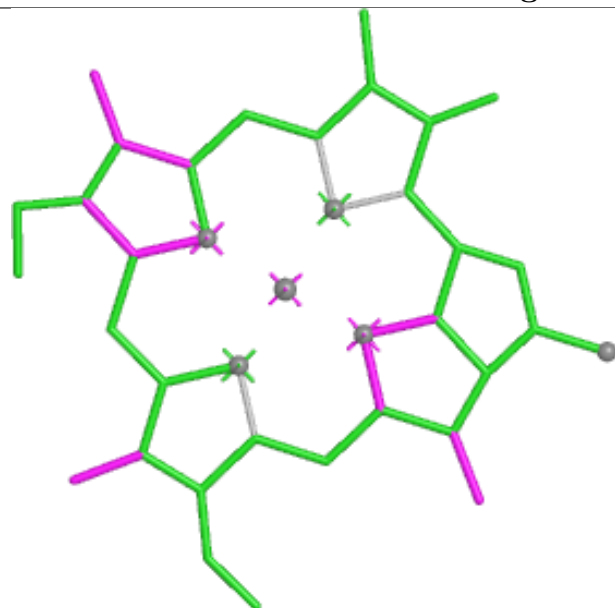
Torsions



Rings



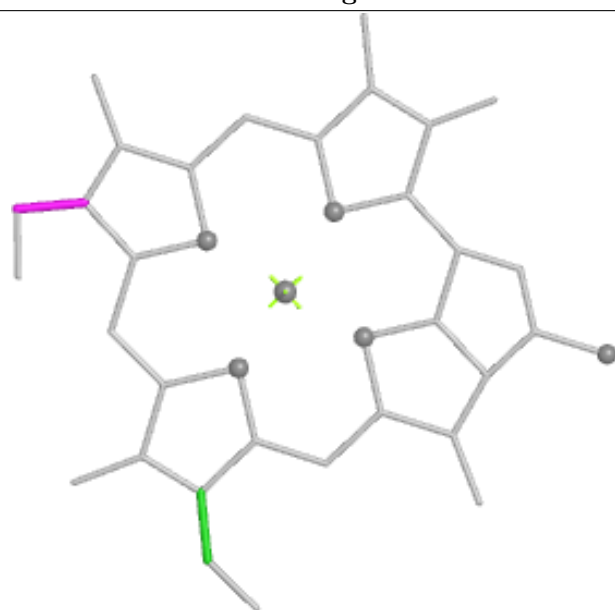
Ligand CLA 7 311



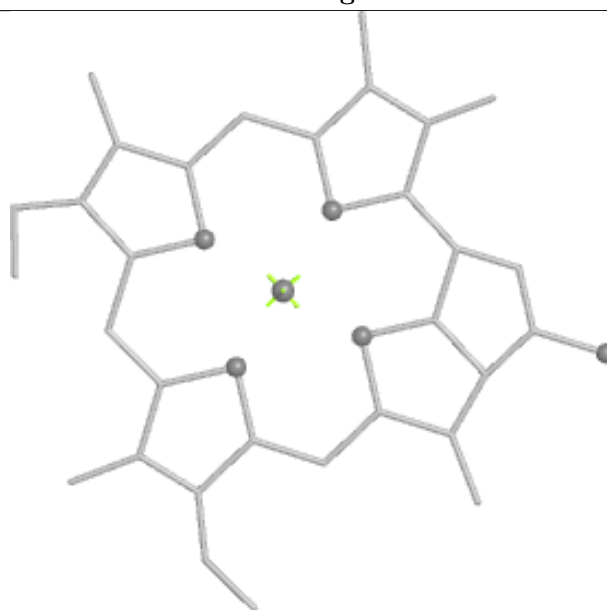
Bond lengths



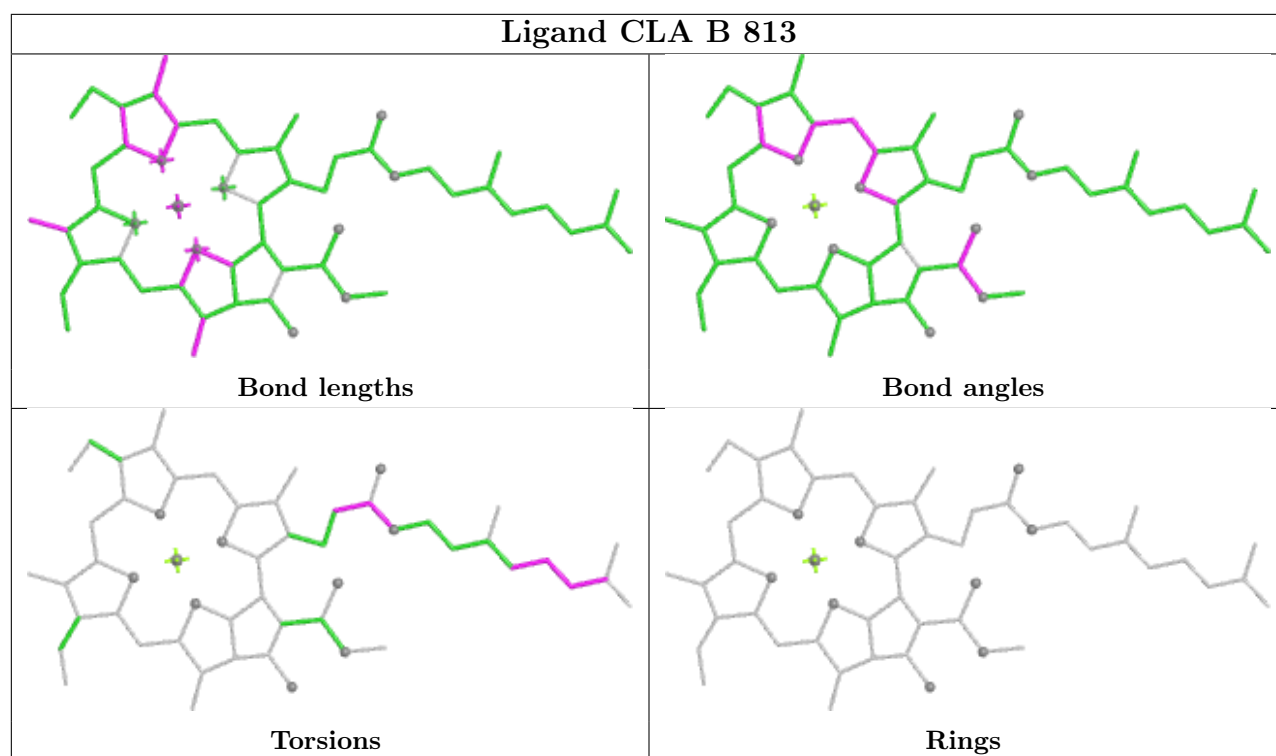
Bond angles

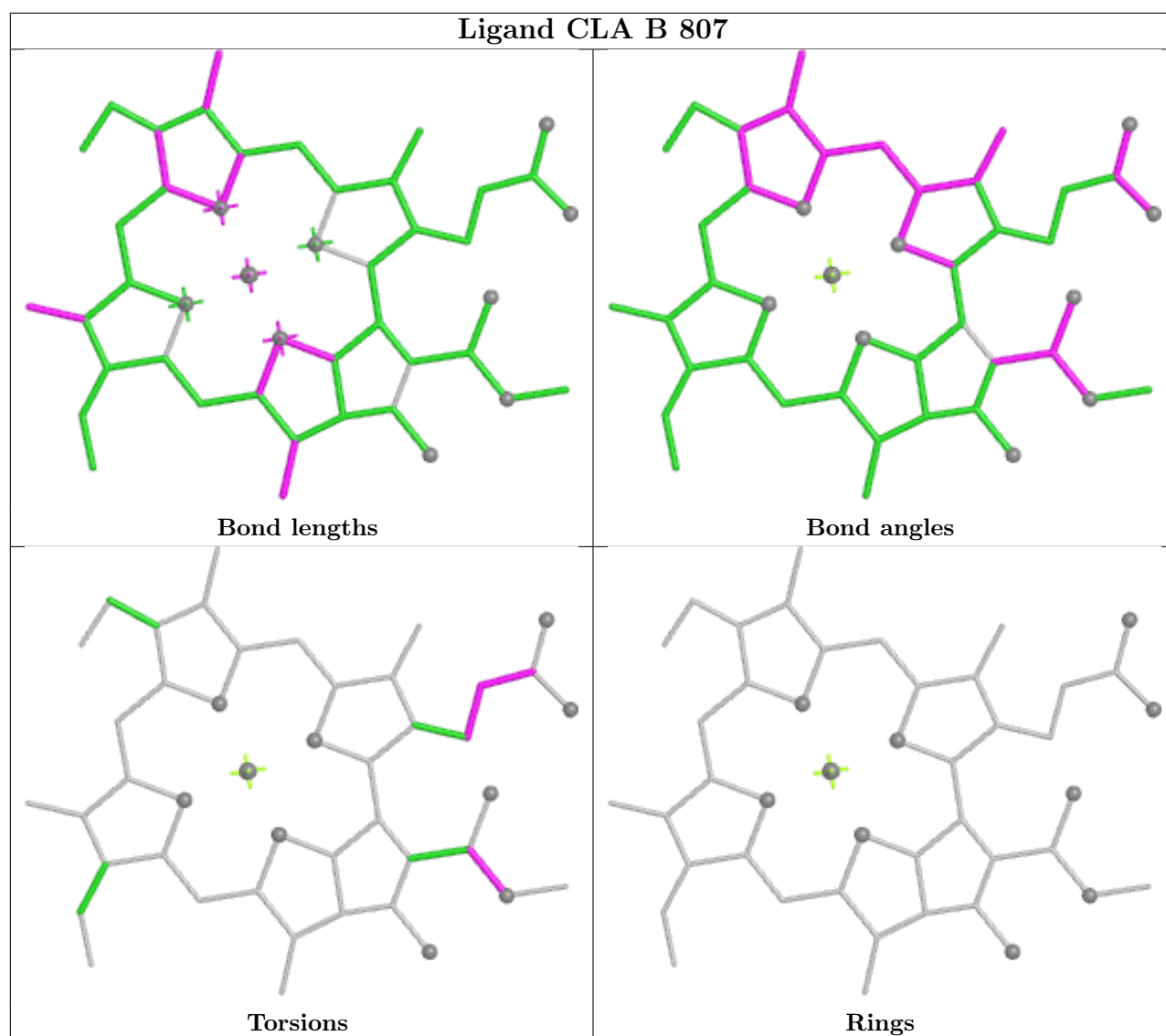


Torsions

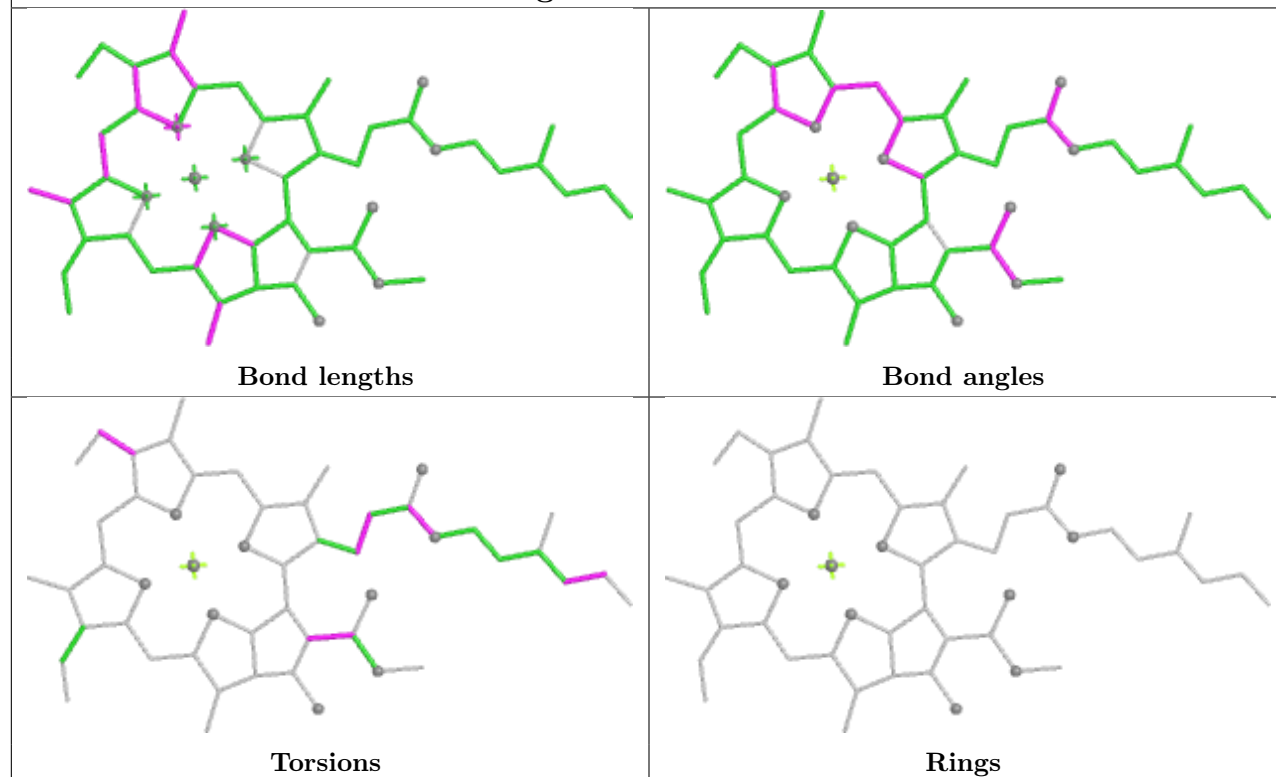


Rings

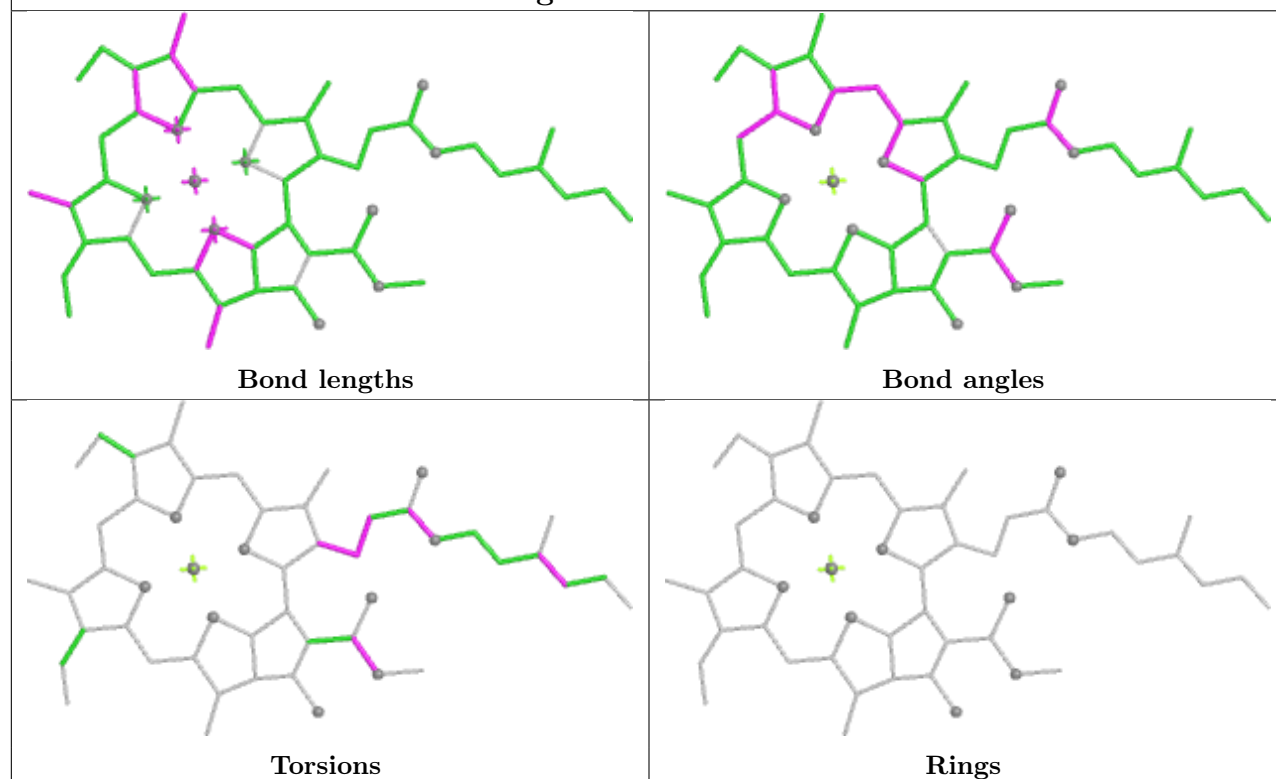




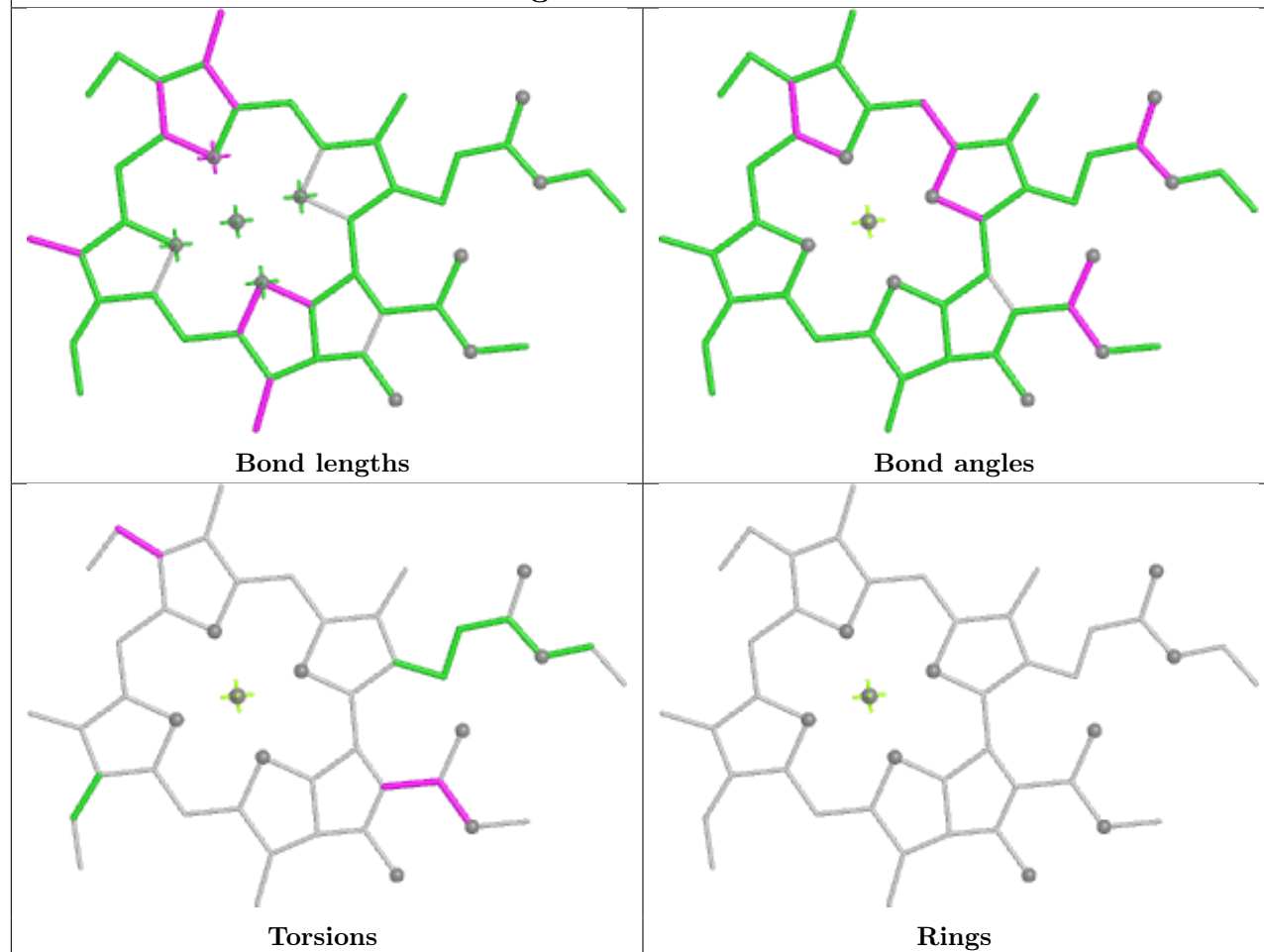
Ligand CLA 8 311



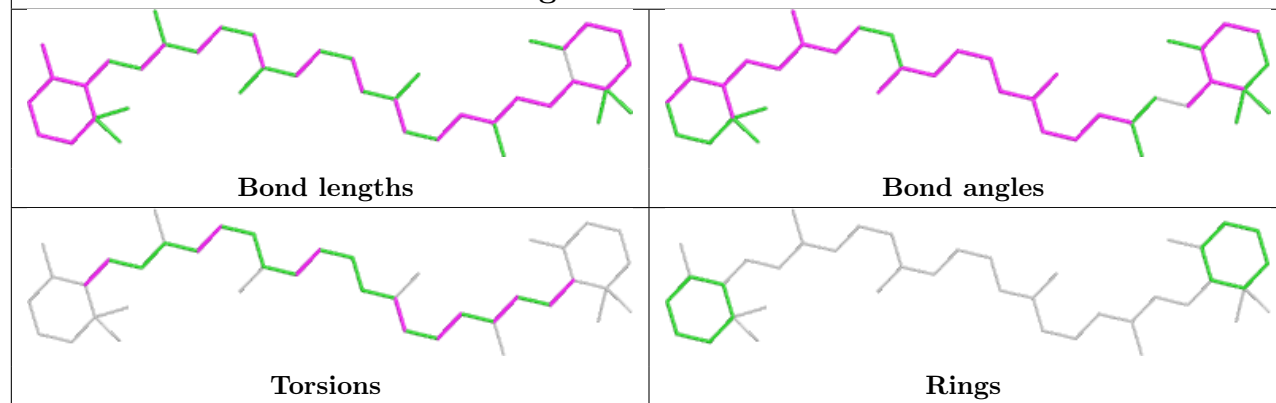
Ligand CLA 9 306

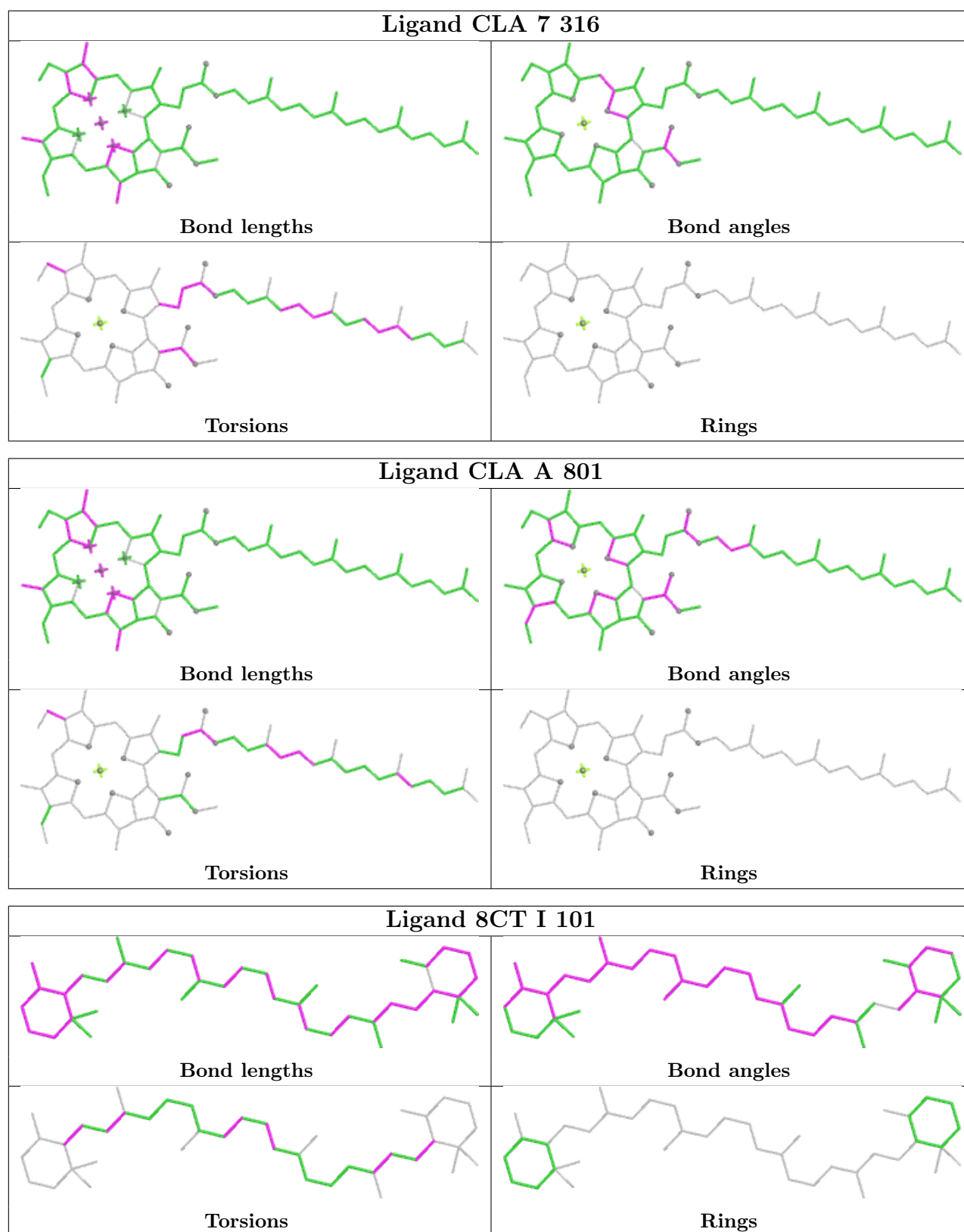


Ligand CLA 7 307

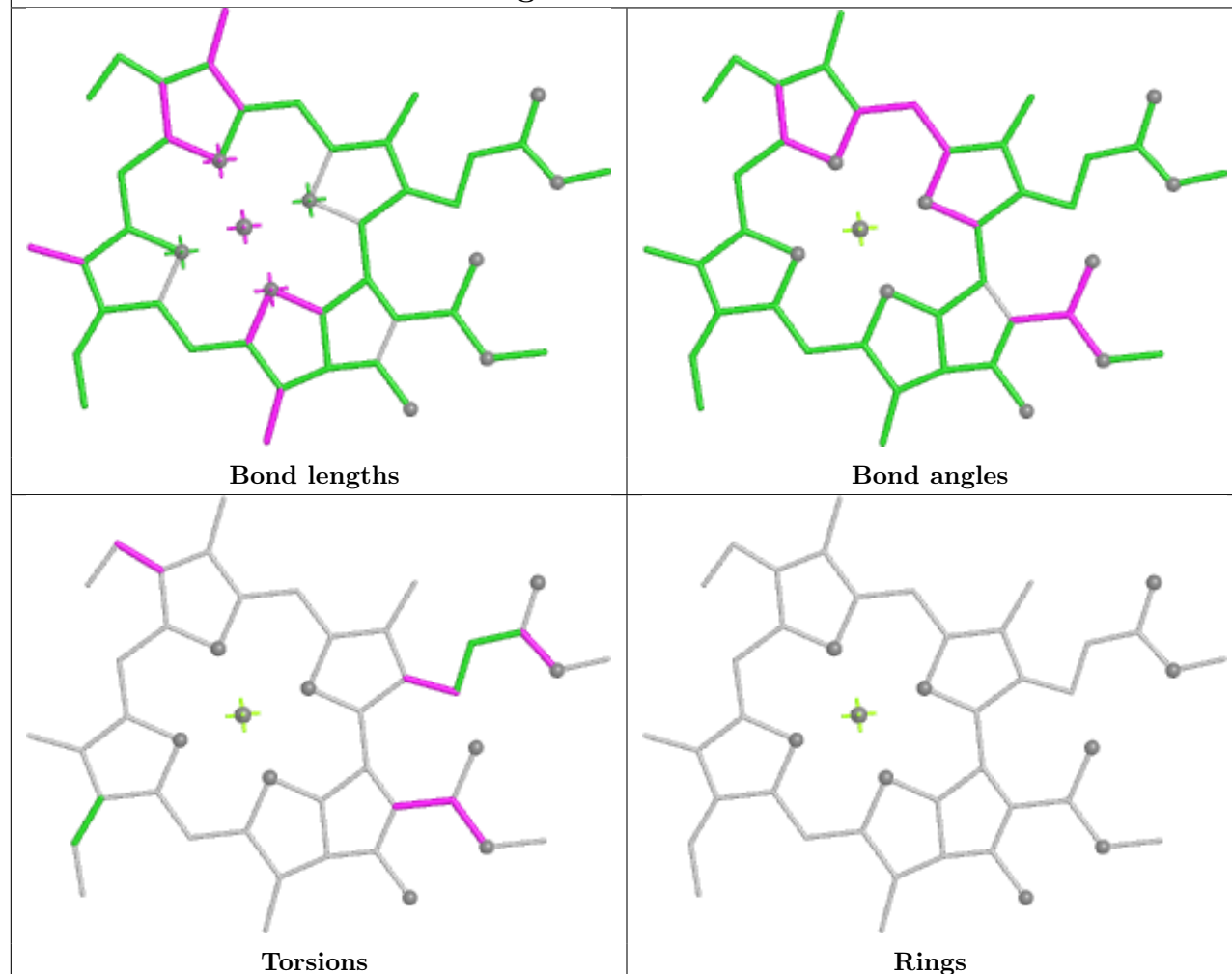


Ligand 8CT 1 316

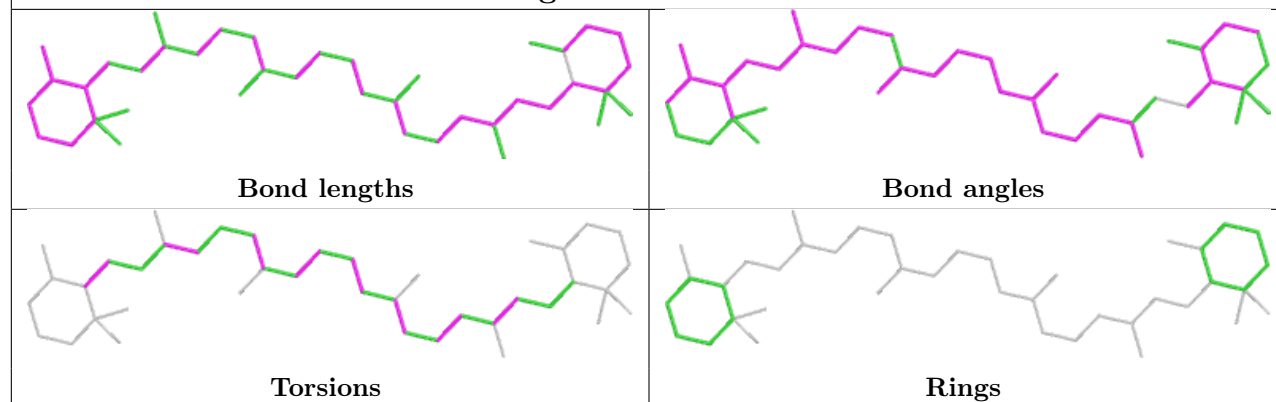




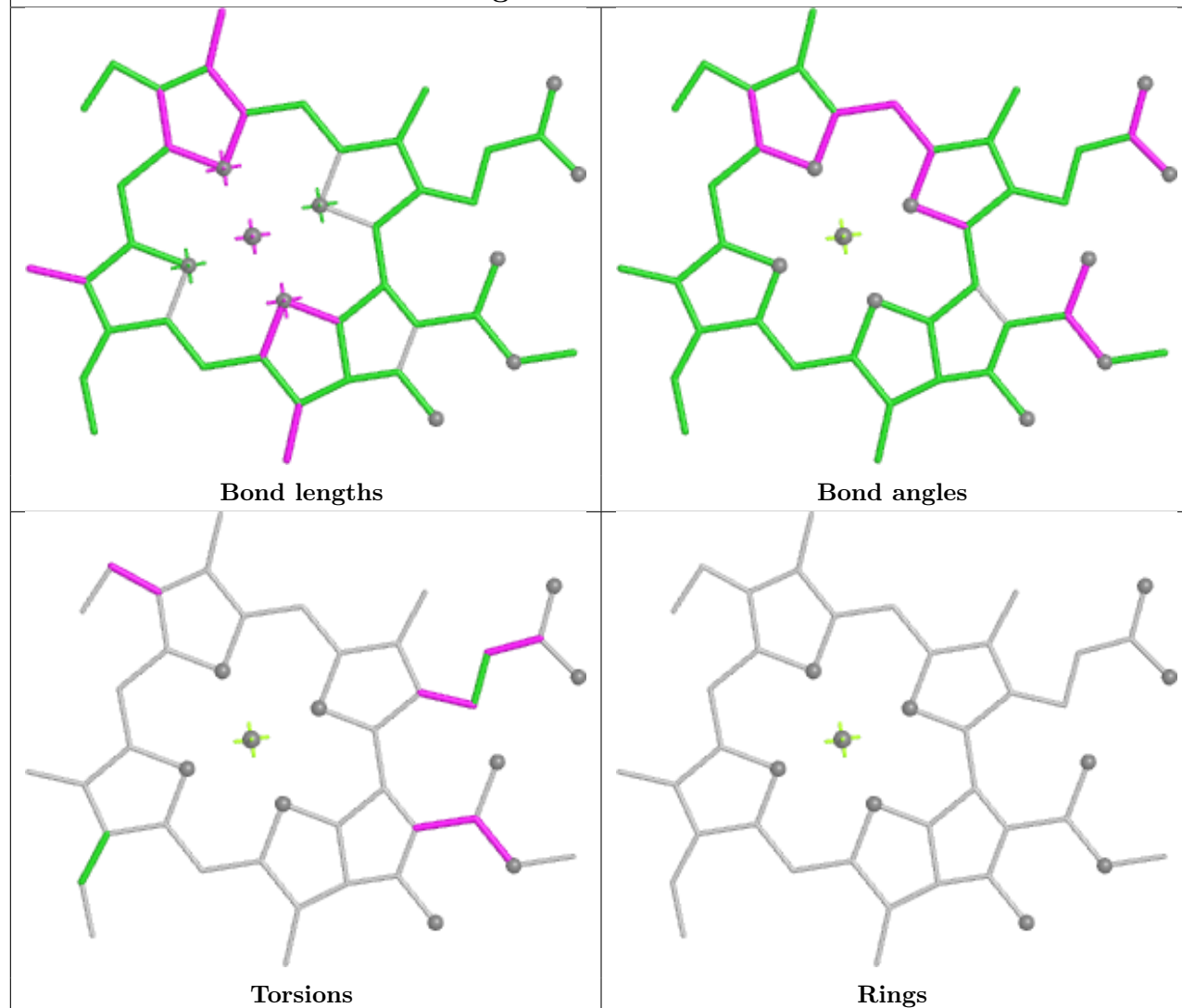
Ligand CLA 1 313



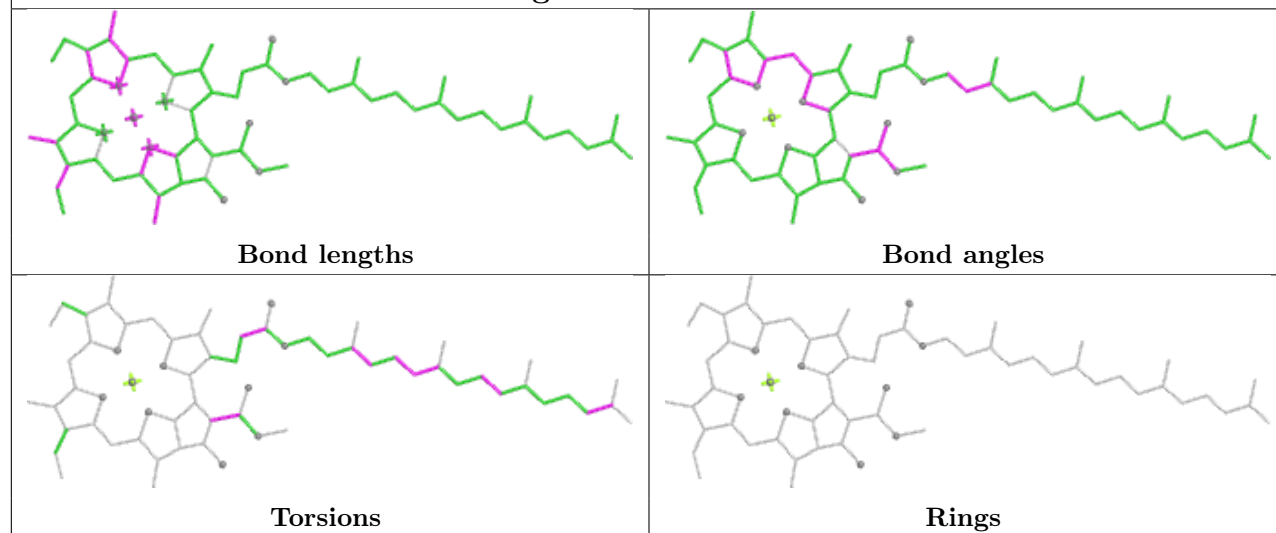
Ligand 8CT 3 316



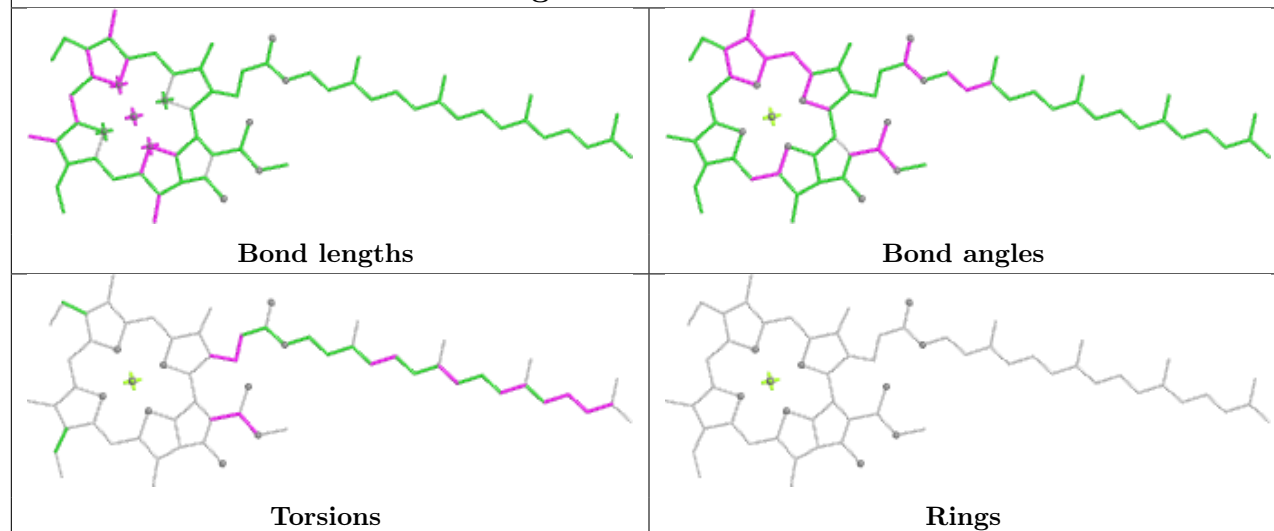
Ligand CLA A 814



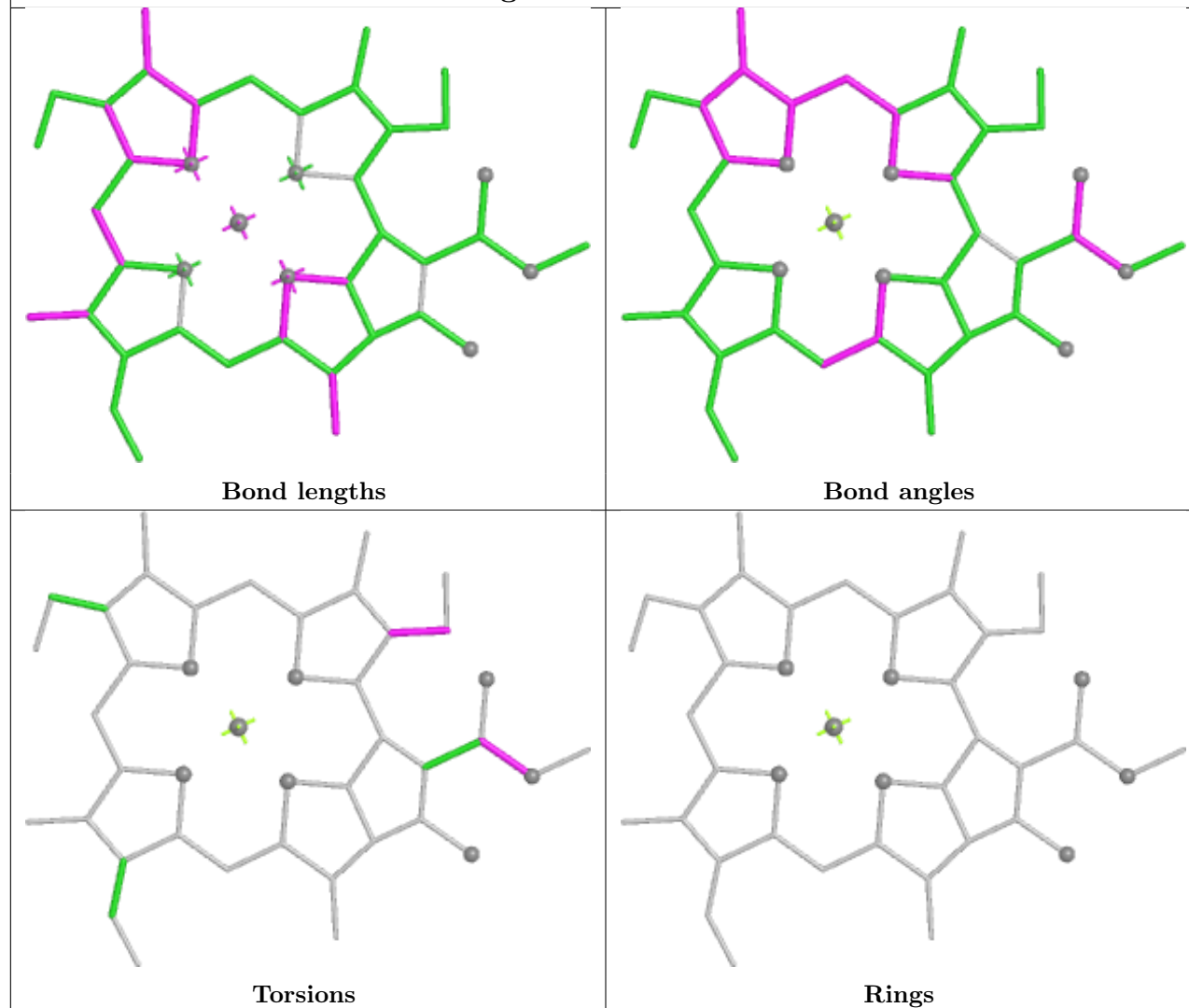
Ligand CLA B 801



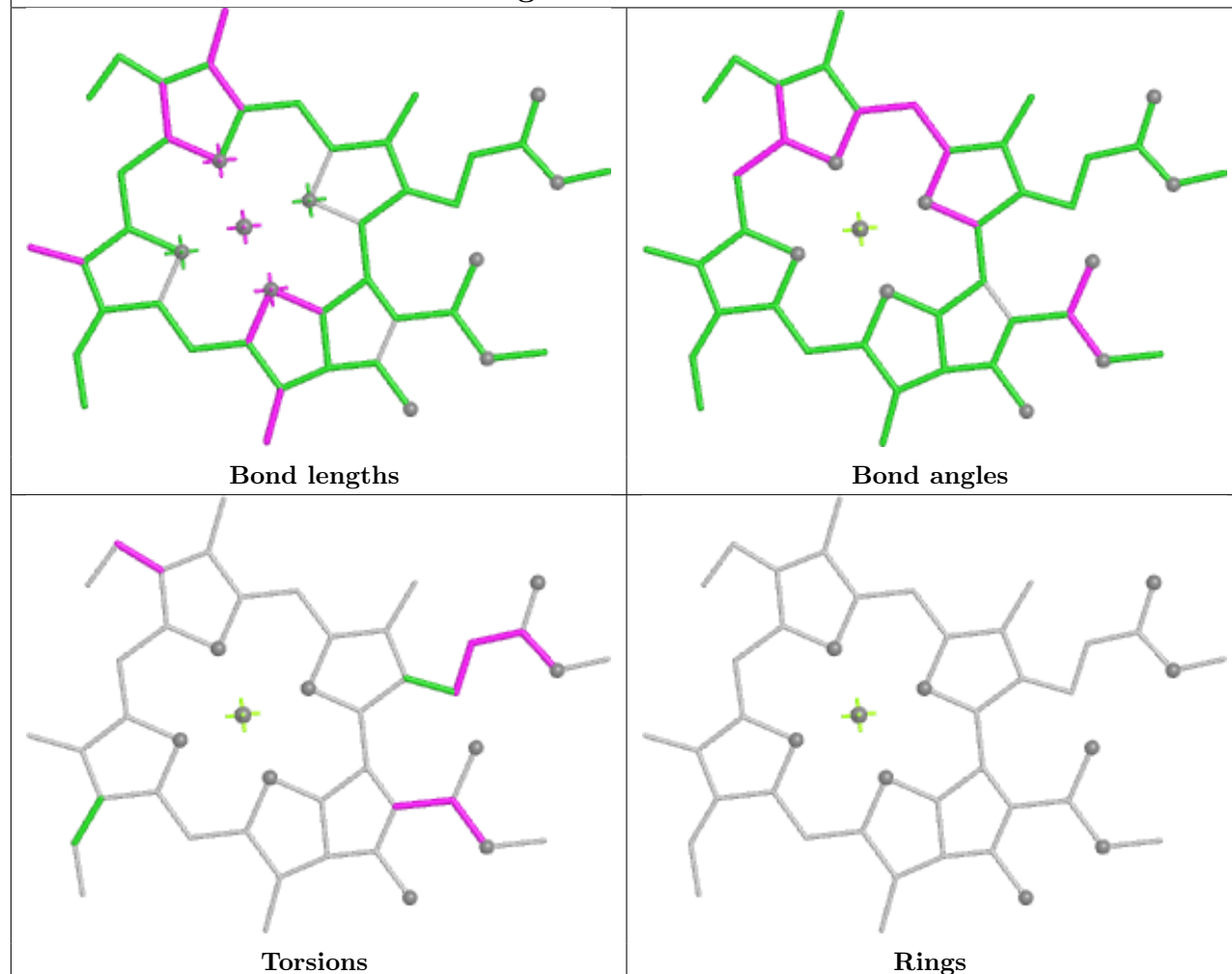
Ligand CLA A 813



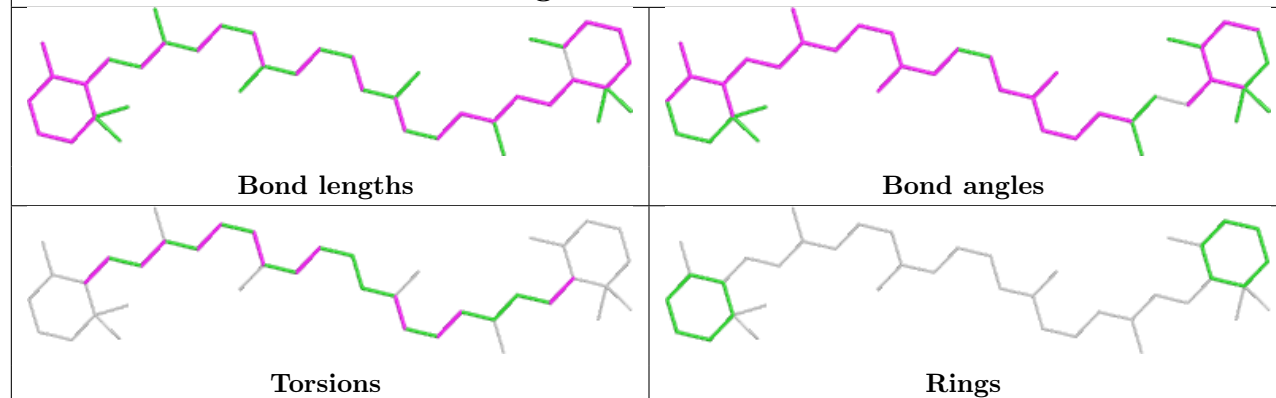
Ligand CLA 7 306



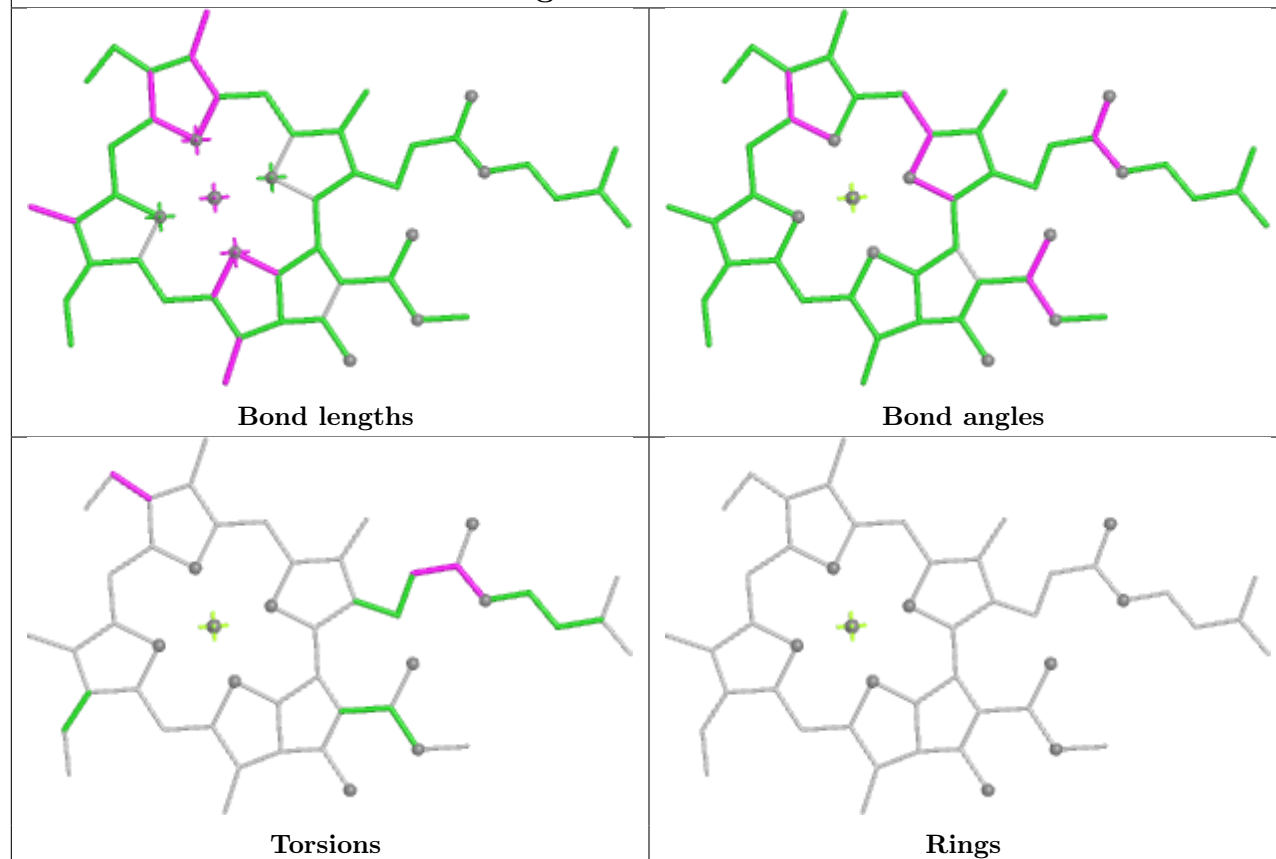
Ligand CLA 5 314



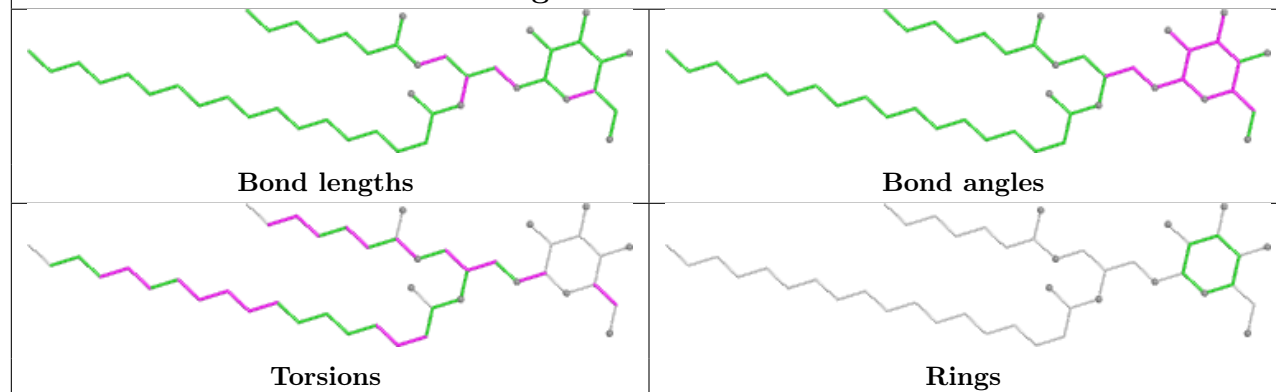
Ligand 8CT A 854



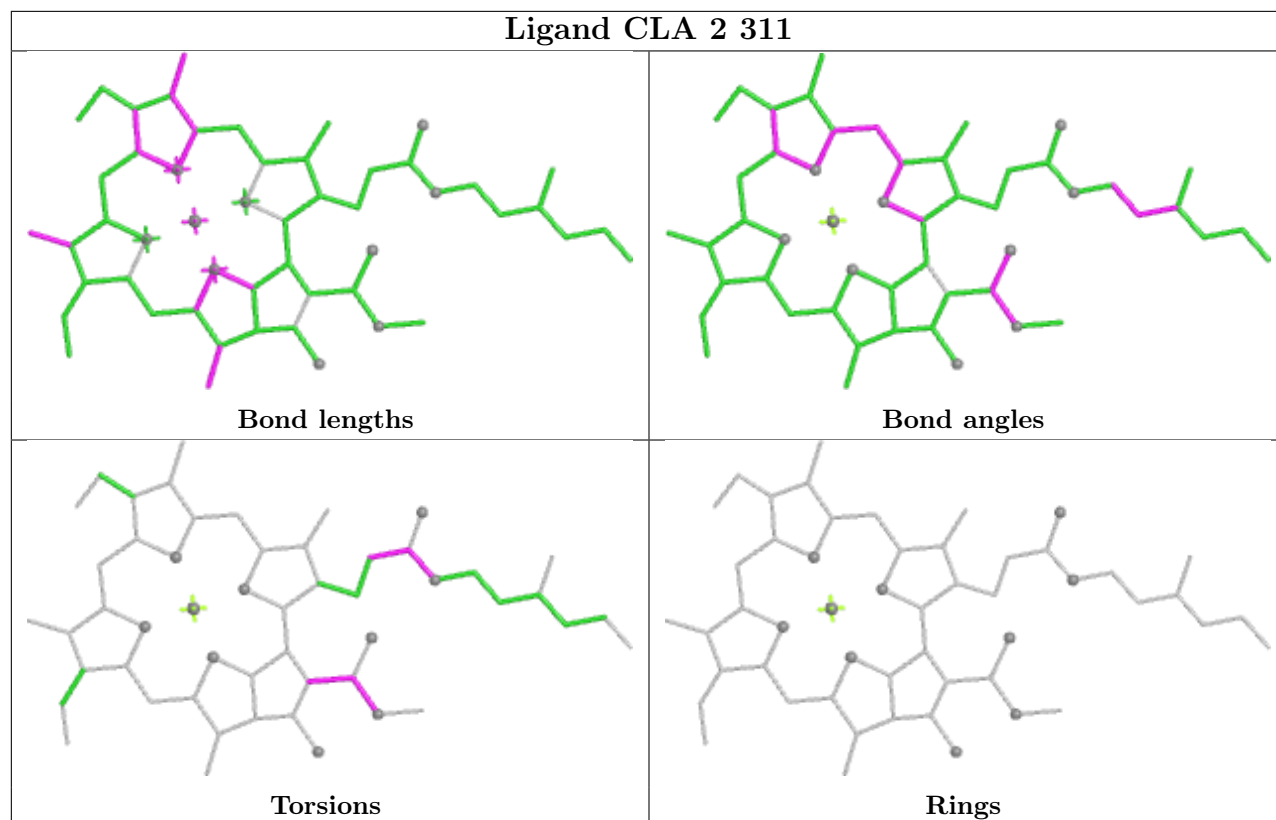
Ligand CLA 7 309



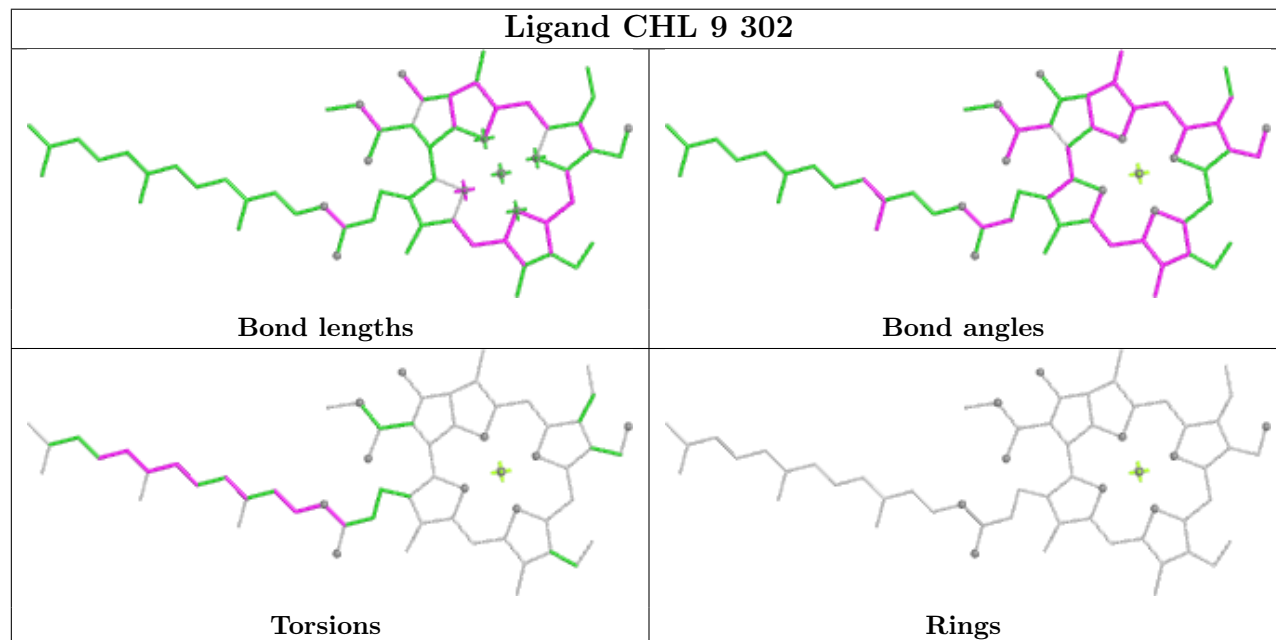
Ligand LMG 4 318



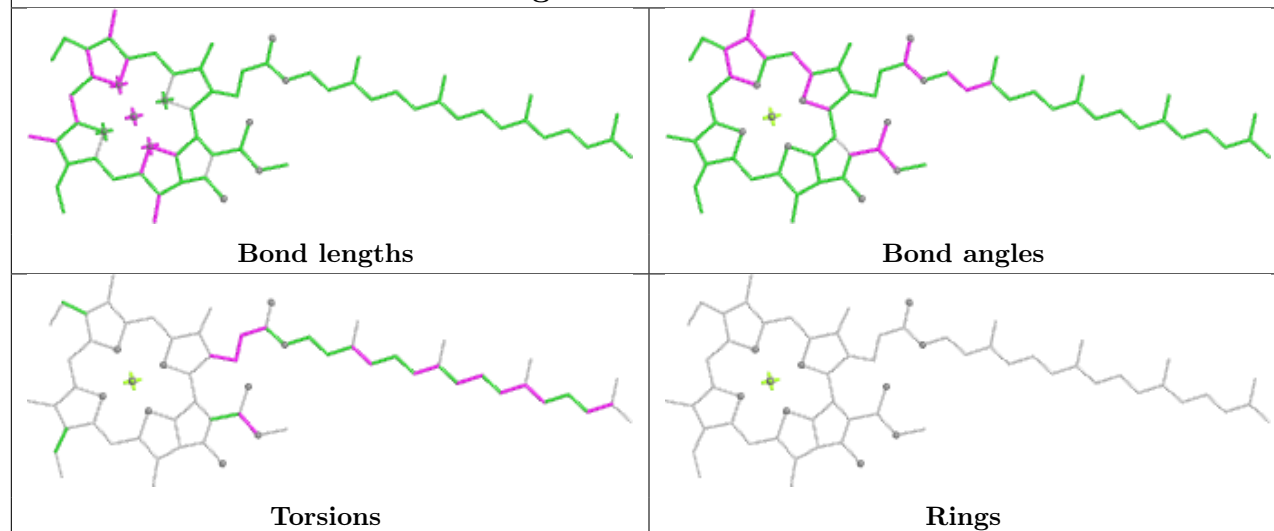
Ligand CLA 2 311



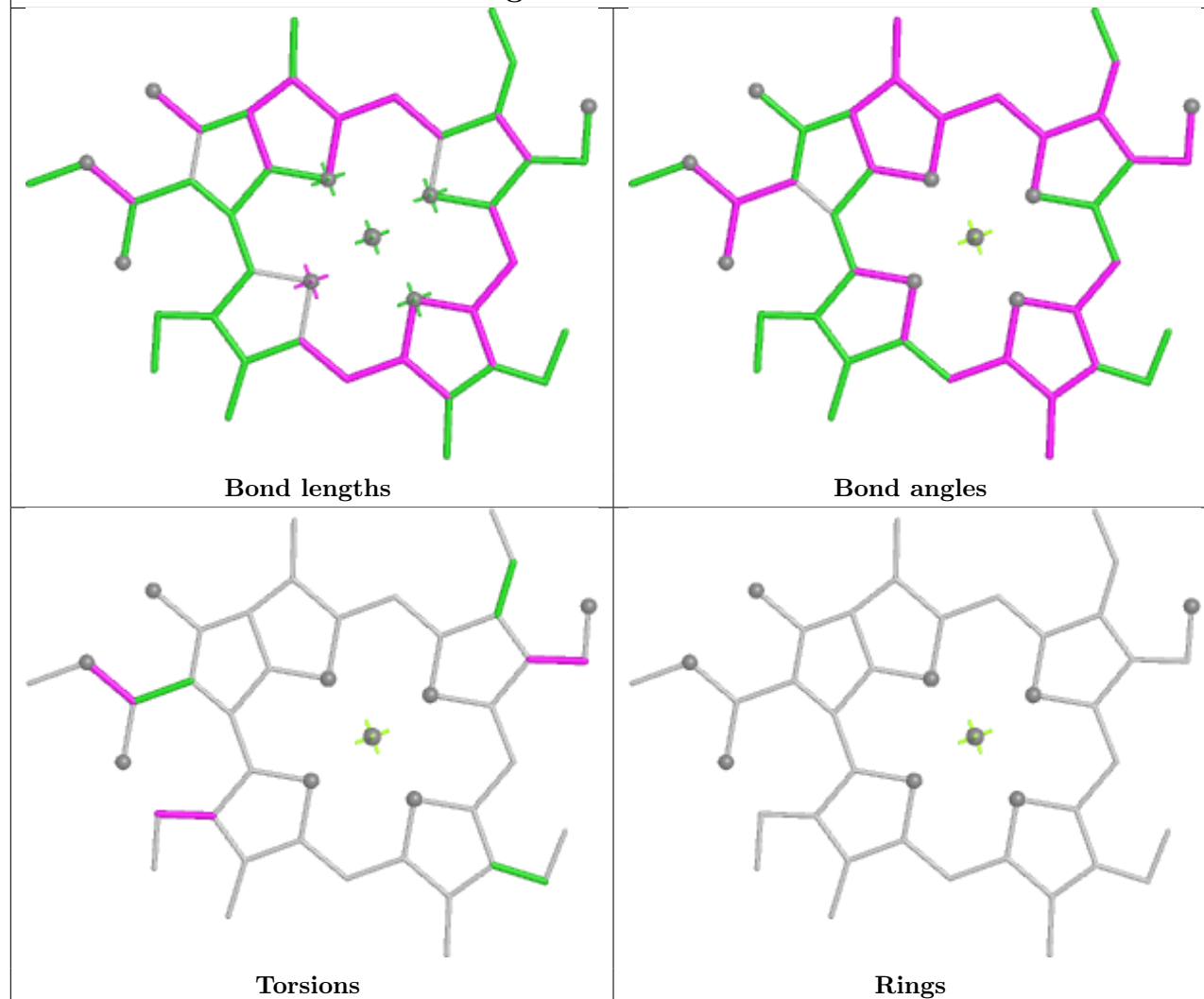
Ligand CHL 9 302

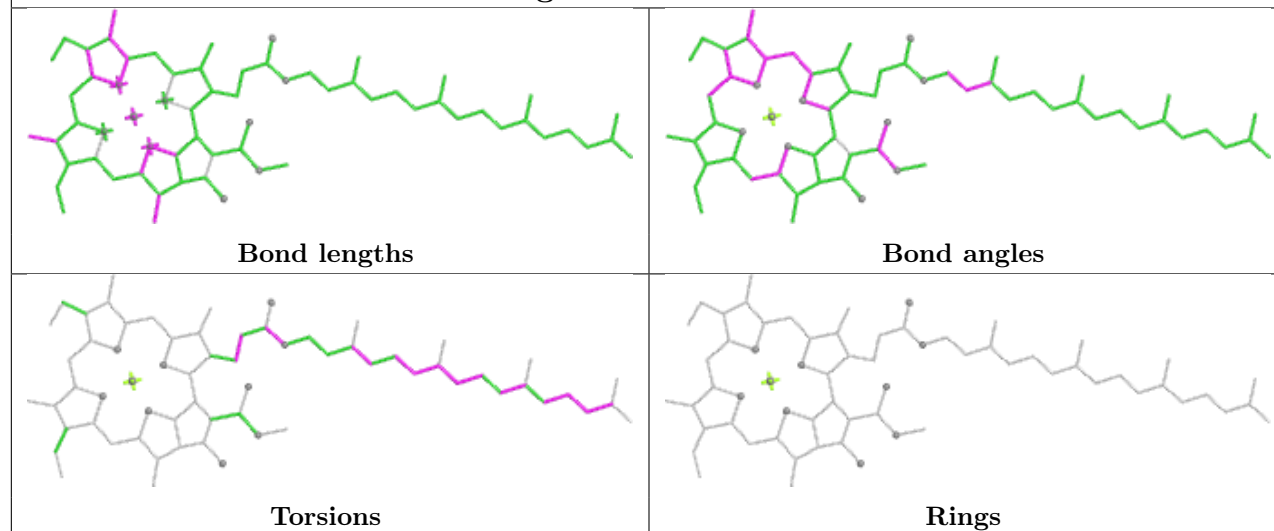
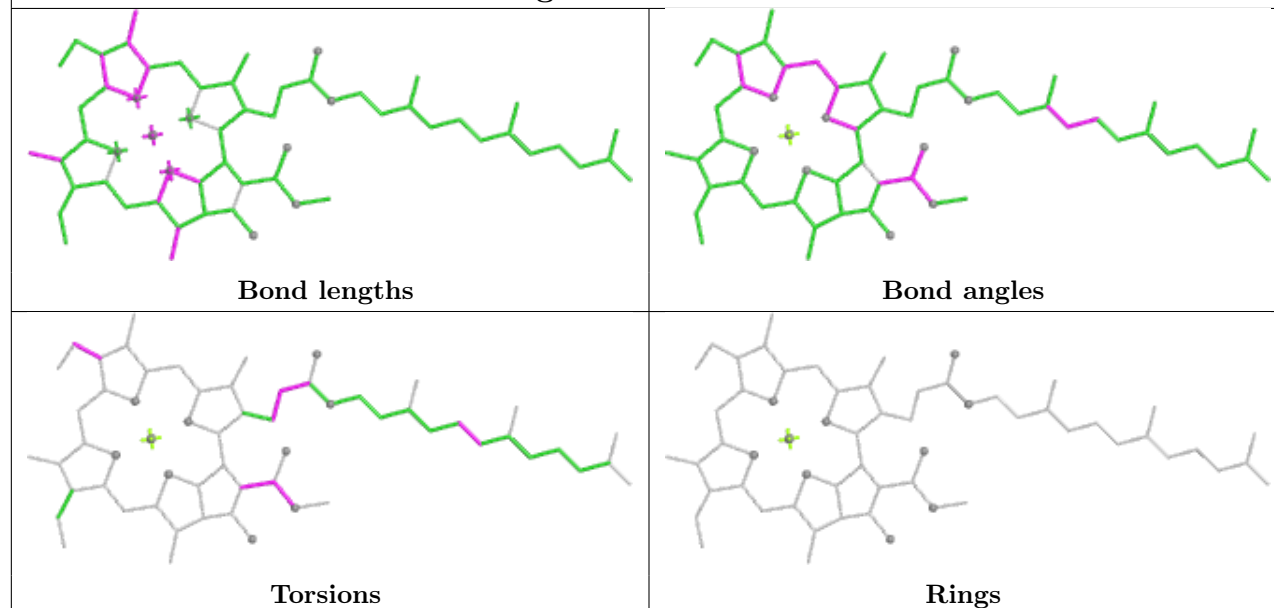


Ligand CLA B 828

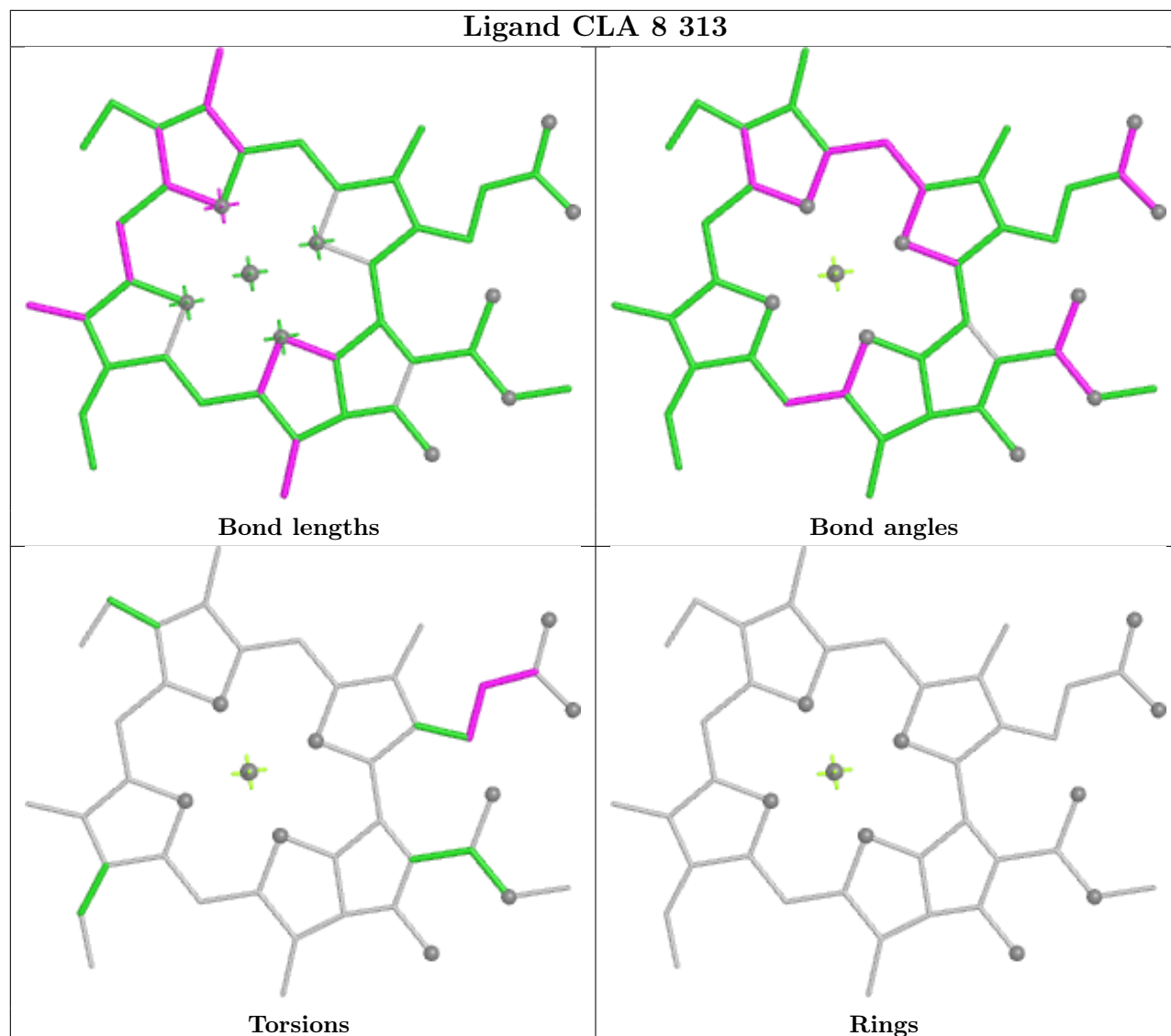


Ligand CHL 6 307

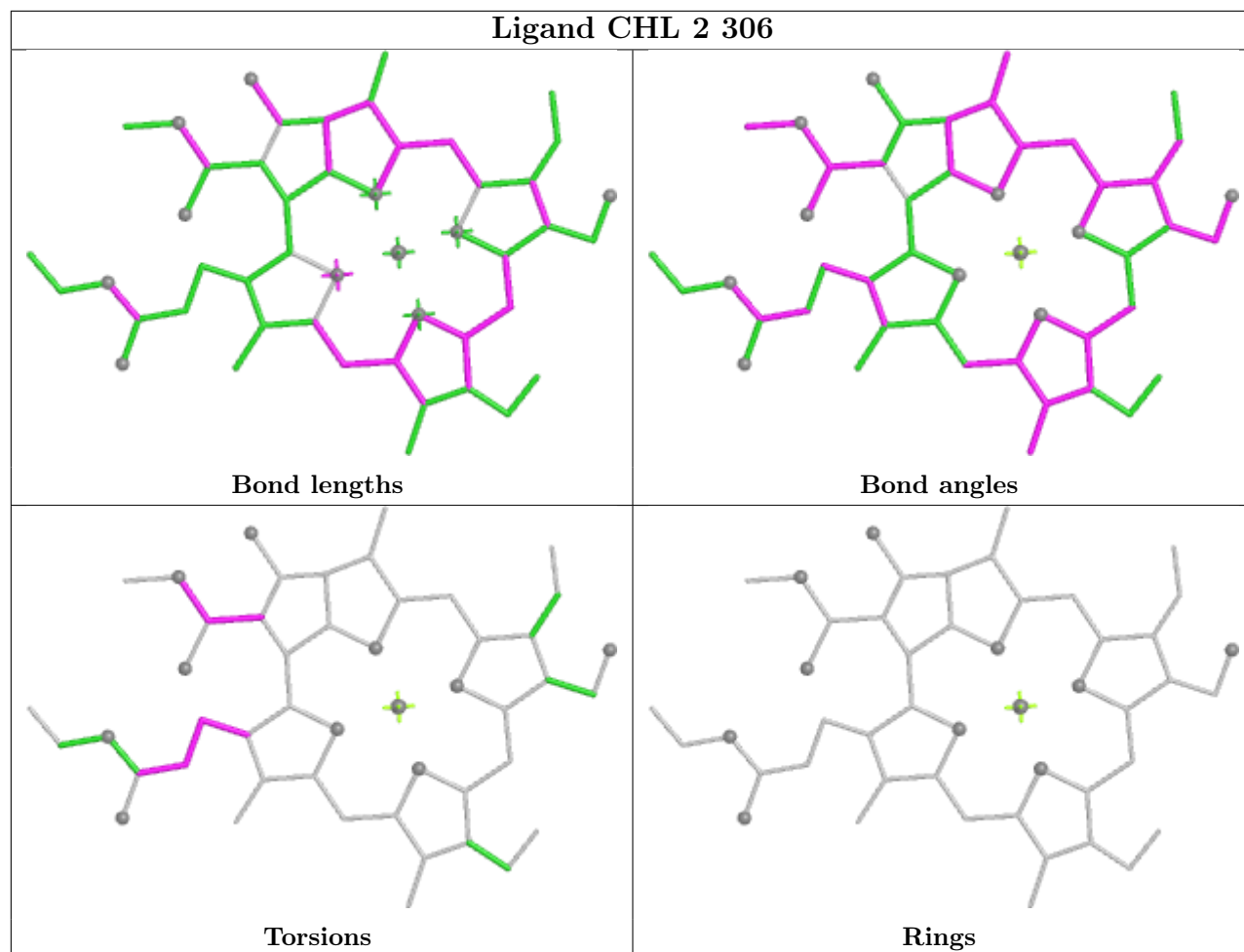


Ligand CLA 2 312**Ligand CLA 4 302**

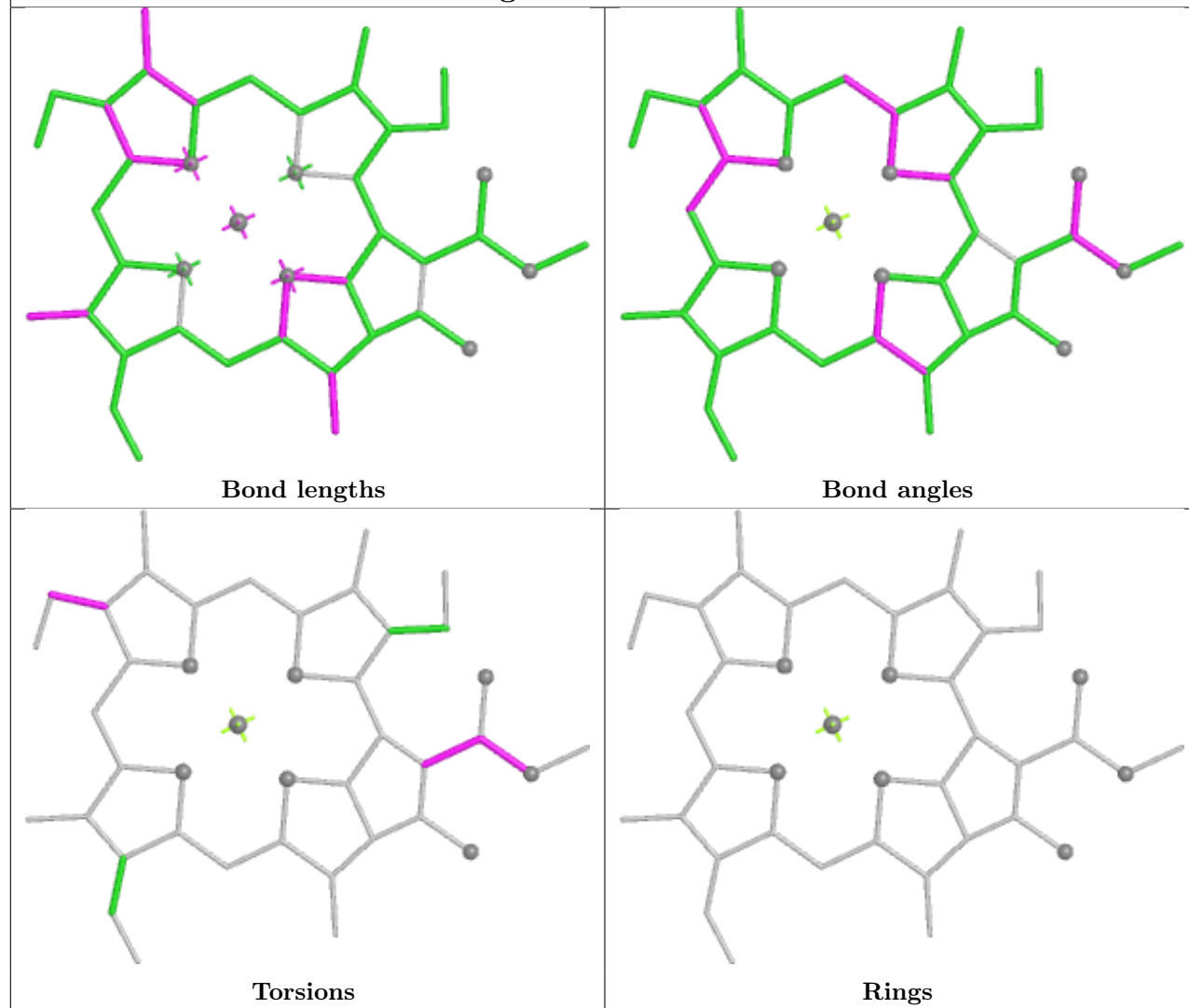
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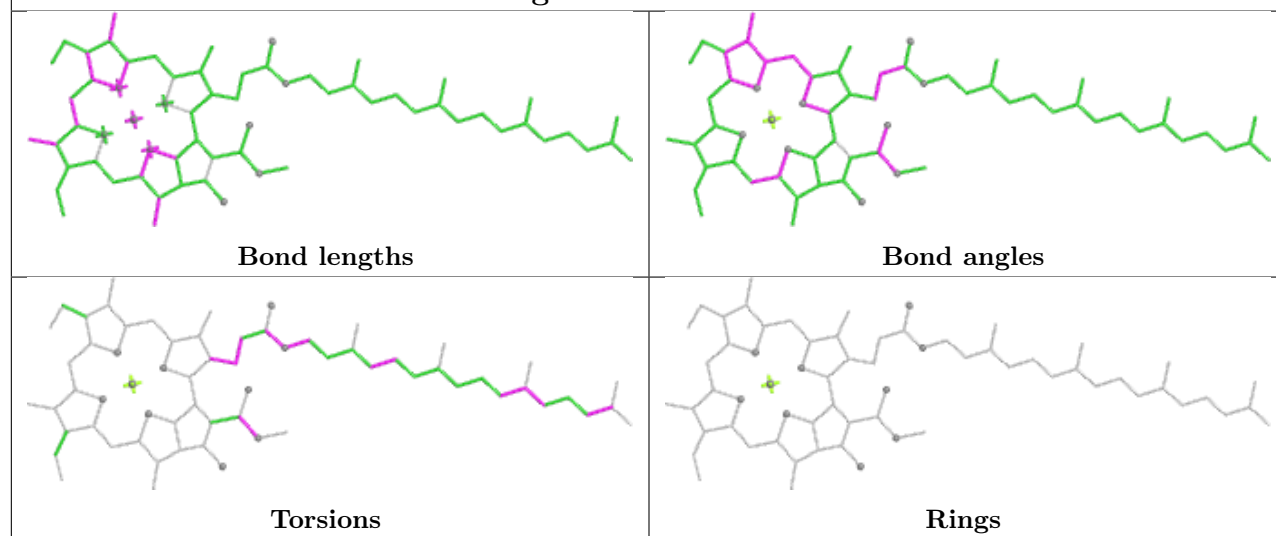
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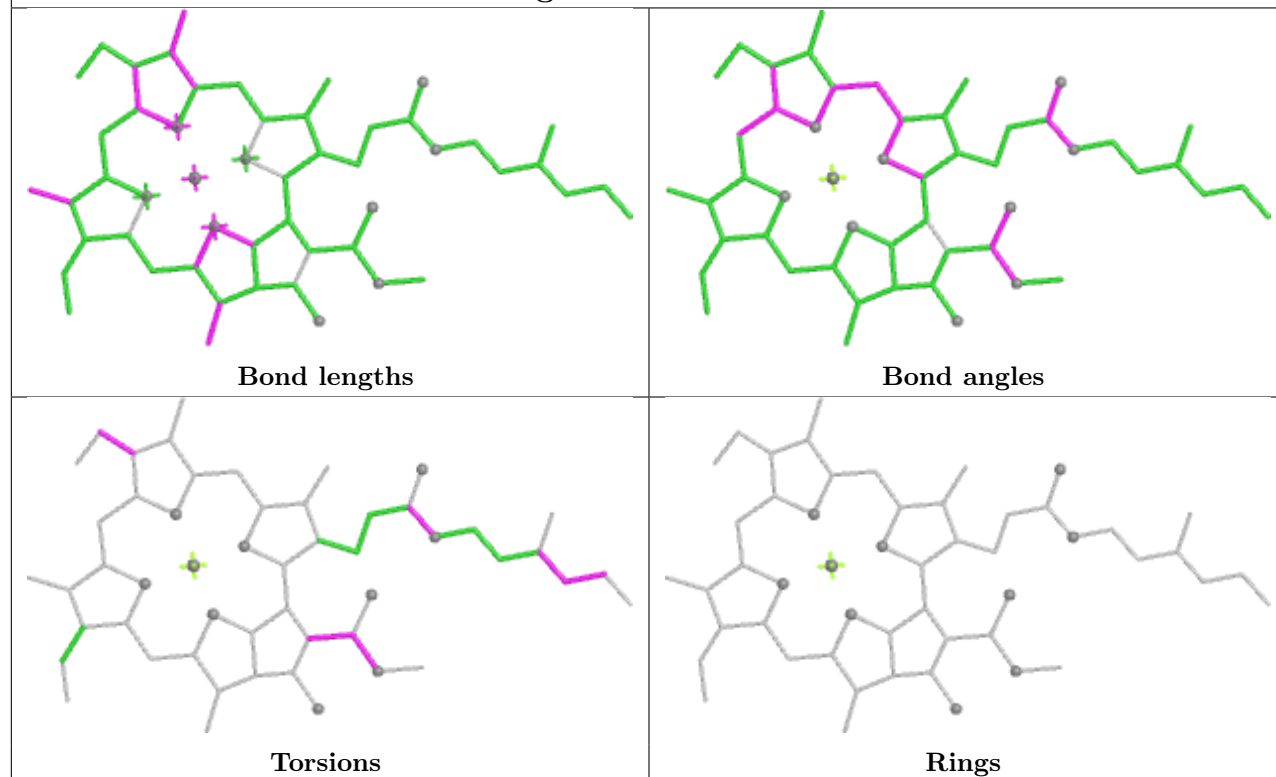
Ligand CLA 3 304



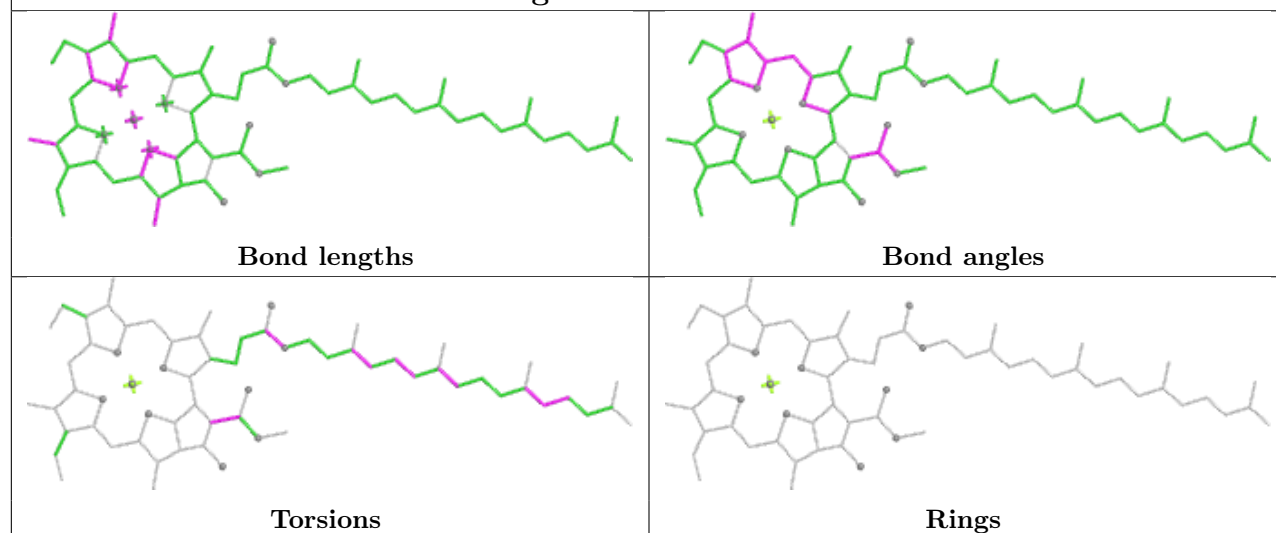
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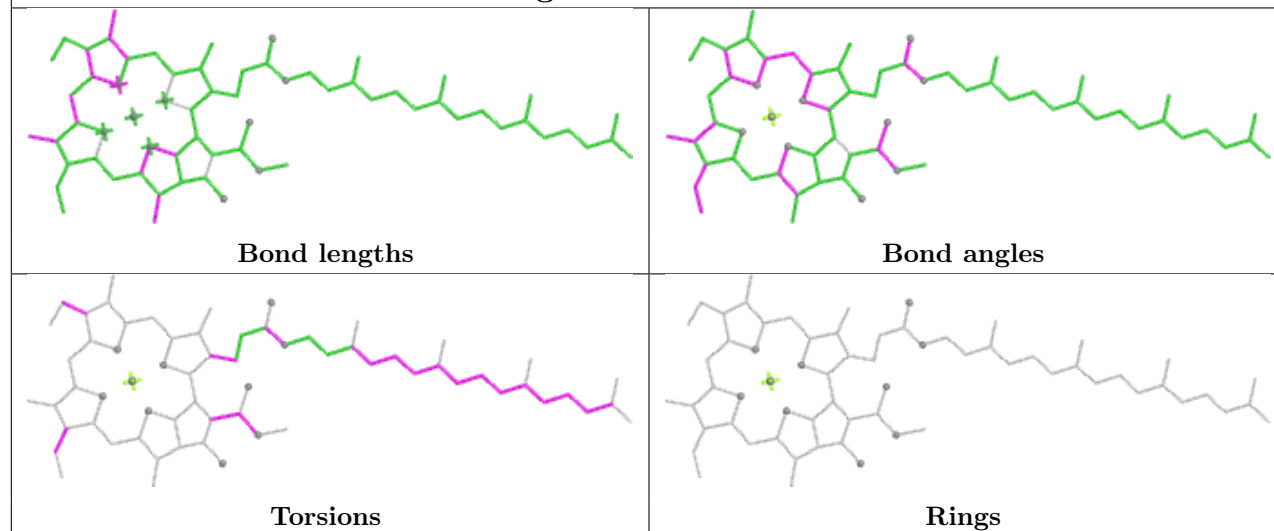
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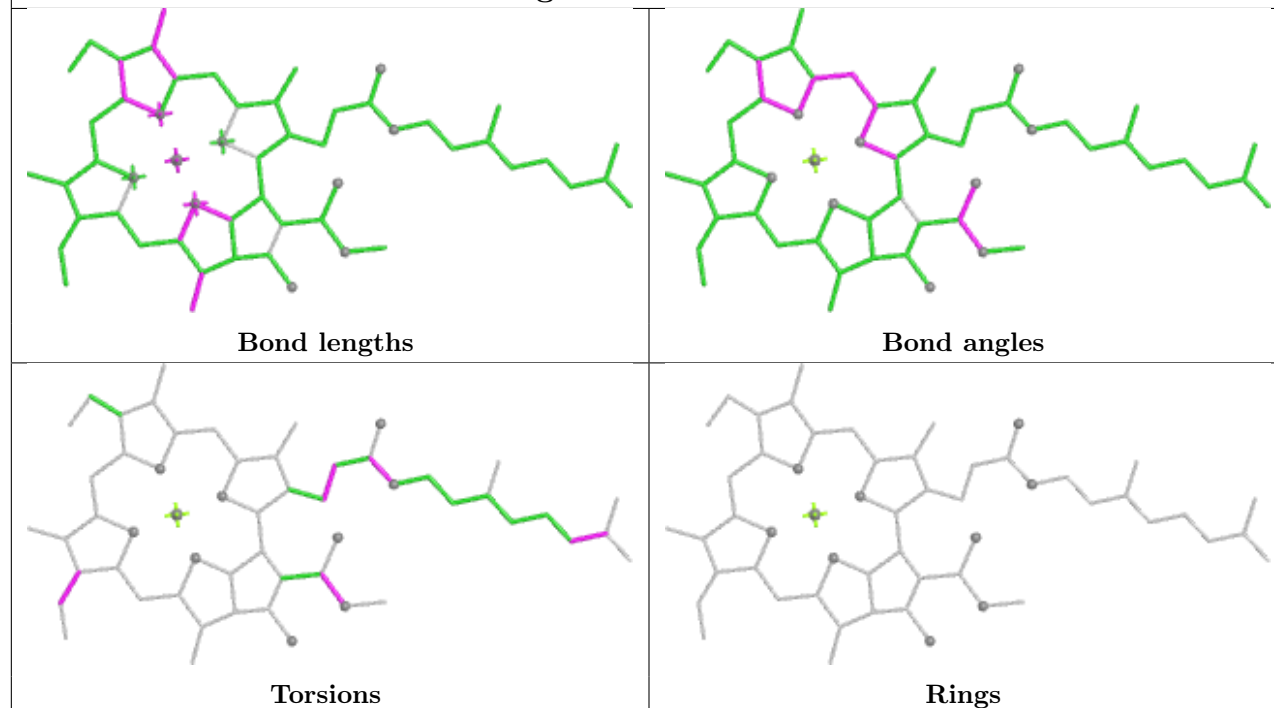
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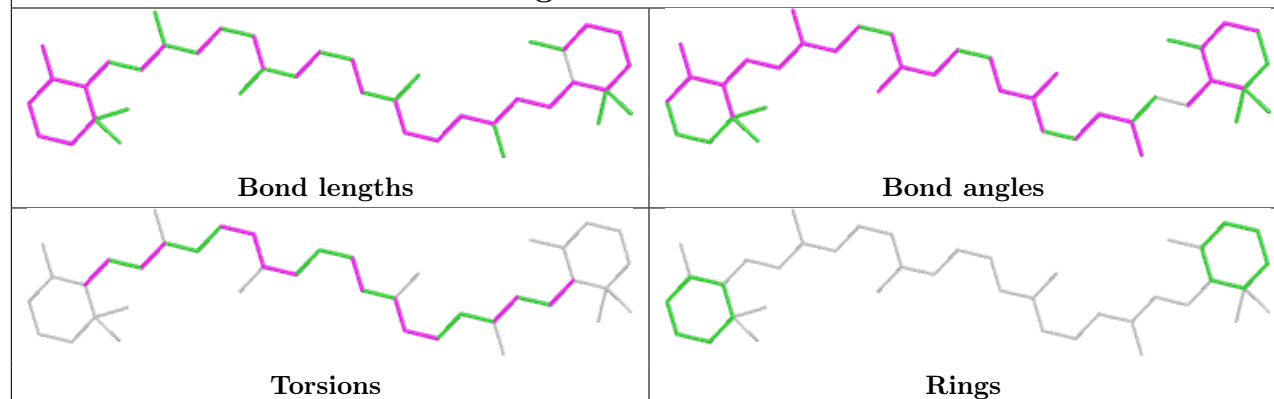
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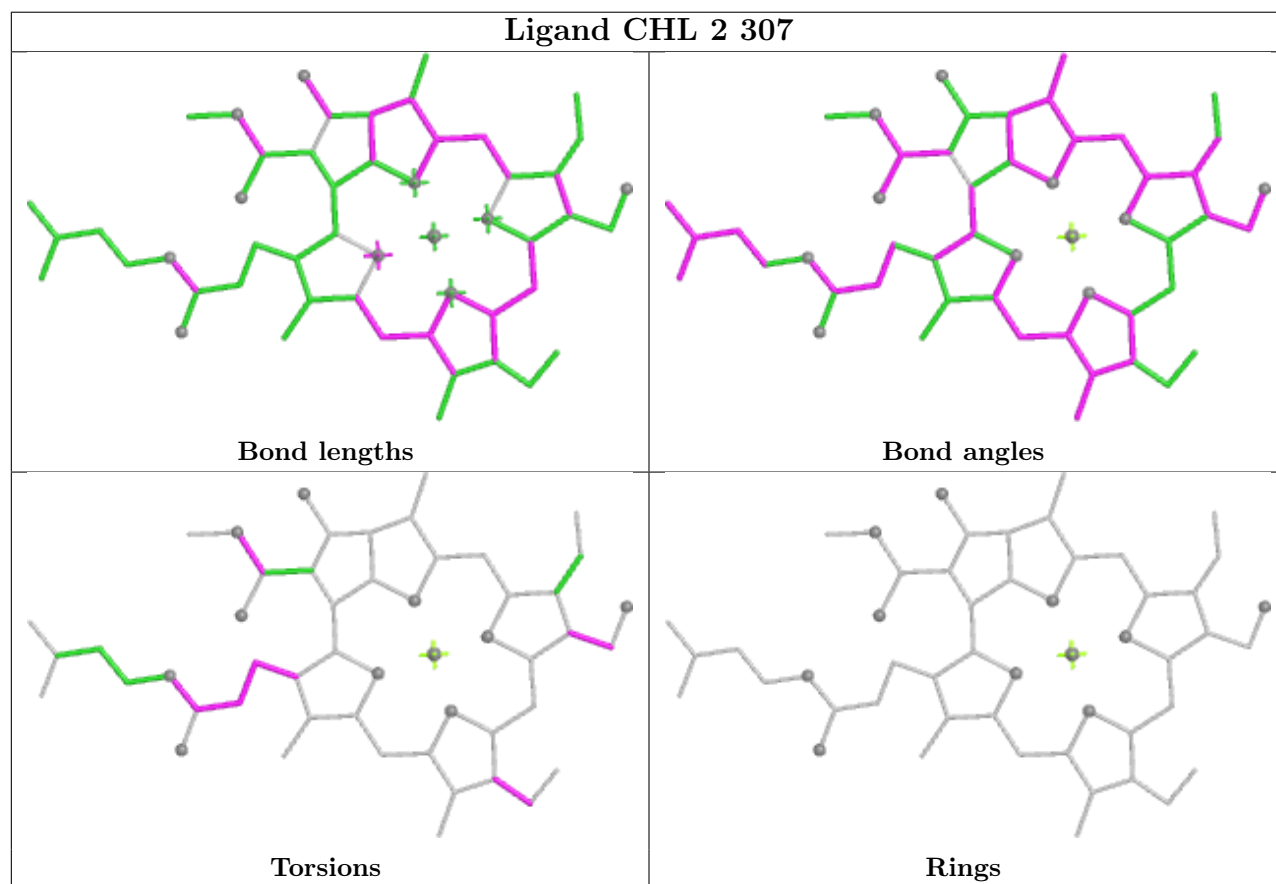
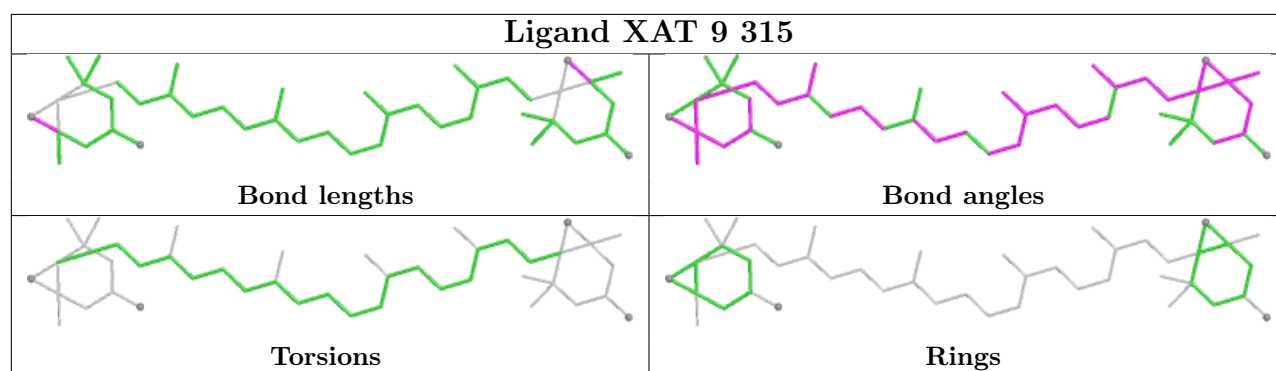


Ligand CLA 8 310

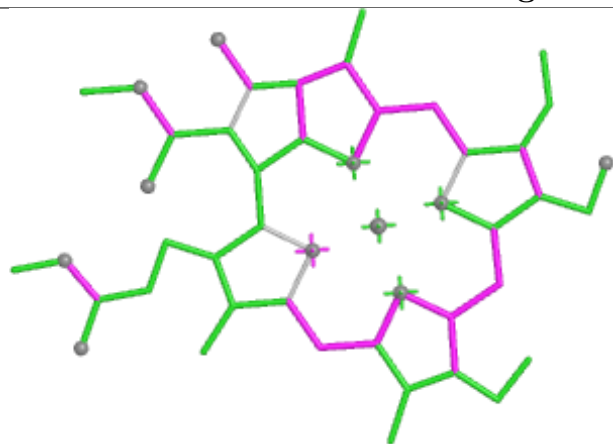


Ligand 8CT B 843

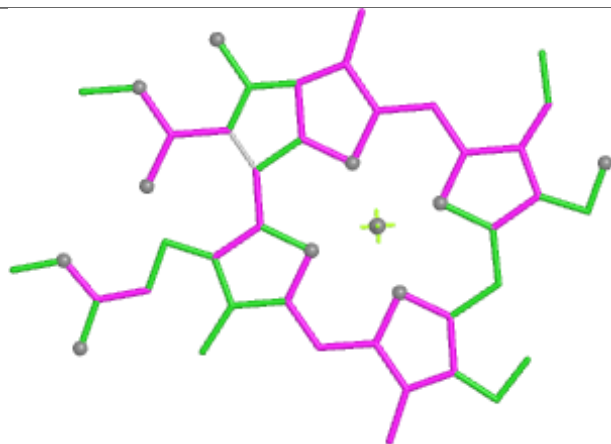




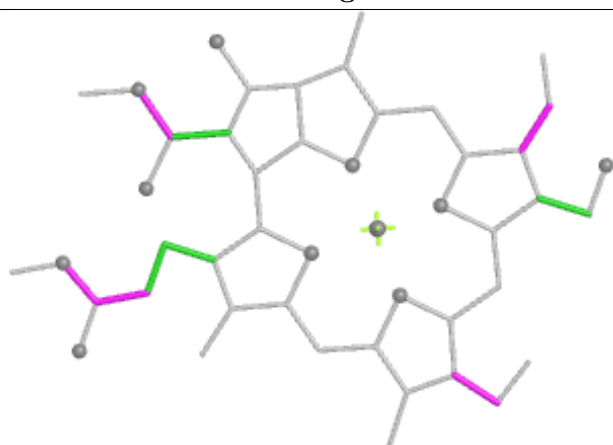
Ligand CHL 7 308



Bond lengths



Bond angles

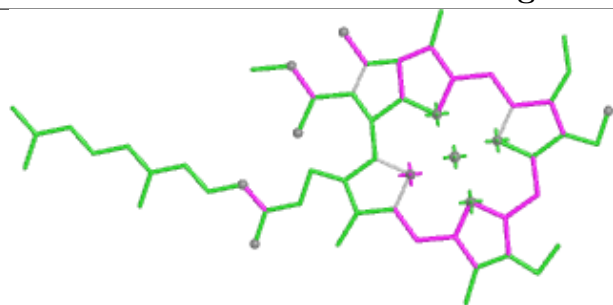


Torsions

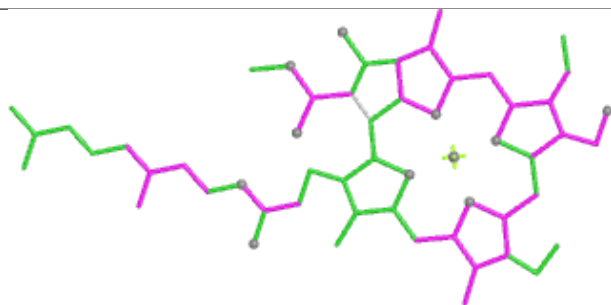


Rings

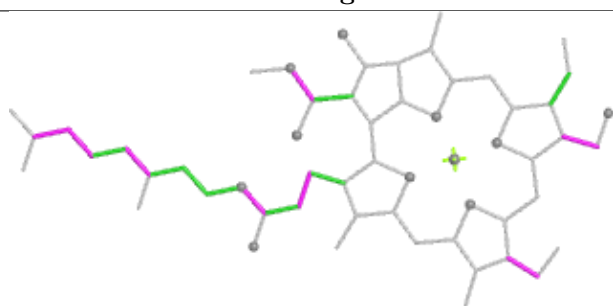
Ligand CHL 4 305



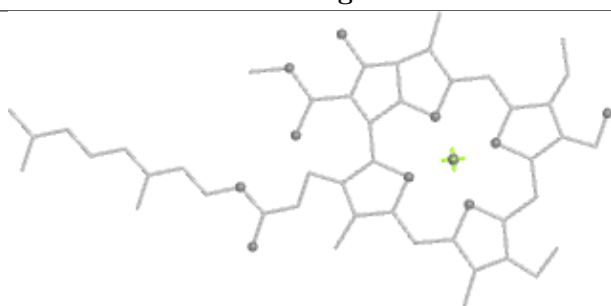
Bond lengths



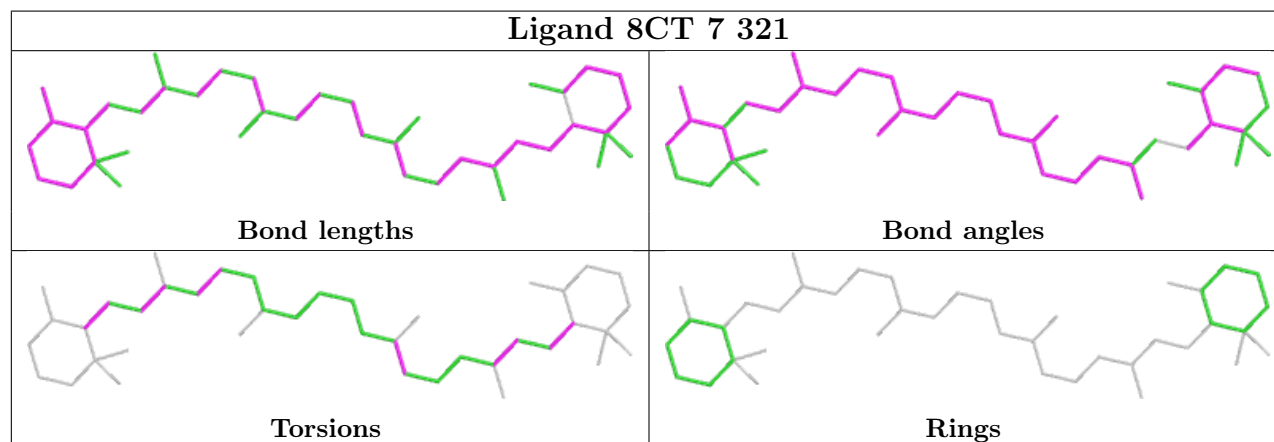
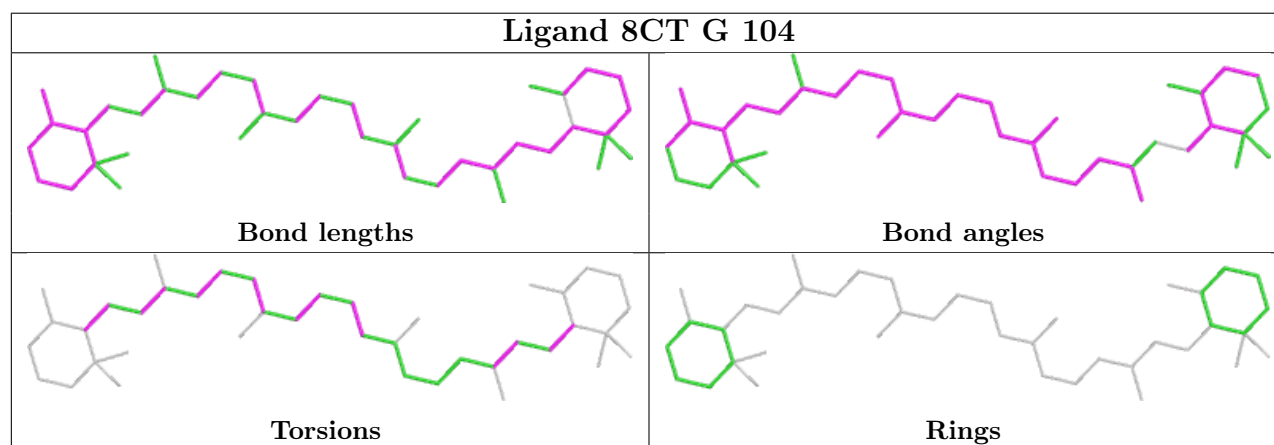
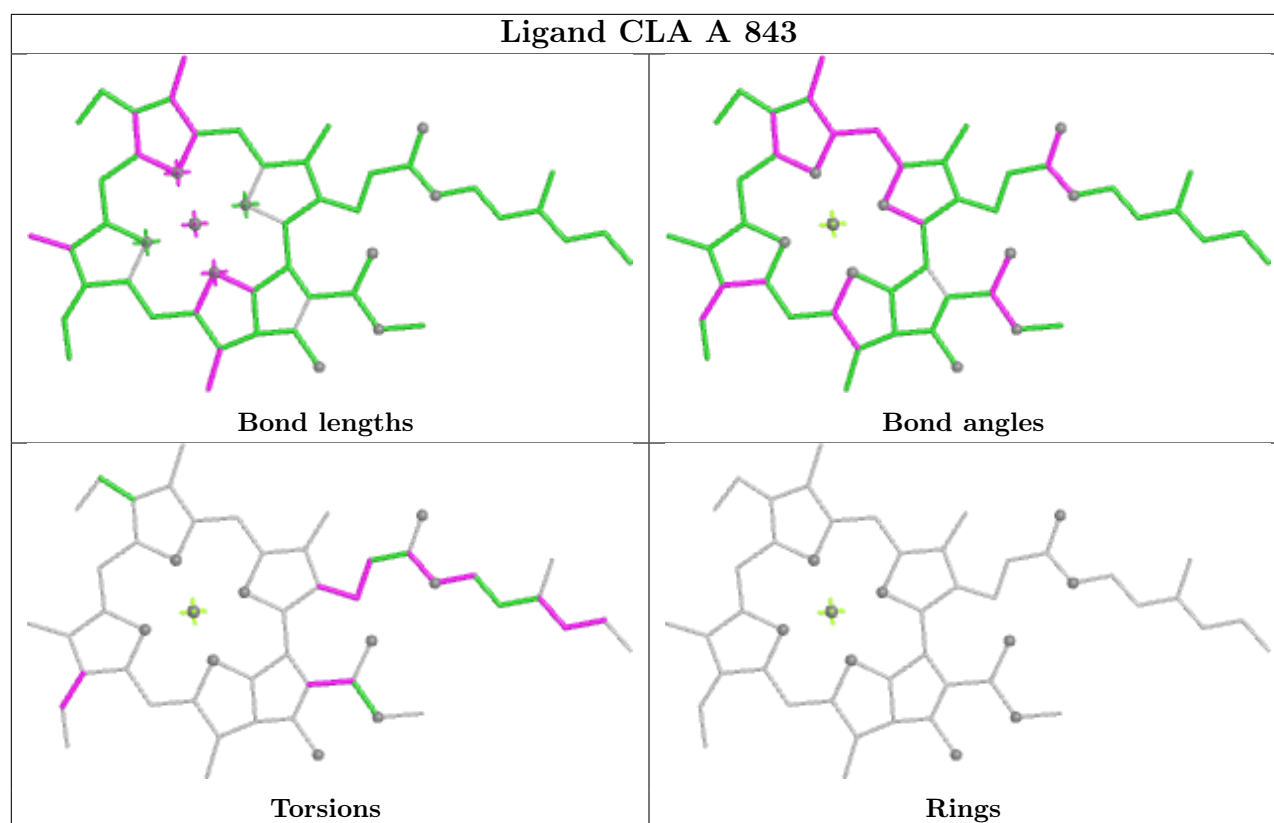
Bond angles



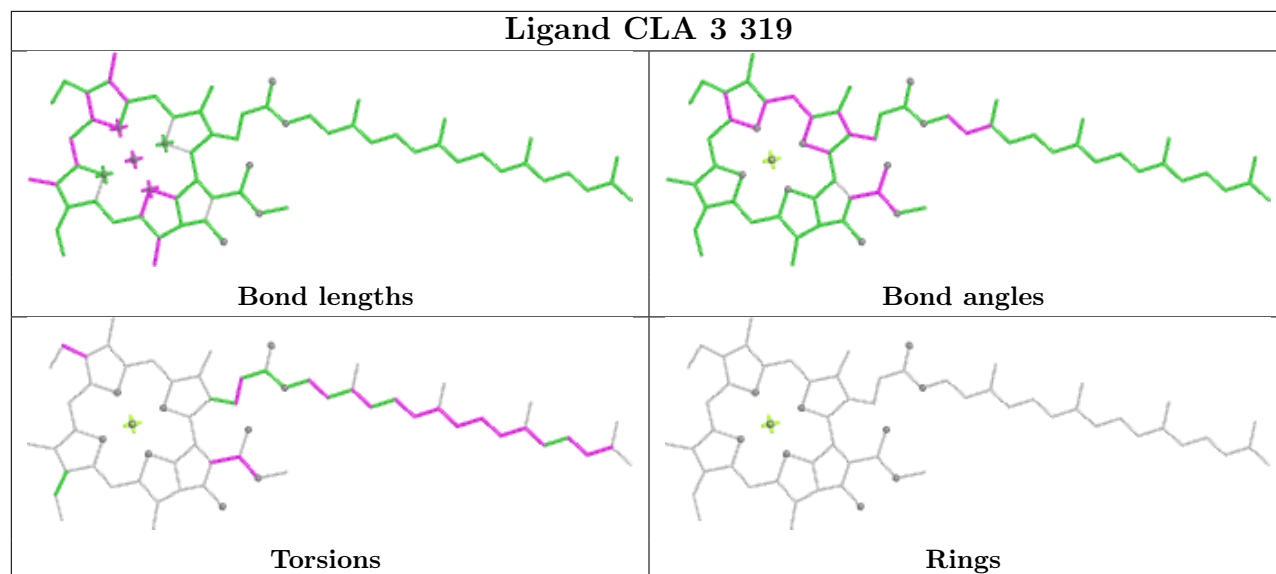
Torsions



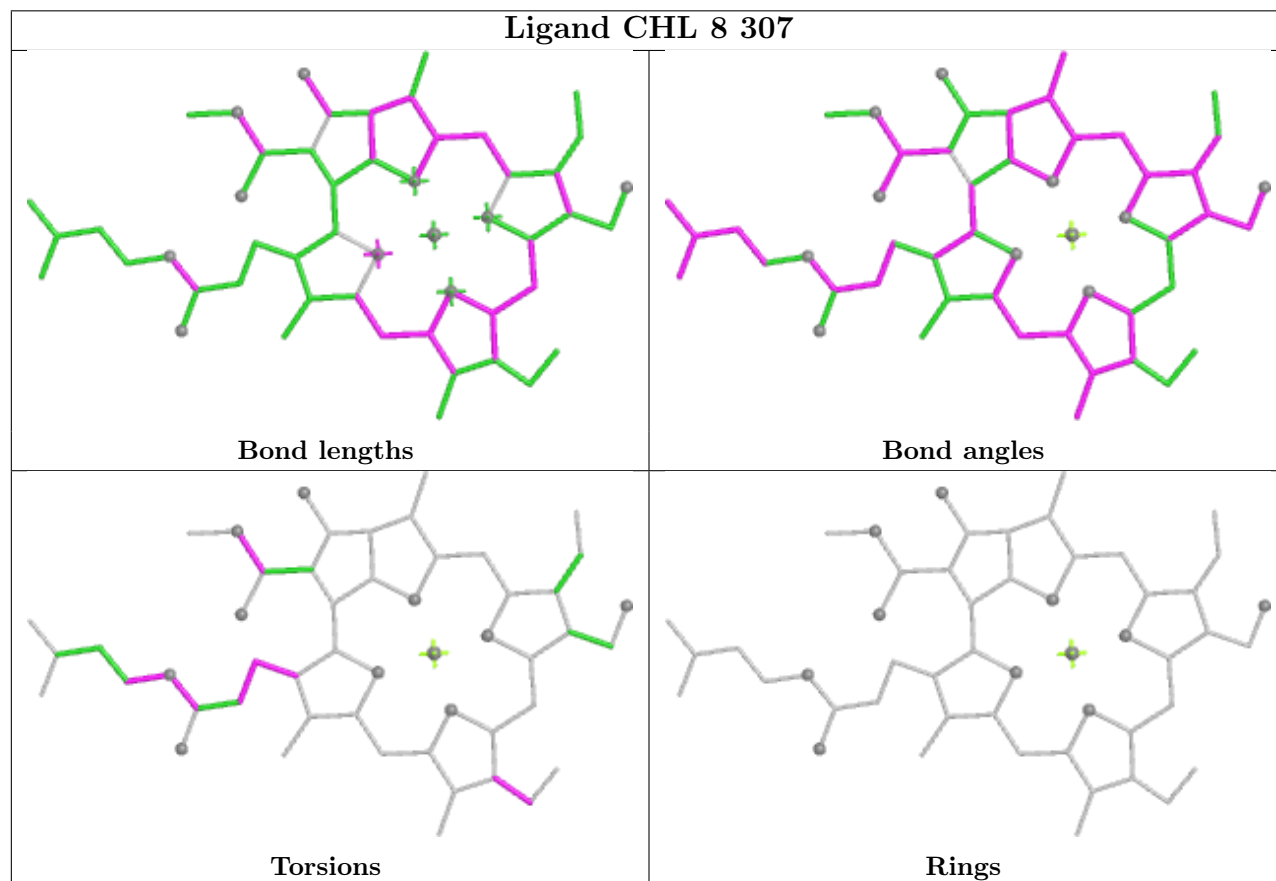
Rings



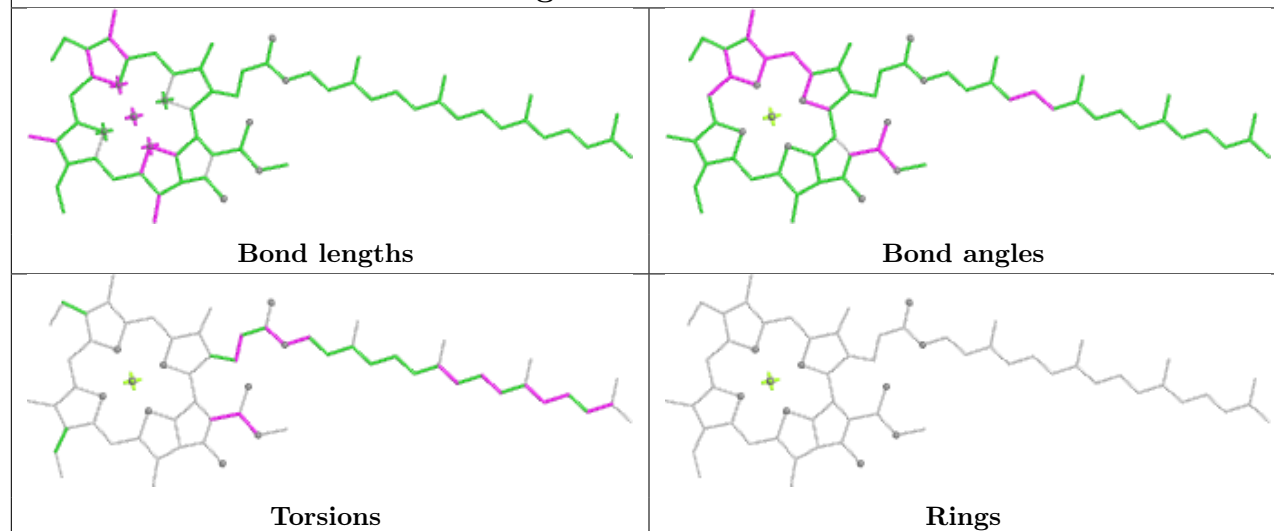
Ligand CLA 3 319



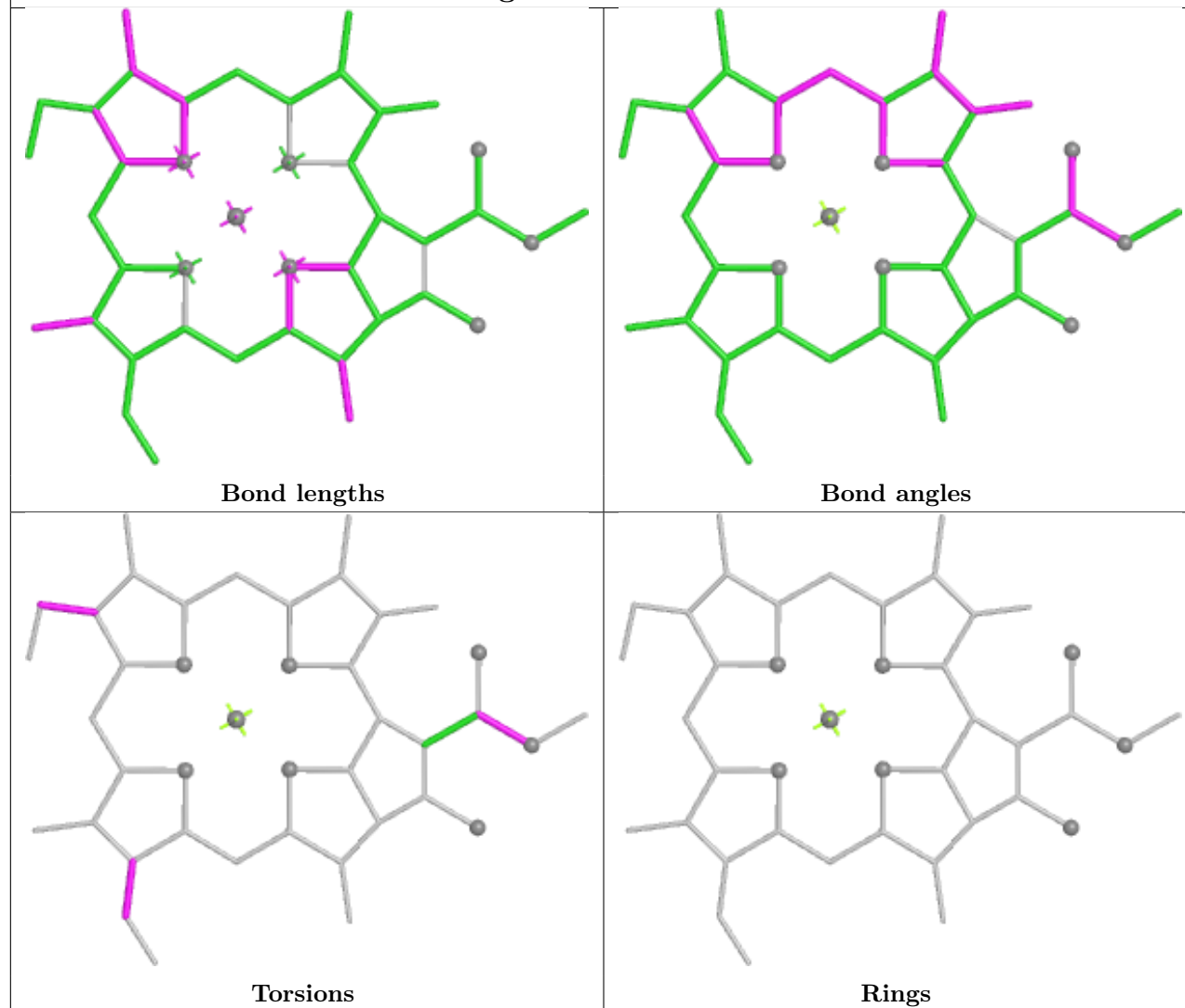
Ligand CHL 8 307

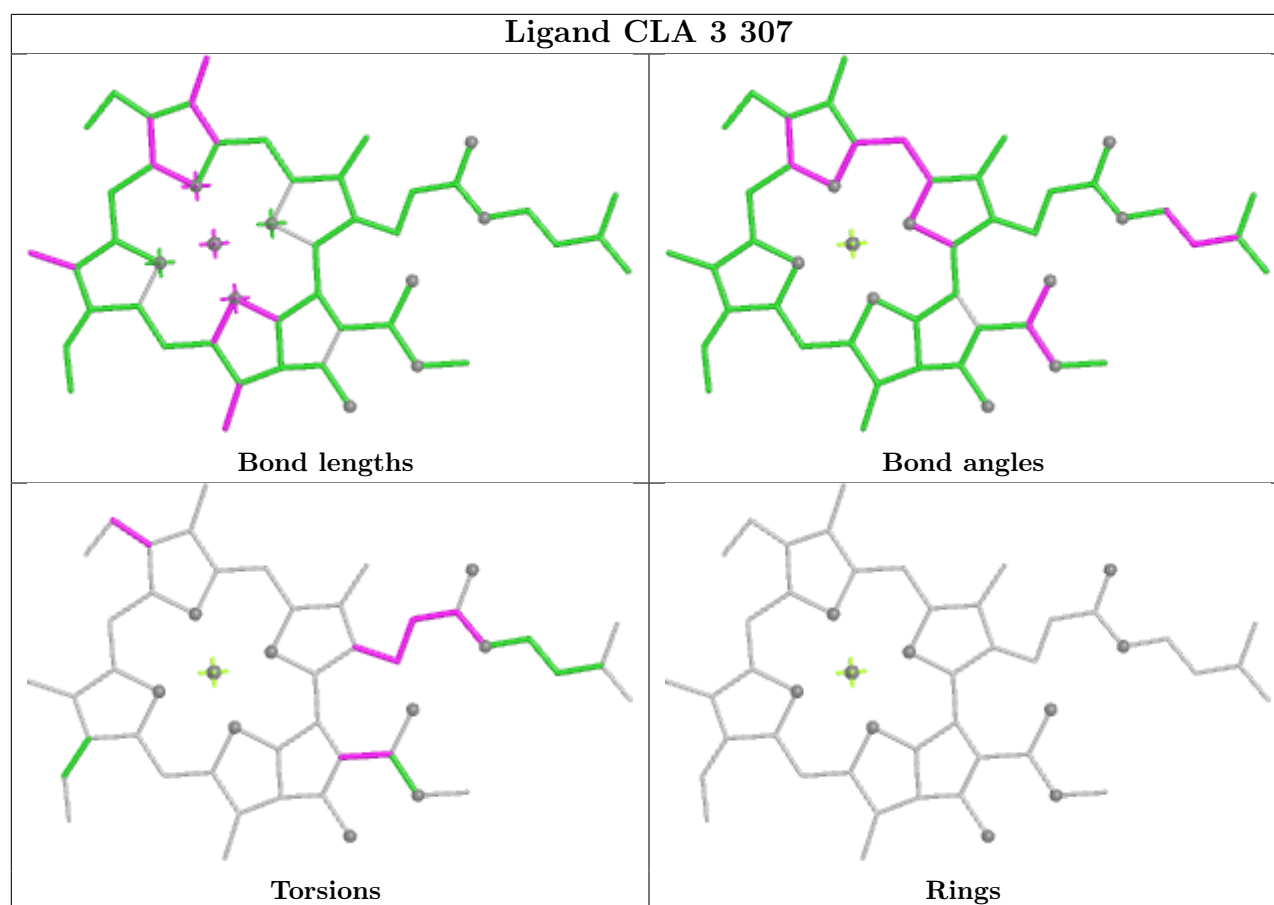


Ligand CLA 6 303

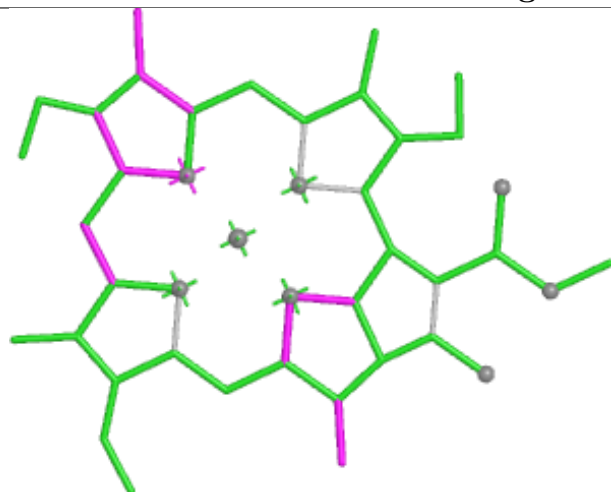


Ligand CLA 2 310

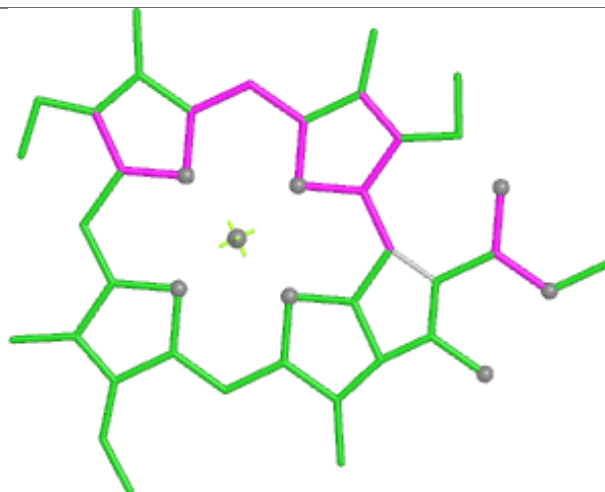




Ligand CLA 5 308



Bond lengths



Bond angles

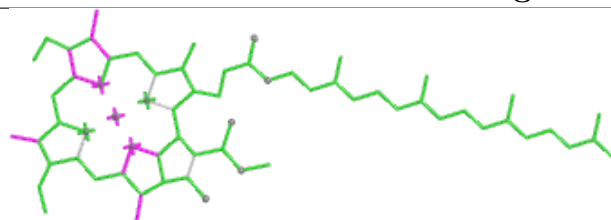


Torsions

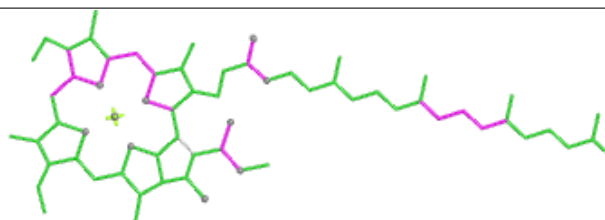


Rings

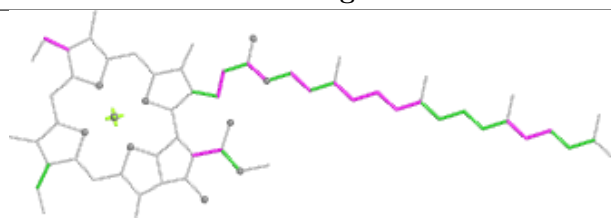
Ligand CLA A 840



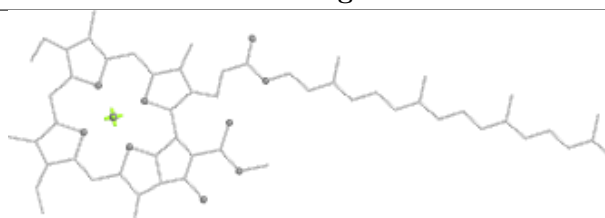
Bond lengths



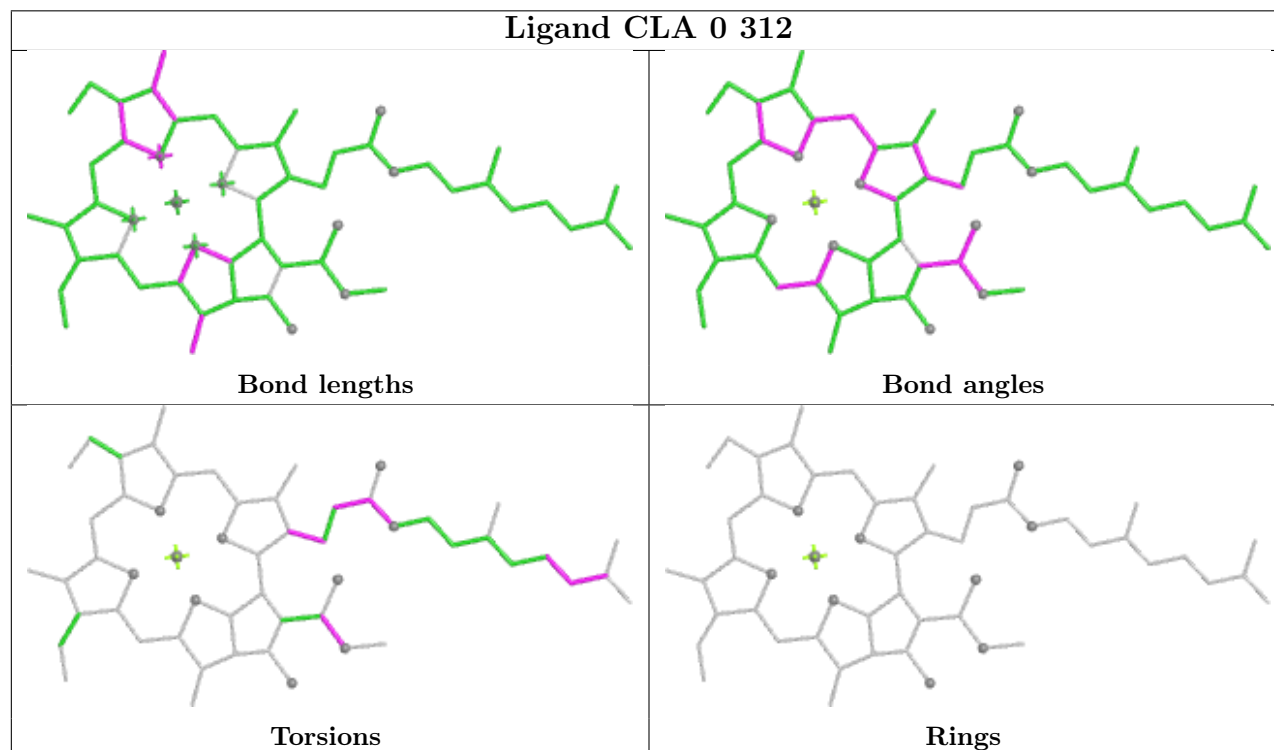
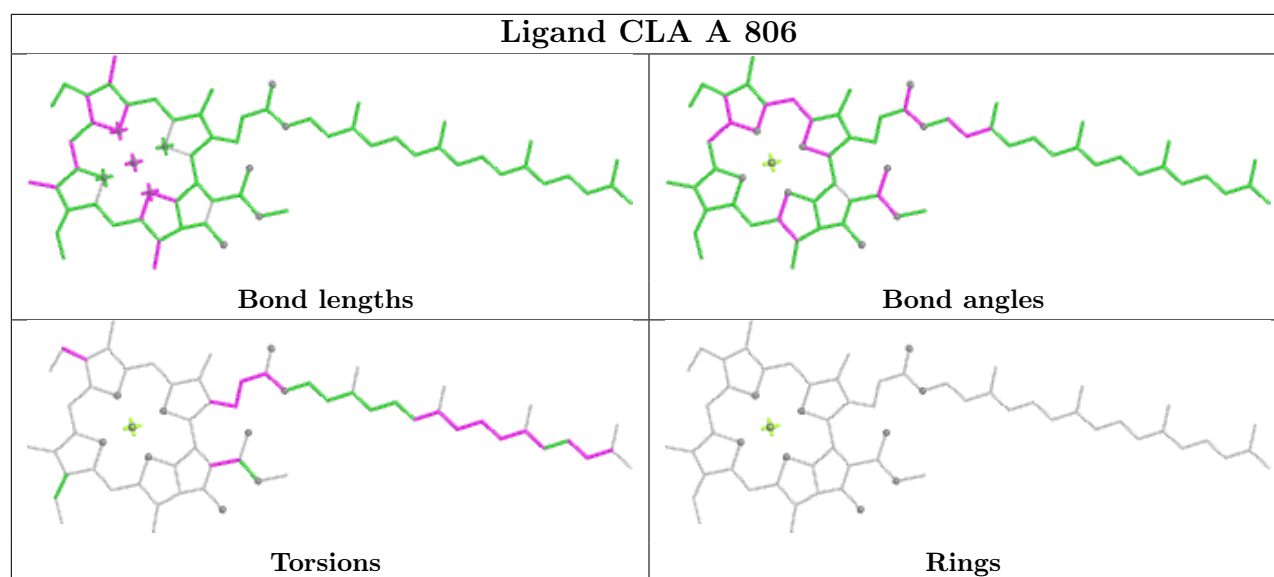
Bond angles

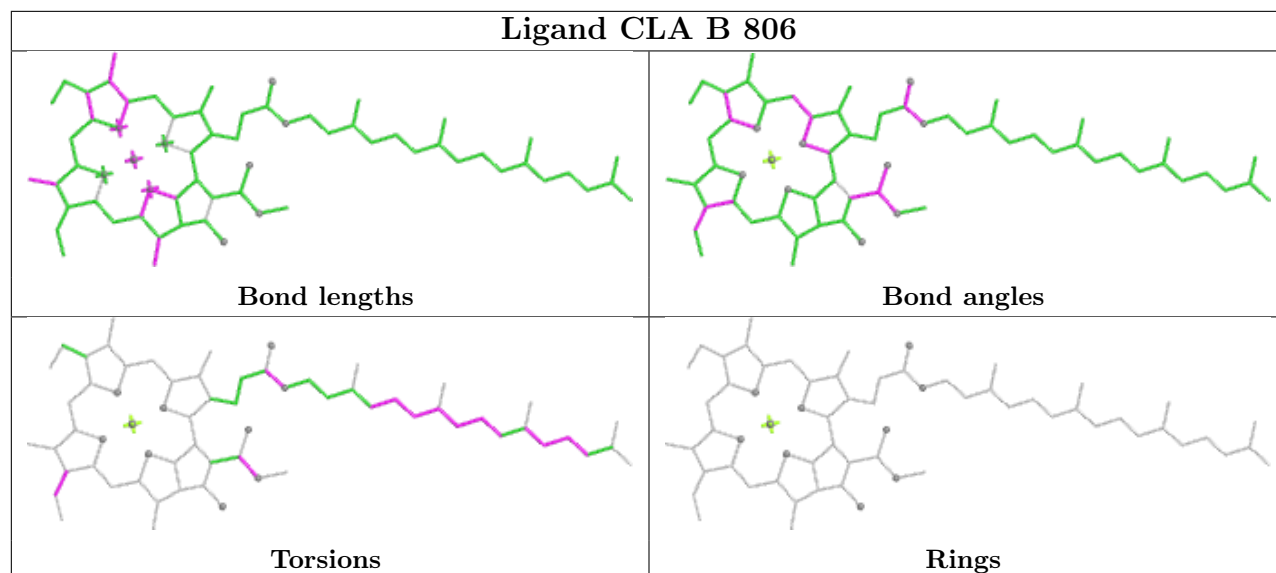
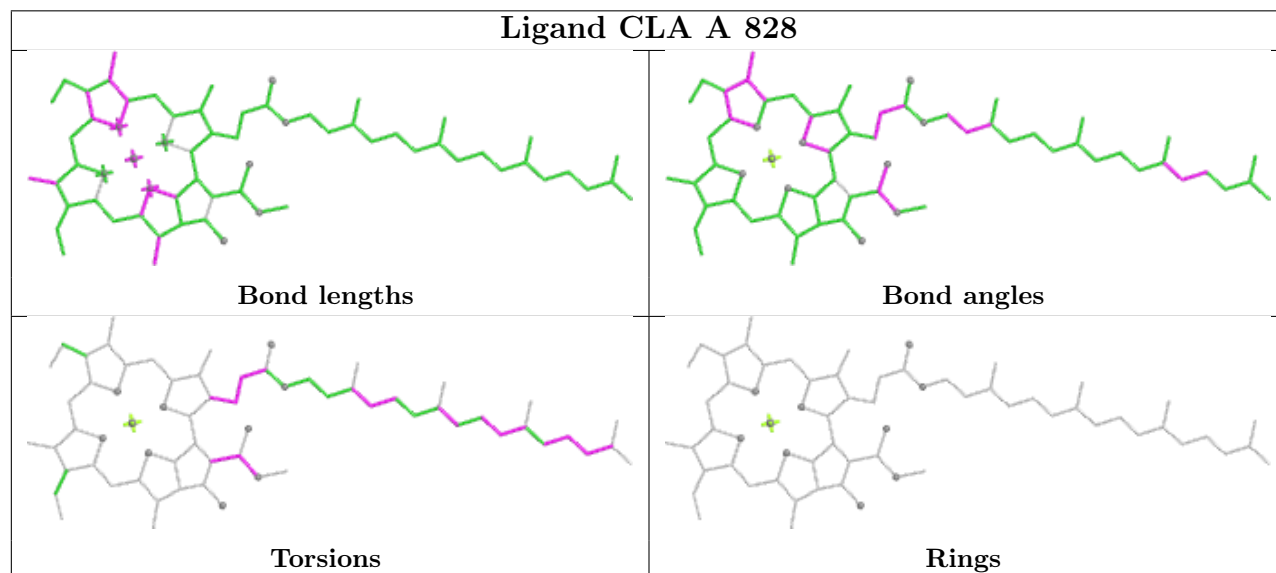
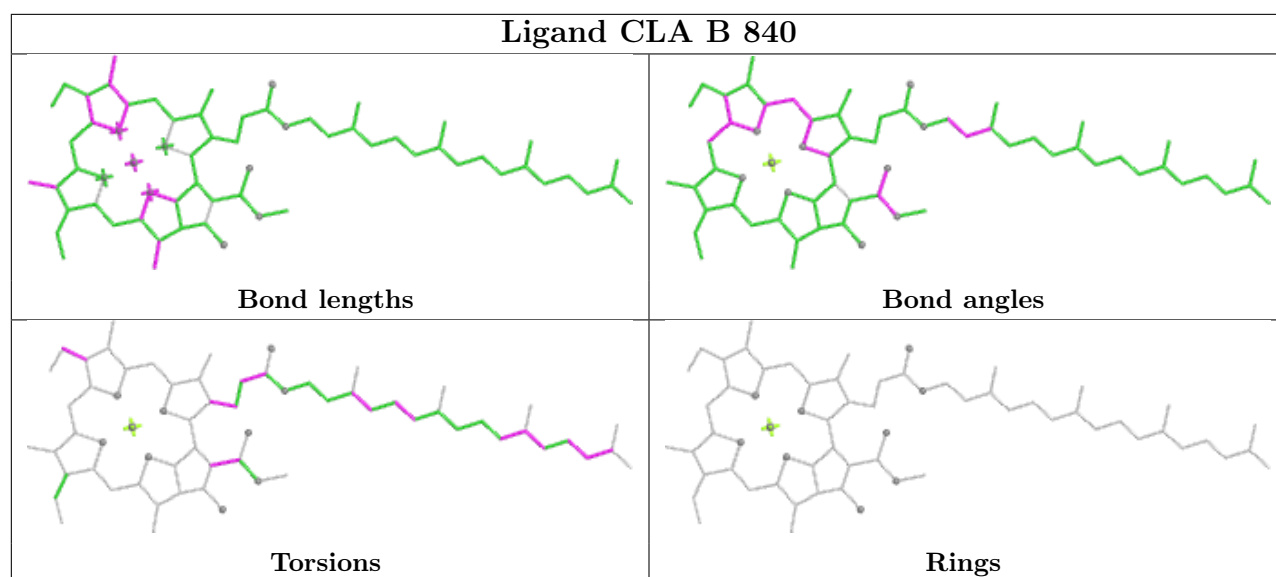


Torsions

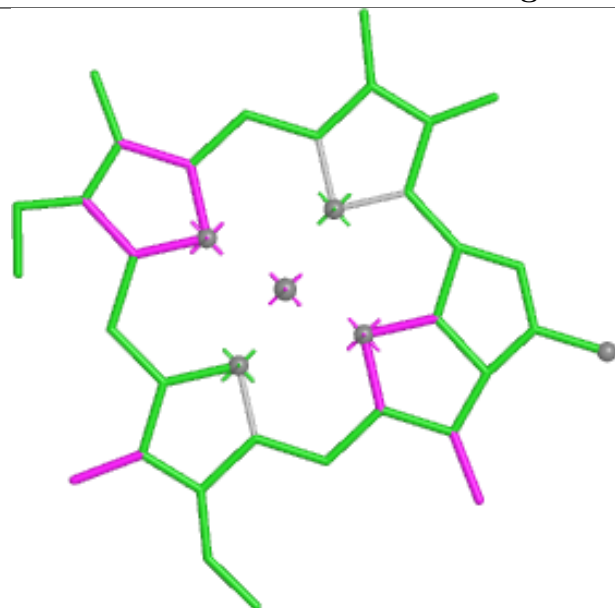


Rings

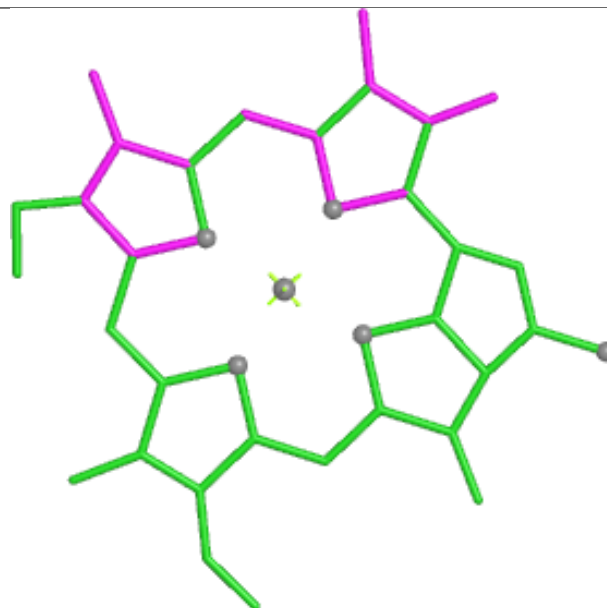




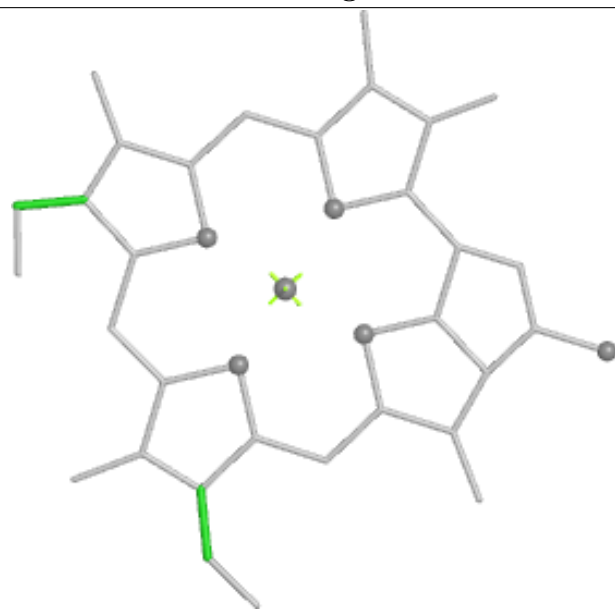
Ligand CLA 3 309



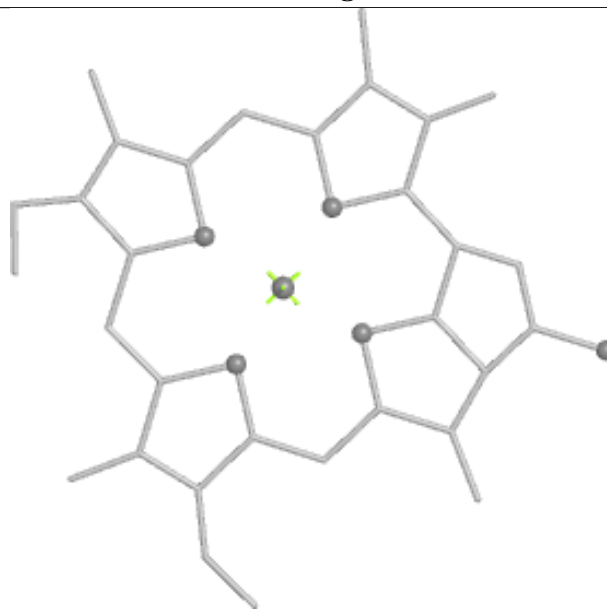
Bond lengths



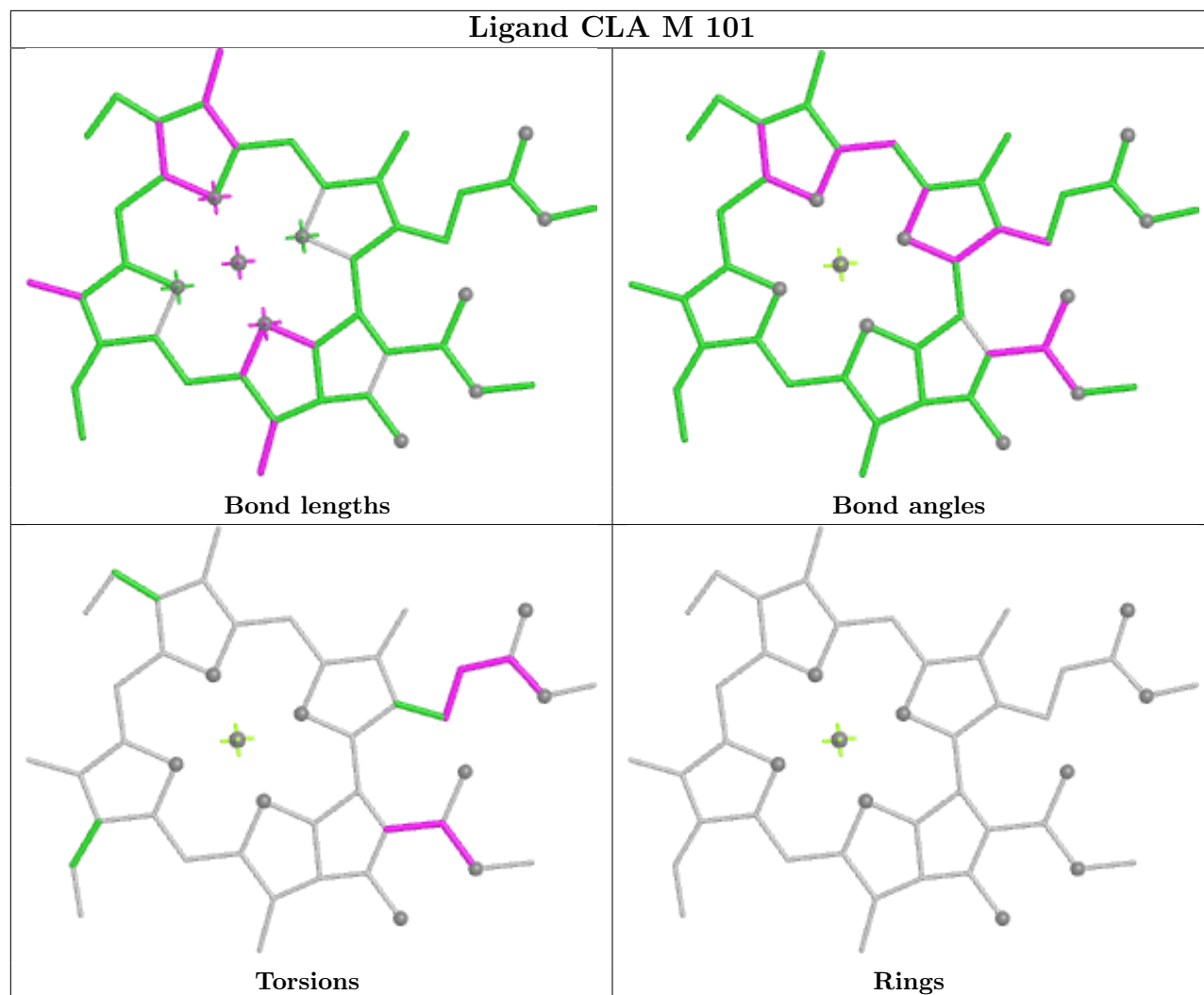
Bond angles



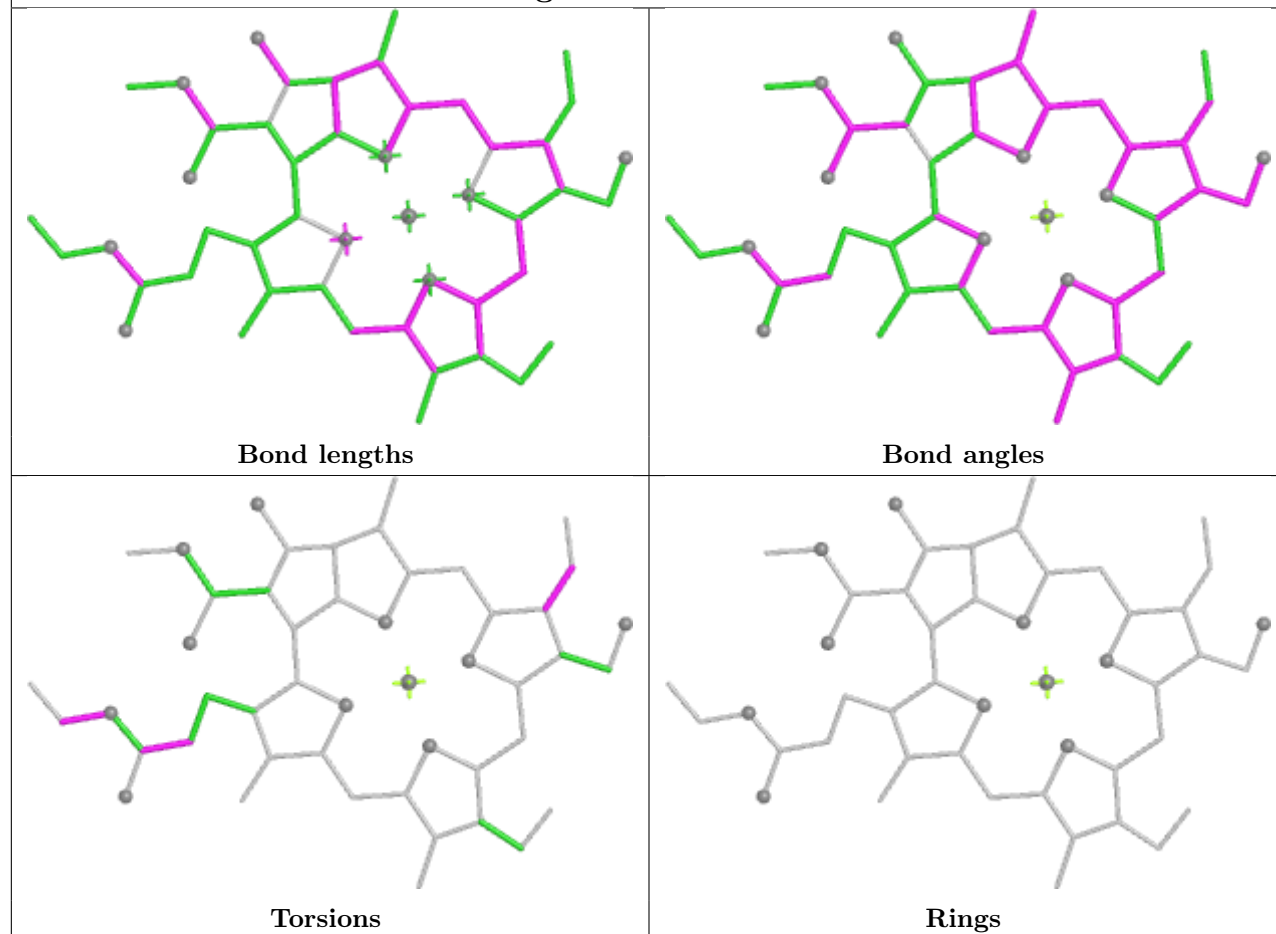
Torsions



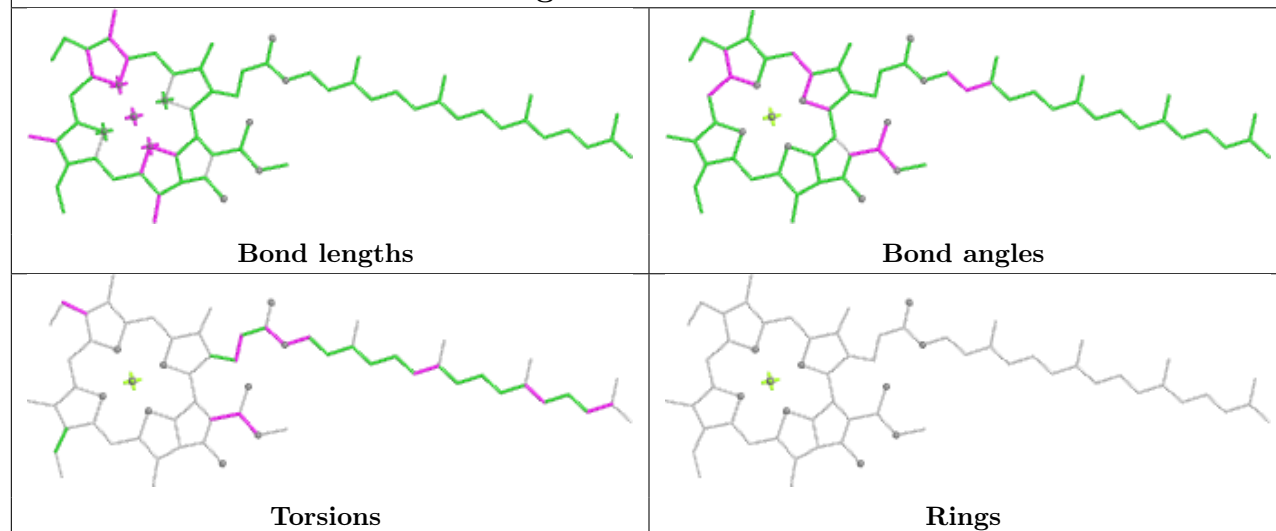
Rings



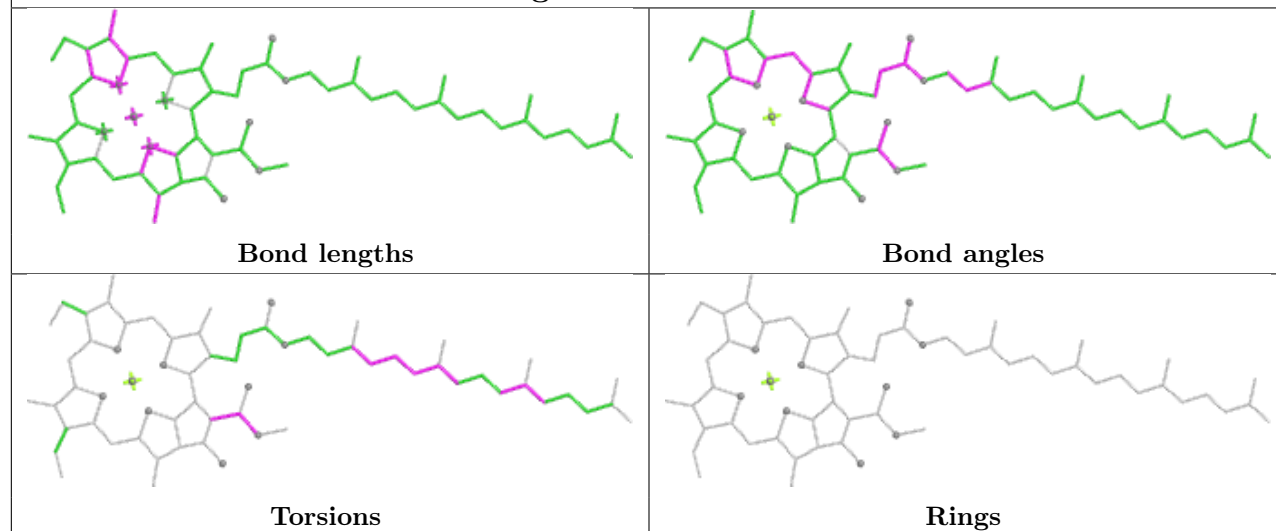
Ligand CHL 0 306



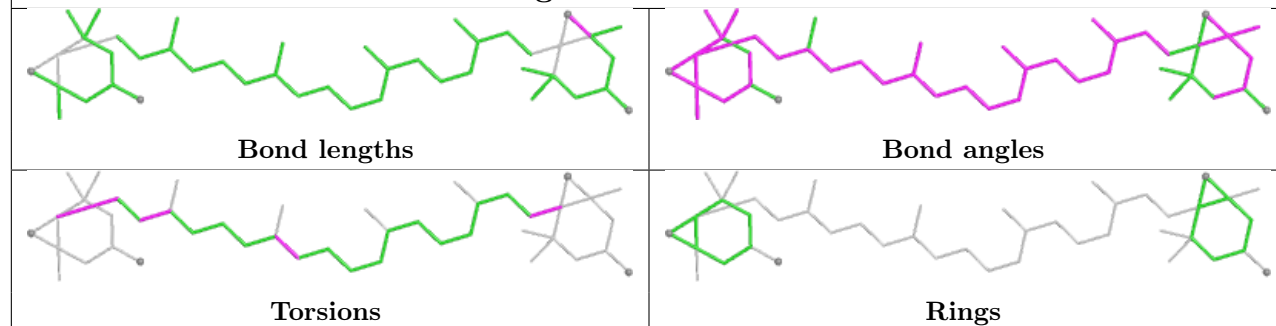
Ligand CLA 9 303



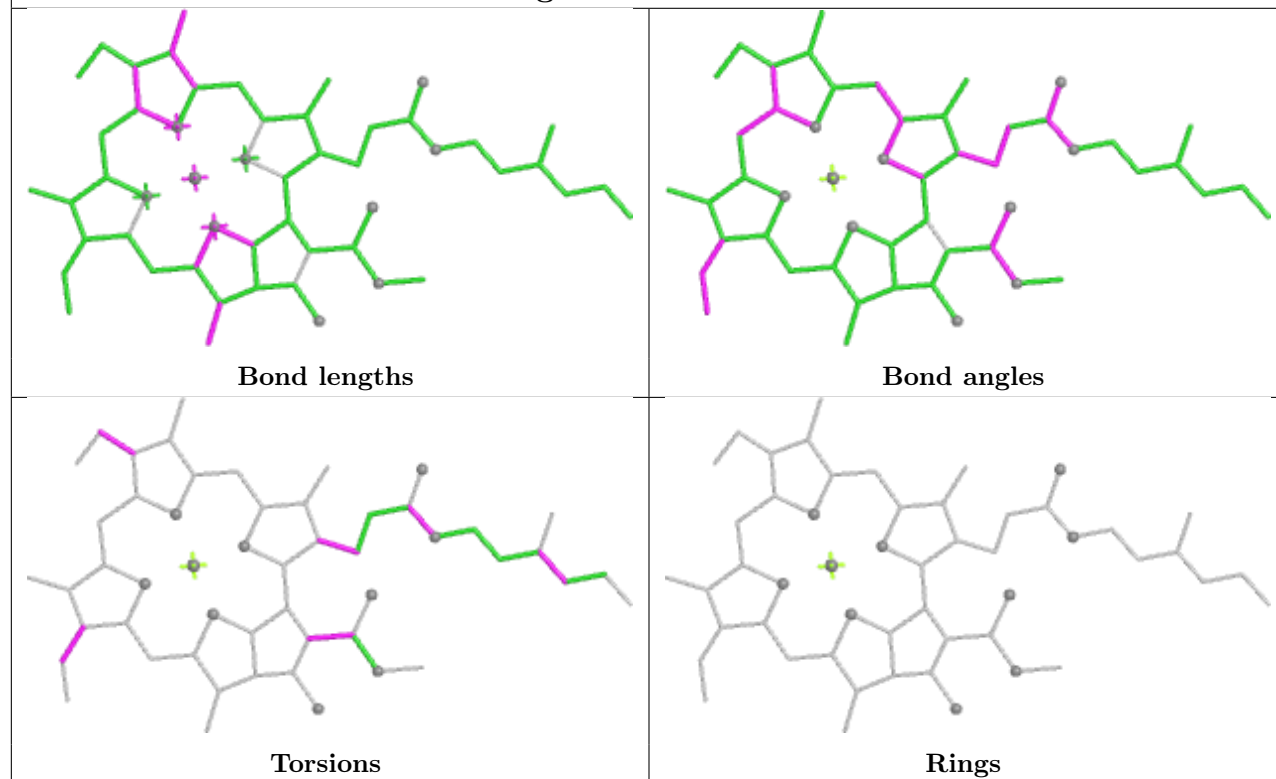
Ligand CLA A 838

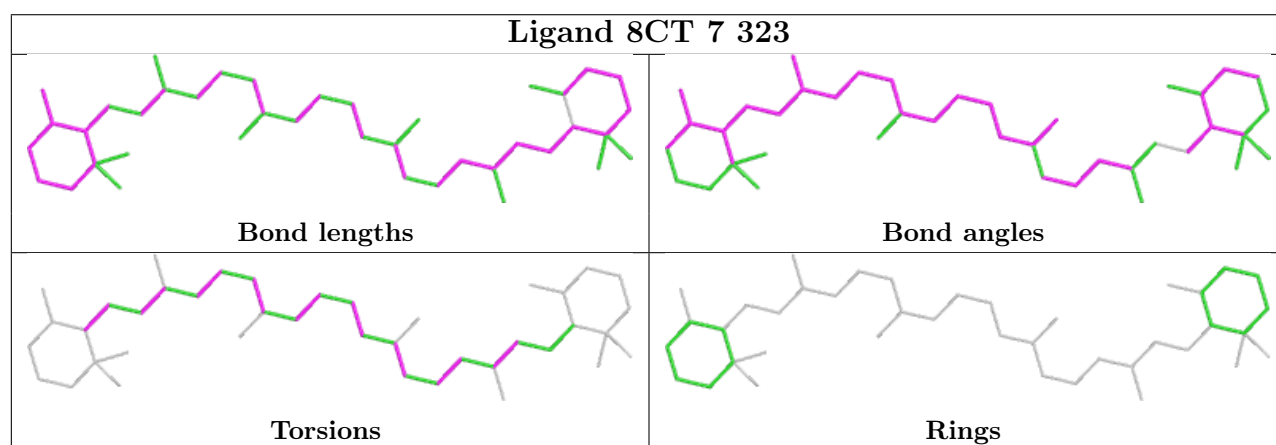
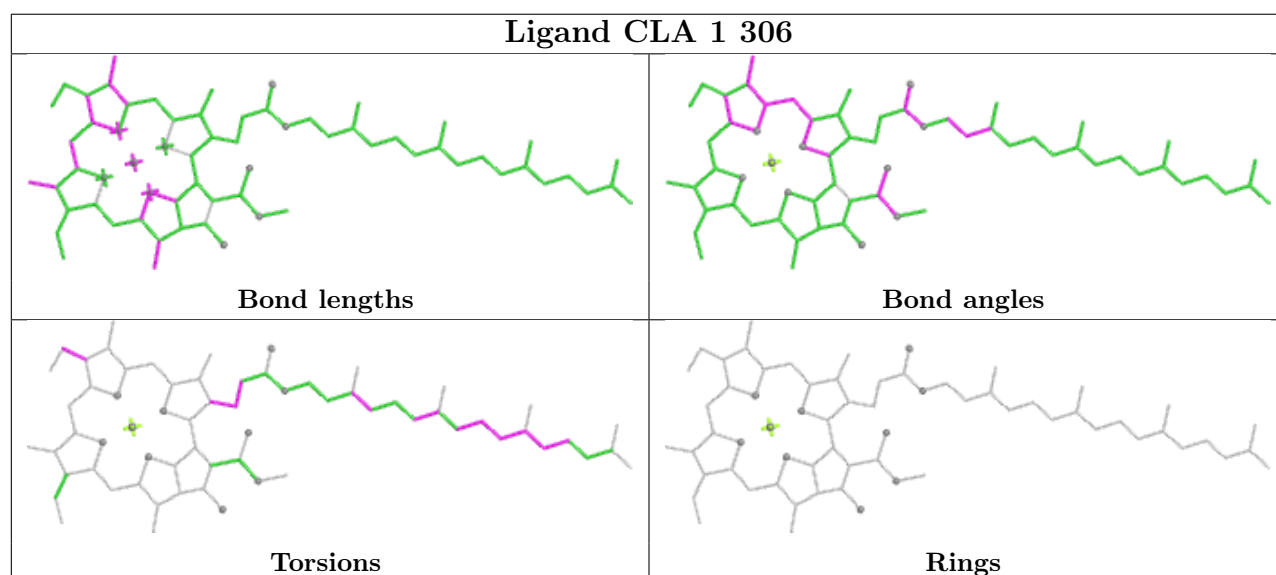
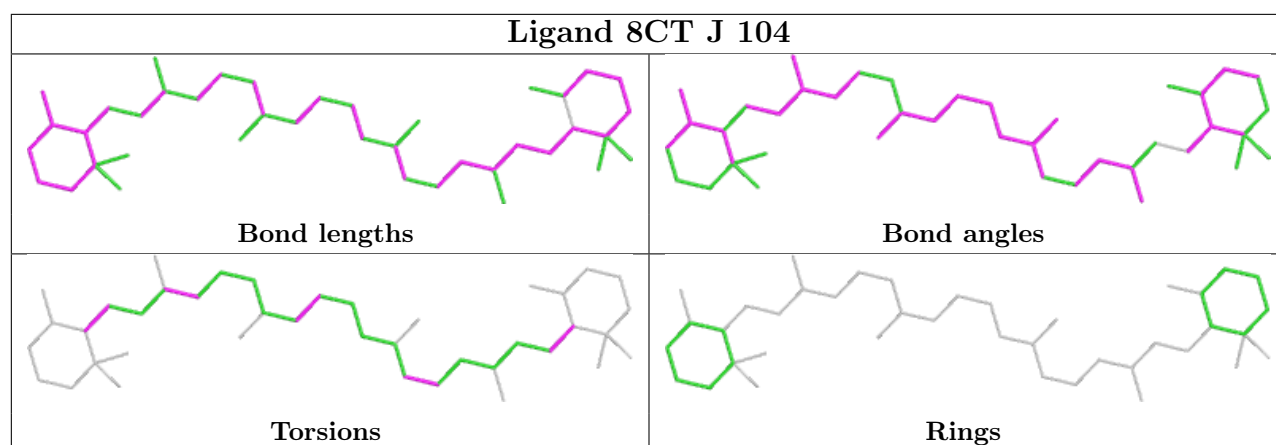


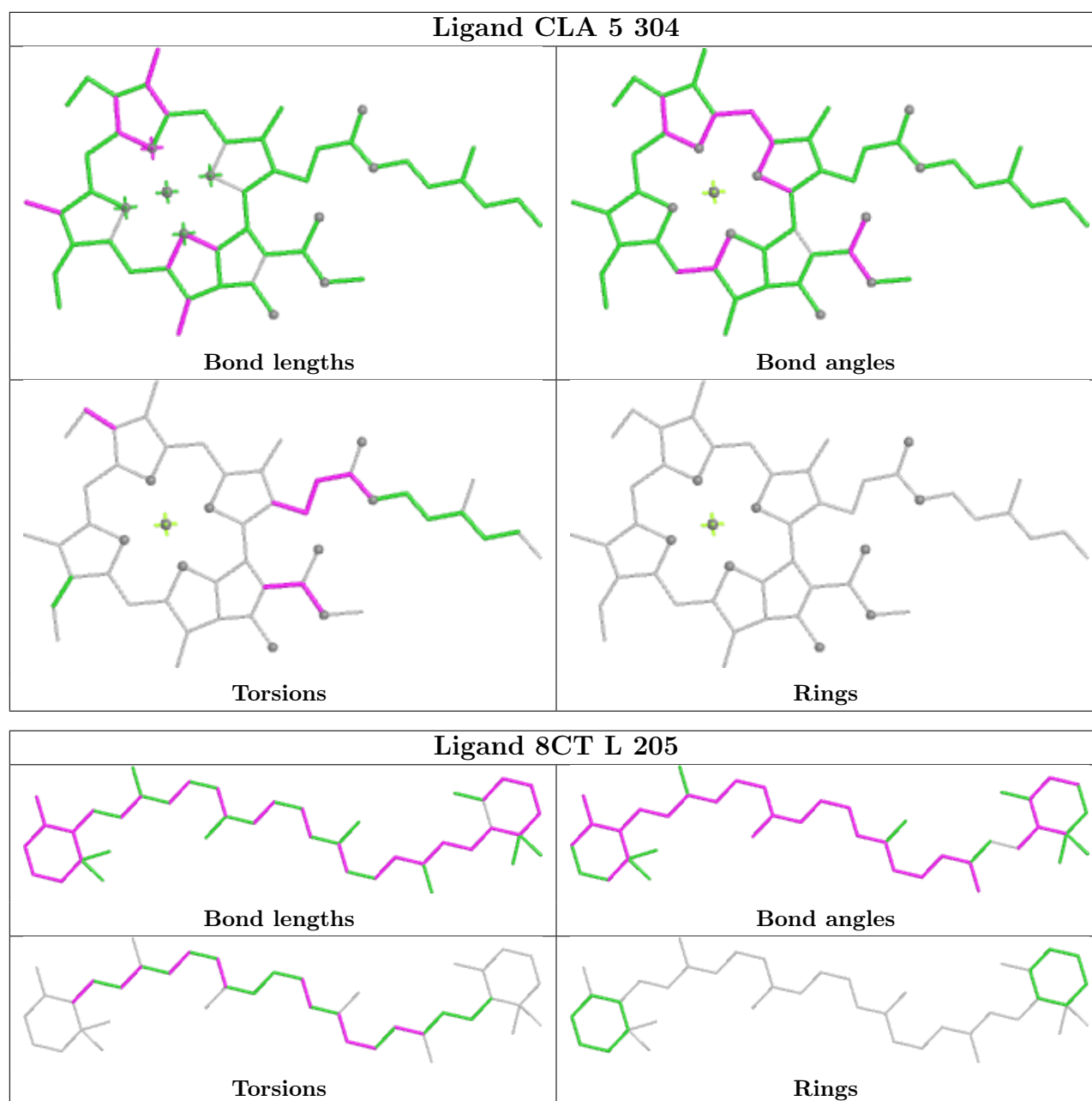
Ligand XAT 8 316



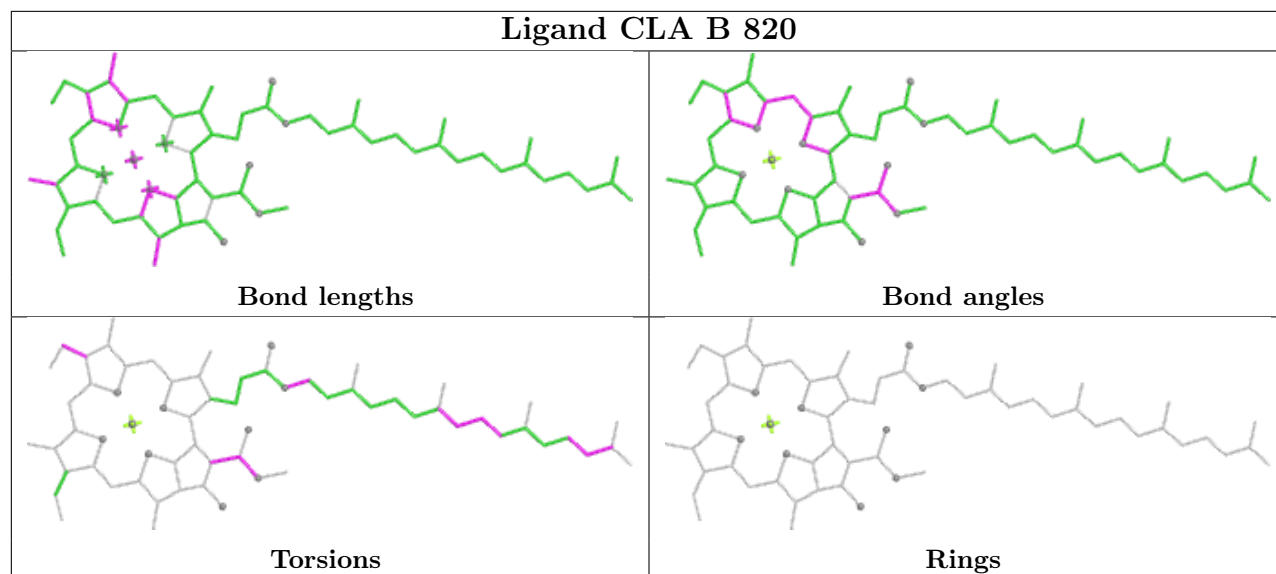
Ligand CLA 0 305



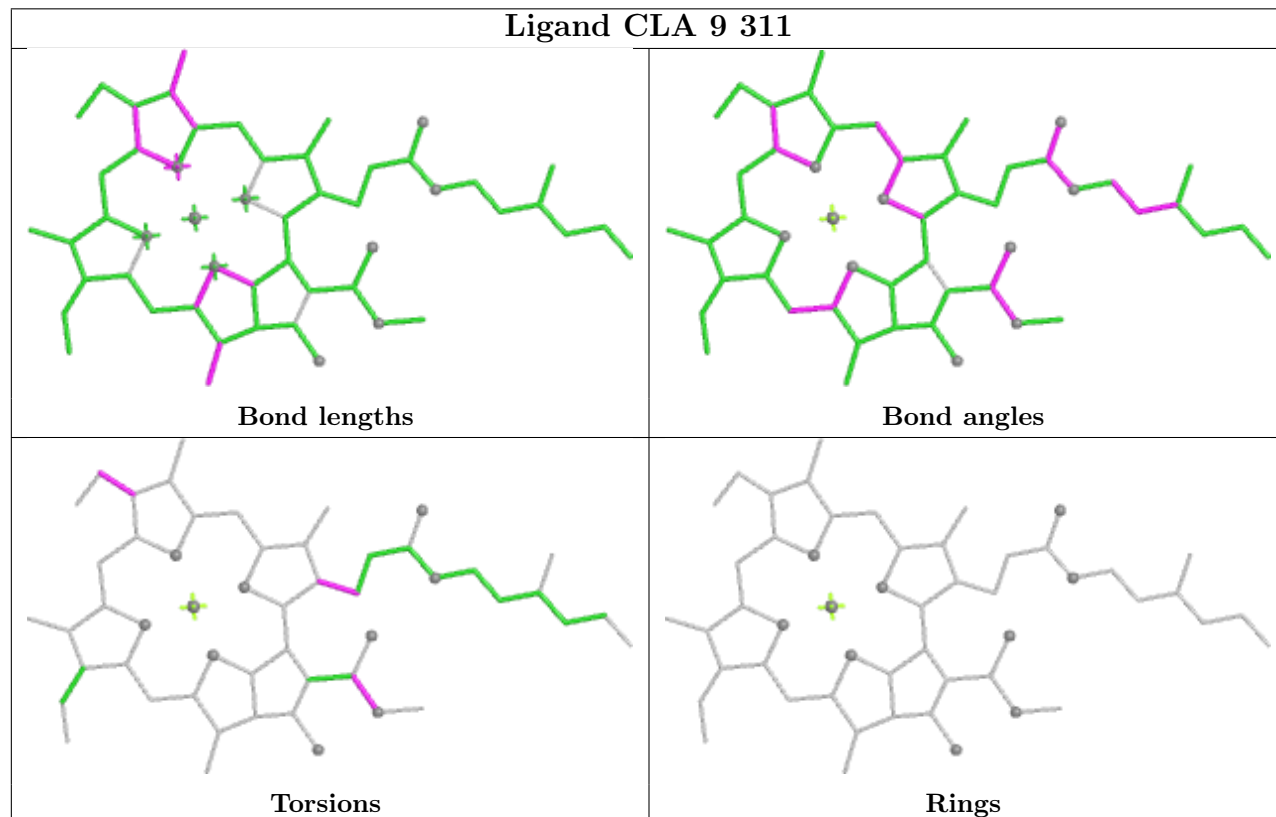




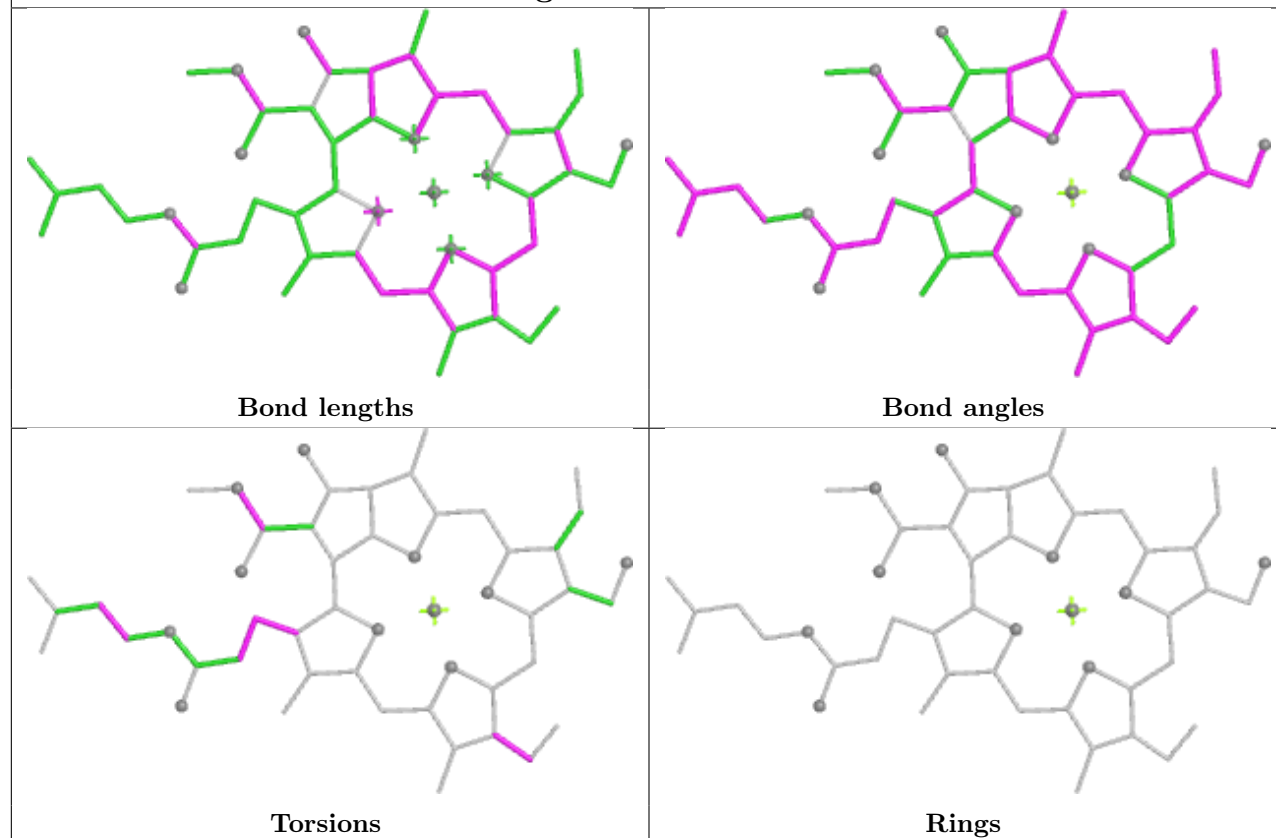
Ligand CLA B 820



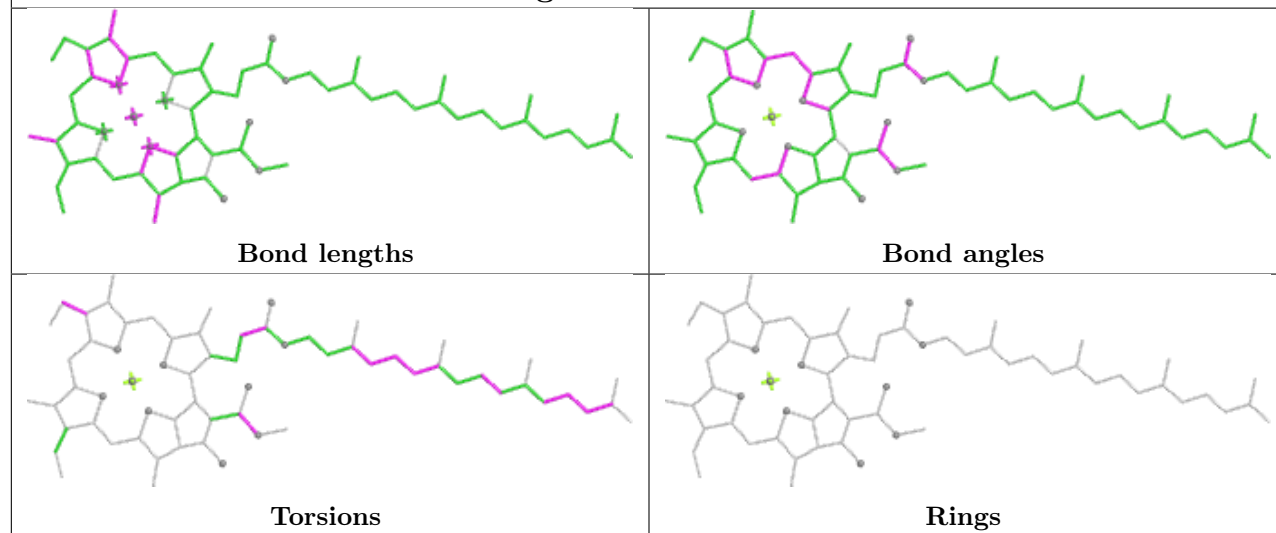
Ligand CLA 9 311



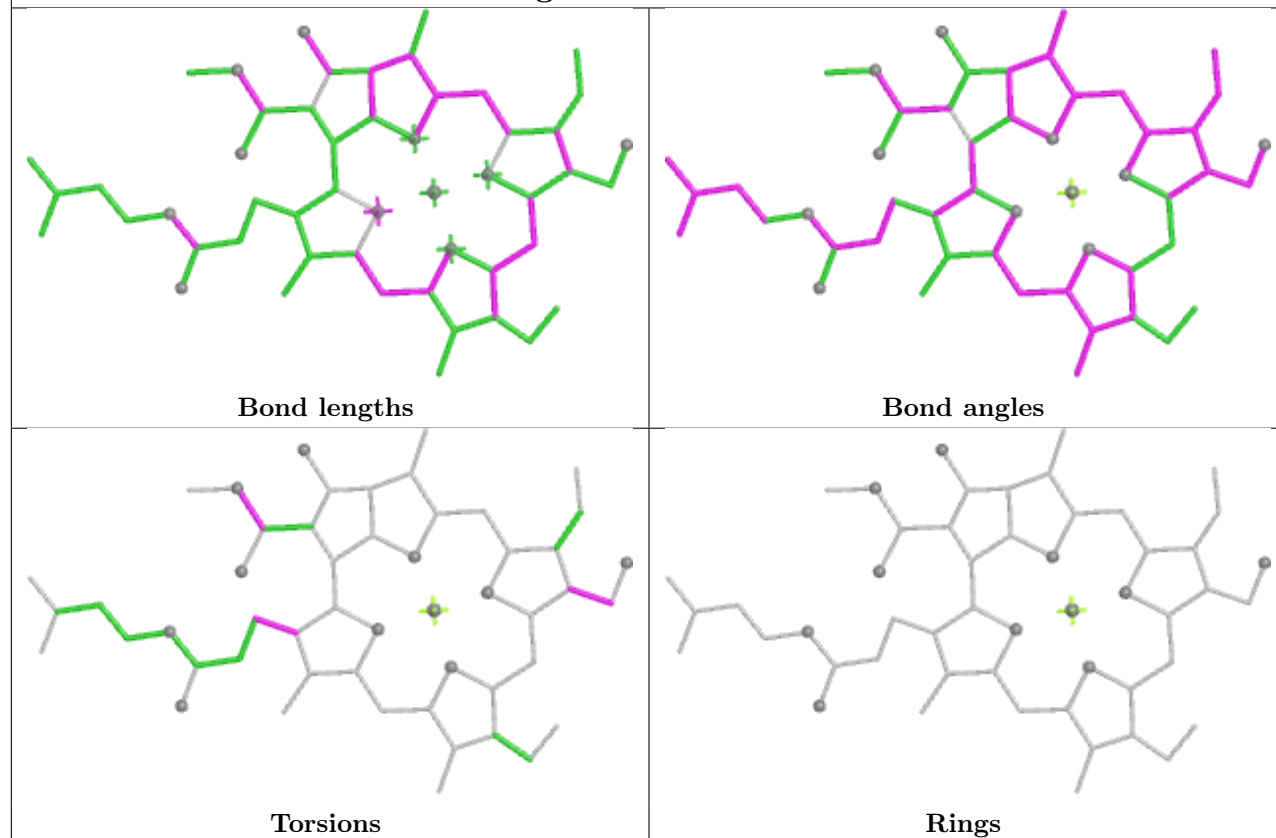
Ligand CHL 6 308



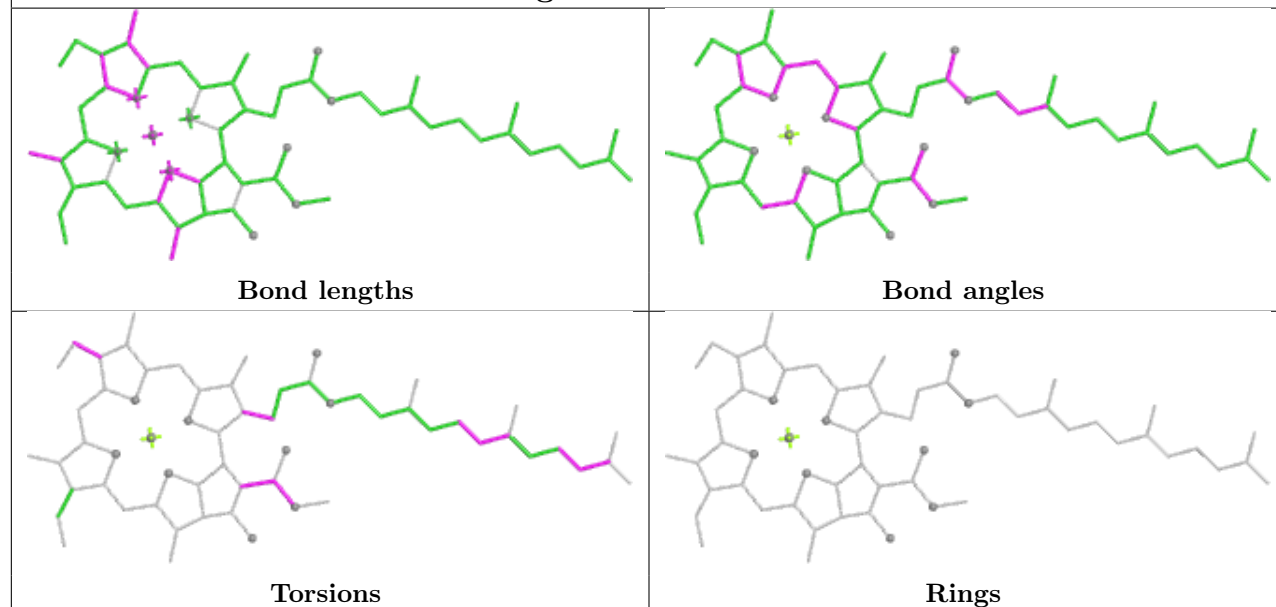
Ligand CLA 6 304



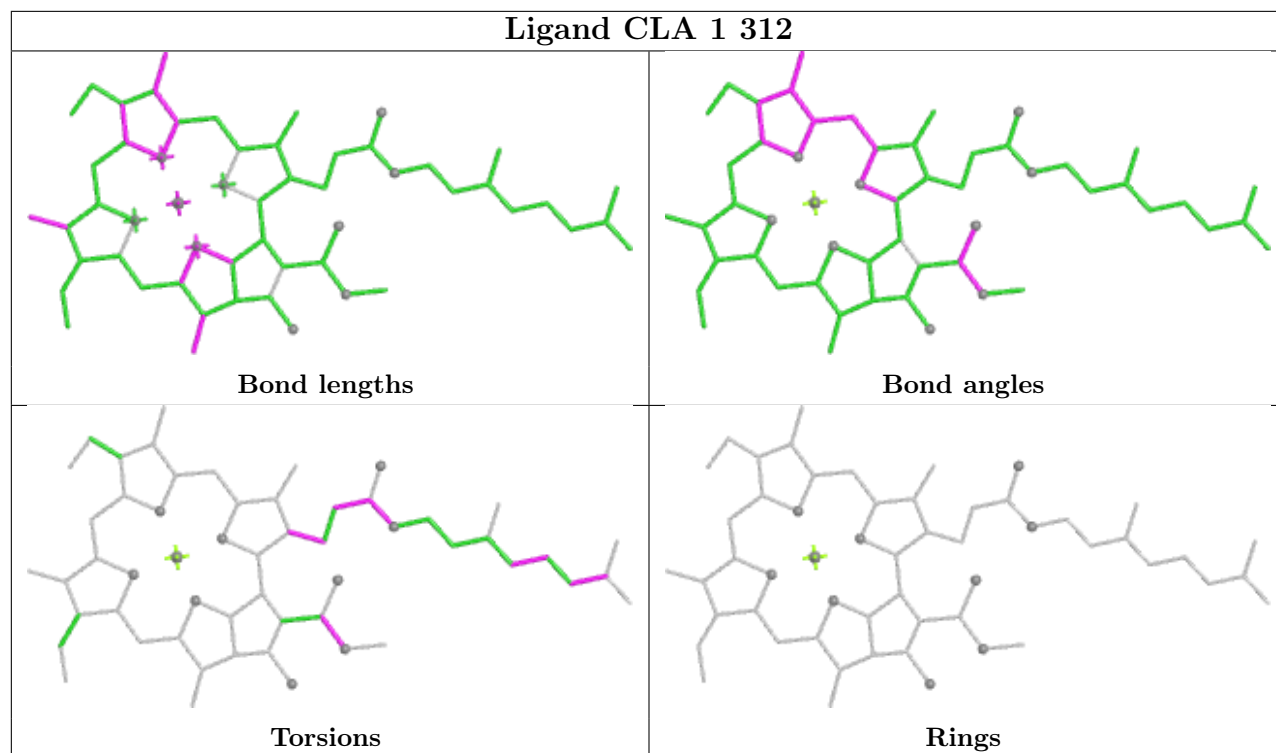
Ligand CHL 4 307



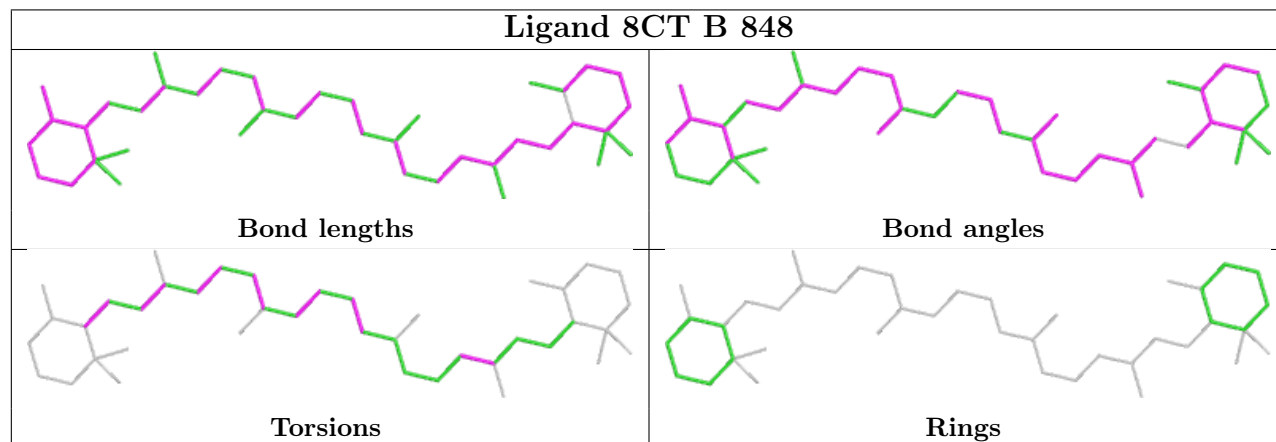
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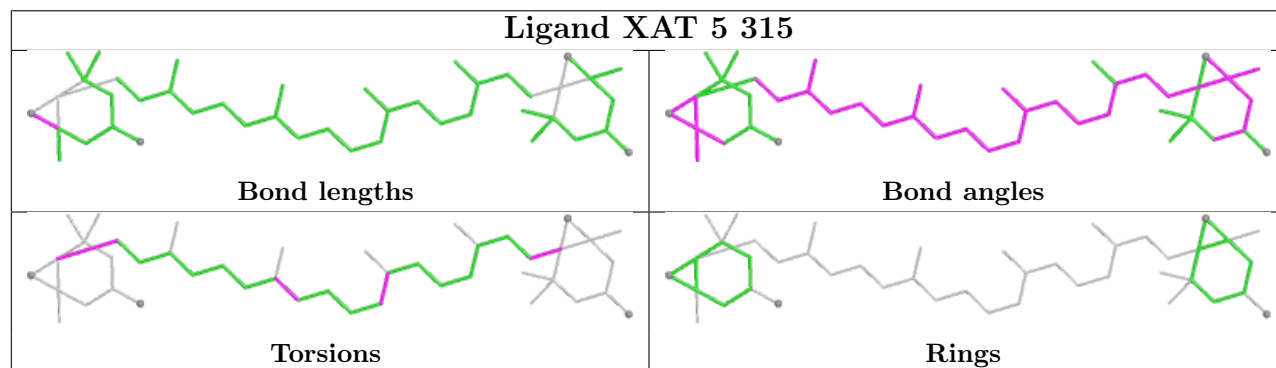
Ligand CLA 1 312



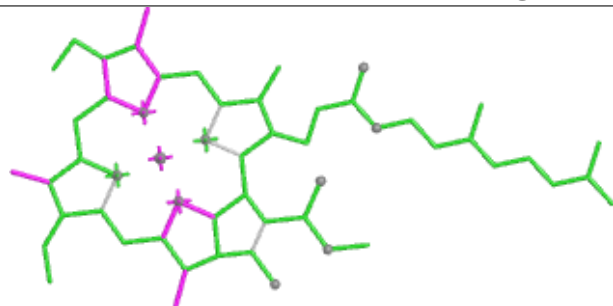
Ligand 8CT B 848



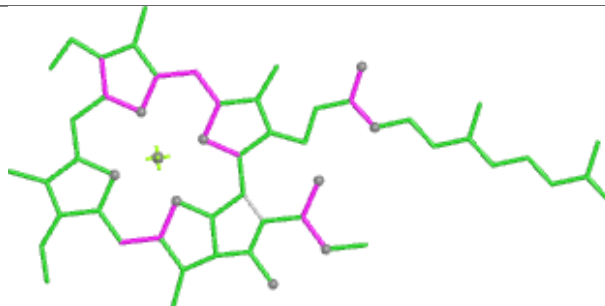
Ligand XAT 5 315



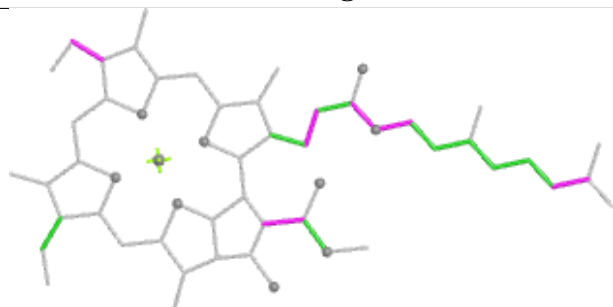
Ligand CLA A 824



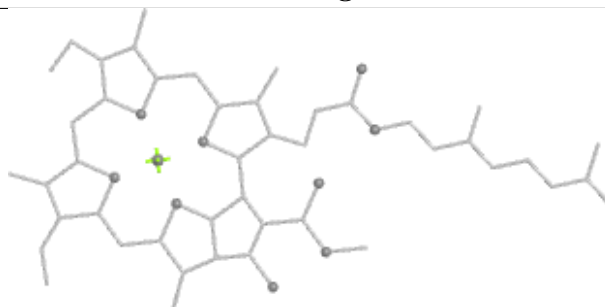
Bond lengths



Bond angles

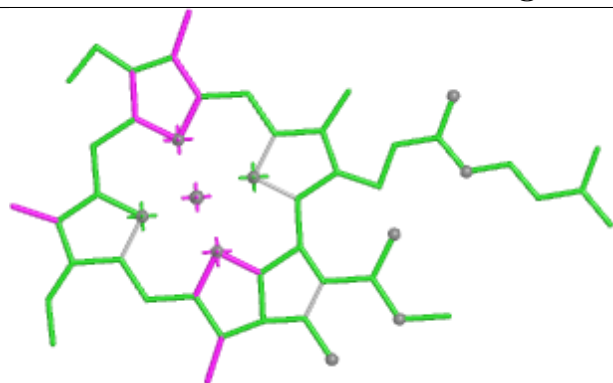


Torsions

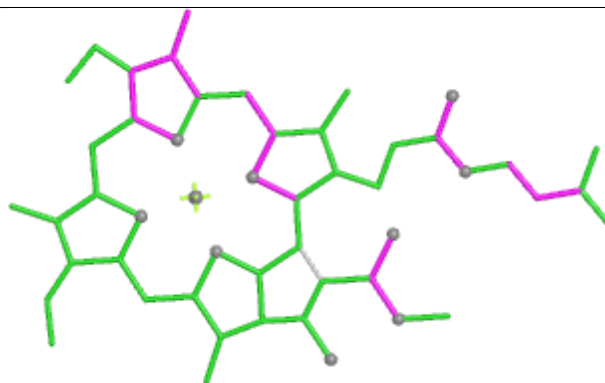


Rings

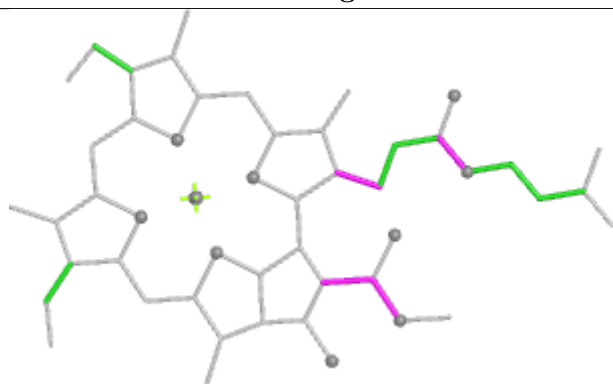
Ligand CLA 7 310



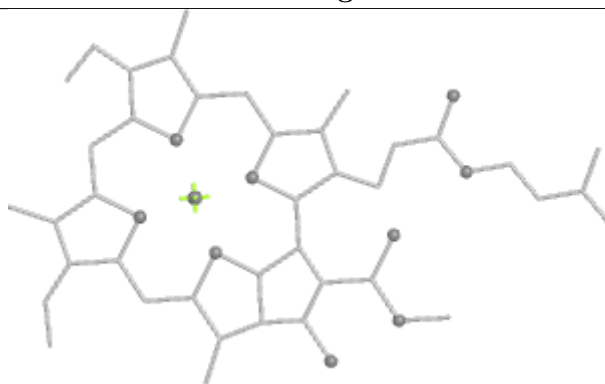
Bond lengths



Bond angles

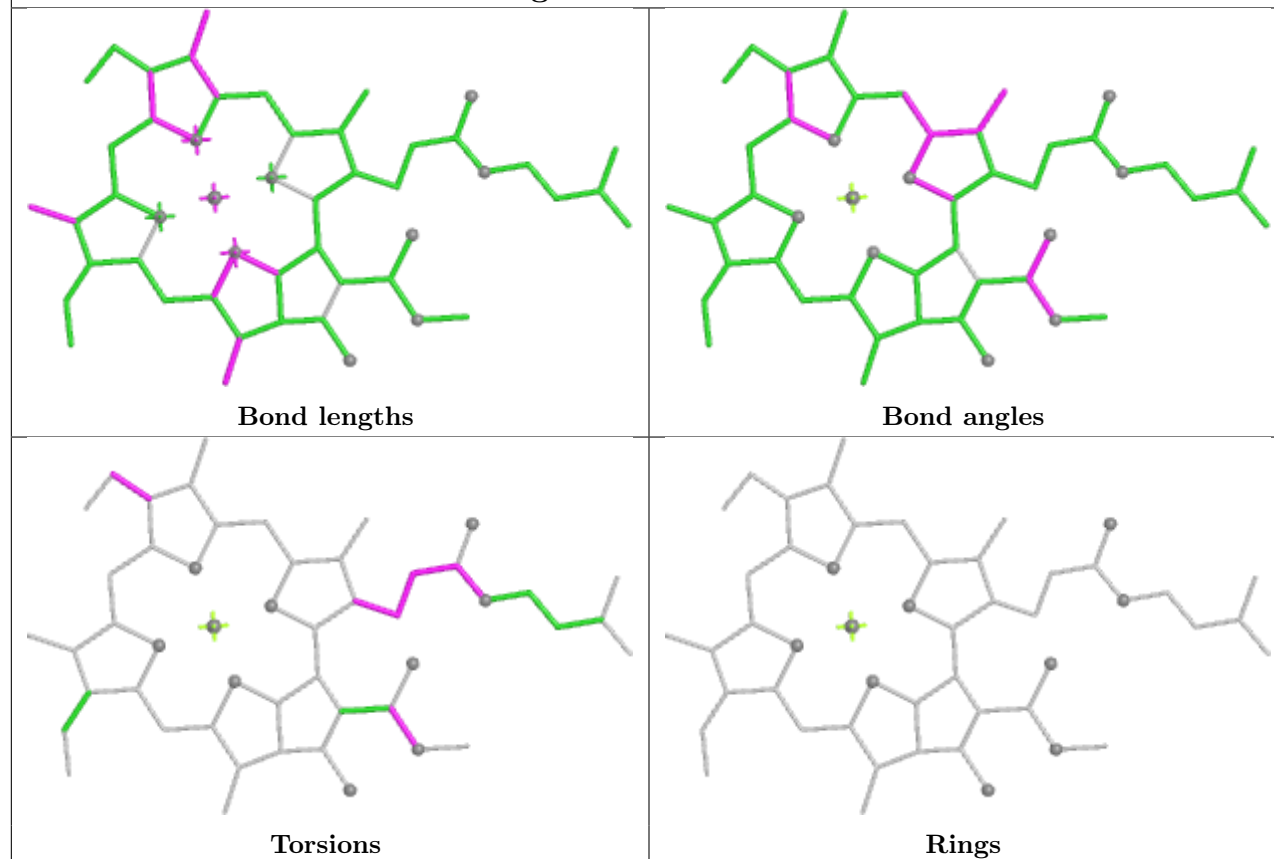


Torsions

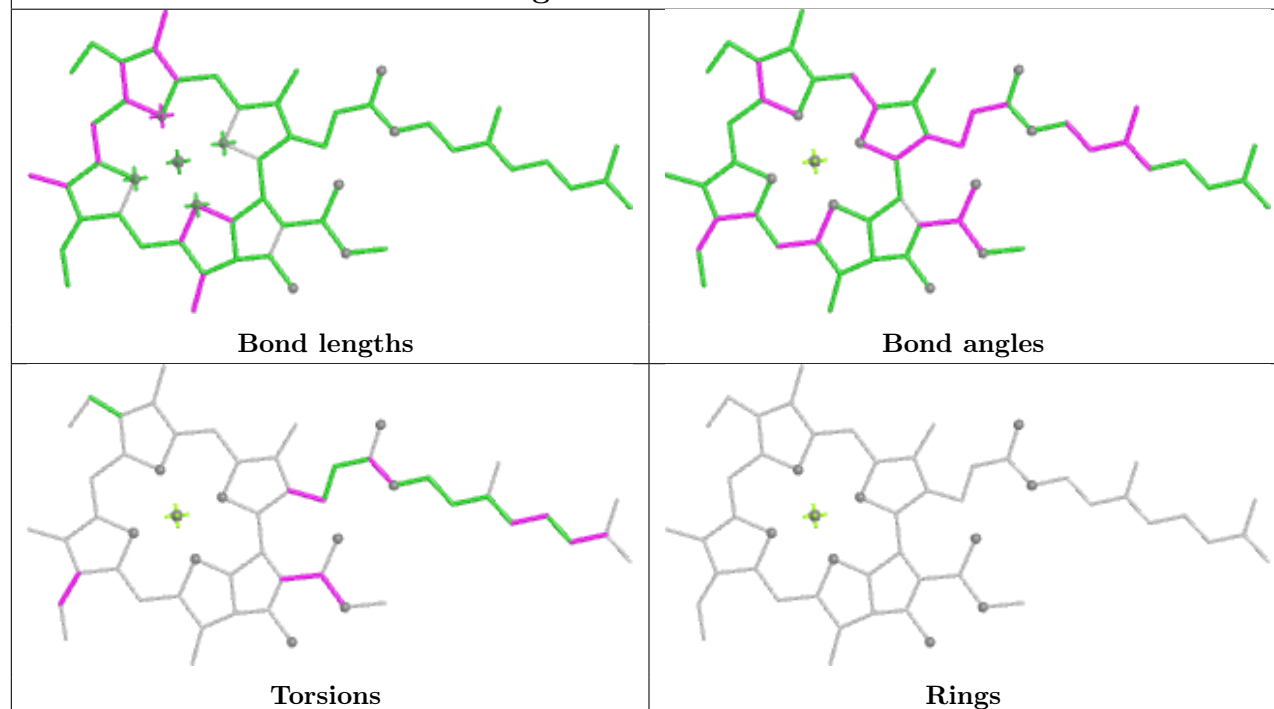


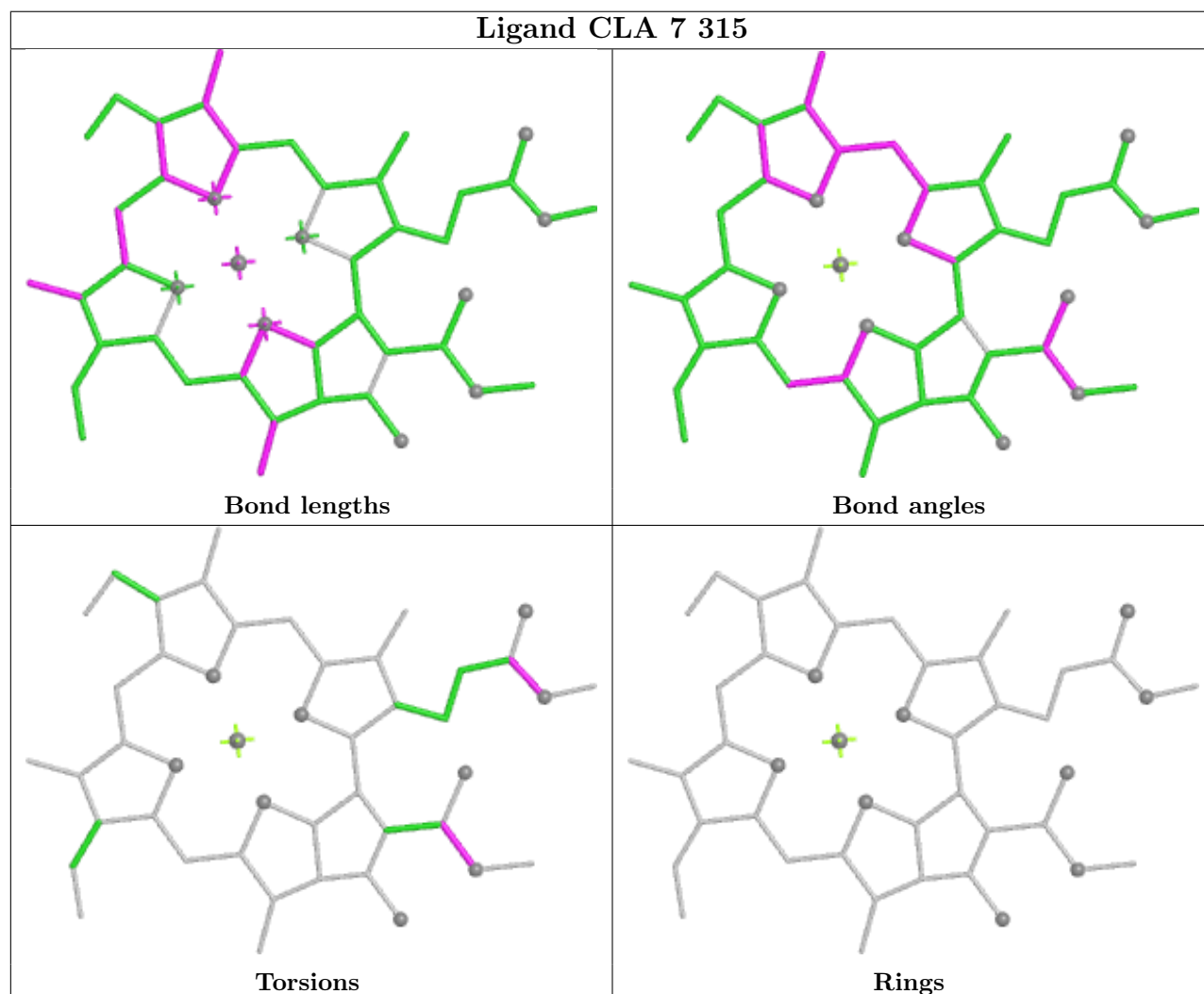
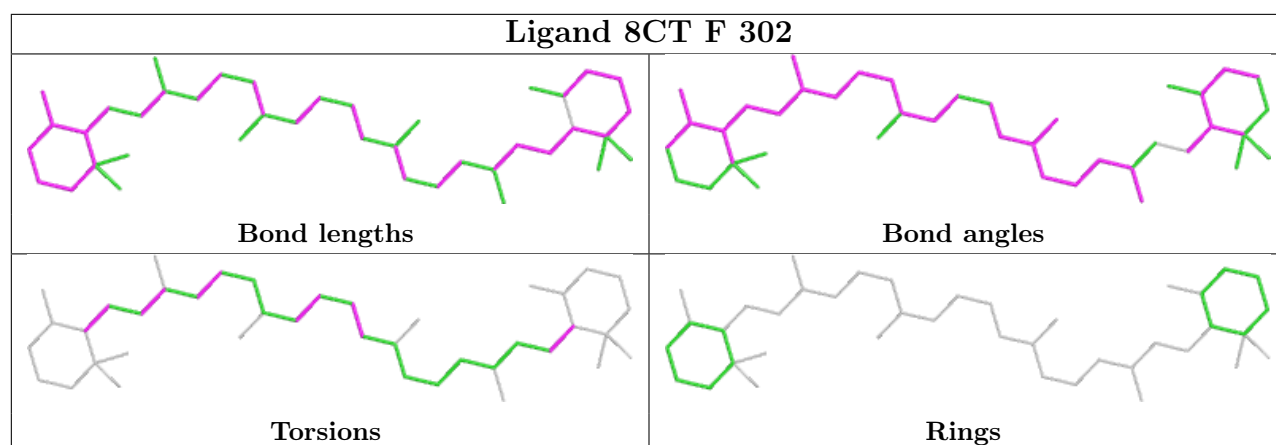
Rings

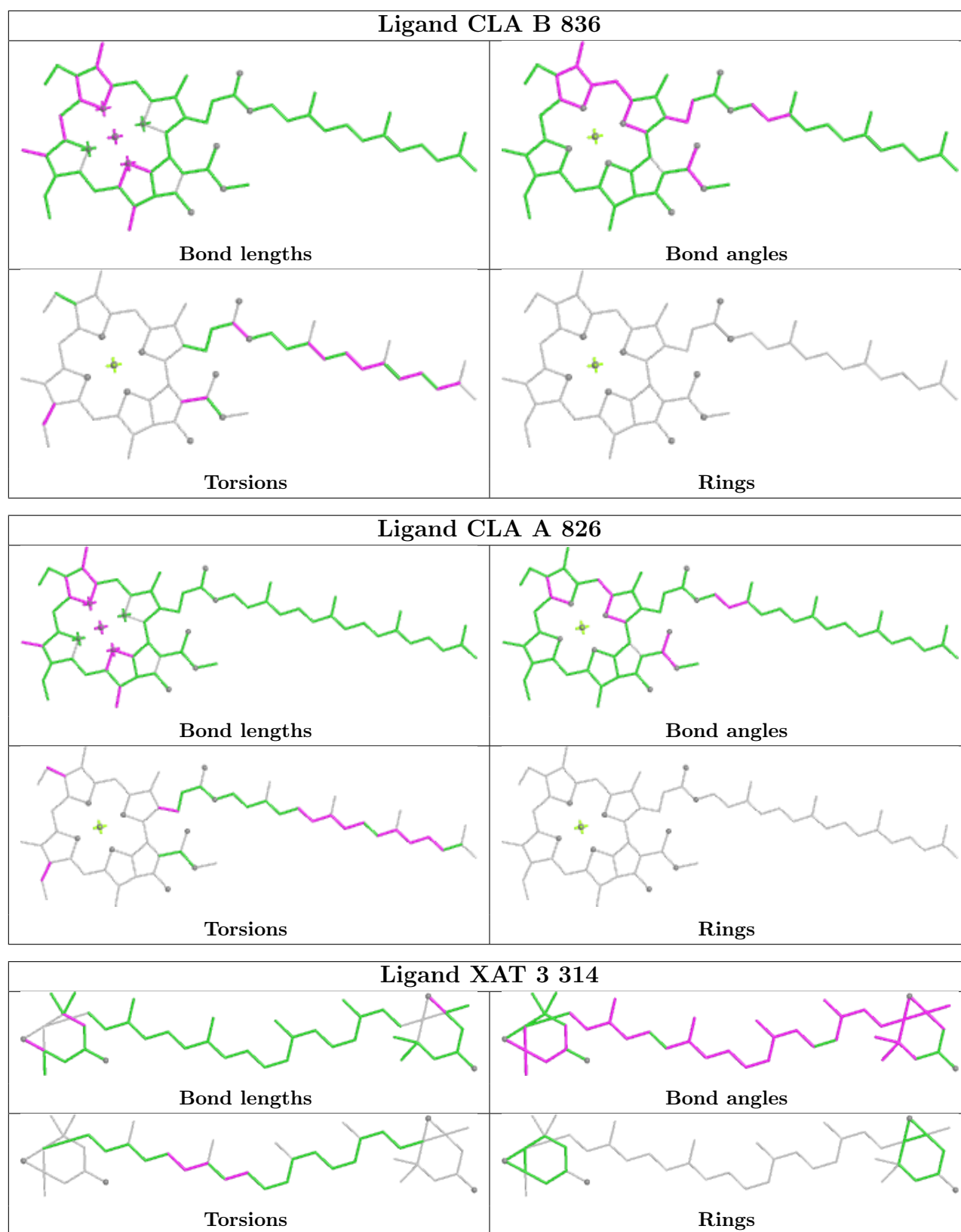
Ligand CLA K 105

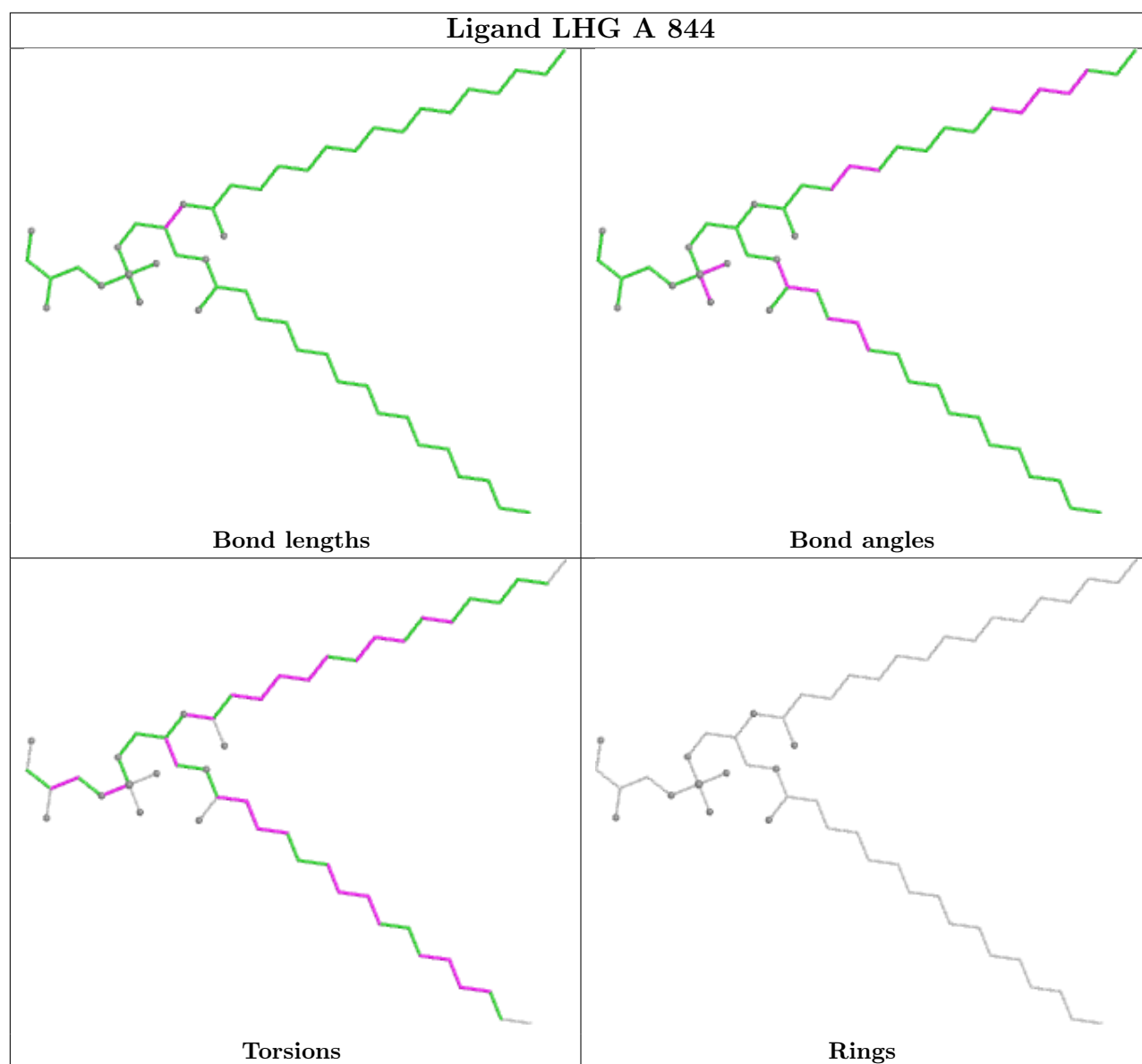


Ligand CLA B 850

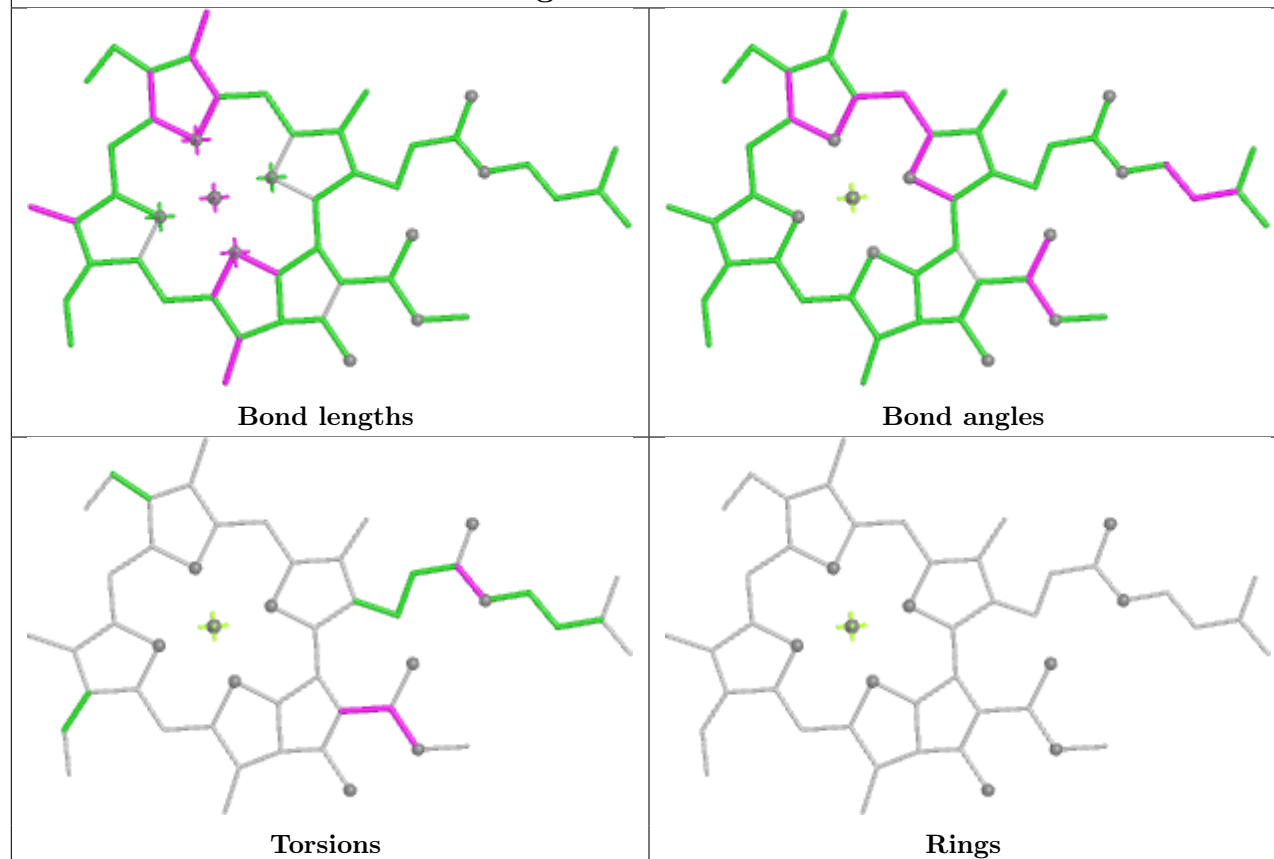




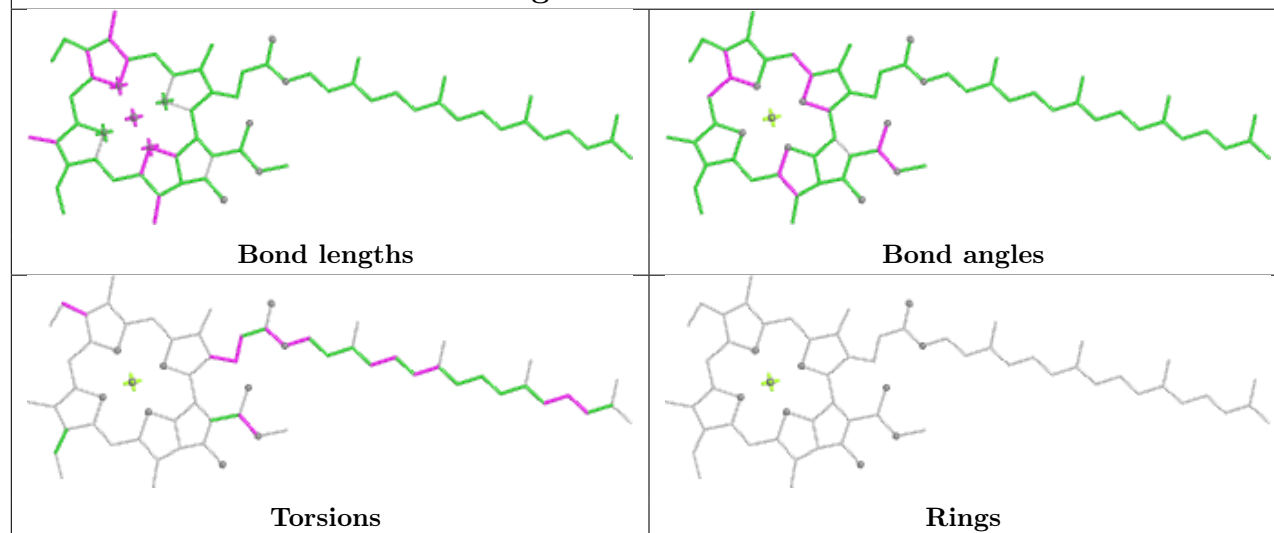




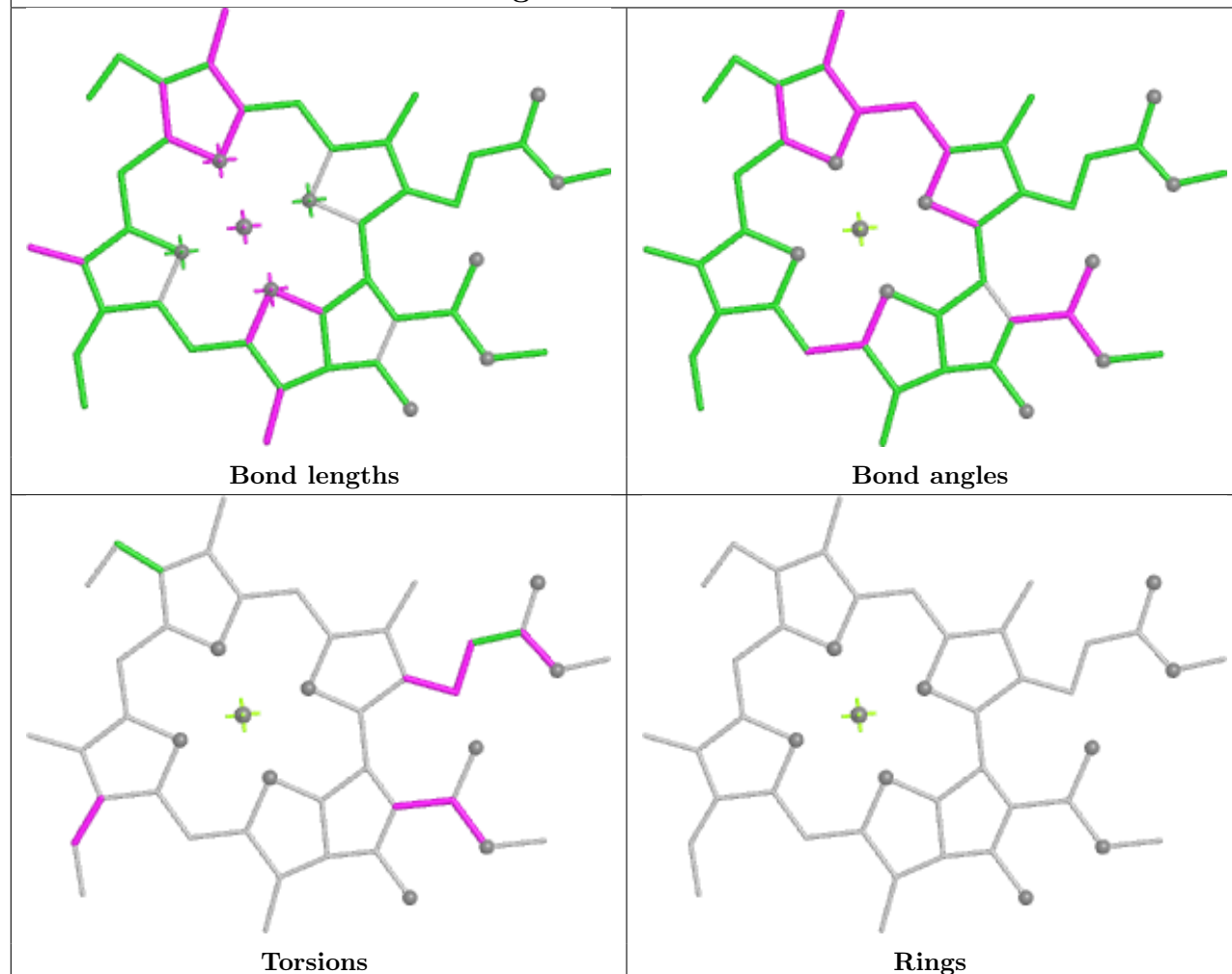
Ligand CLA 2 308



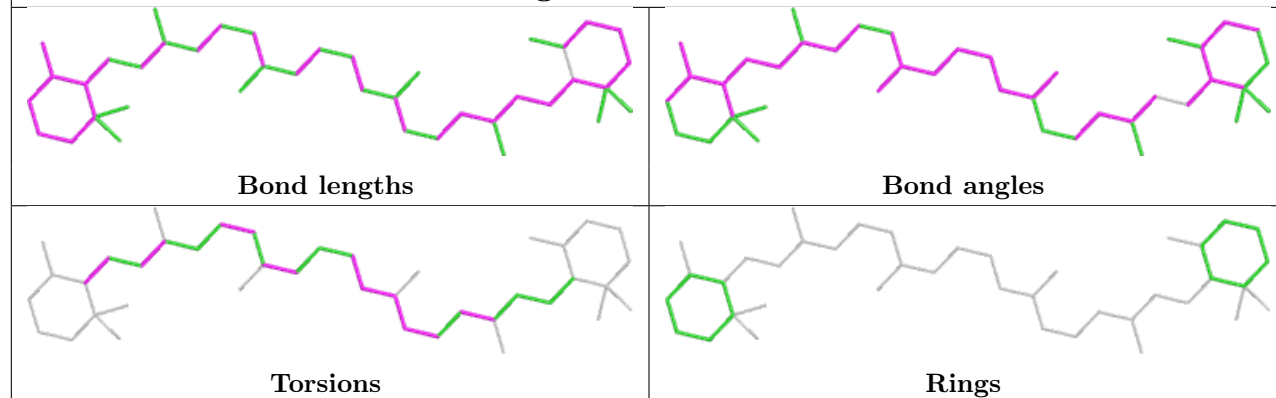
Ligand CLA A 841

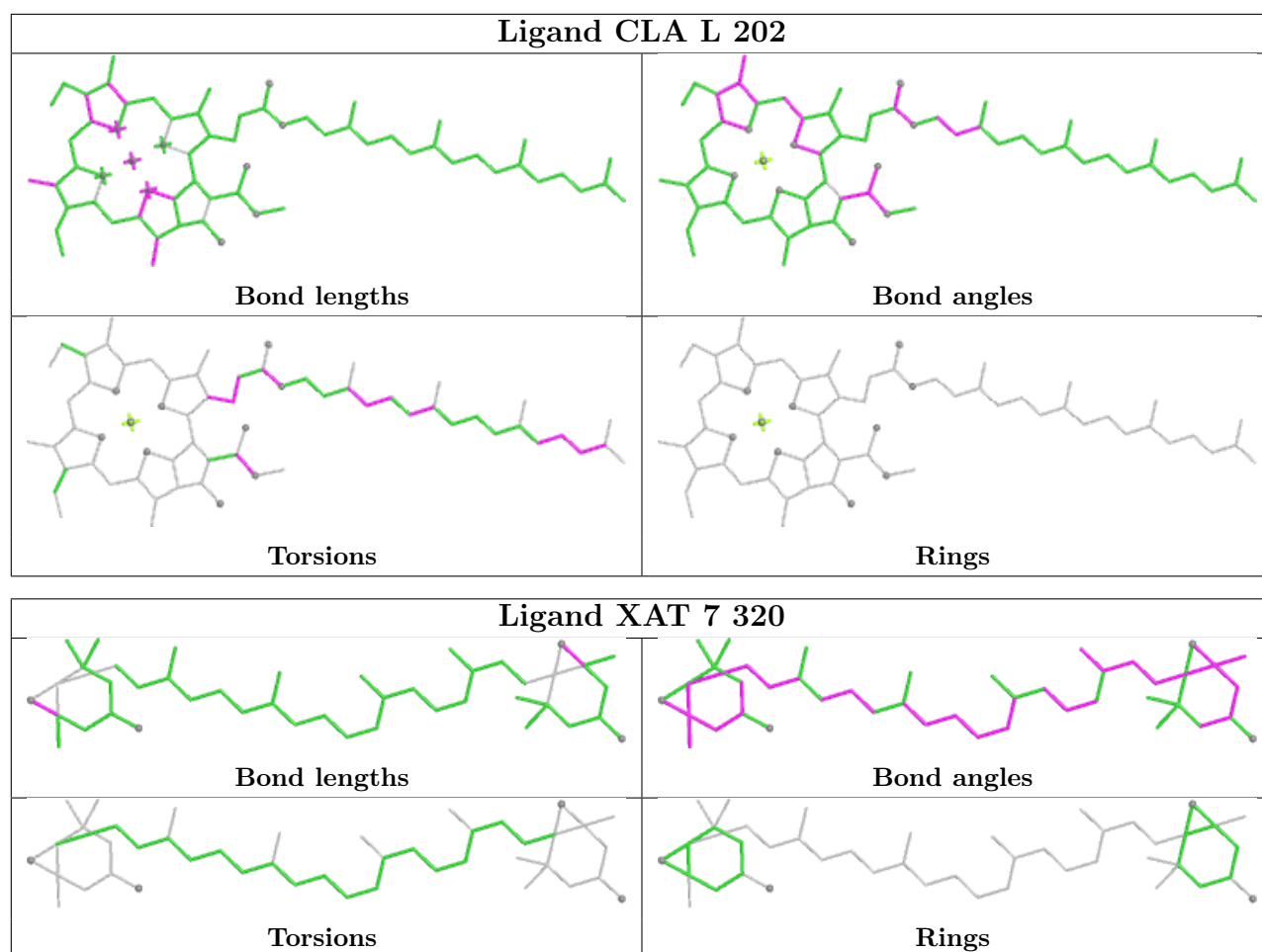


Ligand CLA K 102

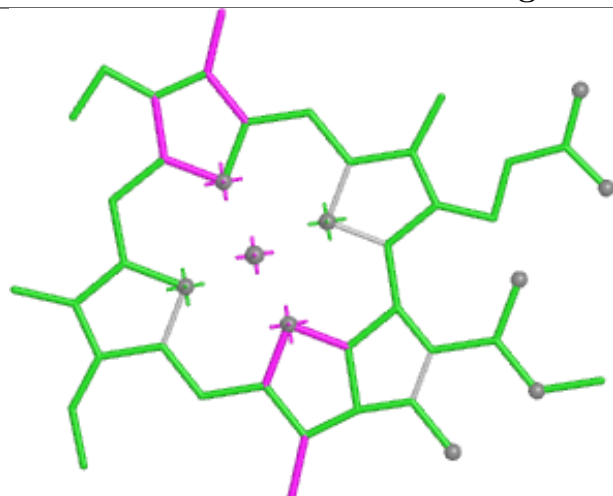


Ligand 8CT B 844

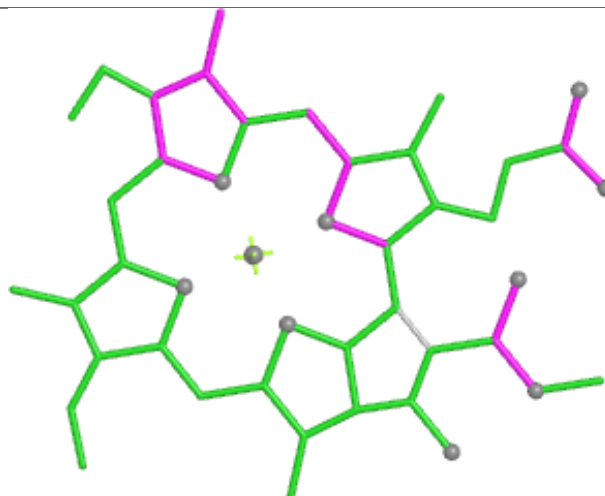




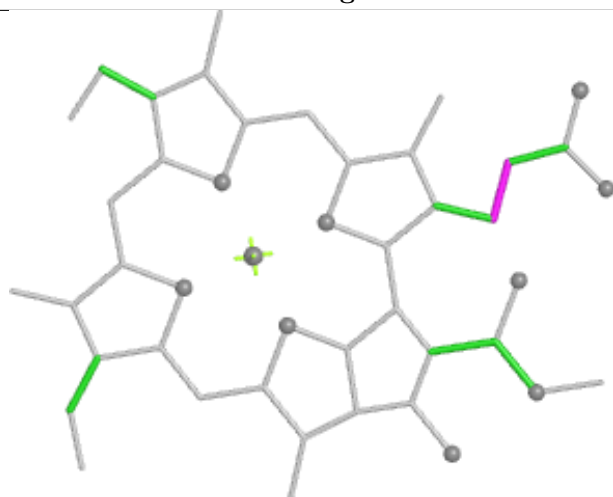
Ligand CLA 5 311



Bond lengths



Bond angles

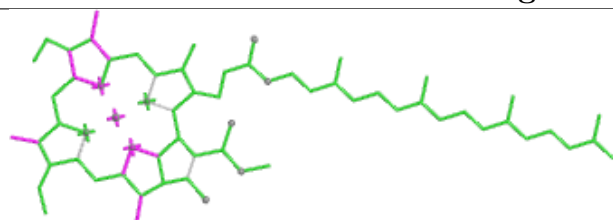


Torsions

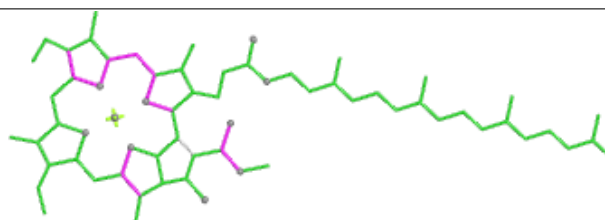


Rings

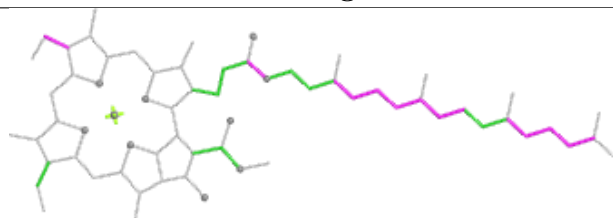
Ligand CLA 9 308



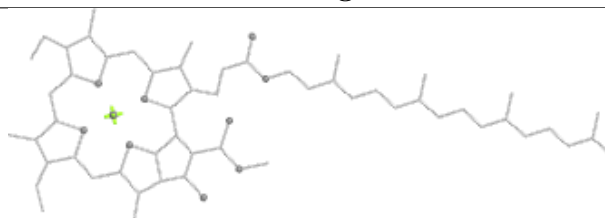
Bond lengths



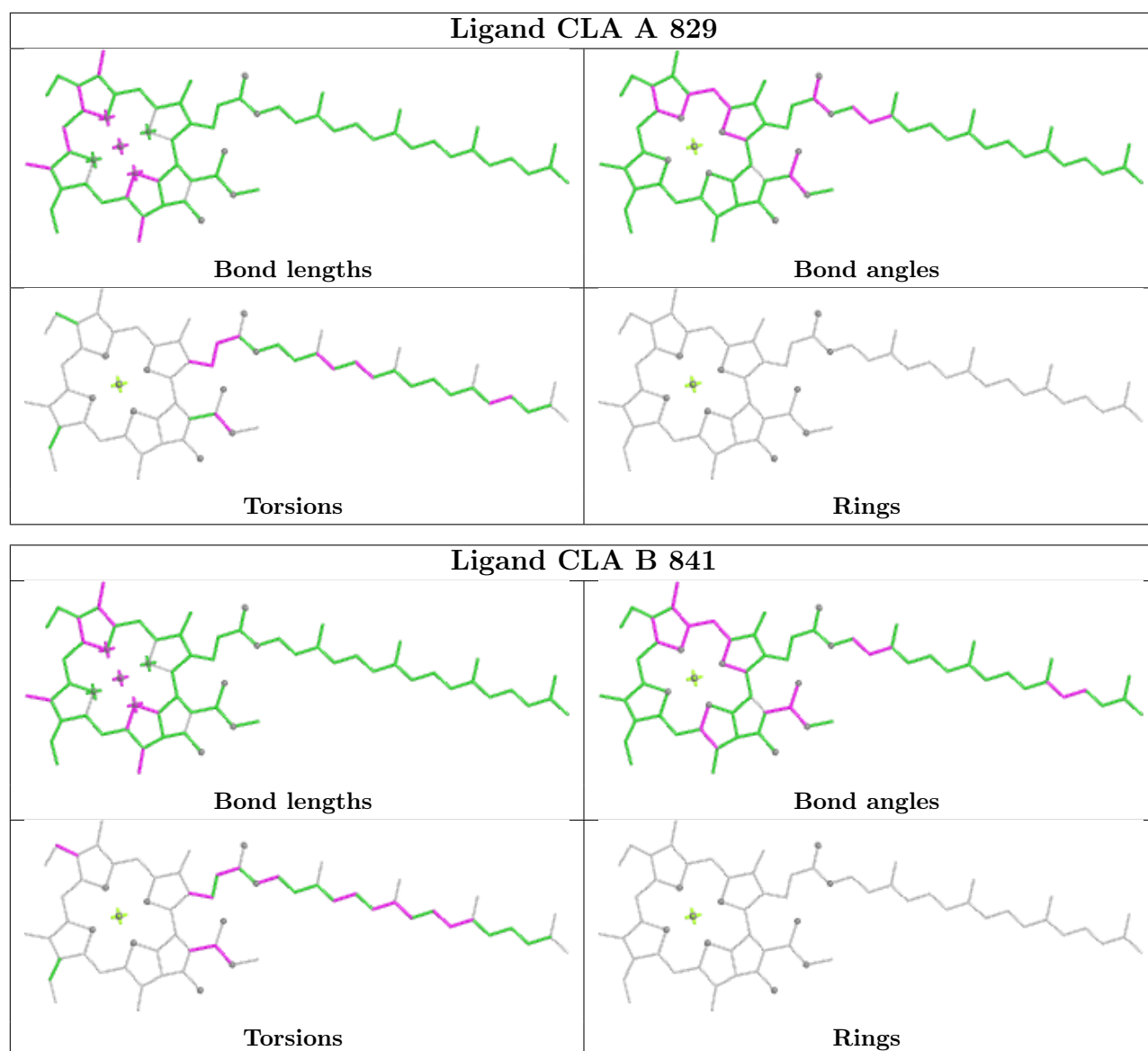
Bond angles



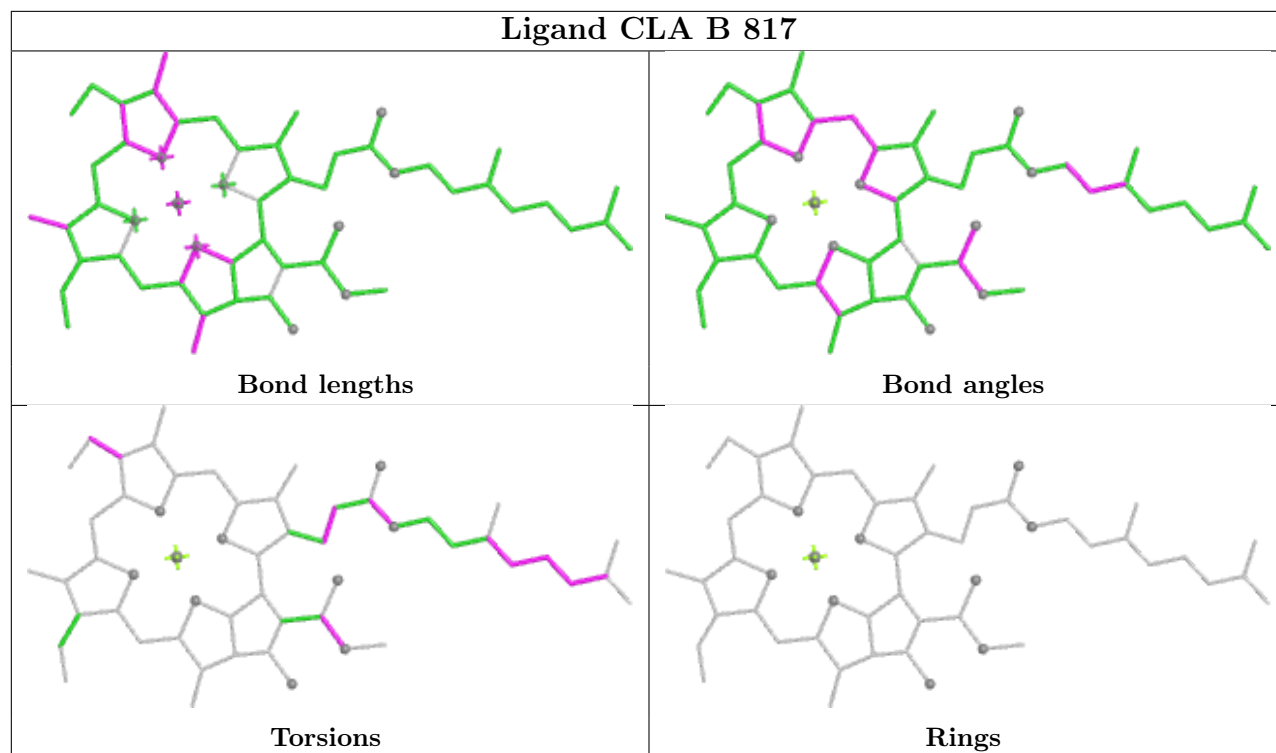
Torsions



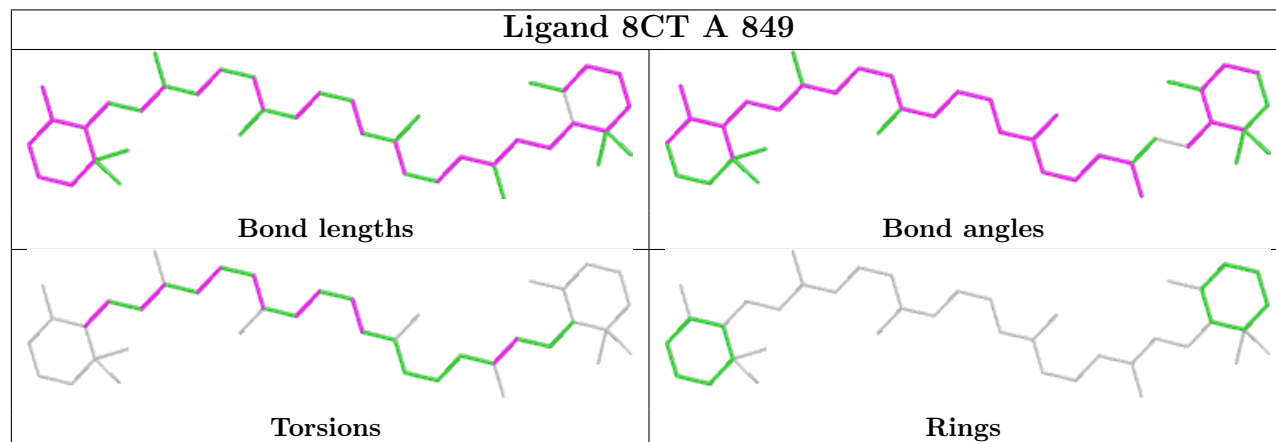
Rings



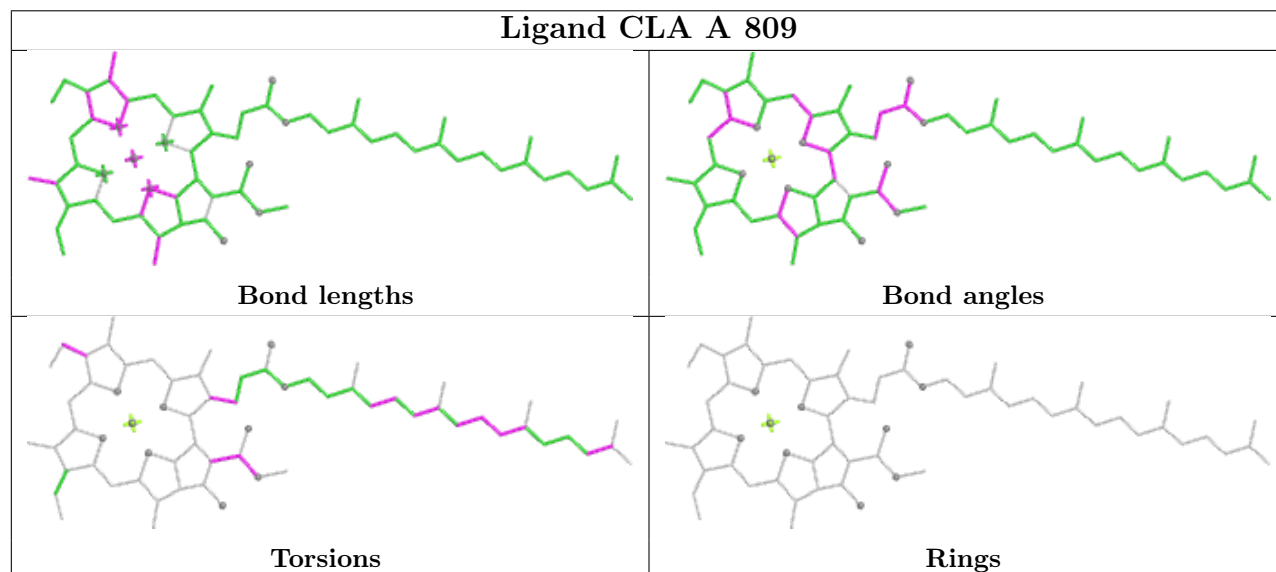
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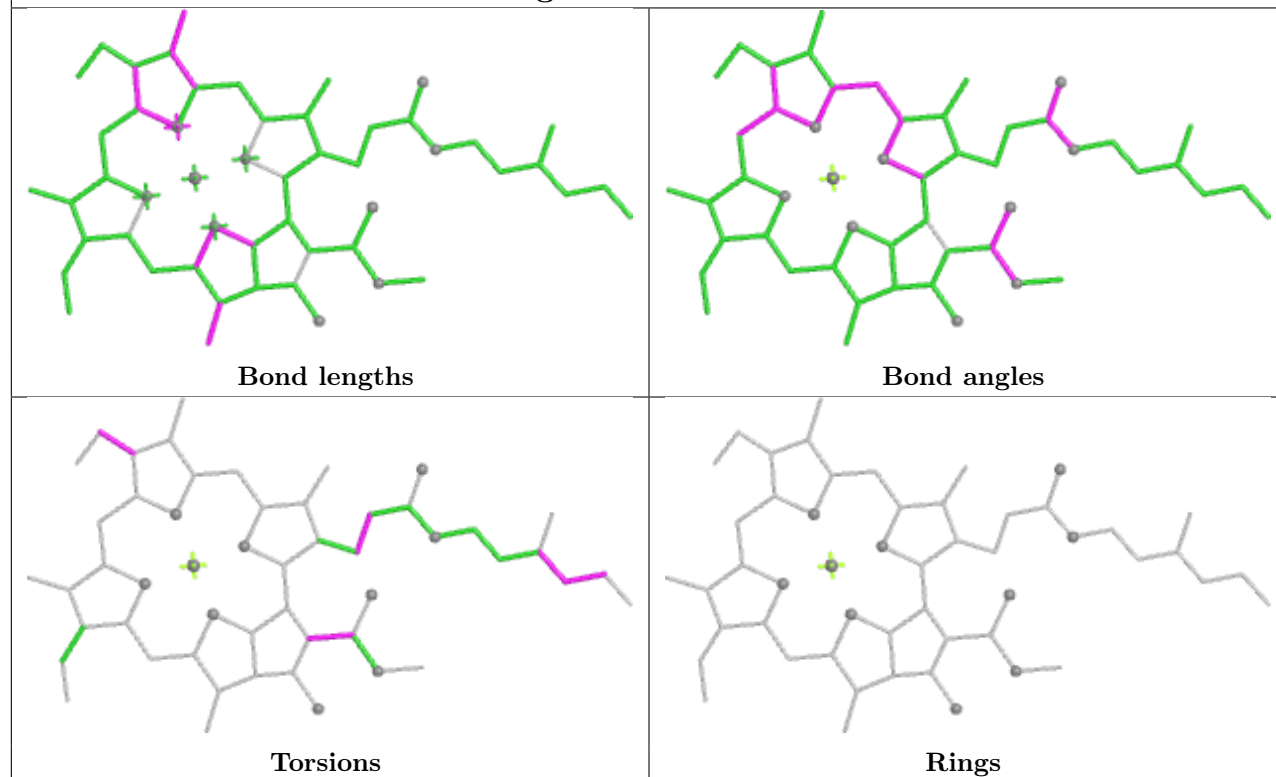
Ligand 8CT A 849



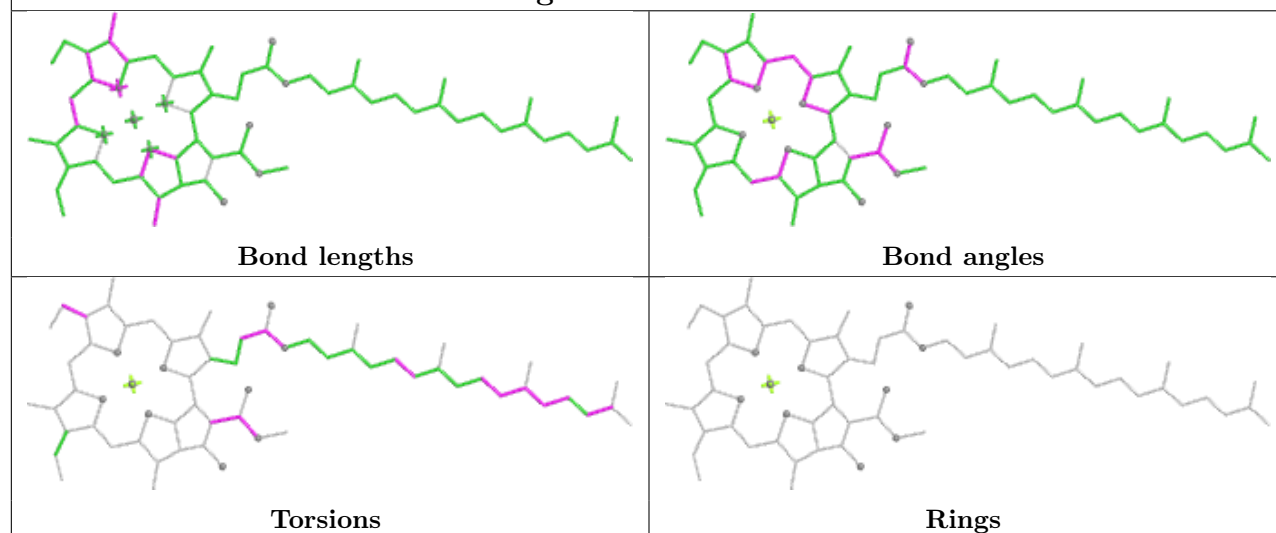
Ligand CLA A 809

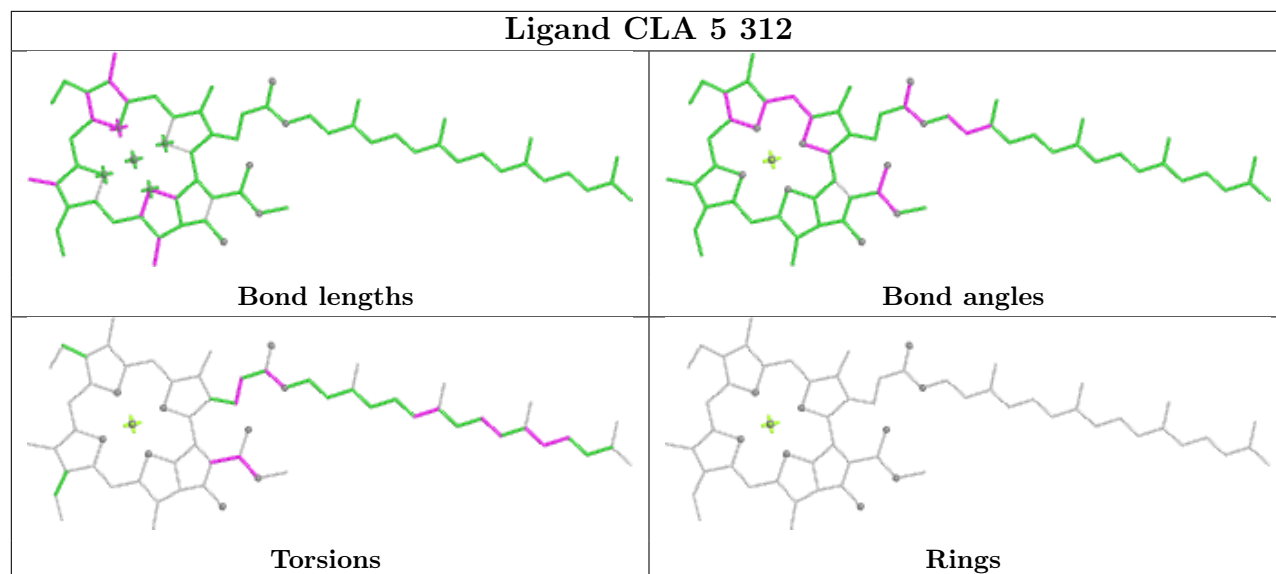
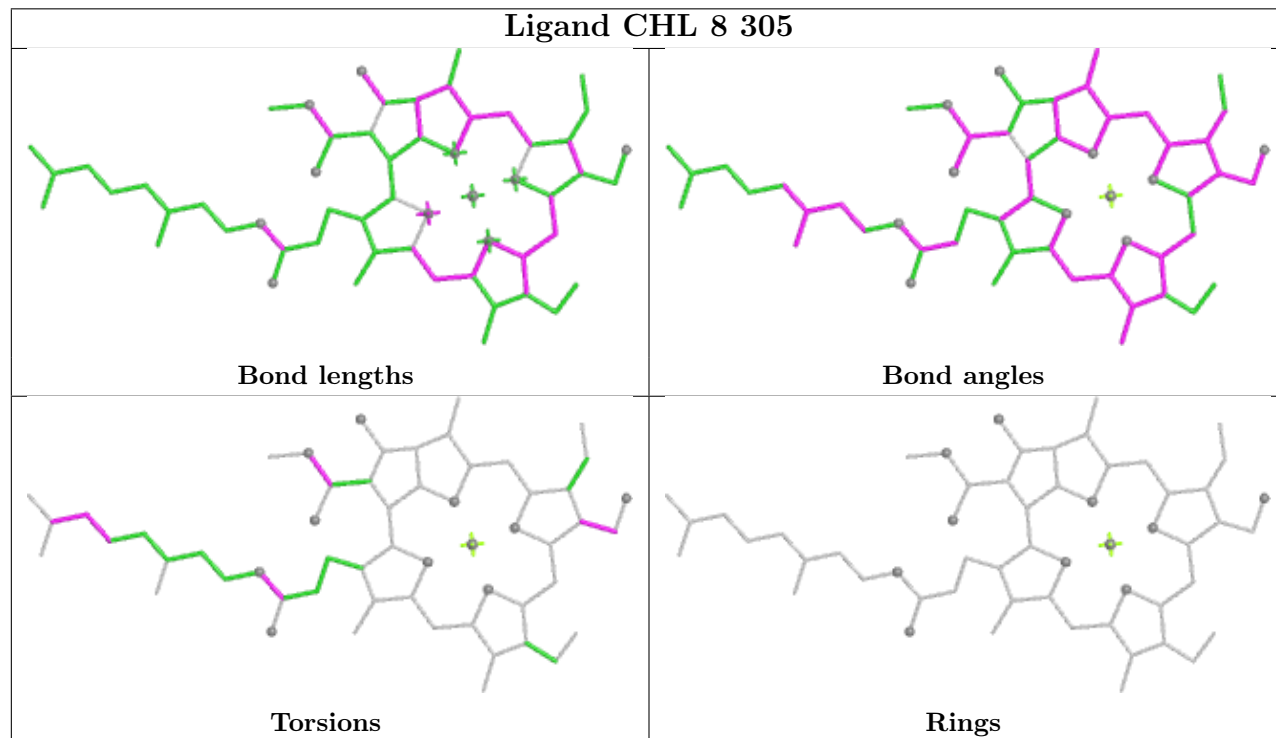


Ligand CLA 5 305

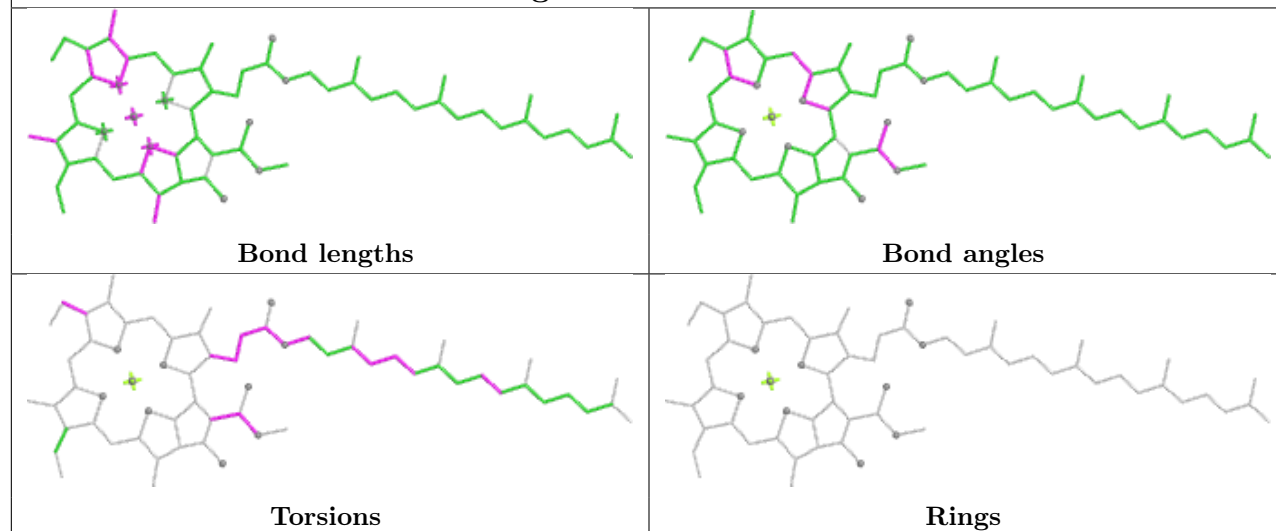


Ligand CLA 5 307

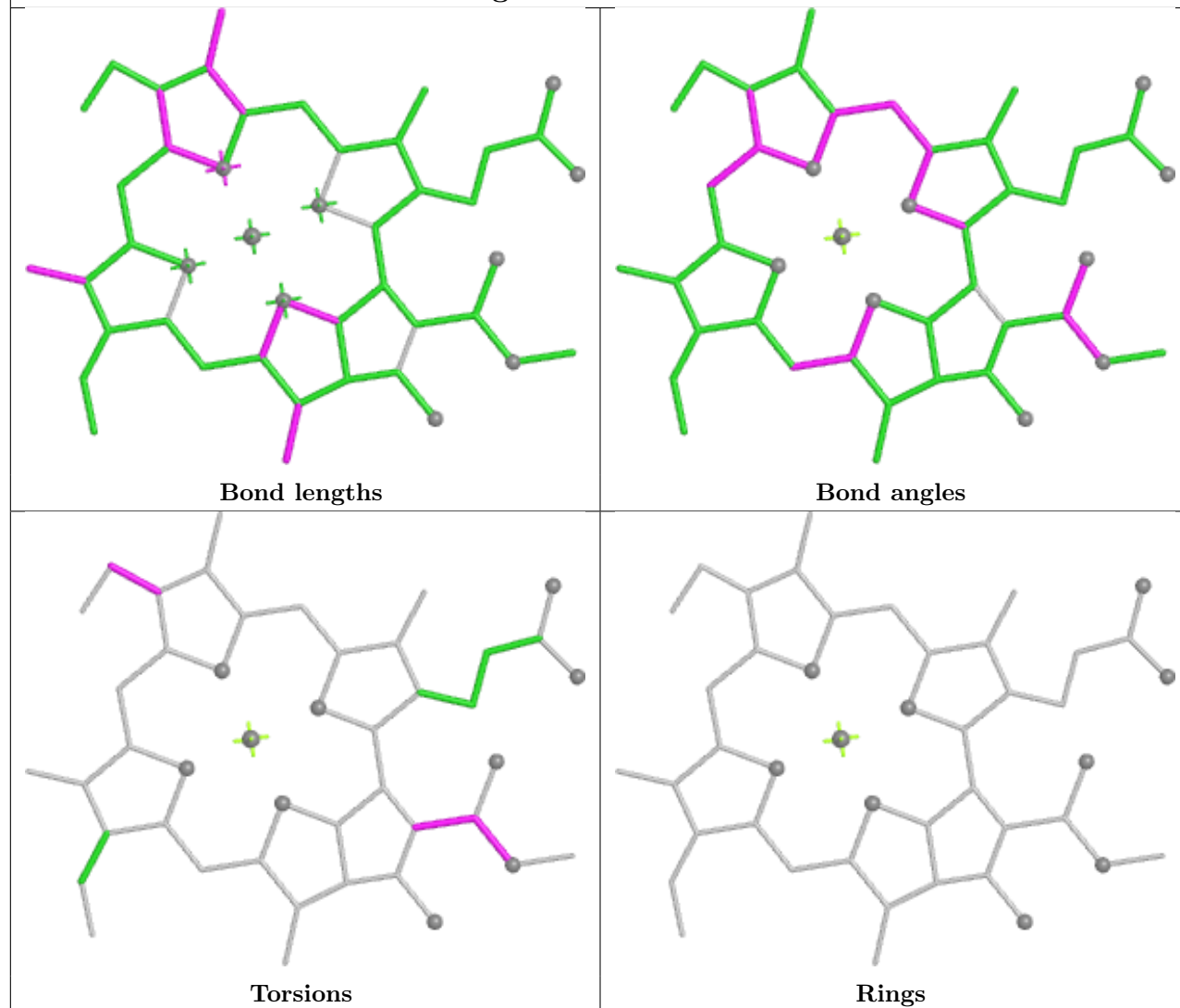


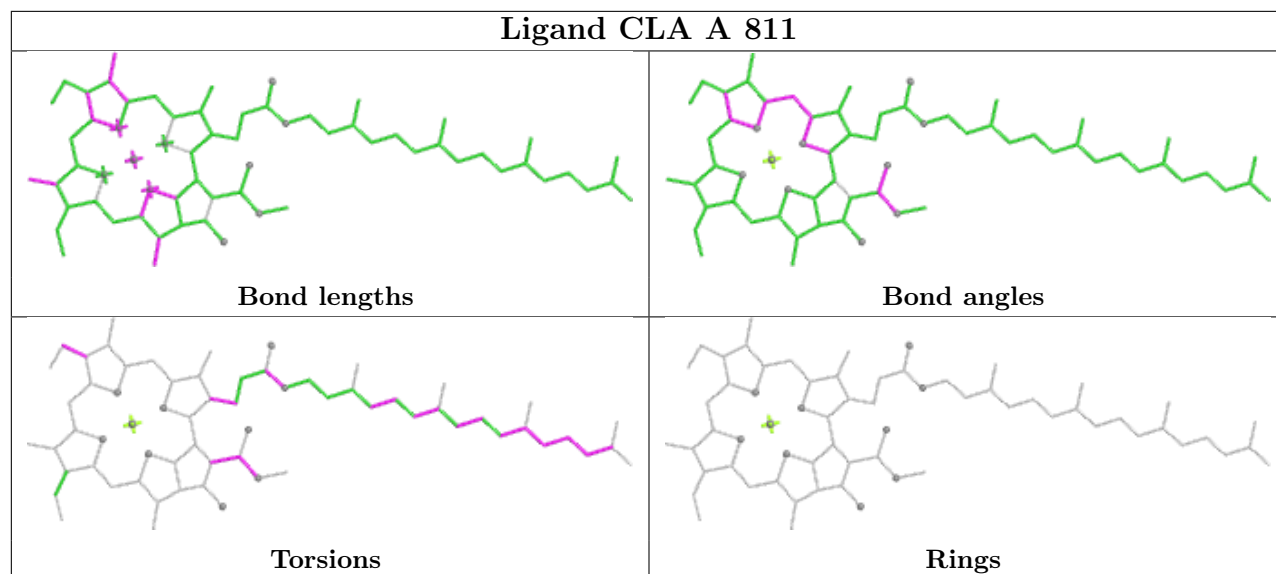
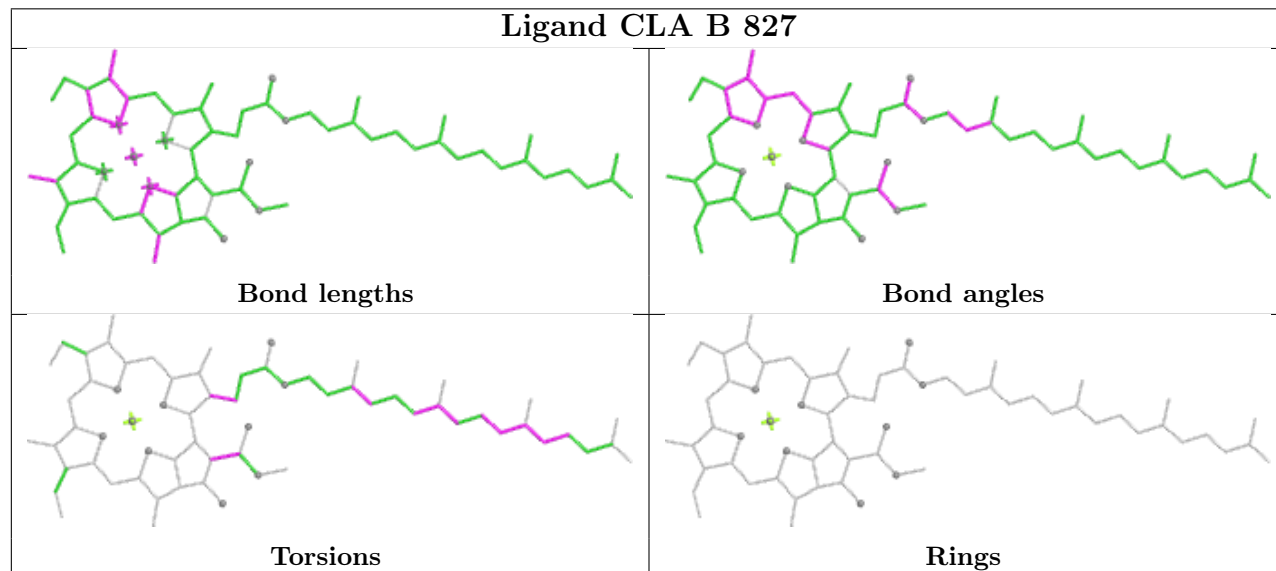
Ligand CLA 5 312**Ligand CHL 8 305**

Ligand CLA A 832

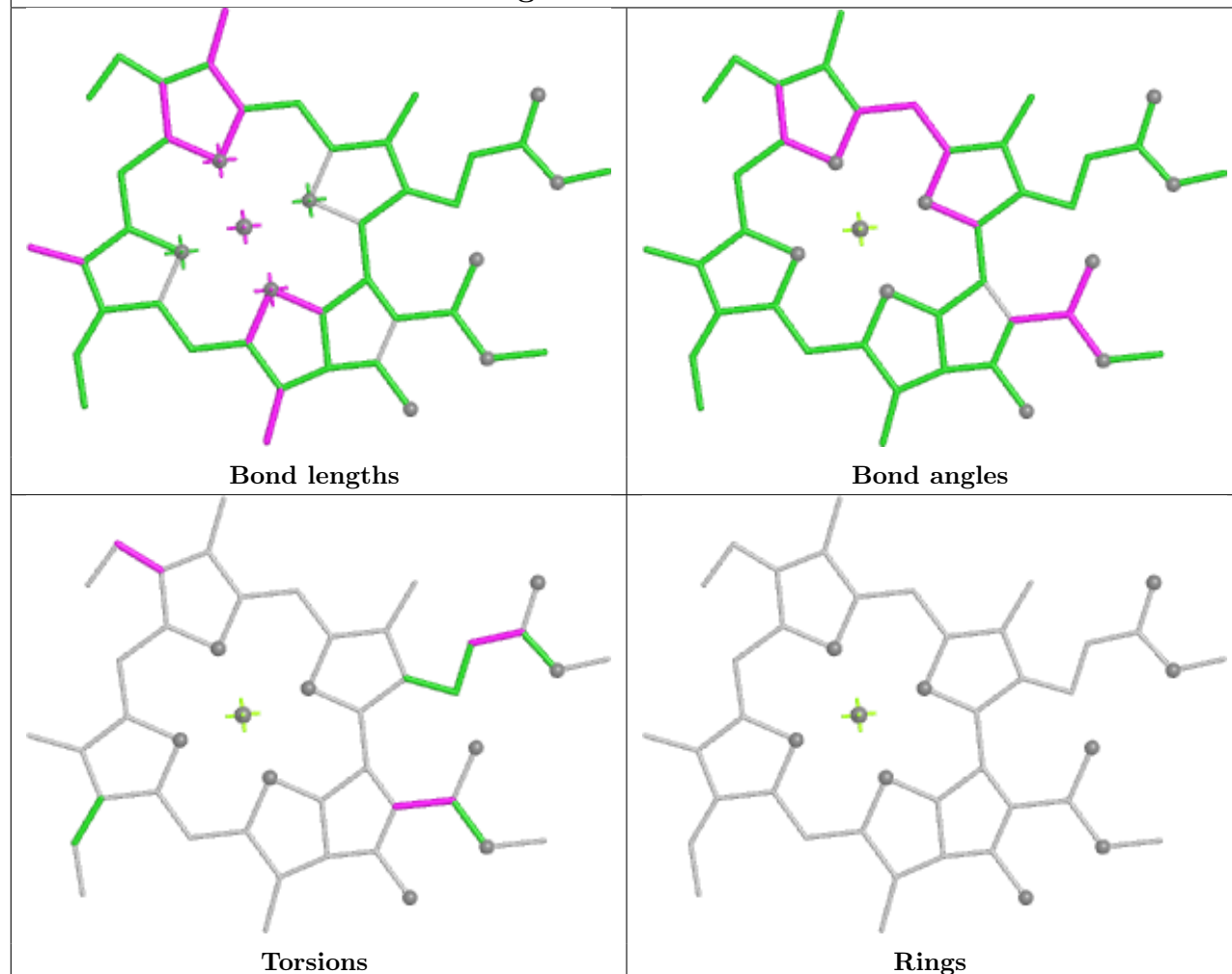


Ligand CLA B 835

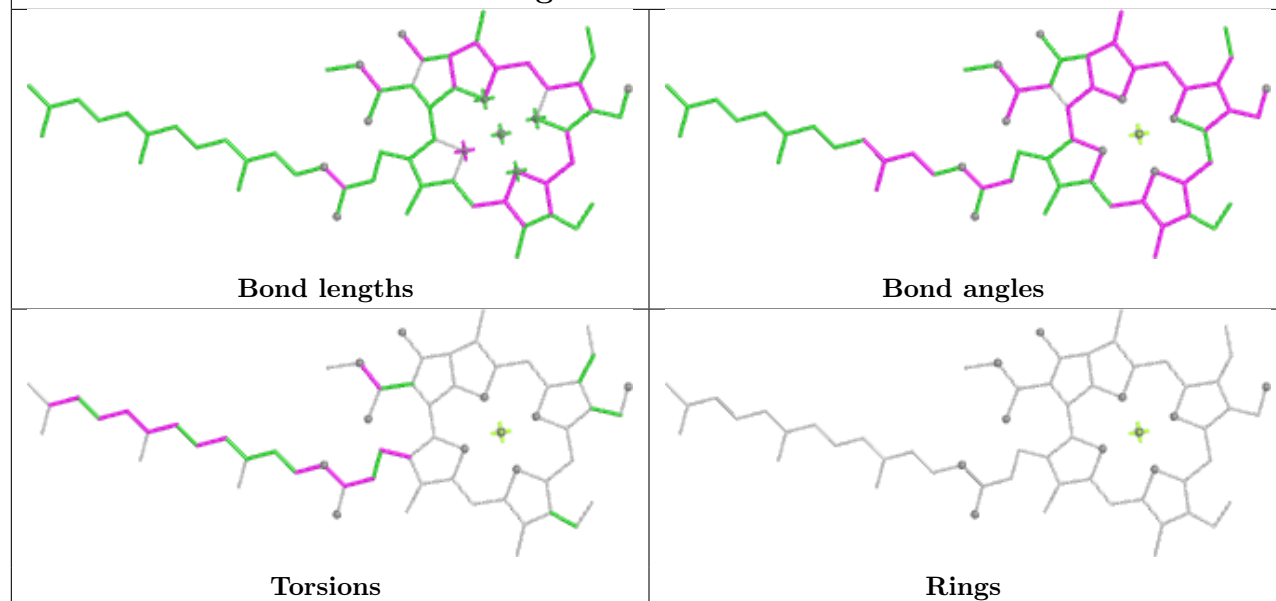


Ligand CLA A 811**Ligand CLA B 827**

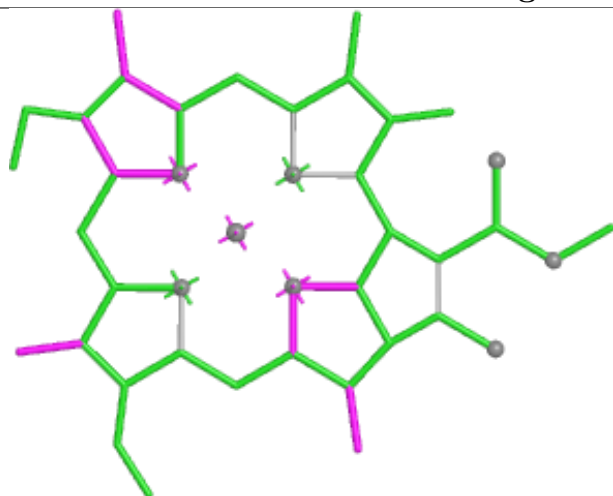
Ligand CLA 8 303



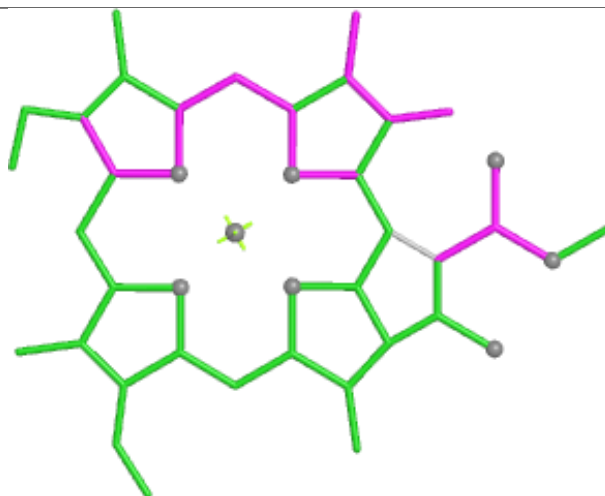
Ligand CHL 0 301



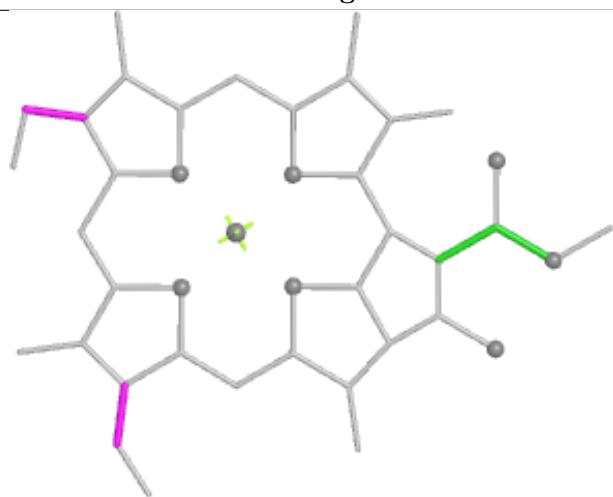
Ligand CLA 1 309



Bond lengths



Bond angles

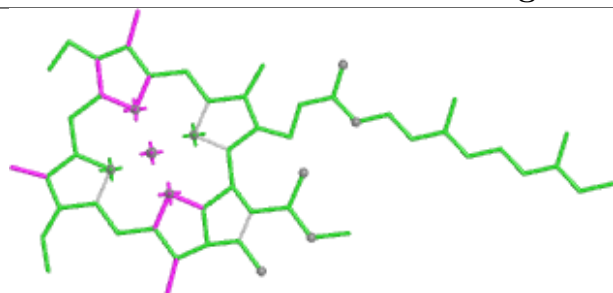


Torsions

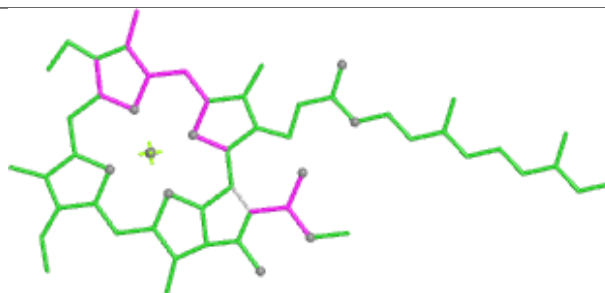


Rings

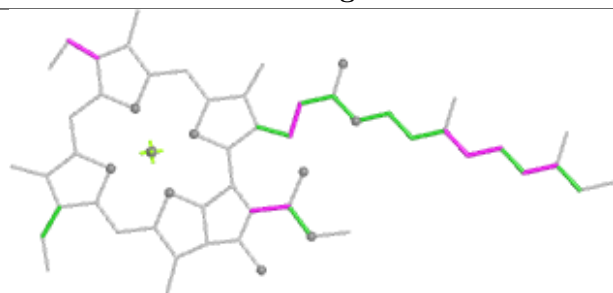
Ligand CLA 4 312



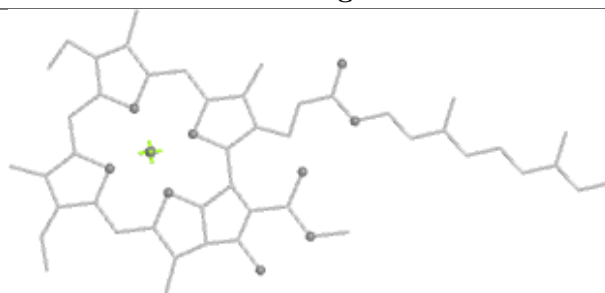
Bond lengths



Bond angles

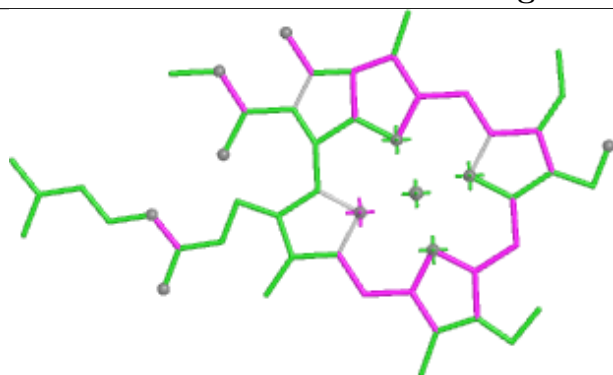


Torsions

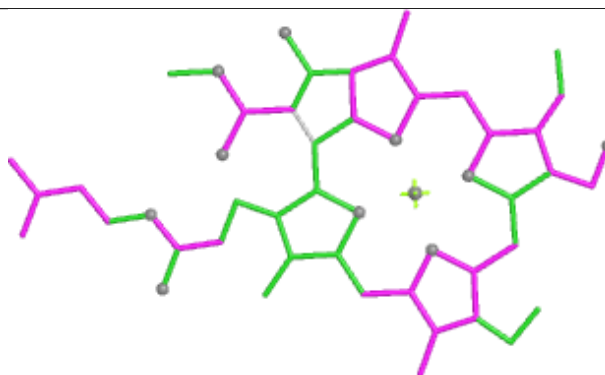


Rings

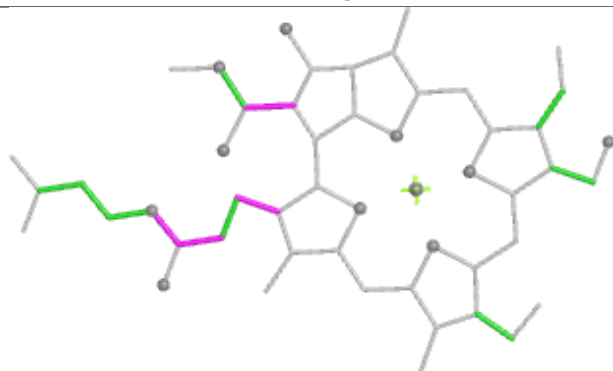
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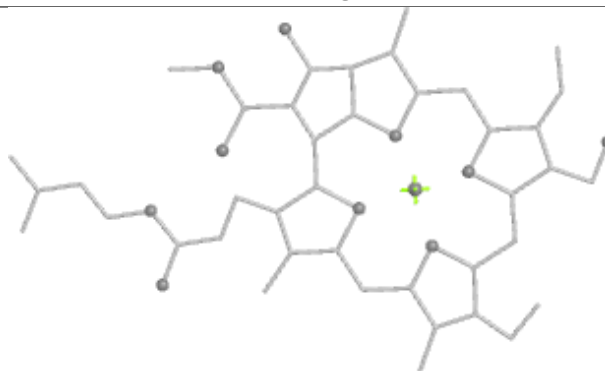
Bond lengths



Bond angles

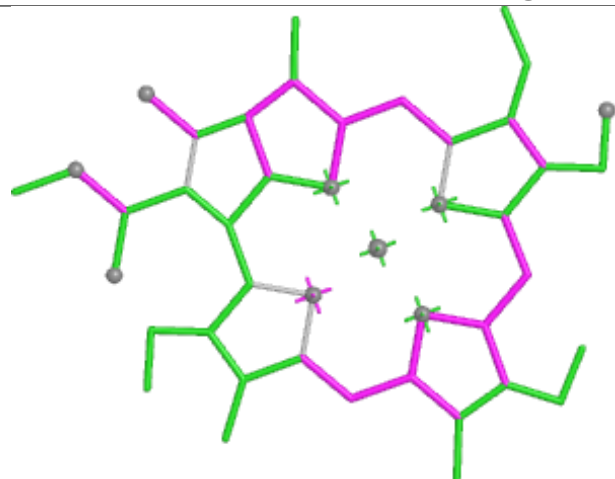


Torsions

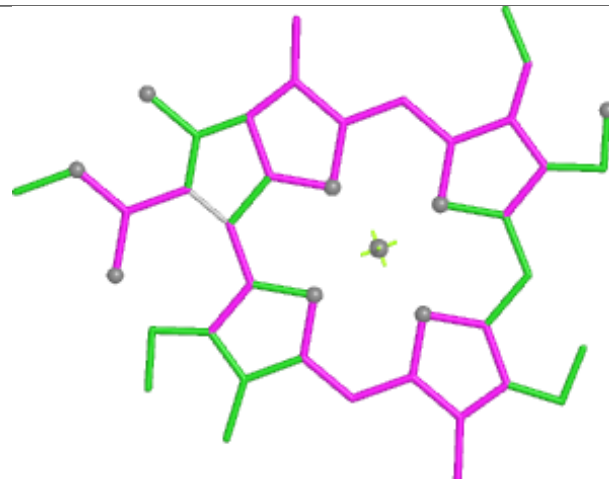


Rings

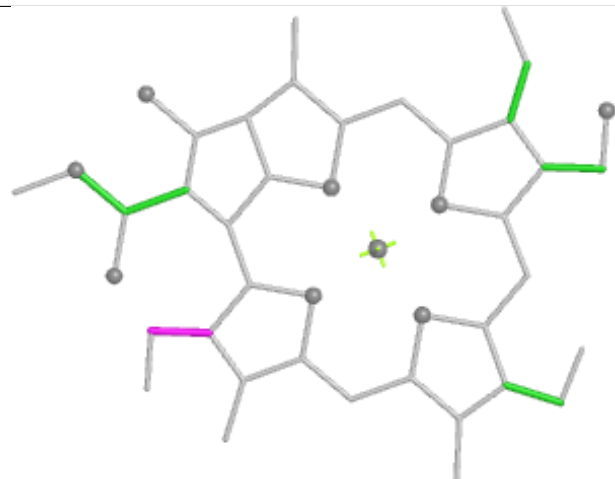
Ligand CHL 6 306



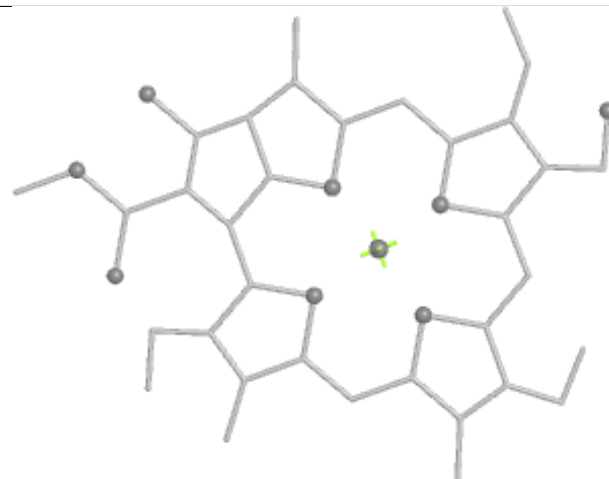
Bond lengths



Bond angles

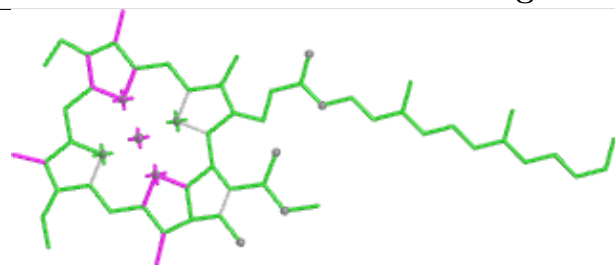


Torsions

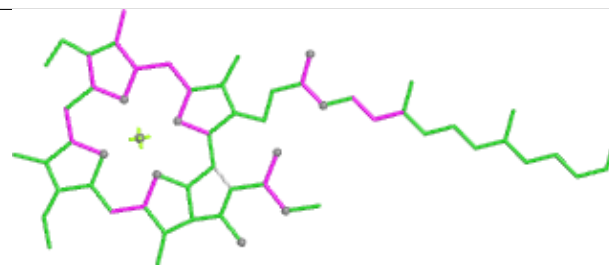


Rings

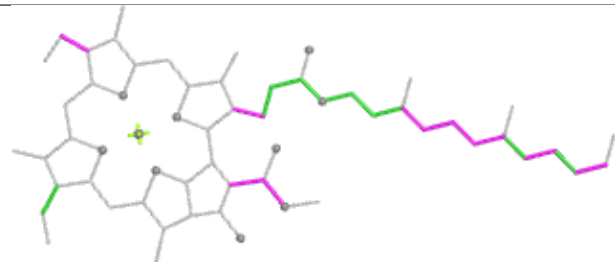
Ligand CLA B 818



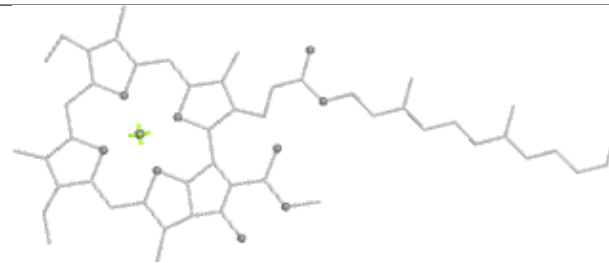
Bond lengths



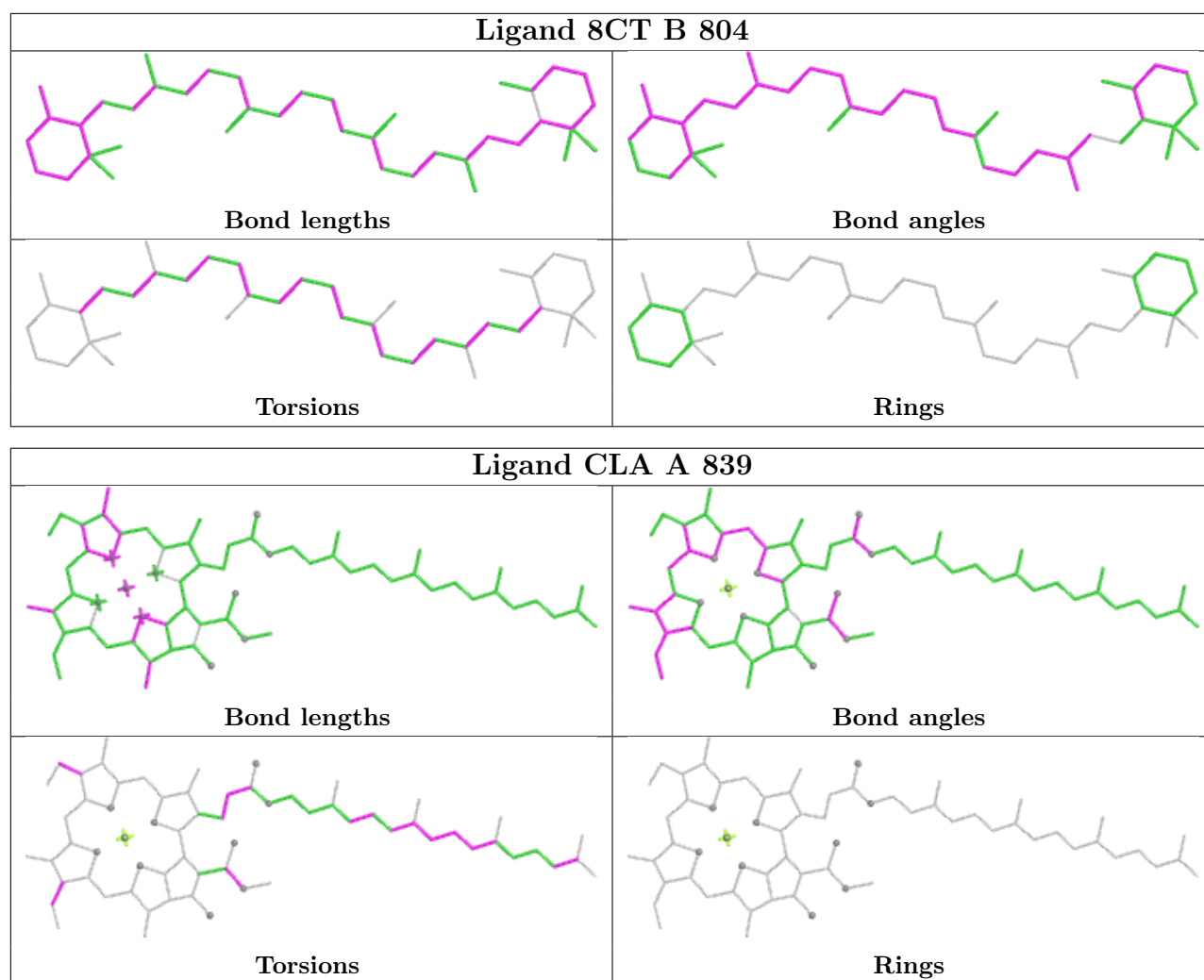
Bond angles



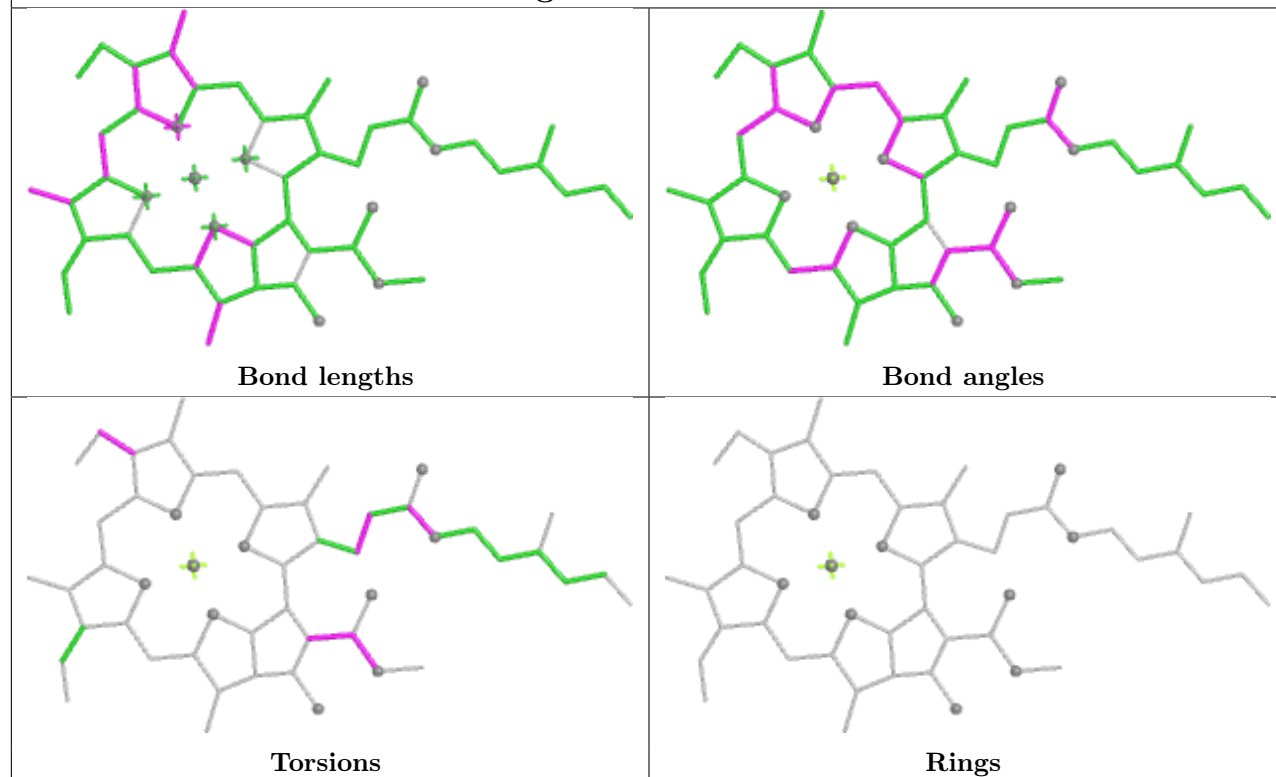
Torsions



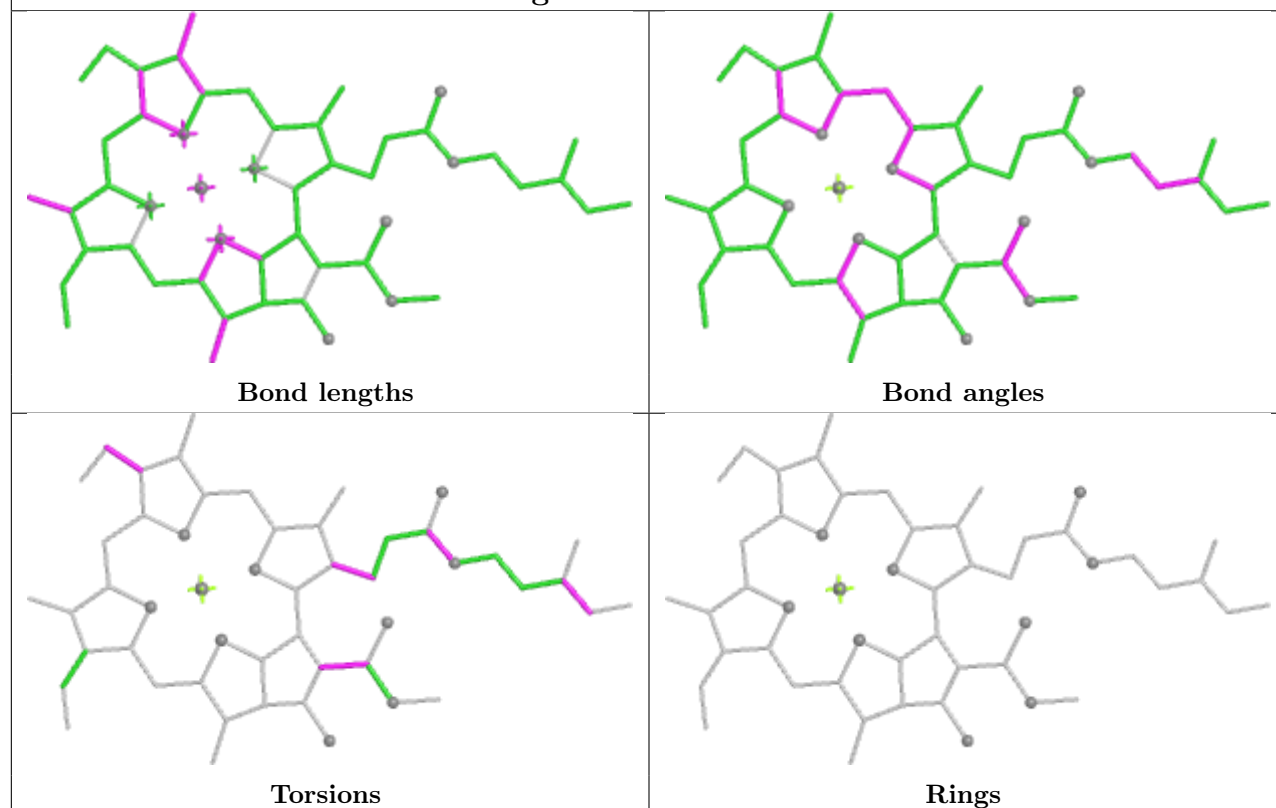
Rings



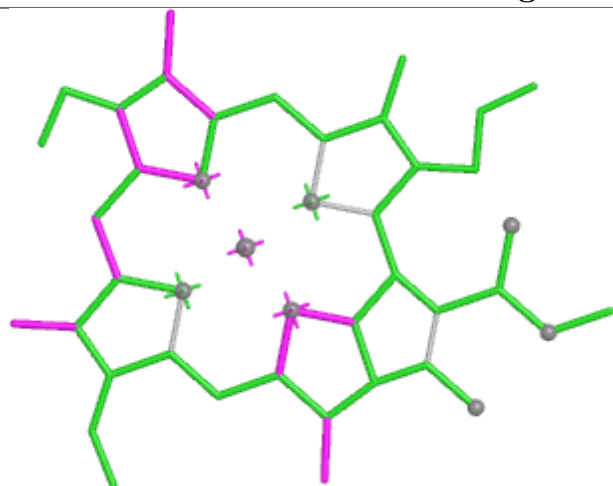
Ligand CLA 9 305



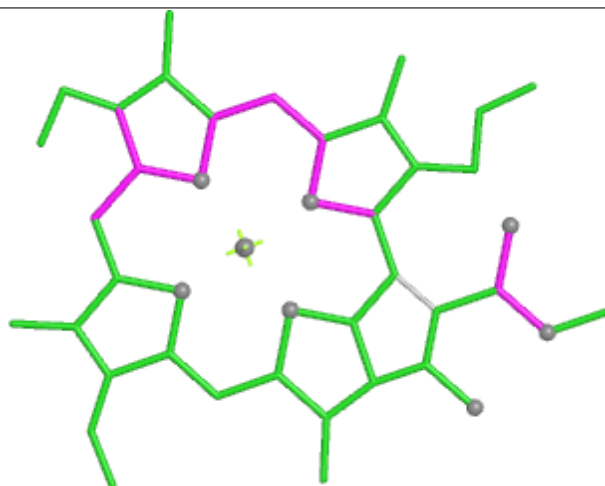
Ligand CLA A 823



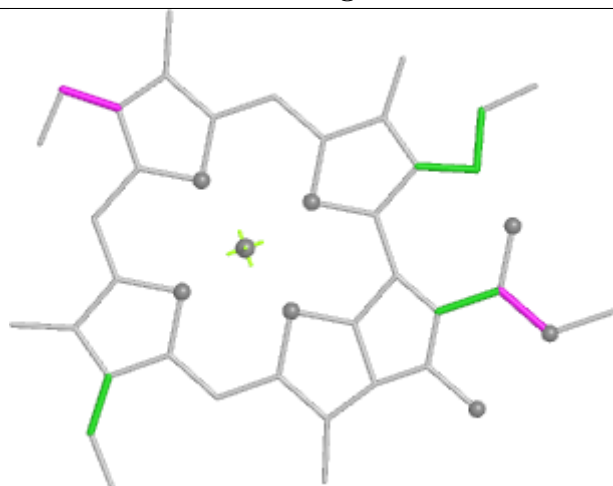
Ligand CLA 2 313



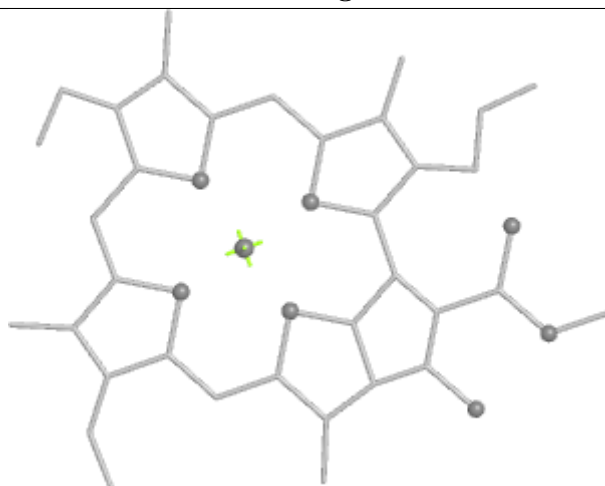
Bond lengths



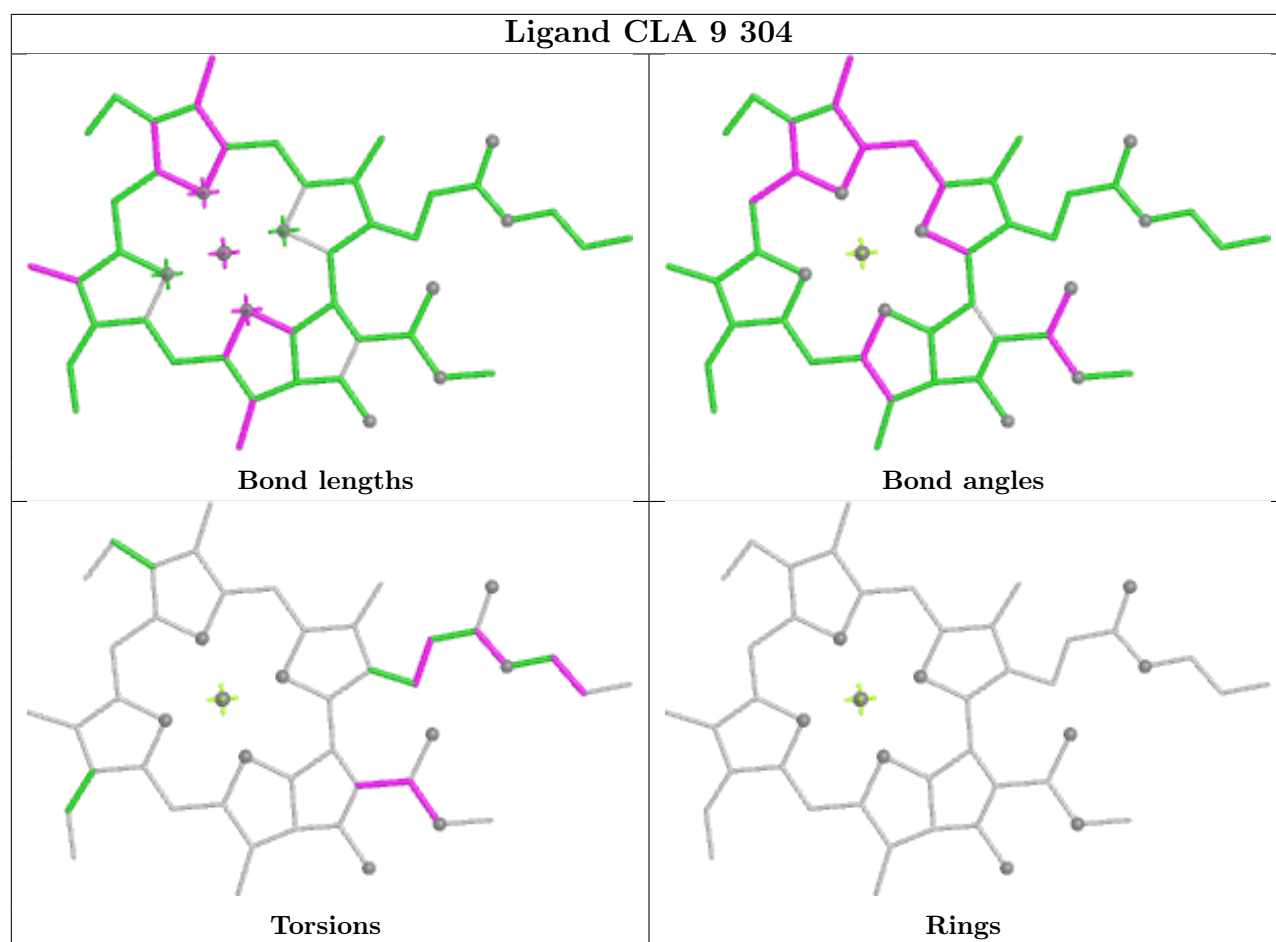
Bond angles



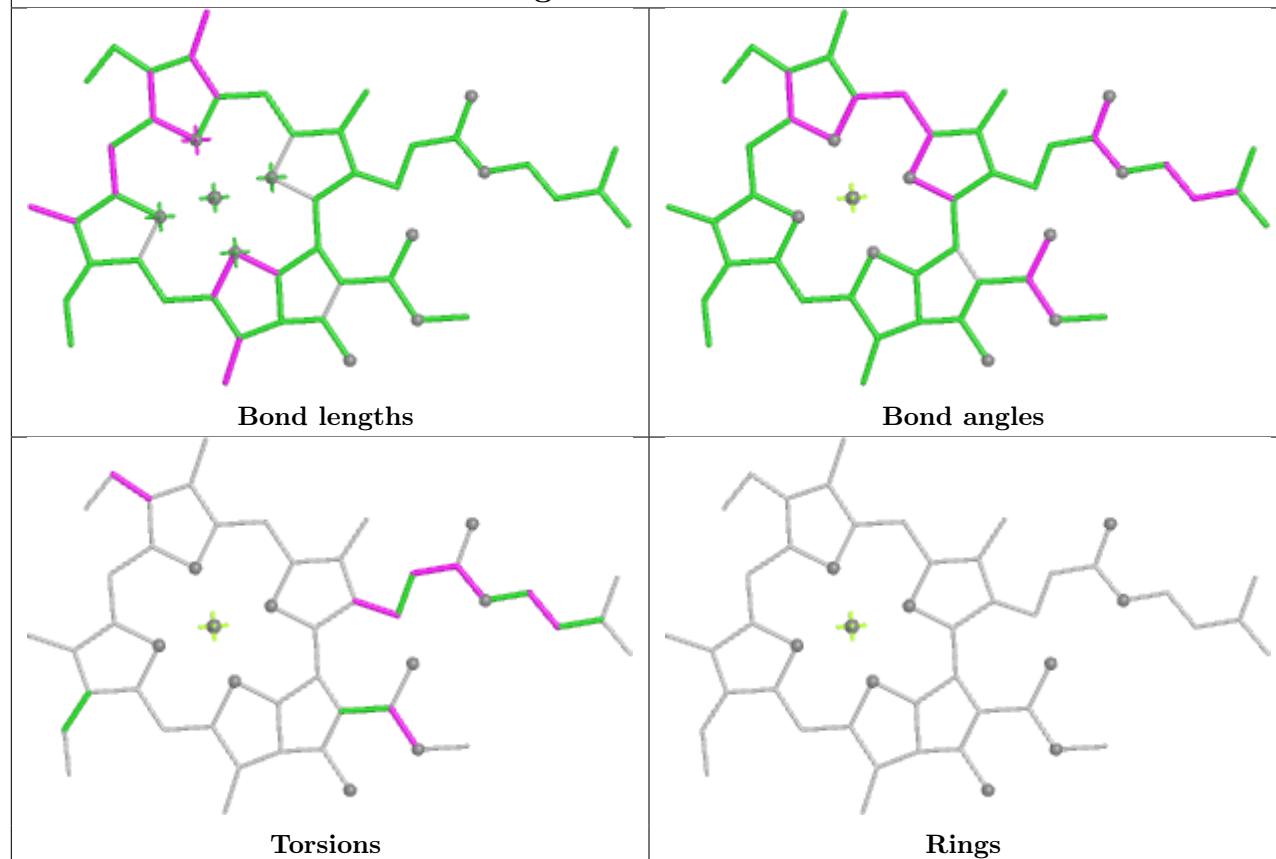
Torsions



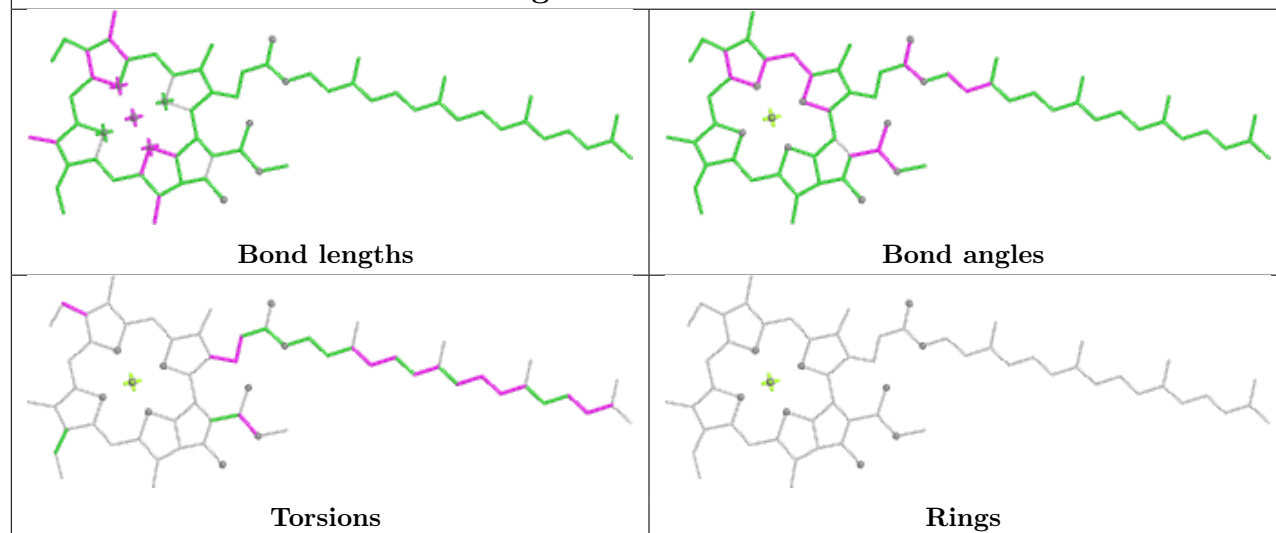
Rings

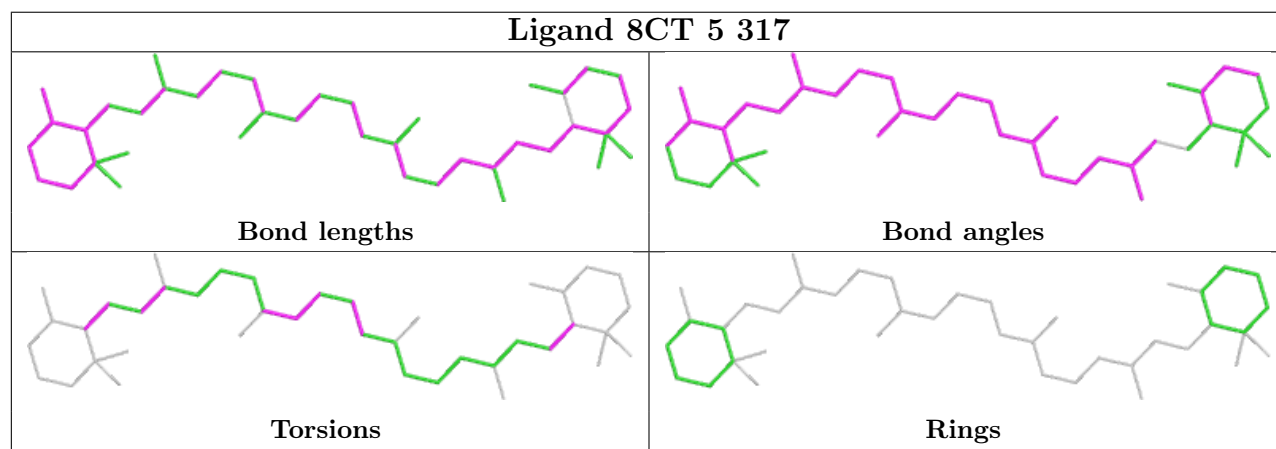
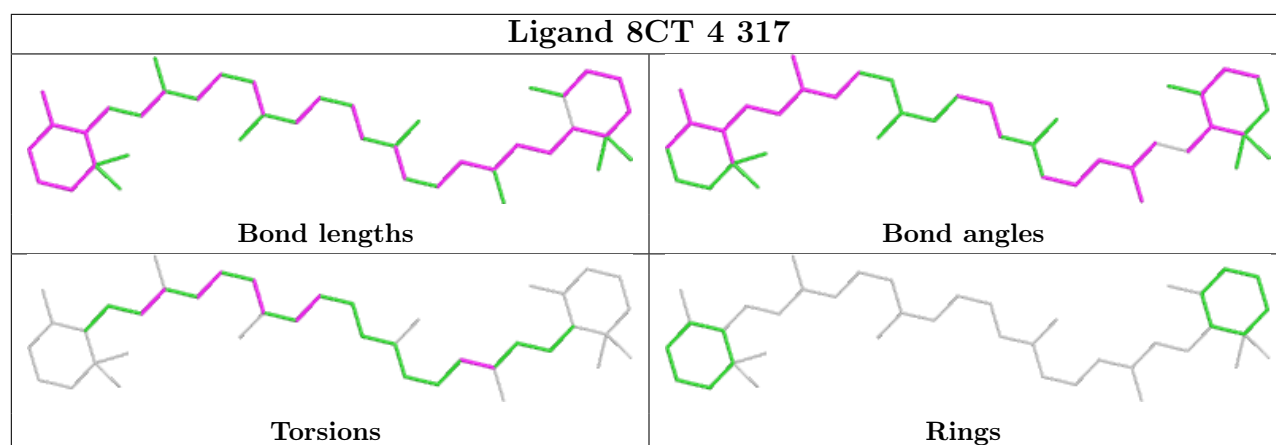


Ligand CLA L 204

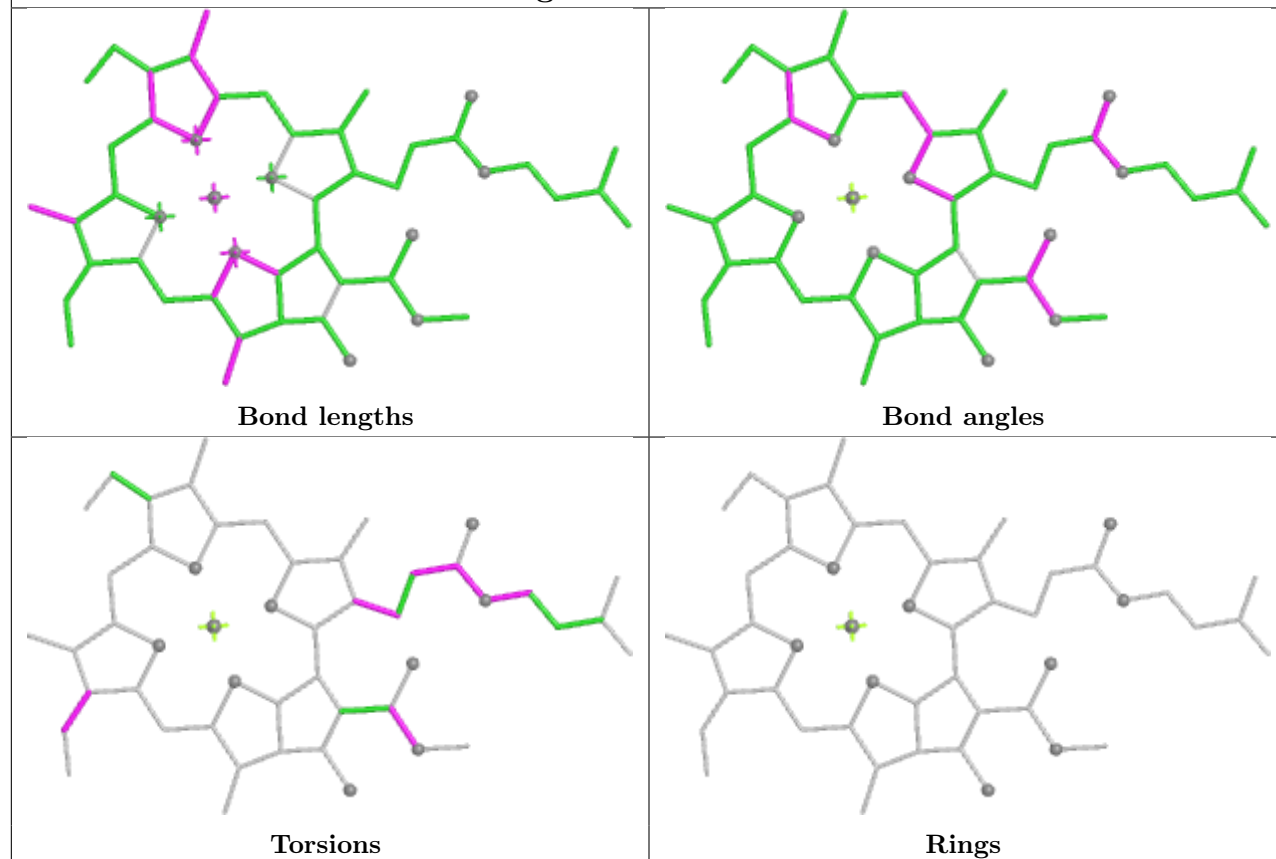


Ligand CLA A 853

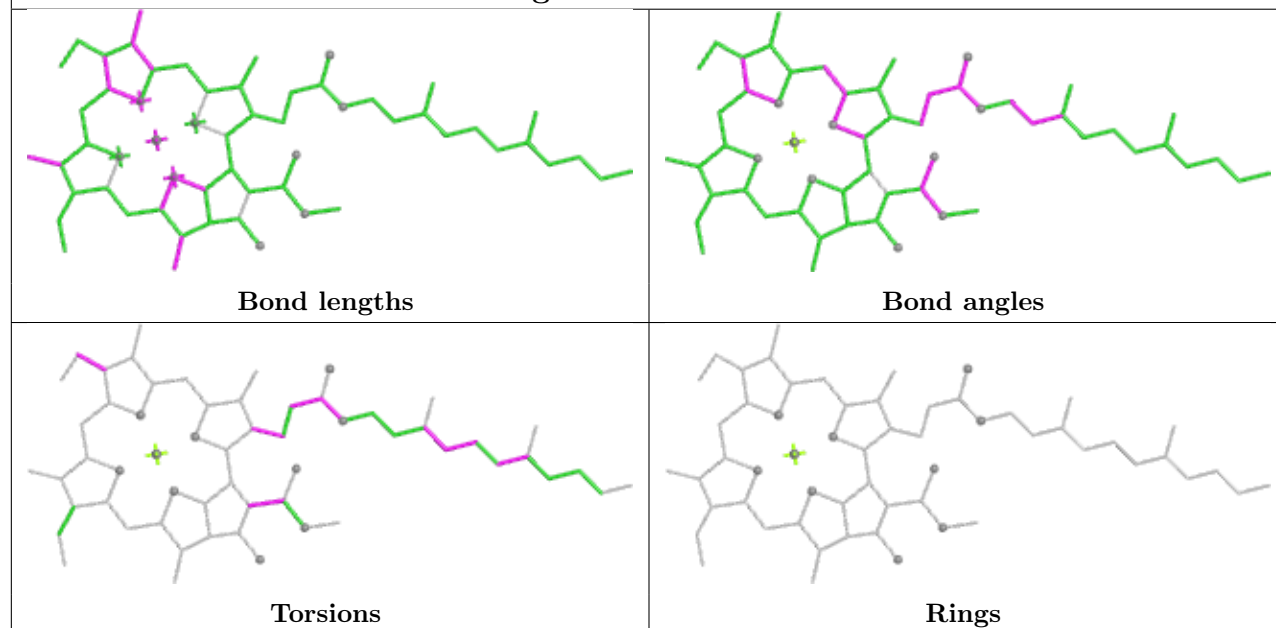




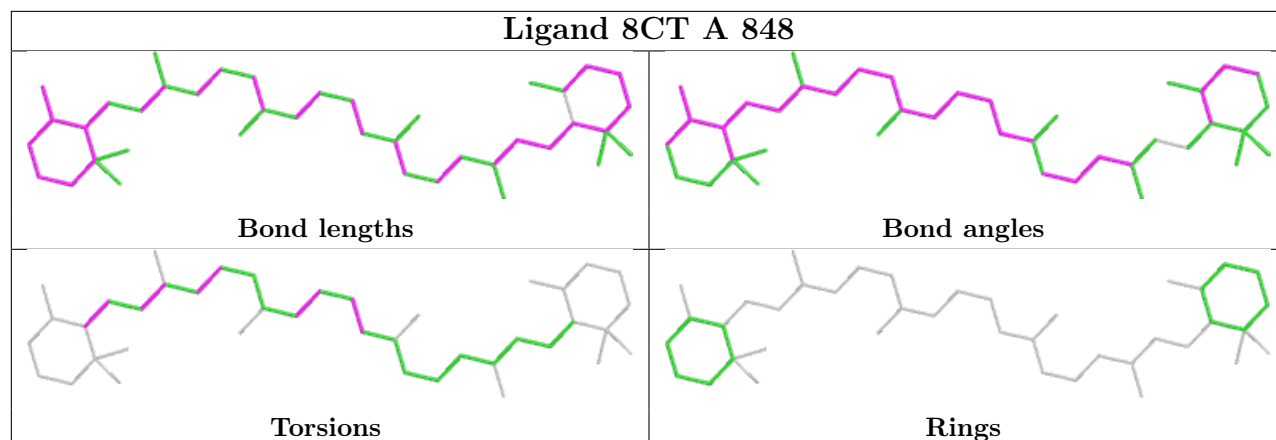
Ligand CLA 6 309



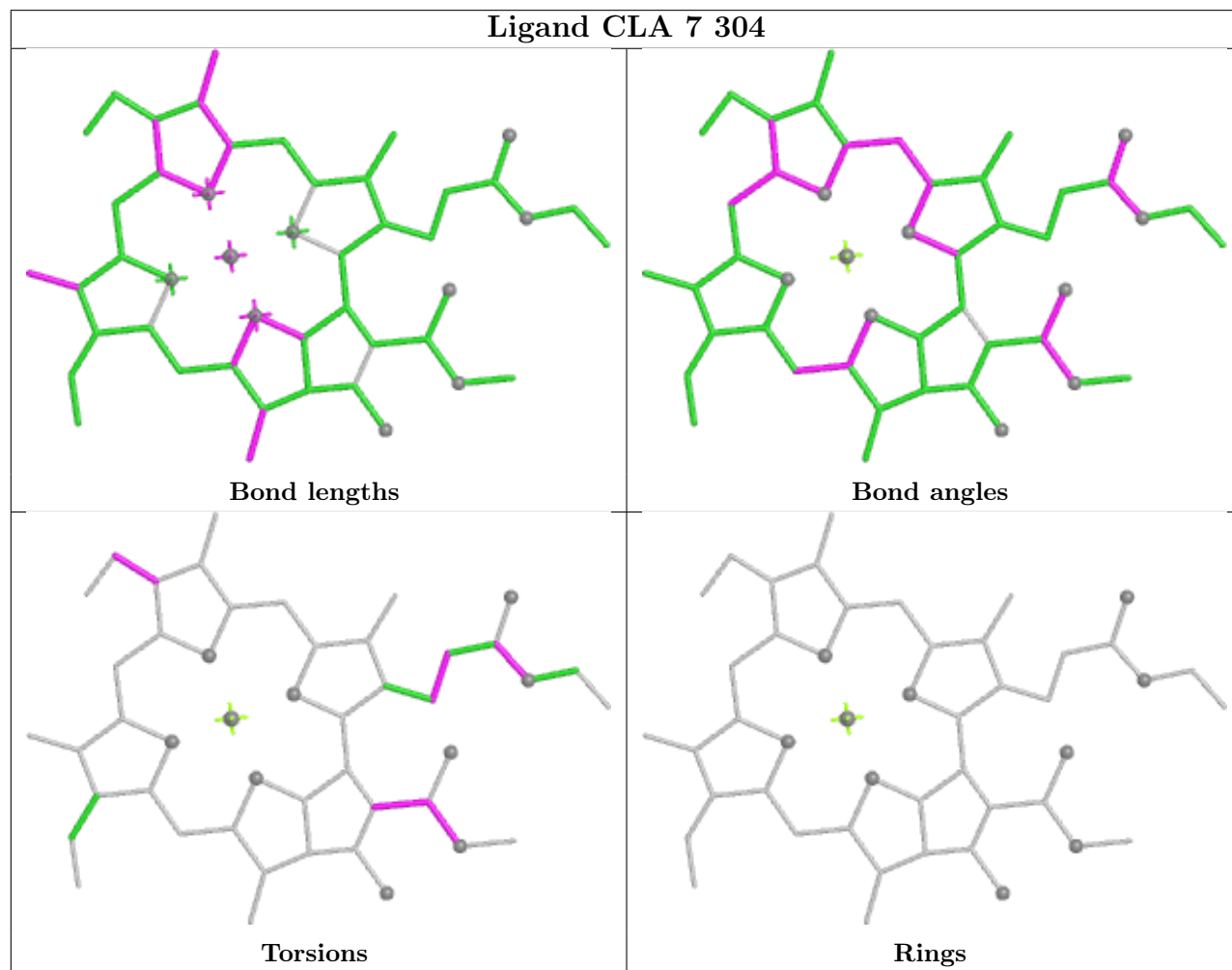
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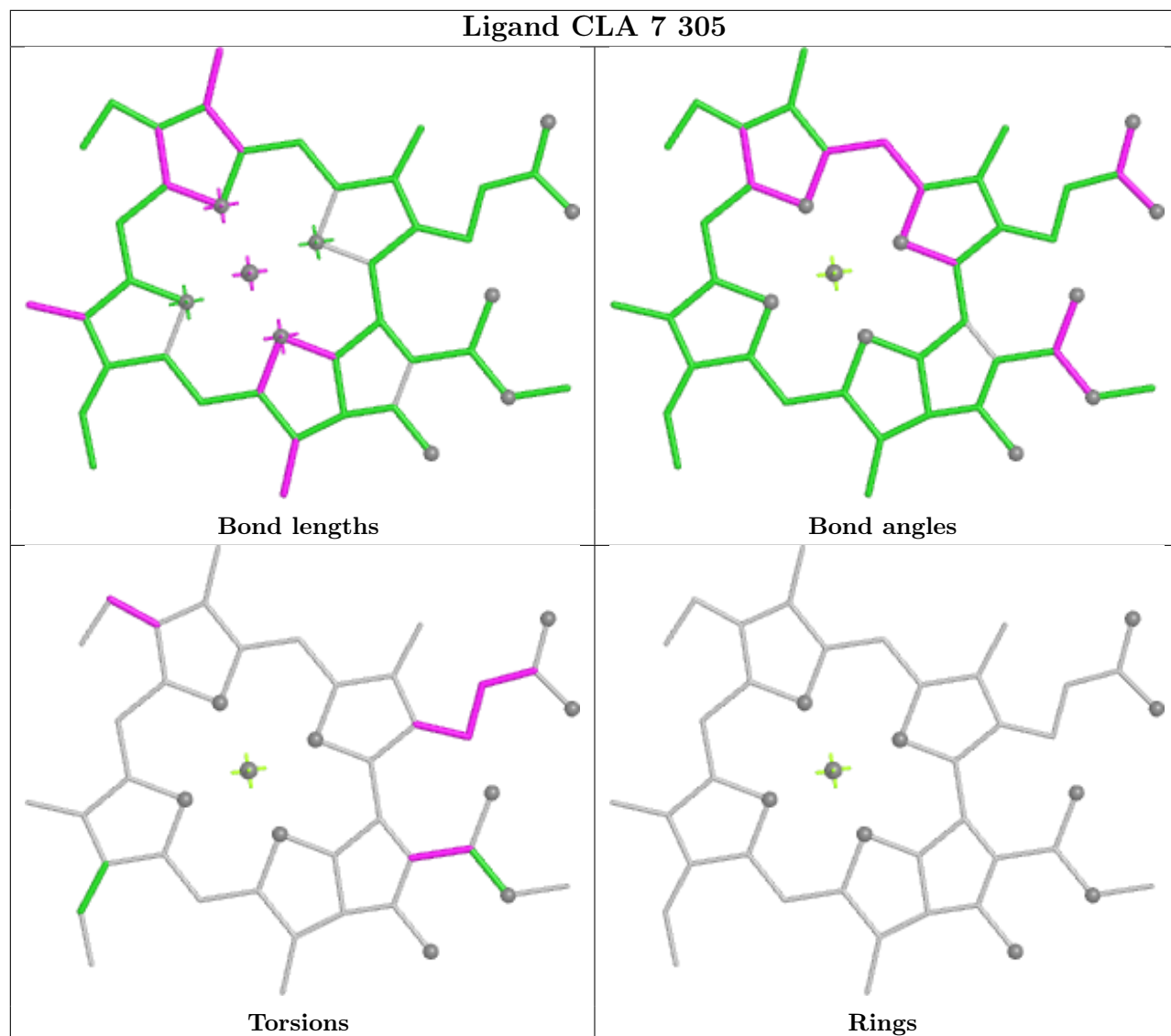
Ligand 8CT A 848

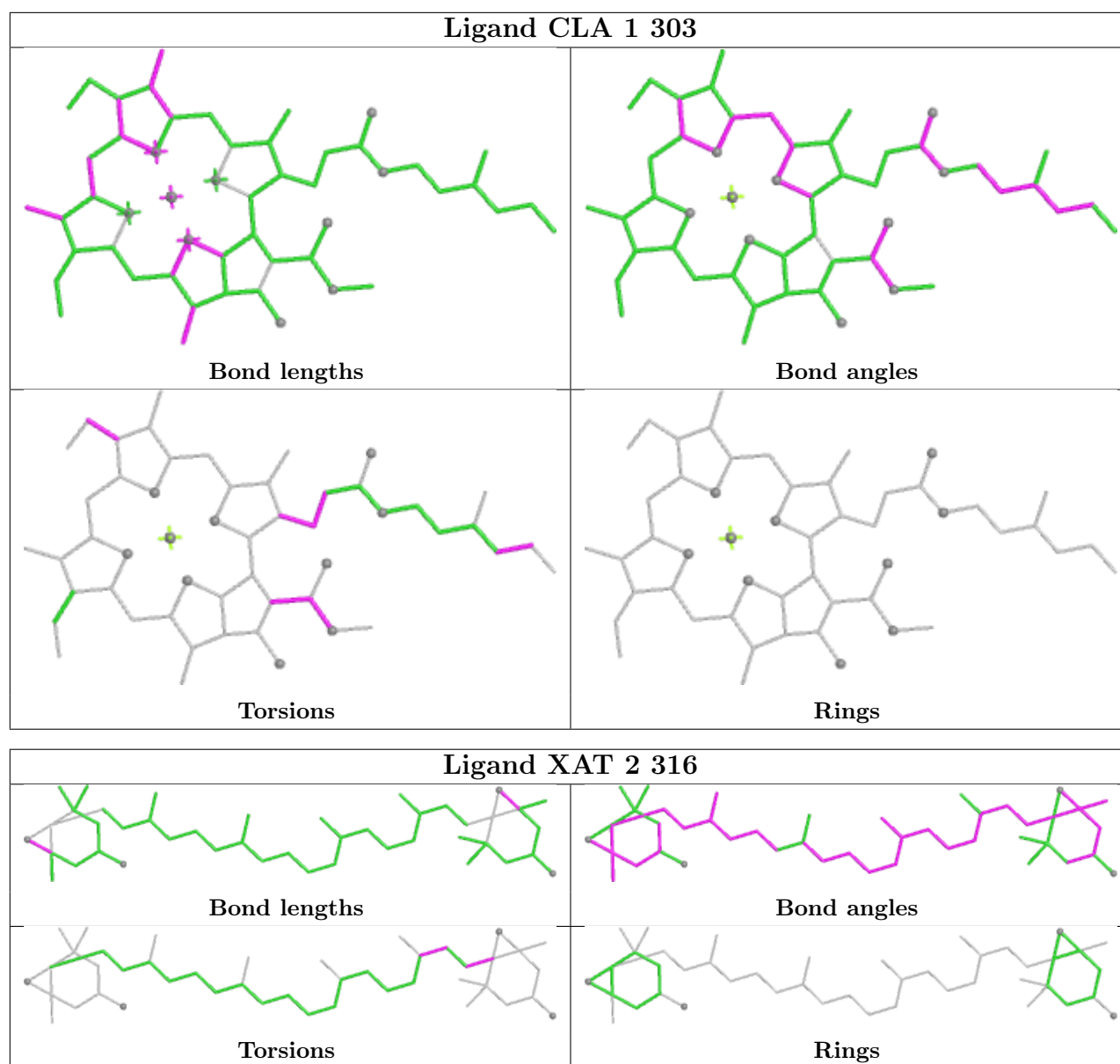


Ligand CLA 7 304

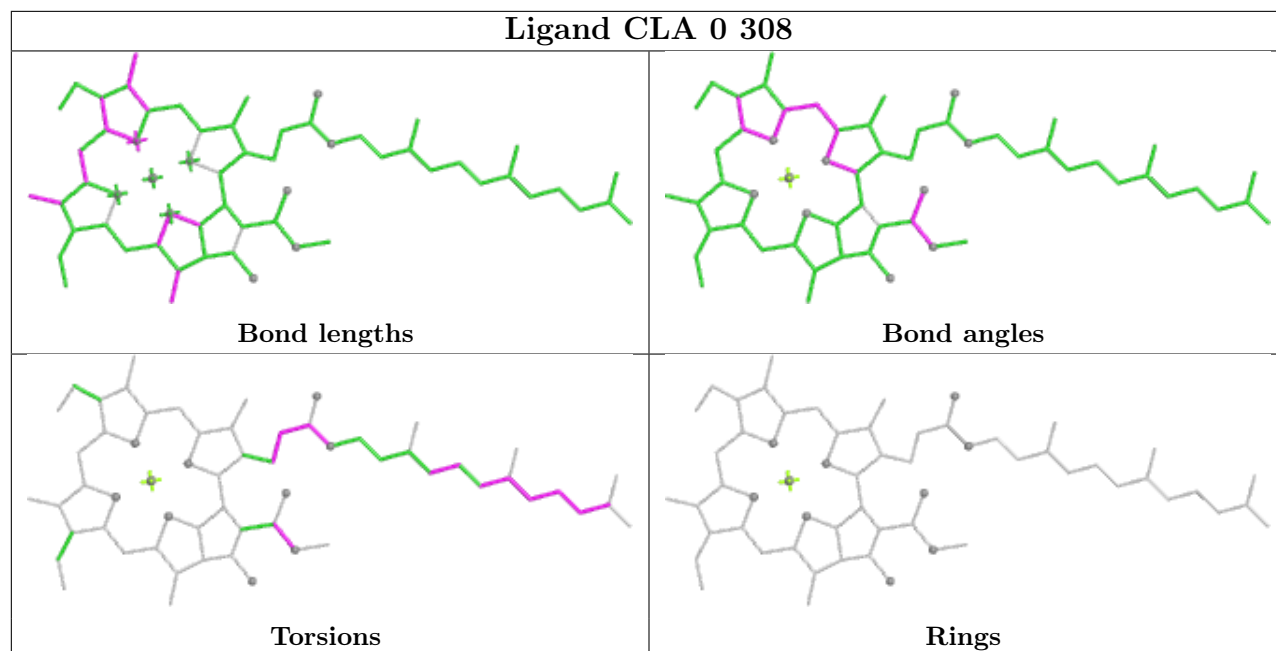


Ligand CLA 7 305

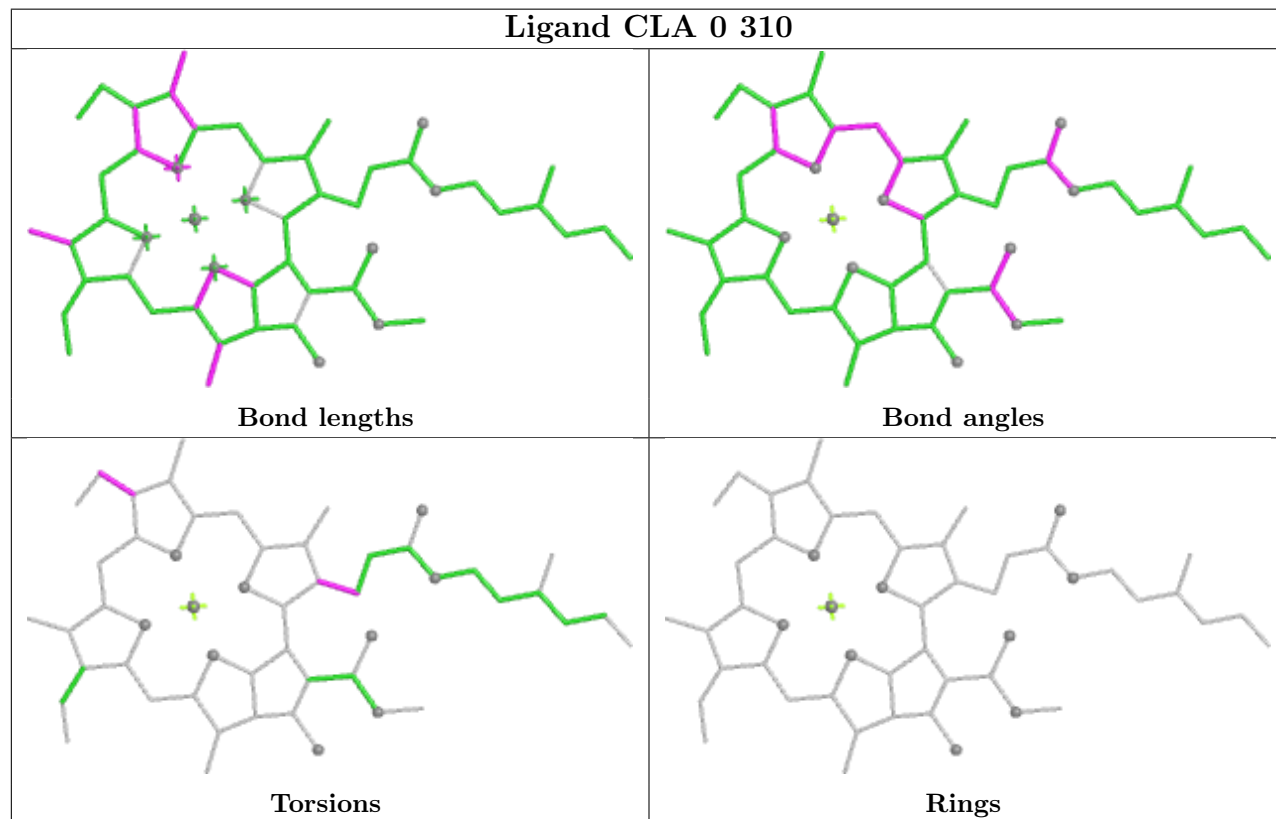




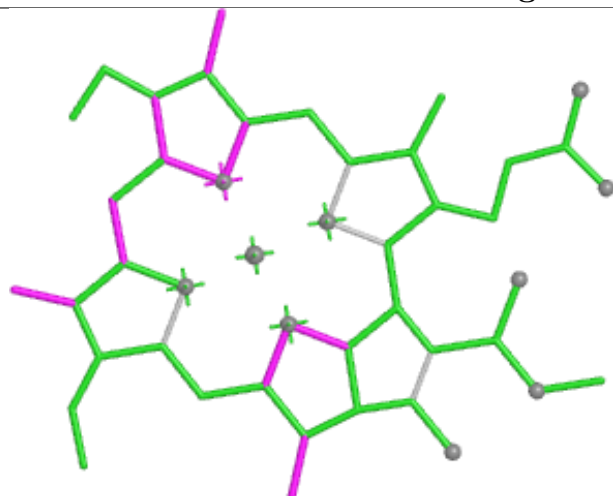
Ligand CLA 0 308



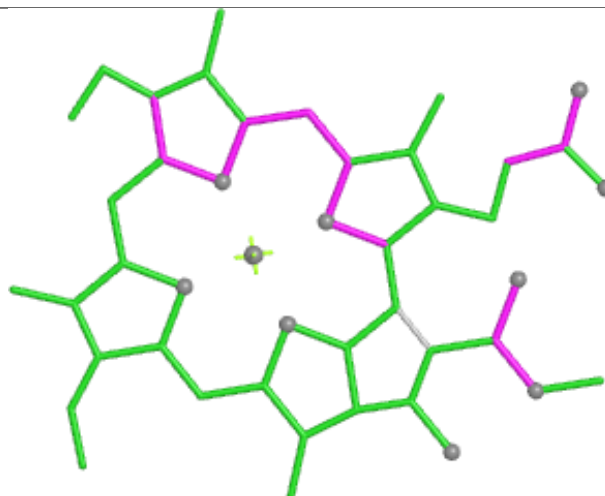
Ligand CLA 0 310



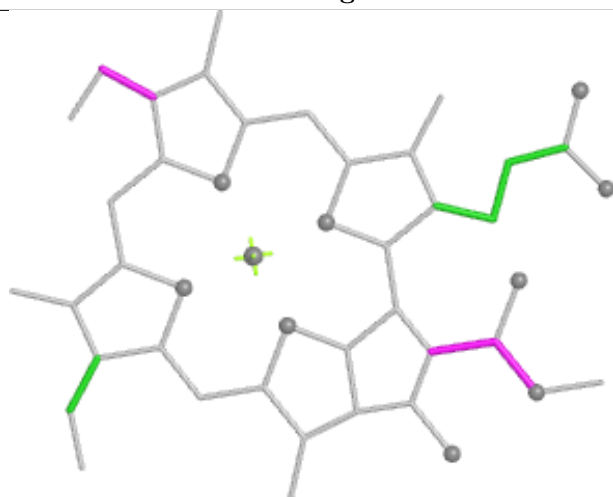
Ligand CLA 3 303



Bond lengths



Bond angles

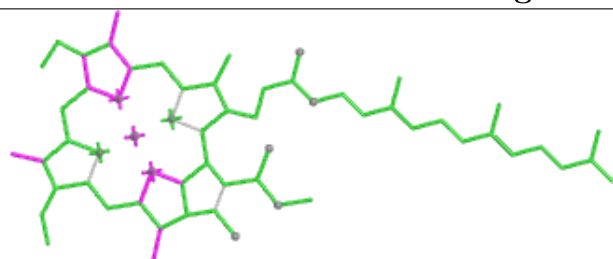


Torsions

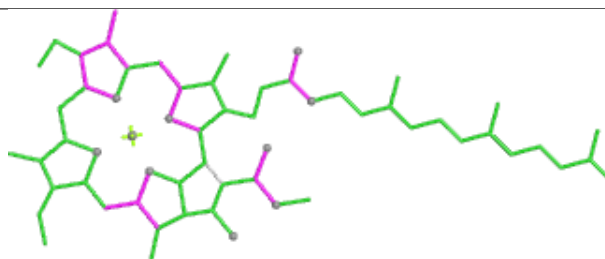


Rings

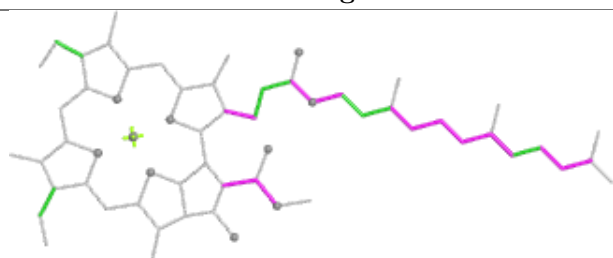
Ligand CLA B 819



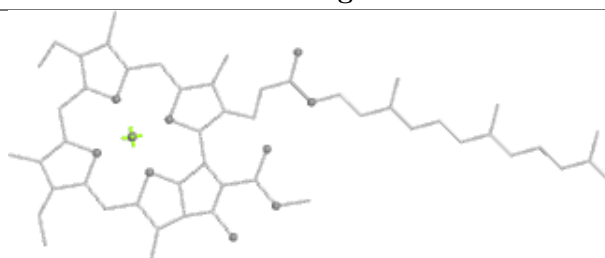
Bond lengths



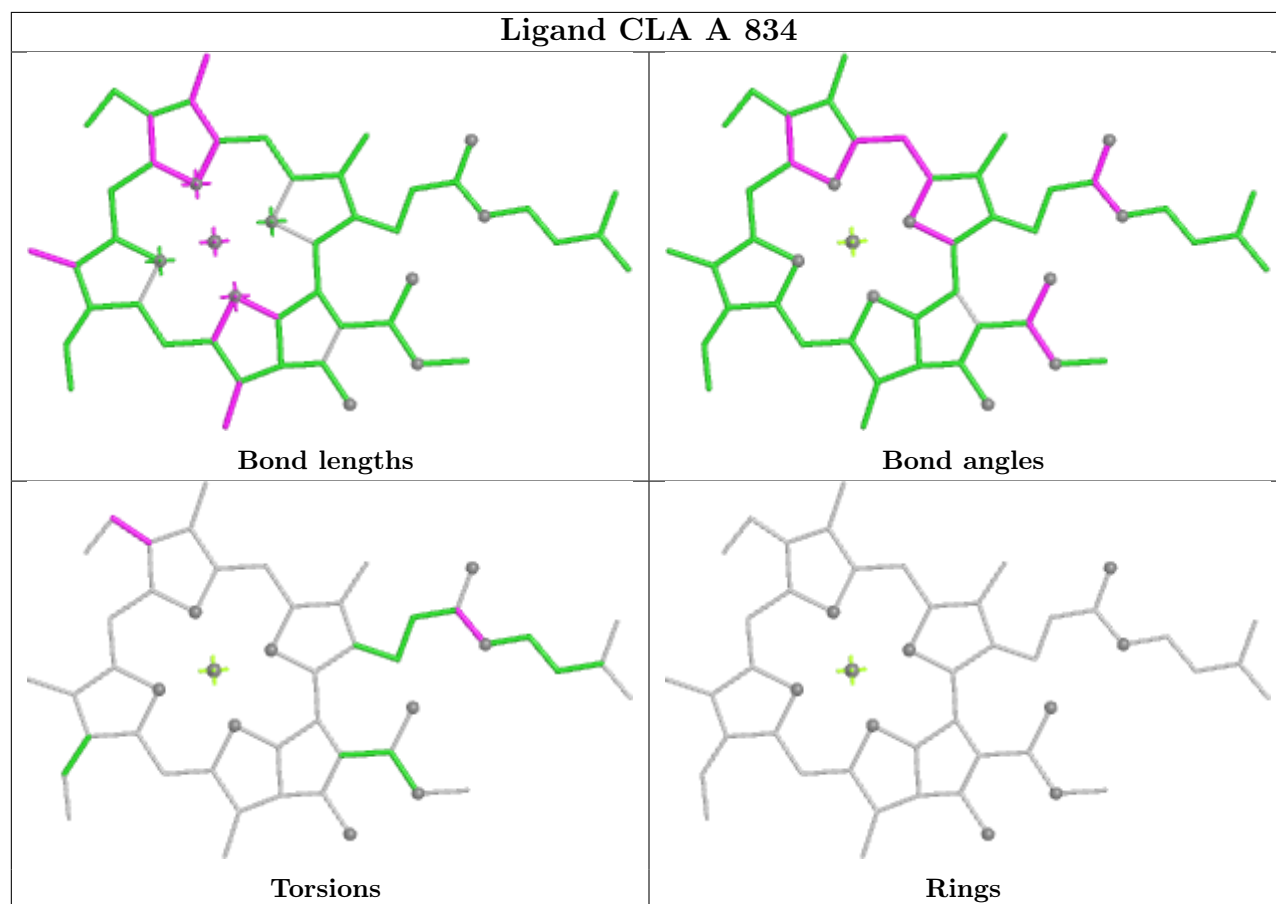
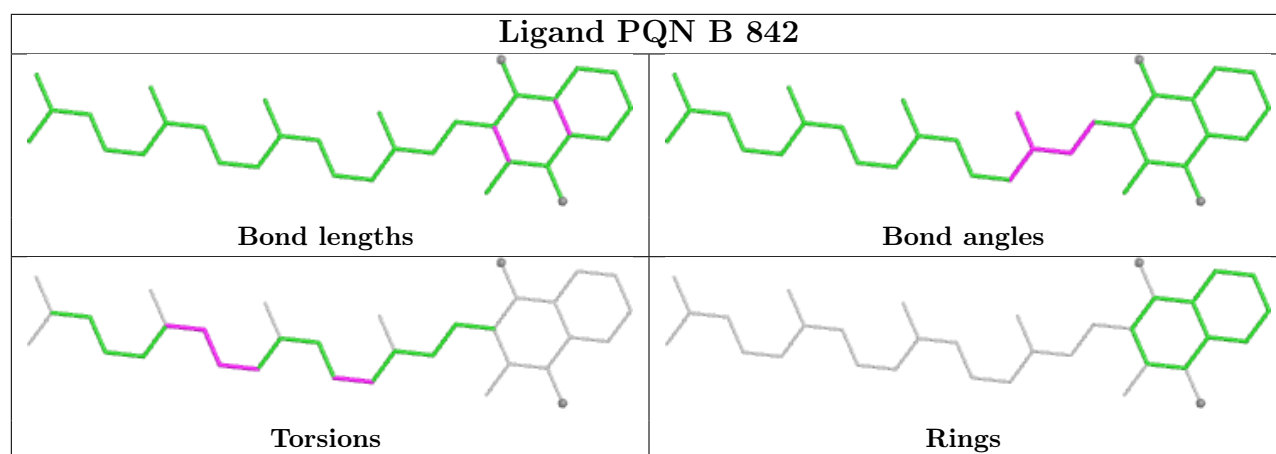
Bond angles

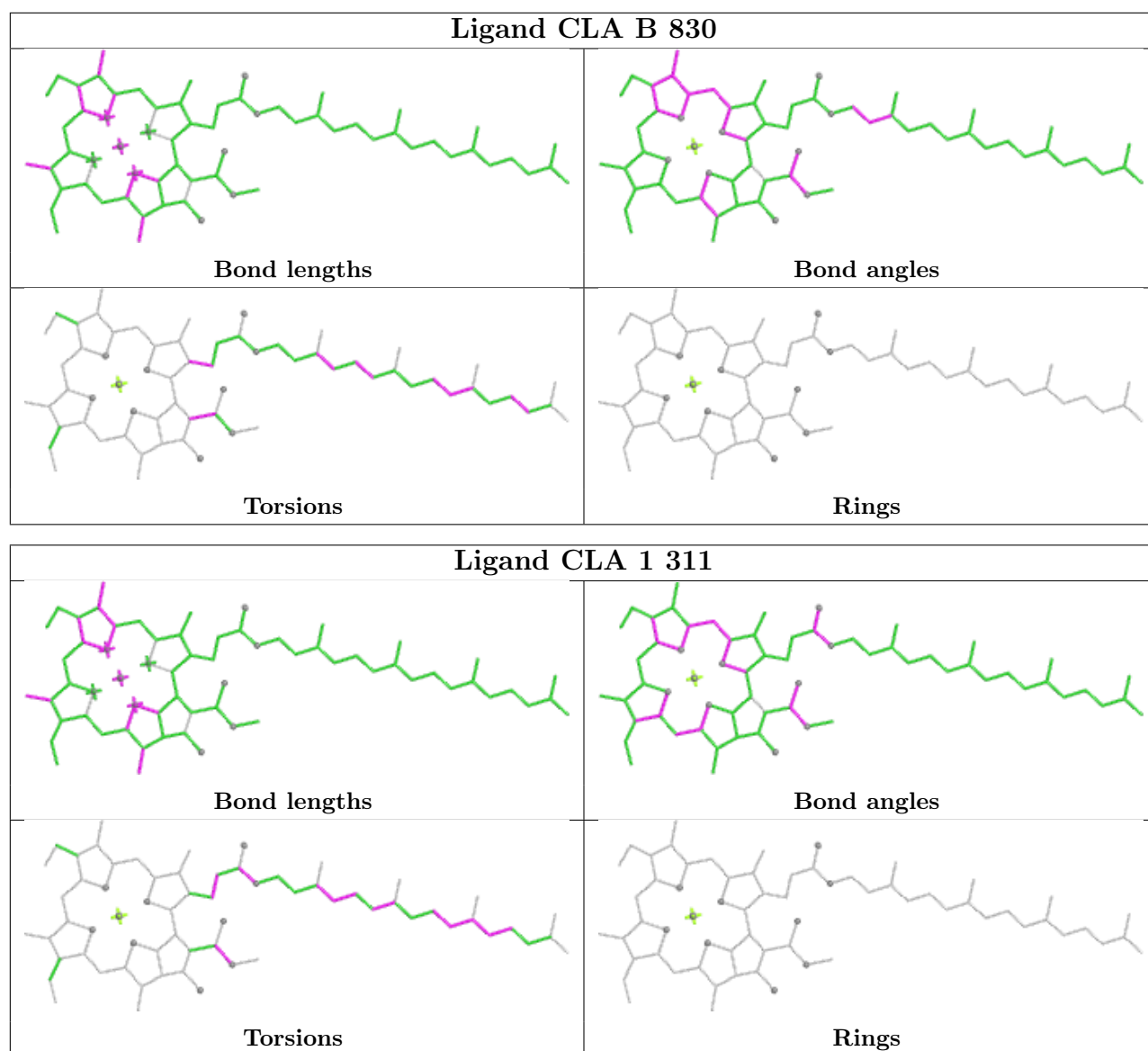


Torsions

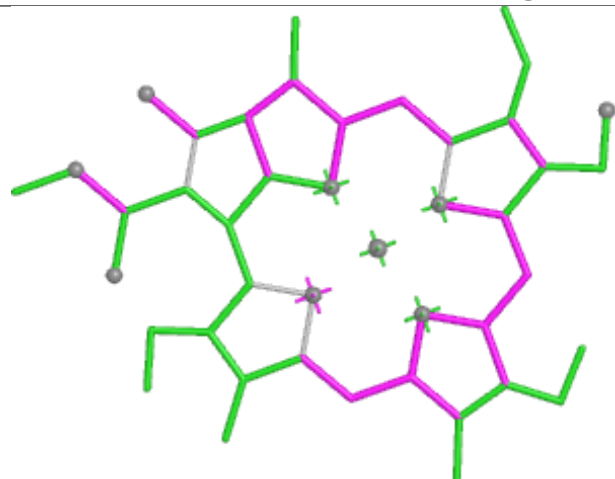


Rings

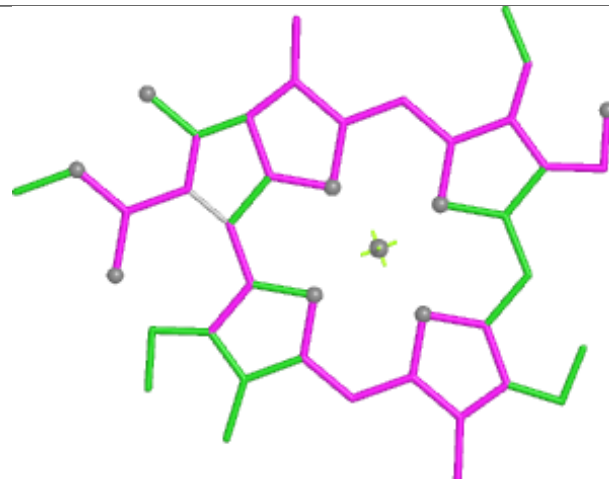




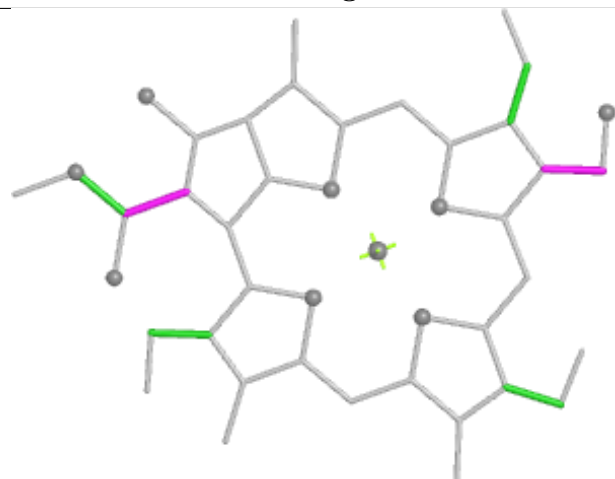
Ligand CHL 2 305



Bond lengths



Bond angles

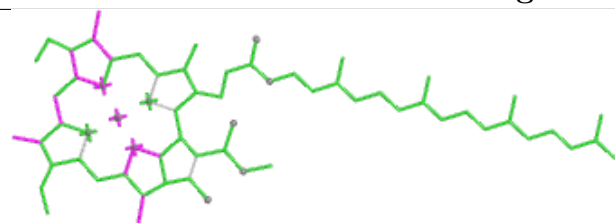


Torsions

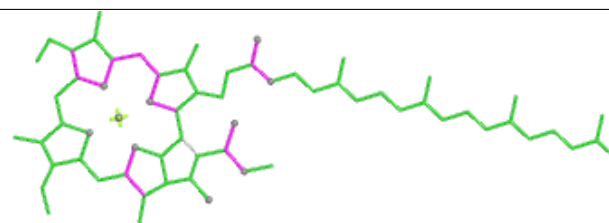


Rings

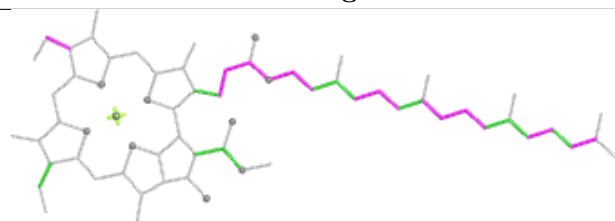
Ligand CLA B 834



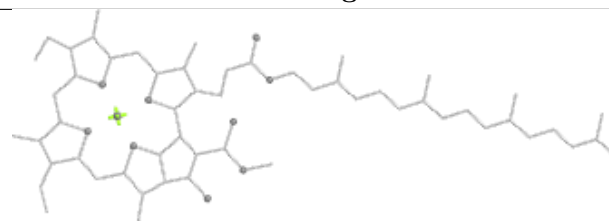
Bond lengths



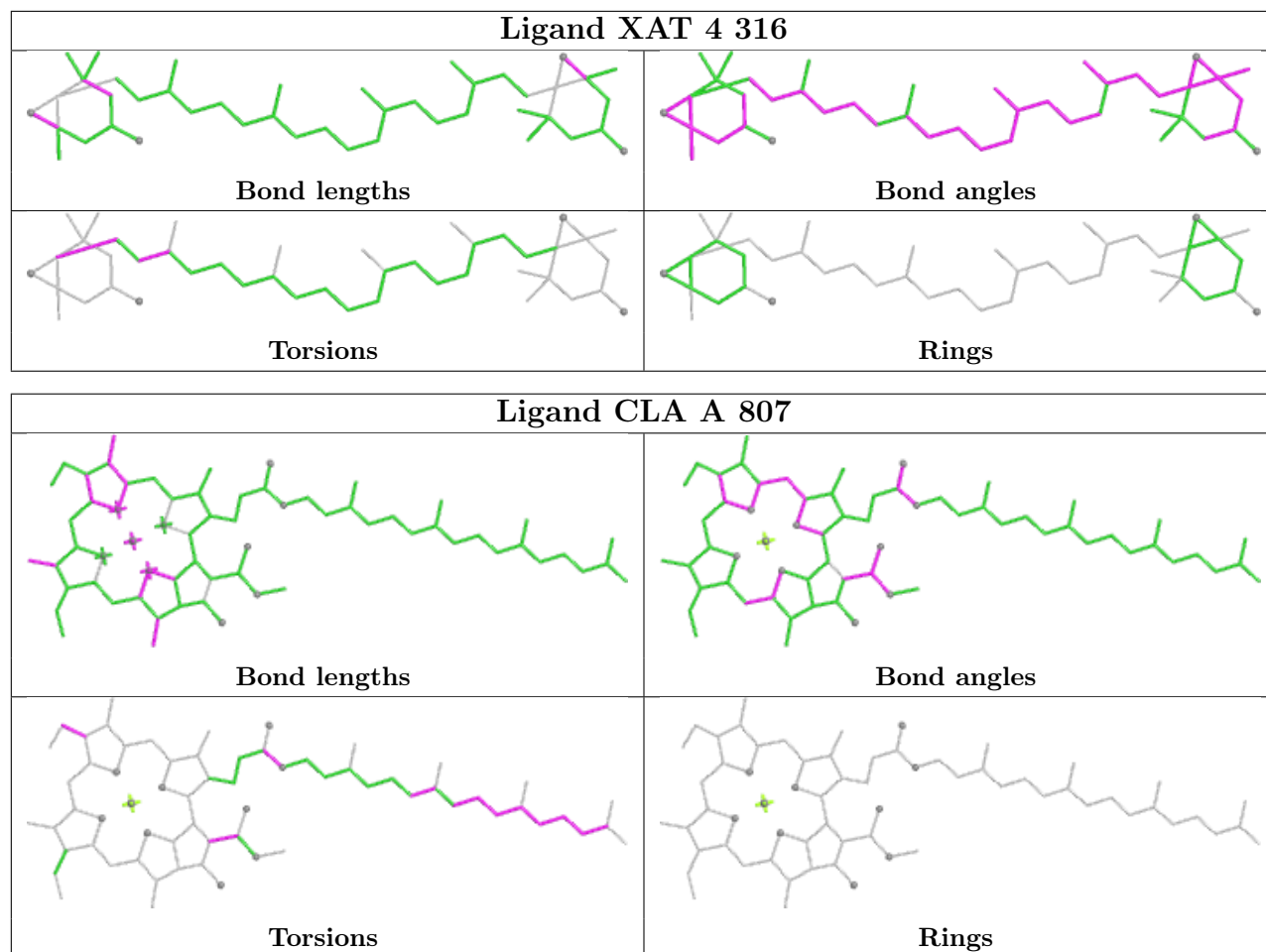
Bond angles

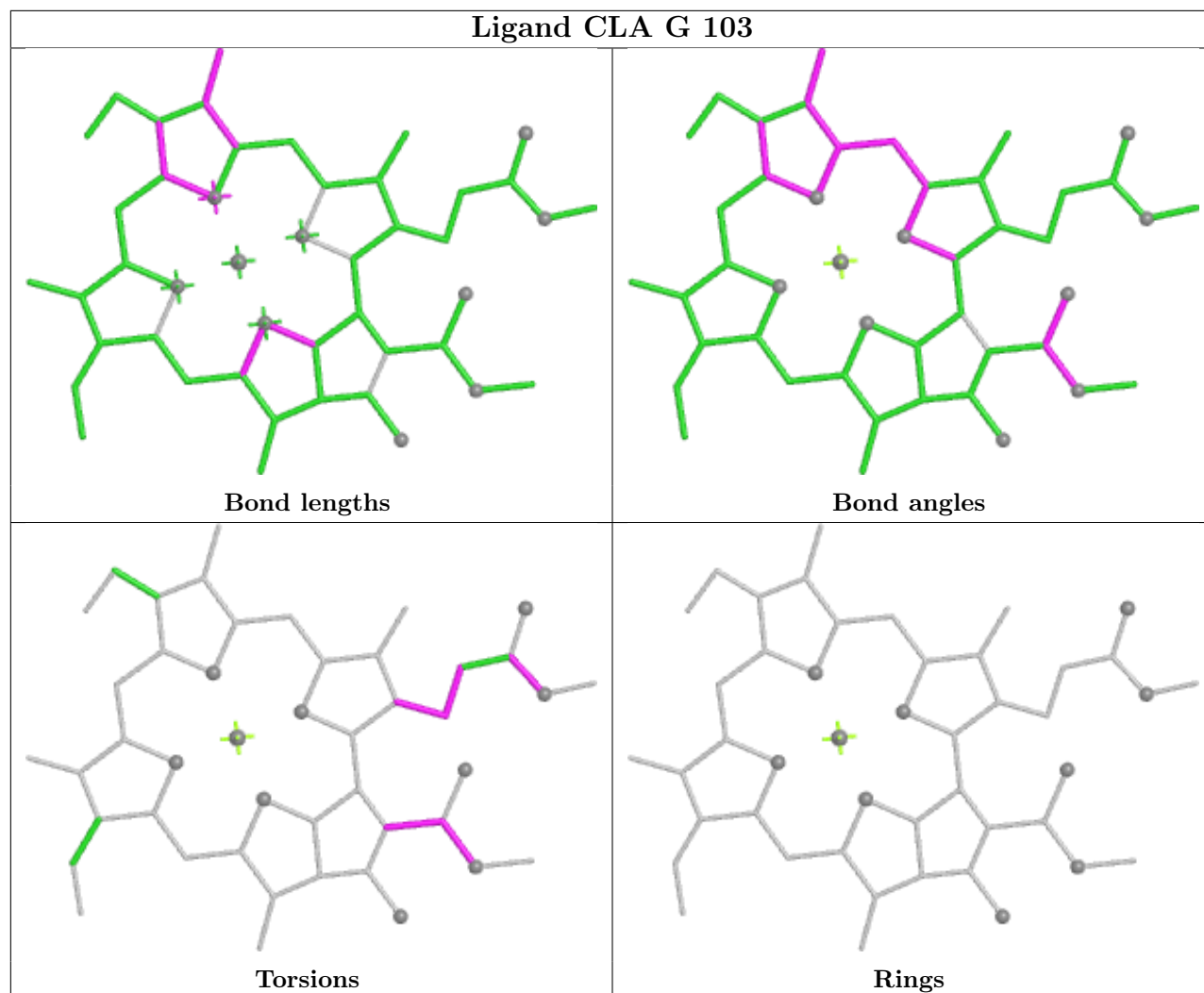


Torsions

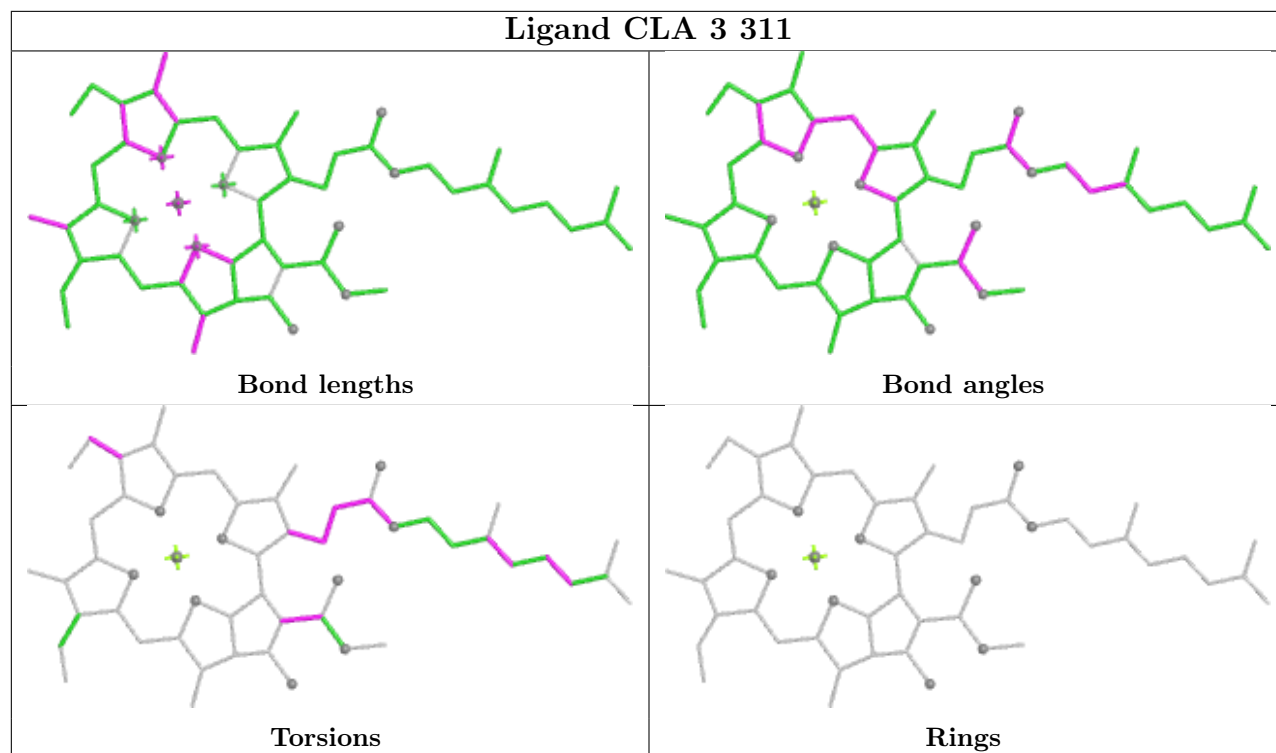


Rings

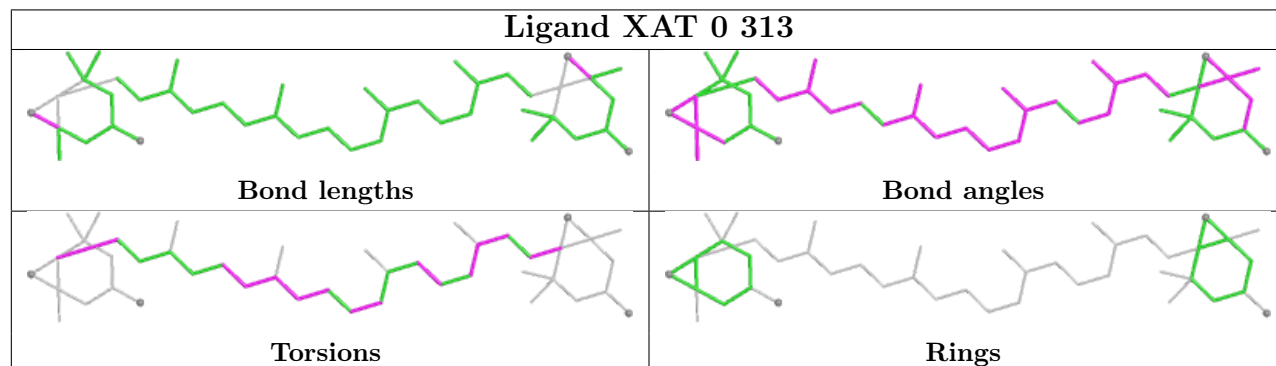




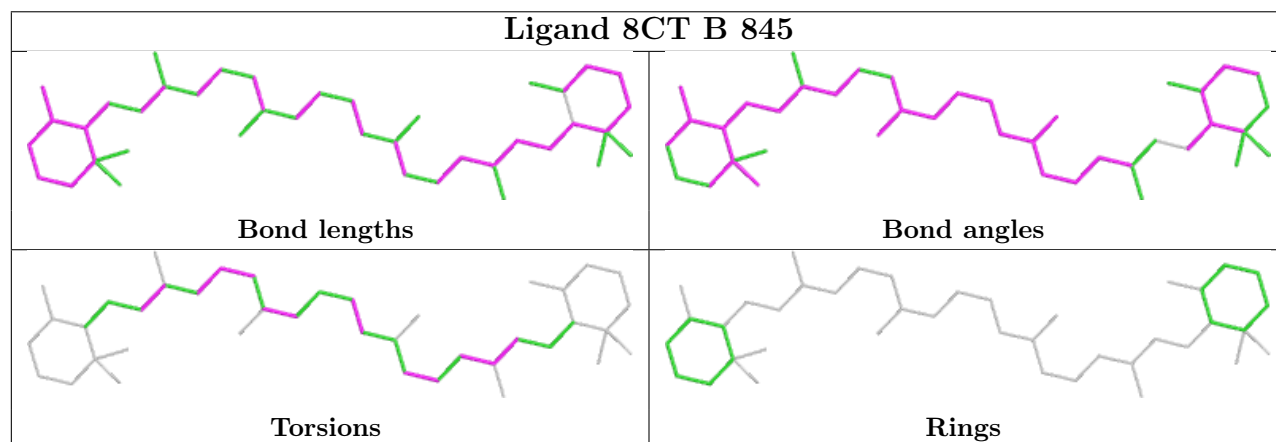
Ligand CLA 3 311

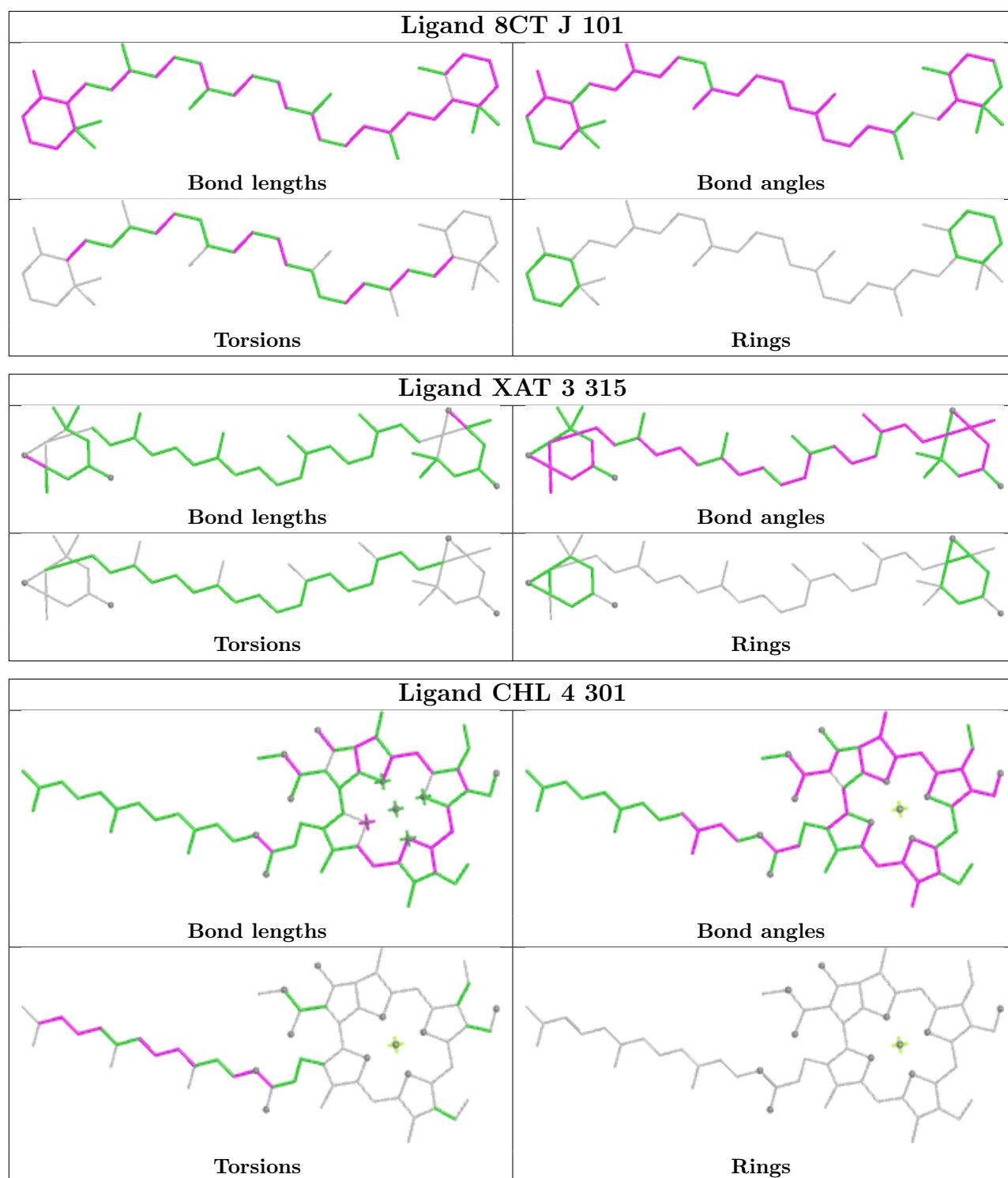


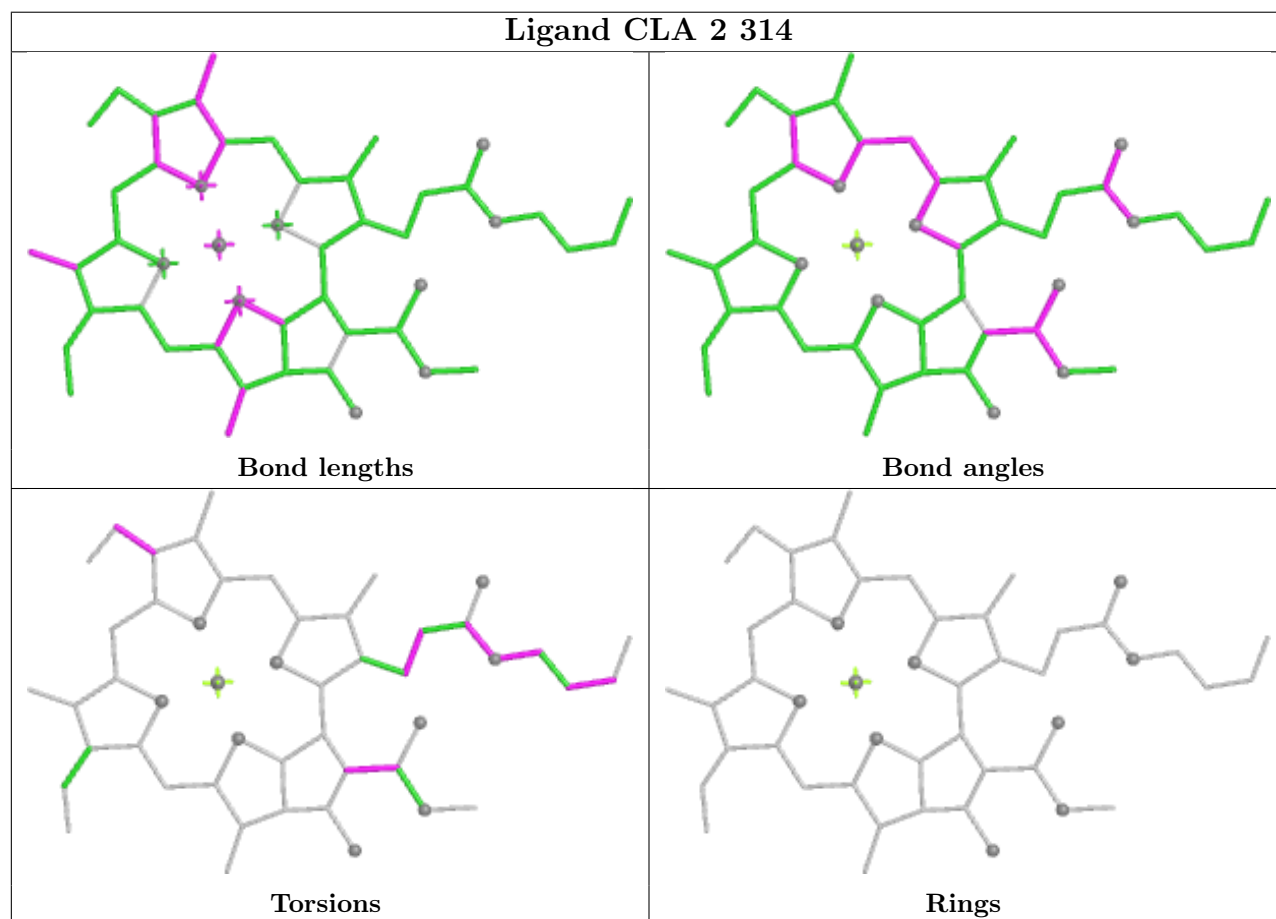
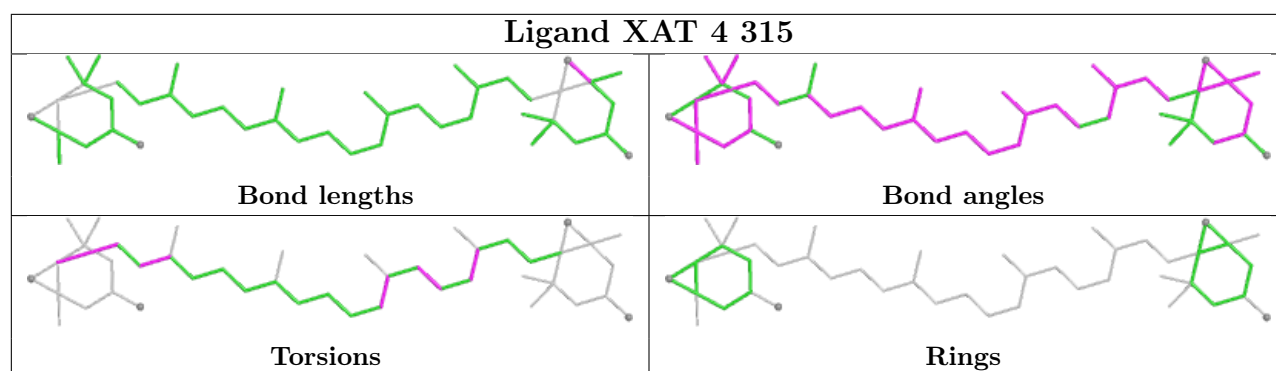
Ligand XAT 0 313

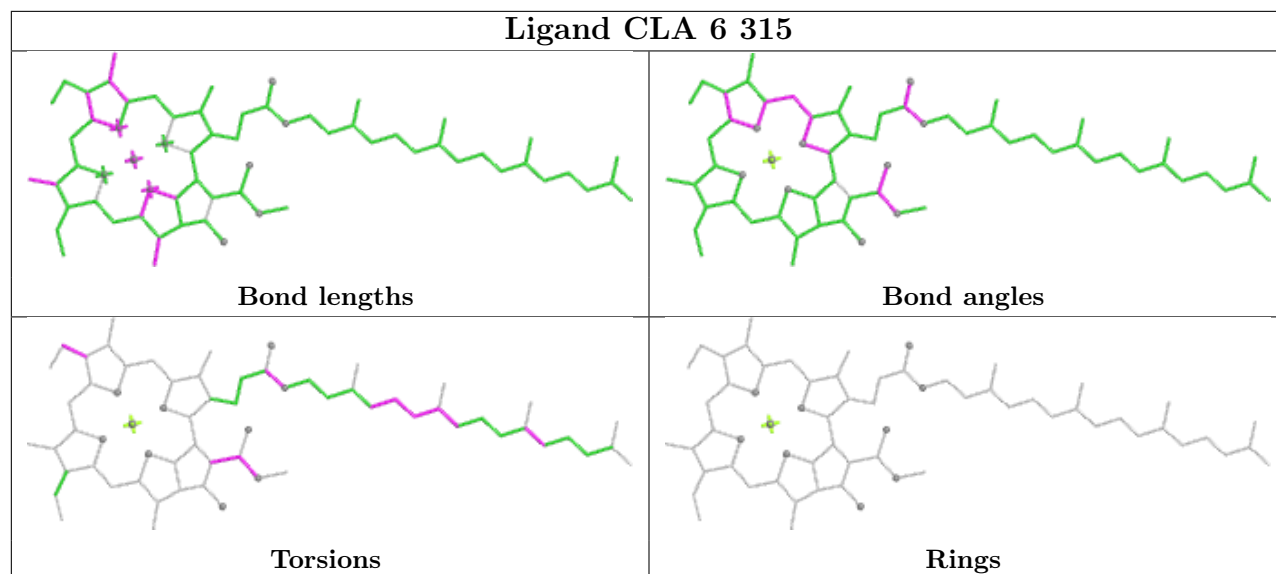
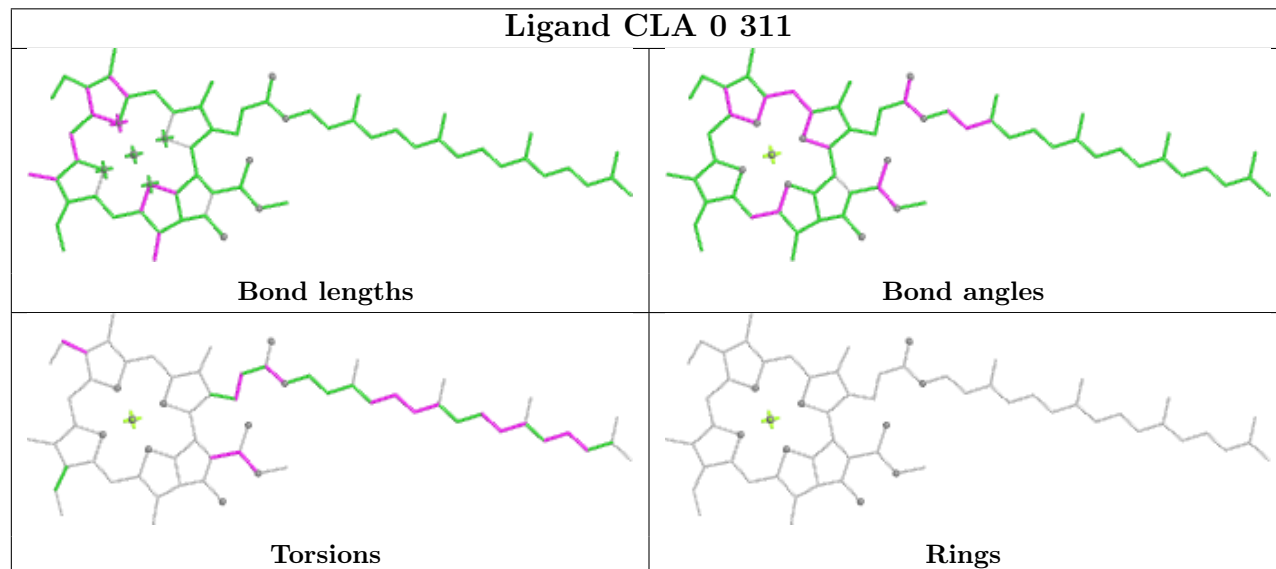


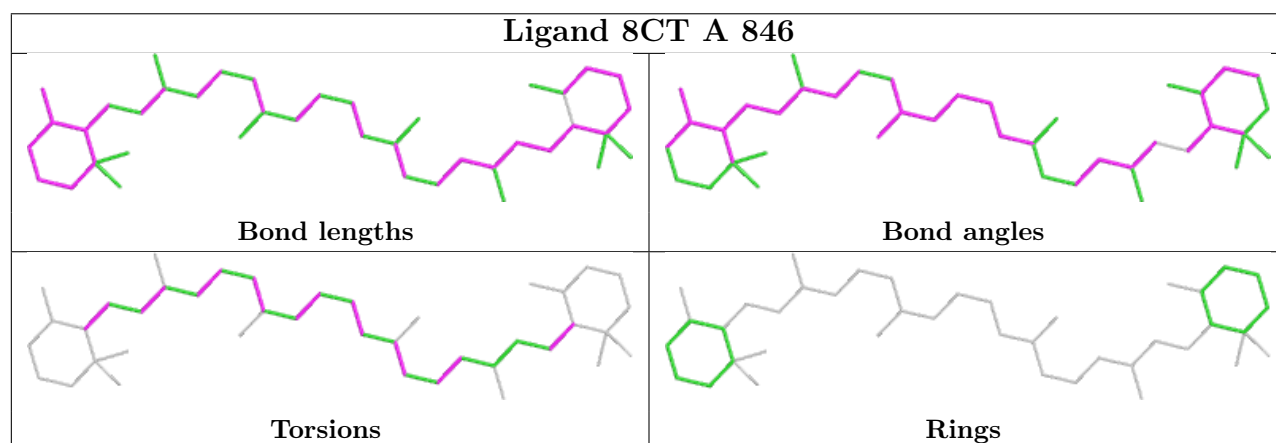
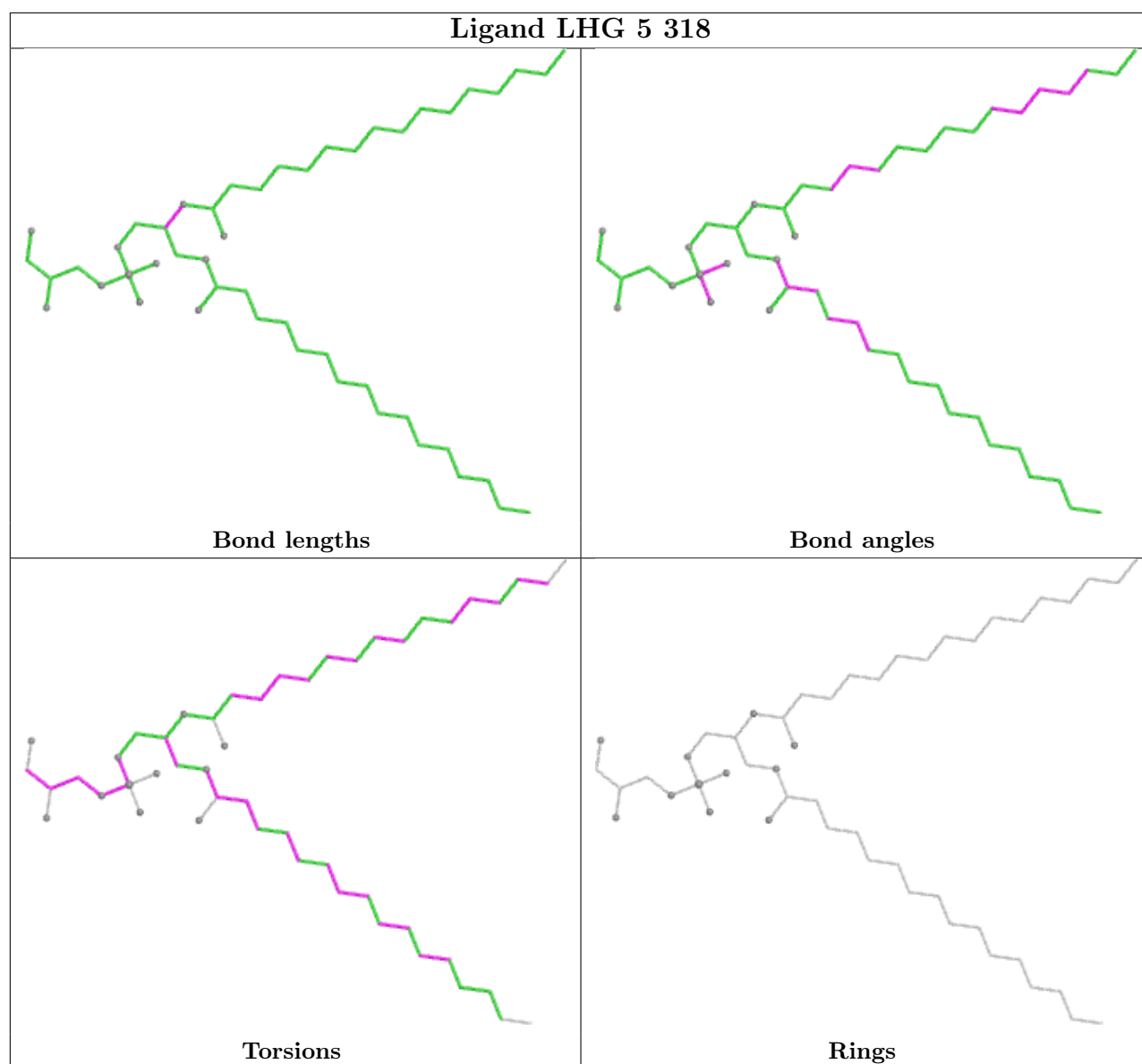
Ligand 8CT B 845



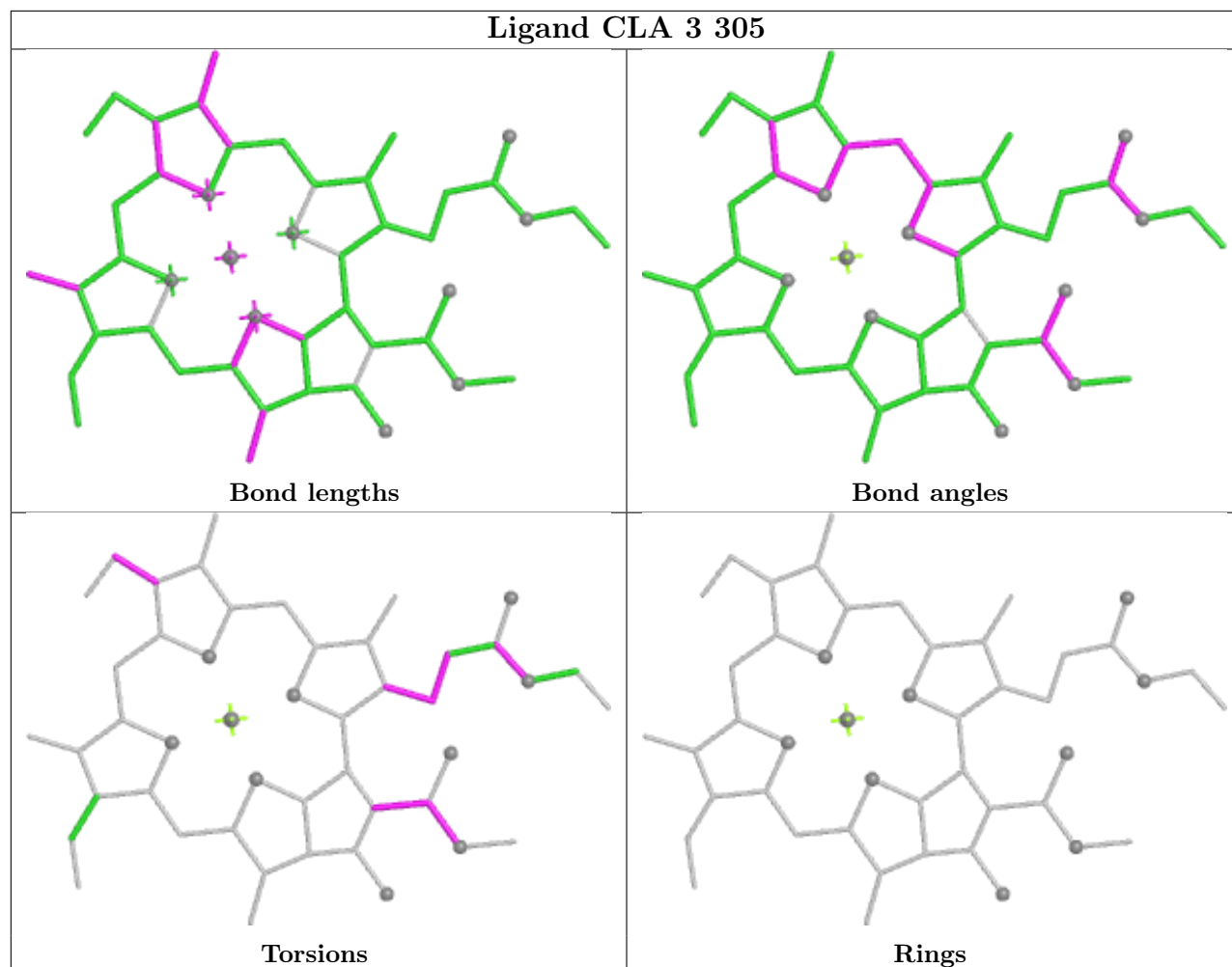




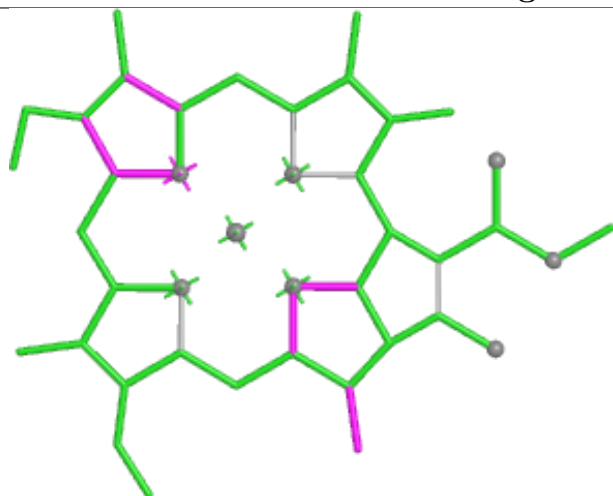
Ligand CLA 6 315**Ligand CLA 0 311**



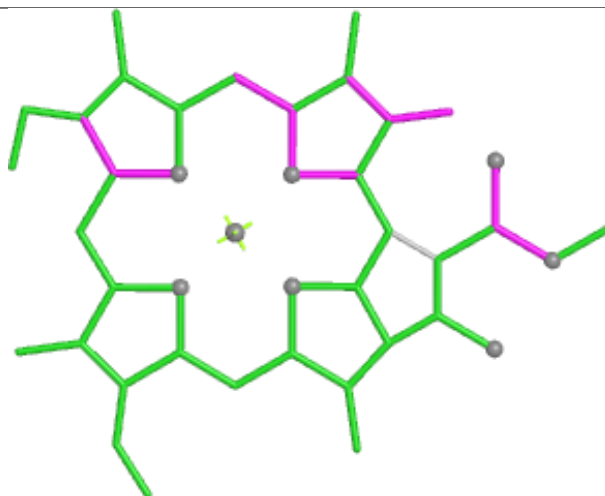
Ligand CLA 3 305



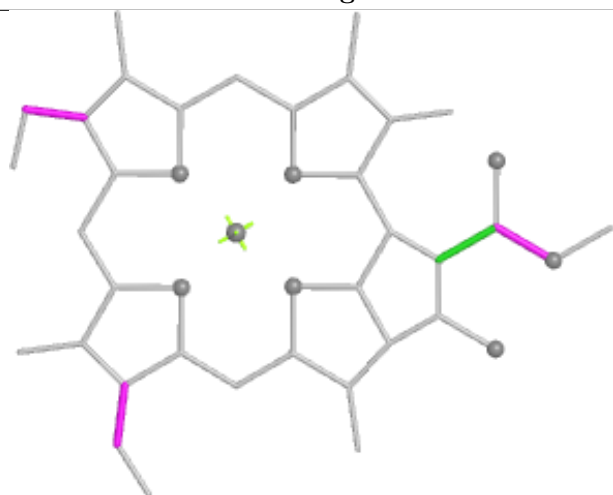
Ligand CLA 9 310



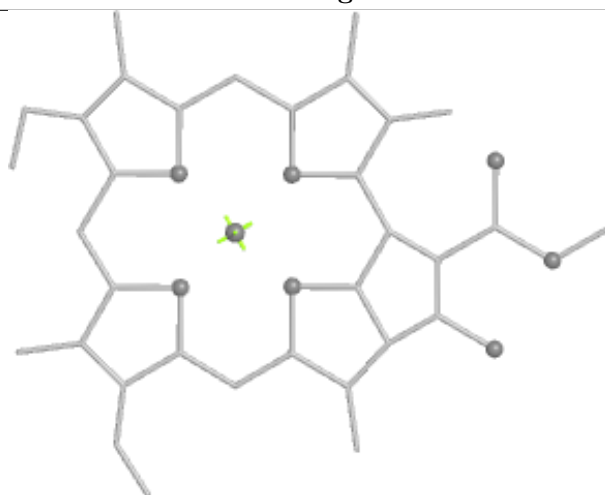
Bond lengths



Bond angles

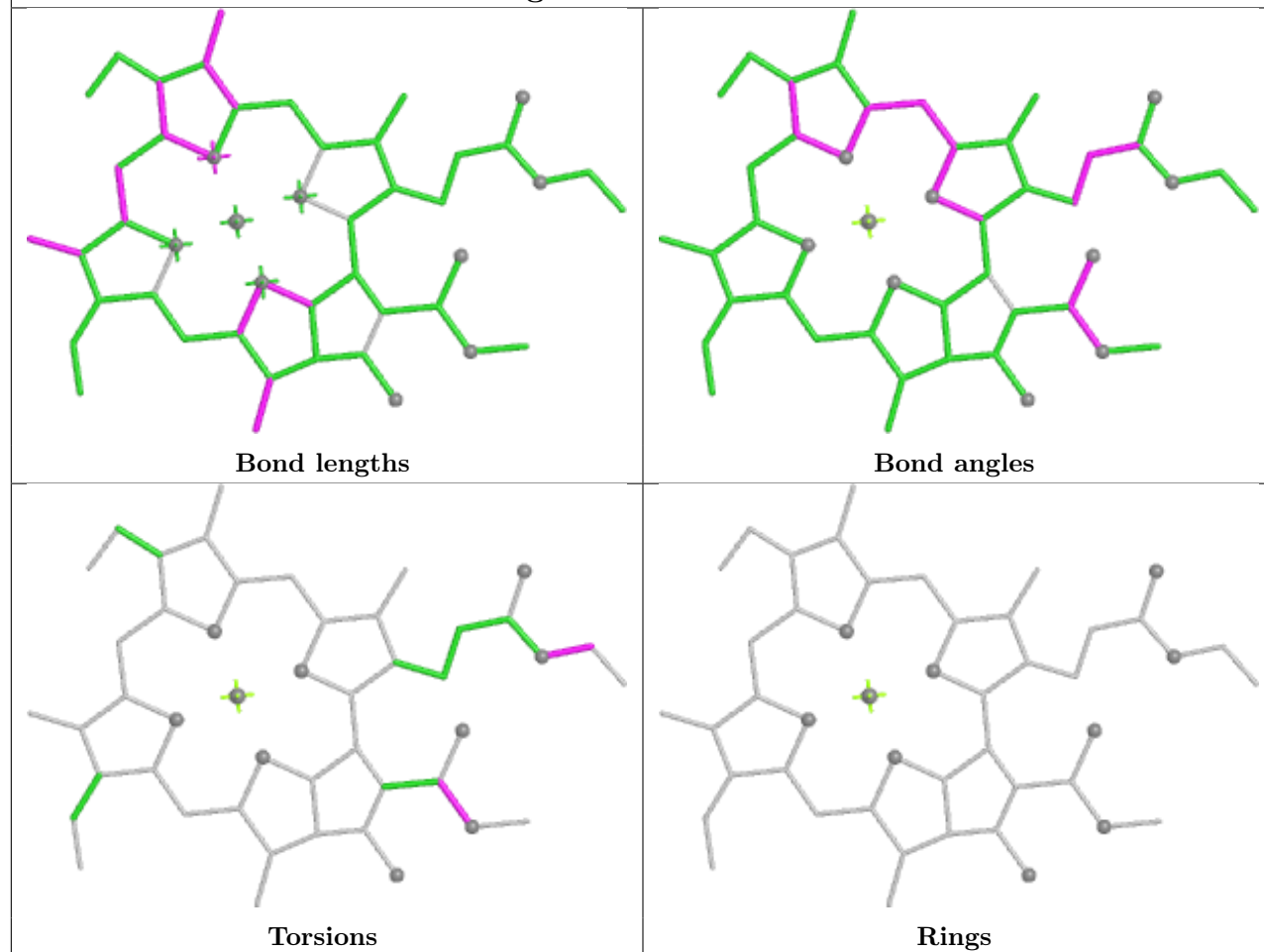


Torsions

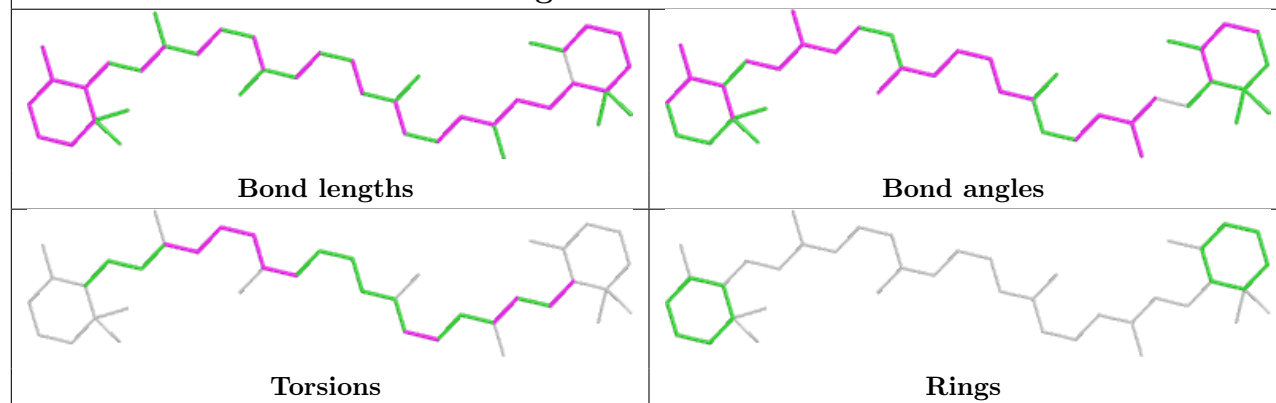


Rings

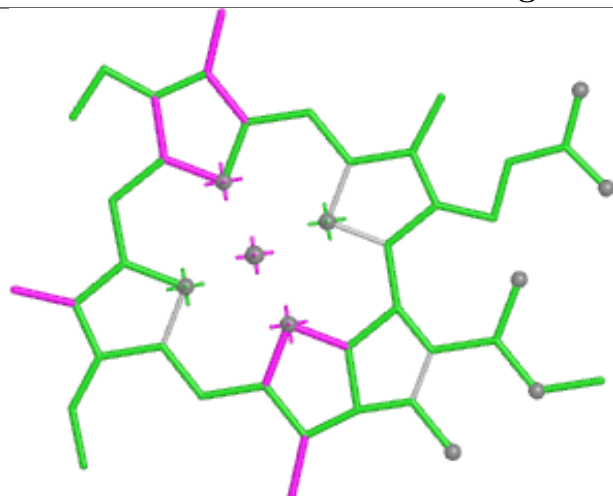
Ligand CLA A 815



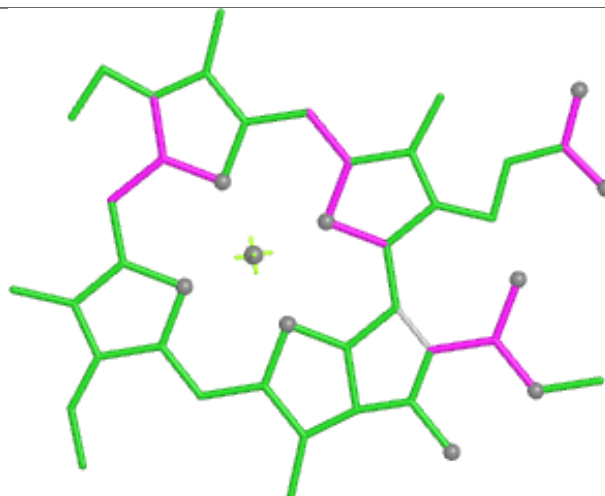
Ligand 8CT B 846



Ligand CLA 6 317



Bond lengths



Bond angles

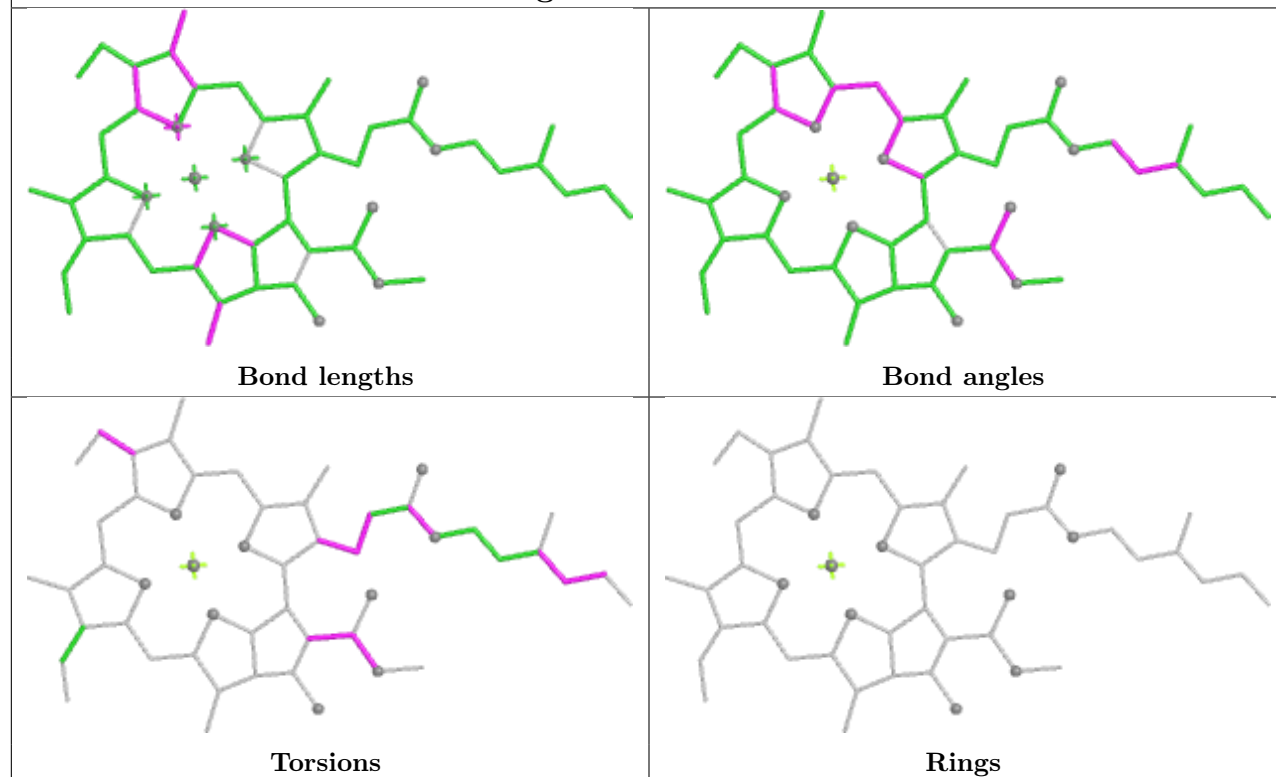


Torsions

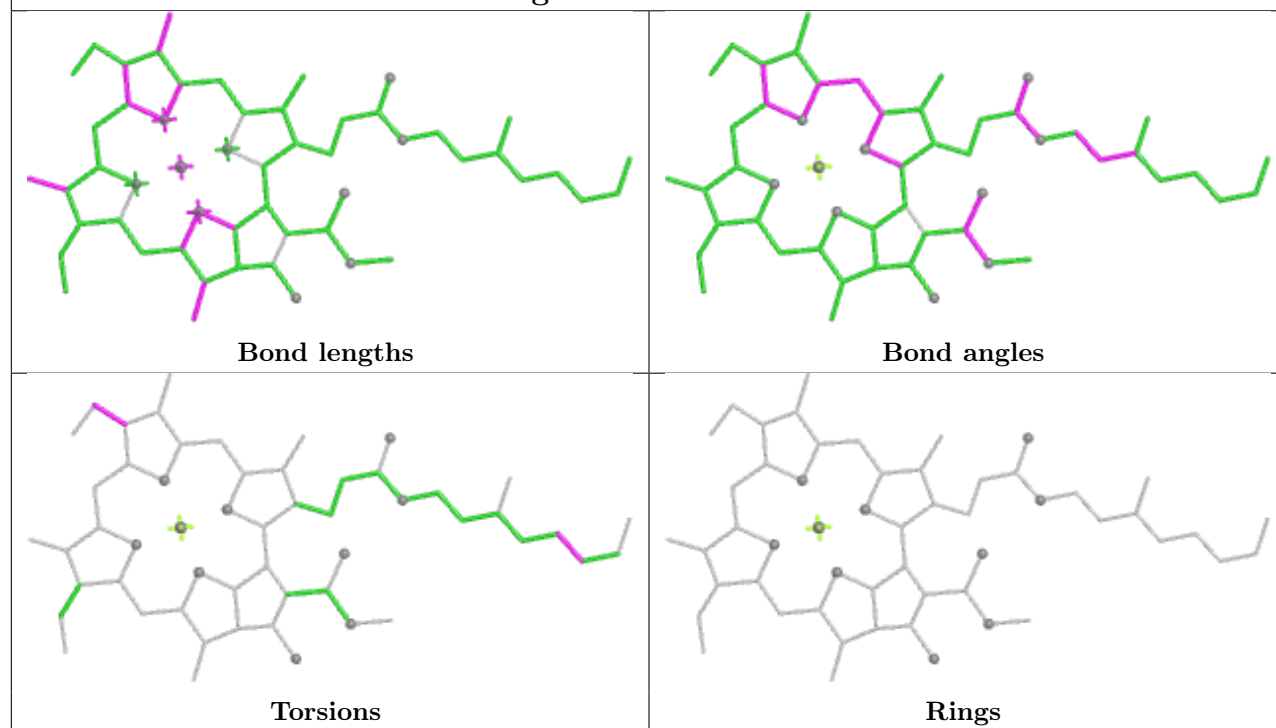


Rings

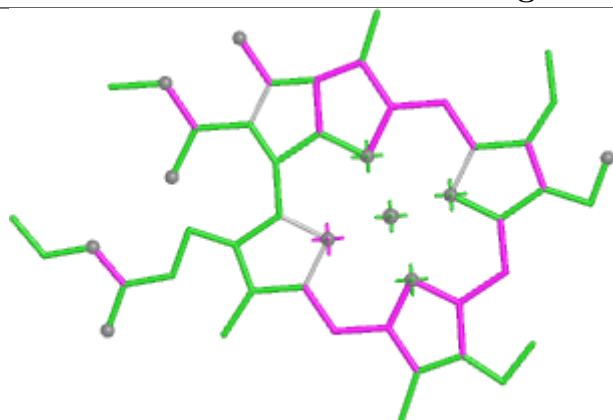
Ligand CLA 0 304



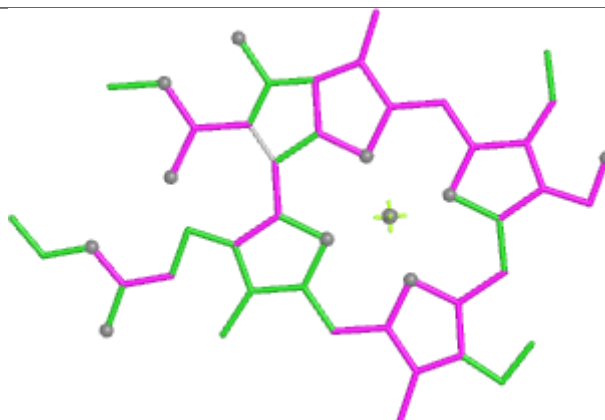
Ligand CLA A 812



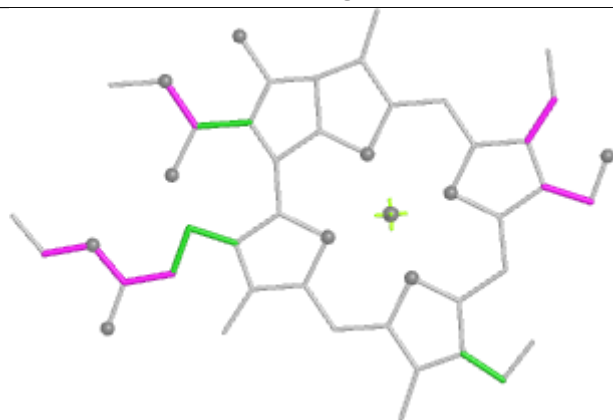
Ligand CHL 9 307



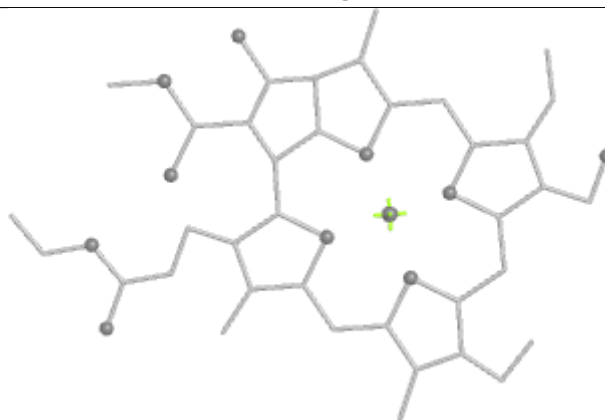
Bond lengths



Bond angles

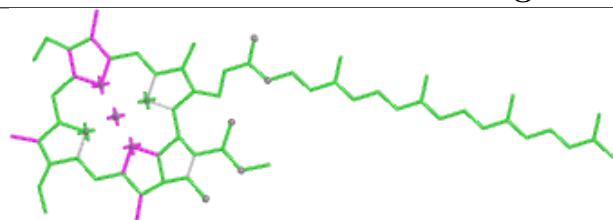


Torsions

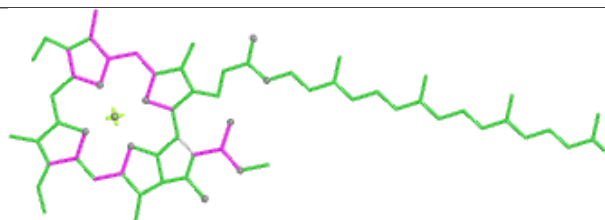


Rings

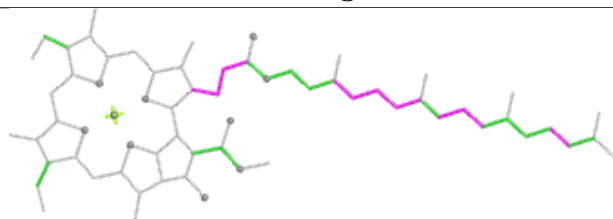
Ligand CLA B 832



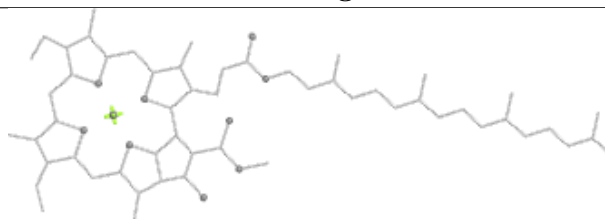
Bond lengths



Bond angles

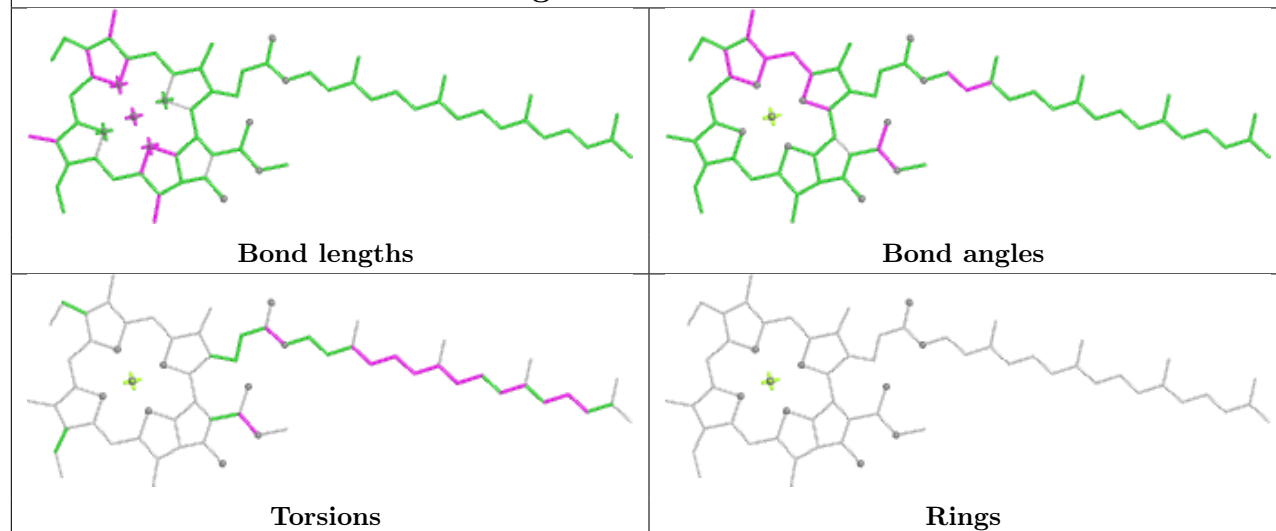


Torsions

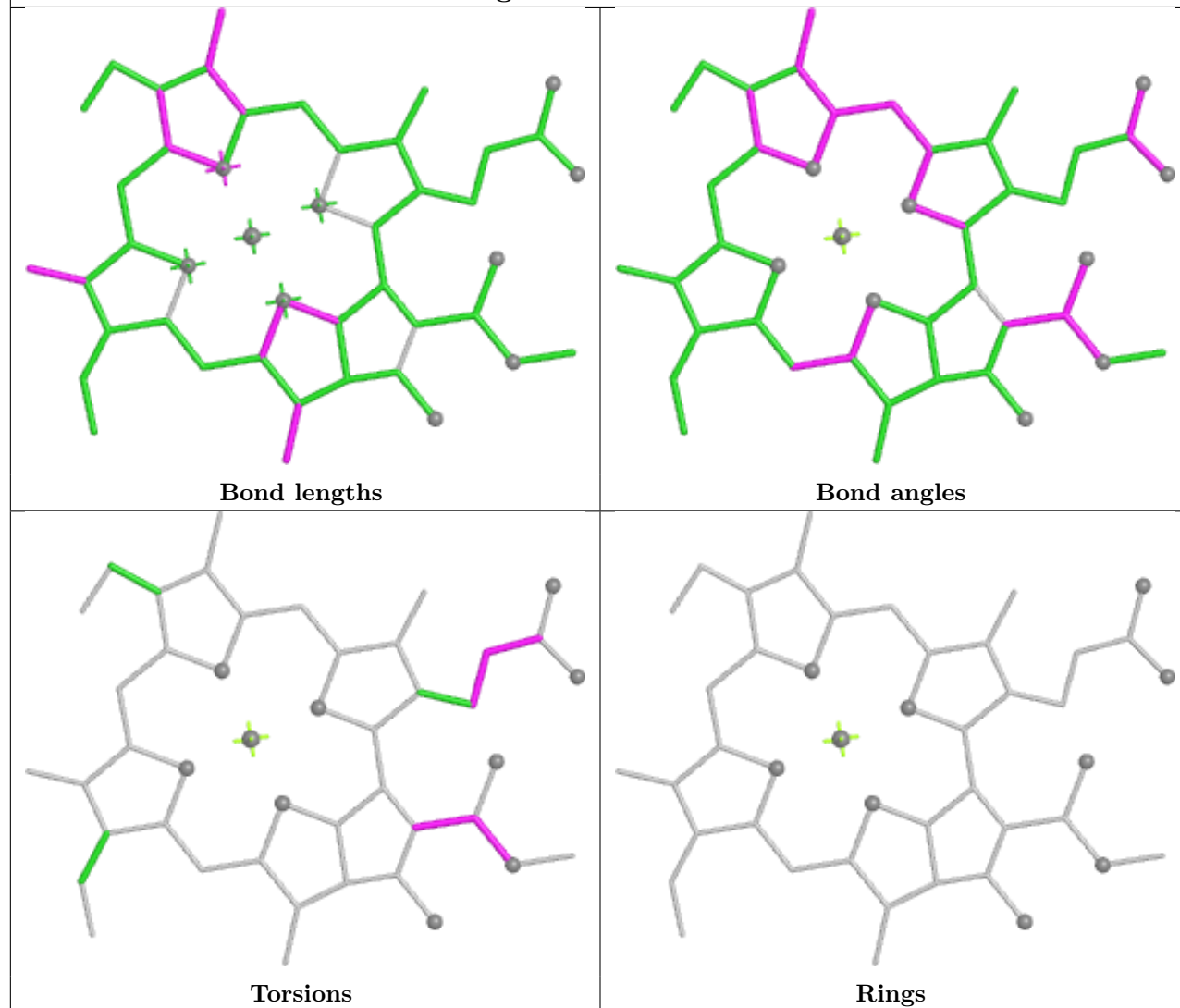


Rings

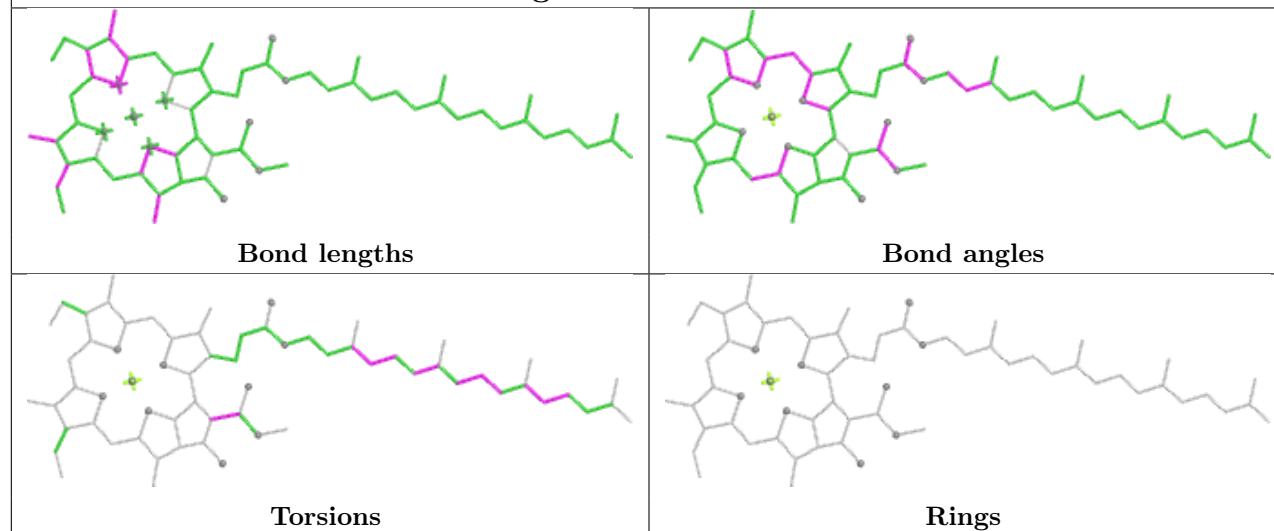
Ligand CLA B 812



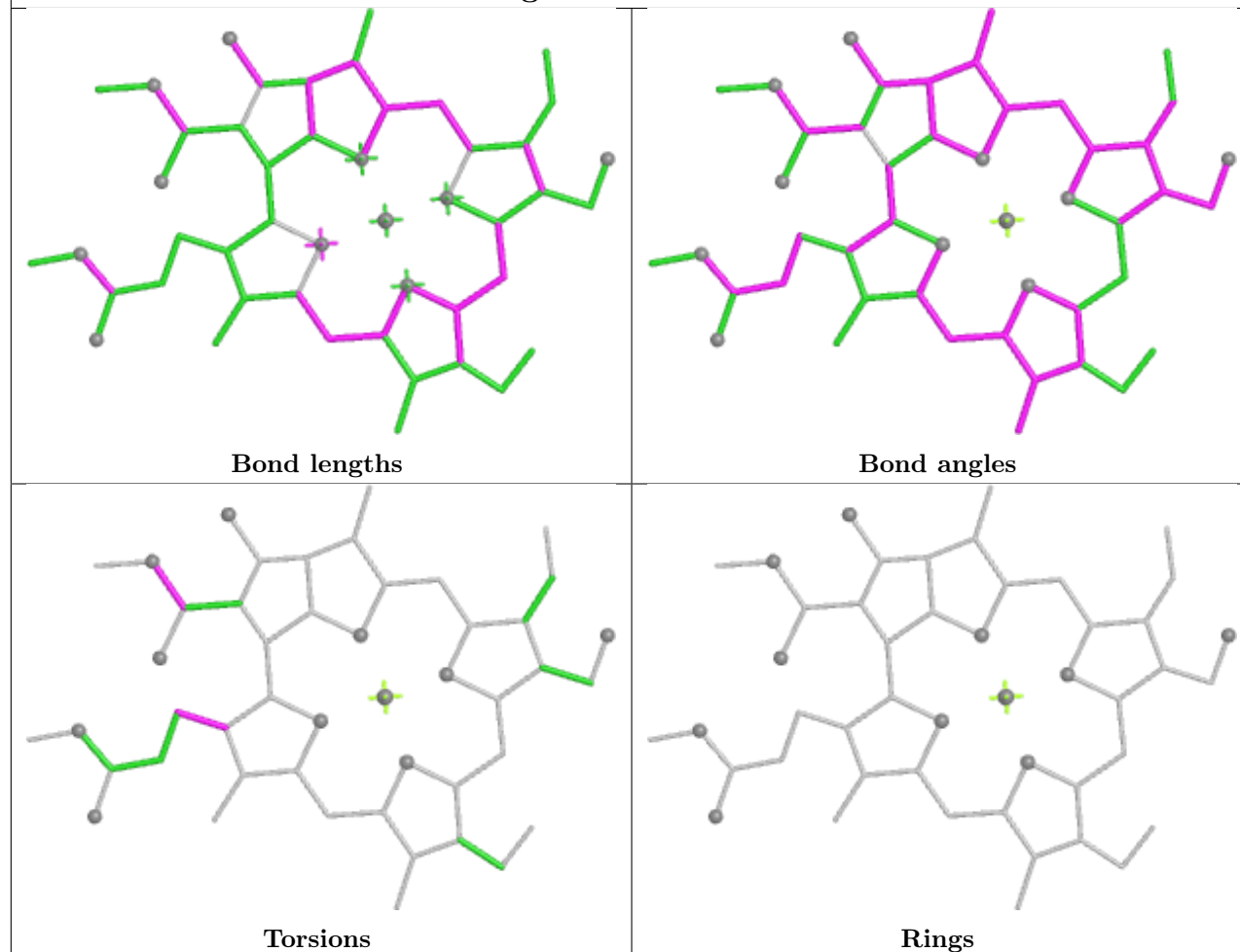
Ligand CLA 3 312



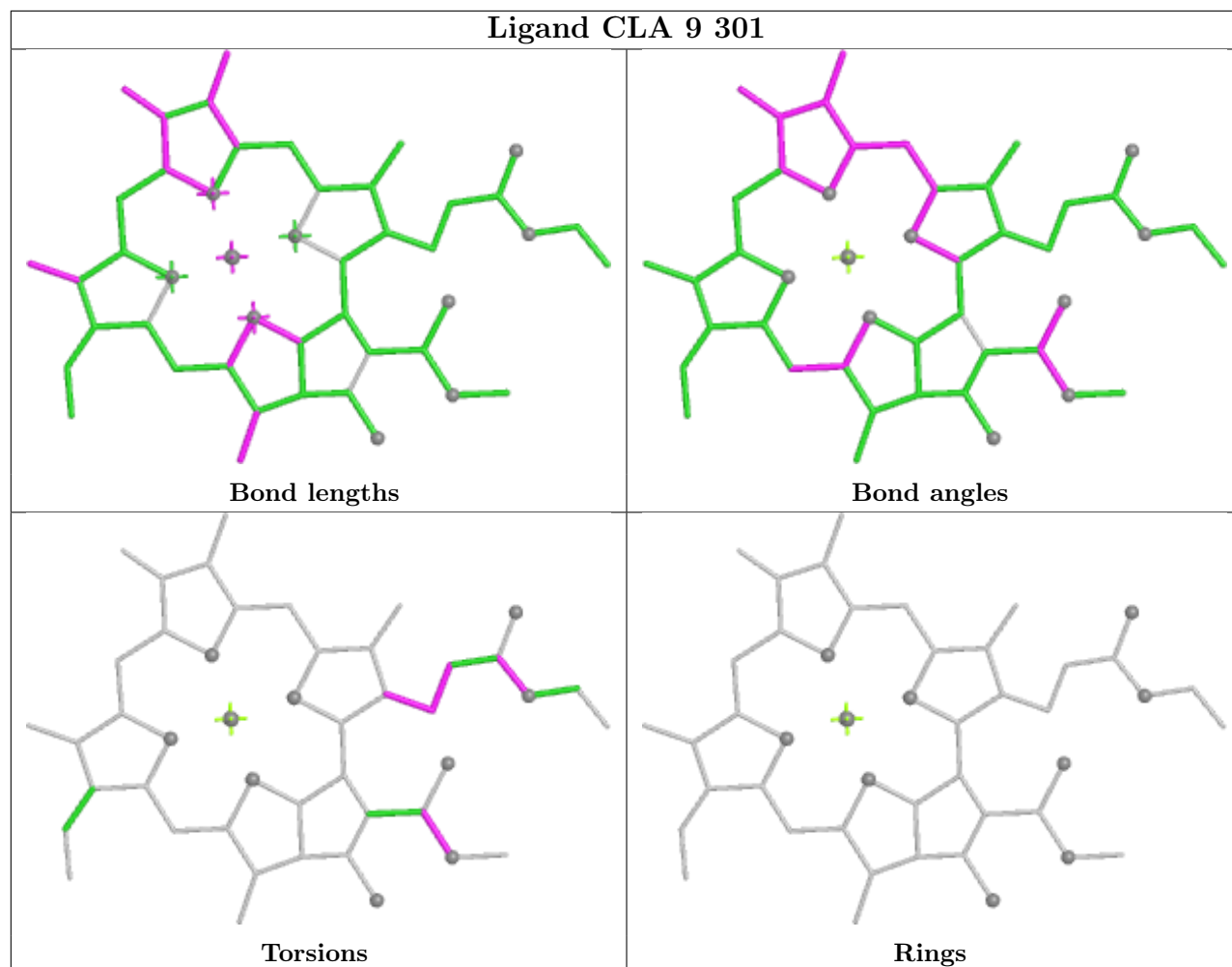
Ligand CLA B 811

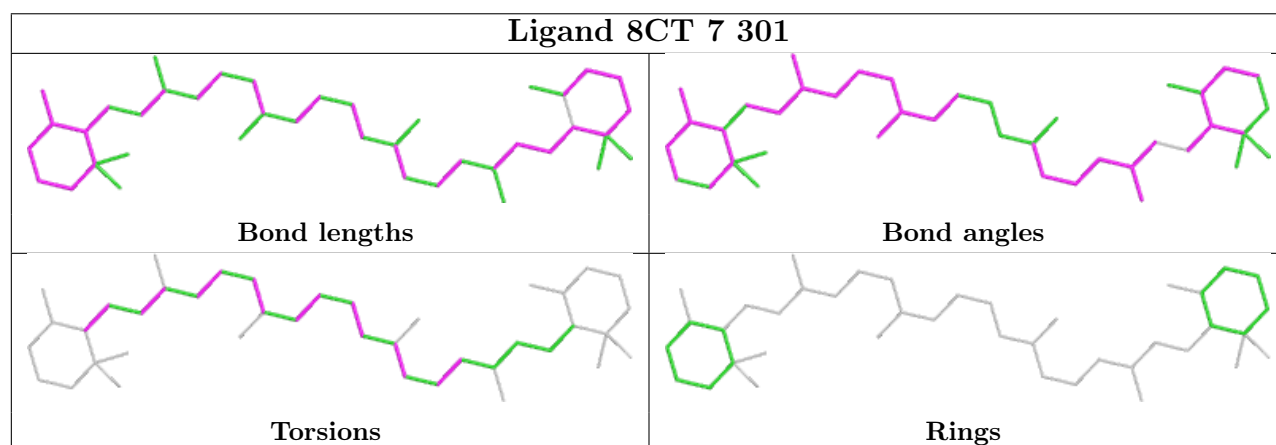
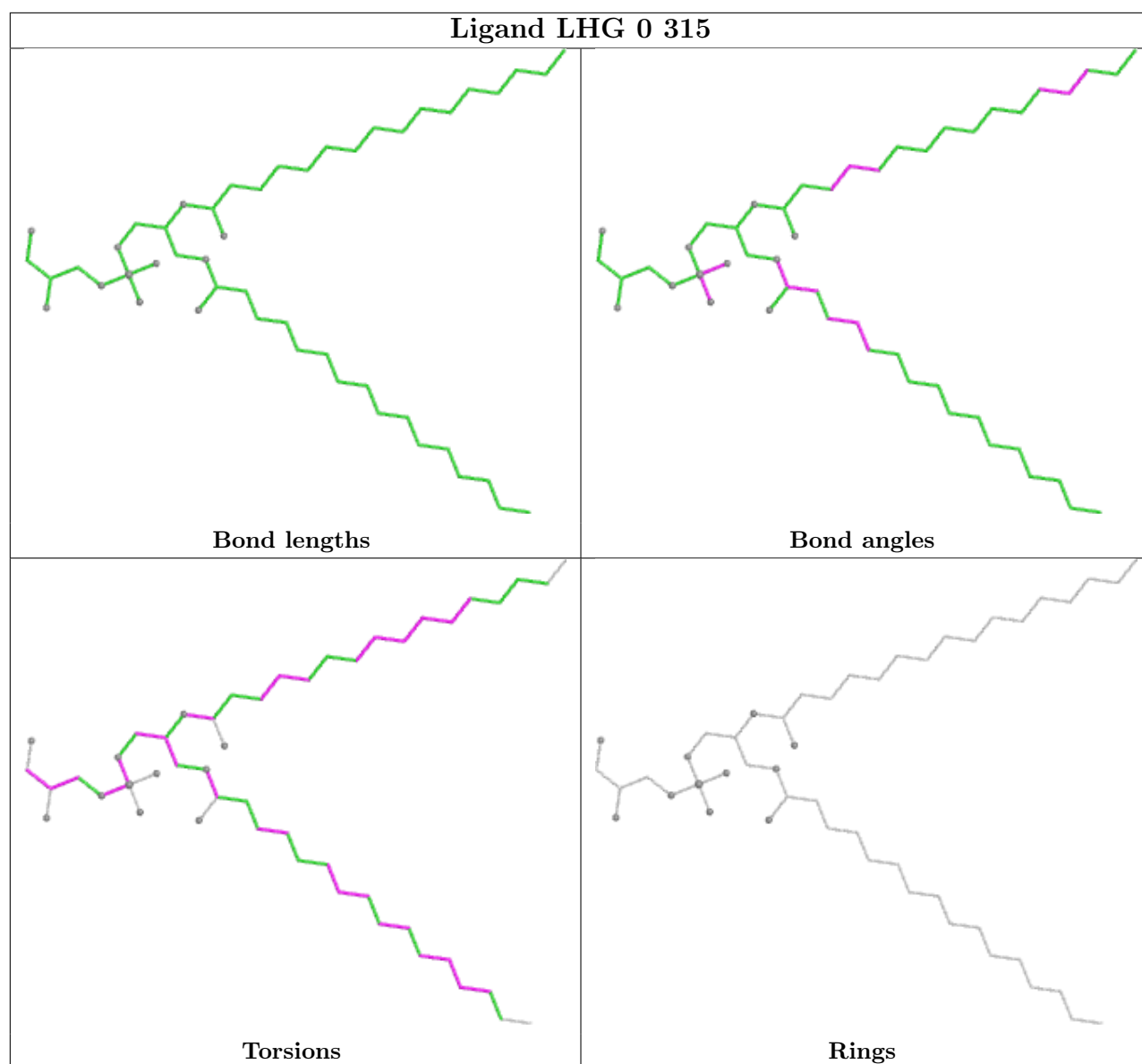


Ligand CHL 3 306

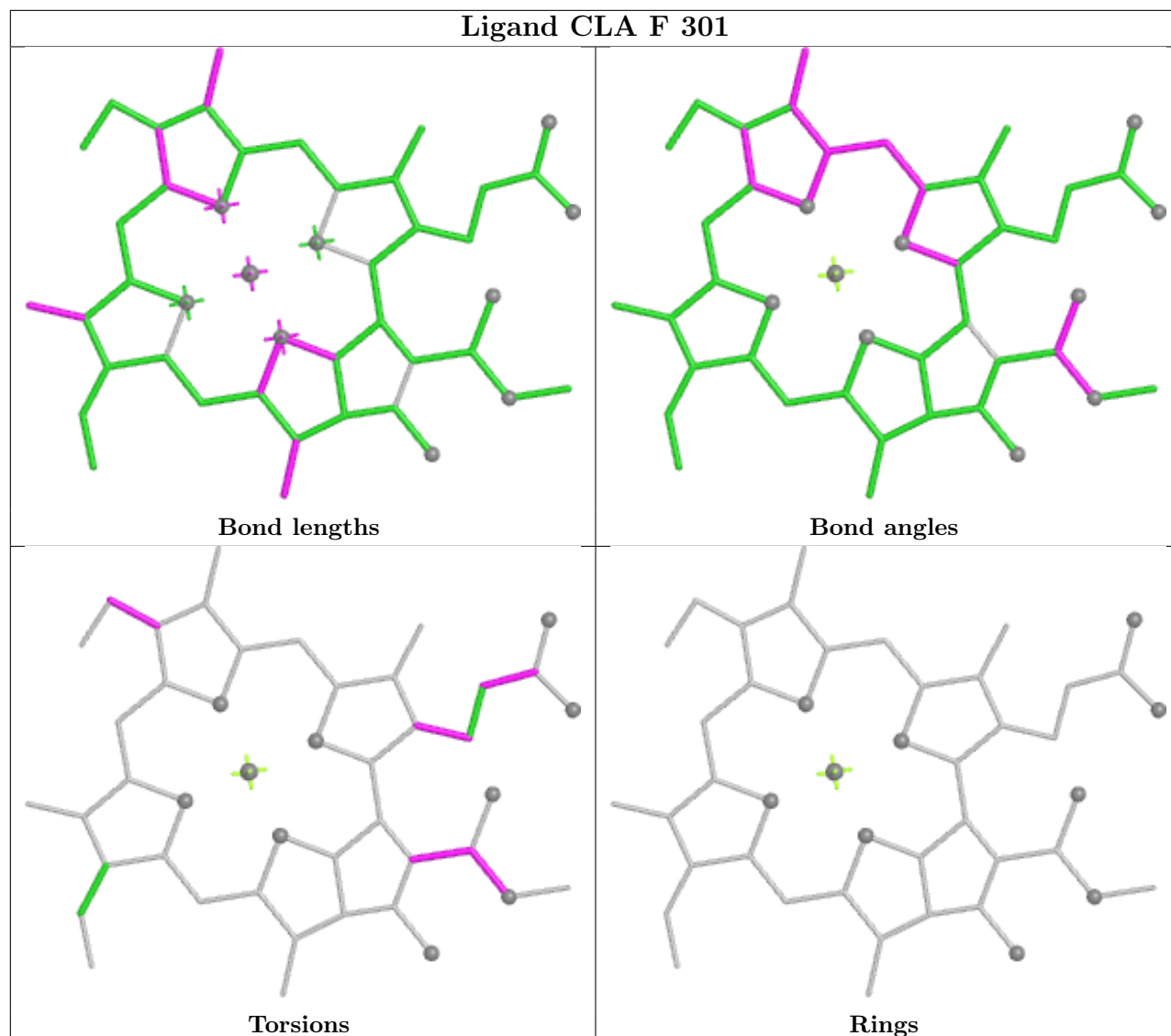


Ligand CLA 9 301

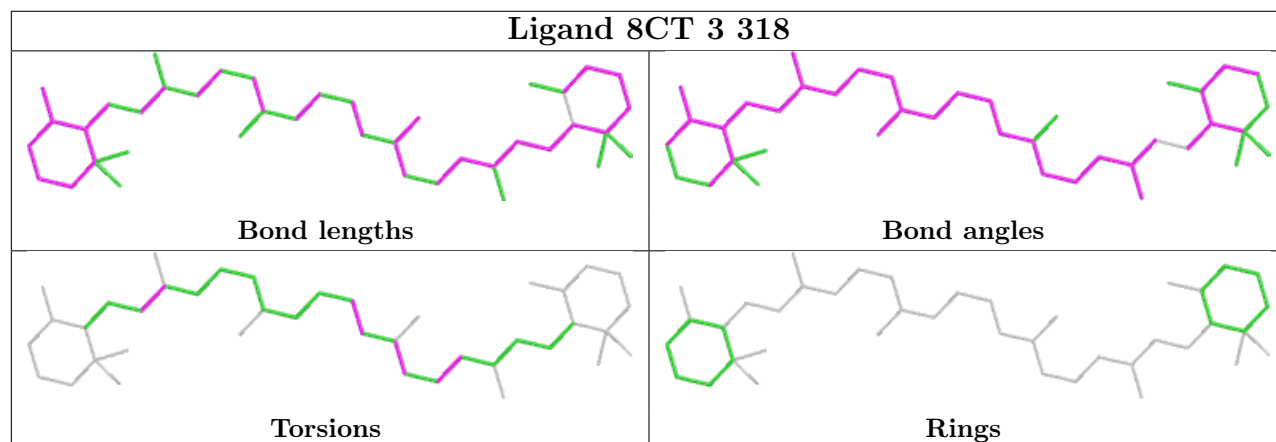




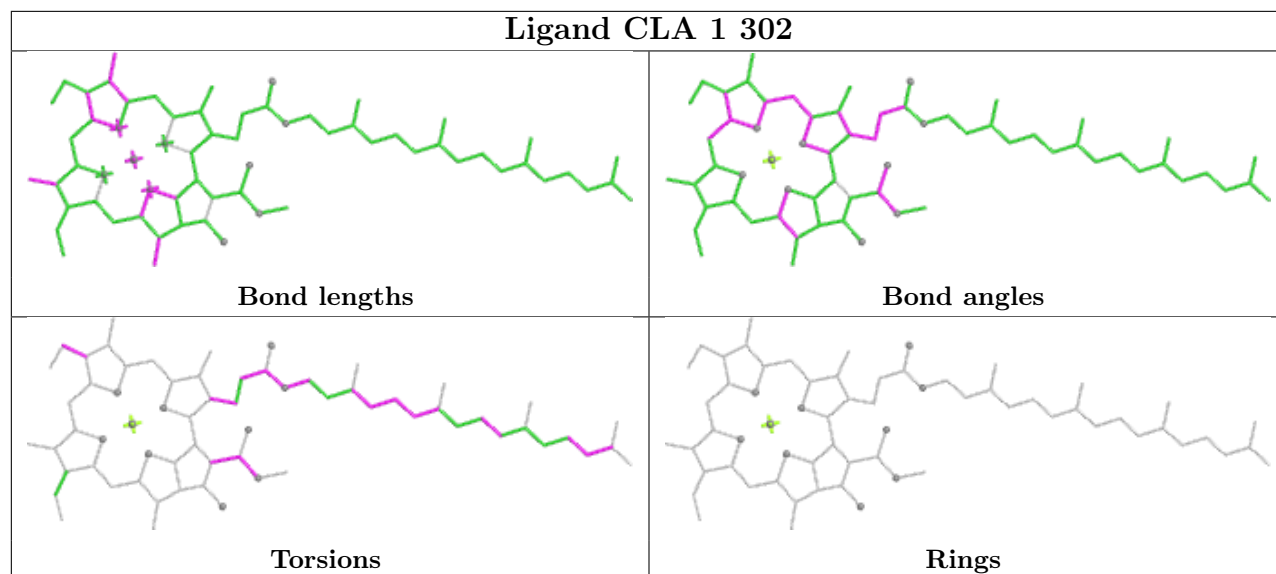
Ligand CLA F 301



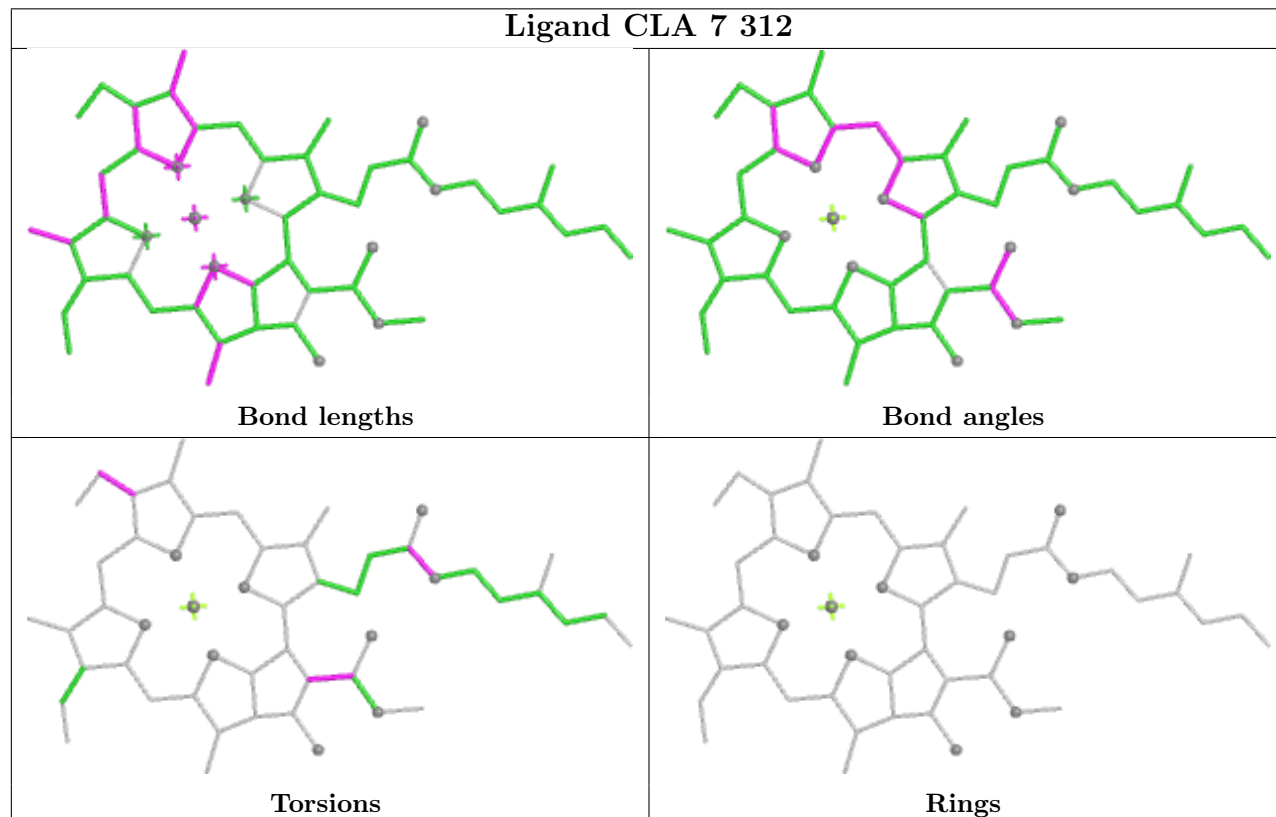
Ligand 8CT 3 318



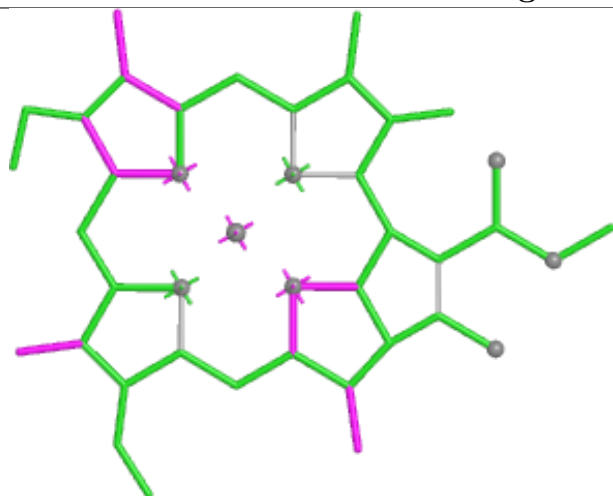
Ligand CLA 1 302



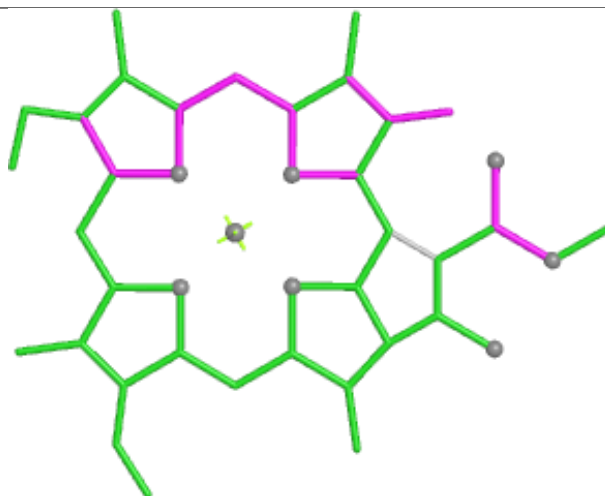
Ligand CLA 7 312



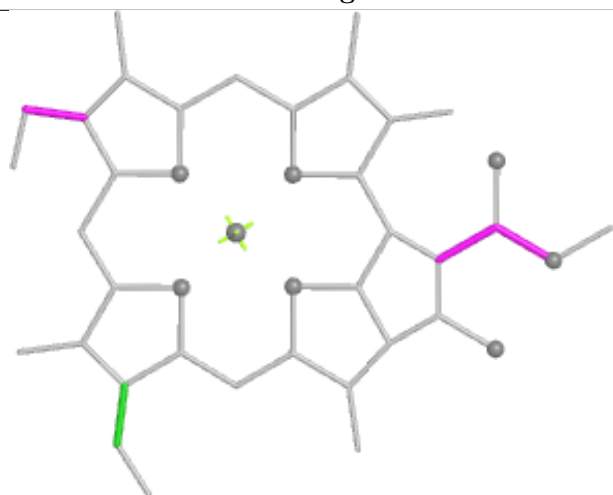
Ligand CLA 5 310



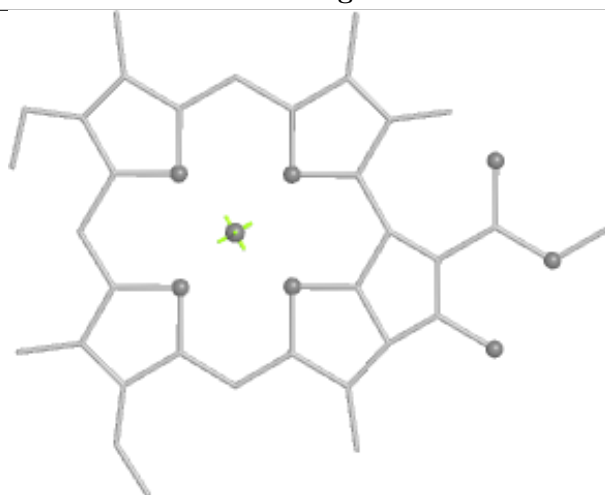
Bond lengths



Bond angles

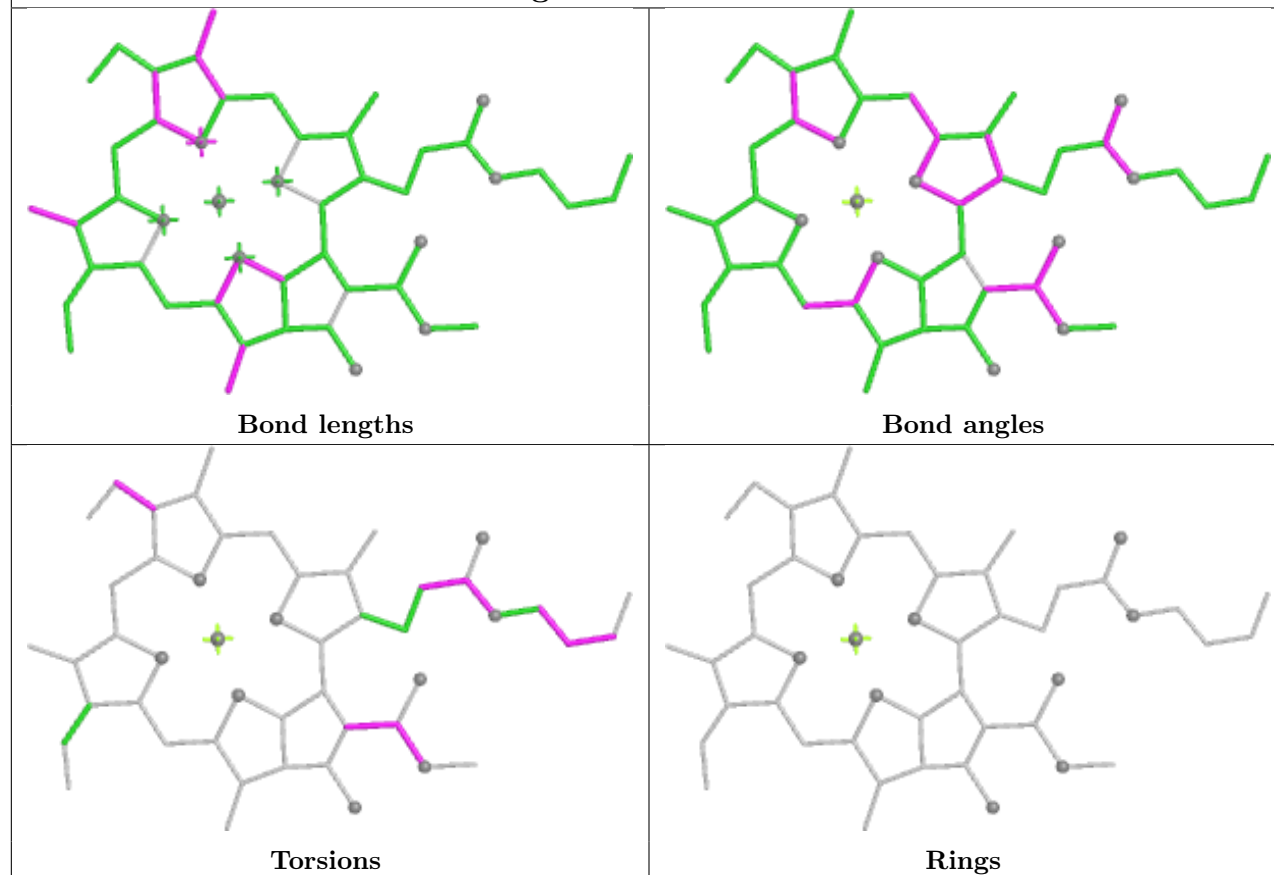


Torsions

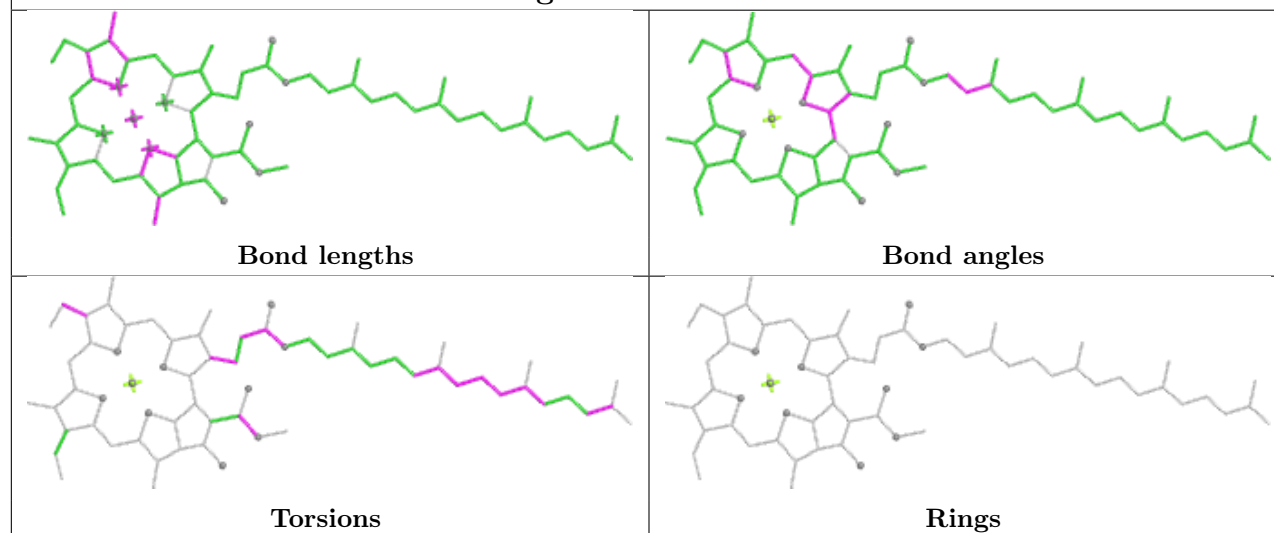


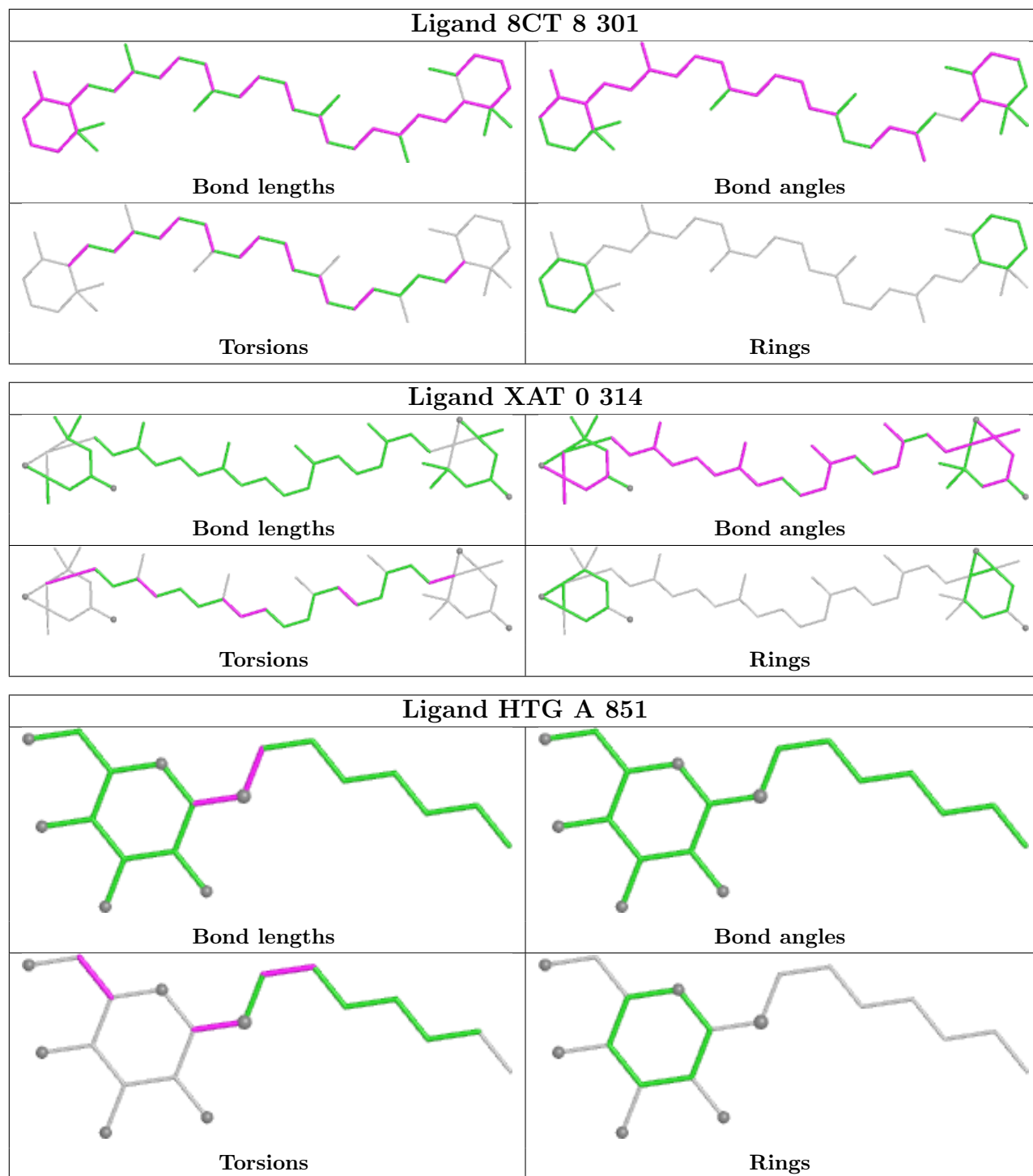
Rings

Ligand CLA A 822

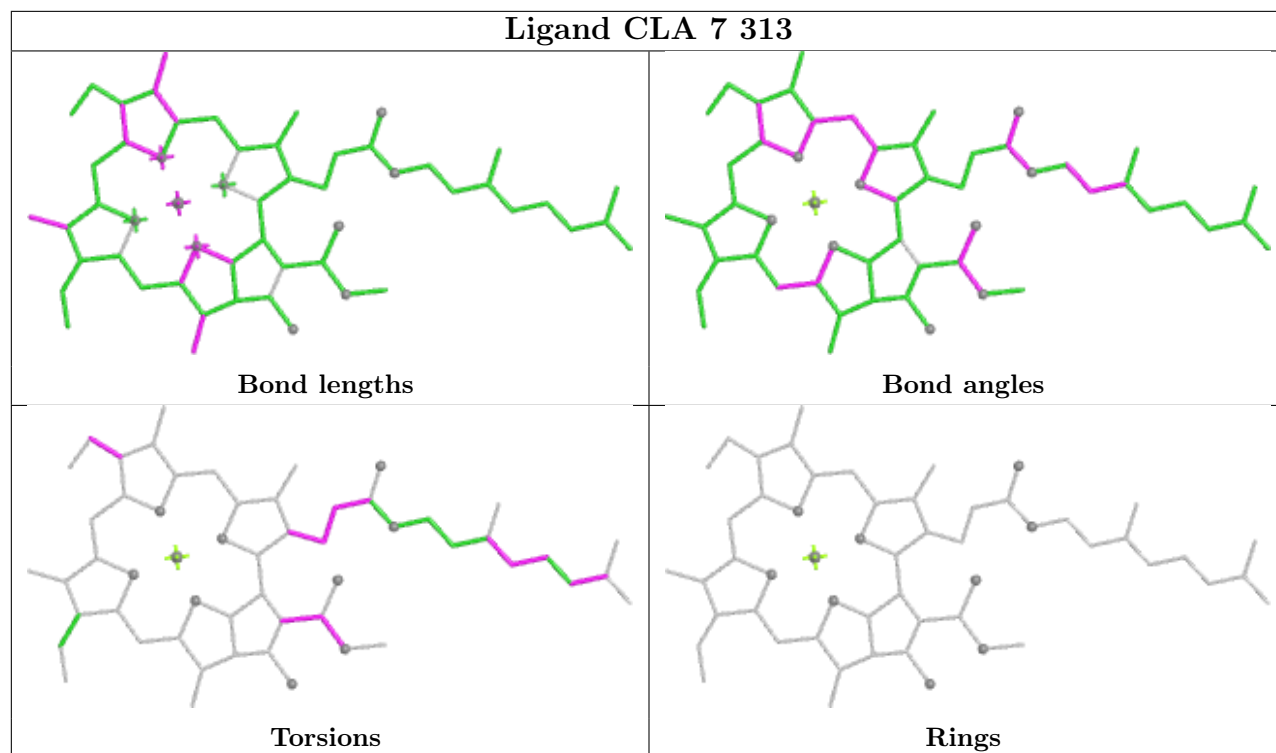


Ligand CLA 7 317

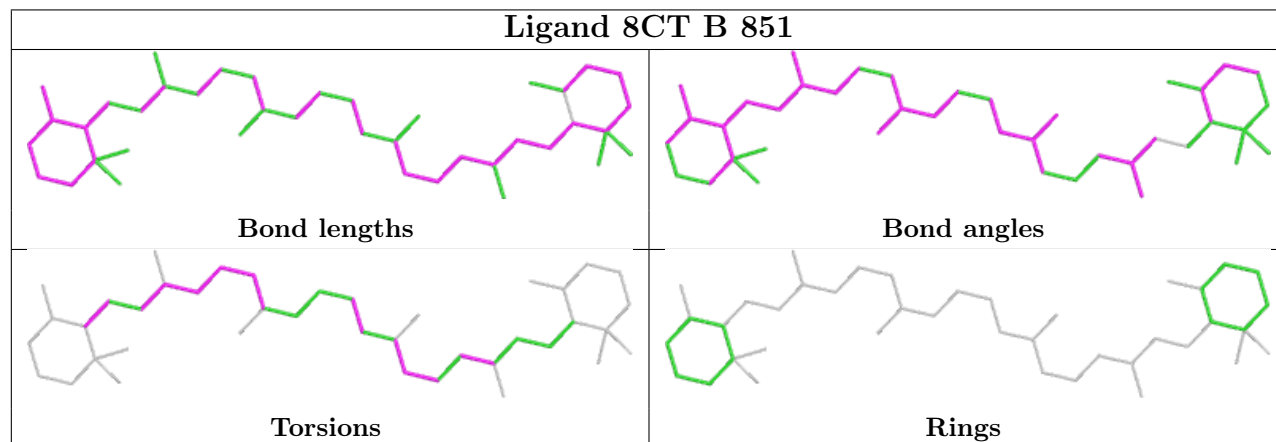




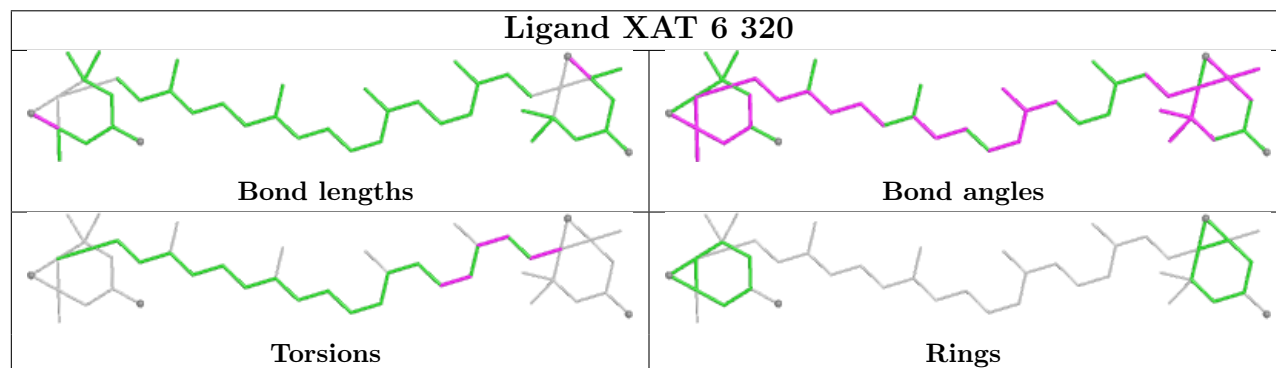
Ligand CLA 7 313



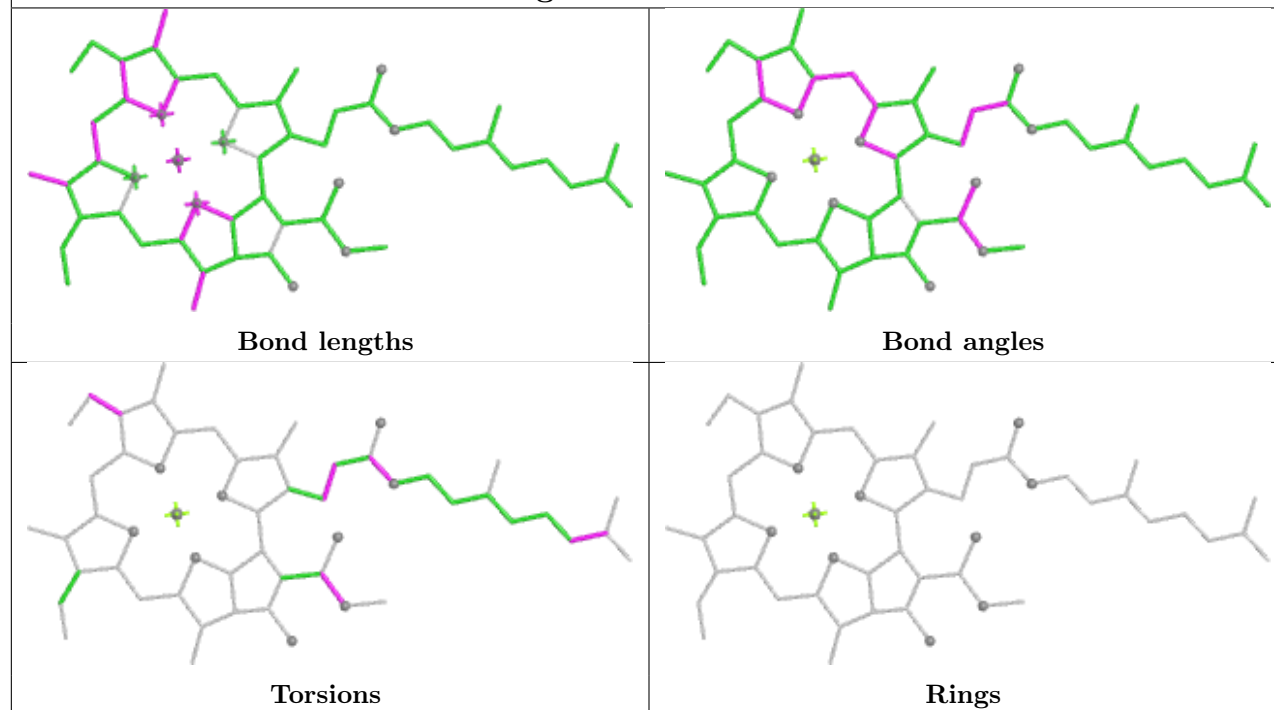
Ligand 8CT B 851



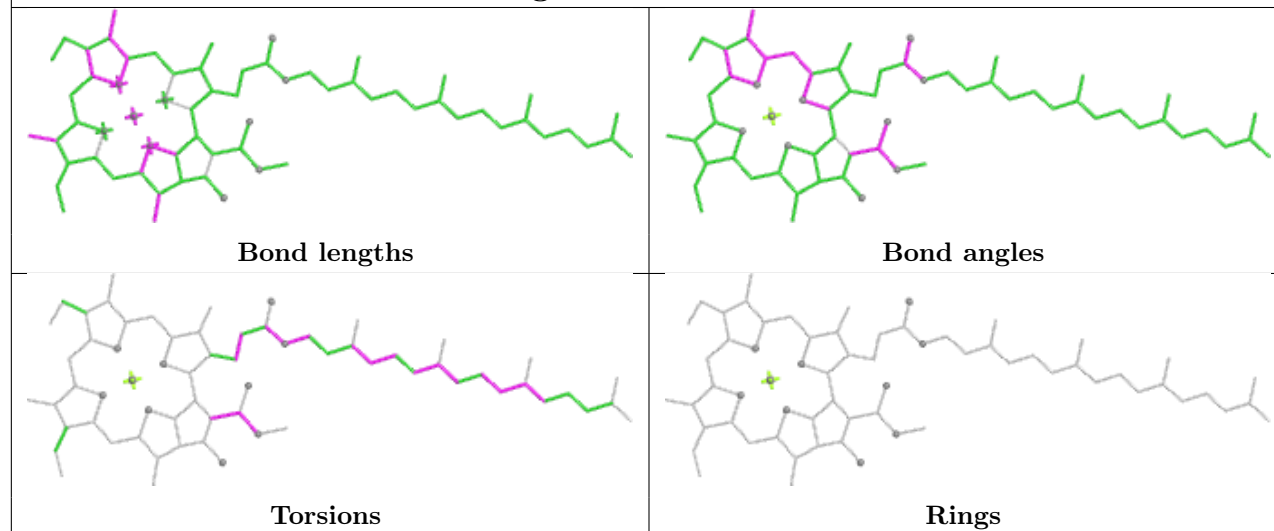
Ligand XAT 6 320



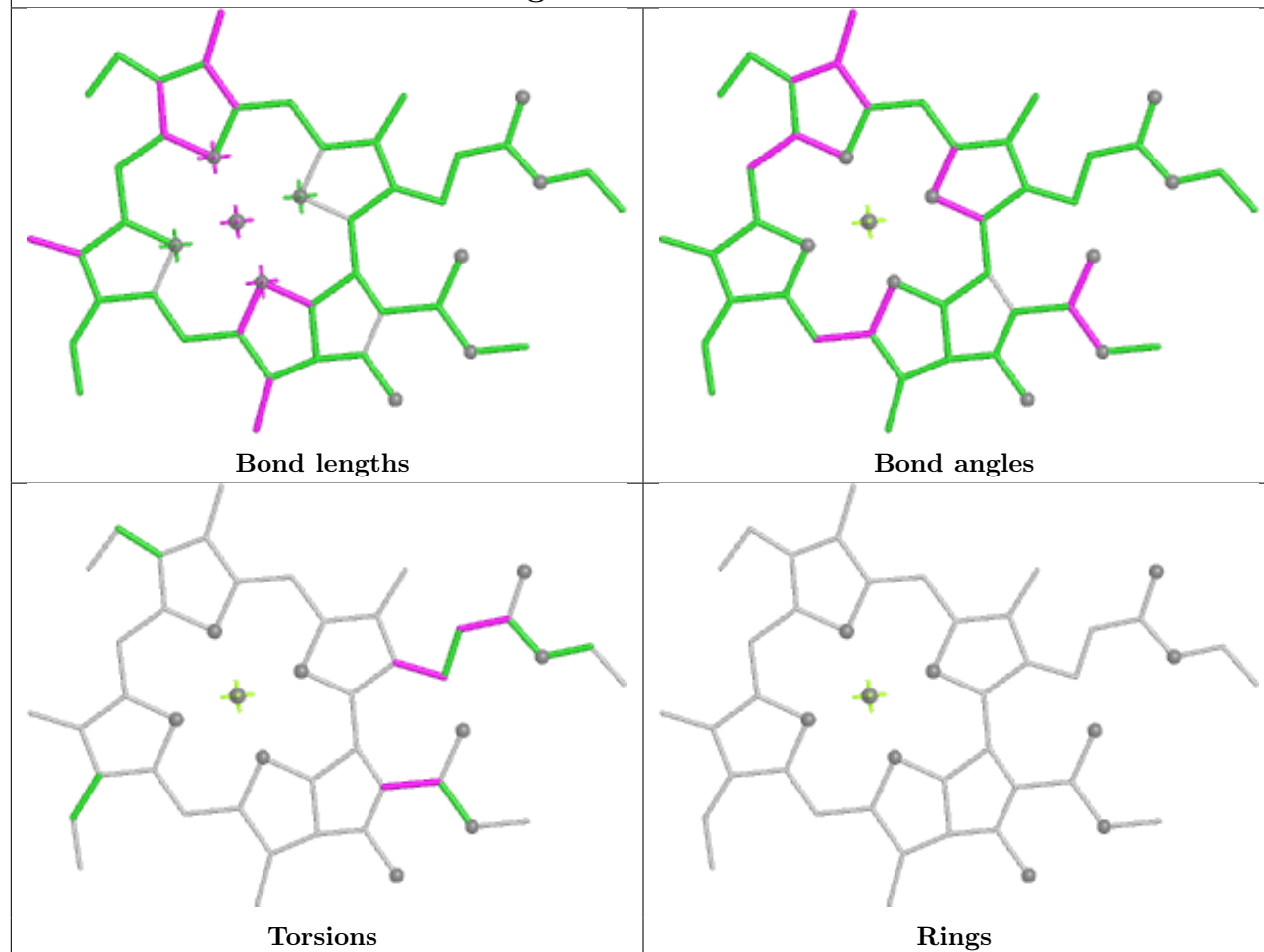
Ligand CLA 4 310



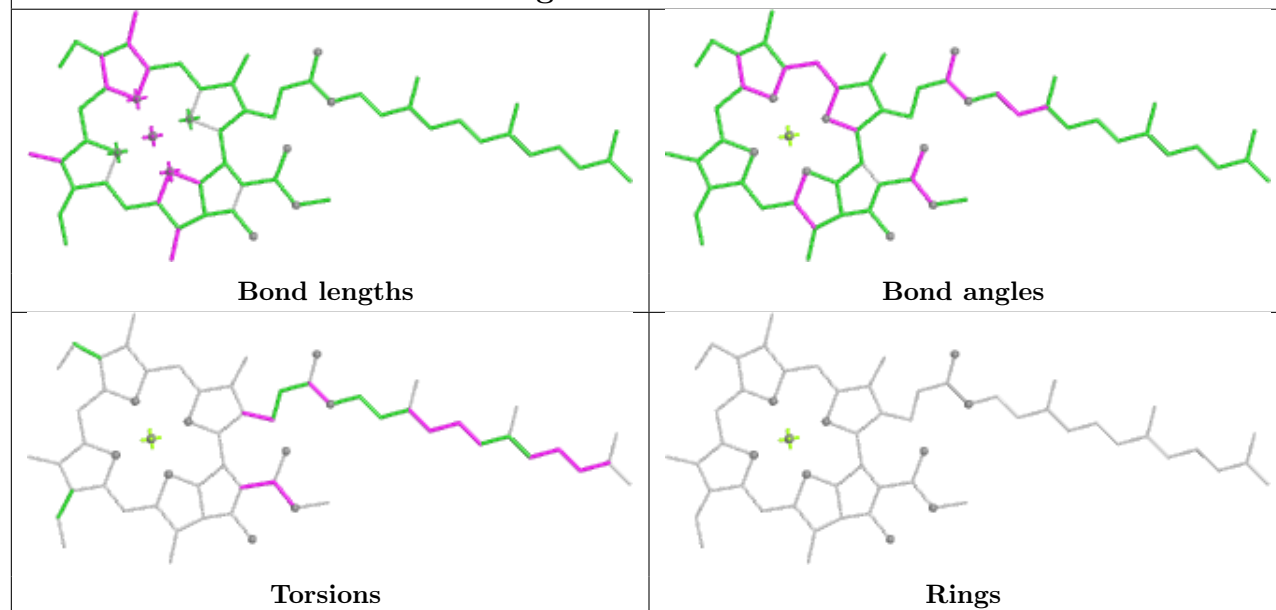
Ligand CLA A 837

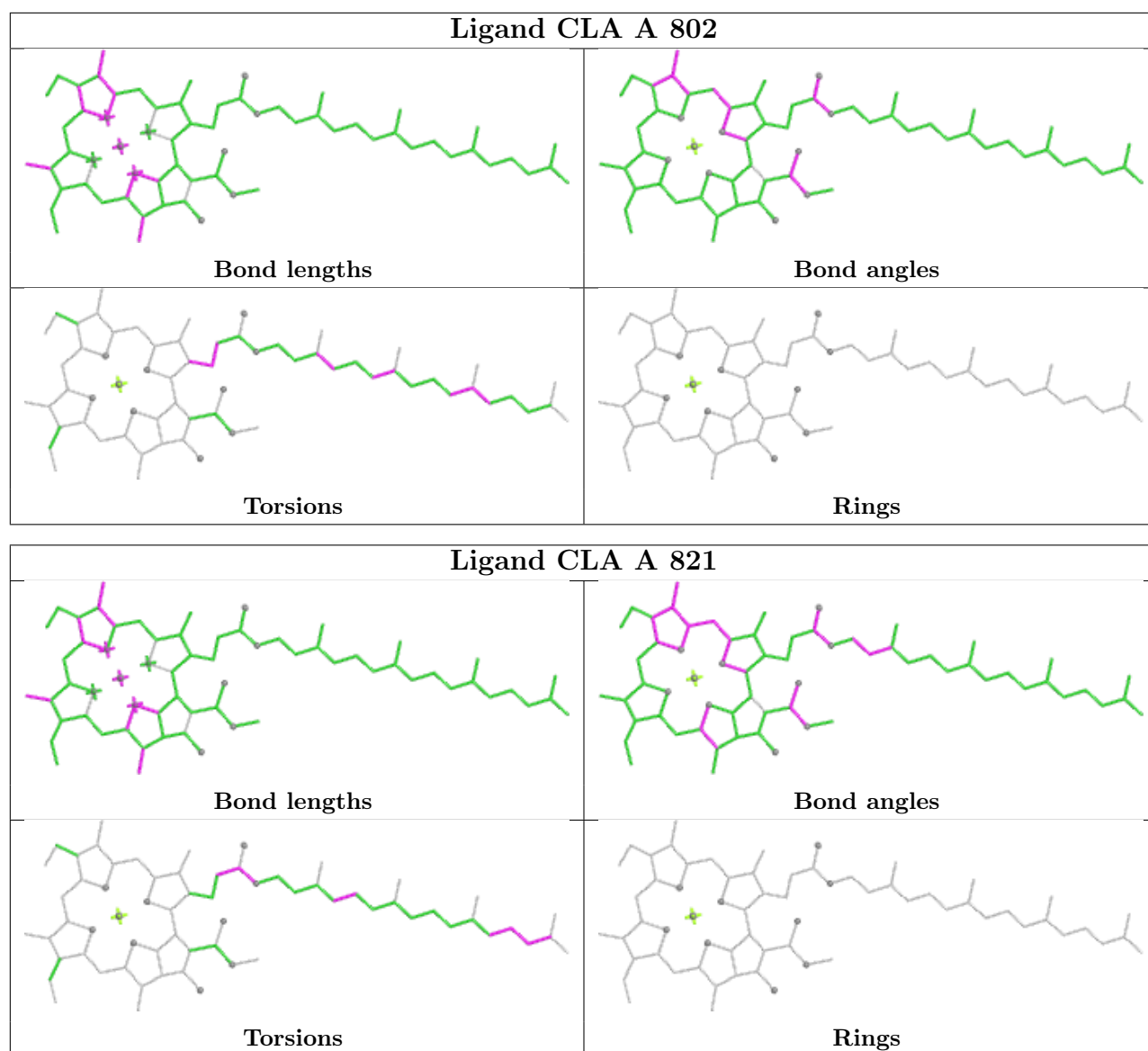


Ligand CLA B 838

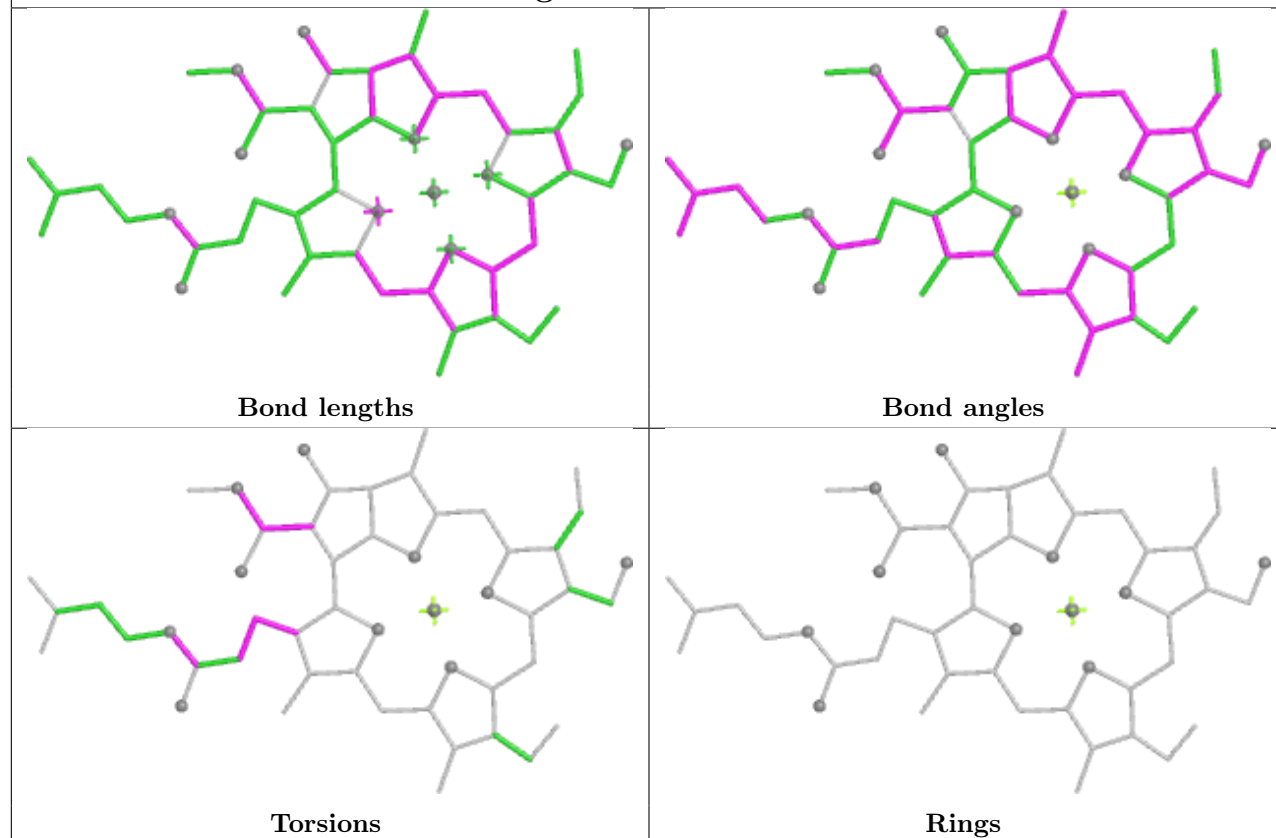


Ligand CLA 4 309

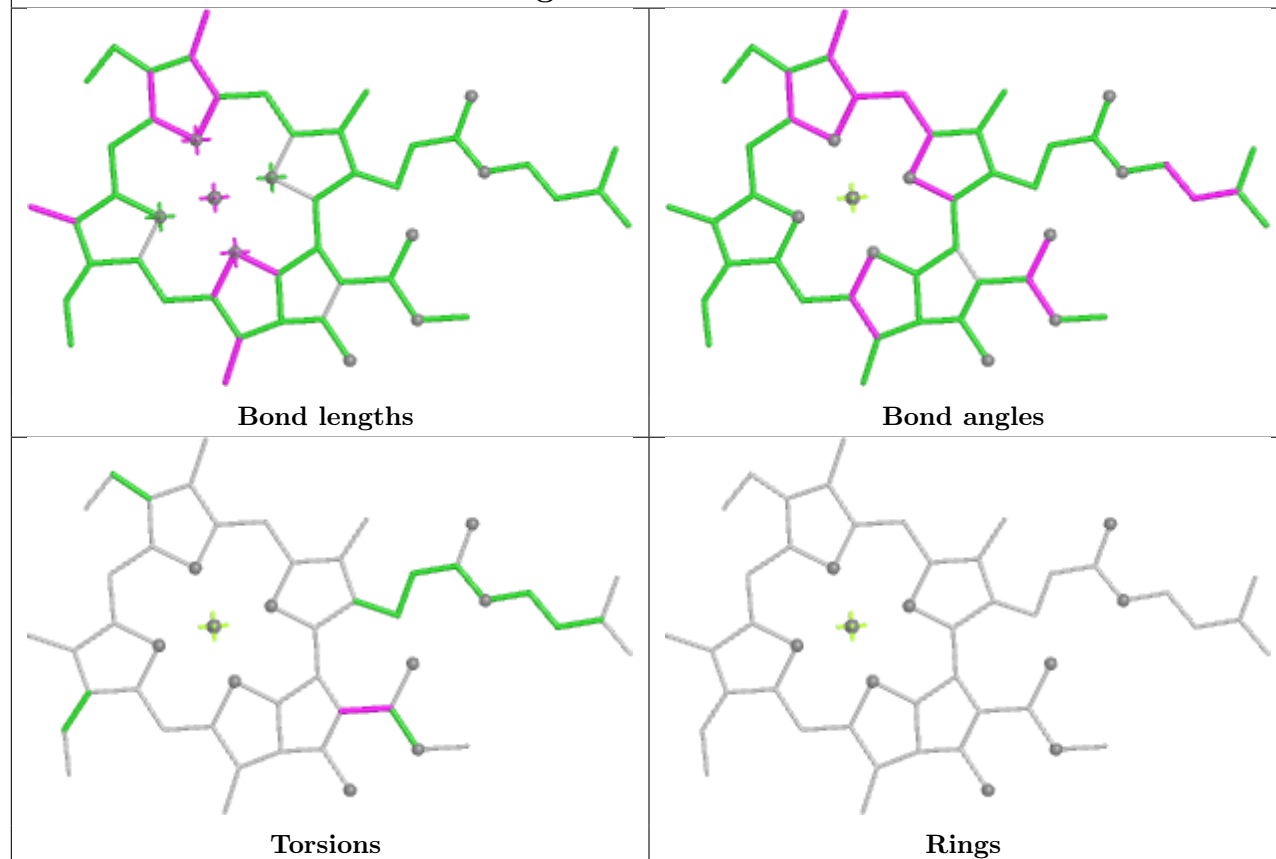


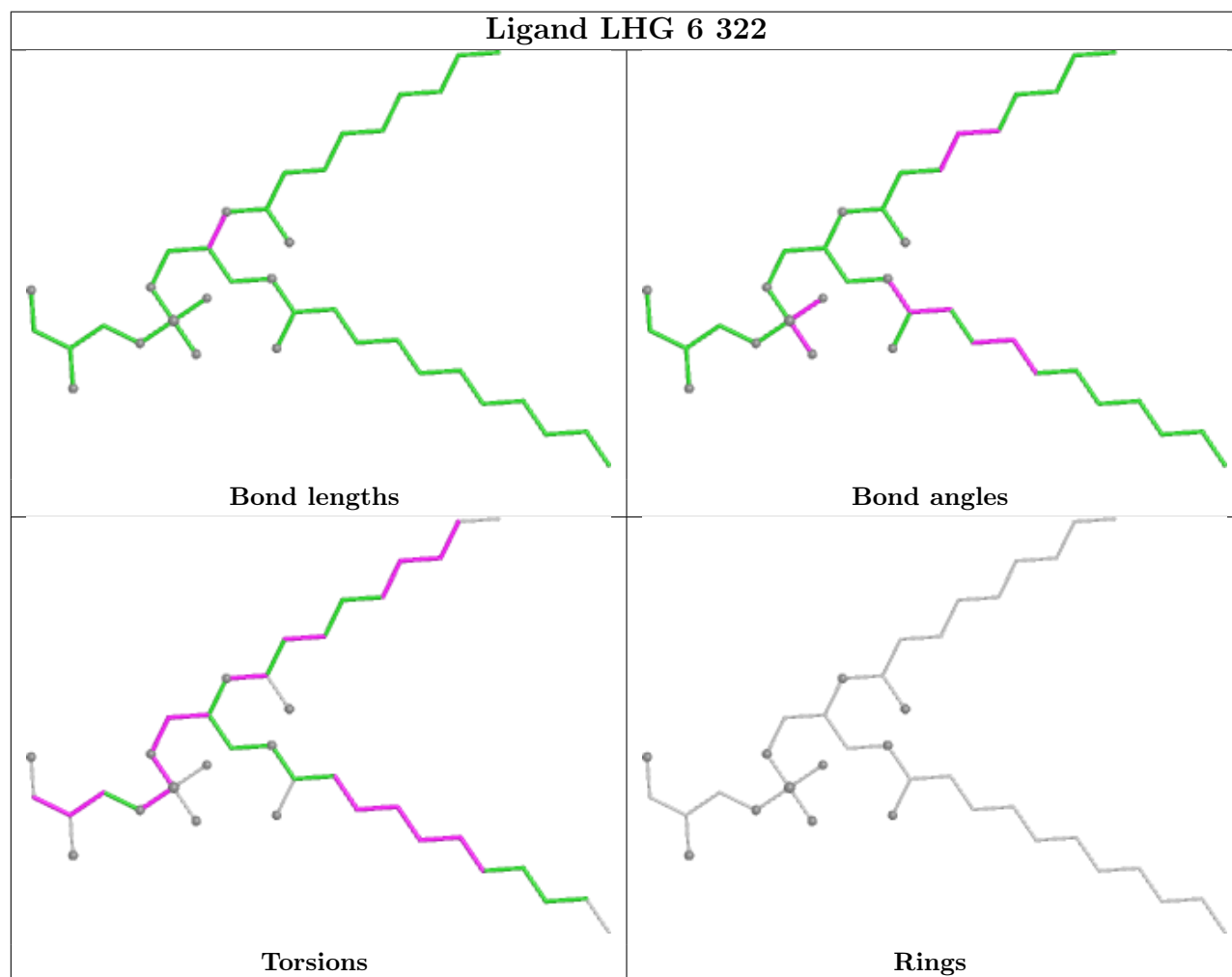
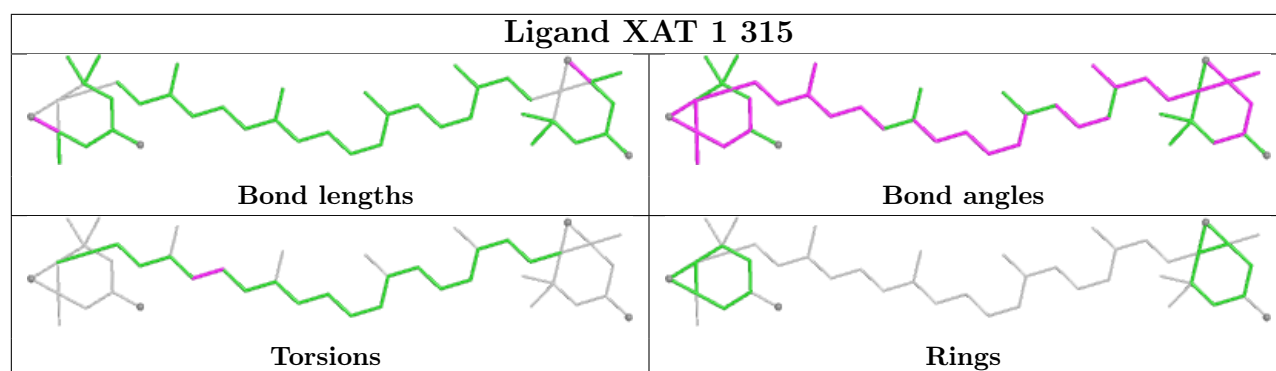


Ligand CHL 8 306

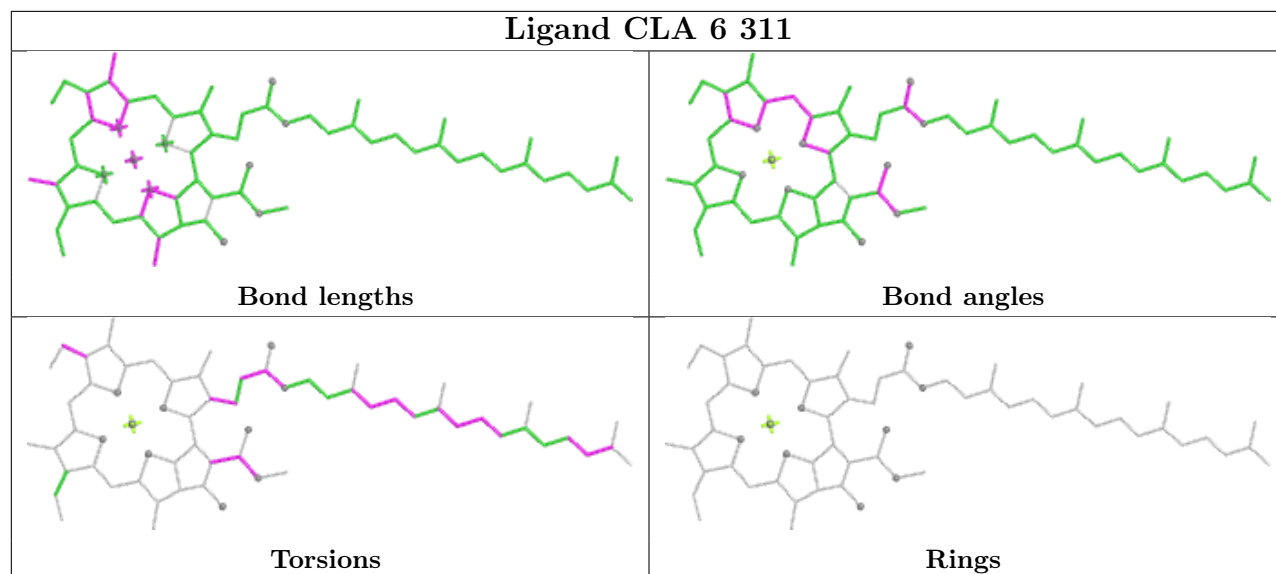


Ligand CLA 4 308

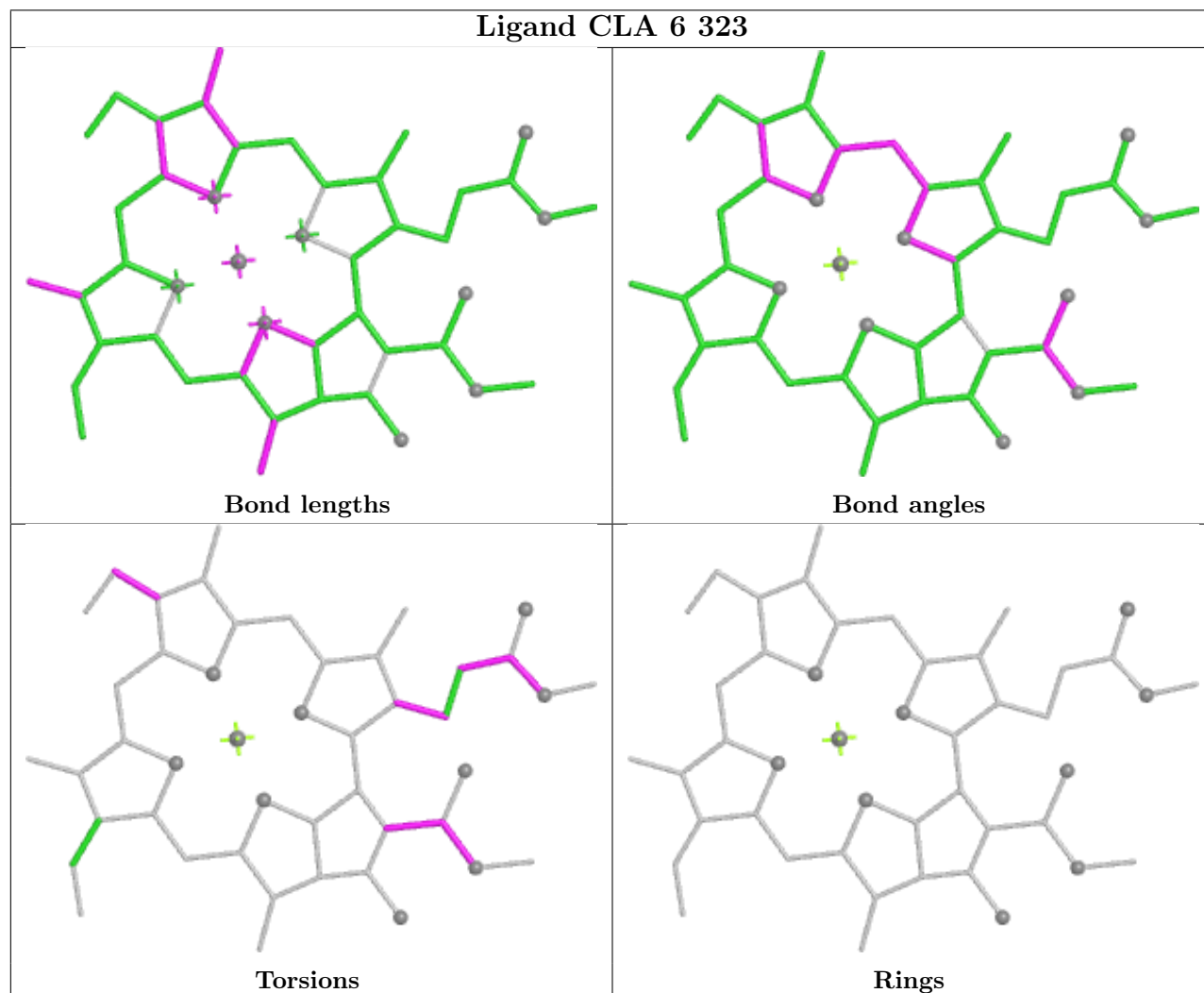


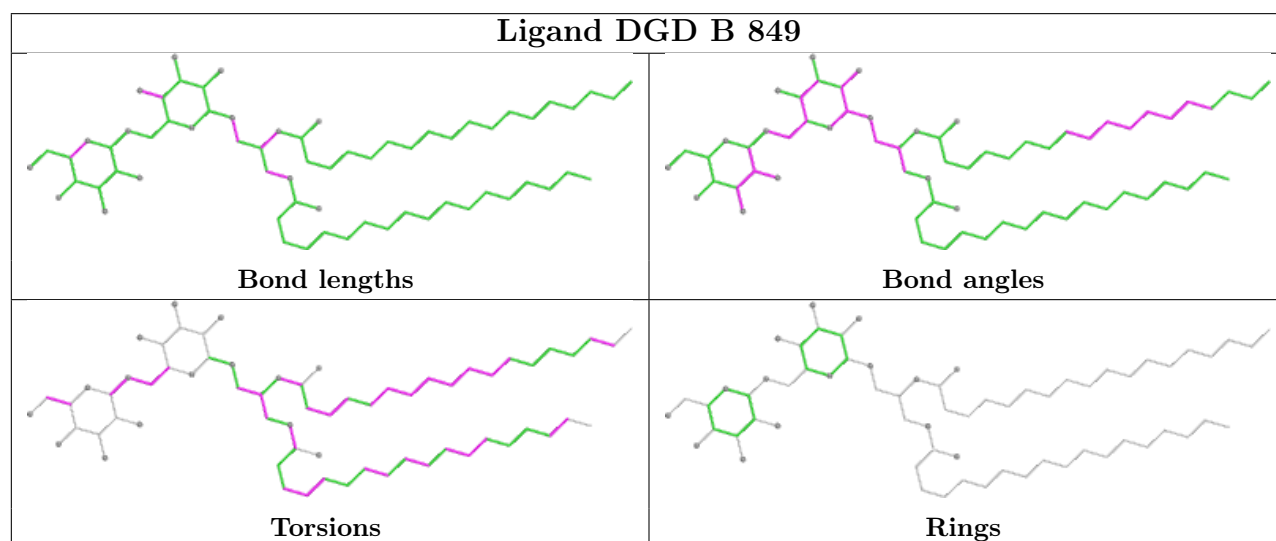
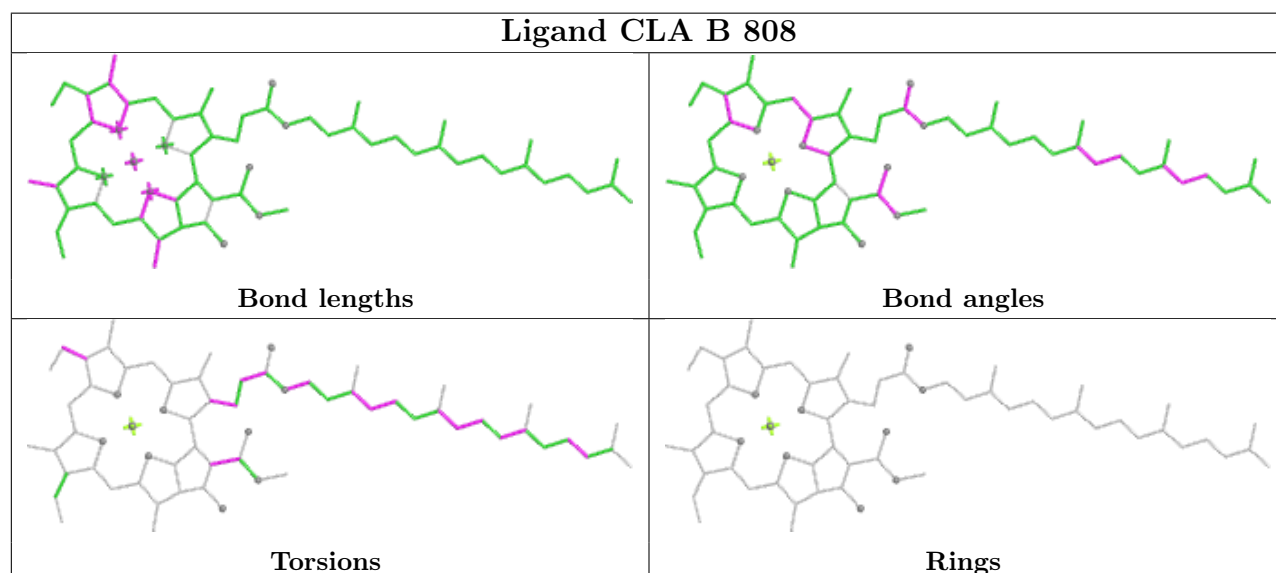
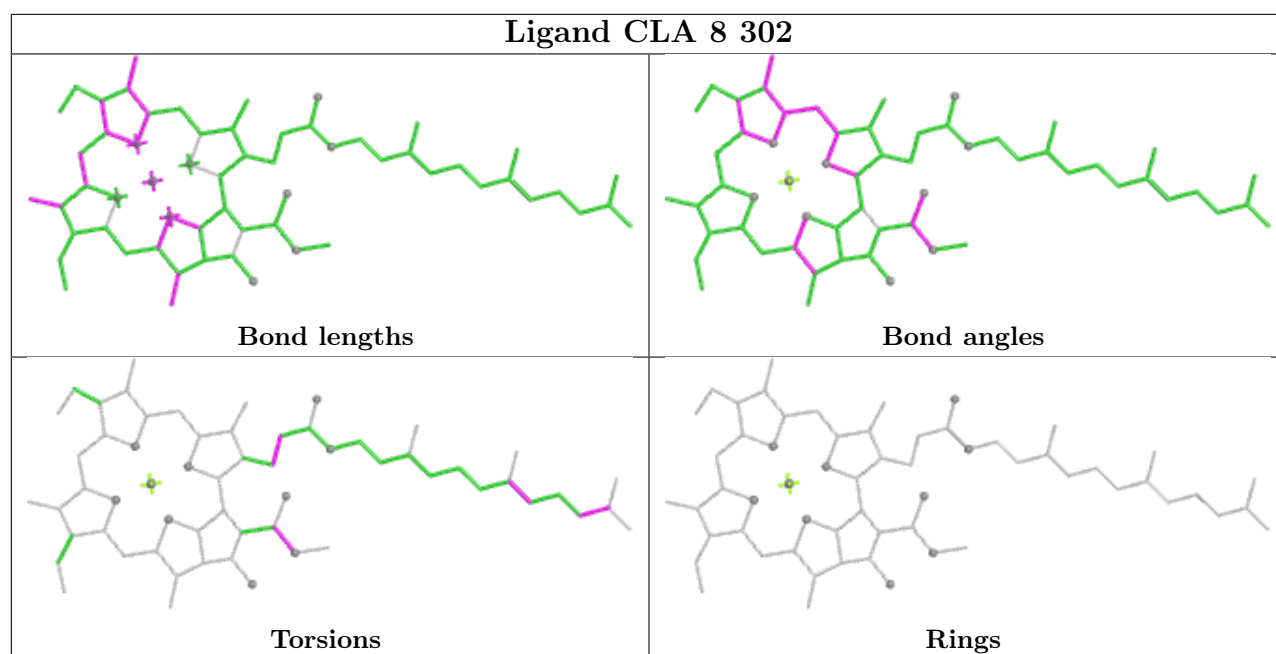


Ligand CLA 6 311

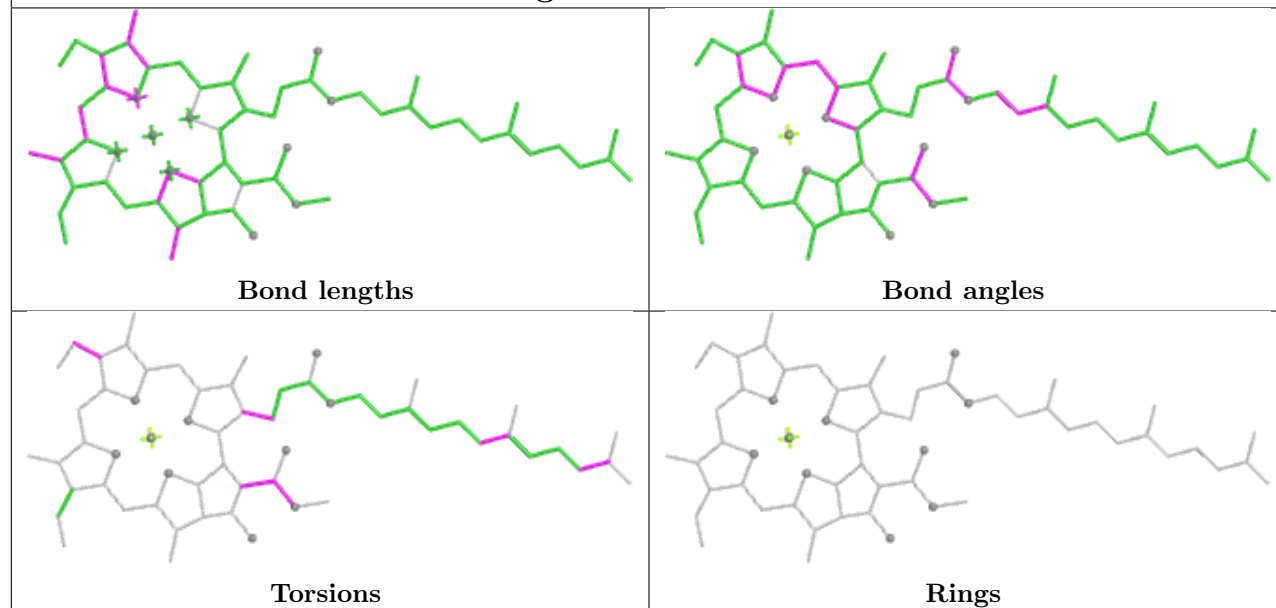


Ligand CLA 6 323

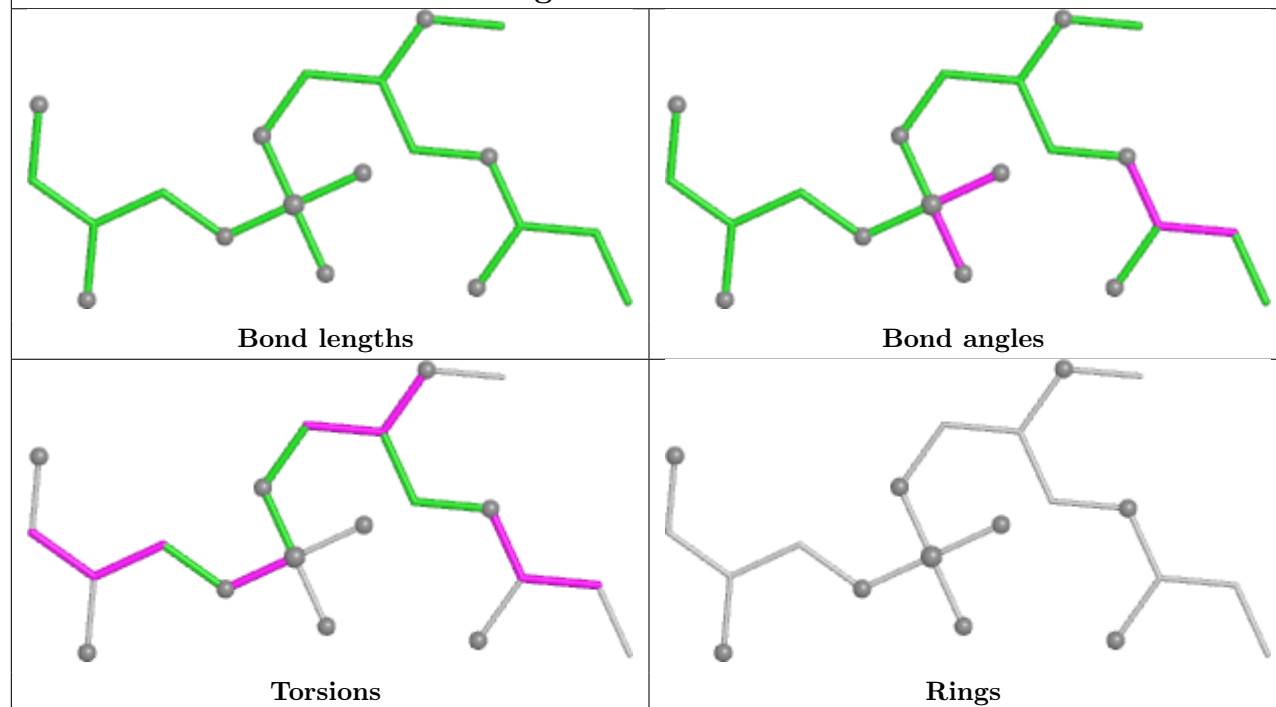


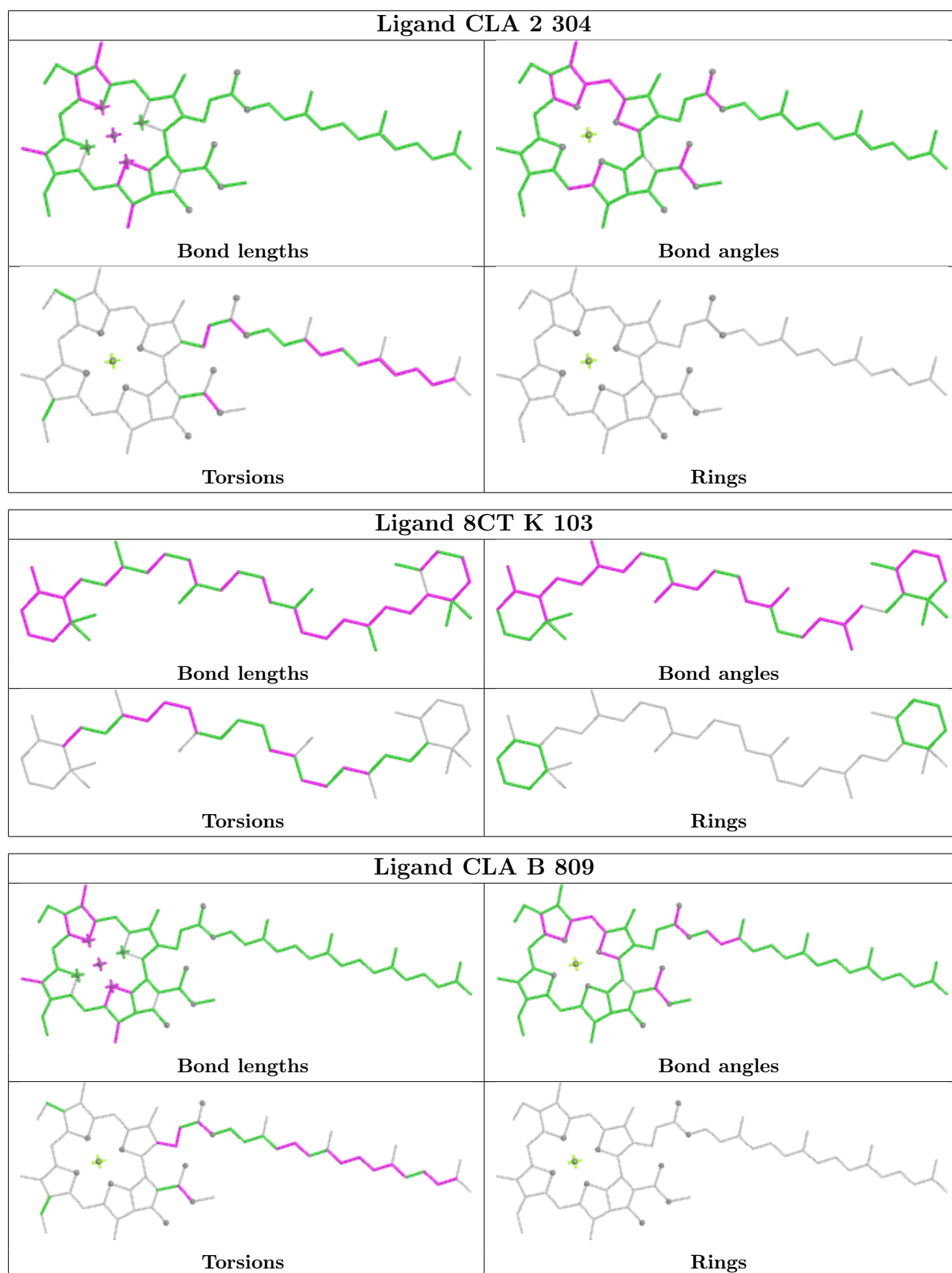


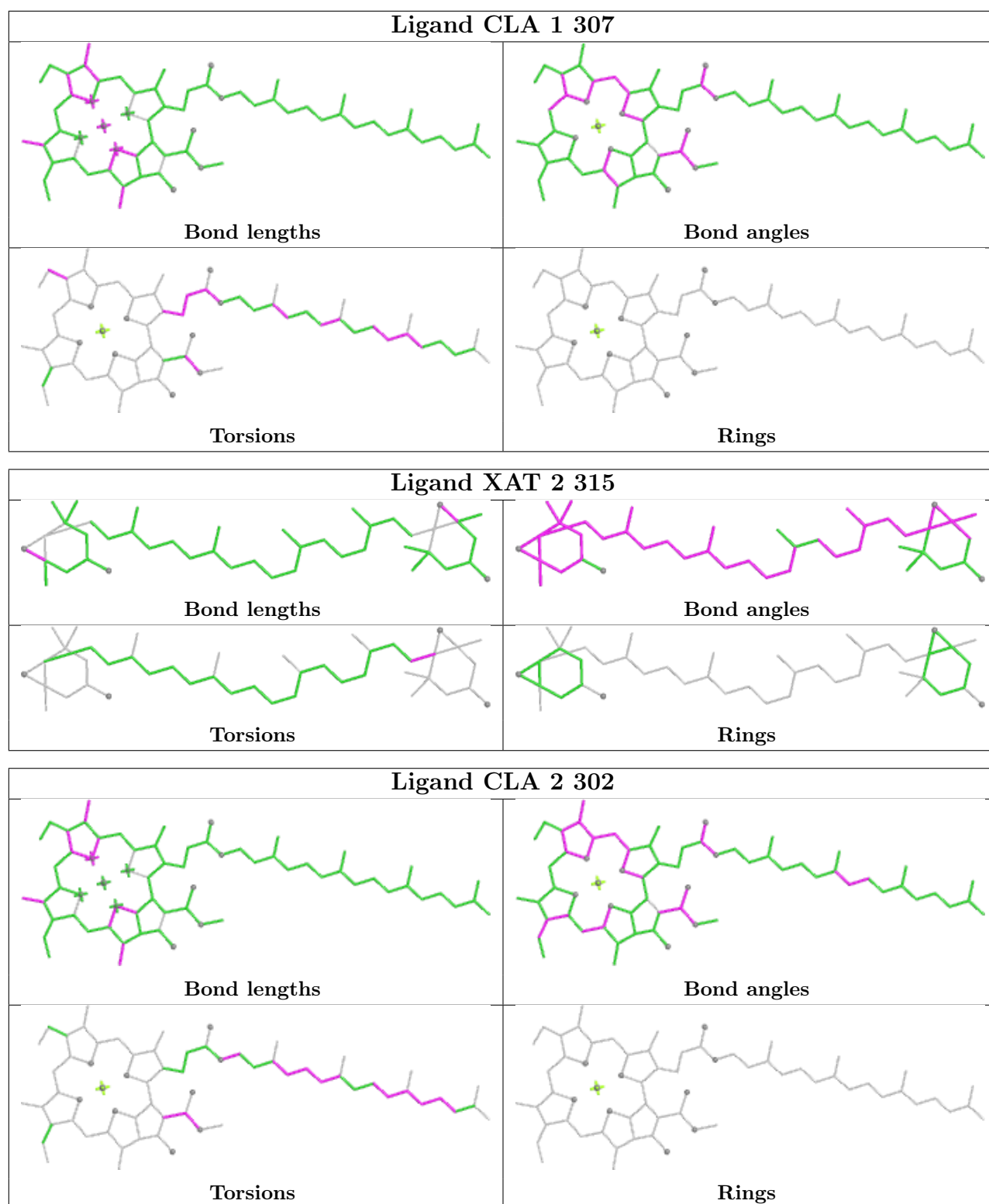
Ligand CLA 5 309



Ligand LHG 3 317







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

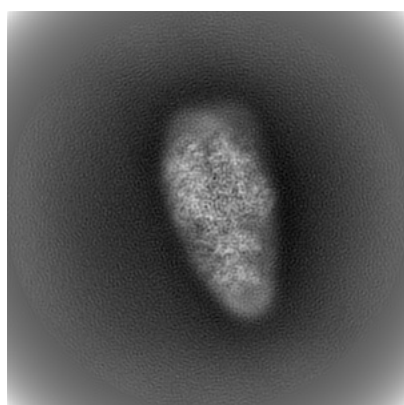
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9670. These allow visual inspection of the internal detail of the map and identification of artifacts.

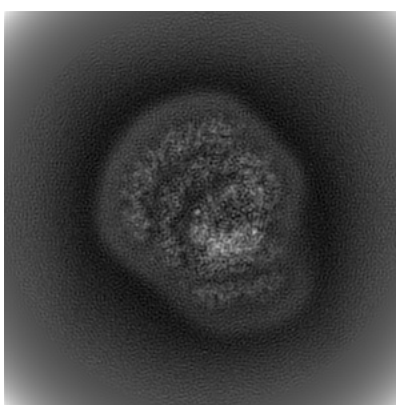
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

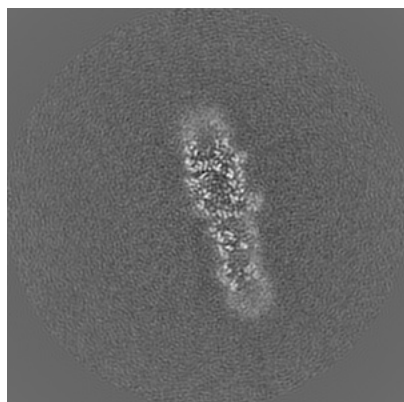


Z

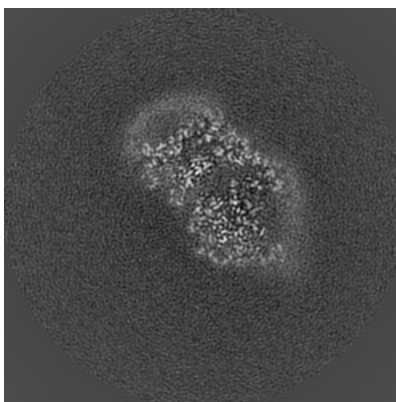
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

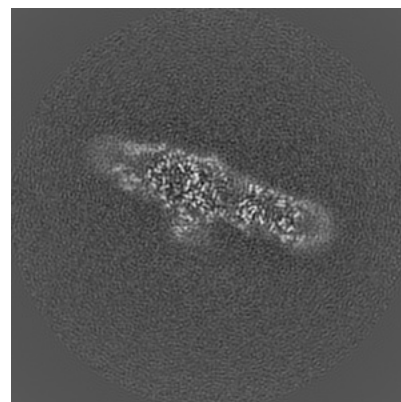
6.2.1 Primary map



X Index: 230



Y Index: 230

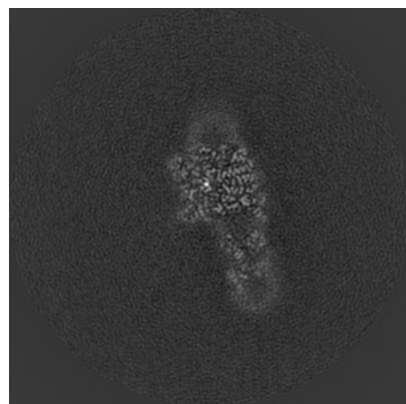


Z Index: 230

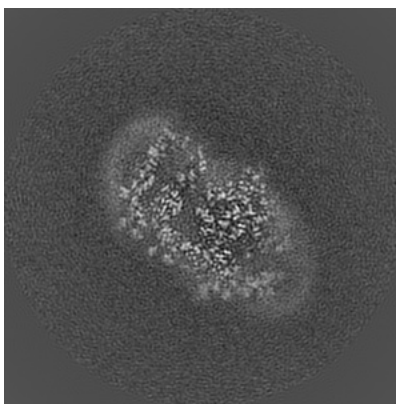
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

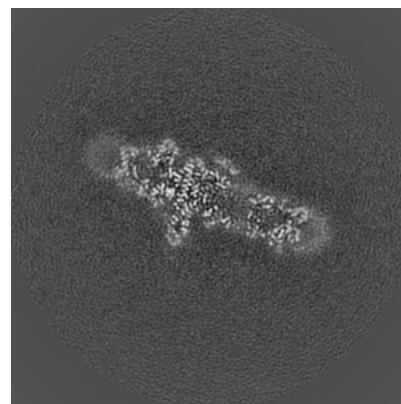
6.3.1 Primary map



X Index: 202



Y Index: 254

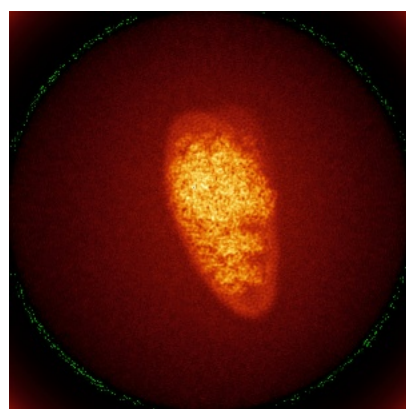


Z Index: 250

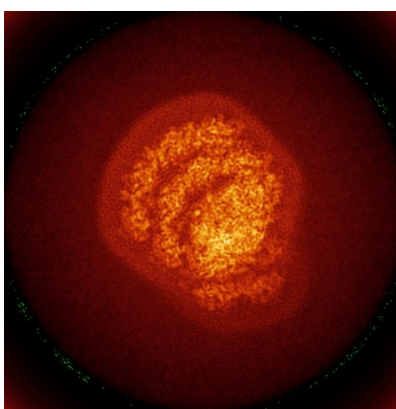
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

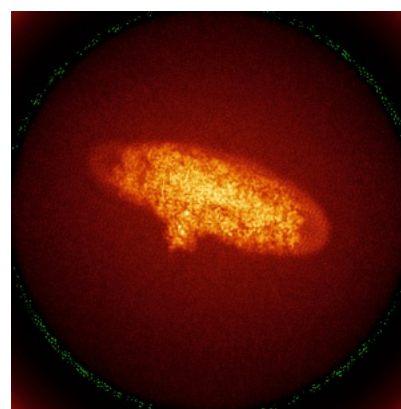
6.4.1 Primary map



X



Y

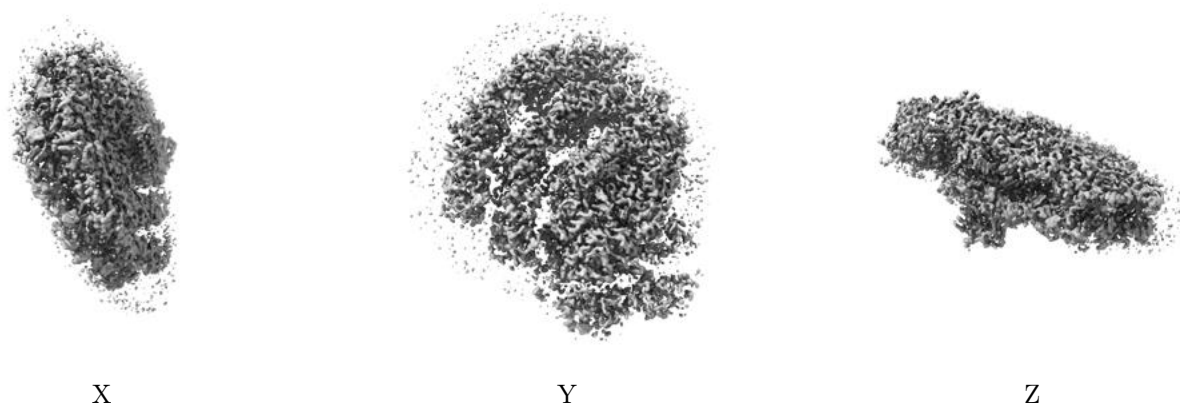


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

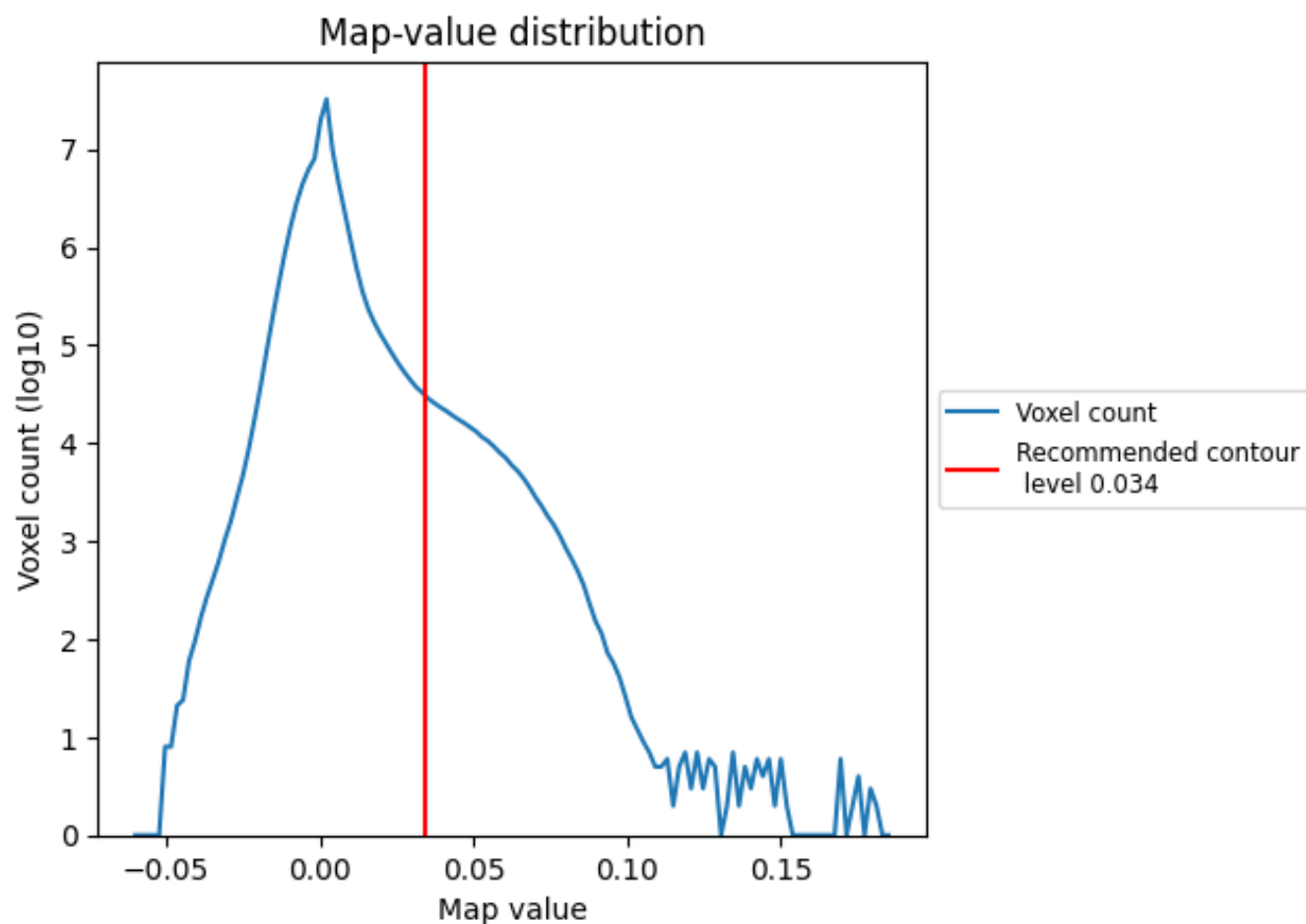
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

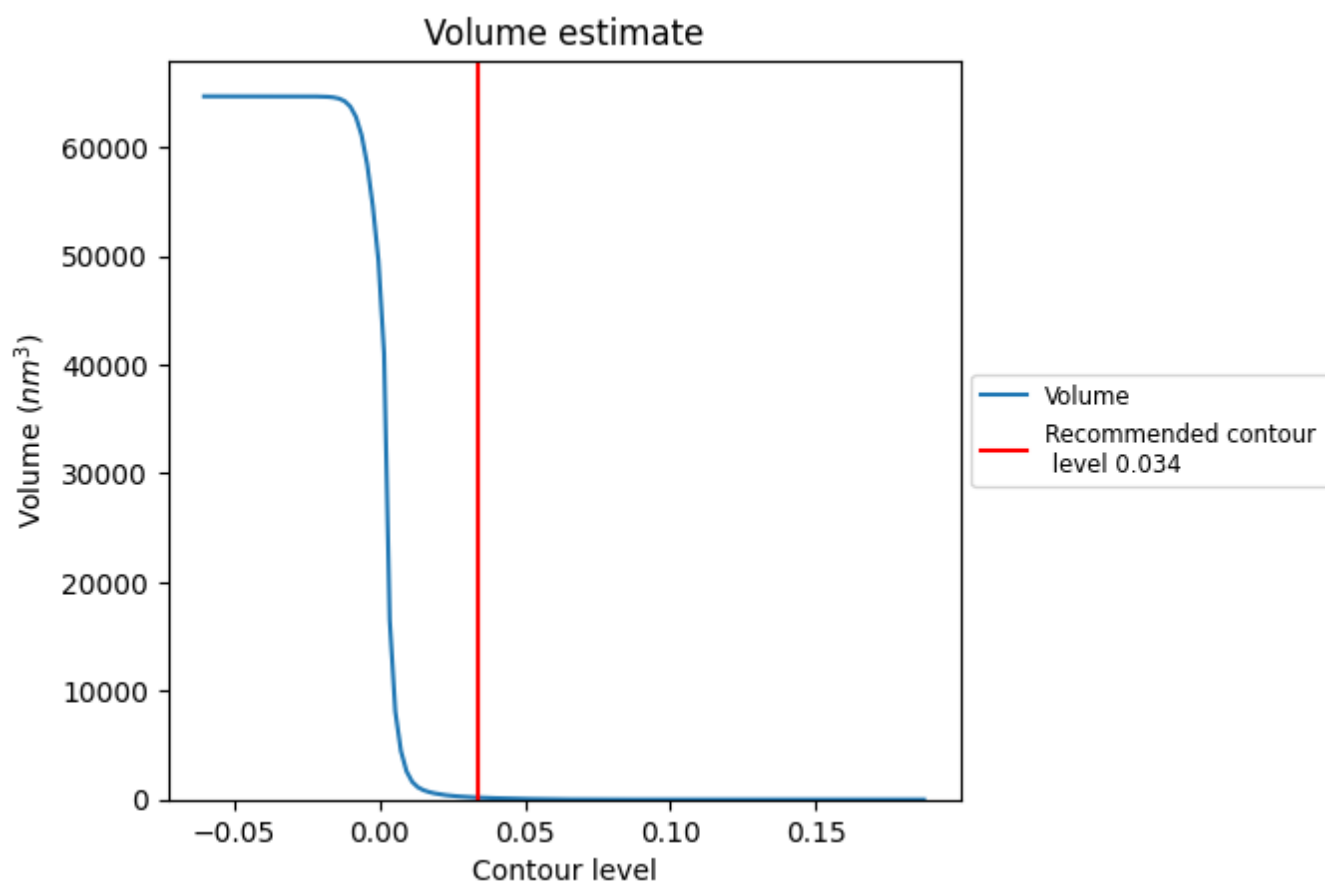
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

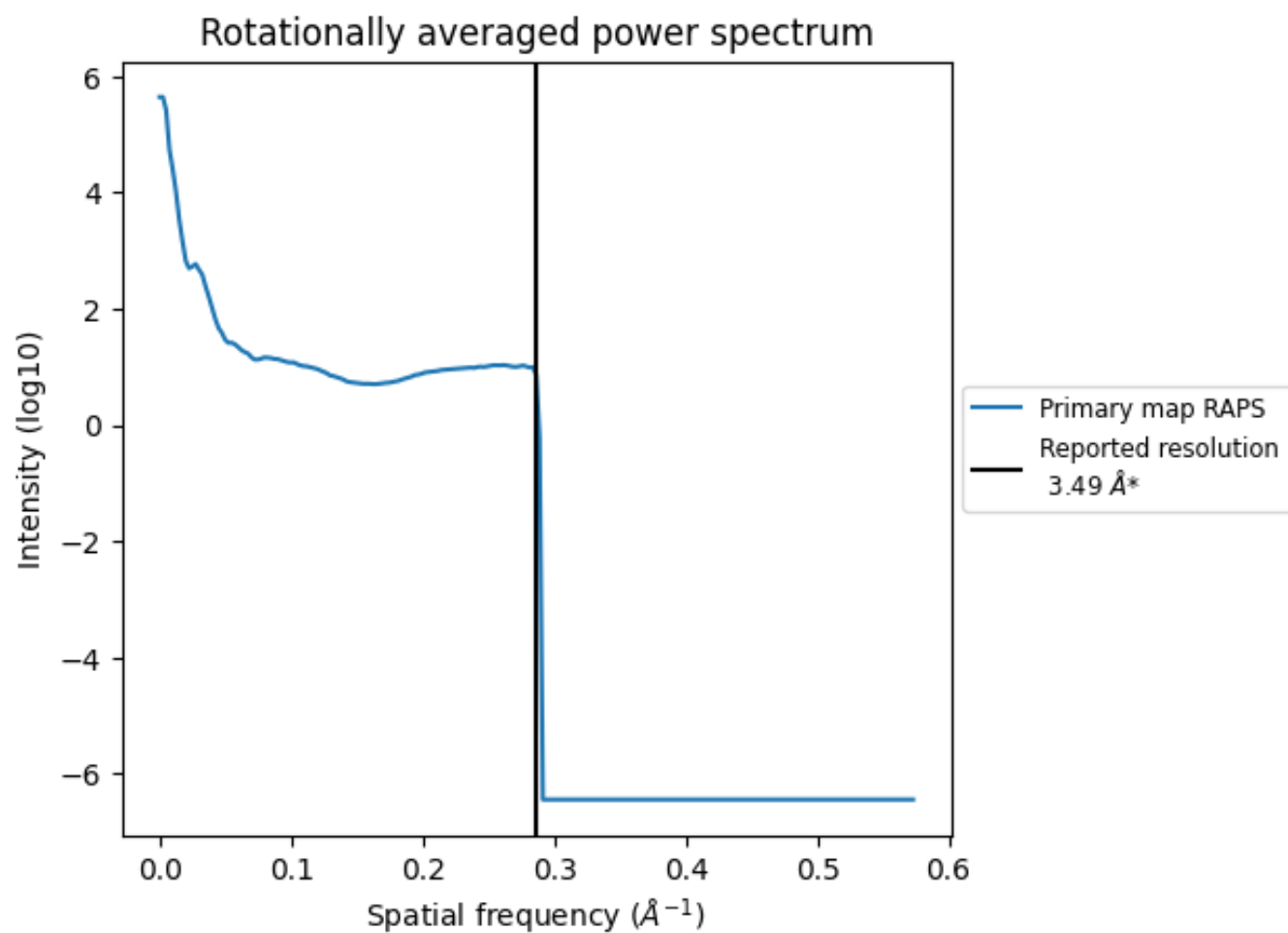
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 186 nm^3 ; this corresponds to an approximate mass of 168 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

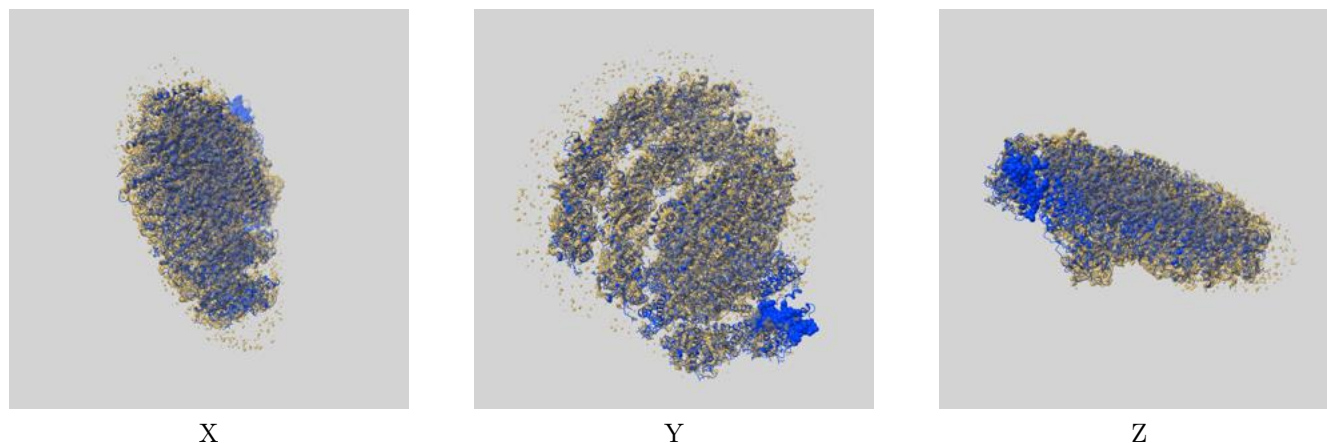
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

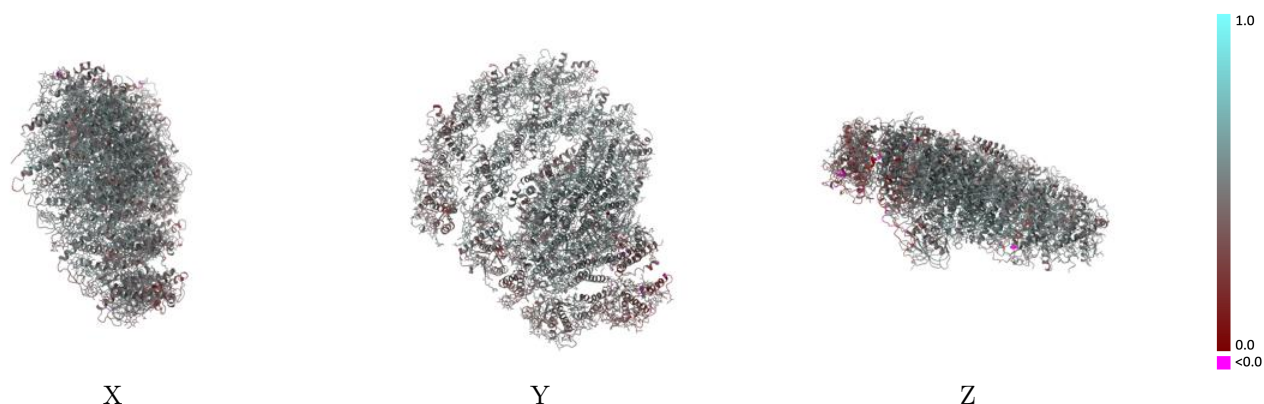
This section contains information regarding the fit between EMDB map EMD-9670 and PDB model 6IGZ. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



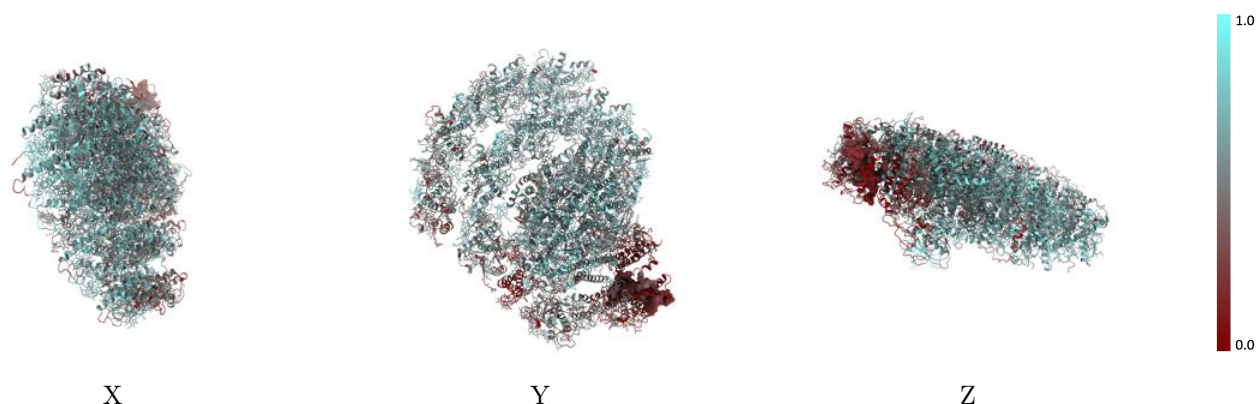
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



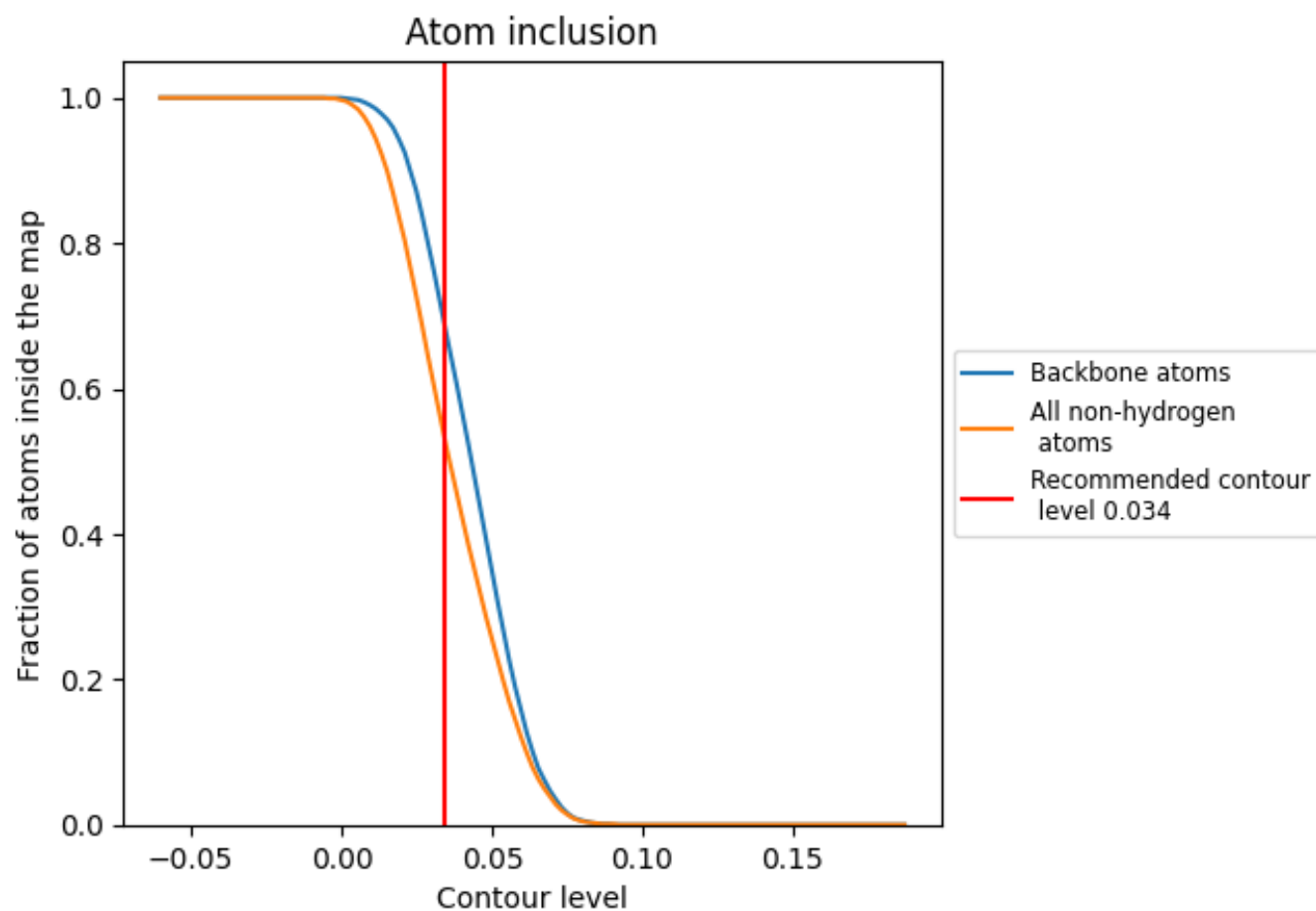
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.034).

9.4 Atom inclusion ⓘ



At the recommended contour level, 69% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5360	0.4750
0	0.2070	0.3440
1	0.5270	0.4620
2	0.6430	0.5160
3	0.6390	0.5010
4	0.5880	0.4810
5	0.4560	0.4250
6	0.5840	0.4770
7	0.5990	0.4760
8	0.5460	0.4490
9	0.4150	0.4280
A	0.6220	0.5250
B	0.6010	0.5160
C	0.7150	0.4740
D	0.5960	0.4680
E	0.5750	0.4740
F	0.5360	0.4700
G	0.1210	0.3640
H	0.0650	0.2890
I	0.4310	0.4880
J	0.4920	0.4980
K	0.4900	0.4400
L	0.2280	0.4030
M	0.5130	0.4760

