



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 07:39 PM JST

PDB ID : 7Y3F
EMDB ID : EMD-33593
Title : Structure of the Anabaena PSI-monomer-IsiA supercomplex
Authors : Nagao, R.; Kato, K.; Hamaguchi, T.; Kawakami, K.; Yonekura, K.; Shen, J.R.
Deposited on : 2022-06-10
Resolution : 2.62 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

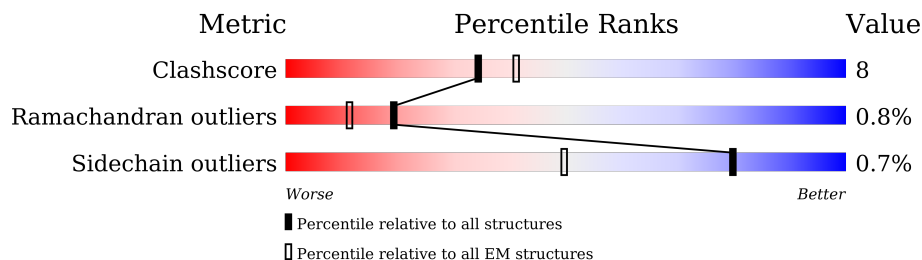
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.62 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	752	 87% 11% .
2	B	741	 88% 11%
3	C	81	 91% 7% .
4	D	139	 92% 5% .
5	E	70	 84% . 13%
6	F	164	 79% 7% 14%
7	I	46	 63% . 33%
8	J	49	 82% 6% 12%

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Mol	Chain	Length	Quality of chain
9	K	82	
10	M	40	
11	X	44	
12	1	476	
13	2	325	
13	3	325	
13	6	325	
14	4	344	
14	5	344	

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
15	CL0	A	801	X	-	-	-
16	CLA	1	501	X	-	-	-
16	CLA	1	502	X	-	-	-
16	CLA	1	503	X	-	-	-
16	CLA	1	505	X	-	-	-
16	CLA	1	506	X	-	-	-
16	CLA	1	507	X	-	-	-
16	CLA	1	508	X	-	-	-
16	CLA	1	509	X	-	-	-
16	CLA	1	510	X	-	-	-
16	CLA	1	511	X	-	-	-
16	CLA	1	512	X	-	-	-
16	CLA	1	513	X	-	-	-
16	CLA	1	514	X	-	-	-
16	CLA	1	515	X	-	-	-
16	CLA	1	521	X	-	-	-
16	CLA	1	525	X	-	-	-
16	CLA	1	526	X	-	-	-
16	CLA	2	401	X	-	-	-
16	CLA	2	402	X	-	-	-
16	CLA	2	403	X	-	-	-
16	CLA	2	404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	2	405	X	-	-	-
16	CLA	2	406	X	-	-	-
16	CLA	3	401	X	-	-	-
16	CLA	4	402	X	-	-	-
16	CLA	4	403	X	-	-	-
16	CLA	4	404	X	-	-	-
16	CLA	4	405	X	-	-	-
16	CLA	4	406	X	-	-	-
16	CLA	4	407	X	-	-	-
16	CLA	4	408	X	-	-	-
16	CLA	4	409	X	-	-	-
16	CLA	4	410	X	-	-	-
16	CLA	4	411	X	-	-	-
16	CLA	5	403	X	-	-	-
16	CLA	5	404	X	-	-	-
16	CLA	5	405	X	-	-	-
16	CLA	5	406	X	-	-	-
16	CLA	5	407	X	-	-	-
16	CLA	5	408	X	-	-	-
16	CLA	5	409	X	-	-	-
16	CLA	5	410	X	-	-	-
16	CLA	5	411	X	-	-	-
16	CLA	5	412	X	-	-	-
16	CLA	5	413	X	-	-	-
16	CLA	5	414	X	-	-	-
16	CLA	5	415	X	-	-	-
16	CLA	5	416	X	-	-	-
16	CLA	5	417	X	-	-	-
16	CLA	5	418	X	-	-	-
16	CLA	5	419	X	-	-	-
16	CLA	5	421	X	-	-	-
16	CLA	5	422	X	-	-	-
16	CLA	6	401	X	-	-	-
16	CLA	6	402	X	-	-	-
16	CLA	6	403	X	-	-	-
16	CLA	6	404	X	-	-	-
16	CLA	6	405	X	-	-	-
16	CLA	6	406	X	-	-	-
16	CLA	6	407	X	-	-	-
16	CLA	6	408	X	-	-	-
16	CLA	6	409	X	-	-	-
16	CLA	A	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	803	X	-	-	-
16	CLA	A	804	X	-	-	-
16	CLA	A	805	X	-	-	-
16	CLA	A	806	X	-	-	-
16	CLA	A	807	X	-	-	-
16	CLA	A	808	X	-	-	-
16	CLA	A	809	X	-	-	-
16	CLA	A	811	X	-	-	-
16	CLA	A	812	X	-	-	-
16	CLA	A	813	X	-	-	-
16	CLA	A	814	X	-	-	-
16	CLA	A	815	X	-	-	-
16	CLA	A	816	X	-	-	-
16	CLA	A	819	X	-	-	-
16	CLA	A	820	X	-	-	-
16	CLA	A	822	X	-	-	-
16	CLA	A	826	X	-	-	-
16	CLA	A	827	X	-	-	-
16	CLA	A	828	X	-	-	-
16	CLA	A	829	X	-	-	-
16	CLA	A	830	X	-	-	-
16	CLA	A	831	X	-	-	-
16	CLA	A	833	X	-	-	-
16	CLA	A	834	X	-	-	-
16	CLA	A	835	X	-	-	-
16	CLA	A	836	X	-	-	-
16	CLA	A	837	X	-	-	-
16	CLA	A	838	X	-	-	-
16	CLA	A	839	X	-	-	-
16	CLA	A	840	X	-	-	-
16	CLA	A	841	X	-	-	-
16	CLA	A	842	X	-	-	-
16	CLA	A	843	X	-	-	-
16	CLA	B	801	X	-	-	-
16	CLA	B	802	X	-	-	-
16	CLA	B	803	X	-	-	-
16	CLA	B	804	X	-	-	-
16	CLA	B	805	X	-	-	-
16	CLA	B	806	X	-	-	-
16	CLA	B	807	X	-	-	-
16	CLA	B	808	X	-	-	-
16	CLA	B	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	810	X	-	-	-
16	CLA	B	811	X	-	-	-
16	CLA	B	812	X	-	-	-
16	CLA	B	813	X	-	-	-
16	CLA	B	814	X	-	-	-
16	CLA	B	817	X	-	-	-
16	CLA	B	818	X	-	-	-
16	CLA	B	819	X	-	-	-
16	CLA	B	822	X	-	-	-
16	CLA	B	823	X	-	-	-
16	CLA	B	824	X	-	-	-
16	CLA	B	825	X	-	-	-
16	CLA	B	826	X	-	-	-
16	CLA	B	827	X	-	-	-
16	CLA	B	828	X	-	-	-
16	CLA	B	829	X	-	-	-
16	CLA	B	830	X	-	-	-
16	CLA	B	831	X	-	-	-
16	CLA	B	832	X	-	-	-
16	CLA	B	833	X	-	-	-
16	CLA	B	834	X	-	-	-
16	CLA	B	835	X	-	-	-
16	CLA	B	836	X	-	-	-
16	CLA	B	837	X	-	-	-
16	CLA	B	838	X	-	-	-
16	CLA	B	839	X	-	-	-
16	CLA	B	840	X	-	-	-
16	CLA	F	201	X	-	-	-
16	CLA	F	204	X	-	-	-
16	CLA	J	101	X	-	-	-
16	CLA	J	102	X	-	-	-
16	CLA	K	101	X	-	-	-
16	CLA	K	103	X	-	-	-
16	CLA	X	101	X	-	-	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 39463 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5824	3821	1003	979	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	367	103	118	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	135	Total	C	N	O	S	0	0
			1043	668	179	195	1		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			490	313	84	93		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	31	Total	C	N	O	0	0
			253	177	35	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	43	Total	C	N	O	0	0
			347	236	52	59		

- Molecule 9 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	72	Total	C	N	O	0	0
			360	216	72	72		

- Molecule 10 is a protein called PsaM.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	30	Total	C	N	O	0	0
			235	157	36	42		

- Molecule 11 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	X	29	Total	C	N	O	0	0
			243	170	37	36		

- Molecule 12 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	466	Total	C	N	O	S	0	0
			3590	2380	578	624	8		

- Molecule 13 is a protein called IsiA.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	2	302	Total	C	N	O	0	0
			1474	870	302	302		
13	3	277	Total	C	N	O	0	0
			1354	800	277	277		

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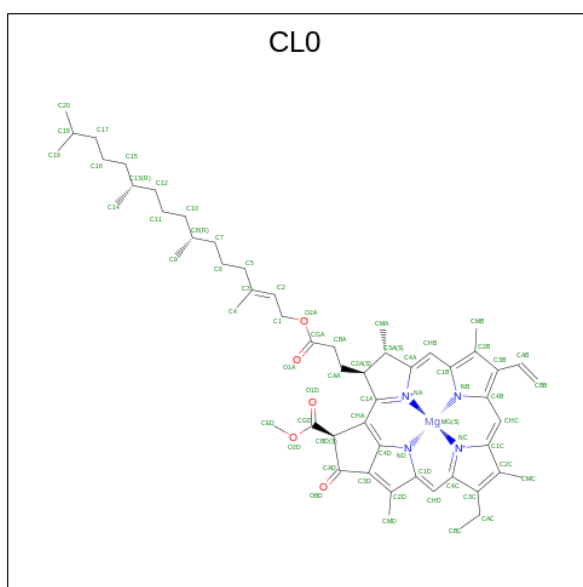
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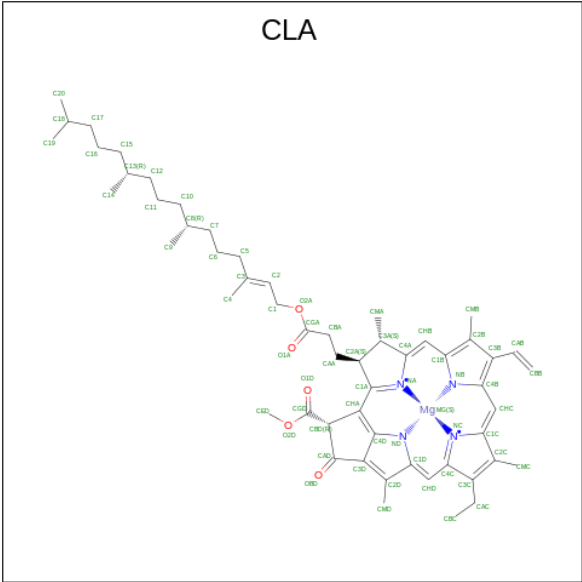
Mol	Chain	Residues	Atoms				AltConf	Trace
13	6	303	Total	C	N	O	0	0
			1479	873	303	303		

- Molecule 14 is a protein called Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	329	Total	C	N	O	S	0	0
			2562	1709	424	425	4		
14	5	332	Total	C	N	O	S	0	0
			2589	1725	429	431	4		

- Molecule 15 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).





Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	F	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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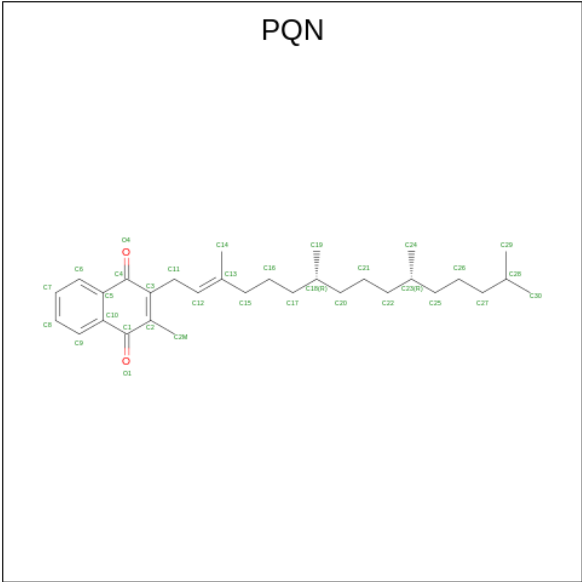
Mol	Chain	Residues	Atoms					AltConf
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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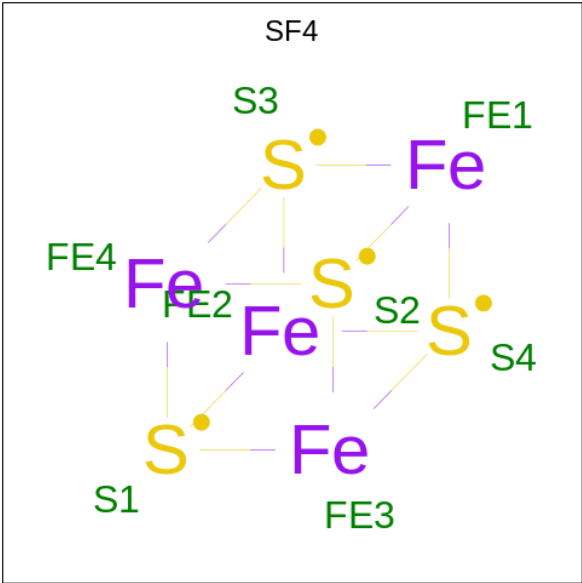
Mol	Chain	Residues	Atoms					AltConf
16	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 17 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



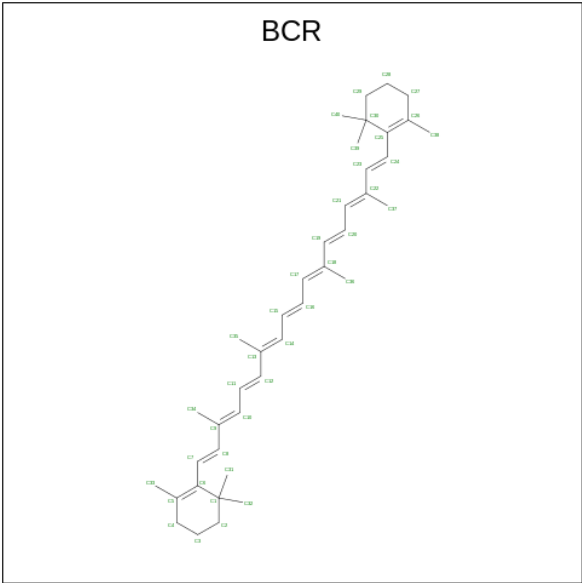
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



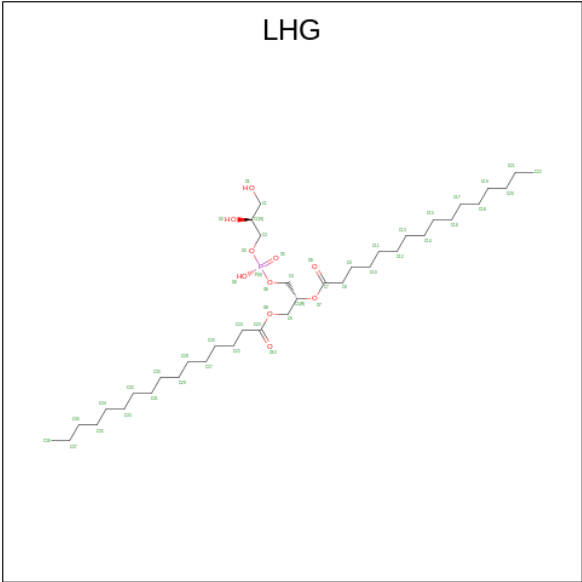
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	

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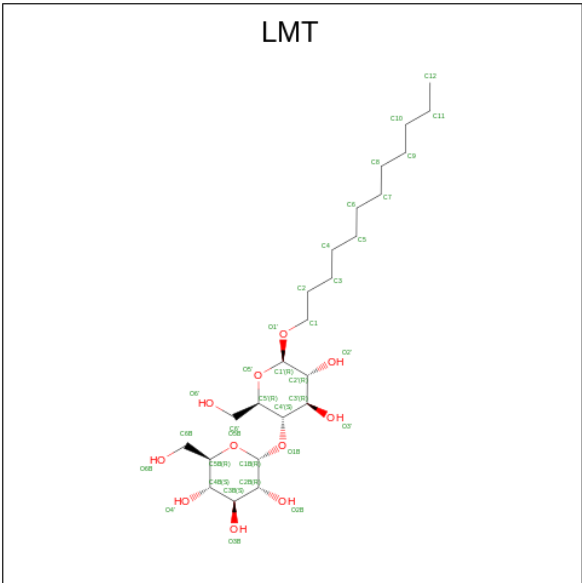
Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	M	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	4	1	Total C 40 40	0
19	5	1	Total C 40 40	0
19	5	1	Total C 40 40	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



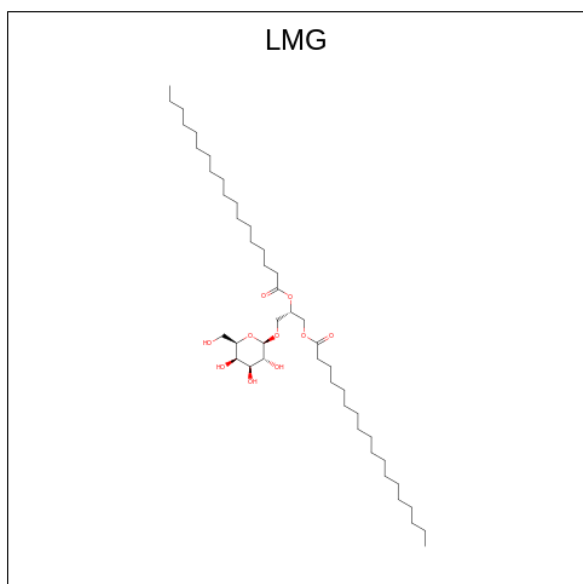
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			27	16	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	F	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			35	24	11	
21	B	1	Total	C	O	0
			35	24	11	
21	B	1	Total	C	O	0
			35	24	11	
21	M	1	Total	C	O	0
			35	24	11	
21	1	1	Total	C	O	0
			35	24	11	
21	5	1	Total	C	O	0
			35	24	11	

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			55	45	10	

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	A	9	Total	O	0
			9	9	
23	B	12	Total	O	0
			12	12	

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Mol	Chain	Residues	Atoms		AltConf
23	F	2	Total 2	O 2	0
23	K	1	Total 1	O 1	0
23	1	2	Total 2	O 2	0

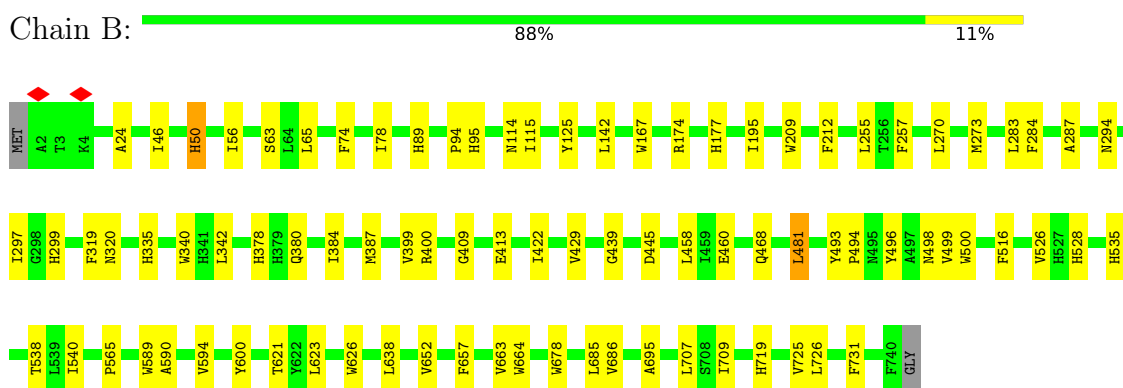
3 Residue-property plots

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.

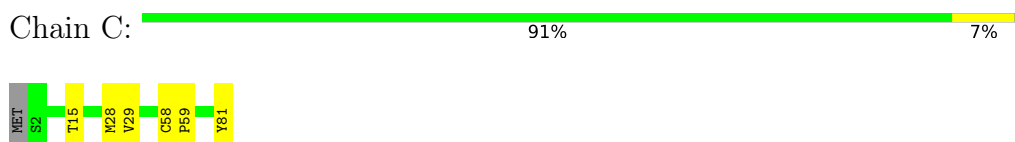
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



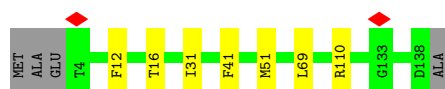
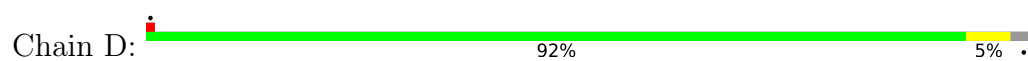
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1



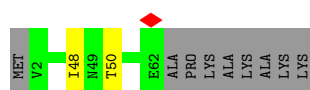
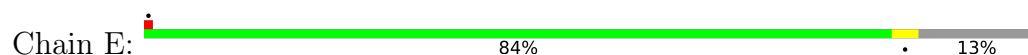
- Molecule 3: Photosystem I iron-sulfur center



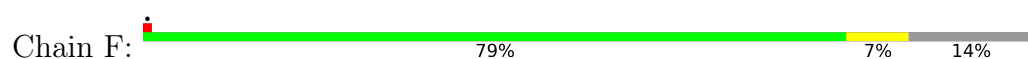
- Molecule 4: Photosystem I reaction center subunit II



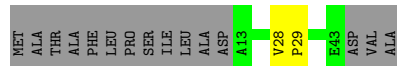
- Molecule 5: Photosystem I reaction center subunit IV



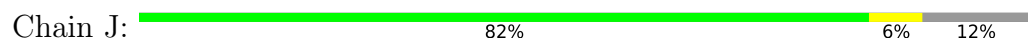
- Molecule 6: Photosystem I reaction center subunit III



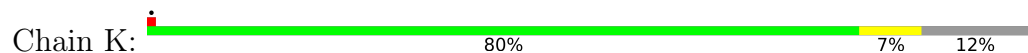
- Molecule 7: Photosystem I reaction center subunit VIII



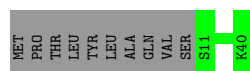
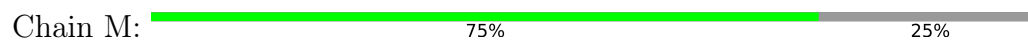
- Molecule 8: Photosystem I reaction center subunit IX



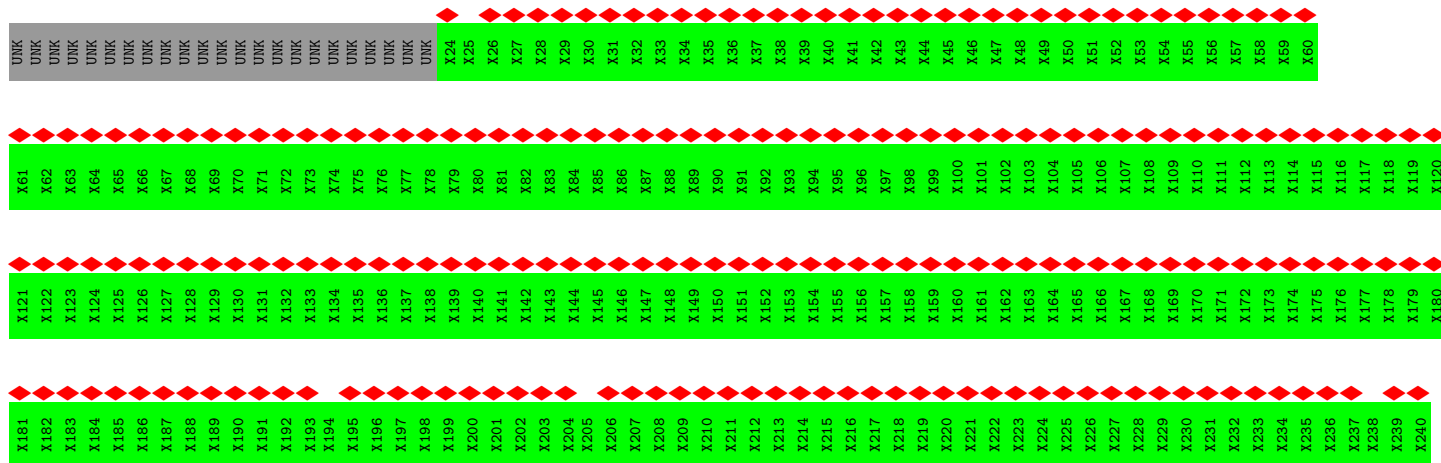
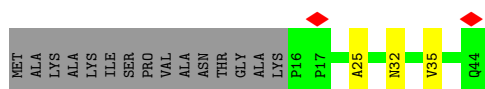
- Molecule 9: Unknown



- Molecule 10: Psam

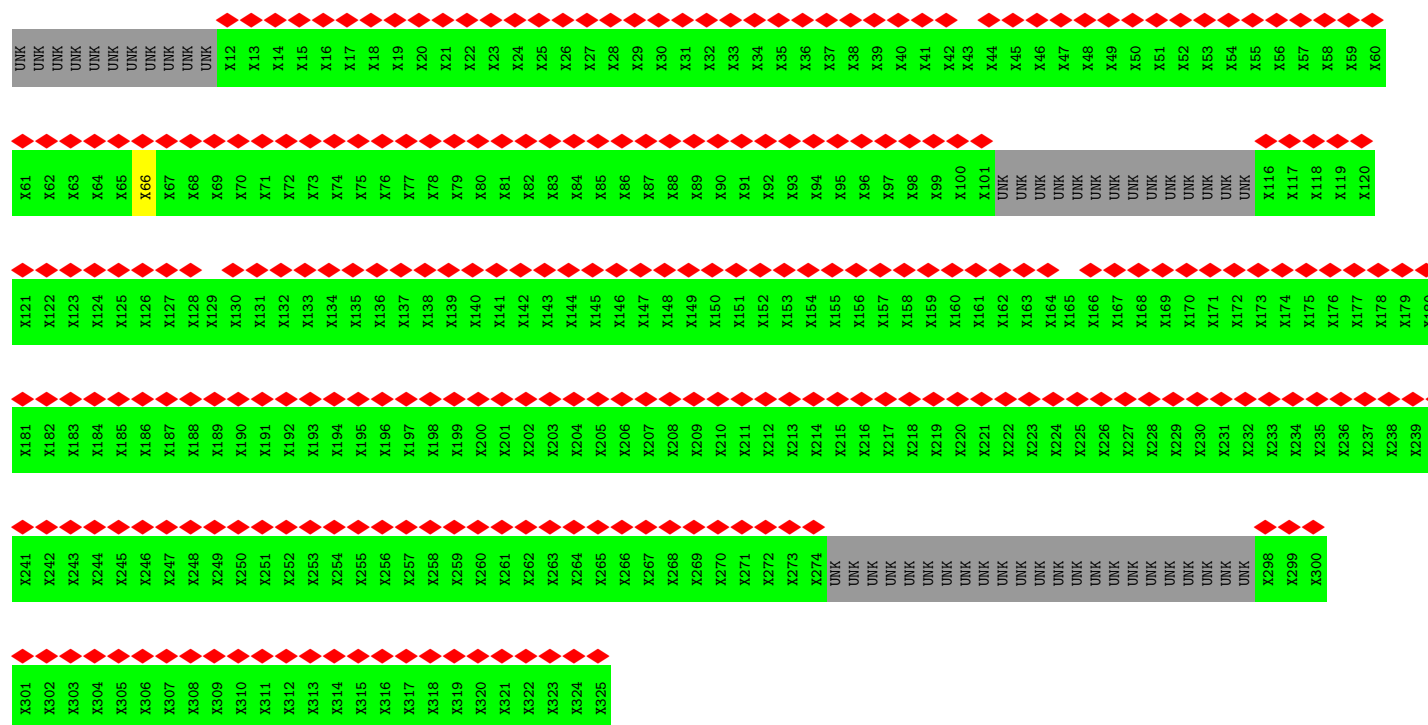
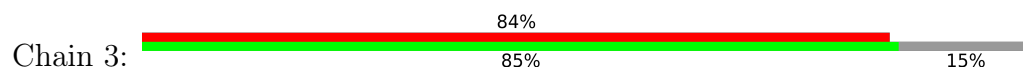


- Molecule 11: Photosystem I 4.8 kDa protein

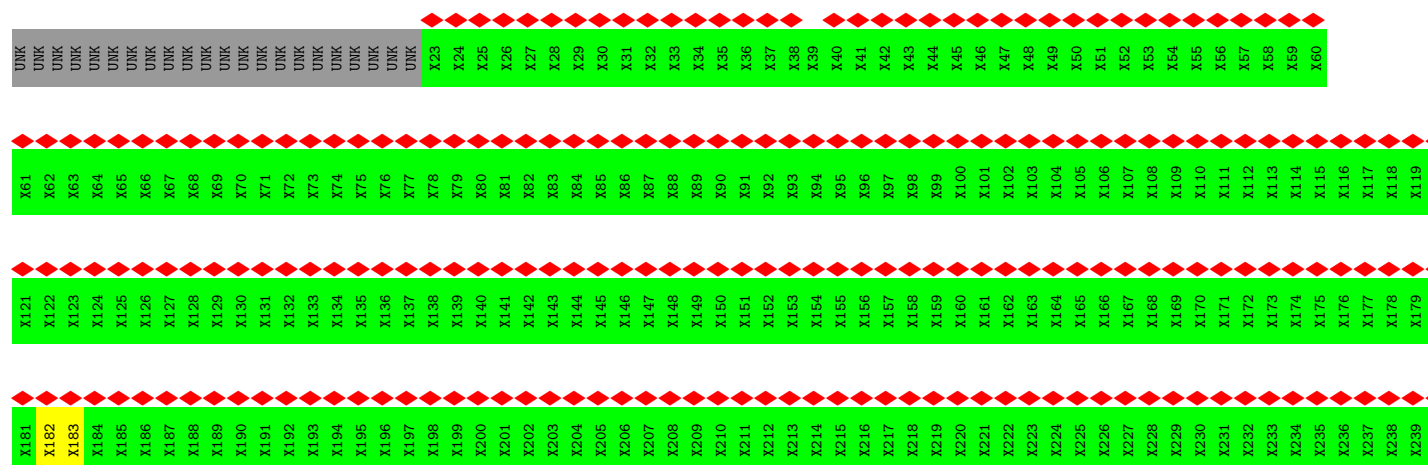
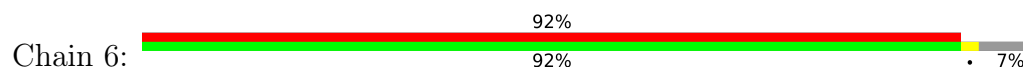


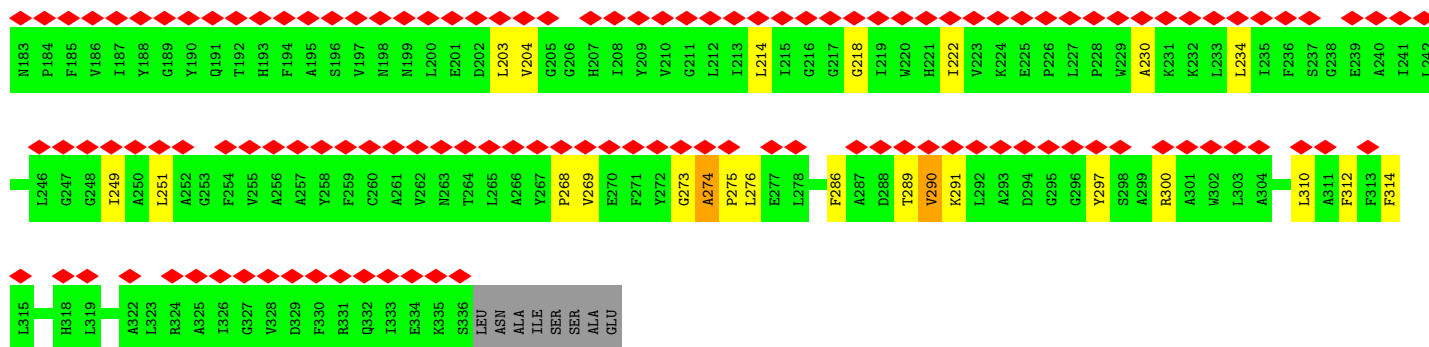


• Molecule 13: IsiA



• Molecule 13: IsiA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	11.70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	229.68001, 229.68001, 229.68001	wwPDB
Map dimensions	232, 232, 232	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.99, 0.99, 0.99	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LHG, CL0, SF4, BCR, LMT, LMG, PQN

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	0.61	0/6023	0.71	0/8216
2	B	0.60	0/6143	0.72	0/8398
3	C	0.63	0/609	0.79	0/826
4	D	0.63	0/1067	0.76	0/1441
5	E	0.64	0/499	0.77	0/677
6	F	0.63	0/1104	0.76	0/1500
7	I	0.63	0/262	0.68	0/358
8	J	0.61	0/358	0.67	0/490
10	M	0.64	0/239	0.68	0/326
11	X	0.59	0/253	0.67	0/347
12	1	0.67	0/3702	0.72	0/5059
14	4	0.68	0/2648	0.79	0/3611
14	5	0.69	0/2676	0.77	0/3649
All	All	0.64	0/25583	0.74	0/34898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5824	0	5701	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5919	0	5676	87	0
3	C	599	0	577	5	0
4	D	1043	0	1049	5	0
5	E	490	0	484	2	0
6	F	1080	0	1076	9	0
7	I	253	0	255	1	0
8	J	347	0	352	3	0
9	K	360	0	77	5	0
10	M	235	0	251	0	0
11	X	243	0	244	2	0
12	1	3590	0	3568	33	0
13	2	1474	0	277	0	0
13	3	1354	0	264	1	0
13	6	1479	0	284	3	0
14	4	2562	0	2544	35	0
14	5	2589	0	2569	38	0
15	A	65	0	72	7	0
16	1	959	0	764	39	0
16	2	270	0	198	8	0
16	3	45	0	33	2	0
16	4	450	0	330	13	0
16	5	851	0	623	46	0
16	6	401	0	293	10	0
16	A	2460	0	2456	138	0
16	B	2489	0	2585	161	0
16	F	96	0	74	8	0
16	J	90	0	66	4	0
16	K	86	0	62	10	0
16	X	45	0	33	2	0
17	A	33	0	46	5	0
17	B	33	0	46	5	0
18	A	8	0	0	0	0
18	C	16	0	0	1	0
19	1	200	0	280	8	0
19	4	40	0	56	3	0
19	5	80	0	112	5	0
19	A	240	0	336	14	0
19	B	280	0	392	15	0
19	F	80	0	112	4	0
19	I	80	0	112	7	0
19	J	80	0	112	4	0
19	K	40	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	M	40	0	56	2	0
20	A	76	0	98	4	0
20	B	49	0	74	3	0
20	F	49	0	74	0	0
21	1	35	0	46	0	0
21	5	35	0	46	0	0
21	A	35	0	46	0	0
21	B	70	0	92	0	0
21	M	35	0	46	2	0
22	B	55	0	86	3	0
23	1	2	0	0	0	0
23	A	9	0	0	0	0
23	B	12	0	0	0	0
23	F	2	0	0	0	0
23	K	1	0	0	0	0
All	All	39463	0	35161	592	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 8.

All (592) 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)
14:5:28:ILE:HD11	16:5:414:CLA:HBC3	1.49	0.94
16:A:804:CLA:H201	16:B:802:CLA:H141	1.49	0.92
16:B:807:CLA:H92	16:B:807:CLA:HMC2	1.56	0.86
14:4:157:VAL:HG11	14:4:208:ILE:HD11	1.64	0.79
14:5:276:LEU:HD23	14:5:300:ARG:HD2	1.66	0.77
16:A:806:CLA:H93	16:A:814:CLA:H42	1.66	0.76
19:1:523:BCR:H403	19:1:523:BCR:H371	1.68	0.75
16:A:823:CLA:HMD2	19:A:846:BCR:H23C	1.69	0.75
14:5:17:ASN:HD22	14:5:20:PHE:HE2	1.36	0.73
1:A:737:ILE:HG21	16:A:829:CLA:HMC2	1.71	0.72
16:A:803:CLA:HMB1	16:A:803:CLA:HBB1	1.73	0.71
12:1:40:LEU:HD11	16:2:406:CLA:HMB2	1.73	0.71
9:K:29:UNK:HA	9:K:65:UNK:CB	2.21	0.70
1:A:430:VAL:HG21	16:A:840:CLA:H201	1.72	0.70
1:A:734:LEU:HD22	16:A:842:CLA:HMA1	1.75	0.69
12:1:30:ALA:HA	16:1:512:CLA:HMB3	1.73	0.69
14:4:166:LEU:HD12	14:4:200:LEU:HD21	1.73	0.69
2:B:342:LEU:HD21	16:B:829:CLA:HBB1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:663:VAL:HG22	16:B:841:CLA:HMB3	1.76	0.68
16:A:802:CLA:HBB1	16:A:802:CLA:HMB1	1.74	0.68
16:A:842:CLA:H41	17:A:844:PQN:H192	1.75	0.68
2:B:257:PHE:CE2	2:B:500:TRP:HE3	2.12	0.68
2:B:319:PHE:HB2	16:B:823:CLA:HMA1	1.77	0.67
16:1:510:CLA:HBB1	16:1:510:CLA:HMB1	1.77	0.67
16:B:821:CLA:HMB1	16:B:821:CLA:HBB1	1.77	0.67
14:5:310:LEU:HD22	16:5:404:CLA:HMC3	1.77	0.67
2:B:384:ILE:HG23	2:B:590:ALA:HB1	1.77	0.67
14:5:274:ALA:HB3	14:5:275:PRO:HD3	1.77	0.66
16:B:832:CLA:CBB	16:B:833:CLA:HMB2	2.25	0.66
16:B:840:CLA:H91	16:B:841:CLA:H203	1.77	0.66
14:4:274:ALA:HB3	14:4:275:PRO:HD3	1.77	0.66
2:B:623:LEU:HD12	16:B:802:CLA:H11	1.78	0.66
1:A:432:ARG:NH2	4:D:12:PHE:O	2.29	0.66
16:B:805:CLA:HMB1	16:B:805:CLA:HBB1	1.77	0.66
12:1:307:PHE:CZ	16:1:511:CLA:HMB3	2.31	0.65
9:K:75:UNK:CB	16:K:103:CLA:C1B	2.74	0.65
14:5:249:ILE:CG2	16:5:404:CLA:HAC1	2.26	0.65
16:B:807:CLA:H202	16:B:827:CLA:H201	1.79	0.65
16:B:823:CLA:HMB1	16:B:823:CLA:HBB1	1.78	0.65
16:A:817:CLA:HBB1	16:A:817:CLA:HMB1	1.78	0.65
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.79	0.64
1:A:547:VAL:HG11	16:A:840:CLA:HMB3	1.79	0.64
2:B:299:HIS:CE1	16:B:822:CLA:HMD1	2.33	0.64
16:B:839:CLA:HBB1	16:B:839:CLA:HMB1	1.80	0.64
16:A:802:CLA:OBD	16:B:801:CLA:HMB3	1.97	0.64
16:B:840:CLA:HBB2	17:B:842:PQN:H141	1.78	0.64
14:5:34:GLN:HB2	16:5:411:CLA:HMB2	1.78	0.64
16:5:408:CLA:HMB1	16:5:408:CLA:HBB1	1.79	0.64
1:A:122:VAL:HB	16:B:833:CLA:HMD1	1.78	0.63
1:A:457:ILE:HG22	16:A:835:CLA:HBC2	1.80	0.63
16:A:833:CLA:HMB1	16:A:833:CLA:HBB1	1.80	0.63
14:4:23:LEU:HD22	14:4:26:LEU:HB2	1.80	0.63
16:A:826:CLA:HBB1	16:A:826:CLA:HMB1	1.81	0.63
16:A:831:CLA:HMB1	16:A:831:CLA:HBB1	1.80	0.63
15:A:801:CL0:H13	16:B:802:CLA:OBD	1.99	0.63
16:B:804:CLA:HMB1	16:B:804:CLA:HBB1	1.81	0.62
16:K:101:CLA:HBC3	19:K:102:BCR:H312	1.81	0.62
16:A:815:CLA:HBB1	16:A:815:CLA:HMB1	1.81	0.62
16:B:802:CLA:HMB1	16:B:802:CLA:HBB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:813:CLA:H92	16:B:824:CLA:H11	1.81	0.62
14:5:249:ILE:HG22	16:5:404:CLA:HAC1	1.82	0.62
16:A:833:CLA:H91	19:1:523:BCR:C29	2.29	0.61
1:A:662:TYR:OH	2:B:445:ASP:OD2	2.13	0.61
17:A:844:PQN:H141	16:F:201:CLA:HBB2	1.82	0.61
16:B:825:CLA:H92	16:B:839:CLA:H41	1.81	0.61
16:A:834:CLA:HBB2	12:1:391:LEU:HD13	1.82	0.61
16:A:822:CLA:HMB2	16:A:826:CLA:HMA3	1.81	0.61
16:B:825:CLA:HMB1	16:B:825:CLA:HBB1	1.83	0.61
16:B:814:CLA:HMB1	16:B:814:CLA:HBB1	1.83	0.61
16:A:806:CLA:HBB1	16:A:806:CLA:HMB1	1.83	0.61
16:A:837:CLA:HBB1	16:A:837:CLA:HMB1	1.82	0.61
19:A:851:BCR:H362	16:B:802:CLA:C4	2.31	0.61
16:B:822:CLA:HBB1	16:B:822:CLA:HMB1	1.82	0.60
16:4:405:CLA:HBB1	16:4:405:CLA:HMB1	1.84	0.60
19:A:851:BCR:H292	16:B:832:CLA:HMB3	1.82	0.60
14:4:312:PHE:CE1	16:4:411:CLA:HMC2	2.36	0.60
16:A:805:CLA:HMA2	16:A:812:CLA:HMD2	1.84	0.60
16:A:807:CLA:HED1	16:A:831:CLA:H2	1.84	0.59
12:1:307:PHE:CE2	16:1:511:CLA:HMB3	2.37	0.59
16:A:834:CLA:C3B	16:A:835:CLA:HMB2	2.32	0.59
2:B:663:VAL:CG2	16:B:841:CLA:HMB3	2.33	0.59
1:A:599:MET:HG2	16:A:827:CLA:HBC1	1.84	0.59
14:4:30:ALA:HA	16:4:408:CLA:HMB3	1.85	0.58
1:A:349:TRP:HB3	16:A:806:CLA:HAC1	1.85	0.58
2:B:257:PHE:HE2	2:B:500:TRP:HE3	1.49	0.58
14:5:312:PHE:CE2	16:5:419:CLA:HMC2	2.39	0.58
16:A:829:CLA:H93	19:J:103:BCR:H361	1.86	0.58
16:A:839:CLA:H93	16:1:520:CLA:H191	1.85	0.58
2:B:458:LEU:HD22	2:B:621:THR:HG21	1.85	0.58
1:A:320:HIS:HB3	1:A:325:ILE:HD11	1.85	0.57
2:B:460:GLU:HG3	6:F:28:LEU:HD11	1.85	0.57
2:B:78:ILE:HD12	2:B:125:TYR:CD1	2.39	0.57
3:C:59:PRO:O	5:E:48:ILE:HD13	2.04	0.57
8:J:28:ILE:HA	16:J:101:CLA:HBB2	1.85	0.57
16:A:809:CLA:H142	16:B:802:CLA:H201	1.86	0.57
16:B:806:CLA:HMB2	16:B:829:CLA:HBB2	1.86	0.57
14:4:65:ILE:HB	14:4:303:LEU:HD21	1.87	0.57
16:A:841:CLA:HMB1	16:A:841:CLA:HBB1	1.86	0.56
1:A:59:PHE:CD2	16:A:806:CLA:HMC2	2.41	0.56
1:A:719:LEU:HD11	16:A:842:CLA:HMD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:825:CLA:H42	20:B:850:LHG:H381	1.86	0.56
1:A:396:TRP:HB3	16:A:829:CLA:HMC3	1.86	0.56
16:A:805:CLA:HMB1	16:A:805:CLA:HBB1	1.88	0.56
16:A:833:CLA:H91	19:1:523:BCR:H291	1.86	0.56
2:B:65:LEU:HD12	2:B:142:LEU:HD12	1.87	0.56
16:A:809:CLA:HBB1	16:A:809:CLA:HMB1	1.87	0.56
19:A:851:BCR:H362	16:B:802:CLA:H42	1.87	0.56
14:4:171:THR:HG23	14:4:173:VAL:HG12	1.88	0.56
16:F:201:CLA:HMC2	19:F:202:BCR:H381	1.87	0.56
14:5:251:LEU:HD21	16:5:407:CLA:HMC1	1.86	0.56
2:B:167:TRP:CZ2	16:B:811:CLA:HMA1	2.40	0.56
1:A:741:TRP:CZ2	16:A:829:CLA:H42	2.41	0.55
16:B:801:CLA:HBB1	16:B:801:CLA:HHC	1.88	0.55
16:B:830:CLA:H142	16:B:839:CLA:H93	1.89	0.55
1:A:737:ILE:HG23	16:A:829:CLA:HBB1	1.87	0.55
16:A:809:CLA:HMC2	16:A:829:CLA:C14	2.37	0.55
9:K:25:UNK:HA	9:K:69:UNK:CB	2.36	0.55
12:1:34:HIS:HB2	16:1:510:CLA:HMB2	1.89	0.55
12:1:390:LYS:HB2	16:1:521:CLA:HMB3	1.88	0.55
1:A:678:PHE:CD2	19:A:851:BCR:H363	2.42	0.55
1:A:540:ALA:HB1	16:A:839:CLA:HMB3	1.89	0.55
16:B:811:CLA:HHC	16:B:811:CLA:HBB1	1.89	0.55
2:B:95:HIS:CE1	16:B:809:CLA:HMB3	2.41	0.54
16:K:101:CLA:HBC3	19:K:102:BCR:C31	2.37	0.54
16:A:843:CLA:HMA1	2:B:695:ALA:CB	2.37	0.54
16:A:827:CLA:HBB2	19:A:850:BCR:H311	1.89	0.54
2:B:257:PHE:CE2	2:B:500:TRP:HB3	2.41	0.54
16:B:806:CLA:HBB1	19:B:844:BCR:H402	1.89	0.54
16:B:840:CLA:CBB	17:B:842:PQN:H141	2.37	0.54
16:B:819:CLA:HMB1	16:B:824:CLA:HMA3	1.89	0.54
16:A:834:CLA:HMB2	19:I:102:BCR:C35	2.38	0.54
2:B:115:ILE:O	16:B:808:CLA:HMD3	2.08	0.54
16:K:101:CLA:HHC	16:K:101:CLA:HBB1	1.90	0.54
16:K:101:CLA:HBC2	16:K:101:CLA:HHD	1.90	0.53
1:A:119:TRP:CD2	16:A:810:CLA:HED3	2.43	0.53
2:B:177:HIS:CG	16:B:813:CLA:HMC2	2.42	0.53
1:A:203:GLN:HB3	16:A:821:CLA:HBC3	1.91	0.53
12:1:203:VAL:HG12	12:1:269:ASN:HD21	1.73	0.53
2:B:384:ILE:HD13	16:B:825:CLA:HAC2	1.90	0.53
16:B:835:CLA:HMB1	19:B:847:BCR:HC31	1.91	0.53
1:A:714:ILE:CD1	6:F:122:ILE:HG23	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:803:CLA:HMB1	16:B:803:CLA:HBB1	1.89	0.53
19:B:853:BCR:H363	19:F:202:BCR:HC21	1.90	0.53
1:A:691:ARG:HG3	1:A:719:LEU:O	2.08	0.53
16:A:810:CLA:HHC	16:A:810:CLA:HBB1	1.91	0.53
4:D:16:THR:HA	12:1:341:GLY:O	2.09	0.53
19:I:102:BCR:H331	19:I:102:BCR:C8	2.37	0.53
14:4:324:ARG:HG2	14:4:329:ASP:HB3	1.90	0.53
2:B:422:ILE:HG23	16:B:839:CLA:HBB2	1.91	0.53
2:B:335:HIS:CE1	16:B:829:CLA:HED1	2.43	0.52
16:B:813:CLA:H91	16:B:828:CLA:HBC1	1.91	0.52
14:5:251:LEU:HD21	16:5:407:CLA:CMC	2.39	0.52
19:A:846:BCR:C13	19:K:102:BCR:H323	2.40	0.52
13:3:66:UNK:CB	16:3:401:CLA:HED3	2.40	0.52
16:A:831:CLA:H91	20:A:852:LHG:H331	1.91	0.52
16:A:810:CLA:CBB	16:B:833:CLA:HBC2	2.39	0.52
16:B:806:CLA:HBB1	16:B:806:CLA:HHC	1.91	0.52
16:A:827:CLA:CBB	19:A:850:BCR:H311	2.40	0.52
16:5:414:CLA:HHC	16:5:414:CLA:HBB1	1.93	0.52
16:A:822:CLA:CMB	16:A:826:CLA:HMA3	2.40	0.51
2:B:378:HIS:HE2	16:B:828:CLA:C1B	2.23	0.51
12:1:128:PHE:CD1	16:1:514:CLA:HMB2	2.45	0.51
16:5:422:CLA:HMD2	13:6:320:UNK:HA	1.92	0.51
16:A:819:CLA:CAC	16:A:822:CLA:H191	2.40	0.51
3:C:29:VAL:HG12	4:D:110:ARG:HB3	1.92	0.51
16:A:822:CLA:H202	16:A:828:CLA:HMB2	1.90	0.51
2:B:74:PHE:CZ	2:B:78:ILE:HD11	2.46	0.51
2:B:409:GLY:N	2:B:413:GLU:OE1	2.38	0.51
16:B:813:CLA:H91	16:B:828:CLA:CBC	2.40	0.51
12:1:28:LEU:HD22	12:1:118:LEU:HD11	1.92	0.51
12:1:149:LEU:HD11	16:1:508:CLA:HED1	1.93	0.51
14:4:40:LEU:HD11	16:5:419:CLA:HMB2	1.93	0.51
16:1:508:CLA:HHC	16:1:508:CLA:HBB1	1.92	0.51
16:B:818:CLA:HBB1	16:B:818:CLA:HHC	1.92	0.51
6:F:76:VAL:HG12	6:F:86:PHE:HB2	1.91	0.51
19:1:523:BCR:H331	19:1:523:BCR:C8	2.40	0.51
14:4:157:VAL:HG11	14:4:208:ILE:CD1	2.40	0.51
16:F:201:CLA:HHC	16:F:201:CLA:HBB1	1.93	0.51
16:1:520:CLA:HMB3	16:1:521:CLA:HBC2	1.93	0.51
14:4:108:LEU:C	14:4:108:LEU:HD12	2.31	0.51
14:5:268:PRO:O	14:5:269:VAL:HG22	2.11	0.51
16:B:841:CLA:HHC	16:B:841:CLA:HBB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:412:LEU:HD22	12:1:458:SER:HB2	1.92	0.51
16:A:836:CLA:HHC	16:A:836:CLA:HBB1	1.92	0.50
15:A:801:CL0:CED	15:A:801:CL0:H36	2.41	0.50
16:A:842:CLA:HHC	16:A:842:CLA:HBB1	1.93	0.50
12:1:13:TRP:HA	16:1:512:CLA:HMD3	1.92	0.50
16:A:810:CLA:HBB2	16:B:833:CLA:CHD	2.42	0.50
16:5:404:CLA:HBB1	16:5:404:CLA:HHC	1.94	0.50
16:5:406:CLA:HMD3	16:6:409:CLA:HED3	1.94	0.50
16:A:813:CLA:HHC	16:A:813:CLA:HBB1	1.92	0.50
16:A:834:CLA:HMC2	16:1:521:CLA:HBB2	1.94	0.50
16:A:829:CLA:H201	19:J:103:BCR:H12C	1.93	0.50
14:4:67:LEU:HD11	14:4:89:TYR:CD2	2.46	0.50
16:A:825:CLA:HBB1	16:A:825:CLA:HHC	1.93	0.50
16:A:831:CLA:H41	20:A:852:LHG:H101	1.93	0.50
2:B:287:ALA:HB2	16:B:819:CLA:HBC2	1.93	0.50
16:B:812:CLA:HHC	16:B:812:CLA:HBB1	1.93	0.50
14:5:310:LEU:HB3	16:5:404:CLA:HBC2	1.93	0.50
16:B:819:CLA:CMB	16:B:824:CLA:HMA3	2.42	0.50
16:B:825:CLA:H141	11:X:35:VAL:HG21	1.94	0.50
16:J:101:CLA:HBB1	16:J:101:CLA:HHC	1.93	0.50
16:A:830:CLA:HHC	16:A:830:CLA:HBB1	1.93	0.50
19:A:846:BCR:C12	19:K:102:BCR:H323	2.42	0.50
2:B:195:ILE:HD13	16:B:815:CLA:CAC	2.42	0.49
14:5:276:LEU:HD12	14:5:286:PHE:HB3	1.94	0.49
14:4:195:ALA:HB1	14:4:262:VAL:CG2	2.42	0.49
16:5:407:CLA:HHC	16:5:407:CLA:HBB1	1.92	0.49
2:B:399:VAL:HG13	2:B:400:ARG:HG3	1.95	0.49
16:B:810:CLA:HMD3	19:I:101:BCR:H403	1.94	0.49
1:A:222:ALA:HB3	1:A:223:PRO:HD3	1.93	0.49
16:B:816:CLA:HMC1	16:B:816:CLA:HBC2	1.93	0.49
16:5:409:CLA:HHC	16:5:409:CLA:HBB1	1.94	0.49
2:B:707:LEU:HD11	16:B:841:CLA:HMD3	1.94	0.49
16:B:827:CLA:H203	22:B:849:LMG:H261	1.95	0.49
16:1:513:CLA:HHC	16:1:513:CLA:HBB1	1.95	0.49
14:4:122:THR:HG21	14:4:128:PHE:HB2	1.93	0.49
1:A:601:ASN:HD21	15:A:801:CL0:H68	1.78	0.49
15:A:801:CL0:H15	15:A:801:CL0:H11	1.94	0.49
14:4:200:LEU:HD23	14:4:204:VAL:HG23	1.94	0.49
2:B:142:LEU:HD21	19:B:845:BCR:H24C	1.94	0.49
2:B:319:PHE:O	2:B:319:PHE:CD2	2.66	0.49
2:B:340:TRP:HE1	16:B:824:CLA:C2B	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:CYS:HA	18:C:102:SF4:S4	2.53	0.49
16:1:510:CLA:HMB3	16:1:511:CLA:HAA1	1.94	0.49
16:A:834:CLA:HHC	16:A:834:CLA:HBB1	1.95	0.49
12:1:362:ILE:HB	16:1:520:CLA:HMD1	1.95	0.49
14:4:108:LEU:HD11	16:5:407:CLA:H3A	1.95	0.49
19:4:401:BCR:H331	19:4:401:BCR:C8	2.42	0.49
15:A:801:CL0:CGD	15:A:801:CL0:H8	2.43	0.49
16:A:832:CLA:HMB2	16:A:833:CLA:C1D	2.43	0.49
16:A:839:CLA:HHC	16:A:839:CLA:HBB1	1.95	0.49
2:B:493:TYR:O	2:B:496:TYR:CZ	2.66	0.48
2:B:678:TRP:CZ2	17:B:842:PQN:H2M3	2.48	0.48
16:B:808:CLA:HHC	16:B:808:CLA:HBB1	1.95	0.48
14:5:87:TYR:N	14:5:88:PRO:HD2	2.28	0.48
14:5:122:THR:HG21	14:5:128:PHE:HB2	1.95	0.48
1:A:220:VAL:HG13	1:A:240:PRO:HB3	1.96	0.48
17:B:842:PQN:H301	22:B:849:LMG:H181	1.95	0.48
2:B:46:ILE:HG23	2:B:50:HIS:CE1	2.49	0.48
16:X:101:CLA:HHC	16:X:101:CLA:HBB1	1.95	0.48
1:A:538:ILE:HG23	15:A:801:CL0:H67	1.96	0.48
16:B:823:CLA:HAB	16:B:830:CLA:HMD2	1.96	0.48
16:1:504:CLA:HHC	16:1:504:CLA:HBB1	1.96	0.48
16:B:813:CLA:H92	16:B:824:CLA:C1	2.43	0.48
16:B:831:CLA:HMB1	16:B:831:CLA:HBB1	1.94	0.48
16:2:403:CLA:HHC	16:2:403:CLA:HBB1	1.95	0.48
1:A:175:PHE:HD2	16:A:811:CLA:HBC3	1.79	0.48
2:B:89:HIS:CE1	2:B:114:ASN:HD22	2.31	0.48
2:B:498:ASN:ND2	16:B:835:CLA:O1D	2.46	0.48
14:4:211:GLY:O	14:4:215:ILE:HD12	2.14	0.48
14:5:203:LEU:CD1	16:5:403:CLA:HMA3	2.43	0.48
16:6:403:CLA:HHC	16:6:403:CLA:HBB1	1.95	0.48
6:F:88:ILE:HG12	16:J:102:CLA:HMB3	1.96	0.48
14:5:289:THR:O	14:5:290:VAL:HG12	2.14	0.48
16:A:811:CLA:HHC	16:A:811:CLA:HBB1	1.96	0.48
16:B:832:CLA:CAD	16:B:832:CLA:H93	2.44	0.48
2:B:707:LEU:HD21	17:B:842:PQN:H151	1.96	0.48
1:A:217:LEU:HA	1:A:221:SER:HB2	1.95	0.47
1:A:355:THR:HG23	19:A:849:BCR:H342	1.95	0.47
12:1:177:ILE:HG21	12:1:210:VAL:HG21	1.96	0.47
16:2:401:CLA:HHC	16:2:401:CLA:HBB1	1.96	0.47
1:A:75:ALA:HB2	1:A:181:TYR:HB2	1.96	0.47
16:2:405:CLA:HHC	16:2:405:CLA:HBB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5:13:TRP:HA	16:5:413:CLA:HMD3	1.95	0.47
16:A:819:CLA:HBB1	16:A:819:CLA:HHC	1.97	0.47
16:A:831:CLA:H143	20:A:852:LHG:H372	1.95	0.47
19:B:853:BCR:C8	19:B:853:BCR:H331	2.44	0.47
17:A:844:PQN:H141	16:F:201:CLA:CBB	2.44	0.47
2:B:516:PHE:CE2	16:B:826:CLA:HMC3	2.49	0.47
2:B:623:LEU:HD12	16:B:802:CLA:C1	2.44	0.47
16:B:834:CLA:HHC	16:B:834:CLA:HBB1	1.96	0.47
19:K:102:BCR:HC8	19:K:102:BCR:H311	1.95	0.47
16:K:103:CLA:HHC	16:K:103:CLA:HBB1	1.95	0.47
14:5:218:GLY:O	14:5:222:ILE:HD12	2.14	0.47
16:5:416:CLA:HHC	16:5:416:CLA:HBB1	1.95	0.47
16:A:804:CLA:HHC	16:A:804:CLA:HBB1	1.97	0.47
16:2:404:CLA:HHC	16:2:404:CLA:HBB1	1.97	0.47
19:5:420:BCR:C8	19:5:420:BCR:H331	2.44	0.47
16:A:823:CLA:HHC	16:A:823:CLA:HBB1	1.96	0.47
16:A:802:CLA:HAA2	16:A:802:CLA:HBD	1.97	0.47
16:A:824:CLA:HHC	16:A:824:CLA:HBB1	1.97	0.47
2:B:270:LEU:HD23	2:B:273:MET:HE3	1.95	0.47
16:B:807:CLA:HAA2	16:B:809:CLA:HED1	1.97	0.47
16:B:827:CLA:CGA	16:B:827:CLA:H3A	2.45	0.47
8:J:19:PRO:HB2	19:J:104:BCR:H391	1.96	0.47
16:2:402:CLA:HHC	16:2:402:CLA:HBB1	1.97	0.47
14:4:258:TYR:O	14:4:262:VAL:HG22	2.14	0.47
2:B:439:GLY:HA3	16:B:833:CLA:CBB	2.44	0.47
16:B:808:CLA:H92	16:B:829:CLA:H202	1.97	0.47
16:1:502:CLA:HHC	16:1:502:CLA:HBB1	1.97	0.47
14:4:157:VAL:CG1	14:4:208:ILE:HD11	2.41	0.47
16:5:405:CLA:HHC	16:5:405:CLA:HBB1	1.97	0.47
1:A:172:LEU:O	16:A:811:CLA:HBC2	2.15	0.47
6:F:34:ASN:ND2	6:F:67:GLY:O	2.48	0.47
16:1:519:CLA:HHC	16:1:519:CLA:HBB1	1.97	0.47
14:4:17:ASN:HD21	16:4:408:CLA:C1C	2.27	0.47
16:4:404:CLA:HHC	16:4:404:CLA:HBB1	1.96	0.47
16:5:403:CLA:HHC	16:5:403:CLA:HBB1	1.97	0.47
13:6:259:UNK:O	13:6:263:UNK:CB	2.63	0.47
20:A:853:LHG:HC62	16:1:501:CLA:CHB	2.44	0.47
16:2:406:CLA:HHC	16:2:406:CLA:HBB1	1.97	0.47
1:A:506:VAL:HG11	16:A:819:CLA:H42	1.97	0.46
16:A:812:CLA:HHC	16:A:812:CLA:HBB1	1.97	0.46
16:5:422:CLA:HHC	16:5:422:CLA:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:6:405:CLA:HHC	16:6:405:CLA:HBB1	1.96	0.46
1:A:75:ALA:HB3	16:A:812:CLA:HMD3	1.98	0.46
2:B:384:ILE:HG13	2:B:594:VAL:HB	1.96	0.46
2:B:726:LEU:HD23	16:B:827:CLA:H41	1.98	0.46
14:5:314:PHE:CE2	16:5:412:CLA:HMB3	2.50	0.46
16:A:803:CLA:HMC2	16:B:802:CLA:CAC	2.44	0.46
16:A:809:CLA:HMC2	16:A:829:CLA:H142	1.97	0.46
16:A:814:CLA:HHC	16:A:814:CLA:HBB1	1.97	0.46
16:A:833:CLA:H91	19:1:523:BCR:H292	1.97	0.46
21:M:101:LMT:H91	19:M:102:BCR:HC21	1.97	0.46
12:1:19:ARG:NH1	16:1:512:CLA:HMD1	2.30	0.46
1:A:353:LEU:N	16:A:806:CLA:HMD3	2.31	0.46
16:A:821:CLA:HHC	16:A:821:CLA:HBB1	1.97	0.46
14:5:177:VAL:HG21	14:5:204:VAL:HG21	1.98	0.46
1:A:203:GLN:OE1	1:A:310:HIS:CE1	2.69	0.46
1:A:401:LEU:HD21	16:A:807:CLA:H142	1.96	0.46
16:A:841:CLA:HBB2	6:F:104:GLY:HA3	1.96	0.46
2:B:257:PHE:CD2	2:B:499:VAL:HG23	2.51	0.46
16:4:411:CLA:HBB1	16:4:411:CLA:HHC	1.97	0.46
14:5:28:ILE:CD1	16:5:414:CLA:HBC3	2.33	0.46
16:5:415:CLA:HHC	16:5:415:CLA:HBB1	1.98	0.46
1:A:694:TRP:CZ2	17:A:844:PQN:H2M3	2.51	0.46
2:B:725:VAL:HG21	16:B:827:CLA:HMC2	1.97	0.46
16:1:503:CLA:HHC	16:1:503:CLA:HBB1	1.97	0.46
1:A:359:PHE:CD2	16:A:826:CLA:HMB2	2.50	0.46
16:A:811:CLA:HBB2	16:A:814:CLA:HMA3	1.96	0.46
16:B:807:CLA:H201	21:M:101:LMT:H123	1.98	0.46
14:4:258:TYR:HB2	19:4:401:BCR:H312	1.97	0.46
16:6:409:CLA:HHC	16:6:409:CLA:HBB1	1.97	0.46
2:B:56:ILE:HG13	19:M:102:BCR:H343	1.97	0.46
16:1:514:CLA:HHC	16:1:514:CLA:HBB1	1.97	0.46
14:4:195:ALA:HB1	14:4:262:VAL:HG23	1.98	0.46
1:A:203:GLN:HG3	1:A:309:GLY:HA3	1.96	0.46
16:B:803:CLA:CBA	16:B:803:CLA:HED3	2.46	0.46
16:B:806:CLA:CBB	19:B:844:BCR:H402	2.46	0.46
14:4:312:PHE:CD1	16:4:411:CLA:HMC2	2.51	0.46
16:4:402:CLA:HHC	16:4:402:CLA:HBB1	1.97	0.46
16:6:404:CLA:HHC	16:6:404:CLA:HBB1	1.97	0.46
16:6:406:CLA:HHC	16:6:406:CLA:HBB1	1.97	0.46
2:B:209:TRP:CE2	16:B:814:CLA:H42	2.51	0.45
16:1:525:CLA:HHC	16:1:525:CLA:HBB1	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:526:CLA:HHC	16:1:526:CLA:HBB1	1.98	0.45
16:4:403:CLA:HHC	16:4:403:CLA:HBB1	1.96	0.45
16:4:407:CLA:HHC	16:4:407:CLA:HBB1	1.98	0.45
16:6:402:CLA:HHC	16:6:402:CLA:HBB1	1.99	0.45
1:A:510:PHE:CE2	16:A:828:CLA:HMC3	2.51	0.45
12:1:98:VAL:HG11	19:1:517:BCR:H353	1.97	0.45
16:3:401:CLA:HHC	16:3:401:CLA:HBB1	1.97	0.45
14:5:146:LEU:HD21	16:5:408:CLA:CAB	2.46	0.45
16:5:418:CLA:HHC	16:5:418:CLA:HBB1	1.97	0.45
1:A:20:ASP:N	1:A:21:PRO:HD3	2.32	0.45
16:A:820:CLA:CAD	16:A:830:CLA:H41	2.47	0.45
16:A:840:CLA:HHC	16:A:840:CLA:HBB1	1.98	0.45
2:B:565:PRO:HB3	2:B:709:ILE:HB	1.97	0.45
6:F:139:TRP:N	6:F:140:PRO:CD	2.79	0.45
16:J:102:CLA:HHC	16:J:102:CLA:HBB1	1.97	0.45
14:5:312:PHE:CD2	16:5:419:CLA:HMC2	2.51	0.45
16:6:401:CLA:HHC	16:6:401:CLA:HBB1	1.97	0.45
16:A:828:CLA:HHC	16:A:828:CLA:HBB1	1.99	0.45
16:A:841:CLA:HMC3	16:F:201:CLA:C4D	2.47	0.45
1:A:427:LEU:O	1:A:430:VAL:HG22	2.17	0.45
2:B:500:TRP:CD1	16:B:834:CLA:HED1	2.52	0.45
2:B:652:VAL:HA	16:B:809:CLA:HAC1	1.99	0.45
19:F:202:BCR:H332	19:J:103:BCR:HC32	1.98	0.45
16:F:204:CLA:HHC	16:F:204:CLA:HBB1	1.99	0.45
16:1:506:CLA:HHC	16:1:506:CLA:HBB1	1.98	0.45
16:4:409:CLA:HHC	16:4:409:CLA:HBB1	1.97	0.45
19:5:402:BCR:HC8	19:5:402:BCR:H331	1.98	0.45
16:5:412:CLA:HHC	16:5:412:CLA:HBB1	1.97	0.45
2:B:319:PHE:CD2	16:B:823:CLA:HMB3	2.52	0.45
1:A:376:PRO:HG3	16:A:820:CLA:HBA2	1.98	0.45
19:A:846:BCR:C8	19:A:846:BCR:H331	2.46	0.45
16:B:839:CLA:HBC2	16:X:101:CLA:HBC3	1.98	0.45
12:1:359:ASN:HB3	16:1:519:CLA:HAC1	1.99	0.45
16:1:509:CLA:HMD2	19:1:516:BCR:HC7	1.99	0.45
16:1:511:CLA:HHC	16:1:511:CLA:HBB1	1.99	0.45
16:4:410:CLA:HHC	16:4:410:CLA:HBB1	1.98	0.45
16:5:421:CLA:HHC	16:5:421:CLA:HBB1	1.97	0.45
14:4:47:TRP:CZ3	19:5:402:BCR:H323	2.51	0.45
14:5:276:LEU:HD23	14:5:300:ARG:CD	2.40	0.45
16:5:406:CLA:HHC	16:5:406:CLA:HBB1	1.98	0.45
16:6:407:CLA:HHC	16:6:407:CLA:HBB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:663:VAL:HG12	2:B:719:HIS:O	2.17	0.45
16:B:818:CLA:H61	16:B:818:CLA:H41	1.77	0.45
16:1:515:CLA:HHC	16:1:515:CLA:HBB1	1.98	0.45
16:A:834:CLA:H112	16:B:841:CLA:H92	1.99	0.44
2:B:294:ASN:ND2	16:B:812:CLA:HMA2	2.31	0.44
12:1:380:HIS:HA	12:1:383:PHE:CE1	2.52	0.44
16:1:512:CLA:HBB1	16:1:512:CLA:HHC	1.99	0.44
14:5:230:ALA:O	14:5:234:LEU:HG	2.17	0.44
14:5:314:PHE:CZ	16:5:412:CLA:HMB3	2.52	0.44
16:5:404:CLA:CAB	16:5:412:CLA:HMC3	2.48	0.44
16:B:839:CLA:H193	11:X:25:ALA:HB1	1.98	0.44
12:1:228:ILE:HG13	12:1:229:LEU:HG	1.98	0.44
16:6:408:CLA:HHC	16:6:408:CLA:HBB1	1.98	0.44
1:A:461:THR:HG21	16:B:809:CLA:CBB	2.47	0.44
16:A:829:CLA:H62	16:A:829:CLA:H41	1.78	0.44
2:B:638:LEU:HD22	2:B:731:PHE:HA	1.99	0.44
16:A:841:CLA:H172	6:F:104:GLY:HA2	2.00	0.44
16:A:843:CLA:HMD3	2:B:685:LEU:HD13	1.98	0.44
16:B:809:CLA:HHC	16:B:809:CLA:HBB1	2.00	0.44
16:B:826:CLA:HHC	16:B:826:CLA:HBB1	1.99	0.44
3:C:15:THR:HG22	3:C:28:MET:HG3	2.00	0.44
16:5:417:CLA:HHC	16:5:417:CLA:HBB1	1.99	0.44
2:B:24:ALA:O	16:B:804:CLA:HMD3	2.18	0.44
16:B:820:CLA:HHC	16:B:820:CLA:HBB1	1.98	0.44
19:B:843:BCR:HC41	19:B:845:BCR:H322	2.00	0.44
16:A:839:CLA:HMB2	16:A:840:CLA:C3D	2.47	0.44
8:J:17:THR:HG22	8:J:19:PRO:HD2	1.99	0.44
12:1:191:LEU:HD22	16:1:515:CLA:HMA3	1.99	0.44
14:5:146:LEU:HD22	14:5:214:LEU:HD11	2.00	0.44
16:5:410:CLA:HMD3	16:5:417:CLA:HBC1	2.00	0.44
1:A:265:PHE:HA	16:K:101:CLA:HAC2	1.99	0.44
1:A:320:HIS:CB	1:A:325:ILE:HD11	2.48	0.44
16:5:419:CLA:HBB1	16:5:419:CLA:HHC	1.99	0.44
16:A:802:CLA:C3C	16:B:803:CLA:HMC2	2.48	0.44
16:A:832:CLA:HMB2	16:A:833:CLA:C2D	2.48	0.44
14:4:324:ARG:HA	14:4:329:ASP:HB3	2.00	0.44
16:4:408:CLA:HHC	16:4:408:CLA:HBB1	1.99	0.44
14:5:275:PRO:O	14:5:276:LEU:HD22	2.18	0.44
1:A:536:HIS:CG	16:A:839:CLA:HED2	2.53	0.44
1:A:574:PRO:HB3	1:A:721:ILE:HB	2.00	0.44
16:A:803:CLA:HMC2	16:B:802:CLA:HAC1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:843:CLA:HHC	16:A:843:CLA:HBB1	2.00	0.44
2:B:526:VAL:HG23	16:B:801:CLA:H143	2.00	0.44
16:B:834:CLA:H61	16:B:834:CLA:H41	1.81	0.44
16:1:509:CLA:HHC	16:1:509:CLA:HBB1	1.99	0.44
14:4:159:LYS:HA	14:4:163:TRP:HB2	2.00	0.44
14:5:109:PHE:HB2	16:5:421:CLA:HBA1	2.00	0.44
14:5:159:LYS:HA	14:5:163:TRP:HB2	2.00	0.44
16:A:841:CLA:H2	16:B:832:CLA:H42	2.00	0.43
17:A:844:PQN:H292	16:F:204:CLA:HBC1	2.00	0.43
1:A:121:ILE:O	1:A:124:GLN:HG2	2.18	0.43
1:A:589:TRP:CD1	16:A:831:CLA:HMD1	2.53	0.43
16:A:819:CLA:HAC2	16:A:822:CLA:H191	2.00	0.43
2:B:174:ARG:HB2	16:B:813:CLA:HBC2	2.00	0.43
16:B:807:CLA:HMA1	16:B:808:CLA:CHB	2.48	0.43
16:A:803:CLA:H141	16:A:804:CLA:H191	2.00	0.43
16:A:818:CLA:HMD1	16:A:837:CLA:O2D	2.18	0.43
16:A:843:CLA:HMC3	16:B:840:CLA:ND	2.34	0.43
2:B:257:PHE:HE2	2:B:500:TRP:CE3	2.32	0.43
2:B:481:LEU:HB3	16:B:834:CLA:HMD3	2.00	0.43
16:B:826:CLA:HBC3	16:B:826:CLA:HHD	1.99	0.43
16:B:830:CLA:HMA1	16:B:831:CLA:HED2	2.00	0.43
1:A:682:PHE:HZ	16:A:842:CLA:HBC2	1.83	0.43
2:B:283:LEU:HG	16:B:819:CLA:HMC1	1.98	0.43
16:B:828:CLA:H192	19:B:844:BCR:H352	1.99	0.43
16:A:839:CLA:C9	16:1:520:CLA:H191	2.48	0.43
16:B:830:CLA:CBB	16:B:839:CLA:HAB	2.48	0.43
12:1:28:LEU:O	12:1:32:ILE:HD12	2.18	0.43
12:1:335:LEU:HD11	12:1:342:ASN:HB3	2.00	0.43
14:4:23:LEU:HD23	14:4:24:SER:H	1.83	0.43
14:4:315:LEU:HD11	19:4:401:BCR:C35	2.48	0.43
1:A:393:HIS:CE1	16:A:829:CLA:ND	2.86	0.43
16:A:816:CLA:HHC	16:A:816:CLA:HBB1	2.01	0.43
16:A:834:CLA:HMB2	19:I:102:BCR:H352	2.00	0.43
2:B:174:ARG:HD2	16:B:824:CLA:HMD1	2.01	0.43
16:B:830:CLA:C14	16:B:839:CLA:H93	2.48	0.43
16:B:838:CLA:H42	16:B:838:CLA:C4C	2.48	0.43
14:4:289:THR:O	14:4:290:VAL:HG22	2.18	0.43
2:B:726:LEU:CD2	16:B:827:CLA:H41	2.49	0.43
16:B:838:CLA:H93	16:B:839:CLA:HBC1	1.99	0.43
16:B:830:CLA:HMB2	16:B:831:CLA:C3D	2.48	0.43
12:1:45:MET:HA	12:1:48:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:HB3	16:A:821:CLA:CBC	2.48	0.43
1:A:430:VAL:HA	1:A:433:HIS:CE1	2.53	0.43
1:A:743:PHE:CD2	15:A:801:CL0:H25	2.54	0.43
16:A:807:CLA:H43	16:A:807:CLA:HED3	2.01	0.43
16:A:822:CLA:H202	16:A:828:CLA:CMB	2.49	0.43
2:B:297:ILE:HB	16:B:821:CLA:HMD1	2.01	0.43
16:B:817:CLA:HHC	16:B:817:CLA:HBB1	2.01	0.43
12:1:270:ASP:HB3	12:1:281:LEU:HD21	2.01	0.43
1:A:349:TRP:CH2	16:A:826:CLA:H143	2.54	0.42
1:A:576:ASP:OD2	1:A:580:ARG:NH2	2.52	0.42
16:A:802:CLA:H171	16:B:810:CLA:HMC2	2.01	0.42
2:B:429:VAL:HG11	2:B:535:HIS:CD2	2.53	0.42
2:B:538:THR:HG21	16:B:839:CLA:HMB3	2.00	0.42
4:D:31:ILE:HG21	4:D:69:LEU:HD23	1.99	0.42
14:4:47:TRP:CH2	19:5:402:BCR:H323	2.54	0.42
19:A:849:BCR:H21C	16:1:501:CLA:HMB1	2.01	0.42
16:B:828:CLA:H203	19:B:845:BCR:H15C	2.01	0.42
4:D:41:PHE:CD1	4:D:51:MET:HG3	2.54	0.42
12:1:239:VAL:HG23	12:1:240:LEU:HG	2.00	0.42
1:A:262:THR:N	1:A:263:PRO:CD	2.82	0.42
2:B:257:PHE:HD1	16:B:817:CLA:HMB1	1.84	0.42
16:B:810:CLA:HHC	16:B:810:CLA:HBB1	2.00	0.42
16:B:817:CLA:H43	16:B:834:CLA:HED3	2.00	0.42
9:K:71:UNK:CB	16:K:103:CLA:HBC2	2.48	0.42
16:K:101:CLA:HMB2	19:K:102:BCR:C15	2.49	0.42
12:1:39:ILE:HD11	16:1:504:CLA:C3C	2.49	0.42
2:B:664:TRP:CE3	16:B:801:CLA:HMA1	2.53	0.42
12:1:157:VAL:HG11	12:1:214:ILE:HD11	2.00	0.42
12:1:266:VAL:HA	12:1:273:TYR:CD1	2.55	0.42
19:1:517:BCR:H321	19:1:517:BCR:C8	2.50	0.42
1:A:204:VAL:HG22	16:A:821:CLA:HBC1	2.00	0.42
1:A:453:PHE:CZ	1:A:457:ILE:HD11	2.54	0.42
16:A:807:CLA:HHC	16:A:807:CLA:HBB1	2.01	0.42
2:B:320:ASN:ND2	20:B:850:LHG:O4	2.53	0.42
12:1:44:ALA:HB1	16:2:406:CLA:HMA1	2.01	0.42
16:B:808:CLA:C1A	16:B:808:CLA:CGA	2.97	0.42
16:A:818:CLA:CHD	16:A:819:CLA:HBB2	2.50	0.42
2:B:528:HIS:CE1	19:B:853:BCR:H322	2.54	0.42
16:B:818:CLA:O1A	16:B:828:CLA:HMD1	2.19	0.42
16:B:838:CLA:C1A	16:B:838:CLA:CGA	2.97	0.42
16:B:839:CLA:H43	19:B:847:BCR:C10	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5:23:LEU:HB3	14:5:24:SER:H	1.76	0.42
14:5:290:VAL:O	14:5:290:VAL:HG22	2.19	0.42
1:A:734:LEU:CD2	16:A:842:CLA:HMA1	2.47	0.42
16:B:815:CLA:HHC	16:B:815:CLA:HBB1	2.01	0.42
16:B:835:CLA:HHC	16:B:835:CLA:HBB1	2.02	0.42
1:A:318:ILE:CD1	16:A:821:CLA:HMA2	2.49	0.42
1:A:343:GLU:N	1:A:343:GLU:OE1	2.52	0.42
2:B:589:TRP:CH2	16:B:802:CLA:HAB	2.55	0.42
2:B:626:TRP:CZ2	16:B:801:CLA:H142	2.55	0.42
1:A:428:ASP:O	1:A:432:ARG:HG3	2.20	0.42
2:B:526:VAL:HG21	2:B:600:TYR:HB2	2.02	0.42
16:B:804:CLA:HAB	16:B:806:CLA:CAD	2.50	0.42
16:B:830:CLA:H92	20:B:850:LHG:H101	2.02	0.42
16:B:838:CLA:HHC	16:B:838:CLA:HBB1	2.01	0.42
19:I:102:BCR:C18	16:1:520:CLA:HBB2	2.50	0.42
14:4:108:LEU:HD11	16:5:407:CLA:CMA	2.49	0.42
1:A:197:MET:HE1	16:A:826:CLA:H142	2.00	0.41
1:A:494:ALA:N	1:A:495:PRO:HD2	2.35	0.41
2:B:212:PHE:O	16:B:815:CLA:HED1	2.20	0.41
16:B:807:CLA:HHC	16:B:807:CLA:HBB1	2.01	0.41
9:K:75:UNK:CB	16:K:103:CLA:NB	2.83	0.41
1:A:392:THR:HG23	1:A:607:ILE:HG21	2.02	0.41
2:B:340:TRP:CE2	16:B:826:CLA:H91	2.55	0.41
2:B:686:VAL:HG11	3:C:81:TYR:CG	2.55	0.41
16:B:825:CLA:H161	16:B:834:CLA:H142	2.01	0.41
14:5:20:PHE:O	14:5:23:LEU:HB2	2.21	0.41
16:A:815:CLA:HMB1	19:A:848:BCR:H362	2.02	0.41
16:A:820:CLA:HHC	16:A:820:CLA:HBB1	2.02	0.41
2:B:94:PRO:HG2	16:B:810:CLA:HMB2	2.02	0.41
16:B:822:CLA:HBC2	16:B:823:CLA:CGA	2.50	0.41
13:6:182:UNK:O	13:6:183:UNK:CB	2.68	0.41
16:A:825:CLA:HMA1	16:1:501:CLA:CBB	2.50	0.41
16:B:821:CLA:HMD2	19:B:843:BCR:H24C	2.03	0.41
5:E:48:ILE:HD12	5:E:50:THR:O	2.20	0.41
19:F:202:BCR:H331	19:F:202:BCR:C8	2.49	0.41
14:5:13:TRP:HZ3	16:5:413:CLA:HBC1	1.85	0.41
1:A:506:VAL:HG13	16:A:836:CLA:HED3	2.03	0.41
16:A:809:CLA:C14	16:B:802:CLA:H201	2.50	0.41
1:A:372:TYR:OH	16:A:838:CLA:HBC3	2.20	0.41
2:B:468:GLN:NE2	16:B:837:CLA:HMD1	2.36	0.41
1:A:203:GLN:NE2	1:A:309:GLY:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:HG22	1:A:603:LEU:HD13	2.02	0.41
16:A:833:CLA:HBB1	16:A:843:CLA:HAA2	2.02	0.41
2:B:63:SER:HB2	16:B:807:CLA:C4B	2.51	0.41
16:B:810:CLA:H91	19:I:102:BCR:HC31	2.03	0.41
16:B:827:CLA:H193	19:I:101:BCR:H342	2.03	0.41
16:B:838:CLA:HMB2	16:B:839:CLA:C2D	2.51	0.41
14:4:28:ILE:O	14:4:32:VAL:HG12	2.21	0.41
14:5:30:ALA:HA	16:5:413:CLA:HMB3	2.01	0.41
1:A:87:TRP:HA	16:A:808:CLA:CBB	2.50	0.41
16:B:809:CLA:H91	16:B:829:CLA:H162	2.03	0.41
14:4:67:LEU:HD11	14:4:89:TYR:CG	2.55	0.41
1:A:465:LEU:HG	16:B:809:CLA:HMC3	2.02	0.41
1:A:710:VAL:O	16:F:201:CLA:HMD3	2.20	0.41
16:A:833:CLA:HMC2	16:A:839:CLA:H203	2.03	0.41
16:B:820:CLA:HAA1	16:B:820:CLA:HBD	2.03	0.41
16:B:829:CLA:H41	16:B:829:CLA:H61	1.87	0.41
12:1:427:PHE:CZ	12:1:433:PRO:HG3	2.56	0.41
1:A:678:PHE:CG	19:A:851:BCR:H363	2.56	0.40
16:B:809:CLA:H142	22:B:849:LMG:H221	2.02	0.40
19:5:402:BCR:H331	19:5:402:BCR:C8	2.50	0.40
1:A:363:LEU:CD1	16:A:820:CLA:H192	2.51	0.40
16:A:841:CLA:H202	6:F:107:TYR:CD2	2.56	0.40
2:B:195:ILE:HD11	2:B:255:LEU:HD21	2.04	0.40
2:B:284:PHE:HE1	16:B:819:CLA:CBB	2.34	0.40
2:B:380:GLN:HA	2:B:380:GLN:OE1	2.20	0.40
2:B:638:LEU:HD21	2:B:657:PHE:CD1	2.56	0.40
16:B:839:CLA:H43	19:B:847:BCR:C11	2.51	0.40
7:I:28:VAL:HB	7:I:29:PRO:HD3	2.02	0.40
16:5:414:CLA:HED2	16:5:415:CLA:HBB2	2.03	0.40
1:A:708:LEU:HD11	16:B:831:CLA:HHB	2.04	0.40
16:B:812:CLA:C3D	16:B:813:CLA:HMC3	2.52	0.40
16:1:501:CLA:HBB1	16:1:501:CLA:HHC	2.03	0.40
14:5:31:HIS:CG	16:5:414:CLA:HMD1	2.57	0.40
1:A:600:TYR:HB2	1:A:733:LEU:CD2	2.51	0.40
16:A:803:CLA:HMD1	2:B:540:ILE:HG12	2.03	0.40
16:A:833:CLA:H62	16:A:833:CLA:H41	1.94	0.40
16:B:806:CLA:HMC2	19:B:844:BCR:H401	2.02	0.40
12:1:64:LEU:HD13	12:1:67:LEU:HD12	2.04	0.40
16:5:413:CLA:HHC	16:5:413:CLA:HBB1	2.04	0.40
2:B:387:MET:HE1	19:B:847:BCR:H361	2.02	0.40
14:4:108:LEU:HD11	16:5:407:CLA:HMA1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	740/752 (98%)	714 (96%)	26 (4%)	0	100	100
2	B	737/741 (100%)	713 (97%)	22 (3%)	2 (0%)	37	57
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	133/139 (96%)	130 (98%)	3 (2%)	0	100	100
5	E	59/70 (84%)	59 (100%)	0	0	100	100
6	F	139/164 (85%)	137 (99%)	1 (1%)	1 (1%)	19	36
7	I	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
8	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
10	M	28/40 (70%)	28 (100%)	0	0	100	100
11	X	27/44 (61%)	26 (96%)	1 (4%)	0	100	100
12	1	464/476 (98%)	446 (96%)	18 (4%)	0	100	100
14	4	327/344 (95%)	290 (89%)	26 (8%)	11 (3%)	3	4
14	5	330/344 (96%)	289 (88%)	31 (9%)	10 (3%)	3	5
All	All	3132/3290 (95%)	2976 (95%)	132 (4%)	24 (1%)	19	32

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	481	LEU
14	4	274	ALA
14	5	274	ALA
6	F	26	ALA
14	4	24	SER
14	5	24	SER
2	B	494	PRO

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Mol	Chain	Res	Type
14	4	22	ASN
14	4	83	VAL
14	4	127	LYS
14	4	290	VAL
14	4	291	LYS
14	4	297	TYR
14	5	127	LYS
14	5	291	LYS
14	4	57	ILE
14	5	22	ASN
14	5	57	ILE
14	5	83	VAL
14	5	290	VAL
14	5	297	TYR
14	5	273	GLY
14	4	273	GLY
14	4	268	PRO

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	595/605 (98%)	593 (100%)	2 (0%)	91	97
2	B	601/602 (100%)	600 (100%)	1 (0%)	92	98
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	108/110 (98%)	108 (100%)	0	100	100
5	E	54/60 (90%)	54 (100%)	0	100	100
6	F	110/129 (85%)	110 (100%)	0	100	100
7	I	28/39 (72%)	28 (100%)	0	100	100
8	J	38/42 (90%)	38 (100%)	0	100	100
10	M	25/34 (74%)	25 (100%)	0	100	100
11	X	24/34 (71%)	23 (96%)	1 (4%)	25	48
12	1	364/373 (98%)	363 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	4	252/266 (95%)	244 (97%)	8 (3%)	34	59
14	5	256/266 (96%)	252 (98%)	4 (2%)	58	78
All	All	2523/2629 (96%)	2506 (99%)	17 (1%)	80	92

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	372	TYR
2	B	50	HIS
11	X	32	ASN
12	1	336	ASP
14	4	12	ASP
14	4	23	LEU
14	4	24	SER
14	4	69	HIS
14	4	108	LEU
14	4	119	LYS
14	4	136	LYS
14	4	200	LEU
14	5	24	SER
14	5	37	LEU
14	5	58	PRO
14	5	144	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	HIS
1	A	311	GLN
2	B	294	ASN
2	B	619	ASN
4	D	39	GLN
6	F	38	GLN
12	1	269	ASN
14	5	133	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

201 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	$\# Z > 2$
21	LMT	M	101	-	36,36,36	0.47	0	47,47,47	0.67	0
16	CLA	B	822	23	55,63,73	2.22	16 (29%)	64,101,113	2.83	27 (42%)
16	CLA	1	514	-	45,53,73	2.52	17 (37%)	52,89,113	3.22	22 (42%)
19	BCR	B	847	-	41,41,41	1.62	10 (24%)	56,56,56	1.35	7 (12%)
16	CLA	1	512	12	45,53,73	2.44	16 (35%)	52,89,113	3.22	26 (50%)
16	CLA	B	816	-	55,63,73	2.08	14 (25%)	64,101,113	3.12	27 (42%)
16	CLA	5	417	14	45,53,73	2.53	17 (37%)	52,89,113	3.19	24 (46%)
16	CLA	6	404	-	45,53,73	2.55	17 (37%)	52,89,113	3.20	23 (44%)
16	CLA	5	413	14	45,53,73	2.52	17 (37%)	52,89,113	3.20	23 (44%)
16	CLA	B	836	23	45,53,73	2.44	16 (35%)	52,89,113	3.16	24 (46%)
19	BCR	1	518	-	41,41,41	1.72	8 (19%)	56,56,56	1.49	10 (17%)
16	CLA	4	402	-	45,53,73	2.51	17 (37%)	52,89,113	3.27	23 (44%)
16	CLA	B	839	-	65,73,73	1.92	18 (27%)	76,113,113	2.83	27 (35%)
16	CLA	1	513	-	45,53,73	2.48	16 (35%)	52,89,113	3.11	23 (44%)
19	BCR	I	101	-	41,41,41	1.64	9 (21%)	56,56,56	1.42	9 (16%)
16	CLA	A	840	-	65,73,73	1.88	18 (27%)	76,113,113	2.86	24 (31%)
16	CLA	6	405	-	45,53,73	2.55	17 (37%)	52,89,113	3.15	25 (48%)
16	CLA	B	818	-	65,73,73	1.86	14 (21%)	76,113,113	2.87	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	2	402	-	45,53,73	2.55	17 (37%)	52,89,113	3.15	22 (42%)
16	CLA	B	837	-	60,68,73	2.01	16 (26%)	70,107,113	2.79	26 (37%)
16	CLA	A	819	-	54,62,73	2.13	16 (29%)	62,99,113	2.94	25 (40%)
16	CLA	B	828	-	65,73,73	1.90	15 (23%)	76,113,113	2.59	25 (32%)
16	CLA	B	813	-	65,73,73	1.90	15 (23%)	76,113,113	2.83	23 (30%)
19	BCR	J	103	-	41,41,41	1.60	8 (19%)	56,56,56	1.31	7 (12%)
16	CLA	B	817	-	59,67,73	2.02	16 (27%)	68,105,113	2.91	27 (39%)
16	CLA	K	101	-	42,49,73	2.31	15 (35%)	48,83,113	3.12	21 (43%)
16	CLA	A	807	-	65,73,73	1.93	16 (24%)	76,113,113	2.77	25 (32%)
19	BCR	A	847	-	41,41,41	1.64	8 (19%)	56,56,56	1.27	7 (12%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
16	CLA	B	832	-	65,73,73	1.87	15 (23%)	76,113,113	2.93	24 (31%)
16	CLA	B	823	-	65,73,73	1.97	15 (23%)	76,113,113	2.85	33 (43%)
19	BCR	K	102	-	41,41,41	1.65	8 (19%)	56,56,56	1.38	9 (16%)
19	BCR	F	205	-	41,41,41	1.65	8 (19%)	56,56,56	1.32	8 (14%)
16	CLA	A	817	23	49,57,73	2.33	16 (32%)	55,93,113	3.07	24 (43%)
16	CLA	A	821	-	50,58,73	2.25	17 (34%)	58,95,113	3.11	25 (43%)
19	BCR	M	102	-	41,41,41	1.65	8 (19%)	56,56,56	1.35	8 (14%)
16	CLA	6	409	13	45,53,73	2.55	17 (37%)	52,89,113	3.17	23 (44%)
20	LHG	A	853	16	26,26,48	0.32	0	29,32,54	0.48	0
16	CLA	J	102	-	45,53,73	2.43	16 (35%)	52,89,113	3.18	24 (46%)
16	CLA	K	103	23	45,53,73	2.39	17 (37%)	52,89,113	3.23	24 (46%)
16	CLA	1	515	12	45,53,73	2.56	16 (35%)	52,89,113	3.18	23 (44%)
16	CLA	J	101	8	45,53,73	2.39	16 (35%)	52,89,113	3.13	24 (46%)
16	CLA	B	802	23	65,73,73	1.93	18 (27%)	76,113,113	2.85	30 (39%)
16	CLA	1	519	12	65,73,73	2.08	14 (21%)	76,113,113	2.69	26 (34%)
19	BCR	A	849	-	41,41,41	1.66	7 (17%)	56,56,56	1.58	11 (19%)
16	CLA	B	805	-	65,73,73	1.93	15 (23%)	76,113,113	2.83	29 (38%)
16	CLA	A	830	-	65,73,73	1.93	15 (23%)	76,113,113	2.61	21 (27%)
16	CLA	A	828	-	65,73,73	1.91	17 (26%)	76,113,113	2.78	25 (32%)
16	CLA	B	827	-	65,73,73	1.94	16 (24%)	76,113,113	2.97	28 (36%)
16	CLA	2	403	-	45,53,73	2.54	17 (37%)	52,89,113	3.16	23 (44%)
16	CLA	5	407	-	45,53,73	2.51	16 (35%)	52,89,113	3.16	24 (46%)
16	CLA	A	806	-	65,73,73	1.89	16 (24%)	76,113,113	2.87	28 (36%)
16	CLA	5	411	-	45,53,73	2.45	16 (35%)	52,89,113	3.08	23 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMT	1	524	-	36,36,36	0.53	1 (2%)	47,47,47	0.64	1 (2%)
19	BCR	B	848	-	41,41,41	1.65	11 (26%)	56,56,56	1.36	9 (16%)
20	LHG	B	850	-	48,48,48	0.27	0	51,54,54	0.33	0
16	CLA	B	819	23	65,73,73	2.02	15 (23%)	76,113,113	2.69	29 (38%)
16	CLA	6	403	-	45,53,73	2.52	17 (37%)	52,89,113	3.14	24 (46%)
16	CLA	A	843	23	65,73,73	1.97	16 (24%)	76,113,113	2.79	27 (35%)
16	CLA	4	409	-	45,53,73	2.53	17 (37%)	52,89,113	3.25	22 (42%)
16	CLA	5	421	-	45,53,73	2.53	17 (37%)	52,89,113	3.15	25 (48%)
16	CLA	4	410	14	45,53,73	2.56	17 (37%)	52,89,113	3.19	22 (42%)
16	CLA	A	815	-	45,53,73	2.36	18 (40%)	52,89,113	3.15	24 (46%)
16	CLA	A	810	1	65,73,73	1.98	17 (26%)	76,113,113	2.71	26 (34%)
16	CLA	B	830	-	65,73,73	1.96	16 (24%)	76,113,113	2.59	27 (35%)
16	CLA	6	401	-	45,53,73	2.56	17 (37%)	52,89,113	3.16	23 (44%)
16	CLA	5	405	-	45,53,73	2.52	17 (37%)	52,89,113	3.30	23 (44%)
16	CLA	1	508	-	45,53,73	2.43	17 (37%)	52,89,113	3.12	25 (48%)
16	CLA	A	805	16	54,62,73	2.15	14 (25%)	62,99,113	3.02	29 (46%)
16	CLA	1	511	-	51,59,73	2.32	16 (31%)	59,96,113	3.03	27 (45%)
16	CLA	5	412	-	45,53,73	2.52	16 (35%)	52,89,113	3.19	24 (46%)
21	LMT	5	401	-	36,36,36	0.43	0	47,47,47	0.75	1 (2%)
16	CLA	A	836	-	51,59,73	2.17	17 (33%)	59,96,113	3.00	26 (44%)
16	CLA	B	840	23	65,73,73	1.93	16 (24%)	76,113,113	2.63	24 (31%)
16	CLA	A	834	-	65,73,73	1.87	14 (21%)	76,113,113	2.69	29 (38%)
19	BCR	A	846	-	41,41,41	1.62	9 (21%)	56,56,56	1.35	10 (17%)
19	BCR	J	104	-	41,41,41	1.58	9 (21%)	56,56,56	1.38	9 (16%)
20	LHG	A	852	-	48,48,48	0.30	0	51,54,54	0.50	0
16	CLA	4	404	-	45,53,73	2.57	17 (37%)	52,89,113	3.17	23 (44%)
16	CLA	5	409	-	45,53,73	2.45	17 (37%)	52,89,113	3.27	22 (42%)
16	CLA	1	501	20	45,53,73	2.34	16 (35%)	52,89,113	3.12	26 (50%)
16	CLA	5	414	-	45,53,73	2.44	17 (37%)	52,89,113	3.06	22 (42%)
16	CLA	A	820	-	65,73,73	1.91	16 (24%)	76,113,113	2.85	28 (36%)
16	CLA	6	408	-	41,49,73	2.59	16 (39%)	47,84,113	3.34	22 (46%)
17	PQN	B	842	-	34,34,34	1.66	2 (5%)	42,45,45	0.83	1 (2%)
16	CLA	B	807	-	65,73,73	1.94	16 (24%)	76,113,113	2.66	25 (32%)
19	BCR	A	848	-	41,41,41	1.65	10 (24%)	56,56,56	1.34	9 (16%)
17	PQN	A	844	-	34,34,34	1.56	2 (5%)	42,45,45	1.12	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	SF4	A	845	1,2	0,12,12	-	-	-		
16	CLA	A	804	-	65,73,73	1.89	15 (23%)	76,113,113	2.78	27 (35%)
16	CLA	X	101	11	45,53,73	2.37	18 (40%)	52,89,113	3.12	22 (42%)
16	CLA	A	813	-	54,62,73	2.15	17 (31%)	62,99,113	2.98	27 (43%)
16	CLA	5	406	-	45,53,73	2.54	17 (37%)	52,89,113	3.21	24 (46%)
16	CLA	5	415	-	45,53,73	2.53	17 (37%)	52,89,113	3.36	22 (42%)
16	CLA	A	809	1	65,73,73	2.02	15 (23%)	76,113,113	2.75	31 (40%)
16	CLA	1	507	-	45,53,73	2.55	16 (35%)	52,89,113	3.20	22 (42%)
16	CLA	A	814	-	65,73,73	1.95	16 (24%)	76,113,113	2.67	25 (32%)
16	CLA	A	842	-	65,73,73	1.96	17 (26%)	76,113,113	2.77	24 (31%)
16	CLA	3	401	-	45,53,73	2.55	17 (37%)	52,89,113	3.17	22 (42%)
16	CLA	1	505	-	45,53,73	2.52	17 (37%)	52,89,113	3.19	23 (44%)
16	CLA	A	802	23	65,73,73	1.85	16 (24%)	76,113,113	2.81	28 (36%)
16	CLA	2	405	-	45,53,73	2.55	16 (35%)	52,89,113	3.15	23 (44%)
16	CLA	B	806	-	65,73,73	1.90	16 (24%)	76,113,113	2.71	27 (35%)
16	CLA	4	408	14	45,53,73	2.52	17 (37%)	52,89,113	3.14	22 (42%)
19	BCR	B	844	-	41,41,41	1.67	9 (21%)	56,56,56	1.33	8 (14%)
16	CLA	B	812	-	45,53,73	2.36	16 (35%)	52,89,113	3.27	27 (51%)
16	CLA	A	832	-	50,58,73	2.11	15 (30%)	58,95,113	3.14	28 (48%)
16	CLA	2	404	-	45,53,73	2.53	17 (37%)	52,89,113	3.19	22 (42%)
16	CLA	A	826	23	65,73,73	2.00	18 (27%)	76,113,113	2.64	30 (39%)
16	CLA	5	408	-	45,53,73	2.56	17 (37%)	52,89,113	3.31	22 (42%)
16	CLA	A	823	-	49,57,73	2.20	16 (32%)	55,93,113	3.38	25 (45%)
16	CLA	A	808	-	51,59,73	2.22	15 (29%)	59,96,113	3.09	25 (42%)
16	CLA	4	407	14	45,53,73	2.54	16 (35%)	52,89,113	3.25	25 (48%)
19	BCR	B	843	-	41,41,41	1.64	8 (19%)	56,56,56	1.35	8 (14%)
16	CLA	5	403	-	45,53,73	2.51	16 (35%)	52,89,113	3.28	21 (40%)
19	BCR	5	402	-	41,41,41	1.67	8 (19%)	56,56,56	1.41	8 (14%)
21	LMT	B	851	-	36,36,36	0.51	1 (2%)	47,47,47	0.69	1 (2%)
19	BCR	A	850	-	41,41,41	1.61	12 (29%)	56,56,56	1.30	7 (12%)
19	BCR	F	202	-	41,41,41	1.63	10 (24%)	56,56,56	1.32	8 (14%)
16	CLA	B	810	-	65,73,73	1.92	16 (24%)	76,113,113	2.85	25 (32%)
19	BCR	4	401	-	41,41,41	1.67	8 (19%)	56,56,56	1.48	9 (16%)
16	CLA	A	811	-	45,53,73	2.29	16 (35%)	52,89,113	3.20	26 (50%)
16	CLA	A	829	-	65,73,73	1.91	15 (23%)	76,113,113	2.82	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	824	-	51,59,73	2.22	16 (31%)	59,96,113	3.14	25 (42%)
16	CLA	F	204	23	45,53,73	2.38	16 (35%)	52,89,113	3.19	23 (44%)
16	CLA	5	419	-	45,53,73	2.50	17 (37%)	52,89,113	3.21	22 (42%)
16	CLA	1	502	-	45,53,73	2.50	16 (35%)	52,89,113	3.28	22 (42%)
21	LMT	B	852	-	36,36,36	0.49	0	47,47,47	0.94	3 (6%)
16	CLA	6	406	-	45,53,73	2.55	17 (37%)	52,89,113	3.14	23 (44%)
16	CLA	6	407	-	45,53,73	2.55	17 (37%)	52,89,113	3.18	22 (42%)
16	CLA	B	808	-	65,73,73	1.86	16 (24%)	76,113,113	2.92	29 (38%)
16	CLA	5	404	-	45,53,73	2.42	17 (37%)	52,89,113	3.15	20 (38%)
16	CLA	A	833	-	65,73,73	2.05	18 (27%)	76,113,113	2.78	29 (38%)
16	CLA	B	824	2	65,73,73	1.91	16 (24%)	76,113,113	2.78	28 (36%)
16	CLA	A	827	23	55,63,73	2.12	15 (27%)	64,101,113	2.93	23 (35%)
16	CLA	1	520	-	65,73,73	1.94	14 (21%)	76,113,113	2.80	27 (35%)
16	CLA	1	521	23	52,60,73	2.31	16 (30%)	60,97,113	3.01	25 (41%)
16	CLA	1	510	-	45,53,73	2.48	16 (35%)	52,89,113	3.13	24 (46%)
16	CLA	5	410	-	45,53,73	2.49	17 (37%)	52,89,113	3.19	23 (44%)
19	BCR	B	845	-	41,41,41	1.60	8 (19%)	56,56,56	1.36	8 (14%)
16	CLA	F	201	23	51,59,73	2.15	16 (31%)	59,96,113	2.85	24 (40%)
16	CLA	A	825	-	47,55,73	2.29	18 (38%)	54,91,113	3.17	21 (38%)
16	CLA	B	815	-	45,53,73	2.37	14 (31%)	52,89,113	3.22	25 (48%)
19	BCR	B	846	-	41,41,41	1.58	10 (24%)	56,56,56	1.32	7 (12%)
16	CLA	A	831	-	65,73,73	1.93	16 (24%)	76,113,113	2.86	23 (30%)
16	CLA	1	504	-	45,53,73	2.44	17 (37%)	52,89,113	3.43	23 (44%)
16	CLA	A	822	23	65,73,73	1.97	15 (23%)	76,113,113	2.65	26 (34%)
16	CLA	5	422	-	45,53,73	2.54	16 (35%)	52,89,113	3.17	23 (44%)
16	CLA	A	835	-	65,73,73	1.88	14 (21%)	76,113,113	2.81	28 (36%)
16	CLA	A	816	-	45,53,73	2.36	14 (31%)	52,89,113	3.18	25 (48%)
16	CLA	6	402	-	45,53,73	2.54	17 (37%)	52,89,113	3.16	23 (44%)
19	BCR	A	851	-	41,41,41	1.69	8 (19%)	56,56,56	1.40	10 (17%)
16	CLA	5	418	-	45,53,73	2.54	17 (37%)	52,89,113	3.14	24 (46%)
19	BCR	5	420	-	41,41,41	1.71	8 (19%)	56,56,56	1.33	9 (16%)
16	CLA	1	506	-	45,53,73	2.47	16 (35%)	52,89,113	3.17	23 (44%)
19	BCR	1	517	-	41,41,41	1.74	8 (19%)	56,56,56	1.53	9 (16%)
16	CLA	B	804	2	54,62,73	2.18	16 (29%)	62,99,113	2.91	30 (48%)
16	CLA	A	839	-	65,73,73	1.92	16 (24%)	76,113,113	2.85	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	803	-	65,73,73	1.91	15 (23%)	76,113,113	2.55	28 (36%)
22	LMG	B	849	-	55,55,55	0.24	0	63,63,63	0.39	0
16	CLA	4	403	-	45,53,73	2.52	16 (35%)	52,89,113	3.28	22 (42%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
16	CLA	B	809	2	65,73,73	1.84	15 (23%)	76,113,113	2.69	27 (35%)
16	CLA	4	406	-	45,53,73	2.47	16 (35%)	52,89,113	3.15	21 (40%)
16	CLA	B	835	23	45,53,73	2.33	17 (37%)	52,89,113	3.16	20 (38%)
15	CL0	A	801	-	65,73,73	1.97	18 (27%)	76,113,113	2.85	30 (39%)
16	CLA	1	526	-	45,53,73	2.53	17 (37%)	52,89,113	3.20	23 (44%)
16	CLA	4	411	-	45,53,73	2.55	17 (37%)	52,89,113	3.20	23 (44%)
19	BCR	1	523	-	41,41,41	1.61	10 (24%)	56,56,56	1.35	8 (14%)
16	CLA	A	837	1	45,53,73	2.38	17 (37%)	52,89,113	3.24	24 (46%)
16	CLA	2	401	-	45,53,73	2.54	16 (35%)	52,89,113	3.24	21 (40%)
16	CLA	2	406	-	45,53,73	2.53	17 (37%)	52,89,113	3.17	21 (40%)
19	BCR	I	102	-	41,41,41	1.69	7 (17%)	56,56,56	1.68	12 (21%)
19	BCR	1	516	-	41,41,41	1.66	7 (17%)	56,56,56	1.53	10 (17%)
16	CLA	4	405	-	45,53,73	2.55	17 (37%)	52,89,113	3.24	25 (48%)
16	CLA	1	509	-	45,53,73	2.37	15 (33%)	52,89,113	3.24	24 (46%)
20	LHG	F	203	-	48,48,48	0.27	0	51,54,54	0.37	0
16	CLA	B	829	-	65,73,73	1.90	17 (26%)	76,113,113	2.81	28 (36%)
16	CLA	B	826	-	65,73,73	1.92	16 (24%)	76,113,113	2.82	23 (30%)
16	CLA	5	416	-	41,49,73	2.57	17 (41%)	47,84,113	3.37	23 (48%)
16	CLA	B	838	-	65,73,73	1.88	15 (23%)	76,113,113	2.70	27 (35%)
16	CLA	A	803	-	65,73,73	1.96	14 (21%)	76,113,113	2.72	30 (39%)
16	CLA	A	838	-	51,59,73	2.18	17 (33%)	59,96,113	3.10	25 (42%)
16	CLA	1	503	-	51,59,73	2.36	16 (31%)	59,96,113	2.97	27 (45%)
16	CLA	B	834	-	65,73,73	1.93	17 (26%)	76,113,113	2.66	28 (36%)
19	BCR	B	853	-	41,41,41	1.65	9 (21%)	56,56,56	1.29	7 (12%)
16	CLA	A	812	16	65,73,73	1.87	16 (24%)	76,113,113	2.77	29 (38%)
16	CLA	B	821	-	45,53,73	2.44	15 (33%)	52,89,113	3.17	25 (48%)
16	CLA	B	801	-	65,73,73	1.90	16 (24%)	76,113,113	2.89	30 (39%)
21	LMT	A	854	-	36,36,36	0.42	0	47,47,47	0.99	4 (8%)
16	CLA	A	818	-	54,62,73	2.14	15 (27%)	62,99,113	3.15	22 (35%)
16	CLA	B	833	-	58,66,73	2.02	17 (29%)	67,104,113	2.90	27 (40%)
16	CLA	A	841	-	65,73,73	1.95	17 (26%)	76,113,113	2.80	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	820	-	47,55,73	2.35	16 (34%)	54,91,113	3.23	27 (50%)
16	CLA	B	814	-	56,64,73	2.12	16 (28%)	65,102,113	2.99	25 (38%)
16	CLA	B	841	-	65,73,73	1.90	18 (27%)	76,113,113	2.86	23 (30%)
16	CLA	B	831	-	65,73,73	2.03	17 (26%)	76,113,113	2.77	29 (38%)
16	CLA	1	525	-	45,53,73	2.52	16 (35%)	52,89,113	3.13	24 (46%)
19	BCR	1	522	-	41,41,41	1.64	9 (21%)	56,56,56	1.23	9 (16%)
16	CLA	B	811	-	65,73,73	1.93	15 (23%)	76,113,113	2.68	25 (32%)
16	CLA	B	825	23	65,73,73	2.00	15 (23%)	76,113,113	2.81	33 (43%)

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
21	LMT	M	101	-	-	4/21/61/61	0/2/2/2
16	CLA	B	822	23	1/1/13/20	10/25/103/115	-
16	CLA	1	514	-	1/1/11/20	5/13/91/115	-
19	BCR	B	847	-	-	7/29/63/63	0/2/2/2
16	CLA	1	512	12	1/1/11/20	5/13/91/115	-
16	CLA	B	816	-	-	6/25/103/115	-
16	CLA	5	417	14	1/1/11/20	6/13/91/115	-
16	CLA	6	404	-	1/1/11/20	5/13/91/115	-
16	CLA	5	413	14	1/1/11/20	4/13/91/115	-
16	CLA	B	836	23	1/1/11/20	4/13/91/115	-
19	BCR	1	518	-	-	6/29/63/63	0/2/2/2
16	CLA	4	402	-	1/1/11/20	6/13/91/115	-
16	CLA	B	839	-	1/1/15/20	9/37/115/115	-
16	CLA	1	513	-	1/1/11/20	2/13/91/115	-
19	BCR	I	101	-	-	1/29/63/63	0/2/2/2
16	CLA	A	840	-	1/1/15/20	11/37/115/115	-
16	CLA	6	405	-	1/1/11/20	5/13/91/115	-
16	CLA	B	818	-	1/1/15/20	12/37/115/115	-
16	CLA	2	402	-	1/1/11/20	5/13/91/115	-
16	CLA	B	837	-	1/1/14/20	7/31/109/115	-
16	CLA	A	819	-	1/1/12/20	6/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	828	-	1/1/15/20	10/37/115/115	-
16	CLA	B	813	-	1/1/15/20	9/37/115/115	-
19	BCR	J	103	-	-	8/29/63/63	0/2/2/2
16	CLA	B	817	-	1/1/13/20	5/30/108/115	-
16	CLA	K	101	-	1/1/9/20	3/7/81/115	-
16	CLA	A	807	-	1/1/15/20	9/37/115/115	-
19	BCR	A	847	-	-	5/29/63/63	0/2/2/2
18	SF4	C	101	3	-	-	0/6/5/5
16	CLA	B	832	-	1/1/15/20	9/37/115/115	-
16	CLA	B	823	-	1/1/15/20	8/37/115/115	-
19	BCR	K	102	-	-	12/29/63/63	0/2/2/2
19	BCR	F	205	-	-	2/29/63/63	0/2/2/2
16	CLA	A	817	23	-	4/18/96/115	-
16	CLA	A	821	-	-	7/19/97/115	-
19	BCR	M	102	-	-	10/29/63/63	0/2/2/2
16	CLA	6	409	13	1/1/11/20	5/13/91/115	-
20	LHG	A	853	16	-	8/31/31/53	-
16	CLA	J	102	-	1/1/11/20	5/13/91/115	-
16	CLA	K	103	23	1/1/11/20	3/13/91/115	-
16	CLA	1	515	12	1/1/11/20	5/13/91/115	-
16	CLA	J	101	8	1/1/11/20	8/13/91/115	-
16	CLA	B	802	23	1/1/15/20	8/37/115/115	-
16	CLA	1	519	12	-	11/37/115/115	-
19	BCR	A	849	-	-	16/29/63/63	0/2/2/2
16	CLA	B	805	-	1/1/15/20	11/37/115/115	-
16	CLA	A	830	-	1/1/15/20	9/37/115/115	-
16	CLA	A	828	-	1/1/15/20	6/37/115/115	-
16	CLA	B	827	-	1/1/15/20	11/37/115/115	-
16	CLA	2	403	-	1/1/11/20	2/13/91/115	-
16	CLA	5	407	-	1/1/11/20	3/13/91/115	-
16	CLA	A	806	-	1/1/15/20	13/37/115/115	-
16	CLA	5	411	-	1/1/11/20	5/13/91/115	-
21	LMT	1	524	-	-	7/21/61/61	0/2/2/2
19	BCR	B	848	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	B	850	-	-	15/53/53/53	-
16	CLA	B	819	23	1/1/15/20	10/37/115/115	-
16	CLA	6	403	-	1/1/11/20	4/13/91/115	-
16	CLA	A	843	23	1/1/15/20	10/37/115/115	-
16	CLA	4	409	-	1/1/11/20	3/13/91/115	-
16	CLA	5	421	-	1/1/11/20	7/13/91/115	-
16	CLA	4	410	14	1/1/11/20	5/13/91/115	-
16	CLA	A	815	-	1/1/11/20	2/13/91/115	-
16	CLA	6	401	-	1/1/11/20	6/13/91/115	-
16	CLA	B	830	-	1/1/15/20	11/37/115/115	-
16	CLA	A	810	1	-	12/37/115/115	-
16	CLA	5	405	-	1/1/11/20	2/13/91/115	-
16	CLA	1	508	-	1/1/11/20	6/13/91/115	-
16	CLA	A	805	16	1/1/12/20	8/24/102/115	-
16	CLA	1	511	-	1/1/12/20	7/21/99/115	-
16	CLA	5	412	-	1/1/11/20	5/13/91/115	-
21	LMT	5	401	-	-	3/21/61/61	0/2/2/2
16	CLA	A	836	-	1/1/12/20	5/21/99/115	-
16	CLA	B	840	23	1/1/15/20	11/37/115/115	-
16	CLA	A	834	-	1/1/15/20	7/37/115/115	-
19	BCR	A	846	-	-	9/29/63/63	0/2/2/2
19	BCR	J	104	-	-	11/29/63/63	0/2/2/2
20	LHG	A	852	-	-	21/53/53/53	-
16	CLA	4	404	-	1/1/11/20	1/13/91/115	-
16	CLA	5	409	-	1/1/11/20	6/13/91/115	-
16	CLA	1	501	20	1/1/11/20	5/13/91/115	-
16	CLA	5	414	-	1/1/11/20	7/13/91/115	-
16	CLA	A	820	-	1/1/15/20	14/37/115/115	-
16	CLA	6	408	-	1/1/10/20	2/8/86/115	-
17	PQN	B	842	-	-	2/23/43/43	0/2/2/2
16	CLA	B	807	-	1/1/15/20	5/37/115/115	-
19	BCR	A	848	-	-	3/29/63/63	0/2/2/2
17	PQN	A	844	-	-	3/23/43/43	0/2/2/2
18	SF4	A	845	1,2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	804	-	1/1/15/20	11/37/115/115	-
16	CLA	X	101	11	1/1/11/20	7/13/91/115	-
16	CLA	A	813	-	1/1/12/20	11/24/102/115	-
16	CLA	5	406	-	1/1/11/20	5/13/91/115	-
16	CLA	5	415	-	1/1/11/20	5/13/91/115	-
16	CLA	A	809	1	1/1/15/20	11/37/115/115	-
16	CLA	1	507	-	1/1/11/20	6/13/91/115	-
16	CLA	A	814	-	1/1/15/20	15/37/115/115	-
16	CLA	A	842	-	1/1/15/20	8/37/115/115	-
16	CLA	3	401	-	1/1/11/20	5/13/91/115	-
16	CLA	1	505	-	1/1/11/20	3/13/91/115	-
16	CLA	A	802	23	1/1/15/20	3/37/115/115	-
16	CLA	2	405	-	1/1/11/20	5/13/91/115	-
16	CLA	B	806	-	1/1/15/20	11/37/115/115	-
16	CLA	4	408	14	1/1/11/20	4/13/91/115	-
19	BCR	B	844	-	-	6/29/63/63	0/2/2/2
16	CLA	B	812	-	1/1/11/20	0/13/91/115	-
16	CLA	A	832	-	-	3/19/97/115	-
16	CLA	2	404	-	1/1/11/20	5/13/91/115	-
16	CLA	A	826	23	1/1/15/20	11/37/115/115	-
16	CLA	5	408	-	1/1/11/20	4/13/91/115	-
16	CLA	A	823	-	-	10/18/96/115	-
16	CLA	A	808	-	1/1/12/20	4/21/99/115	-
16	CLA	4	407	14	1/1/11/20	5/13/91/115	-
19	BCR	B	843	-	-	8/29/63/63	0/2/2/2
16	CLA	5	403	-	1/1/11/20	6/13/91/115	-
19	BCR	5	402	-	-	4/29/63/63	0/2/2/2
21	LMT	B	851	-	-	6/21/61/61	0/2/2/2
19	BCR	A	850	-	-	6/29/63/63	0/2/2/2
19	BCR	F	202	-	-	4/29/63/63	0/2/2/2
16	CLA	B	810	-	1/1/15/20	10/37/115/115	-
19	BCR	4	401	-	-	19/29/63/63	0/2/2/2
16	CLA	A	811	-	1/1/11/20	2/13/91/115	-
16	CLA	A	829	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	824	-	-	7/21/99/115	-
16	CLA	F	204	23	1/1/11/20	0/13/91/115	-
16	CLA	5	419	-	1/1/11/20	5/13/91/115	-
16	CLA	1	502	-	1/1/11/20	6/13/91/115	-
21	LMT	B	852	-	-	5/21/61/61	0/2/2/2
16	CLA	6	406	-	1/1/11/20	2/13/91/115	-
16	CLA	6	407	-	1/1/11/20	5/13/91/115	-
16	CLA	B	808	-	1/1/15/20	10/37/115/115	-
16	CLA	5	404	-	1/1/11/20	4/13/91/115	-
16	CLA	A	833	-	1/1/15/20	10/37/115/115	-
16	CLA	B	824	2	1/1/15/20	10/37/115/115	-
16	CLA	A	827	23	1/1/13/20	5/25/103/115	-
16	CLA	1	521	23	1/1/12/20	6/22/100/115	-
16	CLA	5	410	-	1/1/11/20	2/13/91/115	-
16	CLA	1	510	-	1/1/11/20	5/13/91/115	-
16	CLA	1	520	-	-	9/37/115/115	-
19	BCR	B	845	-	-	9/29/63/63	0/2/2/2
16	CLA	F	201	23	1/1/12/20	8/21/99/115	-
16	CLA	A	825	-	-	7/16/94/115	-
16	CLA	B	815	-	-	4/13/91/115	-
19	BCR	B	846	-	-	6/29/63/63	0/2/2/2
16	CLA	A	831	-	1/1/15/20	5/37/115/115	-
16	CLA	1	504	-	-	5/13/91/115	-
16	CLA	A	822	23	1/1/15/20	10/37/115/115	-
16	CLA	5	422	-	1/1/11/20	6/13/91/115	-
16	CLA	A	835	-	1/1/15/20	11/37/115/115	-
16	CLA	A	816	-	1/1/11/20	3/13/91/115	-
16	CLA	6	402	-	1/1/11/20	6/13/91/115	-
19	BCR	A	851	-	-	9/29/63/63	0/2/2/2
16	CLA	5	418	-	1/1/11/20	6/13/91/115	-
19	BCR	5	420	-	-	9/29/63/63	0/2/2/2
16	CLA	1	506	-	1/1/11/20	6/13/91/115	-
19	BCR	1	517	-	-	12/29/63/63	0/2/2/2
16	CLA	B	804	2	1/1/12/20	6/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	839	-	1/1/15/20	10/37/115/115	-
16	CLA	B	803	-	1/1/15/20	8/37/115/115	-
22	LMG	B	849	-	-	16/50/70/70	0/1/1/1
16	CLA	4	403	-	1/1/11/20	5/13/91/115	-
18	SF4	C	102	3	-	-	0/6/5/5
16	CLA	B	809	2	1/1/15/20	10/37/115/115	-
16	CLA	4	406	-	1/1/11/20	6/13/91/115	-
16	CLA	B	835	23	1/1/11/20	6/13/91/115	-
15	CL0	A	801	-	2/2/20/25	2/37/135/135	-
16	CLA	1	526	-	1/1/11/20	6/13/91/115	-
16	CLA	4	411	-	1/1/11/20	7/13/91/115	-
19	BCR	1	523	-	-	5/29/63/63	0/2/2/2
16	CLA	A	837	1	1/1/11/20	7/13/91/115	-
16	CLA	2	401	-	1/1/11/20	5/13/91/115	-
16	CLA	2	406	-	1/1/11/20	7/13/91/115	-
19	BCR	I	102	-	-	7/29/63/63	0/2/2/2
19	BCR	1	516	-	-	11/29/63/63	0/2/2/2
16	CLA	4	405	-	1/1/11/20	2/13/91/115	-
16	CLA	1	509	-	1/1/11/20	5/13/91/115	-
20	LHG	F	203	-	-	20/53/53/53	-
16	CLA	B	829	-	1/1/15/20	19/37/115/115	-
16	CLA	B	826	-	1/1/15/20	10/37/115/115	-
16	CLA	5	416	-	1/1/10/20	4/8/86/115	-
16	CLA	B	838	-	1/1/15/20	8/37/115/115	-
16	CLA	A	803	-	1/1/15/20	11/37/115/115	-
16	CLA	A	838	-	1/1/12/20	7/21/99/115	-
16	CLA	1	503	-	1/1/12/20	7/21/99/115	-
16	CLA	B	834	-	1/1/15/20	7/37/115/115	-
19	BCR	B	853	-	-	6/29/63/63	0/2/2/2
16	CLA	A	812	16	1/1/15/20	7/37/115/115	-
16	CLA	B	821	-	-	3/13/91/115	-
16	CLA	B	801	-	1/1/15/20	11/37/115/115	-
21	LMT	A	854	-	-	6/21/61/61	0/2/2/2
16	CLA	A	818	-	-	1/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	833	-	1/1/13/20	10/29/107/115	-
16	CLA	A	841	-	1/1/15/20	8/37/115/115	-
16	CLA	1	525	-	1/1/11/20	8/13/91/115	-
16	CLA	B	814	-	1/1/13/20	9/27/105/115	-
16	CLA	B	820	-	-	5/16/94/115	-
16	CLA	B	831	-	1/1/15/20	7/37/115/115	-
16	CLA	B	841	-	-	8/37/115/115	-
19	BCR	1	522	-	-	4/29/63/63	0/2/2/2
16	CLA	B	811	-	1/1/15/20	5/37/115/115	-
16	CLA	B	825	23	1/1/15/20	14/37/115/115	-

All (2785) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	842	PQN	C3-C2	7.90	1.49	1.35
17	A	844	PQN	C3-C2	7.37	1.48	1.35
16	B	822	CLA	C3B-C2B	6.39	1.49	1.40
16	A	837	CLA	C3B-C2B	6.33	1.49	1.40
16	A	826	CLA	C3B-C2B	6.27	1.49	1.40
15	A	801	CL0	C3B-C2B	6.26	1.49	1.40
16	A	809	CLA	C3B-C2B	6.25	1.49	1.40
16	A	817	CLA	C3B-C2B	6.25	1.49	1.40
16	B	821	CLA	C3B-C2B	6.24	1.49	1.40
16	5	408	CLA	C3B-C2B	6.18	1.49	1.40
16	B	825	CLA	C3B-C2B	6.15	1.48	1.40
16	A	833	CLA	C3B-C2B	6.15	1.48	1.40
16	A	803	CLA	C3B-C2B	6.14	1.48	1.40
16	B	814	CLA	C3B-C2B	6.13	1.48	1.40
16	1	507	CLA	C3B-C2B	6.12	1.48	1.40
16	B	823	CLA	C3B-C2B	6.11	1.48	1.40
16	4	404	CLA	C3B-C2B	6.10	1.48	1.40
16	2	401	CLA	C3B-C2B	6.09	1.48	1.40
16	5	422	CLA	C3B-C2B	6.08	1.48	1.40
16	1	502	CLA	C3B-C2B	6.08	1.48	1.40
16	5	417	CLA	C3B-C2B	6.07	1.48	1.40
16	6	404	CLA	C3B-C2B	6.07	1.48	1.40
16	2	403	CLA	C3B-C2B	6.07	1.48	1.40
16	4	405	CLA	C3B-C2B	6.06	1.48	1.40
16	6	401	CLA	C3B-C2B	6.06	1.48	1.40
16	4	411	CLA	C3B-C2B	6.06	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	6	405	CLA	C3B-C2B	6.06	1.48	1.40
16	5	421	CLA	C3B-C2B	6.05	1.48	1.40
16	3	401	CLA	C3B-C2B	6.05	1.48	1.40
16	2	402	CLA	C3B-C2B	6.05	1.48	1.40
16	2	405	CLA	C3B-C2B	6.04	1.48	1.40
16	4	407	CLA	C3B-C2B	6.02	1.48	1.40
16	4	403	CLA	C3B-C2B	5.98	1.48	1.40
16	B	831	CLA	C3B-C2B	5.98	1.48	1.40
16	5	418	CLA	C3B-C2B	5.98	1.48	1.40
16	6	408	CLA	C3B-C2B	5.96	1.48	1.40
16	4	409	CLA	C3B-C2B	5.96	1.48	1.40
16	5	416	CLA	C3B-C2B	5.95	1.48	1.40
16	1	515	CLA	C3B-C2B	5.94	1.48	1.40
16	A	805	CLA	C3B-C2B	5.94	1.48	1.40
16	6	409	CLA	C3B-C2B	5.94	1.48	1.40
16	6	407	CLA	C3B-C2B	5.94	1.48	1.40
16	4	410	CLA	C3B-C2B	5.93	1.48	1.40
16	2	404	CLA	C3B-C2B	5.93	1.48	1.40
16	1	503	CLA	C3B-C2B	5.92	1.48	1.40
16	6	406	CLA	C3B-C2B	5.92	1.48	1.40
16	1	519	CLA	C3B-C2B	5.92	1.48	1.40
16	5	405	CLA	C3B-C2B	5.92	1.48	1.40
16	5	403	CLA	C3B-C2B	5.89	1.48	1.40
16	1	513	CLA	C3B-C2B	5.88	1.48	1.40
16	A	815	CLA	C3B-C2B	5.88	1.48	1.40
16	5	412	CLA	C3B-C2B	5.87	1.48	1.40
16	4	402	CLA	C3B-C2B	5.87	1.48	1.40
16	1	525	CLA	C3B-C2B	5.87	1.48	1.40
16	1	505	CLA	C3B-C2B	5.86	1.48	1.40
16	5	415	CLA	C3B-C2B	5.86	1.48	1.40
16	6	403	CLA	C3B-C2B	5.83	1.48	1.40
16	5	409	CLA	C3B-C2B	5.80	1.48	1.40
16	2	406	CLA	C3B-C2B	5.79	1.48	1.40
16	5	406	CLA	C3B-C2B	5.77	1.48	1.40
16	1	526	CLA	C3B-C2B	5.77	1.48	1.40
16	1	504	CLA	C3B-C2B	5.77	1.48	1.40
16	1	508	CLA	C3B-C2B	5.77	1.48	1.40
16	A	841	CLA	C3B-C2B	5.76	1.48	1.40
16	5	407	CLA	C3B-C2B	5.74	1.48	1.40
16	B	812	CLA	C3B-C2B	5.74	1.48	1.40
16	5	414	CLA	C3B-C2B	5.74	1.48	1.40
16	B	820	CLA	C3B-C2B	5.69	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	506	CLA	C3B-C2B	5.68	1.48	1.40
16	1	510	CLA	C3B-C2B	5.68	1.48	1.40
16	1	514	CLA	C3B-C2B	5.68	1.48	1.40
16	6	402	CLA	C3B-C2B	5.68	1.48	1.40
16	1	521	CLA	CHC-C1C	5.64	1.49	1.35
16	B	805	CLA	C3B-C2B	5.63	1.48	1.40
16	5	419	CLA	C3B-C2B	5.62	1.48	1.40
16	4	408	CLA	C3B-C2B	5.60	1.48	1.40
16	K	103	CLA	C3B-C2B	5.60	1.48	1.40
16	1	519	CLA	C3C-C2C	5.56	1.48	1.36
16	A	831	CLA	C3B-C2B	5.55	1.48	1.40
16	A	813	CLA	C3B-C2B	5.54	1.48	1.40
16	5	407	CLA	C3C-C2C	5.54	1.48	1.36
16	A	822	CLA	CHC-C1C	5.53	1.49	1.35
16	5	404	CLA	C3B-C2B	5.53	1.48	1.40
16	B	836	CLA	C3B-C2B	5.53	1.48	1.40
16	A	827	CLA	CHC-C1C	5.52	1.49	1.35
16	B	802	CLA	C3B-C2B	5.52	1.48	1.40
16	B	827	CLA	C3B-C2B	5.50	1.48	1.40
16	5	413	CLA	C3B-C2B	5.49	1.48	1.40
16	5	404	CLA	O2D-CGD	5.49	1.46	1.33
16	5	410	CLA	C3C-C2C	5.48	1.48	1.36
16	A	818	CLA	CHC-C1C	5.47	1.49	1.35
16	5	408	CLA	O2D-CGD	5.46	1.46	1.33
16	1	503	CLA	O2D-CGD	5.46	1.46	1.33
16	X	101	CLA	C3B-C2B	5.44	1.47	1.40
16	5	416	CLA	C1D-ND	5.43	1.44	1.37
16	5	419	CLA	O2D-CGD	5.42	1.46	1.33
16	1	505	CLA	CHC-C1C	5.42	1.48	1.35
16	1	514	CLA	C3C-C2C	5.41	1.48	1.36
16	6	402	CLA	C3C-C2C	5.41	1.48	1.36
16	5	415	CLA	C1D-ND	5.41	1.44	1.37
16	6	407	CLA	C3C-C2C	5.41	1.48	1.36
16	A	824	CLA	C3B-C2B	5.41	1.47	1.40
16	J	102	CLA	C3B-C2B	5.41	1.47	1.40
16	4	408	CLA	C3C-C2C	5.41	1.48	1.36
16	5	411	CLA	CHC-C1C	5.40	1.48	1.35
16	B	804	CLA	C3B-C2B	5.40	1.47	1.40
16	6	405	CLA	C1D-ND	5.40	1.44	1.37
16	5	416	CLA	C3C-C2C	5.40	1.48	1.36
16	4	405	CLA	C1D-ND	5.40	1.44	1.37
16	5	406	CLA	O2D-CGD	5.40	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	405	CLA	C1D-ND	5.40	1.44	1.37
16	5	418	CLA	C1D-ND	5.39	1.44	1.37
16	5	415	CLA	C3C-C2C	5.39	1.48	1.36
16	4	405	CLA	O2D-CGD	5.39	1.46	1.33
16	4	411	CLA	C1D-ND	5.39	1.44	1.37
16	4	408	CLA	O2D-CGD	5.39	1.46	1.33
16	6	406	CLA	C1D-ND	5.38	1.44	1.37
16	1	525	CLA	C3C-C2C	5.38	1.48	1.36
16	5	421	CLA	C3C-C2C	5.38	1.48	1.36
16	5	415	CLA	O2D-CGD	5.38	1.46	1.33
16	1	506	CLA	O2D-CGD	5.38	1.46	1.33
16	6	404	CLA	O2D-CGD	5.38	1.46	1.33
16	2	405	CLA	C3C-C2C	5.38	1.48	1.36
16	B	804	CLA	C3C-C2C	5.38	1.48	1.36
16	4	403	CLA	O2D-CGD	5.37	1.46	1.33
16	B	813	CLA	CHC-C1C	5.37	1.48	1.35
16	5	408	CLA	C1D-ND	5.37	1.44	1.37
16	6	401	CLA	C3C-C2C	5.37	1.48	1.36
16	2	401	CLA	C1D-ND	5.37	1.44	1.37
16	5	407	CLA	O2D-CGD	5.37	1.46	1.33
16	2	405	CLA	O2D-CGD	5.36	1.46	1.33
16	5	422	CLA	C3C-C2C	5.36	1.48	1.36
16	6	409	CLA	O2D-CGD	5.36	1.46	1.33
16	1	520	CLA	CHC-C1C	5.36	1.48	1.35
16	K	101	CLA	C3B-C2B	5.36	1.47	1.40
16	4	409	CLA	CHC-C1C	5.36	1.48	1.35
16	A	809	CLA	CHC-C1C	5.36	1.48	1.35
16	5	403	CLA	C1D-ND	5.36	1.44	1.37
16	2	406	CLA	C1D-ND	5.36	1.44	1.37
16	2	402	CLA	O2D-CGD	5.36	1.46	1.33
16	6	409	CLA	C3C-C2C	5.36	1.48	1.36
16	4	410	CLA	C1D-ND	5.35	1.44	1.37
16	A	816	CLA	C3B-C2B	5.35	1.47	1.40
16	B	819	CLA	CHC-C1C	5.35	1.48	1.35
16	2	402	CLA	C3C-C2C	5.34	1.48	1.36
16	1	515	CLA	C1D-ND	5.34	1.44	1.37
16	B	839	CLA	C3B-C2B	5.34	1.47	1.40
16	2	404	CLA	C1D-ND	5.34	1.44	1.37
16	5	422	CLA	C1D-ND	5.34	1.44	1.37
16	2	402	CLA	C1D-ND	5.34	1.44	1.37
16	4	404	CLA	O2D-CGD	5.34	1.46	1.33
16	F	204	CLA	C3B-C2B	5.34	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	405	CLA	C1D-ND	5.34	1.44	1.37
16	3	401	CLA	C3C-C2C	5.33	1.48	1.36
16	2	406	CLA	C3C-C2C	5.33	1.48	1.36
16	B	810	CLA	C3B-C2B	5.33	1.47	1.40
16	5	413	CLA	CHC-C1C	5.33	1.48	1.35
16	B	824	CLA	CHC-C1C	5.33	1.48	1.35
16	6	403	CLA	C1D-ND	5.33	1.44	1.37
16	1	515	CLA	O2D-CGD	5.33	1.46	1.33
16	1	510	CLA	C1D-ND	5.33	1.44	1.37
16	4	404	CLA	C1D-ND	5.33	1.44	1.37
16	4	403	CLA	C3C-C2C	5.33	1.48	1.36
16	6	404	CLA	C1D-ND	5.33	1.44	1.37
16	X	101	CLA	C3C-C2C	5.33	1.48	1.36
16	3	401	CLA	C1D-ND	5.32	1.44	1.37
16	6	408	CLA	C1D-ND	5.32	1.44	1.37
16	5	410	CLA	O2D-CGD	5.32	1.46	1.33
16	6	401	CLA	O2D-CGD	5.32	1.46	1.33
16	4	404	CLA	C3C-C2C	5.32	1.48	1.36
16	6	405	CLA	O2D-CGD	5.32	1.46	1.33
16	1	512	CLA	O2D-CGD	5.32	1.46	1.33
16	6	406	CLA	O2D-CGD	5.32	1.46	1.33
16	4	407	CLA	C1D-ND	5.32	1.44	1.37
16	A	829	CLA	CHC-C1C	5.32	1.48	1.35
16	A	842	CLA	C3B-C2B	5.32	1.47	1.40
16	5	408	CLA	C3C-C2C	5.31	1.48	1.36
16	1	511	CLA	C3B-C2B	5.31	1.47	1.40
16	A	828	CLA	CHC-C1C	5.31	1.48	1.35
16	1	505	CLA	C3C-C2C	5.31	1.48	1.36
16	6	407	CLA	O2D-CGD	5.31	1.46	1.33
16	6	407	CLA	C1D-ND	5.31	1.44	1.37
16	6	406	CLA	C3C-C2C	5.31	1.48	1.36
16	6	408	CLA	O2D-CGD	5.31	1.46	1.33
16	6	405	CLA	C3C-C2C	5.31	1.48	1.36
16	4	403	CLA	C1D-ND	5.31	1.44	1.37
16	A	825	CLA	O2D-CGD	5.30	1.46	1.33
16	6	409	CLA	C1D-ND	5.30	1.44	1.37
16	2	403	CLA	O2D-CGD	5.30	1.46	1.33
16	5	416	CLA	O2D-CGD	5.30	1.46	1.33
16	A	807	CLA	C3C-C2C	5.30	1.48	1.36
16	6	408	CLA	C3C-C2C	5.30	1.48	1.36
16	5	412	CLA	CHC-C1C	5.30	1.48	1.35
16	B	826	CLA	C3B-C2B	5.30	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	6	402	CLA	C1D-ND	5.30	1.44	1.37
16	4	402	CLA	C1D-ND	5.30	1.44	1.37
16	4	411	CLA	CHC-C1C	5.29	1.48	1.35
16	5	418	CLA	O2D-CGD	5.29	1.46	1.33
16	5	405	CLA	C3C-C2C	5.29	1.48	1.36
16	5	410	CLA	C3B-C2B	5.29	1.47	1.40
16	4	410	CLA	CHC-C1C	5.29	1.48	1.35
16	6	402	CLA	O2D-CGD	5.29	1.46	1.33
16	4	406	CLA	CHC-C1C	5.29	1.48	1.35
16	5	417	CLA	CHC-C1C	5.29	1.48	1.35
16	5	406	CLA	C3C-C2C	5.29	1.48	1.36
16	4	410	CLA	C3C-C2C	5.29	1.48	1.36
16	1	525	CLA	O2D-CGD	5.28	1.46	1.33
16	5	413	CLA	O2D-CGD	5.28	1.46	1.33
16	J	102	CLA	O2D-CGD	5.28	1.46	1.33
16	6	401	CLA	C1D-ND	5.28	1.44	1.37
16	1	513	CLA	C3C-C2C	5.28	1.47	1.36
16	4	402	CLA	O2D-CGD	5.27	1.46	1.33
16	A	819	CLA	CHC-C1C	5.27	1.48	1.35
16	A	838	CLA	CHC-C1C	5.27	1.48	1.35
16	5	411	CLA	O2D-CGD	5.27	1.46	1.33
16	1	512	CLA	C3C-C2C	5.27	1.47	1.36
16	B	819	CLA	C3C-C2C	5.27	1.47	1.36
16	B	837	CLA	CHC-C1C	5.27	1.48	1.35
16	B	832	CLA	CHC-C1C	5.27	1.48	1.35
16	B	836	CLA	CHC-C1C	5.27	1.48	1.35
16	5	412	CLA	C1D-ND	5.27	1.44	1.37
16	4	409	CLA	O2D-CGD	5.27	1.46	1.33
16	1	507	CLA	O2D-CGD	5.27	1.46	1.33
16	2	401	CLA	O2D-CGD	5.26	1.46	1.33
16	2	406	CLA	O2D-CGD	5.26	1.46	1.33
16	4	407	CLA	CHC-C1C	5.26	1.48	1.35
16	1	526	CLA	C1D-ND	5.26	1.44	1.37
16	2	401	CLA	C3C-C2C	5.26	1.47	1.36
16	4	410	CLA	O2D-CGD	5.26	1.46	1.33
16	2	404	CLA	O2D-CGD	5.26	1.46	1.33
16	1	515	CLA	C3C-C2C	5.26	1.47	1.36
16	6	404	CLA	CHC-C1C	5.26	1.48	1.35
16	4	407	CLA	O2D-CGD	5.26	1.46	1.33
16	4	407	CLA	C3C-C2C	5.26	1.47	1.36
16	6	403	CLA	O2D-CGD	5.26	1.46	1.33
16	4	402	CLA	C3C-C2C	5.26	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3	401	CLA	O2D-CGD	5.26	1.46	1.33
16	5	418	CLA	C3C-C2C	5.26	1.47	1.36
16	1	519	CLA	O2D-CGD	5.25	1.46	1.33
16	1	515	CLA	CHC-C1C	5.25	1.48	1.35
16	5	405	CLA	O2D-CGD	5.25	1.46	1.33
16	1	514	CLA	O2D-CGD	5.25	1.46	1.33
16	1	521	CLA	C1D-ND	5.25	1.44	1.37
16	4	409	CLA	C3C-C2C	5.25	1.47	1.36
16	B	803	CLA	C3B-C2B	5.25	1.47	1.40
16	6	404	CLA	C3C-C2C	5.25	1.47	1.36
16	5	417	CLA	O2D-CGD	5.25	1.46	1.33
16	B	830	CLA	O2D-CGD	5.25	1.46	1.33
16	5	413	CLA	C3C-C2C	5.25	1.47	1.36
16	6	401	CLA	CHC-C1C	5.25	1.48	1.35
16	A	806	CLA	C3B-C2B	5.24	1.47	1.40
16	5	421	CLA	O2D-CGD	5.24	1.46	1.33
16	5	422	CLA	O2D-CGD	5.24	1.46	1.33
16	2	403	CLA	C1D-ND	5.24	1.44	1.37
16	4	411	CLA	O2D-CGD	5.24	1.46	1.33
16	A	802	CLA	C3B-C2B	5.24	1.47	1.40
16	6	407	CLA	CHC-C1C	5.24	1.48	1.35
16	1	502	CLA	O2D-CGD	5.24	1.46	1.33
16	2	404	CLA	CHC-C1C	5.23	1.48	1.35
16	1	525	CLA	CHC-C1C	5.23	1.48	1.35
16	2	401	CLA	CHC-C1C	5.23	1.48	1.35
16	K	103	CLA	C3C-C2C	5.23	1.47	1.36
16	1	521	CLA	C3C-C2C	5.23	1.47	1.36
16	B	828	CLA	CHC-C1C	5.23	1.48	1.35
16	5	403	CLA	C3C-C2C	5.22	1.47	1.36
16	1	526	CLA	C3C-C2C	5.22	1.47	1.36
16	A	824	CLA	C3C-C2C	5.22	1.47	1.36
16	1	507	CLA	C1D-ND	5.22	1.44	1.37
16	5	406	CLA	CHC-C1C	5.22	1.48	1.35
16	A	835	CLA	O2D-CGD	5.22	1.45	1.33
16	4	411	CLA	C3C-C2C	5.22	1.47	1.36
16	B	816	CLA	CHC-C1C	5.22	1.48	1.35
16	2	404	CLA	C3C-C2C	5.22	1.47	1.36
16	1	526	CLA	O2D-CGD	5.22	1.45	1.33
16	2	403	CLA	C3C-C2C	5.22	1.47	1.36
16	5	411	CLA	C3C-C2C	5.21	1.47	1.36
16	1	502	CLA	C3C-C2C	5.21	1.47	1.36
16	B	826	CLA	CHC-C1C	5.21	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	6	408	CLA	CHC-C1C	5.21	1.48	1.35
16	K	103	CLA	CHC-C1C	5.21	1.48	1.35
16	6	406	CLA	CHC-C1C	5.21	1.48	1.35
16	4	404	CLA	CHC-C1C	5.21	1.48	1.35
16	5	422	CLA	CHC-C1C	5.20	1.48	1.35
16	A	810	CLA	C3B-C2B	5.20	1.47	1.40
16	B	840	CLA	CHC-C1C	5.20	1.48	1.35
16	5	421	CLA	CHC-C1C	5.20	1.48	1.35
16	5	403	CLA	O2D-CGD	5.20	1.45	1.33
16	5	406	CLA	C1D-ND	5.19	1.44	1.37
16	4	405	CLA	C3C-C2C	5.19	1.47	1.36
16	5	417	CLA	C1D-ND	5.19	1.44	1.37
16	1	505	CLA	O2D-CGD	5.19	1.45	1.33
16	1	501	CLA	CHC-C1C	5.19	1.48	1.35
16	A	808	CLA	O2D-CGD	5.19	1.45	1.33
16	1	514	CLA	C1D-ND	5.19	1.44	1.37
16	B	817	CLA	CHC-C1C	5.19	1.48	1.35
16	5	419	CLA	CHC-C1C	5.18	1.48	1.35
16	5	412	CLA	O2D-CGD	5.18	1.45	1.33
16	4	406	CLA	C1D-ND	5.18	1.44	1.37
16	1	501	CLA	O2D-CGD	5.18	1.45	1.33
16	5	414	CLA	O2D-CGD	5.18	1.45	1.33
16	4	406	CLA	O2D-CGD	5.18	1.45	1.33
16	4	408	CLA	C1D-ND	5.18	1.44	1.37
16	A	827	CLA	C3C-C2C	5.18	1.47	1.36
16	5	403	CLA	CHC-C1C	5.17	1.48	1.35
16	B	815	CLA	C3C-C2C	5.17	1.47	1.36
16	4	403	CLA	CHC-C1C	5.17	1.48	1.35
16	1	511	CLA	C1D-ND	5.17	1.44	1.37
16	1	512	CLA	CHC-C1C	5.17	1.48	1.35
16	B	838	CLA	CHC-C1C	5.17	1.48	1.35
16	B	835	CLA	CHC-C1C	5.17	1.48	1.35
16	4	408	CLA	CHC-C1C	5.17	1.48	1.35
16	5	418	CLA	CHC-C1C	5.17	1.48	1.35
16	1	519	CLA	C1D-ND	5.17	1.44	1.37
16	4	409	CLA	C1D-ND	5.17	1.44	1.37
16	1	505	CLA	C1D-ND	5.17	1.44	1.37
16	2	405	CLA	CHC-C1C	5.16	1.48	1.35
16	A	839	CLA	CHC-C1C	5.16	1.48	1.35
16	4	406	CLA	C3C-C2C	5.16	1.47	1.36
16	F	204	CLA	CHC-C1C	5.16	1.48	1.35
16	3	401	CLA	CHC-C1C	5.16	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	804	CLA	C3B-C2B	5.16	1.47	1.40
16	5	409	CLA	O2D-CGD	5.16	1.45	1.33
16	5	421	CLA	C1D-ND	5.16	1.44	1.37
16	5	412	CLA	C3C-C2C	5.16	1.47	1.36
16	A	816	CLA	C3C-C2C	5.15	1.47	1.36
16	J	101	CLA	O2D-CGD	5.15	1.45	1.33
16	1	504	CLA	C1D-ND	5.15	1.44	1.37
16	B	824	CLA	O2D-CGD	5.15	1.45	1.33
16	1	511	CLA	C3C-C2C	5.15	1.47	1.36
16	2	402	CLA	CHC-C1C	5.15	1.48	1.35
16	1	503	CLA	C3C-C2C	5.15	1.47	1.36
16	1	526	CLA	CHC-C1C	5.15	1.48	1.35
16	6	409	CLA	CHC-C1C	5.14	1.48	1.35
16	1	508	CLA	C3C-C2C	5.14	1.47	1.36
16	6	402	CLA	CHC-C1C	5.14	1.48	1.35
16	B	830	CLA	C3C-C2C	5.14	1.47	1.36
16	5	417	CLA	C3C-C2C	5.14	1.47	1.36
16	B	821	CLA	CHC-C1C	5.14	1.48	1.35
16	B	822	CLA	C3C-C2C	5.14	1.47	1.36
16	B	836	CLA	O2D-CGD	5.14	1.45	1.33
16	1	507	CLA	C3C-C2C	5.14	1.47	1.36
16	1	509	CLA	C3B-C2B	5.14	1.47	1.40
16	5	419	CLA	C1D-ND	5.14	1.44	1.37
16	6	403	CLA	C3C-C2C	5.14	1.47	1.36
16	A	840	CLA	C3C-C2C	5.14	1.47	1.36
16	B	810	CLA	O2D-CGD	5.13	1.45	1.33
16	6	405	CLA	CHC-C1C	5.13	1.48	1.35
16	A	839	CLA	C3B-C2B	5.13	1.47	1.40
16	A	825	CLA	C3C-C2C	5.13	1.47	1.36
16	A	843	CLA	C3B-C2B	5.13	1.47	1.40
16	A	823	CLA	CHC-C1C	5.13	1.48	1.35
16	2	403	CLA	CHC-C1C	5.13	1.48	1.35
16	5	415	CLA	CHC-C1C	5.13	1.48	1.35
16	A	807	CLA	C3B-C2B	5.12	1.47	1.40
16	5	414	CLA	C3C-C2C	5.12	1.47	1.36
16	5	409	CLA	C1D-ND	5.12	1.44	1.37
16	1	510	CLA	O2D-CGD	5.12	1.45	1.33
16	4	402	CLA	CHC-C1C	5.12	1.48	1.35
16	1	511	CLA	O2D-CGD	5.12	1.45	1.33
16	B	827	CLA	CHC-C1C	5.12	1.48	1.35
16	1	504	CLA	C3C-C2C	5.12	1.47	1.36
16	A	810	CLA	CHC-C1C	5.12	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	814	CLA	CHC-C1C	5.12	1.48	1.35
16	B	831	CLA	O2D-CGD	5.11	1.45	1.33
16	1	504	CLA	O2D-CGD	5.11	1.45	1.33
16	2	406	CLA	CHC-C1C	5.11	1.48	1.35
16	5	405	CLA	CHC-C1C	5.11	1.48	1.35
16	1	502	CLA	C1D-ND	5.11	1.44	1.37
16	1	519	CLA	CHC-C1C	5.10	1.48	1.35
16	1	513	CLA	O2D-CGD	5.10	1.45	1.33
16	1	506	CLA	CHC-C1C	5.10	1.48	1.35
16	1	520	CLA	C3C-C2C	5.09	1.47	1.36
16	A	834	CLA	C3B-C2B	5.09	1.47	1.40
16	B	815	CLA	CHC-C1C	5.09	1.48	1.35
16	A	821	CLA	C3B-C2B	5.09	1.47	1.40
16	B	840	CLA	O2D-CGD	5.09	1.45	1.33
16	1	506	CLA	C3C-C2C	5.09	1.47	1.36
16	B	819	CLA	O2D-CGD	5.09	1.45	1.33
16	J	101	CLA	C3B-C2B	5.09	1.47	1.40
16	B	813	CLA	C3C-C2C	5.09	1.47	1.36
16	5	410	CLA	CHC-C1C	5.08	1.48	1.35
16	5	408	CLA	CHC-C1C	5.08	1.48	1.35
16	5	416	CLA	CHC-C1C	5.08	1.48	1.35
16	A	836	CLA	O2D-CGD	5.08	1.45	1.33
16	A	840	CLA	O2D-CGD	5.08	1.45	1.33
16	A	821	CLA	C3C-C2C	5.08	1.47	1.36
16	A	830	CLA	C3B-C2B	5.07	1.47	1.40
16	B	833	CLA	CHC-C1C	5.07	1.48	1.35
16	A	833	CLA	C3C-C2C	5.07	1.47	1.36
16	A	830	CLA	CHC-C1C	5.07	1.48	1.35
16	B	834	CLA	CHC-C1C	5.07	1.48	1.35
16	1	514	CLA	CHC-C1C	5.07	1.48	1.35
16	B	822	CLA	O2D-CGD	5.07	1.45	1.33
15	A	801	CL0	C3C-C2C	5.07	1.47	1.36
16	5	419	CLA	C3C-C2C	5.06	1.47	1.36
16	A	819	CLA	C3B-C2B	5.06	1.47	1.40
16	5	413	CLA	C1D-ND	5.06	1.44	1.37
16	B	835	CLA	C3C-C2C	5.06	1.47	1.36
16	B	817	CLA	C3C-C2C	5.05	1.47	1.36
16	J	102	CLA	CHC-C1C	5.05	1.47	1.35
16	B	831	CLA	C3C-C2C	5.05	1.47	1.36
16	B	820	CLA	O2D-CGD	5.05	1.45	1.33
16	B	810	CLA	CHC-C1C	5.05	1.47	1.35
16	1	502	CLA	CHC-C1C	5.05	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	503	CLA	CHC-C1C	5.05	1.47	1.35
16	1	508	CLA	O2D-CGD	5.05	1.45	1.33
16	B	837	CLA	C3C-C2C	5.04	1.47	1.36
16	B	812	CLA	O2D-CGD	5.04	1.45	1.33
16	B	827	CLA	O2D-CGD	5.04	1.45	1.33
16	B	826	CLA	C3C-C2C	5.04	1.47	1.36
16	1	525	CLA	C1D-ND	5.04	1.44	1.37
16	B	841	CLA	C3B-C2B	5.04	1.47	1.40
16	K	101	CLA	C3C-C2C	5.04	1.47	1.36
16	B	807	CLA	C3C-C2C	5.04	1.47	1.36
16	5	410	CLA	C1D-ND	5.03	1.44	1.37
16	1	509	CLA	CHC-C1C	5.03	1.47	1.35
16	A	833	CLA	O2D-CGD	5.03	1.45	1.33
16	A	808	CLA	CHC-C1C	5.02	1.47	1.35
16	1	512	CLA	C1D-ND	5.02	1.44	1.37
16	A	841	CLA	O2D-CGD	5.02	1.45	1.33
16	B	820	CLA	CHC-C1C	5.02	1.47	1.35
16	A	814	CLA	CHC-C1C	5.02	1.47	1.35
16	A	826	CLA	O2D-CGD	5.02	1.45	1.33
16	A	808	CLA	C3B-C2B	5.02	1.47	1.40
16	F	201	CLA	C3B-C2B	5.02	1.47	1.40
16	5	407	CLA	C1D-ND	5.02	1.44	1.37
16	1	509	CLA	C3C-C2C	5.02	1.47	1.36
16	A	843	CLA	CHC-C1C	5.02	1.47	1.35
16	A	814	CLA	C3C-C2C	5.01	1.47	1.36
16	1	510	CLA	CHC-C1C	5.01	1.47	1.35
16	A	813	CLA	O2D-CGD	5.01	1.45	1.33
16	A	816	CLA	CHC-C1C	5.01	1.47	1.35
16	A	805	CLA	CHC-C1C	5.00	1.47	1.35
16	B	816	CLA	C3C-C2C	5.00	1.47	1.36
17	B	842	PQN	C10-C5	5.00	1.49	1.40
16	X	101	CLA	CHC-C1C	5.00	1.47	1.35
16	A	824	CLA	CHC-C1C	5.00	1.47	1.35
16	1	507	CLA	O2A-CGA	5.00	1.47	1.30
16	A	841	CLA	C3C-C2C	5.00	1.47	1.36
16	A	806	CLA	O2D-CGD	5.00	1.45	1.33
16	B	841	CLA	C3C-C2C	5.00	1.47	1.36
16	1	504	CLA	CHC-C1C	4.99	1.47	1.35
16	A	836	CLA	C3C-C2C	4.99	1.47	1.36
16	A	843	CLA	O2D-CGD	4.99	1.45	1.33
16	J	101	CLA	CHC-C1C	4.99	1.47	1.35
16	A	835	CLA	C3C-C2C	4.99	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	818	CLA	C3B-C2B	4.99	1.47	1.40
16	4	406	CLA	C3B-C2B	4.99	1.47	1.40
16	B	804	CLA	O2D-CGD	4.99	1.45	1.33
16	1	513	CLA	CHC-C1C	4.99	1.47	1.35
16	4	405	CLA	CHC-C1C	4.98	1.47	1.35
16	B	841	CLA	O2D-CGD	4.98	1.45	1.33
16	A	824	CLA	O2D-CGD	4.98	1.45	1.33
16	1	510	CLA	C3C-C2C	4.98	1.47	1.36
16	A	817	CLA	O2D-CGD	4.98	1.45	1.33
16	6	403	CLA	CHC-C1C	4.98	1.47	1.35
16	B	823	CLA	O2D-CGD	4.97	1.45	1.33
16	B	839	CLA	O2D-CGD	4.97	1.45	1.33
16	A	821	CLA	CHC-C1C	4.97	1.47	1.35
16	A	818	CLA	O2D-CGD	4.97	1.45	1.33
16	A	840	CLA	CHC-C1C	4.97	1.47	1.35
16	B	809	CLA	CHC-C1C	4.97	1.47	1.35
16	B	832	CLA	C3C-C2C	4.97	1.47	1.36
16	A	830	CLA	O2D-CGD	4.96	1.45	1.33
16	B	833	CLA	O2D-CGD	4.96	1.45	1.33
16	A	807	CLA	CHC-C1C	4.96	1.47	1.35
16	B	809	CLA	C3C-C2C	4.96	1.47	1.36
16	B	838	CLA	C3C-C2C	4.96	1.47	1.36
16	B	816	CLA	O2D-CGD	4.96	1.45	1.33
16	A	830	CLA	C3C-C2C	4.96	1.47	1.36
16	A	813	CLA	CHC-C1C	4.96	1.47	1.35
16	A	832	CLA	CHC-C1C	4.95	1.47	1.35
16	B	834	CLA	C3C-C2C	4.95	1.47	1.36
16	A	811	CLA	C3C-C2C	4.95	1.47	1.36
16	F	204	CLA	O2D-CGD	4.95	1.45	1.33
16	5	409	CLA	CHC-C1C	4.95	1.47	1.35
16	B	834	CLA	O2D-CGD	4.95	1.45	1.33
16	A	810	CLA	C3C-C2C	4.95	1.47	1.36
16	A	803	CLA	C3C-C2C	4.95	1.47	1.36
16	A	829	CLA	O2D-CGD	4.95	1.45	1.33
16	1	501	CLA	C3B-C2B	4.94	1.47	1.40
16	A	811	CLA	O2D-CGD	4.94	1.45	1.33
16	B	830	CLA	CHC-C1C	4.94	1.47	1.35
16	A	820	CLA	CHC-C1C	4.94	1.47	1.35
16	A	829	CLA	C3C-C2C	4.94	1.47	1.36
16	J	102	CLA	C3C-C2C	4.93	1.47	1.36
16	B	840	CLA	C3C-C2C	4.93	1.47	1.36
16	B	821	CLA	C3C-C2C	4.93	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	802	CLA	O2D-CGD	4.93	1.45	1.33
16	J	101	CLA	C3C-C2C	4.93	1.47	1.36
16	B	825	CLA	CHC-C1C	4.93	1.47	1.35
16	1	511	CLA	CHC-C1C	4.92	1.47	1.35
16	B	806	CLA	O2D-CGD	4.92	1.45	1.33
16	A	823	CLA	C3B-C2B	4.91	1.47	1.40
16	B	827	CLA	C3C-C2C	4.91	1.47	1.36
16	5	409	CLA	C3C-C2C	4.90	1.47	1.36
16	B	829	CLA	CHC-C1C	4.90	1.47	1.35
16	A	832	CLA	O2D-CGD	4.90	1.45	1.33
16	A	832	CLA	C3C-C2C	4.90	1.47	1.36
16	A	804	CLA	CHC-C1C	4.90	1.47	1.35
16	A	818	CLA	C3B-C2B	4.90	1.47	1.40
16	B	836	CLA	C3C-C2C	4.90	1.47	1.36
16	B	818	CLA	CHC-C1C	4.89	1.47	1.35
16	1	509	CLA	O2D-CGD	4.89	1.45	1.33
16	A	822	CLA	C3C-C2C	4.89	1.47	1.36
16	1	521	CLA	C3B-C2B	4.89	1.47	1.40
16	B	808	CLA	C3B-C2B	4.89	1.47	1.40
16	A	816	CLA	O2D-CGD	4.89	1.45	1.33
16	B	825	CLA	O2D-CGD	4.89	1.45	1.33
16	B	820	CLA	C3C-C2C	4.89	1.47	1.36
16	5	407	CLA	CHC-C1C	4.89	1.47	1.35
16	A	837	CLA	C3C-C2C	4.89	1.47	1.36
16	A	822	CLA	O2D-CGD	4.89	1.45	1.33
16	A	804	CLA	O2D-CGD	4.89	1.45	1.33
16	B	815	CLA	C3B-C2B	4.89	1.47	1.40
16	A	828	CLA	C3B-C2B	4.88	1.47	1.40
16	B	821	CLA	O2D-CGD	4.88	1.45	1.33
16	F	204	CLA	C3C-C2C	4.88	1.47	1.36
16	B	822	CLA	CHC-C1C	4.88	1.47	1.35
16	1	507	CLA	CHC-C1C	4.88	1.47	1.35
16	5	411	CLA	C1D-ND	4.87	1.43	1.37
16	A	838	CLA	C3C-C2C	4.87	1.47	1.36
16	B	817	CLA	C3B-C2B	4.87	1.47	1.40
16	B	831	CLA	CHC-C1C	4.87	1.47	1.35
16	A	838	CLA	C1D-ND	4.86	1.43	1.37
16	5	411	CLA	C3B-C2B	4.86	1.47	1.40
16	A	812	CLA	C3B-C2B	4.86	1.47	1.40
16	K	101	CLA	CHC-C1C	4.85	1.47	1.35
16	A	821	CLA	O2D-CGD	4.85	1.45	1.33
16	1	508	CLA	C1D-ND	4.85	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	838	CLA	O2D-CGD	4.85	1.45	1.33
16	1	508	CLA	CHC-C1C	4.85	1.47	1.35
16	A	823	CLA	O2D-CGD	4.85	1.45	1.33
16	A	827	CLA	C3B-C2B	4.84	1.47	1.40
15	A	801	CL0	O2D-CGD	4.84	1.45	1.33
16	B	829	CLA	C3C-C2C	4.84	1.47	1.36
16	A	814	CLA	C3B-C2B	4.84	1.47	1.40
16	1	503	CLA	C1D-ND	4.84	1.43	1.37
16	A	825	CLA	CHC-C1C	4.84	1.47	1.35
16	B	806	CLA	C3B-C2B	4.84	1.47	1.40
16	B	825	CLA	C1D-ND	4.83	1.43	1.37
16	1	501	CLA	C3C-C2C	4.83	1.47	1.36
16	A	812	CLA	C3C-C2C	4.83	1.47	1.36
16	B	811	CLA	C3C-C2C	4.83	1.47	1.36
16	A	812	CLA	CHC-C1C	4.82	1.47	1.35
16	A	834	CLA	CHC-C1C	4.82	1.47	1.35
16	B	812	CLA	CHC-C1C	4.82	1.47	1.35
16	F	201	CLA	O2A-CGA	4.82	1.47	1.33
16	A	817	CLA	C3C-C2C	4.81	1.47	1.36
16	1	513	CLA	C1D-ND	4.81	1.43	1.37
16	5	414	CLA	CHC-C1C	4.81	1.47	1.35
16	1	506	CLA	C1D-ND	4.81	1.43	1.37
16	B	817	CLA	O2D-CGD	4.80	1.44	1.33
16	A	842	CLA	C1D-ND	4.80	1.43	1.37
16	B	801	CLA	C1D-ND	4.80	1.43	1.37
16	A	834	CLA	C3C-C2C	4.80	1.46	1.36
16	B	840	CLA	C3B-C2B	4.80	1.47	1.40
16	B	837	CLA	O2D-CGD	4.79	1.44	1.33
16	A	839	CLA	C3C-C2C	4.79	1.46	1.36
16	A	803	CLA	CHC-C1C	4.79	1.47	1.35
16	A	815	CLA	O2D-CGD	4.79	1.44	1.33
16	B	836	CLA	C1D-ND	4.79	1.43	1.37
16	B	803	CLA	O2D-CGD	4.78	1.44	1.33
16	B	814	CLA	C3C-C2C	4.78	1.46	1.36
16	B	807	CLA	O2D-CGD	4.78	1.44	1.33
16	B	821	CLA	C1D-ND	4.78	1.43	1.37
16	A	819	CLA	O2D-CGD	4.78	1.44	1.33
16	B	811	CLA	O2D-CGD	4.77	1.44	1.33
16	B	833	CLA	C3C-C2C	4.77	1.46	1.36
16	1	512	CLA	C3B-C2B	4.77	1.47	1.40
16	A	828	CLA	O2D-CGD	4.77	1.44	1.33
16	F	201	CLA	C3C-C2C	4.77	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	815	CLA	CHC-C1C	4.77	1.47	1.35
16	B	825	CLA	C3C-C2C	4.77	1.46	1.36
16	B	839	CLA	CHC-C1C	4.77	1.47	1.35
16	B	831	CLA	C1D-ND	4.76	1.43	1.37
16	B	828	CLA	C3C-C2C	4.76	1.46	1.36
17	A	844	PQN	C10-C5	4.76	1.48	1.40
16	B	812	CLA	O2A-CGA	4.76	1.46	1.30
16	A	821	CLA	C1D-ND	4.76	1.43	1.37
16	B	820	CLA	C1D-ND	4.76	1.43	1.37
16	A	828	CLA	C3C-C2C	4.75	1.46	1.36
16	B	807	CLA	CHC-C1C	4.75	1.47	1.35
16	B	815	CLA	O2D-CGD	4.75	1.44	1.33
16	B	806	CLA	CHC-C1C	4.75	1.47	1.35
16	F	204	CLA	C1D-ND	4.75	1.43	1.37
16	A	808	CLA	C3C-C2C	4.75	1.46	1.36
16	B	802	CLA	C3C-C2C	4.74	1.46	1.36
16	A	814	CLA	C1D-ND	4.74	1.43	1.37
16	A	807	CLA	O2D-CGD	4.74	1.44	1.33
16	A	842	CLA	C3C-C2C	4.74	1.46	1.36
16	B	801	CLA	O2D-CGD	4.74	1.44	1.33
16	A	842	CLA	O2D-CGD	4.73	1.44	1.33
16	B	815	CLA	O2A-CGA	4.73	1.46	1.30
16	B	824	CLA	C3C-C2C	4.73	1.46	1.36
16	A	826	CLA	C1D-ND	4.73	1.43	1.37
16	5	414	CLA	C1D-ND	4.72	1.43	1.37
16	B	823	CLA	C3C-C2C	4.72	1.46	1.36
16	B	830	CLA	C3B-C2B	4.72	1.46	1.40
16	A	838	CLA	O2D-CGD	4.72	1.44	1.33
16	B	812	CLA	C3C-C2C	4.72	1.46	1.36
16	A	815	CLA	O2A-CGA	4.72	1.46	1.30
16	F	201	CLA	O2D-CGD	4.72	1.44	1.33
16	B	815	CLA	C1D-ND	4.71	1.43	1.37
16	A	815	CLA	C3C-C2C	4.71	1.46	1.36
16	1	520	CLA	O2D-CGD	4.71	1.44	1.33
16	A	823	CLA	C3C-C2C	4.71	1.46	1.36
16	B	835	CLA	O2A-CGA	4.71	1.46	1.30
16	B	811	CLA	C3B-C2B	4.70	1.46	1.40
16	A	810	CLA	O2D-CGD	4.70	1.44	1.33
16	5	404	CLA	C1D-ND	4.70	1.43	1.37
16	B	811	CLA	CHC-C1C	4.70	1.47	1.35
16	A	840	CLA	C3B-C2B	4.70	1.46	1.40
16	K	103	CLA	C1D-ND	4.70	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	835	CLA	C3B-C2B	4.69	1.46	1.40
16	A	809	CLA	O2D-CGD	4.69	1.44	1.33
16	B	807	CLA	C1D-ND	4.69	1.43	1.37
16	B	839	CLA	C3C-C2C	4.69	1.46	1.36
16	A	820	CLA	O2D-CGD	4.69	1.44	1.33
16	A	806	CLA	CHC-C1C	4.69	1.47	1.35
16	B	819	CLA	C3B-C2B	4.68	1.46	1.40
16	B	804	CLA	CHC-C1C	4.68	1.47	1.35
16	B	818	CLA	C3C-C2C	4.68	1.46	1.36
16	A	843	CLA	C3C-C2C	4.68	1.46	1.36
16	A	820	CLA	C3C-C2C	4.68	1.46	1.36
16	J	102	CLA	O2A-CGA	4.67	1.46	1.30
16	X	101	CLA	O2D-CGD	4.67	1.44	1.33
16	K	101	CLA	O2A-CGA	4.67	1.46	1.30
16	B	819	CLA	C1D-ND	4.67	1.43	1.37
16	A	816	CLA	O2A-CGA	4.67	1.46	1.30
16	A	809	CLA	C1D-ND	4.66	1.43	1.37
16	A	826	CLA	C3C-C2C	4.66	1.46	1.36
16	1	520	CLA	C3B-C2B	4.66	1.46	1.40
16	A	837	CLA	O2A-CGA	4.65	1.46	1.30
16	5	404	CLA	CHC-C1C	4.65	1.46	1.35
16	1	509	CLA	O2A-CGA	4.65	1.46	1.30
16	1	521	CLA	O2D-CGD	4.65	1.44	1.33
16	B	836	CLA	O2A-CGA	4.65	1.46	1.30
16	A	820	CLA	C3B-C2B	4.65	1.46	1.40
16	B	808	CLA	CHC-C1C	4.65	1.46	1.35
16	A	836	CLA	C3B-C2B	4.65	1.46	1.40
16	A	837	CLA	O2D-CGD	4.65	1.44	1.33
16	A	837	CLA	CHC-C1C	4.64	1.46	1.35
16	B	833	CLA	C3B-C2B	4.64	1.46	1.40
16	A	829	CLA	C1D-ND	4.64	1.43	1.37
16	B	832	CLA	C3B-C2B	4.64	1.46	1.40
16	B	801	CLA	C3C-C2C	4.64	1.46	1.36
16	B	821	CLA	O2A-CGA	4.64	1.46	1.30
16	B	826	CLA	O2D-CGD	4.64	1.44	1.33
16	1	506	CLA	O2A-CGA	4.64	1.46	1.30
16	B	829	CLA	O2D-CGD	4.64	1.44	1.33
16	A	838	CLA	C3B-C2B	4.64	1.46	1.40
16	B	805	CLA	O2D-CGD	4.63	1.44	1.33
16	J	101	CLA	O2A-CGA	4.63	1.46	1.30
16	A	833	CLA	CHC-C1C	4.63	1.46	1.35
16	1	512	CLA	O2A-CGA	4.63	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	404	CLA	C3C-C2C	4.63	1.46	1.36
16	A	834	CLA	O2D-CGD	4.63	1.44	1.33
16	B	828	CLA	O2D-CGD	4.63	1.44	1.33
16	A	811	CLA	CHC-C1C	4.62	1.46	1.35
16	B	834	CLA	C3B-C2B	4.62	1.46	1.40
16	1	521	CLA	O2A-CGA	4.62	1.46	1.33
16	A	839	CLA	C1D-ND	4.62	1.43	1.37
16	1	526	CLA	O2A-CGA	4.62	1.46	1.30
16	A	802	CLA	C3C-C2C	4.61	1.46	1.36
16	1	513	CLA	O2A-CGA	4.61	1.46	1.30
16	B	835	CLA	O2D-CGD	4.60	1.44	1.33
16	A	805	CLA	C1D-ND	4.60	1.43	1.37
16	A	818	CLA	C1D-ND	4.60	1.43	1.37
16	K	103	CLA	O2A-CGA	4.60	1.46	1.30
16	A	805	CLA	C3C-C2C	4.60	1.46	1.36
16	A	836	CLA	CHC-C1C	4.59	1.46	1.35
16	A	825	CLA	C3B-C2B	4.59	1.46	1.40
16	A	831	CLA	O2D-CGD	4.59	1.44	1.33
16	B	828	CLA	C3B-C2B	4.59	1.46	1.40
16	5	414	CLA	O2A-CGA	4.59	1.46	1.30
16	A	817	CLA	CHC-C1C	4.58	1.46	1.35
16	B	802	CLA	CHC-C1C	4.58	1.46	1.35
16	A	817	CLA	O2A-CGA	4.58	1.46	1.33
16	B	828	CLA	O2A-CGA	4.58	1.46	1.33
16	B	806	CLA	C3C-C2C	4.58	1.46	1.36
16	A	803	CLA	O2D-CGD	4.58	1.44	1.33
16	B	801	CLA	C3B-C2B	4.58	1.46	1.40
16	J	101	CLA	C1D-ND	4.57	1.43	1.37
16	A	817	CLA	C1D-ND	4.57	1.43	1.37
16	A	818	CLA	C3C-C2C	4.57	1.46	1.36
16	A	831	CLA	C3C-C2C	4.57	1.46	1.36
16	A	802	CLA	O2D-CGD	4.57	1.44	1.33
16	B	808	CLA	O2D-CGD	4.57	1.44	1.33
16	A	841	CLA	C1D-ND	4.57	1.43	1.37
16	A	811	CLA	O2A-CGA	4.57	1.46	1.30
16	B	826	CLA	C1D-ND	4.56	1.43	1.37
16	4	405	CLA	CHD-C1D	4.56	1.47	1.38
16	B	809	CLA	O2D-CGD	4.55	1.44	1.33
16	5	413	CLA	O2A-CGA	4.55	1.46	1.30
16	5	410	CLA	O2A-CGA	4.55	1.46	1.30
16	J	102	CLA	C1D-ND	4.55	1.43	1.37
16	B	805	CLA	C3C-C2C	4.55	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	832	CLA	O2D-CGD	4.55	1.44	1.33
16	1	501	CLA	C1D-ND	4.55	1.43	1.37
16	F	204	CLA	O2A-CGA	4.55	1.46	1.30
16	4	404	CLA	O2A-CGA	4.55	1.46	1.30
16	4	410	CLA	CHD-C1D	4.55	1.47	1.38
16	4	403	CLA	O2A-CGA	4.55	1.46	1.30
19	1	517	BCR	C14-C13	4.54	1.41	1.35
16	1	510	CLA	O2A-CGA	4.54	1.46	1.30
16	1	508	CLA	O2A-CGA	4.54	1.46	1.30
16	B	824	CLA	C3B-C2B	4.54	1.46	1.40
16	1	502	CLA	O2A-CGA	4.54	1.46	1.30
16	1	514	CLA	O2A-CGA	4.54	1.46	1.30
16	4	404	CLA	CHD-C1D	4.54	1.47	1.38
16	5	407	CLA	O2A-CGA	4.54	1.46	1.30
16	4	407	CLA	O2A-CGA	4.54	1.46	1.30
16	A	808	CLA	C1D-ND	4.54	1.43	1.37
16	5	419	CLA	O2A-CGA	4.54	1.46	1.30
19	5	420	BCR	C10-C9	4.53	1.41	1.35
16	F	201	CLA	CHC-C1C	4.53	1.46	1.35
16	B	804	CLA	C1D-ND	4.53	1.43	1.37
16	2	406	CLA	O2A-CGA	4.53	1.46	1.30
16	1	505	CLA	O2A-CGA	4.53	1.46	1.30
16	5	417	CLA	O2A-CGA	4.53	1.46	1.30
16	4	408	CLA	O2A-CGA	4.53	1.46	1.30
16	B	812	CLA	C1D-ND	4.53	1.43	1.37
16	2	404	CLA	O2A-CGA	4.52	1.46	1.30
16	4	410	CLA	O2A-CGA	4.52	1.46	1.30
16	A	807	CLA	C1D-ND	4.52	1.43	1.37
16	A	836	CLA	O2A-CGA	4.52	1.46	1.33
16	A	806	CLA	O2A-CGA	4.52	1.46	1.33
16	B	822	CLA	C1D-ND	4.52	1.43	1.37
16	5	412	CLA	O2A-CGA	4.52	1.45	1.30
16	2	401	CLA	O2A-CGA	4.52	1.45	1.30
16	5	403	CLA	O2A-CGA	4.52	1.45	1.30
16	4	411	CLA	O2A-CGA	4.52	1.45	1.30
16	4	402	CLA	O2A-CGA	4.52	1.45	1.30
16	5	415	CLA	O2A-CGA	4.52	1.45	1.30
16	6	401	CLA	O2A-CGA	4.52	1.45	1.30
16	4	405	CLA	O2A-CGA	4.51	1.45	1.30
16	A	804	CLA	C1D-ND	4.51	1.43	1.37
16	1	515	CLA	O2A-CGA	4.51	1.45	1.30
16	6	406	CLA	O2A-CGA	4.51	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	819	CLA	C3C-C2C	4.51	1.46	1.36
16	5	413	CLA	CHD-C1D	4.51	1.47	1.38
16	1	509	CLA	C1D-ND	4.51	1.43	1.37
16	A	839	CLA	O2D-CGD	4.51	1.44	1.33
16	5	418	CLA	O2A-CGA	4.51	1.45	1.30
16	A	813	CLA	C1D-ND	4.51	1.43	1.37
16	B	811	CLA	C1D-ND	4.51	1.43	1.37
16	A	842	CLA	CHC-C1C	4.51	1.46	1.35
16	5	404	CLA	O2A-CGA	4.51	1.45	1.30
16	5	409	CLA	O2A-CGA	4.51	1.45	1.30
16	B	803	CLA	CHC-C1C	4.51	1.46	1.35
16	A	813	CLA	O2A-CGA	4.51	1.46	1.33
16	6	408	CLA	CHD-C1D	4.51	1.47	1.38
16	6	405	CLA	O2A-CGA	4.51	1.45	1.30
19	I	102	BCR	C21-C22	4.51	1.41	1.35
16	4	409	CLA	O2A-CGA	4.51	1.45	1.30
16	2	403	CLA	O2A-CGA	4.50	1.45	1.30
16	5	408	CLA	O2A-CGA	4.50	1.45	1.30
16	1	526	CLA	CHD-C1D	4.50	1.47	1.38
16	6	407	CLA	O2A-CGA	4.50	1.45	1.30
16	B	817	CLA	O2A-CGA	4.50	1.46	1.33
16	A	813	CLA	C3C-C2C	4.50	1.46	1.36
19	A	851	BCR	C14-C13	4.50	1.41	1.35
16	B	837	CLA	C1D-ND	4.50	1.43	1.37
16	5	422	CLA	O2A-CGA	4.50	1.45	1.30
16	A	835	CLA	CHC-C1C	4.50	1.46	1.35
16	6	403	CLA	O2A-CGA	4.50	1.45	1.30
16	2	402	CLA	O2A-CGA	4.50	1.45	1.30
16	A	833	CLA	O2A-CGA	4.50	1.46	1.33
16	2	405	CLA	O2A-CGA	4.50	1.45	1.30
16	4	406	CLA	O2A-CGA	4.50	1.45	1.30
16	K	103	CLA	O2D-CGD	4.50	1.44	1.33
16	3	401	CLA	O2A-CGA	4.50	1.45	1.30
16	5	407	CLA	CHD-C1D	4.50	1.47	1.38
16	6	409	CLA	O2A-CGA	4.49	1.45	1.30
16	6	403	CLA	CHD-C1D	4.49	1.47	1.38
16	6	402	CLA	O2A-CGA	4.49	1.45	1.30
16	X	101	CLA	O2A-CGA	4.49	1.45	1.30
16	B	816	CLA	C1D-ND	4.49	1.43	1.37
16	B	818	CLA	O2D-CGD	4.49	1.44	1.33
16	5	405	CLA	O2A-CGA	4.49	1.45	1.30
16	6	404	CLA	O2A-CGA	4.49	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	827	CLA	O2D-CGD	4.49	1.44	1.33
16	2	402	CLA	CHD-C1D	4.48	1.47	1.38
16	6	406	CLA	CHD-C1D	4.48	1.47	1.38
16	B	818	CLA	C1D-ND	4.48	1.43	1.37
16	B	816	CLA	C3B-C2B	4.48	1.46	1.40
16	6	402	CLA	CHD-C1D	4.48	1.47	1.38
16	A	819	CLA	C1D-ND	4.48	1.43	1.37
16	B	827	CLA	C1D-ND	4.48	1.43	1.37
16	2	403	CLA	CHD-C1D	4.48	1.47	1.38
16	6	407	CLA	CHD-C1D	4.47	1.47	1.38
16	5	421	CLA	CHD-C1D	4.47	1.47	1.38
16	A	812	CLA	O2D-CGD	4.47	1.44	1.33
16	B	814	CLA	O2D-CGD	4.47	1.44	1.33
16	5	411	CLA	O2A-CGA	4.47	1.45	1.30
16	6	409	CLA	CHD-C1D	4.47	1.47	1.38
16	A	814	CLA	O2A-CGA	4.46	1.46	1.33
16	A	819	CLA	O2A-CGA	4.46	1.46	1.33
16	A	837	CLA	C1D-ND	4.46	1.43	1.37
19	1	516	BCR	C14-C13	4.46	1.41	1.35
16	6	404	CLA	CHD-C1D	4.46	1.47	1.38
16	5	406	CLA	O2A-CGA	4.46	1.45	1.30
16	5	421	CLA	O2A-CGA	4.46	1.45	1.30
16	A	816	CLA	C1D-ND	4.46	1.43	1.37
16	B	841	CLA	CHC-C1C	4.46	1.46	1.35
16	5	406	CLA	CHD-C1D	4.45	1.47	1.38
16	B	810	CLA	C3C-C2C	4.45	1.46	1.36
19	1	516	BCR	C10-C9	4.44	1.41	1.35
16	A	824	CLA	O2A-CGA	4.44	1.46	1.33
16	K	101	CLA	C1D-ND	4.44	1.43	1.37
16	B	823	CLA	CHC-C1C	4.44	1.46	1.35
16	5	416	CLA	CHD-C1D	4.44	1.47	1.38
16	6	405	CLA	CHD-C1D	4.44	1.47	1.38
16	B	841	CLA	O2A-CGA	4.44	1.46	1.33
16	5	417	CLA	CHD-C1D	4.44	1.47	1.38
16	A	818	CLA	O2A-CGA	4.44	1.46	1.33
16	1	503	CLA	CHD-C1D	4.44	1.47	1.38
19	1	517	BCR	C21-C22	4.43	1.41	1.35
16	1	507	CLA	CHD-C1D	4.43	1.47	1.38
16	A	832	CLA	O2A-CGA	4.43	1.46	1.33
16	A	831	CLA	O2A-CGA	4.43	1.46	1.33
16	1	501	CLA	O2A-CGA	4.43	1.45	1.30
16	B	814	CLA	C1D-ND	4.43	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	815	CLA	CHD-C1D	4.43	1.47	1.38
16	B	820	CLA	O2A-CGA	4.43	1.46	1.33
16	4	408	CLA	CHD-C1D	4.43	1.47	1.38
16	1	515	CLA	CHD-C1D	4.43	1.47	1.38
16	B	805	CLA	O2A-CGA	4.43	1.46	1.33
16	B	823	CLA	O2A-CGA	4.43	1.46	1.33
16	6	401	CLA	CHD-C1D	4.43	1.47	1.38
16	1	511	CLA	CHD-C1D	4.43	1.47	1.38
16	A	805	CLA	O2D-CGD	4.43	1.44	1.33
16	A	820	CLA	C1D-ND	4.42	1.43	1.37
16	2	406	CLA	CHD-C1D	4.42	1.47	1.38
16	1	504	CLA	O2A-CGA	4.42	1.45	1.30
16	3	401	CLA	CHD-C1D	4.42	1.47	1.38
16	5	408	CLA	CHD-C1D	4.42	1.47	1.38
16	1	514	CLA	CHD-C1D	4.42	1.47	1.38
16	B	801	CLA	CHC-C1C	4.42	1.46	1.35
16	5	422	CLA	CHD-C1D	4.41	1.47	1.38
16	A	825	CLA	O2A-CGA	4.41	1.46	1.33
16	1	525	CLA	CHD-C1D	4.41	1.47	1.38
16	2	405	CLA	CHD-C1D	4.41	1.47	1.38
16	4	411	CLA	CHD-C1D	4.40	1.46	1.38
16	A	805	CLA	O2A-CGA	4.40	1.46	1.33
16	B	805	CLA	CHC-C1C	4.40	1.46	1.35
16	B	829	CLA	O2A-CGA	4.40	1.46	1.33
16	5	413	CLA	CHD-C4C	4.40	1.49	1.39
16	A	809	CLA	C3C-C2C	4.39	1.46	1.36
16	B	830	CLA	C1D-ND	4.39	1.43	1.37
16	1	520	CLA	C1D-ND	4.39	1.43	1.37
16	5	418	CLA	CHD-C1D	4.39	1.46	1.38
16	J	102	CLA	CHD-C1D	4.39	1.46	1.38
16	1	511	CLA	O2A-CGA	4.39	1.46	1.33
16	B	816	CLA	O2A-CGA	4.39	1.46	1.33
16	A	823	CLA	O2A-CGA	4.38	1.46	1.33
16	A	810	CLA	C1D-ND	4.38	1.43	1.37
16	A	827	CLA	C1D-ND	4.38	1.43	1.37
16	2	404	CLA	CHD-C1D	4.38	1.46	1.38
16	B	833	CLA	O2A-CGA	4.38	1.46	1.33
16	A	804	CLA	C3C-C2C	4.38	1.46	1.36
16	B	803	CLA	C3C-C2C	4.37	1.46	1.36
16	A	811	CLA	C1D-ND	4.37	1.43	1.37
16	4	409	CLA	CHD-C1D	4.37	1.46	1.38
16	A	831	CLA	CHC-C1C	4.37	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	830	CLA	O2A-CGA	4.37	1.46	1.33
16	A	808	CLA	O2A-CGA	4.36	1.46	1.33
16	1	519	CLA	O2A-CGA	4.36	1.46	1.33
16	B	822	CLA	O2A-CGA	4.36	1.46	1.33
16	1	521	CLA	CHD-C1D	4.36	1.46	1.38
16	A	814	CLA	O2D-CGD	4.36	1.43	1.33
16	B	810	CLA	C1D-ND	4.35	1.43	1.37
16	A	804	CLA	O2A-CGA	4.35	1.46	1.33
16	A	810	CLA	O2A-CGA	4.35	1.46	1.33
16	1	520	CLA	O2A-CGA	4.35	1.46	1.33
16	4	406	CLA	CHD-C1D	4.35	1.46	1.38
16	B	813	CLA	O2D-CGD	4.35	1.43	1.33
16	1	505	CLA	CHD-C1D	4.34	1.46	1.38
16	B	813	CLA	C3B-C2B	4.34	1.46	1.40
16	B	810	CLA	O2A-CGA	4.34	1.46	1.33
19	5	420	BCR	C14-C13	4.33	1.41	1.35
16	4	407	CLA	CHD-C1D	4.33	1.46	1.38
19	1	518	BCR	C10-C9	4.33	1.41	1.35
15	A	801	CL0	CHC-C1C	4.33	1.46	1.35
16	5	411	CLA	CHD-C1D	4.33	1.46	1.38
16	B	808	CLA	C3C-C2C	4.33	1.45	1.36
16	B	835	CLA	C3B-C2B	4.33	1.46	1.40
16	B	831	CLA	O2A-CGA	4.32	1.46	1.33
16	2	401	CLA	CHD-C1D	4.32	1.46	1.38
16	B	811	CLA	O2A-CGA	4.31	1.45	1.33
16	5	412	CLA	CHD-C1D	4.31	1.46	1.38
16	B	808	CLA	O2A-CGA	4.31	1.45	1.33
16	B	806	CLA	C1D-ND	4.31	1.43	1.37
16	B	802	CLA	O2A-CGA	4.31	1.45	1.33
16	6	403	CLA	CHD-C4C	4.30	1.49	1.39
16	5	419	CLA	CHD-C1D	4.30	1.46	1.38
16	6	405	CLA	CHD-C4C	4.30	1.49	1.39
19	A	849	BCR	C10-C9	4.30	1.41	1.35
16	5	408	CLA	CHD-C4C	4.30	1.49	1.39
16	B	834	CLA	O2A-CGA	4.30	1.45	1.33
16	6	408	CLA	CHD-C4C	4.29	1.49	1.39
16	5	404	CLA	CHD-C4C	4.29	1.49	1.39
16	4	405	CLA	CHD-C4C	4.29	1.49	1.39
16	B	809	CLA	O2A-CGA	4.29	1.45	1.33
16	A	831	CLA	C1D-ND	4.29	1.43	1.37
16	A	833	CLA	C1D-ND	4.29	1.43	1.37
15	A	801	CL0	O2A-CGA	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	827	CLA	O2A-CGA	4.29	1.45	1.33
16	A	823	CLA	C1D-ND	4.29	1.43	1.37
16	A	840	CLA	O2A-CGA	4.29	1.45	1.33
16	6	401	CLA	CHD-C4C	4.29	1.49	1.39
16	5	405	CLA	CHD-C1D	4.29	1.46	1.38
16	5	419	CLA	CHD-C4C	4.28	1.49	1.39
16	4	410	CLA	CHD-C4C	4.28	1.49	1.39
16	A	841	CLA	CHC-C1C	4.28	1.45	1.35
16	6	407	CLA	CHD-C4C	4.28	1.49	1.39
16	A	843	CLA	CHD-C1D	4.28	1.46	1.38
19	1	518	BCR	C14-C13	4.28	1.41	1.35
16	1	525	CLA	O2A-CGA	4.28	1.45	1.30
16	5	421	CLA	CHD-C4C	4.28	1.49	1.39
16	A	802	CLA	CHC-C1C	4.28	1.45	1.35
16	4	402	CLA	CHD-C1D	4.28	1.46	1.38
16	5	403	CLA	CHD-C1D	4.28	1.46	1.38
16	B	838	CLA	C1D-ND	4.28	1.43	1.37
16	1	526	CLA	CHD-C4C	4.28	1.49	1.39
16	A	842	CLA	O2A-CGA	4.27	1.45	1.33
16	1	515	CLA	CHD-C4C	4.27	1.49	1.39
16	B	804	CLA	O2A-CGA	4.27	1.45	1.33
16	A	824	CLA	C1D-ND	4.27	1.43	1.37
16	6	402	CLA	CHD-C4C	4.27	1.49	1.39
16	5	406	CLA	CHD-C4C	4.27	1.49	1.39
16	2	403	CLA	CHD-C4C	4.27	1.49	1.39
16	A	827	CLA	O2A-CGA	4.27	1.45	1.33
16	1	503	CLA	CHD-C4C	4.27	1.49	1.39
16	A	811	CLA	C3B-C2B	4.26	1.46	1.40
16	2	405	CLA	CHD-C4C	4.26	1.49	1.39
16	5	415	CLA	CHD-C1D	4.26	1.46	1.38
16	B	835	CLA	C1D-ND	4.26	1.43	1.37
16	5	417	CLA	CHD-C4C	4.26	1.49	1.39
16	5	422	CLA	CHD-C4C	4.26	1.49	1.39
16	A	822	CLA	C3B-C2B	4.26	1.46	1.40
16	4	411	CLA	CHD-C4C	4.26	1.49	1.39
16	1	510	CLA	CHD-C1D	4.26	1.46	1.38
16	A	836	CLA	C1D-ND	4.26	1.43	1.37
16	B	805	CLA	C1D-ND	4.25	1.43	1.37
16	B	819	CLA	CHD-C1D	4.25	1.46	1.38
16	B	819	CLA	CHD-C4C	4.25	1.48	1.39
16	5	410	CLA	CHD-C1D	4.25	1.46	1.38
16	A	806	CLA	C3C-C2C	4.25	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	409	CLA	CHD-C1D	4.25	1.46	1.38
16	B	839	CLA	O2A-CGA	4.25	1.45	1.33
16	4	404	CLA	CHD-C4C	4.25	1.48	1.39
16	4	409	CLA	CHD-C4C	4.25	1.48	1.39
16	1	503	CLA	O2A-CGA	4.25	1.45	1.33
16	4	402	CLA	CHD-C4C	4.25	1.48	1.39
16	B	840	CLA	C1D-ND	4.24	1.43	1.37
16	A	838	CLA	O2A-CGA	4.24	1.45	1.33
16	4	408	CLA	CHD-C4C	4.24	1.48	1.39
16	1	512	CLA	CHD-C1D	4.24	1.46	1.38
16	6	409	CLA	CHD-C4C	4.24	1.48	1.39
16	1	514	CLA	CHD-C4C	4.24	1.48	1.39
19	F	205	BCR	C21-C22	4.24	1.41	1.35
16	6	404	CLA	CHD-C4C	4.23	1.48	1.39
16	B	807	CLA	CHD-C1D	4.23	1.46	1.38
16	3	401	CLA	CHD-C4C	4.23	1.48	1.39
16	B	807	CLA	C3B-C2B	4.23	1.46	1.40
16	6	406	CLA	CHD-C4C	4.22	1.48	1.39
16	1	511	CLA	CHD-C4C	4.22	1.48	1.39
16	1	525	CLA	CHD-C4C	4.22	1.48	1.39
16	B	832	CLA	O2A-CGA	4.22	1.45	1.33
16	B	836	CLA	CHD-C1D	4.22	1.46	1.38
16	4	403	CLA	CHD-C1D	4.21	1.46	1.38
16	2	404	CLA	CHD-C4C	4.21	1.48	1.39
16	5	410	CLA	CHD-C4C	4.21	1.48	1.39
16	1	505	CLA	CHD-C4C	4.21	1.48	1.39
16	A	826	CLA	CHC-C1C	4.21	1.45	1.35
16	B	831	CLA	CHD-C1D	4.21	1.46	1.38
16	B	814	CLA	O2A-CGA	4.21	1.45	1.33
16	5	418	CLA	CHD-C4C	4.21	1.48	1.39
16	4	407	CLA	CHD-C4C	4.21	1.48	1.39
16	5	416	CLA	CHD-C4C	4.20	1.48	1.39
16	B	801	CLA	CHD-C1D	4.20	1.46	1.38
16	A	803	CLA	O2A-CGA	4.20	1.45	1.33
16	2	406	CLA	CHD-C4C	4.19	1.48	1.39
16	A	812	CLA	O2A-CGA	4.19	1.45	1.33
16	A	826	CLA	O2A-CGA	4.19	1.45	1.33
16	5	407	CLA	CHD-C4C	4.19	1.48	1.39
16	2	401	CLA	CHD-C4C	4.19	1.48	1.39
16	4	406	CLA	CHD-C4C	4.19	1.48	1.39
16	2	402	CLA	CHD-C4C	4.18	1.48	1.39
16	4	403	CLA	CHD-C4C	4.18	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	506	CLA	CHD-C1D	4.18	1.46	1.38
16	B	811	CLA	CHD-C1D	4.18	1.46	1.38
16	5	412	CLA	CHD-C4C	4.17	1.48	1.39
16	B	806	CLA	O2A-CGA	4.17	1.45	1.33
16	B	838	CLA	CHD-C1D	4.17	1.46	1.38
16	1	502	CLA	CHD-C4C	4.17	1.48	1.39
16	B	819	CLA	O2A-CGA	4.17	1.45	1.33
16	5	414	CLA	CHD-C1D	4.16	1.46	1.38
16	1	507	CLA	CHD-C4C	4.16	1.48	1.39
16	5	403	CLA	CHD-C4C	4.16	1.48	1.39
16	B	826	CLA	O2A-CGA	4.16	1.45	1.33
16	A	835	CLA	O2A-CGA	4.16	1.45	1.33
16	1	513	CLA	CHD-C1D	4.15	1.46	1.38
16	A	816	CLA	CHD-C1D	4.15	1.46	1.38
19	5	402	BCR	C10-C9	4.15	1.41	1.35
16	1	510	CLA	CHD-C4C	4.15	1.48	1.39
19	I	102	BCR	C14-C13	4.15	1.41	1.35
16	B	837	CLA	O2A-CGA	4.15	1.45	1.33
16	A	821	CLA	O2A-CGA	4.14	1.45	1.33
16	A	822	CLA	CHD-C4C	4.14	1.48	1.39
16	X	101	CLA	C1D-ND	4.14	1.42	1.37
16	A	828	CLA	C1D-ND	4.14	1.42	1.37
16	B	813	CLA	C1D-ND	4.13	1.42	1.37
16	5	404	CLA	CHD-C1D	4.13	1.46	1.38
16	5	411	CLA	CHD-C4C	4.13	1.48	1.39
16	5	415	CLA	CHD-C4C	4.13	1.48	1.39
19	1	517	BCR	C17-C18	4.13	1.41	1.35
16	A	822	CLA	O2A-CGA	4.12	1.45	1.33
16	A	809	CLA	CHD-C1D	4.12	1.46	1.38
19	K	102	BCR	C21-C22	4.12	1.41	1.35
16	1	512	CLA	CHD-C4C	4.12	1.48	1.39
16	A	843	CLA	O2A-CGA	4.12	1.45	1.33
16	A	830	CLA	O2A-CGA	4.12	1.45	1.33
16	B	803	CLA	O2A-CGA	4.12	1.45	1.33
16	B	836	CLA	CHD-C4C	4.12	1.48	1.39
16	B	837	CLA	C3B-C2B	4.11	1.46	1.40
16	J	101	CLA	CHD-C1D	4.11	1.46	1.38
16	B	805	CLA	CHD-C1D	4.11	1.46	1.38
16	B	809	CLA	C1D-ND	4.11	1.42	1.37
19	A	847	BCR	C10-C9	4.11	1.41	1.35
16	A	806	CLA	C1D-ND	4.11	1.42	1.37
19	1	518	BCR	C21-C22	4.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	405	CLA	CHD-C4C	4.11	1.48	1.39
16	A	802	CLA	CHD-C1D	4.11	1.46	1.38
16	A	843	CLA	C1D-ND	4.10	1.42	1.37
19	1	517	BCR	C10-C9	4.10	1.41	1.35
16	B	835	CLA	CHD-C1D	4.10	1.46	1.38
16	1	501	CLA	CHD-C1D	4.10	1.46	1.38
16	B	824	CLA	O2A-CGA	4.10	1.45	1.33
16	J	102	CLA	CHD-C4C	4.10	1.48	1.39
16	A	809	CLA	O2A-CGA	4.10	1.45	1.33
16	A	824	CLA	CHD-C1D	4.10	1.46	1.38
16	A	821	CLA	CHD-C4C	4.09	1.48	1.39
16	A	834	CLA	O2A-CGA	4.09	1.45	1.33
16	A	817	CLA	CHD-C1D	4.09	1.46	1.38
16	1	502	CLA	CHD-C1D	4.08	1.46	1.38
19	I	101	BCR	C10-C9	4.08	1.41	1.35
16	A	803	CLA	CHD-C4C	4.08	1.48	1.39
16	A	832	CLA	C1D-ND	4.08	1.42	1.37
16	A	842	CLA	CHD-C1D	4.07	1.46	1.38
16	B	830	CLA	CHD-C1D	4.07	1.46	1.38
16	A	838	CLA	CHD-C1D	4.07	1.46	1.38
19	1	518	BCR	C17-C18	4.07	1.41	1.35
16	5	409	CLA	CHD-C4C	4.07	1.48	1.39
16	B	824	CLA	C1D-ND	4.07	1.42	1.37
16	A	834	CLA	C1D-ND	4.06	1.42	1.37
16	1	520	CLA	CHD-C4C	4.06	1.48	1.39
16	B	821	CLA	CHD-C1D	4.05	1.46	1.38
16	B	823	CLA	C1D-ND	4.05	1.42	1.37
16	B	838	CLA	C3B-C2B	4.05	1.46	1.40
16	1	509	CLA	CHD-C1D	4.05	1.46	1.38
16	B	807	CLA	O2A-CGA	4.05	1.45	1.33
16	A	828	CLA	O2A-CGA	4.04	1.45	1.33
15	A	801	CL0	CHD-C1D	4.04	1.46	1.38
16	A	822	CLA	C1D-ND	4.04	1.42	1.37
16	A	829	CLA	O2A-CGA	4.04	1.45	1.33
16	1	504	CLA	CHD-C1D	4.04	1.46	1.38
16	B	822	CLA	CHD-C1D	4.04	1.46	1.38
16	A	827	CLA	CHD-C4C	4.03	1.48	1.39
16	1	506	CLA	CHD-C4C	4.03	1.48	1.39
19	A	851	BCR	C10-C9	4.03	1.41	1.35
16	A	829	CLA	CHD-C1D	4.03	1.46	1.38
16	A	841	CLA	O2A-CGA	4.03	1.45	1.33
16	A	810	CLA	CHD-C1D	4.03	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	402	BCR	C14-C13	4.03	1.41	1.35
16	A	825	CLA	CHD-C1D	4.03	1.46	1.38
16	J	101	CLA	CHD-C4C	4.01	1.48	1.39
16	B	808	CLA	C1D-ND	4.01	1.42	1.37
16	1	508	CLA	CHD-C4C	4.01	1.48	1.39
16	A	820	CLA	CHD-C4C	4.01	1.48	1.39
16	A	835	CLA	C1D-ND	4.01	1.42	1.37
16	B	831	CLA	CHD-C4C	4.01	1.48	1.39
16	B	825	CLA	O2A-CGA	4.01	1.45	1.33
16	B	829	CLA	C1D-ND	4.00	1.42	1.37
16	A	834	CLA	CHD-C1D	4.00	1.46	1.38
16	K	101	CLA	CHD-C4C	4.00	1.48	1.39
16	A	811	CLA	CHD-C1D	4.00	1.46	1.38
16	A	833	CLA	CHD-C1D	4.00	1.46	1.38
16	B	825	CLA	CHD-C1D	4.00	1.46	1.38
16	1	521	CLA	CHD-C4C	4.00	1.48	1.39
16	B	811	CLA	CHD-C4C	4.00	1.48	1.39
16	B	834	CLA	C1D-ND	3.99	1.42	1.37
16	1	508	CLA	CHD-C1D	3.99	1.46	1.38
16	A	808	CLA	CHD-C1D	3.99	1.46	1.38
16	A	839	CLA	CHD-C1D	3.99	1.46	1.38
16	1	519	CLA	CHD-C4C	3.99	1.48	1.39
19	B	844	BCR	C17-C18	3.98	1.41	1.35
16	A	808	CLA	C3D-C2D	3.98	1.50	1.39
16	B	801	CLA	O2A-CGA	3.98	1.45	1.33
19	B	844	BCR	C10-C9	3.97	1.41	1.35
16	A	809	CLA	CHD-C4C	3.97	1.48	1.39
19	F	205	BCR	C10-C9	3.97	1.41	1.35
16	B	806	CLA	CHD-C1D	3.97	1.46	1.38
16	1	504	CLA	CHD-C4C	3.97	1.48	1.39
16	B	833	CLA	C1D-ND	3.96	1.42	1.37
16	A	829	CLA	C3B-C2B	3.96	1.45	1.40
16	A	820	CLA	CHD-C1D	3.96	1.46	1.38
19	B	845	BCR	C17-C18	3.96	1.41	1.35
16	A	821	CLA	CHD-C1D	3.95	1.46	1.38
16	B	839	CLA	C1D-ND	3.95	1.42	1.37
16	B	816	CLA	CHD-C4C	3.95	1.48	1.39
19	4	401	BCR	C10-C9	3.95	1.41	1.35
19	1	523	BCR	C10-C9	3.95	1.41	1.35
16	A	812	CLA	C1D-ND	3.95	1.42	1.37
16	X	101	CLA	CHD-C4C	3.95	1.48	1.39
16	B	840	CLA	O2A-CGA	3.95	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	519	CLA	OBD-CAD	3.94	1.29	1.22
19	4	401	BCR	C21-C22	3.94	1.41	1.35
16	B	839	CLA	CHD-C1D	3.94	1.46	1.38
16	1	513	CLA	CHD-C4C	3.93	1.48	1.39
19	A	848	BCR	C10-C9	3.93	1.41	1.35
16	A	816	CLA	CHD-C4C	3.93	1.48	1.39
16	B	830	CLA	CHD-C4C	3.93	1.48	1.39
16	B	834	CLA	CHD-C1D	3.93	1.46	1.38
19	B	845	BCR	C10-C9	3.93	1.41	1.35
16	B	820	CLA	CHD-C1D	3.93	1.46	1.38
16	A	815	CLA	C1D-ND	3.93	1.42	1.37
16	A	843	CLA	CHD-C4C	3.92	1.48	1.39
19	5	402	BCR	C21-C22	3.92	1.41	1.35
19	I	102	BCR	C10-C9	3.92	1.41	1.35
16	F	204	CLA	CHD-C1D	3.91	1.46	1.38
16	1	519	CLA	CHD-C1D	3.91	1.46	1.38
16	B	832	CLA	CHD-C4C	3.91	1.48	1.39
16	X	101	CLA	CHD-C1D	3.91	1.46	1.38
16	A	811	CLA	CHD-C4C	3.91	1.48	1.39
16	A	825	CLA	C1D-ND	3.91	1.42	1.37
16	B	818	CLA	CHD-C1D	3.91	1.46	1.38
16	B	840	CLA	CHD-C1D	3.90	1.46	1.38
16	A	817	CLA	CHD-C4C	3.90	1.48	1.39
16	B	804	CLA	CHD-C4C	3.90	1.48	1.39
16	B	821	CLA	CHD-C4C	3.90	1.48	1.39
16	B	841	CLA	C1D-ND	3.90	1.42	1.37
16	B	823	CLA	C3D-C2D	3.90	1.49	1.39
19	B	853	BCR	C10-C9	3.90	1.40	1.35
16	1	509	CLA	CHD-C4C	3.89	1.48	1.39
16	A	819	CLA	CHD-C1D	3.89	1.45	1.38
16	A	805	CLA	C3D-C2D	3.89	1.49	1.39
16	B	804	CLA	CHD-C1D	3.89	1.45	1.38
15	A	801	CL0	C1D-ND	3.89	1.42	1.37
16	A	814	CLA	CHD-C1D	3.89	1.45	1.38
16	B	802	CLA	CHD-C1D	3.88	1.45	1.38
16	A	831	CLA	C3D-C2D	3.88	1.49	1.39
16	A	839	CLA	O2A-CGA	3.88	1.44	1.33
16	B	820	CLA	CHD-C4C	3.87	1.48	1.39
16	A	826	CLA	CHD-C1D	3.87	1.45	1.38
16	A	839	CLA	CHD-C4C	3.87	1.48	1.39
16	A	823	CLA	CHD-C4C	3.87	1.48	1.39
16	A	832	CLA	C3B-C2B	3.87	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	414	CLA	CHD-C4C	3.87	1.48	1.39
16	K	101	CLA	CHD-C1D	3.87	1.45	1.38
16	B	822	CLA	C3D-C2D	3.87	1.49	1.39
16	A	807	CLA	O2A-CGA	3.87	1.44	1.33
16	1	503	CLA	C3D-C2D	3.87	1.49	1.39
16	5	413	CLA	OBD-CAD	3.86	1.29	1.22
16	B	813	CLA	O2A-CGA	3.86	1.44	1.33
16	A	836	CLA	CHD-C1D	3.86	1.45	1.38
16	B	837	CLA	CHD-C4C	3.86	1.48	1.39
16	1	501	CLA	CHD-C4C	3.86	1.48	1.39
16	1	509	CLA	C3D-C2D	3.86	1.49	1.39
16	B	818	CLA	O2A-CGA	3.86	1.44	1.33
16	A	830	CLA	CHD-C1D	3.86	1.45	1.38
16	B	838	CLA	CHD-C4C	3.85	1.48	1.39
16	1	506	CLA	OBD-CAD	3.85	1.29	1.22
16	4	405	CLA	C3D-C2D	3.85	1.49	1.39
16	B	805	CLA	CHD-C4C	3.85	1.48	1.39
16	6	408	CLA	C3D-C2D	3.85	1.49	1.39
16	A	813	CLA	CHD-C1D	3.85	1.45	1.38
16	1	515	CLA	C3D-C2D	3.85	1.49	1.39
19	B	843	BCR	C10-C9	3.85	1.40	1.35
16	B	814	CLA	CHD-C1D	3.85	1.45	1.38
16	B	817	CLA	C1D-ND	3.85	1.42	1.37
16	1	513	CLA	OBD-CAD	3.85	1.29	1.22
16	A	838	CLA	CHD-C4C	3.84	1.48	1.39
16	F	201	CLA	C1D-ND	3.84	1.42	1.37
16	K	101	CLA	C3D-C2D	3.84	1.49	1.39
16	6	402	CLA	C3D-C2D	3.84	1.49	1.39
16	A	807	CLA	CHD-C1D	3.84	1.45	1.38
16	4	404	CLA	C3D-C2D	3.84	1.49	1.39
16	1	520	CLA	CHD-C1D	3.83	1.45	1.38
16	5	414	CLA	C3D-C2D	3.83	1.49	1.39
16	A	823	CLA	CHD-C1D	3.83	1.45	1.38
16	B	815	CLA	CHD-C4C	3.83	1.48	1.39
16	B	839	CLA	CHD-C4C	3.83	1.48	1.39
16	4	409	CLA	C3D-C2D	3.83	1.49	1.39
16	6	407	CLA	OBD-CAD	3.83	1.29	1.22
19	M	102	BCR	C21-C22	3.82	1.40	1.35
16	B	823	CLA	CHD-C1D	3.82	1.45	1.38
16	1	507	CLA	C3D-C2D	3.82	1.49	1.39
16	A	833	CLA	CHD-C4C	3.82	1.48	1.39
16	5	419	CLA	OBD-CAD	3.82	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	502	CLA	C3D-C2D	3.82	1.49	1.39
16	6	404	CLA	C3D-C2D	3.82	1.49	1.39
19	A	846	BCR	C14-C13	3.82	1.40	1.35
16	6	403	CLA	C3D-C2D	3.82	1.49	1.39
16	F	201	CLA	CHD-C1D	3.82	1.45	1.38
16	5	403	CLA	C3D-C2D	3.82	1.49	1.39
16	2	402	CLA	C3D-C2D	3.81	1.49	1.39
16	6	401	CLA	OBD-CAD	3.81	1.29	1.22
16	B	803	CLA	CHD-C1D	3.81	1.45	1.38
16	3	401	CLA	C3D-C2D	3.81	1.49	1.39
16	6	409	CLA	OBD-CAD	3.81	1.29	1.22
16	A	815	CLA	C3D-C2D	3.80	1.49	1.39
16	A	802	CLA	O2A-CGA	3.80	1.44	1.33
19	5	402	BCR	C17-C18	3.80	1.40	1.35
16	A	803	CLA	C3D-C2D	3.80	1.49	1.39
16	6	409	CLA	C3D-C2D	3.80	1.49	1.39
19	A	849	BCR	C17-C18	3.80	1.40	1.35
16	5	416	CLA	C3D-C2D	3.80	1.49	1.39
19	1	516	BCR	C21-C22	3.80	1.40	1.35
16	5	418	CLA	OBD-CAD	3.80	1.29	1.22
16	5	408	CLA	C3D-C2D	3.80	1.49	1.39
16	6	406	CLA	C3D-C2D	3.80	1.49	1.39
16	1	526	CLA	OBD-CAD	3.80	1.29	1.22
16	B	828	CLA	CHD-C1D	3.80	1.45	1.38
16	A	837	CLA	CHD-C1D	3.80	1.45	1.38
16	2	406	CLA	C3D-C2D	3.80	1.49	1.39
16	A	841	CLA	C3D-C2D	3.79	1.49	1.39
19	M	102	BCR	C14-C13	3.79	1.40	1.35
16	5	406	CLA	OBD-CAD	3.79	1.29	1.22
16	6	404	CLA	OBD-CAD	3.79	1.29	1.22
16	5	406	CLA	C3D-C2D	3.79	1.49	1.39
19	5	420	BCR	C17-C18	3.79	1.40	1.35
16	B	829	CLA	CHD-C4C	3.79	1.47	1.39
16	4	406	CLA	C3D-C2D	3.79	1.49	1.39
16	A	819	CLA	CHD-C4C	3.79	1.47	1.39
16	5	416	CLA	OBD-CAD	3.79	1.29	1.22
16	2	401	CLA	C3D-C2D	3.79	1.49	1.39
19	J	104	BCR	C10-C9	3.79	1.40	1.35
16	A	817	CLA	OBD-CAD	3.79	1.29	1.22
16	B	814	CLA	CHD-C4C	3.79	1.47	1.39
16	4	406	CLA	OBD-CAD	3.79	1.29	1.22
16	3	401	CLA	OBD-CAD	3.79	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4	410	CLA	OBD-CAD	3.78	1.29	1.22
16	5	415	CLA	OBD-CAD	3.78	1.29	1.22
16	4	402	CLA	C3D-C2D	3.78	1.49	1.39
16	4	403	CLA	OBD-CAD	3.78	1.29	1.22
16	4	407	CLA	OBD-CAD	3.78	1.29	1.22
16	5	411	CLA	OBD-CAD	3.78	1.29	1.22
16	5	419	CLA	C3D-C2D	3.78	1.49	1.39
16	2	403	CLA	OBD-CAD	3.78	1.29	1.22
16	B	825	CLA	CHD-C4C	3.78	1.47	1.39
16	B	829	CLA	C3B-C2B	3.78	1.45	1.40
19	K	102	BCR	C10-C9	3.78	1.40	1.35
16	5	410	CLA	OBD-CAD	3.78	1.29	1.22
16	A	834	CLA	CHD-C4C	3.78	1.47	1.39
16	5	418	CLA	C3D-C2D	3.78	1.49	1.39
16	4	408	CLA	C3D-C2D	3.78	1.49	1.39
16	A	808	CLA	CHD-C4C	3.78	1.47	1.39
16	1	508	CLA	OBD-CAD	3.78	1.29	1.22
16	A	810	CLA	CHD-C4C	3.77	1.47	1.39
16	4	409	CLA	OBD-CAD	3.77	1.29	1.22
16	4	402	CLA	OBD-CAD	3.77	1.29	1.22
16	K	103	CLA	CHD-C1D	3.77	1.45	1.38
16	4	404	CLA	OBD-CAD	3.77	1.29	1.22
16	2	404	CLA	C3D-C2D	3.77	1.49	1.39
16	2	401	CLA	OBD-CAD	3.77	1.29	1.22
16	A	824	CLA	CHD-C4C	3.77	1.47	1.39
16	1	525	CLA	OBD-CAD	3.77	1.29	1.22
16	2	403	CLA	C3D-C2D	3.77	1.49	1.39
16	2	406	CLA	OBD-CAD	3.77	1.29	1.22
16	1	515	CLA	OBD-CAD	3.76	1.29	1.22
16	B	818	CLA	CHD-C4C	3.76	1.47	1.39
16	4	411	CLA	C3D-C2D	3.76	1.49	1.39
16	2	405	CLA	OBD-CAD	3.76	1.29	1.22
16	5	421	CLA	OBD-CAD	3.76	1.29	1.22
16	5	417	CLA	OBD-CAD	3.76	1.29	1.22
16	5	405	CLA	OBD-CAD	3.76	1.29	1.22
16	4	405	CLA	OBD-CAD	3.76	1.29	1.22
16	6	403	CLA	OBD-CAD	3.76	1.29	1.22
16	6	407	CLA	C3D-C2D	3.76	1.49	1.39
16	5	409	CLA	C3D-C2D	3.76	1.49	1.39
16	5	413	CLA	C3D-C2D	3.75	1.49	1.39
16	2	402	CLA	OBD-CAD	3.75	1.28	1.22
16	1	505	CLA	C3D-C2D	3.75	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	807	CLA	CHD-C4C	3.75	1.47	1.39
16	A	830	CLA	C1D-ND	3.75	1.42	1.37
16	A	804	CLA	CHD-C4C	3.75	1.47	1.39
16	1	514	CLA	OBD-CAD	3.75	1.28	1.22
16	6	402	CLA	OBD-CAD	3.75	1.28	1.22
16	6	405	CLA	OBD-CAD	3.75	1.28	1.22
16	A	840	CLA	C1D-ND	3.75	1.42	1.37
16	1	512	CLA	OBD-CAD	3.75	1.28	1.22
16	2	405	CLA	C3D-C2D	3.75	1.49	1.39
16	B	806	CLA	CHD-C4C	3.75	1.47	1.39
16	A	842	CLA	C3D-C2D	3.75	1.49	1.39
16	2	404	CLA	OBD-CAD	3.74	1.28	1.22
16	6	408	CLA	OBD-CAD	3.74	1.28	1.22
16	B	838	CLA	O2A-CGA	3.74	1.44	1.33
19	B	843	BCR	C14-C13	3.74	1.40	1.35
16	1	514	CLA	C3D-C2D	3.74	1.49	1.39
16	A	830	CLA	OBD-CAD	3.74	1.28	1.22
16	A	821	CLA	C3D-C2D	3.74	1.49	1.39
16	5	408	CLA	OBD-CAD	3.74	1.28	1.22
16	A	818	CLA	CHD-C4C	3.74	1.47	1.39
16	A	826	CLA	C3D-C2D	3.74	1.49	1.39
16	B	833	CLA	C3D-C2D	3.74	1.49	1.39
16	1	511	CLA	OBD-CAD	3.74	1.28	1.22
16	B	822	CLA	CHD-C4C	3.74	1.47	1.39
16	A	814	CLA	CHD-C4C	3.74	1.47	1.39
16	A	835	CLA	OBD-CAD	3.73	1.28	1.22
16	A	812	CLA	CHD-C4C	3.73	1.47	1.39
16	1	510	CLA	C3D-C2D	3.73	1.49	1.39
16	1	502	CLA	OBD-CAD	3.73	1.28	1.22
16	6	405	CLA	C3D-C2D	3.73	1.49	1.39
16	1	519	CLA	C3D-C2D	3.73	1.49	1.39
16	A	822	CLA	CHD-C1D	3.73	1.45	1.38
16	B	812	CLA	CHD-C4C	3.73	1.47	1.39
16	1	526	CLA	C3D-C2D	3.73	1.49	1.39
16	1	505	CLA	OBD-CAD	3.73	1.28	1.22
16	6	401	CLA	C3D-C2D	3.73	1.49	1.39
19	B	853	BCR	C17-C18	3.73	1.40	1.35
16	4	407	CLA	C3D-C2D	3.73	1.49	1.39
16	B	826	CLA	CHD-C4C	3.72	1.47	1.39
19	J	103	BCR	C14-C13	3.72	1.40	1.35
16	5	404	CLA	OBD-CAD	3.72	1.28	1.22
16	5	411	CLA	C3D-C2D	3.72	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	813	CLA	C3D-C2D	3.72	1.49	1.39
16	1	525	CLA	C3D-C2D	3.72	1.49	1.39
16	6	406	CLA	OBD-CAD	3.72	1.28	1.22
16	5	407	CLA	OBD-CAD	3.71	1.28	1.22
19	A	851	BCR	C17-C18	3.71	1.40	1.35
19	4	401	BCR	C14-C13	3.71	1.40	1.35
16	B	802	CLA	C1D-ND	3.71	1.42	1.37
16	A	836	CLA	C3D-C2D	3.71	1.49	1.39
16	B	823	CLA	CHD-C4C	3.71	1.47	1.39
16	5	412	CLA	C3D-C2D	3.71	1.49	1.39
16	A	833	CLA	C3D-C2D	3.71	1.49	1.39
16	5	415	CLA	C3D-C2D	3.71	1.49	1.39
16	4	411	CLA	OBD-CAD	3.70	1.28	1.22
16	A	809	CLA	C3D-C2D	3.70	1.49	1.39
16	B	811	CLA	C3D-C2D	3.70	1.49	1.39
16	5	405	CLA	C3D-C2D	3.70	1.49	1.39
16	B	837	CLA	CHD-C1D	3.70	1.45	1.38
19	B	848	BCR	C10-C9	3.70	1.40	1.35
19	1	522	BCR	C10-C9	3.70	1.40	1.35
16	K	103	CLA	C3D-C2D	3.69	1.49	1.39
16	B	821	CLA	C3D-C2D	3.69	1.49	1.39
16	A	815	CLA	CHD-C4C	3.69	1.47	1.39
16	B	803	CLA	CHD-C4C	3.69	1.47	1.39
16	B	820	CLA	OBD-CAD	3.69	1.28	1.22
16	1	511	CLA	C3D-C2D	3.69	1.49	1.39
16	1	513	CLA	C3D-C2D	3.69	1.49	1.39
19	B	847	BCR	C14-C13	3.69	1.40	1.35
16	A	828	CLA	CHD-C4C	3.69	1.47	1.39
16	5	403	CLA	OBD-CAD	3.69	1.28	1.22
16	1	507	CLA	OBD-CAD	3.69	1.28	1.22
19	B	844	BCR	C14-C13	3.69	1.40	1.35
16	B	810	CLA	CHD-C4C	3.69	1.47	1.39
19	5	420	BCR	C21-C22	3.69	1.40	1.35
16	A	810	CLA	OBD-CAD	3.69	1.28	1.22
16	B	805	CLA	C3D-C2D	3.69	1.49	1.39
16	4	408	CLA	OBD-CAD	3.69	1.28	1.22
16	A	827	CLA	C3D-C2D	3.68	1.49	1.39
16	B	841	CLA	CHD-C1D	3.68	1.45	1.38
16	A	820	CLA	O2A-CGA	3.68	1.44	1.33
19	J	103	BCR	C8-C9	-3.68	1.38	1.45
16	B	820	CLA	C3D-C2D	3.68	1.49	1.39
19	A	849	BCR	C21-C22	3.67	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	I	102	BCR	C17-C18	3.67	1.40	1.35
16	5	417	CLA	C3D-C2D	3.67	1.49	1.39
16	B	812	CLA	CHD-C1D	3.67	1.45	1.38
16	A	817	CLA	C3D-C2D	3.67	1.49	1.39
16	1	503	CLA	OBD-CAD	3.67	1.28	1.22
16	A	823	CLA	C3D-C2D	3.67	1.49	1.39
16	B	821	CLA	OBD-CAD	3.66	1.28	1.22
16	5	410	CLA	C3D-C2D	3.66	1.49	1.39
16	B	813	CLA	OBD-CAD	3.66	1.28	1.22
16	A	815	CLA	CHD-C1D	3.66	1.45	1.38
19	A	849	BCR	C14-C13	3.65	1.40	1.35
16	B	840	CLA	CHD-C4C	3.65	1.47	1.39
16	B	808	CLA	CHD-C4C	3.65	1.47	1.39
19	B	844	BCR	C21-C22	3.65	1.40	1.35
16	5	409	CLA	OBD-CAD	3.64	1.28	1.22
16	B	815	CLA	OBD-CAD	3.64	1.28	1.22
16	A	841	CLA	CHD-C1D	3.64	1.45	1.38
16	B	835	CLA	CHD-C4C	3.64	1.47	1.39
16	A	840	CLA	CHD-C4C	3.64	1.47	1.39
16	A	807	CLA	CHD-C4C	3.64	1.47	1.39
16	A	825	CLA	C3D-C2D	3.64	1.49	1.39
16	A	835	CLA	C3D-C2D	3.64	1.49	1.39
16	1	521	CLA	C3D-C2D	3.64	1.49	1.39
16	A	818	CLA	CHD-C1D	3.64	1.45	1.38
16	5	422	CLA	C3D-C2D	3.64	1.49	1.39
16	A	805	CLA	CHD-C4C	3.64	1.47	1.39
16	B	817	CLA	CHD-C4C	3.64	1.47	1.39
16	A	837	CLA	CHD-C4C	3.64	1.47	1.39
16	B	836	CLA	OBD-CAD	3.63	1.28	1.22
16	J	102	CLA	C3D-C2D	3.63	1.49	1.39
19	B	845	BCR	C14-C13	3.63	1.40	1.35
16	B	803	CLA	C3D-C2D	3.63	1.49	1.39
16	4	410	CLA	C3D-C2D	3.63	1.49	1.39
16	B	804	CLA	C3D-C2D	3.63	1.49	1.39
16	A	843	CLA	C3D-C2D	3.63	1.49	1.39
16	1	508	CLA	C3D-C2D	3.63	1.49	1.39
16	B	807	CLA	C3D-C2D	3.63	1.49	1.39
16	B	825	CLA	C3D-C2D	3.62	1.49	1.39
16	J	102	CLA	OBD-CAD	3.62	1.28	1.22
16	A	825	CLA	CHD-C4C	3.62	1.47	1.39
16	A	803	CLA	OBD-CAD	3.62	1.28	1.22
16	A	830	CLA	C3D-C2D	3.62	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	802	CLA	C1D-ND	3.62	1.42	1.37
16	B	809	CLA	C3B-C2B	3.62	1.45	1.40
16	B	841	CLA	CHD-C4C	3.62	1.47	1.39
19	B	848	BCR	C21-C22	3.62	1.40	1.35
16	A	804	CLA	CHD-C1D	3.61	1.45	1.38
16	B	817	CLA	CHD-C1D	3.61	1.45	1.38
16	B	816	CLA	CHD-C1D	3.61	1.45	1.38
16	F	204	CLA	CHD-C4C	3.61	1.47	1.39
16	J	101	CLA	OBD-CAD	3.61	1.28	1.22
16	A	842	CLA	CHD-C4C	3.61	1.47	1.39
19	B	843	BCR	C21-C22	3.61	1.40	1.35
16	B	829	CLA	C3D-C2D	3.60	1.49	1.39
16	B	819	CLA	OBD-CAD	3.60	1.28	1.22
16	B	834	CLA	CHD-C4C	3.60	1.47	1.39
16	B	838	CLA	C3D-C2D	3.60	1.48	1.39
16	5	412	CLA	OBD-CAD	3.60	1.28	1.22
16	A	818	CLA	C3D-C2D	3.59	1.48	1.39
16	A	827	CLA	CHD-C1D	3.59	1.45	1.38
16	F	201	CLA	OBD-CAD	3.59	1.28	1.22
16	B	835	CLA	OBD-CAD	3.59	1.28	1.22
16	4	403	CLA	C3D-C2D	3.59	1.48	1.39
16	B	801	CLA	CHD-C4C	3.59	1.47	1.39
16	A	805	CLA	CHD-C1D	3.58	1.45	1.38
16	B	829	CLA	OBD-CAD	3.58	1.28	1.22
16	A	803	CLA	CHD-C1D	3.58	1.45	1.38
16	B	830	CLA	C3D-C2D	3.58	1.48	1.39
16	B	834	CLA	C3D-C2D	3.57	1.48	1.39
16	A	821	CLA	OBD-CAD	3.57	1.28	1.22
16	B	836	CLA	C3D-C2D	3.57	1.48	1.39
19	B	847	BCR	C8-C9	-3.57	1.38	1.45
16	A	832	CLA	CHD-C1D	3.57	1.45	1.38
16	5	421	CLA	C3D-C2D	3.57	1.48	1.39
19	A	846	BCR	C23-C22	-3.57	1.38	1.45
19	I	101	BCR	C17-C18	3.57	1.40	1.35
16	B	812	CLA	C3D-C2D	3.57	1.48	1.39
19	A	850	BCR	C23-C22	-3.57	1.38	1.45
16	B	835	CLA	C3D-C2D	3.57	1.48	1.39
16	A	826	CLA	CHD-C4C	3.56	1.47	1.39
16	A	835	CLA	CHD-C1D	3.56	1.45	1.38
16	B	809	CLA	CHD-C1D	3.56	1.45	1.38
16	B	824	CLA	CHD-C1D	3.56	1.45	1.38
19	K	102	BCR	C14-C13	3.56	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	422	CLA	OBD-CAD	3.56	1.28	1.22
16	K	103	CLA	CHD-C4C	3.56	1.47	1.39
16	A	841	CLA	OBD-CAD	3.56	1.28	1.22
16	B	829	CLA	CHD-C1D	3.56	1.45	1.38
19	F	202	BCR	C10-C9	3.56	1.40	1.35
19	I	101	BCR	C21-C22	3.55	1.40	1.35
19	M	102	BCR	C10-C9	3.55	1.40	1.35
16	B	819	CLA	C3D-C2D	3.55	1.48	1.39
16	B	831	CLA	C3D-C2D	3.55	1.48	1.39
16	1	520	CLA	C3D-C2D	3.55	1.48	1.39
16	A	822	CLA	C1B-NB	-3.55	1.32	1.35
19	4	401	BCR	C17-C18	3.55	1.40	1.35
16	B	802	CLA	C3D-C2D	3.55	1.48	1.39
16	A	836	CLA	CHD-C4C	3.55	1.47	1.39
16	B	813	CLA	CHD-C4C	3.55	1.47	1.39
16	A	829	CLA	CHD-C4C	3.55	1.47	1.39
16	B	832	CLA	C1D-ND	3.55	1.42	1.37
19	K	102	BCR	C17-C18	3.54	1.40	1.35
19	1	523	BCR	C14-C13	3.54	1.40	1.35
16	1	506	CLA	C3D-C2D	3.54	1.48	1.39
16	A	820	CLA	C3D-C2D	3.54	1.48	1.39
16	B	816	CLA	OBD-CAD	3.54	1.28	1.22
16	B	817	CLA	C3D-C2D	3.54	1.48	1.39
16	1	509	CLA	OBD-CAD	3.54	1.28	1.22
16	A	841	CLA	CHD-C4C	3.54	1.47	1.39
16	1	504	CLA	OBD-CAD	3.54	1.28	1.22
16	B	833	CLA	CHD-C1D	3.53	1.45	1.38
16	5	414	CLA	OBD-CAD	3.53	1.28	1.22
16	1	510	CLA	OBD-CAD	3.53	1.28	1.22
16	B	840	CLA	C3D-C2D	3.53	1.48	1.39
16	B	824	CLA	C3D-C2D	3.53	1.48	1.39
16	A	814	CLA	C3D-C2D	3.52	1.48	1.39
16	A	812	CLA	CHD-C1D	3.52	1.45	1.38
19	B	848	BCR	C14-C13	3.52	1.40	1.35
16	B	837	CLA	C3D-C2D	3.52	1.48	1.39
19	1	516	BCR	C17-C18	3.52	1.40	1.35
19	1	522	BCR	C14-C13	3.52	1.40	1.35
16	1	512	CLA	C3D-C2D	3.51	1.48	1.39
16	B	804	CLA	OBD-CAD	3.51	1.28	1.22
16	A	808	CLA	OBD-CAD	3.51	1.28	1.22
16	5	407	CLA	C3D-C2D	3.51	1.48	1.39
19	F	202	BCR	C17-C18	3.51	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	824	CLA	C3D-C2D	3.51	1.48	1.39
16	B	809	CLA	CHD-C4C	3.51	1.47	1.39
16	A	830	CLA	CHD-C4C	3.50	1.47	1.39
16	J	101	CLA	C3D-C2D	3.50	1.48	1.39
16	B	814	CLA	C3D-C2D	3.50	1.48	1.39
19	A	848	BCR	C23-C22	-3.50	1.38	1.45
16	5	404	CLA	C3D-C2D	3.50	1.48	1.39
16	B	813	CLA	CHD-C1D	3.50	1.45	1.38
19	B	846	BCR	C21-C22	3.50	1.40	1.35
16	F	201	CLA	CHD-C4C	3.50	1.47	1.39
15	A	801	CL0	C3D-C2D	3.49	1.48	1.39
16	1	521	CLA	OBD-CAD	3.49	1.28	1.22
19	J	103	BCR	C21-C22	3.49	1.40	1.35
19	A	847	BCR	C21-C22	3.49	1.40	1.35
16	A	816	CLA	OBD-CAD	3.48	1.28	1.22
16	A	822	CLA	C3D-C2D	3.48	1.48	1.39
16	A	840	CLA	CHD-C1D	3.48	1.45	1.38
16	A	812	CLA	C3D-C2D	3.48	1.48	1.39
16	A	813	CLA	C3D-C2D	3.48	1.48	1.39
19	A	847	BCR	C17-C18	3.48	1.40	1.35
19	A	848	BCR	C21-C22	3.47	1.40	1.35
16	B	824	CLA	CHD-C4C	3.47	1.47	1.39
16	A	829	CLA	C3D-C2D	3.47	1.48	1.39
16	A	827	CLA	OBD-CAD	3.47	1.28	1.22
16	B	826	CLA	CHD-C1D	3.47	1.45	1.38
16	B	803	CLA	OBD-CAD	3.47	1.28	1.22
19	1	522	BCR	C23-C22	-3.47	1.38	1.45
16	B	810	CLA	CHD-C1D	3.47	1.45	1.38
16	B	808	CLA	CHD-C1D	3.46	1.45	1.38
16	A	806	CLA	CHD-C4C	3.46	1.47	1.39
16	A	831	CLA	CHD-C4C	3.46	1.47	1.39
19	B	848	BCR	C8-C9	-3.45	1.38	1.45
16	A	837	CLA	OBD-CAD	3.45	1.28	1.22
19	B	853	BCR	C21-C22	3.45	1.40	1.35
16	A	832	CLA	CHD-C4C	3.45	1.47	1.39
16	A	802	CLA	C3D-C2D	3.45	1.48	1.39
16	A	839	CLA	C3D-C2D	3.45	1.48	1.39
16	A	816	CLA	C3D-C2D	3.44	1.48	1.39
16	A	813	CLA	CHD-C4C	3.44	1.47	1.39
16	B	825	CLA	OBD-CAD	3.44	1.28	1.22
16	A	831	CLA	CHD-C1D	3.44	1.45	1.38
16	B	833	CLA	CHD-C4C	3.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	806	CLA	OBD-CAD	3.44	1.28	1.22
16	B	808	CLA	OBD-CAD	3.44	1.28	1.22
19	M	102	BCR	C17-C18	3.44	1.40	1.35
16	F	201	CLA	C3D-C2D	3.43	1.48	1.39
16	B	801	CLA	C3D-C2D	3.43	1.48	1.39
16	1	504	CLA	C3D-C2D	3.43	1.48	1.39
16	B	802	CLA	CHD-C4C	3.43	1.47	1.39
19	B	853	BCR	C14-C13	3.43	1.40	1.35
16	B	822	CLA	OBD-CAD	3.43	1.28	1.22
16	B	826	CLA	C3D-C2D	3.43	1.48	1.39
16	A	843	CLA	OBD-CAD	3.43	1.28	1.22
19	A	848	BCR	C14-C13	3.42	1.40	1.35
19	B	843	BCR	C17-C18	3.42	1.40	1.35
19	F	205	BCR	C14-C13	3.42	1.40	1.35
16	F	204	CLA	C3D-C2D	3.42	1.48	1.39
16	K	103	CLA	OBD-CAD	3.41	1.28	1.22
19	A	846	BCR	C10-C9	3.41	1.40	1.35
16	X	101	CLA	C3D-C2D	3.41	1.48	1.39
16	A	828	CLA	CHD-C1D	3.41	1.45	1.38
16	A	812	CLA	OBD-CAD	3.41	1.28	1.22
19	I	102	BCR	C8-C9	-3.41	1.38	1.45
19	B	847	BCR	C21-C22	3.40	1.40	1.35
16	B	811	CLA	OBD-CAD	3.40	1.28	1.22
16	1	520	CLA	OBD-CAD	3.39	1.28	1.22
16	A	837	CLA	C3D-C2D	3.39	1.48	1.39
19	A	846	BCR	C21-C22	3.39	1.40	1.35
16	A	805	CLA	OBD-CAD	3.39	1.28	1.22
19	M	102	BCR	C8-C9	-3.39	1.38	1.45
16	B	828	CLA	CHD-C4C	3.39	1.47	1.39
16	A	828	CLA	C3D-C2D	3.38	1.48	1.39
19	1	522	BCR	C17-C18	3.38	1.40	1.35
16	B	809	CLA	C3D-C2D	3.38	1.48	1.39
16	A	832	CLA	C3D-C2D	3.37	1.48	1.39
16	A	833	CLA	OBD-CAD	3.37	1.28	1.22
16	B	803	CLA	C1D-ND	3.37	1.41	1.37
16	B	810	CLA	C3D-C2D	3.37	1.48	1.39
16	A	835	CLA	CHD-C4C	3.36	1.46	1.39
16	B	803	CLA	C1B-NB	-3.36	1.32	1.35
16	B	815	CLA	C3D-C2D	3.36	1.48	1.39
19	B	848	BCR	C17-C18	3.36	1.40	1.35
19	A	851	BCR	C23-C22	-3.36	1.38	1.45
16	B	832	CLA	C3D-C2D	3.36	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	828	CLA	C1D-ND	3.36	1.41	1.37
16	A	842	CLA	OBD-CAD	3.36	1.28	1.22
16	B	841	CLA	C3D-C2D	3.35	1.48	1.39
16	1	501	CLA	OBD-CAD	3.35	1.28	1.22
16	B	829	CLA	C1B-NB	-3.35	1.32	1.35
16	A	811	CLA	C3D-C2D	3.34	1.48	1.39
16	B	807	CLA	OBD-CAD	3.34	1.28	1.22
19	J	103	BCR	C10-C9	3.34	1.40	1.35
16	A	807	CLA	C3D-C2D	3.34	1.48	1.39
16	A	802	CLA	CHD-C4C	3.34	1.46	1.39
16	B	827	CLA	CHD-C1D	3.33	1.44	1.38
16	A	838	CLA	C3D-C2D	3.33	1.48	1.39
16	A	804	CLA	OBD-CAD	3.33	1.28	1.22
16	F	204	CLA	OBD-CAD	3.32	1.28	1.22
16	A	836	CLA	OBD-CAD	3.32	1.28	1.22
16	A	840	CLA	C3D-C2D	3.32	1.48	1.39
19	F	205	BCR	C17-C18	3.32	1.40	1.35
15	A	801	CL0	OBD-CAD	3.32	1.28	1.22
16	A	825	CLA	OBD-CAD	3.31	1.28	1.22
16	B	827	CLA	CHD-C4C	3.31	1.46	1.39
19	J	104	BCR	C17-C18	3.30	1.40	1.35
16	A	819	CLA	C3D-C2D	3.29	1.48	1.39
19	F	202	BCR	C14-C13	3.29	1.40	1.35
16	A	818	CLA	OBD-CAD	3.29	1.28	1.22
16	A	831	CLA	C1B-NB	-3.29	1.32	1.35
19	B	846	BCR	C10-C9	3.29	1.40	1.35
16	A	831	CLA	OBD-CAD	3.29	1.28	1.22
16	A	806	CLA	CHD-C1D	3.29	1.44	1.38
16	A	804	CLA	C3D-C2D	3.29	1.48	1.39
16	B	841	CLA	OBD-CAD	3.29	1.28	1.22
16	B	832	CLA	CHD-C1D	3.28	1.44	1.38
19	B	846	BCR	C17-C18	3.28	1.40	1.35
19	I	101	BCR	C14-C13	3.26	1.40	1.35
16	B	806	CLA	C3D-C2D	3.26	1.48	1.39
19	F	202	BCR	C21-C22	3.26	1.40	1.35
16	A	839	CLA	OBD-CAD	3.26	1.28	1.22
16	B	816	CLA	C3D-C2D	3.26	1.48	1.39
16	A	810	CLA	C3D-C2D	3.26	1.48	1.39
16	A	803	CLA	C1D-ND	3.24	1.41	1.37
19	1	523	BCR	C23-C22	-3.24	1.39	1.45
19	A	850	BCR	C17-C18	3.24	1.40	1.35
19	J	104	BCR	C21-C22	3.24	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	833	CLA	OBD-CAD	3.23	1.28	1.22
16	A	811	CLA	OBD-CAD	3.23	1.28	1.22
16	B	806	CLA	OBD-CAD	3.23	1.28	1.22
16	B	837	CLA	C1B-NB	-3.22	1.32	1.35
16	A	826	CLA	C1B-NB	-3.22	1.32	1.35
19	J	104	BCR	C8-C9	-3.22	1.39	1.45
16	B	834	CLA	OBD-CAD	3.22	1.28	1.22
16	A	828	CLA	OBD-CAD	3.21	1.28	1.22
19	F	202	BCR	C23-C22	-3.21	1.39	1.45
16	X	101	CLA	OBD-CAD	3.21	1.28	1.22
16	B	828	CLA	C3D-C2D	3.21	1.47	1.39
19	A	846	BCR	C8-C9	-3.21	1.39	1.45
16	B	830	CLA	OBD-CAD	3.21	1.28	1.22
16	B	827	CLA	C3D-C2D	3.20	1.47	1.39
16	B	824	CLA	OBD-CAD	3.20	1.28	1.22
16	A	802	CLA	OBD-CAD	3.20	1.28	1.22
19	A	849	BCR	C8-C9	-3.20	1.39	1.45
19	A	850	BCR	C21-C22	3.19	1.40	1.35
16	B	823	CLA	OBD-CAD	3.19	1.28	1.22
19	B	847	BCR	C10-C9	3.18	1.40	1.35
19	B	846	BCR	C12-C13	-3.18	1.39	1.45
16	B	832	CLA	C1B-NB	-3.17	1.32	1.35
16	A	834	CLA	C3D-C2D	3.17	1.47	1.39
16	A	806	CLA	C3D-C2D	3.17	1.47	1.39
16	B	828	CLA	OBD-CAD	3.16	1.27	1.22
19	B	846	BCR	C8-C9	-3.16	1.39	1.45
16	A	819	CLA	OBD-CAD	3.16	1.27	1.22
16	A	809	CLA	OBD-CAD	3.16	1.27	1.22
19	4	401	BCR	C8-C9	-3.15	1.39	1.45
16	A	823	CLA	OBD-CAD	3.15	1.27	1.22
19	A	847	BCR	C14-C13	3.15	1.40	1.35
19	A	850	BCR	C14-C13	3.15	1.40	1.35
16	B	839	CLA	C3D-C2D	3.14	1.47	1.39
16	B	802	CLA	OBD-CAD	3.14	1.27	1.22
16	B	840	CLA	OBD-CAD	3.13	1.27	1.22
16	1	501	CLA	C3D-C2D	3.13	1.47	1.39
16	A	807	CLA	OBD-CAD	3.13	1.27	1.22
16	A	826	CLA	OBD-CAD	3.13	1.27	1.22
16	B	801	CLA	OBD-CAD	3.12	1.27	1.22
19	1	522	BCR	C21-C22	3.12	1.39	1.35
16	A	814	CLA	OBD-CAD	3.12	1.27	1.22
16	B	814	CLA	OBD-CAD	3.11	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	839	CLA	OBD-CAD	3.10	1.27	1.22
16	A	815	CLA	OBD-CAD	3.10	1.27	1.22
16	B	828	CLA	C1B-NB	-3.07	1.32	1.35
15	A	801	CL0	CHD-C4C	3.07	1.46	1.39
19	A	847	BCR	C23-C22	-3.07	1.39	1.45
16	B	831	CLA	OBD-CAD	3.06	1.27	1.22
19	A	850	BCR	C8-C9	-3.06	1.39	1.45
16	A	828	CLA	C3D-C4D	-3.04	1.37	1.44
19	I	101	BCR	C23-C22	-3.02	1.39	1.45
19	B	843	BCR	C23-C22	-3.01	1.39	1.45
16	B	810	CLA	OBD-CAD	3.01	1.27	1.22
16	A	838	CLA	OBD-CAD	3.01	1.27	1.22
16	1	521	CLA	C1C-C2C	2.99	1.50	1.44
19	B	844	BCR	C23-C22	-2.98	1.39	1.45
16	B	808	CLA	C3D-C2D	2.98	1.47	1.39
19	A	850	BCR	C12-C13	-2.97	1.39	1.45
16	B	818	CLA	C3D-C2D	2.97	1.47	1.39
19	1	523	BCR	C8-C9	-2.96	1.39	1.45
19	B	845	BCR	C21-C22	2.96	1.39	1.35
19	B	853	BCR	C19-C18	-2.96	1.39	1.45
19	A	848	BCR	C8-C9	-2.96	1.39	1.45
19	A	850	BCR	C10-C9	2.96	1.39	1.35
16	A	834	CLA	C3D-C4D	-2.96	1.37	1.44
16	B	812	CLA	OBD-CAD	2.95	1.27	1.22
19	1	522	BCR	C8-C9	-2.95	1.39	1.45
19	J	104	BCR	C14-C13	2.93	1.39	1.35
19	B	847	BCR	C12-C13	-2.92	1.39	1.45
19	B	847	BCR	C23-C22	-2.91	1.39	1.45
16	A	820	CLA	C3D-C4D	-2.91	1.37	1.44
19	F	202	BCR	C12-C13	-2.91	1.39	1.45
16	B	817	CLA	OBD-CAD	2.91	1.27	1.22
16	A	840	CLA	C3D-C4D	-2.91	1.37	1.44
19	A	847	BCR	C8-C9	-2.91	1.39	1.45
19	K	102	BCR	C23-C22	-2.91	1.39	1.45
16	A	822	CLA	OBD-CAD	2.90	1.27	1.22
16	B	809	CLA	C3D-C4D	-2.90	1.37	1.44
16	B	819	CLA	C1B-NB	-2.90	1.32	1.35
19	K	102	BCR	C8-C9	-2.90	1.39	1.45
19	1	523	BCR	C21-C22	2.90	1.39	1.35
16	B	839	CLA	C3D-C4D	-2.90	1.37	1.44
16	B	837	CLA	OBD-CAD	2.89	1.27	1.22
16	B	827	CLA	C3D-C4D	-2.89	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	822	CLA	C1C-C2C	2.88	1.50	1.44
16	A	833	CLA	C4B-NB	-2.88	1.32	1.35
19	F	205	BCR	C23-C22	-2.88	1.39	1.45
19	1	522	BCR	C12-C13	-2.88	1.39	1.45
16	B	824	CLA	C1C-C2C	2.88	1.50	1.44
16	B	838	CLA	OBD-CAD	2.87	1.27	1.22
16	A	824	CLA	OBD-CAD	2.87	1.27	1.22
19	F	205	BCR	C8-C9	-2.87	1.39	1.45
19	A	848	BCR	C12-C13	-2.86	1.39	1.45
16	A	813	CLA	C3D-C4D	-2.85	1.37	1.44
19	5	402	BCR	C8-C9	-2.85	1.39	1.45
19	B	853	BCR	C8-C9	-2.85	1.39	1.45
19	J	103	BCR	C19-C18	-2.85	1.39	1.45
16	4	411	CLA	C1C-C2C	2.85	1.50	1.44
16	B	809	CLA	OBD-CAD	2.85	1.27	1.22
19	B	848	BCR	C23-C22	-2.85	1.39	1.45
19	B	853	BCR	C23-C22	-2.85	1.39	1.45
19	F	202	BCR	C8-C9	-2.85	1.39	1.45
16	B	817	CLA	C3D-C4D	-2.84	1.37	1.44
16	A	818	CLA	C1C-C2C	2.84	1.50	1.44
19	J	104	BCR	C23-C22	-2.84	1.39	1.45
16	2	401	CLA	C1C-C2C	2.84	1.50	1.44
16	B	833	CLA	C1B-NB	-2.84	1.32	1.35
16	A	810	CLA	C1B-NB	-2.83	1.32	1.35
16	1	514	CLA	C4C-C3C	2.83	1.49	1.45
16	A	832	CLA	C3D-C4D	-2.83	1.37	1.44
19	A	847	BCR	C12-C13	-2.83	1.39	1.45
16	1	520	CLA	C4B-CHC	2.82	1.48	1.41
16	A	833	CLA	C1B-NB	-2.82	1.32	1.35
16	B	812	CLA	C1C-C2C	2.82	1.50	1.44
19	B	844	BCR	C8-C9	-2.82	1.39	1.45
19	B	845	BCR	C23-C22	-2.82	1.39	1.45
19	A	851	BCR	C21-C22	2.82	1.39	1.35
19	J	103	BCR	C23-C22	-2.82	1.39	1.45
16	6	403	CLA	C4C-C3C	2.81	1.49	1.45
16	B	818	CLA	C3D-C4D	-2.81	1.37	1.44
16	A	807	CLA	C3D-C4D	-2.81	1.37	1.44
16	B	830	CLA	C3D-C4D	-2.81	1.37	1.44
19	1	518	BCR	C8-C9	-2.81	1.39	1.45
16	4	410	CLA	C1C-C2C	2.81	1.50	1.44
16	B	823	CLA	C1C-NC	-2.80	1.33	1.37
16	A	829	CLA	C3D-C4D	-2.80	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	523	BCR	C17-C18	2.80	1.39	1.35
16	2	403	CLA	C4C-C3C	2.80	1.49	1.45
16	A	808	CLA	C1C-C2C	2.80	1.50	1.44
19	I	101	BCR	C8-C9	-2.80	1.39	1.45
19	B	846	BCR	C23-C22	-2.79	1.40	1.45
16	B	813	CLA	C4B-CHC	2.79	1.48	1.41
16	B	827	CLA	C1B-NB	-2.79	1.32	1.35
16	1	515	CLA	C4C-C3C	2.78	1.49	1.45
16	5	412	CLA	C1C-C2C	2.78	1.49	1.44
16	J	102	CLA	C1C-C2C	2.78	1.49	1.44
16	A	825	CLA	C1B-NB	-2.78	1.32	1.35
16	2	404	CLA	C1C-C2C	2.77	1.49	1.44
16	1	525	CLA	C1C-C2C	2.77	1.49	1.44
16	B	805	CLA	OBD-CAD	2.77	1.27	1.22
16	4	406	CLA	C4B-CHC	2.76	1.48	1.41
16	A	813	CLA	OBD-CAD	2.76	1.27	1.22
16	6	404	CLA	C1C-C2C	2.76	1.49	1.44
16	4	407	CLA	C1C-C2C	2.76	1.49	1.44
19	1	517	BCR	C8-C9	-2.75	1.40	1.45
16	5	414	CLA	C4C-C3C	2.75	1.49	1.45
16	1	520	CLA	C1C-C2C	2.75	1.49	1.44
16	B	835	CLA	C1B-NB	-2.74	1.32	1.35
16	A	819	CLA	C3D-C4D	-2.74	1.38	1.44
19	A	850	BCR	C19-C18	-2.74	1.40	1.45
19	A	846	BCR	C12-C13	-2.74	1.40	1.45
16	B	818	CLA	OBD-CAD	2.74	1.27	1.22
16	5	408	CLA	C1C-C2C	2.73	1.49	1.44
16	B	811	CLA	C1B-NB	-2.73	1.32	1.35
19	5	420	BCR	C8-C9	-2.73	1.40	1.45
16	B	827	CLA	C1C-NC	-2.73	1.33	1.37
16	1	505	CLA	C1C-C2C	2.73	1.49	1.44
16	1	506	CLA	C1C-C2C	2.73	1.49	1.44
16	5	405	CLA	C1C-C2C	2.73	1.49	1.44
16	6	407	CLA	C1C-C2C	2.72	1.49	1.44
16	B	828	CLA	C3D-C4D	-2.72	1.38	1.44
16	5	417	CLA	C1C-C2C	2.72	1.49	1.44
16	A	810	CLA	C3D-C4D	-2.72	1.38	1.44
19	B	843	BCR	C8-C9	-2.72	1.40	1.45
19	1	523	BCR	C12-C13	-2.72	1.40	1.45
16	4	409	CLA	C1C-C2C	2.72	1.49	1.44
16	B	808	CLA	C1C-NC	-2.72	1.33	1.37
16	B	826	CLA	C3D-C4D	-2.72	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	201	CLA	C3D-C4D	-2.71	1.38	1.44
16	5	406	CLA	C1C-C2C	2.71	1.49	1.44
16	B	812	CLA	C3D-C4D	-2.71	1.38	1.44
16	B	807	CLA	C1B-NB	-2.71	1.32	1.35
16	1	505	CLA	C4B-CHC	2.71	1.48	1.41
19	B	847	BCR	C17-C18	2.70	1.39	1.35
16	A	822	CLA	C3D-C4D	-2.70	1.38	1.44
16	1	515	CLA	C1C-C2C	2.70	1.49	1.44
16	A	833	CLA	C3D-C4D	-2.70	1.38	1.44
16	1	513	CLA	C1C-C2C	2.70	1.49	1.44
16	B	826	CLA	OBD-CAD	2.70	1.27	1.22
16	A	834	CLA	OBD-CAD	2.70	1.27	1.22
16	5	413	CLA	C4B-CHC	2.70	1.48	1.41
16	4	404	CLA	C4C-C3C	2.70	1.49	1.45
16	A	840	CLA	OBD-CAD	2.70	1.27	1.22
16	A	832	CLA	C1B-NB	-2.70	1.32	1.35
19	5	420	BCR	C23-C22	-2.70	1.40	1.45
16	1	504	CLA	C1C-C2C	2.70	1.49	1.44
16	5	411	CLA	C4B-CHC	2.70	1.48	1.41
16	A	807	CLA	C1C-C2C	2.70	1.49	1.44
16	B	802	CLA	C4B-NB	-2.69	1.32	1.35
16	B	813	CLA	C1C-C2C	2.69	1.49	1.44
16	5	419	CLA	C1C-C2C	2.69	1.49	1.44
16	6	401	CLA	C4C-C3C	2.69	1.49	1.45
19	A	846	BCR	C17-C18	2.69	1.39	1.35
19	4	401	BCR	C12-C13	-2.69	1.40	1.45
16	A	843	CLA	C3D-C4D	-2.69	1.38	1.44
16	2	405	CLA	C4C-C3C	2.69	1.49	1.45
16	B	832	CLA	C1C-C2C	2.69	1.49	1.44
16	A	829	CLA	OBD-CAD	2.69	1.27	1.22
16	4	409	CLA	C4B-CHC	2.68	1.48	1.41
16	1	502	CLA	C1C-C2C	2.68	1.49	1.44
16	1	503	CLA	C4C-C3C	2.68	1.49	1.45
16	B	805	CLA	C3D-C4D	-2.68	1.38	1.44
16	B	824	CLA	C4B-CHC	2.68	1.48	1.41
16	5	407	CLA	C4C-C3C	2.68	1.49	1.45
19	4	401	BCR	C23-C22	-2.68	1.40	1.45
16	1	501	CLA	C3D-C4D	-2.68	1.38	1.44
16	K	101	CLA	OBD-CAD	2.67	1.28	1.23
16	K	103	CLA	C1C-C2C	2.67	1.49	1.44
16	A	832	CLA	OBD-CAD	2.67	1.27	1.22
19	1	516	BCR	C8-C9	-2.67	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	851	BCR	C19-C18	-2.67	1.40	1.45
16	6	406	CLA	C4C-C3C	2.67	1.49	1.45
16	5	403	CLA	C1C-C2C	2.67	1.49	1.44
16	6	404	CLA	C4B-CHC	2.67	1.48	1.41
16	5	422	CLA	C1C-C2C	2.67	1.49	1.44
16	4	410	CLA	C4C-C3C	2.67	1.49	1.45
16	6	405	CLA	C4C-C3C	2.66	1.49	1.45
15	A	801	CL0	C4B-NB	-2.66	1.32	1.35
16	F	204	CLA	C1C-C2C	2.66	1.49	1.44
16	B	841	CLA	C3D-C4D	-2.66	1.38	1.44
16	5	417	CLA	C4B-CHC	2.66	1.48	1.41
16	5	412	CLA	C4B-CHC	2.66	1.48	1.41
16	6	408	CLA	C4C-C3C	2.66	1.49	1.45
16	B	807	CLA	C3D-C4D	-2.66	1.38	1.44
16	A	820	CLA	C1B-NB	-2.66	1.32	1.35
16	A	823	CLA	C3D-C4D	-2.65	1.38	1.44
16	1	521	CLA	C4B-CHC	2.65	1.48	1.41
16	B	805	CLA	C1B-NB	-2.65	1.32	1.35
16	6	409	CLA	C1C-C2C	2.65	1.49	1.44
16	A	827	CLA	C1C-C2C	2.65	1.49	1.44
16	A	829	CLA	C1B-NB	-2.65	1.32	1.35
16	A	835	CLA	C1C-NC	-2.65	1.33	1.37
16	4	406	CLA	C1C-C2C	2.65	1.49	1.44
16	4	403	CLA	C1C-C2C	2.65	1.49	1.44
16	B	806	CLA	C4D-CHA	2.65	1.47	1.38
16	A	819	CLA	C4B-CHC	2.65	1.48	1.41
16	6	407	CLA	C4B-CHC	2.65	1.48	1.41
16	4	411	CLA	C4B-CHC	2.65	1.48	1.41
16	B	832	CLA	OBD-CAD	2.64	1.27	1.22
16	A	827	CLA	C4B-CHC	2.64	1.48	1.41
16	6	408	CLA	C1C-C2C	2.64	1.49	1.44
16	4	410	CLA	C4B-CHC	2.64	1.48	1.41
16	A	842	CLA	C3D-C4D	-2.64	1.38	1.44
16	5	422	CLA	C4B-CHC	2.64	1.48	1.41
16	2	402	CLA	C4C-C3C	2.64	1.49	1.45
19	1	517	BCR	C23-C22	-2.64	1.40	1.45
16	K	103	CLA	C4B-CHC	2.63	1.48	1.41
16	A	829	CLA	C1C-C2C	2.63	1.49	1.44
16	4	407	CLA	C4B-CHC	2.63	1.48	1.41
16	5	421	CLA	C4B-CHC	2.63	1.48	1.41
16	1	525	CLA	C4B-CHC	2.63	1.48	1.41
16	B	819	CLA	C3D-C4D	-2.63	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	6	401	CLA	C4B-CHC	2.63	1.48	1.41
19	A	851	BCR	C8-C9	-2.63	1.40	1.45
16	1	507	CLA	C4C-C3C	2.63	1.49	1.45
16	A	835	CLA	C3D-C4D	-2.62	1.38	1.44
16	5	415	CLA	C1C-C2C	2.62	1.49	1.44
19	A	849	BCR	C19-C18	-2.62	1.40	1.45
16	6	408	CLA	C4B-CHC	2.62	1.48	1.41
16	5	422	CLA	C4C-C3C	2.62	1.49	1.45
16	4	403	CLA	C4B-CHC	2.62	1.48	1.41
16	B	834	CLA	C1B-NB	-2.62	1.32	1.35
16	1	510	CLA	C1C-C2C	2.62	1.49	1.44
16	3	401	CLA	C4B-CHC	2.62	1.48	1.41
16	6	402	CLA	C4C-C3C	2.62	1.49	1.45
16	B	827	CLA	C1C-C2C	2.61	1.49	1.44
19	1	518	BCR	C23-C22	-2.61	1.40	1.45
16	6	401	CLA	C1C-C2C	2.61	1.49	1.44
16	1	525	CLA	C4C-C3C	2.61	1.49	1.45
16	A	839	CLA	C3D-C4D	-2.61	1.38	1.44
19	B	845	BCR	C8-C9	-2.61	1.40	1.45
19	A	848	BCR	C19-C18	-2.61	1.40	1.45
16	5	406	CLA	C4C-C3C	2.61	1.49	1.45
16	5	415	CLA	C4B-CHC	2.61	1.48	1.41
16	2	406	CLA	C4C-C3C	2.61	1.49	1.45
16	B	833	CLA	C1C-C2C	2.61	1.49	1.44
16	B	814	CLA	C1C-C2C	2.60	1.49	1.44
16	J	101	CLA	C1C-C2C	2.60	1.49	1.44
16	B	836	CLA	C1C-C2C	2.60	1.49	1.44
16	2	405	CLA	C1C-C2C	2.60	1.49	1.44
16	A	804	CLA	C3D-C4D	-2.60	1.38	1.44
16	2	402	CLA	C1C-C2C	2.60	1.49	1.44
16	5	421	CLA	C4C-C3C	2.60	1.49	1.45
16	2	404	CLA	C4B-CHC	2.60	1.48	1.41
16	B	832	CLA	C3D-C4D	-2.60	1.38	1.44
16	5	404	CLA	C1B-CHB	2.60	1.48	1.41
16	1	507	CLA	C4D-CHA	2.60	1.47	1.38
16	2	402	CLA	C4B-CHC	2.60	1.48	1.41
16	2	405	CLA	C4B-CHC	2.60	1.48	1.41
16	4	408	CLA	C1C-C2C	2.60	1.49	1.44
19	A	849	BCR	C23-C22	-2.59	1.40	1.45
19	M	102	BCR	C23-C22	-2.59	1.40	1.45
16	2	401	CLA	C4B-CHC	2.59	1.48	1.41
16	A	805	CLA	C4B-CHC	2.59	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	101	CLA	C1C-C2C	2.59	1.49	1.44
16	B	828	CLA	C1C-C2C	2.59	1.49	1.44
16	4	404	CLA	C1C-C2C	2.59	1.49	1.44
16	A	806	CLA	C3D-C4D	-2.59	1.38	1.44
16	1	515	CLA	C4B-CHC	2.59	1.48	1.41
16	B	801	CLA	C3D-C4D	-2.59	1.38	1.44
16	K	101	CLA	C3D-C4D	-2.59	1.38	1.44
16	B	816	CLA	C1C-C2C	2.59	1.49	1.44
16	5	418	CLA	C4B-CHC	2.59	1.48	1.41
16	6	406	CLA	C4B-CHC	2.59	1.48	1.41
19	J	103	BCR	C17-C18	2.58	1.39	1.35
16	A	815	CLA	C3D-C4D	-2.58	1.38	1.44
16	5	403	CLA	C4B-CHC	2.58	1.48	1.41
16	6	406	CLA	C4D-CHA	2.58	1.47	1.38
16	A	819	CLA	C1B-NB	-2.58	1.32	1.35
19	5	402	BCR	C23-C22	-2.58	1.40	1.45
16	1	511	CLA	C4D-CHA	2.58	1.47	1.38
16	5	411	CLA	C1C-C2C	2.58	1.49	1.44
16	6	405	CLA	C4B-CHC	2.58	1.48	1.41
16	B	834	CLA	C3D-C4D	-2.58	1.38	1.44
16	B	810	CLA	C1C-C2C	2.58	1.49	1.44
16	F	201	CLA	C1C-C2C	2.58	1.49	1.44
16	B	835	CLA	C1C-C2C	2.58	1.49	1.44
16	B	819	CLA	C1C-C2C	2.58	1.49	1.44
16	6	409	CLA	C4B-CHC	2.57	1.48	1.41
15	A	801	CL0	C1B-NB	-2.57	1.32	1.35
16	A	838	CLA	C3D-C4D	-2.57	1.38	1.44
16	2	405	CLA	C4D-CHA	2.57	1.47	1.38
16	2	403	CLA	C1C-C2C	2.57	1.49	1.44
16	A	814	CLA	C1C-C2C	2.57	1.49	1.44
16	A	841	CLA	C3D-C4D	-2.57	1.38	1.44
16	B	815	CLA	C1C-C2C	2.57	1.49	1.44
16	B	837	CLA	C1C-C2C	2.57	1.49	1.44
19	B	853	BCR	C12-C13	-2.57	1.40	1.45
16	6	406	CLA	C1C-C2C	2.57	1.49	1.44
16	J	102	CLA	C3D-C4D	-2.56	1.38	1.44
16	J	101	CLA	C4B-CHC	2.56	1.48	1.41
16	5	418	CLA	C4D-CHA	2.56	1.47	1.38
19	M	102	BCR	C12-C13	-2.56	1.40	1.45
16	4	405	CLA	C4D-CHA	2.56	1.47	1.38
16	6	405	CLA	C1C-C2C	2.56	1.49	1.44
19	B	848	BCR	C19-C18	-2.56	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	802	CLA	C1C-C2C	2.56	1.49	1.44
16	1	514	CLA	C1C-C2C	2.56	1.49	1.44
16	5	405	CLA	C4B-CHC	2.56	1.48	1.41
16	1	515	CLA	C4D-CHA	2.56	1.47	1.38
16	4	407	CLA	C4D-CHA	2.56	1.47	1.38
16	2	402	CLA	C4D-CHA	2.56	1.47	1.38
16	B	807	CLA	C1C-C2C	2.56	1.49	1.44
16	A	828	CLA	C4B-CHC	2.56	1.48	1.41
16	B	826	CLA	C4B-CHC	2.56	1.48	1.41
16	B	837	CLA	C3D-C4D	-2.56	1.38	1.44
16	4	404	CLA	C4B-CHC	2.56	1.48	1.41
16	B	817	CLA	C1C-C2C	2.56	1.49	1.44
16	A	834	CLA	C1C-C2C	2.55	1.49	1.44
16	A	820	CLA	OBD-CAD	2.55	1.26	1.22
16	K	101	CLA	C4C-C3C	2.55	1.49	1.45
16	B	840	CLA	C3D-C4D	-2.55	1.38	1.44
16	B	822	CLA	C1C-C2C	2.55	1.49	1.44
16	3	401	CLA	C1C-C2C	2.55	1.49	1.44
16	4	403	CLA	C1B-CHB	2.55	1.48	1.41
19	A	851	BCR	C12-C13	-2.55	1.40	1.45
16	5	409	CLA	C1C-C2C	2.55	1.49	1.44
16	A	828	CLA	C1C-C2C	2.55	1.49	1.44
16	B	838	CLA	C4B-CHC	2.55	1.48	1.41
16	4	406	CLA	C4D-CHA	2.55	1.47	1.38
16	4	408	CLA	C4C-C3C	2.55	1.49	1.45
19	1	522	BCR	C19-C18	-2.55	1.40	1.45
16	B	806	CLA	C3D-C4D	-2.55	1.38	1.44
16	1	507	CLA	C1C-C2C	2.55	1.49	1.44
16	5	412	CLA	C4D-CHA	2.55	1.47	1.38
16	2	406	CLA	C1C-C2C	2.55	1.49	1.44
16	1	519	CLA	C4B-CHC	2.55	1.48	1.41
19	1	516	BCR	C23-C22	-2.54	1.40	1.45
16	B	808	CLA	C1B-NB	-2.54	1.32	1.35
16	1	501	CLA	C4D-CHA	2.54	1.47	1.38
16	4	402	CLA	C1C-C2C	2.54	1.49	1.44
16	6	409	CLA	C4C-C3C	2.54	1.49	1.45
16	A	822	CLA	C4B-CHC	2.54	1.48	1.41
16	B	837	CLA	C4B-CHC	2.54	1.48	1.41
16	4	408	CLA	C4B-CHC	2.54	1.48	1.41
16	B	809	CLA	C4B-CHC	2.54	1.48	1.41
16	A	813	CLA	C1C-C2C	2.54	1.49	1.44
16	4	402	CLA	C4B-CHC	2.54	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	6	409	CLA	C4D-CHA	2.54	1.47	1.38
16	1	521	CLA	C3D-C4D	-2.54	1.38	1.44
16	B	812	CLA	C1B-CHB	2.54	1.48	1.41
16	A	814	CLA	C4B-CHC	2.54	1.48	1.41
16	5	418	CLA	C4C-C3C	2.54	1.49	1.45
16	6	403	CLA	C4D-CHA	2.53	1.47	1.38
16	1	512	CLA	C1C-C2C	2.53	1.49	1.44
16	5	414	CLA	C1C-C2C	2.53	1.49	1.44
16	B	836	CLA	C4B-CHC	2.53	1.48	1.41
16	5	418	CLA	C1C-C2C	2.53	1.49	1.44
16	A	816	CLA	C3D-C4D	-2.53	1.38	1.44
16	5	413	CLA	C1C-C2C	2.53	1.49	1.44
16	4	405	CLA	C4C-C3C	2.53	1.49	1.45
16	1	526	CLA	C4B-CHC	2.53	1.48	1.41
16	2	406	CLA	C4B-CHC	2.53	1.48	1.41
19	A	848	BCR	C17-C18	2.53	1.39	1.35
16	2	403	CLA	C4D-CHA	2.53	1.47	1.38
16	2	406	CLA	C1B-CHB	2.53	1.48	1.41
16	B	817	CLA	C1B-NB	-2.52	1.33	1.35
16	A	814	CLA	C3D-C4D	-2.52	1.38	1.44
16	B	825	CLA	C3D-C4D	-2.52	1.38	1.44
16	5	406	CLA	C4B-CHC	2.52	1.48	1.41
16	5	409	CLA	C4C-C3C	2.52	1.49	1.45
16	1	526	CLA	C1C-C2C	2.52	1.49	1.44
16	5	419	CLA	C4B-CHC	2.52	1.48	1.41
16	6	405	CLA	C4D-CHA	2.52	1.47	1.38
16	J	101	CLA	C3D-C4D	-2.52	1.38	1.44
16	6	408	CLA	C1B-CHB	2.52	1.48	1.41
16	A	806	CLA	C4B-NB	-2.51	1.33	1.35
16	B	809	CLA	C1B-NB	-2.51	1.33	1.35
16	1	512	CLA	C4B-CHC	2.51	1.48	1.41
16	6	402	CLA	C4D-CHA	2.51	1.47	1.38
16	A	805	CLA	C4D-CHA	2.51	1.47	1.38
16	5	417	CLA	C4D-CHA	2.51	1.47	1.38
19	K	102	BCR	C12-C13	-2.51	1.40	1.45
16	3	401	CLA	C4C-C3C	2.51	1.49	1.45
19	F	202	BCR	C19-C18	-2.51	1.40	1.45
16	B	810	CLA	C3D-C4D	-2.51	1.38	1.44
19	B	845	BCR	C19-C18	-2.50	1.40	1.45
16	F	204	CLA	C4B-CHC	2.50	1.48	1.41
16	B	820	CLA	C3D-C4D	-2.50	1.38	1.44
16	5	407	CLA	C3D-C4D	-2.50	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	403	CLA	C4B-CHC	2.50	1.48	1.41
16	B	821	CLA	C1C-C2C	2.50	1.49	1.44
16	6	407	CLA	C4C-C3C	2.50	1.49	1.45
16	A	812	CLA	C1B-NB	-2.50	1.33	1.35
16	1	526	CLA	C4C-C3C	2.50	1.49	1.45
16	B	807	CLA	C4D-CHA	2.50	1.47	1.38
16	5	411	CLA	C4D-CHA	2.50	1.47	1.38
16	A	838	CLA	C1C-C2C	2.50	1.49	1.44
16	B	816	CLA	C4B-CHC	2.50	1.47	1.41
16	B	836	CLA	C4D-CHA	2.50	1.47	1.38
16	6	402	CLA	C1C-C2C	2.50	1.49	1.44
16	6	409	CLA	C1B-CHB	2.50	1.47	1.41
16	1	513	CLA	C4B-CHC	2.49	1.47	1.41
16	X	101	CLA	C3D-C4D	-2.49	1.38	1.44
16	3	401	CLA	C4D-CHA	2.49	1.47	1.38
19	J	104	BCR	C19-C18	-2.49	1.40	1.45
16	2	401	CLA	C4D-CHA	2.49	1.47	1.38
16	5	408	CLA	C4B-CHC	2.49	1.47	1.41
16	1	509	CLA	C4B-CHC	2.49	1.47	1.41
16	5	404	CLA	C1B-NB	-2.49	1.33	1.35
16	B	831	CLA	C3D-C4D	-2.49	1.38	1.44
16	1	513	CLA	C4D-CHA	2.49	1.47	1.38
16	5	414	CLA	C4D-CHA	2.49	1.47	1.38
16	5	412	CLA	C1B-CHB	2.49	1.47	1.41
16	1	503	CLA	C4D-CHA	2.49	1.47	1.38
16	B	819	CLA	C4B-CHC	2.48	1.47	1.41
19	F	205	BCR	C12-C13	-2.48	1.40	1.45
16	1	508	CLA	C4C-C3C	2.48	1.49	1.45
19	B	843	BCR	C12-C13	-2.48	1.40	1.45
16	4	410	CLA	C1B-CHB	2.48	1.47	1.41
16	1	510	CLA	C4D-CHA	2.48	1.47	1.38
16	A	813	CLA	C1B-NB	-2.48	1.33	1.35
16	B	826	CLA	C1C-C2C	2.48	1.49	1.44
16	A	817	CLA	C1B-CHB	2.48	1.47	1.41
16	B	802	CLA	C1C-NC	-2.48	1.34	1.37
16	6	401	CLA	C4D-CHA	2.48	1.47	1.38
16	4	411	CLA	C4D-CHA	2.48	1.47	1.38
16	B	835	CLA	C3D-C4D	-2.48	1.38	1.44
16	6	404	CLA	C4D-CHA	2.48	1.47	1.38
19	B	846	BCR	C19-C18	-2.48	1.40	1.45
16	4	404	CLA	C1B-CHB	2.48	1.47	1.41
16	6	402	CLA	C4B-CHC	2.48	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	801	CLA	C1C-C2C	2.48	1.49	1.44
16	5	419	CLA	C1B-CHB	2.48	1.47	1.41
16	1	505	CLA	C4D-CHA	2.48	1.47	1.38
16	A	812	CLA	C3D-C4D	-2.48	1.38	1.44
16	A	802	CLA	C3D-C4D	-2.48	1.38	1.44
16	3	401	CLA	C1B-CHB	2.48	1.47	1.41
16	1	514	CLA	C4B-CHC	2.48	1.47	1.41
16	5	416	CLA	C1B-CHB	2.48	1.47	1.41
16	2	404	CLA	C1B-CHB	2.47	1.47	1.41
16	A	825	CLA	C3D-C4D	-2.47	1.38	1.44
16	F	204	CLA	C3D-C4D	-2.47	1.38	1.44
16	B	804	CLA	C3D-C4D	-2.47	1.38	1.44
16	A	837	CLA	C1B-CHB	2.47	1.47	1.41
16	B	817	CLA	C4B-CHC	2.47	1.47	1.41
16	A	817	CLA	C4C-C3C	2.47	1.49	1.45
16	5	416	CLA	C4C-C3C	2.47	1.49	1.45
16	4	410	CLA	C4D-CHA	2.47	1.47	1.38
16	5	406	CLA	C4D-CHA	2.47	1.47	1.38
16	5	405	CLA	C4C-C3C	2.47	1.49	1.45
16	5	414	CLA	C4B-CHC	2.47	1.47	1.41
16	B	823	CLA	C3D-C4D	-2.47	1.38	1.44
16	5	422	CLA	C4D-CHA	2.47	1.47	1.38
16	6	408	CLA	C4D-CHA	2.47	1.47	1.38
16	1	512	CLA	C3D-C4D	-2.47	1.38	1.44
16	6	403	CLA	C1C-C2C	2.47	1.49	1.44
16	1	502	CLA	C4B-CHC	2.47	1.47	1.41
16	A	837	CLA	C3D-C4D	-2.47	1.38	1.44
16	2	404	CLA	C4D-CHA	2.47	1.47	1.38
16	1	508	CLA	C4D-CHA	2.46	1.47	1.38
16	5	413	CLA	C4C-C3C	2.46	1.49	1.45
16	1	509	CLA	C1C-C2C	2.46	1.49	1.44
16	1	511	CLA	C1B-CHB	2.46	1.47	1.41
19	1	523	BCR	C19-C18	-2.46	1.40	1.45
16	2	402	CLA	C1B-CHB	2.46	1.47	1.41
16	B	824	CLA	C3D-C4D	-2.46	1.38	1.44
16	6	401	CLA	C1B-CHB	2.46	1.47	1.41
16	6	407	CLA	C4D-CHA	2.46	1.47	1.38
16	6	402	CLA	C1B-CHB	2.46	1.47	1.41
16	1	526	CLA	C4D-CHA	2.46	1.47	1.38
16	5	416	CLA	C4B-CHC	2.46	1.47	1.41
16	1	507	CLA	C1B-CHB	2.46	1.47	1.41
16	B	839	CLA	C1C-NC	-2.46	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	817	CLA	C3D-C4D	-2.46	1.38	1.44
16	4	402	CLA	C4D-CHA	2.46	1.47	1.38
16	F	204	CLA	C4D-CHA	2.46	1.47	1.38
16	B	821	CLA	C4D-CHA	2.46	1.47	1.38
16	4	411	CLA	C1B-CHB	2.46	1.47	1.41
16	A	808	CLA	C3D-C4D	-2.46	1.38	1.44
16	6	404	CLA	C4C-C3C	2.46	1.49	1.45
16	4	404	CLA	C4D-CHA	2.45	1.47	1.38
16	A	821	CLA	C3D-C4D	-2.45	1.38	1.44
16	B	815	CLA	C3D-C4D	-2.45	1.38	1.44
16	A	825	CLA	C1C-C2C	2.45	1.49	1.44
16	B	833	CLA	C4B-CHC	2.45	1.47	1.41
16	2	406	CLA	C4D-CHA	2.45	1.47	1.38
16	5	409	CLA	C4D-CHA	2.45	1.47	1.38
16	5	408	CLA	C4C-C3C	2.45	1.49	1.45
16	B	816	CLA	C3D-C4D	-2.45	1.38	1.44
16	A	811	CLA	C1B-NB	-2.45	1.33	1.35
16	2	401	CLA	C1B-CHB	2.45	1.47	1.41
16	B	806	CLA	C1C-C2C	2.45	1.49	1.44
16	A	818	CLA	C4B-CHC	2.45	1.47	1.41
16	B	841	CLA	C1C-NC	-2.45	1.34	1.37
16	6	407	CLA	C1B-CHB	2.45	1.47	1.41
16	4	405	CLA	C1C-C2C	2.45	1.49	1.44
19	B	843	BCR	C19-C18	-2.45	1.40	1.45
16	5	416	CLA	C4D-CHA	2.45	1.47	1.38
16	1	519	CLA	C1C-C2C	2.45	1.49	1.44
16	1	514	CLA	C4D-CHA	2.45	1.47	1.38
16	5	406	CLA	C1B-CHB	2.44	1.47	1.41
16	B	840	CLA	C4B-CHC	2.44	1.47	1.41
19	5	420	BCR	C12-C13	-2.44	1.40	1.45
16	B	840	CLA	C1C-C2C	2.44	1.49	1.44
16	1	506	CLA	C4B-CHC	2.44	1.47	1.41
16	F	204	CLA	C1B-CHB	2.44	1.47	1.41
16	1	502	CLA	C4D-CHA	2.44	1.47	1.38
16	A	802	CLA	C1C-C2C	2.44	1.49	1.44
16	1	504	CLA	C4B-CHC	2.44	1.47	1.41
19	A	847	BCR	C19-C18	-2.44	1.40	1.45
16	A	843	CLA	C1B-NB	-2.44	1.33	1.35
16	4	409	CLA	C4D-CHA	2.44	1.47	1.38
16	B	820	CLA	C4B-CHC	2.44	1.47	1.41
16	5	403	CLA	C4D-CHA	2.44	1.47	1.38
16	5	404	CLA	C3D-C4D	-2.44	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	412	CLA	C4C-C3C	2.44	1.49	1.45
16	6	403	CLA	C4B-CHC	2.44	1.47	1.41
16	5	419	CLA	C4C-C3C	2.44	1.49	1.45
16	5	417	CLA	C1B-CHB	2.44	1.47	1.41
16	4	408	CLA	C1B-CHB	2.44	1.47	1.41
19	5	402	BCR	C12-C13	-2.44	1.40	1.45
16	A	829	CLA	C4B-CHC	2.44	1.47	1.41
16	A	825	CLA	C4D-CHA	2.43	1.47	1.38
16	X	101	CLA	C4C-C3C	2.43	1.49	1.45
16	A	814	CLA	C4C-C3C	2.43	1.49	1.45
16	5	405	CLA	C1B-CHB	2.43	1.47	1.41
16	5	422	CLA	C1B-CHB	2.43	1.47	1.41
16	A	832	CLA	C1C-C2C	2.43	1.49	1.44
16	5	413	CLA	C4D-CHA	2.43	1.47	1.38
16	5	411	CLA	C4C-C3C	2.43	1.49	1.45
19	I	101	BCR	C12-C13	-2.43	1.40	1.45
16	A	815	CLA	C4D-CHA	2.43	1.47	1.38
16	A	830	CLA	C3D-C4D	-2.43	1.38	1.44
16	B	840	CLA	C1C-NC	-2.43	1.34	1.37
16	B	815	CLA	C4B-CHC	2.43	1.47	1.41
16	2	403	CLA	C1B-CHB	2.43	1.47	1.41
16	A	831	CLA	C3D-C4D	-2.43	1.38	1.44
16	B	838	CLA	C3D-C4D	-2.43	1.38	1.44
16	A	810	CLA	C4B-CHC	2.42	1.47	1.41
16	5	415	CLA	C4C-C3C	2.42	1.49	1.45
16	B	811	CLA	C3D-C4D	-2.42	1.38	1.44
16	J	101	CLA	C4C-C3C	2.42	1.49	1.45
16	4	411	CLA	C4C-C3C	2.42	1.49	1.45
16	1	510	CLA	C4B-CHC	2.42	1.47	1.41
16	5	421	CLA	C1B-CHB	2.42	1.47	1.41
16	B	803	CLA	C4D-CHA	2.42	1.47	1.38
19	J	104	BCR	C12-C13	-2.42	1.40	1.45
16	A	817	CLA	C4D-CHA	2.42	1.47	1.38
16	1	511	CLA	C4C-C3C	2.42	1.49	1.45
19	M	102	BCR	C19-C18	-2.42	1.40	1.45
16	4	408	CLA	C4D-CHA	2.42	1.47	1.38
16	A	811	CLA	C3D-C4D	-2.42	1.38	1.44
16	6	404	CLA	C1B-CHB	2.42	1.47	1.41
16	A	815	CLA	C4C-C3C	2.42	1.49	1.45
16	B	829	CLA	C3D-C4D	-2.42	1.38	1.44
16	A	839	CLA	C1C-C2C	2.42	1.49	1.44
16	A	827	CLA	C3D-C4D	-2.42	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	818	CLA	C3D-C4D	-2.42	1.38	1.44
16	1	503	CLA	C4B-CHC	2.41	1.47	1.41
16	B	831	CLA	C4D-CHA	2.41	1.47	1.38
16	4	403	CLA	C4D-CHA	2.41	1.47	1.38
16	4	406	CLA	C4C-C3C	2.41	1.49	1.45
16	6	405	CLA	C1B-CHB	2.41	1.47	1.41
16	A	827	CLA	C4D-CHA	2.41	1.47	1.38
16	J	101	CLA	C4D-CHA	2.41	1.47	1.38
16	B	825	CLA	C4B-CHC	2.41	1.47	1.41
16	K	101	CLA	C4B-CHC	2.41	1.47	1.41
16	5	408	CLA	C4D-CHA	2.41	1.47	1.38
16	A	803	CLA	C1C-NC	-2.41	1.34	1.37
16	B	821	CLA	C4B-CHC	2.41	1.47	1.41
16	1	510	CLA	C1B-CHB	2.41	1.47	1.41
16	A	813	CLA	C1C-NC	-2.41	1.34	1.37
16	5	421	CLA	C1C-C2C	2.40	1.49	1.44
16	1	511	CLA	C1C-C2C	2.40	1.49	1.44
19	A	846	BCR	C19-C18	-2.40	1.40	1.45
16	A	806	CLA	C1B-NB	-2.40	1.33	1.35
16	5	422	CLA	C3D-C4D	-2.40	1.38	1.44
16	A	809	CLA	C3D-C4D	-2.40	1.38	1.44
16	1	504	CLA	C3D-C4D	-2.40	1.38	1.44
16	1	506	CLA	C3D-C4D	-2.40	1.38	1.44
16	5	410	CLA	C4B-CHC	2.40	1.47	1.41
16	A	809	CLA	C4D-CHA	2.40	1.46	1.38
16	B	840	CLA	C4D-CHA	2.40	1.46	1.38
16	6	406	CLA	C1B-CHB	2.40	1.47	1.41
16	A	826	CLA	C1C-C2C	2.40	1.49	1.44
16	5	405	CLA	C4D-CHA	2.40	1.46	1.38
16	5	418	CLA	C1B-CHB	2.40	1.47	1.41
16	A	843	CLA	C1B-CHB	2.39	1.47	1.41
19	1	518	BCR	C12-C13	-2.39	1.40	1.45
16	5	414	CLA	C1B-CHB	2.39	1.47	1.41
16	B	826	CLA	C1B-CHB	2.39	1.47	1.41
16	1	514	CLA	C1B-CHB	2.39	1.47	1.41
16	A	824	CLA	C3D-C4D	-2.39	1.38	1.44
16	B	815	CLA	C4D-CHA	2.39	1.46	1.38
16	A	840	CLA	C4B-CHC	2.39	1.47	1.41
16	A	826	CLA	C4D-CHA	2.39	1.46	1.38
16	A	826	CLA	C3D-C4D	-2.39	1.38	1.44
16	A	815	CLA	C4B-NB	-2.39	1.33	1.35
16	B	820	CLA	C1C-C2C	2.39	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	405	CLA	C1B-CHB	2.39	1.47	1.41
16	1	525	CLA	C3D-C4D	-2.39	1.38	1.44
16	5	404	CLA	C4D-CHA	2.39	1.46	1.38
16	1	519	CLA	C4D-CHA	2.39	1.46	1.38
16	1	502	CLA	C1B-CHB	2.38	1.47	1.41
16	A	828	CLA	C4D-CHA	2.38	1.46	1.38
16	B	835	CLA	C4B-CHC	2.38	1.47	1.41
16	1	520	CLA	C3D-C4D	-2.38	1.38	1.44
16	1	512	CLA	C1B-CHB	2.38	1.47	1.41
16	B	802	CLA	C3D-C4D	-2.38	1.38	1.44
16	F	201	CLA	C4D-CHA	2.38	1.46	1.38
16	1	526	CLA	C1B-CHB	2.38	1.47	1.41
16	A	836	CLA	C3D-C4D	-2.38	1.38	1.44
16	5	408	CLA	C1B-CHB	2.38	1.47	1.41
16	5	407	CLA	C4D-CHA	2.38	1.46	1.38
16	5	417	CLA	C4C-C3C	2.38	1.49	1.45
16	K	101	CLA	C1B-CHB	2.38	1.47	1.41
16	A	842	CLA	C4D-CHA	2.38	1.46	1.38
16	1	525	CLA	C1B-CHB	2.38	1.47	1.41
16	K	103	CLA	C1B-CHB	2.38	1.47	1.41
16	4	407	CLA	C4C-C3C	2.37	1.49	1.45
16	J	102	CLA	C4B-CHC	2.37	1.47	1.41
16	5	419	CLA	C4D-CHA	2.37	1.46	1.38
16	B	803	CLA	C1C-NC	-2.37	1.34	1.37
16	5	413	CLA	C3D-C4D	-2.37	1.38	1.44
16	4	403	CLA	C4C-C3C	2.37	1.49	1.45
16	5	403	CLA	C1B-CHB	2.37	1.47	1.41
16	5	415	CLA	C1B-CHB	2.37	1.47	1.41
16	A	811	CLA	C4D-CHA	2.37	1.46	1.38
16	B	822	CLA	C1B-CHB	2.37	1.47	1.41
16	1	510	CLA	C4C-C3C	2.37	1.49	1.45
16	5	421	CLA	C3D-C4D	-2.37	1.38	1.44
16	B	820	CLA	C4D-CHA	2.37	1.46	1.38
16	4	409	CLA	C4C-C3C	2.37	1.49	1.45
16	B	821	CLA	C1B-CHB	2.37	1.47	1.41
16	A	830	CLA	C1B-NB	-2.37	1.33	1.35
16	A	838	CLA	C4D-CHA	2.37	1.46	1.38
16	B	810	CLA	C4B-CHC	2.37	1.47	1.41
16	B	830	CLA	C4D-CHA	2.37	1.46	1.38
16	B	810	CLA	C1C-NC	-2.37	1.34	1.37
16	6	403	CLA	C1B-CHB	2.36	1.47	1.41
16	1	525	CLA	C4D-CHA	2.36	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	410	CLA	C4D-CHA	2.36	1.46	1.38
16	2	404	CLA	C4C-C3C	2.36	1.49	1.45
16	1	526	CLA	C3D-C4D	-2.36	1.38	1.44
16	A	818	CLA	C1B-NB	-2.36	1.33	1.35
16	B	822	CLA	C4D-CHA	2.36	1.46	1.38
16	B	804	CLA	C4B-CHC	2.36	1.47	1.41
16	A	840	CLA	C4D-CHA	2.36	1.46	1.38
16	1	513	CLA	C1B-CHB	2.36	1.47	1.41
16	J	102	CLA	C4D-CHA	2.36	1.46	1.38
16	A	824	CLA	C4B-CHC	2.36	1.47	1.41
16	A	842	CLA	C1B-CHB	2.36	1.47	1.41
16	5	415	CLA	C4D-CHA	2.35	1.46	1.38
16	K	103	CLA	C4D-CHA	2.35	1.46	1.38
16	1	504	CLA	C4D-CHA	2.35	1.46	1.38
16	B	814	CLA	C4D-CHA	2.35	1.46	1.38
16	A	810	CLA	C1C-C2C	2.35	1.49	1.44
16	B	814	CLA	C4B-CHC	2.35	1.47	1.41
19	B	846	BCR	C14-C13	2.35	1.38	1.35
16	A	823	CLA	C4B-CHC	2.35	1.47	1.41
16	4	402	CLA	C1B-CHB	2.35	1.47	1.41
16	B	825	CLA	C4D-CHA	2.35	1.46	1.38
16	A	831	CLA	C1B-CHB	2.35	1.47	1.41
16	4	409	CLA	C1B-CHB	2.35	1.47	1.41
16	A	819	CLA	C4D-CHA	2.35	1.46	1.38
16	X	101	CLA	C4D-CHA	2.35	1.46	1.38
16	1	505	CLA	C4C-C3C	2.35	1.49	1.45
16	1	521	CLA	C4D-CHA	2.35	1.46	1.38
19	B	845	BCR	C12-C13	-2.35	1.40	1.45
19	I	101	BCR	C19-C18	-2.35	1.40	1.45
16	5	416	CLA	C1C-C2C	2.35	1.49	1.44
16	1	511	CLA	C4B-CHC	2.34	1.47	1.41
16	A	814	CLA	C4D-CHA	2.34	1.46	1.38
16	B	802	CLA	C1B-NB	-2.34	1.33	1.35
16	B	829	CLA	C4D-CHA	2.34	1.46	1.38
16	B	831	CLA	C1C-C2C	2.34	1.49	1.44
15	A	801	CL0	C3D-C4D	-2.34	1.38	1.44
15	A	801	CL0	C1C-NC	-2.34	1.34	1.37
16	1	513	CLA	C4C-C3C	2.34	1.49	1.45
16	5	409	CLA	C4B-CHC	2.34	1.47	1.41
16	1	503	CLA	C1C-C2C	2.34	1.49	1.44
16	1	513	CLA	C3D-C4D	-2.34	1.38	1.44
16	B	808	CLA	C3D-C4D	-2.34	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	823	CLA	C1B-CHB	2.34	1.47	1.41
16	A	804	CLA	C1C-C2C	2.34	1.49	1.44
16	A	839	CLA	C4D-CHA	2.34	1.46	1.38
16	B	805	CLA	C4D-CHA	2.34	1.46	1.38
16	A	824	CLA	C1C-C2C	2.34	1.49	1.44
16	4	405	CLA	C4B-CHC	2.33	1.47	1.41
16	B	822	CLA	C3D-C4D	-2.33	1.38	1.44
16	B	836	CLA	C3D-C4D	-2.33	1.38	1.44
16	A	820	CLA	C4B-CHC	2.33	1.47	1.41
16	A	830	CLA	C1C-C2C	2.33	1.49	1.44
16	B	841	CLA	C4D-CHA	2.33	1.46	1.38
19	B	848	BCR	C12-C13	-2.33	1.40	1.45
16	A	841	CLA	C4B-CHC	2.33	1.47	1.41
16	5	410	CLA	C4C-C3C	2.33	1.49	1.45
16	5	421	CLA	C4D-CHA	2.33	1.46	1.38
16	B	834	CLA	C1C-C2C	2.32	1.49	1.44
16	A	816	CLA	C4D-CHA	2.32	1.46	1.38
16	B	811	CLA	C4D-CHA	2.32	1.46	1.38
16	1	512	CLA	C4D-CHA	2.32	1.46	1.38
16	1	503	CLA	C1B-CHB	2.32	1.47	1.41
16	5	411	CLA	C3D-C4D	-2.32	1.38	1.44
16	A	821	CLA	C1C-C2C	2.32	1.49	1.44
16	A	806	CLA	C1B-CHB	2.32	1.47	1.41
16	A	834	CLA	C4D-CHA	2.32	1.46	1.38
16	B	833	CLA	C4D-CHA	2.32	1.46	1.38
16	B	813	CLA	C3D-C4D	-2.32	1.38	1.44
19	B	847	BCR	C19-C18	-2.32	1.41	1.45
16	A	807	CLA	C1B-NB	-2.32	1.33	1.35
16	A	824	CLA	C1B-NB	-2.32	1.33	1.35
16	A	836	CLA	C1B-NB	-2.32	1.33	1.35
16	A	825	CLA	C4B-CHC	2.32	1.47	1.41
16	1	505	CLA	C1B-CHB	2.32	1.47	1.41
16	B	821	CLA	C3D-C4D	-2.32	1.38	1.44
16	B	818	CLA	C1B-NB	-2.32	1.33	1.35
16	A	830	CLA	C4D-CHA	2.32	1.46	1.38
19	1	516	BCR	C12-C13	-2.31	1.41	1.45
16	4	408	CLA	C3D-C4D	-2.31	1.38	1.44
16	5	407	CLA	C1C-C2C	2.31	1.49	1.44
16	1	511	CLA	C3D-C4D	-2.31	1.39	1.44
16	B	823	CLA	C4D-CHA	2.31	1.46	1.38
16	A	813	CLA	C4B-CHC	2.31	1.47	1.41
16	A	841	CLA	C1C-C2C	2.31	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	823	CLA	C1C-C2C	2.31	1.49	1.44
16	5	417	CLA	C3D-C4D	-2.31	1.39	1.44
16	1	512	CLA	C4C-C3C	2.31	1.49	1.45
16	A	810	CLA	C1C-NC	-2.31	1.34	1.37
16	B	811	CLA	C1C-NC	-2.31	1.34	1.37
16	5	410	CLA	C1B-CHB	2.31	1.47	1.41
19	B	844	BCR	C19-C18	-2.31	1.41	1.45
16	B	809	CLA	C1C-C2C	2.31	1.49	1.44
16	4	407	CLA	C1B-CHB	2.31	1.47	1.41
16	1	509	CLA	C3D-C4D	-2.31	1.39	1.44
16	A	803	CLA	C4B-CHC	2.31	1.47	1.41
16	4	405	CLA	C1B-CHB	2.30	1.47	1.41
16	1	507	CLA	C3D-C4D	-2.30	1.39	1.44
16	1	520	CLA	C4D-CHA	2.30	1.46	1.38
16	A	827	CLA	C1B-NB	-2.30	1.33	1.35
16	1	508	CLA	C1B-CHB	2.30	1.47	1.41
16	A	802	CLA	C1B-CHB	2.30	1.47	1.41
16	5	409	CLA	C1B-CHB	2.30	1.47	1.41
16	A	837	CLA	C4D-CHA	2.30	1.46	1.38
19	5	420	BCR	C19-C18	-2.30	1.41	1.45
16	B	808	CLA	C4D-CHA	2.30	1.46	1.38
16	K	103	CLA	C3D-C4D	-2.30	1.39	1.44
16	A	826	CLA	C1B-CHB	2.30	1.47	1.41
16	1	519	CLA	C3D-C4D	-2.30	1.39	1.44
16	5	412	CLA	C3D-C4D	-2.30	1.39	1.44
16	4	410	CLA	C3D-C4D	-2.29	1.39	1.44
19	B	846	BCR	C15-C14	-2.29	1.36	1.43
16	1	504	CLA	C4C-C3C	2.29	1.49	1.45
16	A	804	CLA	C4D-CHA	2.29	1.46	1.38
15	A	801	CL0	C1C-C2C	2.29	1.49	1.44
16	B	832	CLA	C4B-CHC	2.29	1.47	1.41
16	A	804	CLA	C4B-CHC	2.29	1.47	1.41
16	1	508	CLA	C4B-CHC	2.29	1.47	1.41
16	B	812	CLA	C4D-CHA	2.29	1.46	1.38
16	1	501	CLA	C4B-CHC	2.29	1.47	1.41
16	5	409	CLA	C3D-C4D	-2.29	1.39	1.44
16	A	828	CLA	C1C-NC	-2.28	1.34	1.37
16	B	818	CLA	C4D-CHA	2.28	1.46	1.38
16	A	820	CLA	C1C-NC	-2.28	1.34	1.37
16	B	822	CLA	C4C-C3C	2.28	1.49	1.45
16	6	401	CLA	C3D-C4D	-2.28	1.39	1.44
16	B	837	CLA	C4D-CHA	2.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	842	CLA	C1C-NC	-2.28	1.34	1.37
15	A	801	CL0	C4D-CHA	2.28	1.46	1.38
16	A	819	CLA	C1C-C2C	2.28	1.49	1.44
16	1	509	CLA	C4D-CHA	2.28	1.46	1.38
16	B	833	CLA	C1C-NC	-2.28	1.34	1.37
19	B	844	BCR	C12-C13	-2.27	1.41	1.45
16	B	839	CLA	C4B-CHC	2.27	1.47	1.41
16	X	101	CLA	C4B-CHC	2.27	1.47	1.41
16	1	506	CLA	C4C-C3C	2.27	1.49	1.45
16	B	833	CLA	C3D-C4D	-2.27	1.39	1.44
16	5	413	CLA	C1B-CHB	2.27	1.47	1.41
16	A	836	CLA	C4D-CHA	2.27	1.46	1.38
16	4	403	CLA	C3D-C4D	-2.27	1.39	1.44
16	4	409	CLA	C3D-C4D	-2.27	1.39	1.44
16	1	503	CLA	C3D-C4D	-2.27	1.39	1.44
16	A	809	CLA	C1C-C2C	2.27	1.49	1.44
16	1	506	CLA	C4D-CHA	2.27	1.46	1.38
16	6	409	CLA	C3D-C4D	-2.27	1.39	1.44
16	5	406	CLA	C3D-C4D	-2.27	1.39	1.44
16	A	821	CLA	C4D-CHA	2.27	1.46	1.38
16	B	812	CLA	C4B-CHC	2.27	1.47	1.41
16	A	822	CLA	C4D-CHA	2.27	1.46	1.38
16	5	419	CLA	C3D-C4D	-2.27	1.39	1.44
16	A	815	CLA	C1B-NB	-2.27	1.33	1.35
16	5	404	CLA	C1C-C2C	2.27	1.48	1.44
16	4	404	CLA	C3D-C4D	-2.26	1.39	1.44
16	B	812	CLA	C1C-NC	-2.26	1.34	1.37
16	A	833	CLA	C4B-CHC	2.26	1.47	1.41
16	6	407	CLA	C3D-C4D	-2.26	1.39	1.44
16	A	839	CLA	C1B-CHB	2.26	1.47	1.41
16	5	410	CLA	C1C-C2C	2.26	1.48	1.44
16	A	821	CLA	C4B-CHC	2.26	1.47	1.41
16	5	407	CLA	C1B-CHB	2.26	1.47	1.41
16	2	404	CLA	C3D-C4D	-2.26	1.39	1.44
16	A	835	CLA	C4B-CHC	2.26	1.47	1.41
16	6	404	CLA	C3D-C4D	-2.25	1.39	1.44
16	A	813	CLA	C1B-CHB	2.25	1.47	1.41
16	A	813	CLA	C4D-CHA	2.25	1.46	1.38
19	J	104	BCR	C16-C17	-2.25	1.36	1.43
16	1	506	CLA	C1B-CHB	2.25	1.47	1.41
16	B	804	CLA	C4D-CHA	2.25	1.46	1.38
16	1	514	CLA	C3D-C4D	-2.25	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	834	CLA	C4D-CHA	2.25	1.46	1.38
16	A	842	CLA	C1C-C2C	2.25	1.48	1.44
16	5	410	CLA	C3D-C4D	-2.25	1.39	1.44
16	F	201	CLA	C1B-CHB	2.25	1.47	1.41
16	B	841	CLA	C4C-C3C	2.25	1.48	1.45
16	B	841	CLA	C1C-C2C	2.25	1.48	1.44
16	A	808	CLA	C4B-CHC	2.25	1.47	1.41
16	A	802	CLA	C1C-NC	-2.25	1.34	1.37
16	5	416	CLA	C3D-C4D	-2.25	1.39	1.44
16	B	834	CLA	C4B-CHC	2.25	1.47	1.41
16	B	827	CLA	C4B-CHC	2.25	1.47	1.41
16	A	818	CLA	C4D-CHA	2.25	1.46	1.38
16	B	808	CLA	C4B-CHC	2.25	1.47	1.41
19	4	401	BCR	C19-C18	-2.25	1.41	1.45
16	B	807	CLA	C4C-C3C	2.25	1.48	1.45
16	2	406	CLA	C3D-C4D	-2.25	1.39	1.44
16	B	839	CLA	C4B-NB	-2.25	1.33	1.35
16	A	821	CLA	C4C-C3C	2.25	1.48	1.45
16	B	827	CLA	OBD-CAD	2.24	1.26	1.22
16	B	830	CLA	C1B-NB	-2.24	1.33	1.35
16	A	815	CLA	C4B-CHC	2.24	1.47	1.41
16	B	839	CLA	C4D-CHA	2.24	1.46	1.38
16	6	402	CLA	C3D-C4D	-2.24	1.39	1.44
16	A	815	CLA	C1C-C2C	2.24	1.48	1.44
16	A	842	CLA	C4B-CHC	2.24	1.47	1.41
16	5	414	CLA	C3D-C4D	-2.24	1.39	1.44
16	1	504	CLA	C1B-CHB	2.24	1.47	1.41
16	A	841	CLA	C1B-NB	-2.24	1.33	1.35
16	B	803	CLA	C3D-C4D	-2.24	1.39	1.44
16	A	810	CLA	C4D-CHA	2.24	1.46	1.38
19	B	847	BCR	C11-C10	-2.24	1.36	1.43
16	B	805	CLA	C1C-C2C	2.24	1.48	1.44
16	A	824	CLA	C4D-CHA	2.24	1.46	1.38
16	B	841	CLA	C1B-CHB	2.24	1.47	1.41
16	B	838	CLA	C4D-CHA	2.24	1.46	1.38
16	1	521	CLA	C4C-C3C	2.23	1.48	1.45
16	B	829	CLA	C1C-C2C	2.23	1.48	1.44
16	B	832	CLA	C4D-CHA	2.23	1.46	1.38
16	B	831	CLA	C1C-NC	-2.23	1.34	1.37
16	A	831	CLA	C4D-CHA	2.23	1.46	1.38
16	B	805	CLA	C4C-C3C	2.23	1.48	1.45
16	6	408	CLA	C3D-C4D	-2.23	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	405	CLA	C3D-C4D	-2.23	1.39	1.44
16	A	819	CLA	C1C-NC	-2.23	1.34	1.37
16	A	808	CLA	C4D-CHA	2.23	1.46	1.38
16	B	810	CLA	C1B-CHB	2.23	1.47	1.41
16	B	828	CLA	C4D-CHA	2.22	1.46	1.38
16	B	809	CLA	C4D-CHA	2.22	1.46	1.38
16	B	806	CLA	C1B-NB	-2.22	1.33	1.35
16	B	824	CLA	C1B-NB	-2.22	1.33	1.35
16	1	508	CLA	C1C-C2C	2.22	1.48	1.44
16	A	832	CLA	C4D-CHA	2.22	1.46	1.38
16	4	406	CLA	C3D-C4D	-2.22	1.39	1.44
16	4	405	CLA	C3D-C4D	-2.22	1.39	1.44
16	B	820	CLA	C1B-CHB	2.22	1.47	1.41
16	A	830	CLA	C4B-CHC	2.22	1.47	1.41
16	1	515	CLA	C3D-C4D	-2.22	1.39	1.44
16	5	415	CLA	C3D-C4D	-2.22	1.39	1.44
16	A	829	CLA	C4D-CHA	2.22	1.46	1.38
16	4	411	CLA	C3D-C4D	-2.21	1.39	1.44
16	1	515	CLA	C1B-CHB	2.21	1.47	1.41
16	5	408	CLA	C3D-C4D	-2.21	1.39	1.44
16	B	825	CLA	C1C-C2C	2.21	1.48	1.44
16	B	835	CLA	C4D-CHA	2.21	1.46	1.38
16	A	823	CLA	C4D-CHA	2.21	1.46	1.38
16	1	501	CLA	C1B-NB	-2.21	1.33	1.35
16	X	101	CLA	C1B-CHB	2.21	1.47	1.41
16	1	510	CLA	C3D-C4D	-2.21	1.39	1.44
16	1	502	CLA	C3D-C4D	-2.21	1.39	1.44
16	2	405	CLA	C3D-C4D	-2.21	1.39	1.44
16	3	401	CLA	C3D-C4D	-2.21	1.39	1.44
16	B	802	CLA	C4B-CHC	2.21	1.47	1.41
16	B	828	CLA	C4B-CHC	2.21	1.47	1.41
16	J	101	CLA	C1B-CHB	2.21	1.47	1.41
16	1	508	CLA	C3D-C4D	-2.21	1.39	1.44
16	1	505	CLA	C3D-C4D	-2.20	1.39	1.44
19	B	847	BCR	C16-C17	-2.20	1.36	1.43
16	4	407	CLA	C3D-C4D	-2.20	1.39	1.44
16	A	815	CLA	C1B-CHB	2.20	1.47	1.41
16	B	813	CLA	C4D-CHA	2.20	1.46	1.38
16	6	405	CLA	C3D-C4D	-2.20	1.39	1.44
16	A	808	CLA	C1B-NB	-2.20	1.33	1.35
16	B	802	CLA	C4D-CHA	2.20	1.46	1.38
16	B	822	CLA	C4B-CHC	2.20	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	848	BCR	C20-C21	-2.20	1.36	1.43
16	B	816	CLA	C4D-CHA	2.19	1.46	1.38
16	A	816	CLA	C1C-C2C	2.19	1.48	1.44
16	B	807	CLA	C4B-CHC	2.19	1.47	1.41
16	A	843	CLA	C1C-NC	-2.19	1.34	1.37
16	5	407	CLA	C4B-CHC	2.19	1.47	1.41
16	2	401	CLA	C3D-C4D	-2.19	1.39	1.44
16	5	403	CLA	C3D-C4D	-2.19	1.39	1.44
16	A	838	CLA	C4B-CHC	2.19	1.47	1.41
16	A	841	CLA	C4D-CHA	2.19	1.46	1.38
16	A	802	CLA	C4B-NB	-2.19	1.33	1.35
16	1	507	CLA	C4B-CHC	2.19	1.47	1.41
16	1	521	CLA	C1B-CHB	2.18	1.47	1.41
16	A	825	CLA	C4C-C3C	2.18	1.48	1.45
16	K	103	CLA	C4C-C3C	2.18	1.48	1.45
16	A	839	CLA	C4B-CHC	2.18	1.47	1.41
16	2	403	CLA	C3D-C4D	-2.18	1.39	1.44
19	I	102	BCR	C12-C13	-2.18	1.41	1.45
16	2	401	CLA	C4C-C3C	2.18	1.48	1.45
16	B	819	CLA	C4D-CHA	2.18	1.46	1.38
16	5	404	CLA	C4C-C3C	2.18	1.48	1.45
16	A	821	CLA	C1B-CHB	2.18	1.47	1.41
16	6	408	CLA	C1D-C2D	2.18	1.49	1.45
16	5	418	CLA	C3D-C4D	-2.18	1.39	1.44
16	2	402	CLA	C3D-C4D	-2.18	1.39	1.44
16	B	831	CLA	C1B-CHB	2.18	1.47	1.41
16	A	812	CLA	C4B-CHC	2.18	1.47	1.41
16	A	836	CLA	C1C-C2C	2.18	1.48	1.44
16	A	840	CLA	C1C-NC	-2.18	1.34	1.37
16	A	837	CLA	C4B-CHC	2.18	1.47	1.41
16	6	406	CLA	C3D-C4D	-2.18	1.39	1.44
16	B	826	CLA	C4D-CHA	2.17	1.46	1.38
19	B	846	BCR	C16-C17	-2.17	1.36	1.43
16	B	804	CLA	C1C-C2C	2.17	1.48	1.44
16	K	101	CLA	C1C-NC	-2.17	1.34	1.37
16	B	829	CLA	C1B-CHB	2.17	1.47	1.41
16	6	403	CLA	C3D-C4D	-2.17	1.39	1.44
16	B	814	CLA	C3D-C4D	-2.17	1.39	1.44
16	B	802	CLA	C1B-CHB	2.17	1.47	1.41
16	A	804	CLA	C1B-CHB	2.17	1.47	1.41
16	5	403	CLA	C4C-C3C	2.17	1.48	1.45
16	B	824	CLA	C4D-CHA	2.16	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	817	CLA	C1C-NC	-2.16	1.34	1.37
16	A	833	CLA	C1C-NC	-2.16	1.34	1.37
16	A	809	CLA	C1B-CHB	2.16	1.47	1.41
16	B	801	CLA	C4D-CHA	2.16	1.46	1.38
16	B	837	CLA	C4C-C3C	2.16	1.48	1.45
16	A	807	CLA	C4D-CHA	2.16	1.46	1.38
16	B	835	CLA	C1C-NC	-2.15	1.34	1.37
16	B	804	CLA	C1C-NC	-2.15	1.34	1.37
16	A	837	CLA	C1C-C2C	2.15	1.48	1.44
16	A	817	CLA	C4B-CHC	2.15	1.47	1.41
16	B	803	CLA	C4B-NB	-2.15	1.33	1.35
16	1	502	CLA	C4C-C3C	2.15	1.48	1.45
19	1	523	BCR	C16-C17	-2.15	1.36	1.43
16	A	805	CLA	C3D-C4D	-2.15	1.39	1.44
16	4	402	CLA	C3D-C4D	-2.15	1.39	1.44
16	A	805	CLA	C1B-CHB	2.15	1.47	1.41
16	A	807	CLA	C1C-NC	-2.15	1.34	1.37
19	F	205	BCR	C19-C18	-2.15	1.41	1.45
16	B	829	CLA	C1C-NC	-2.15	1.34	1.37
16	B	806	CLA	C4B-CHC	2.15	1.47	1.41
16	K	103	CLA	C1C-NC	-2.15	1.34	1.37
16	B	827	CLA	C4D-CHA	2.15	1.46	1.38
16	A	838	CLA	C1B-NB	-2.14	1.33	1.35
16	A	835	CLA	C4D-CHA	2.14	1.46	1.38
16	B	804	CLA	C1B-CHB	2.14	1.46	1.41
19	A	850	BCR	C15-C14	-2.14	1.36	1.43
16	A	832	CLA	C4B-CHC	2.14	1.46	1.41
16	4	402	CLA	C4C-C3C	2.14	1.48	1.45
16	A	840	CLA	C1B-NB	-2.14	1.33	1.35
16	A	825	CLA	C1B-CHB	2.13	1.46	1.41
16	2	406	CLA	C1D-C2D	2.13	1.49	1.45
16	A	834	CLA	C4B-CHC	2.13	1.46	1.41
16	A	843	CLA	C4D-CHA	2.13	1.46	1.38
16	A	809	CLA	C4B-CHC	2.13	1.46	1.41
16	B	801	CLA	C4C-C3C	2.13	1.48	1.45
16	A	828	CLA	C1B-CHB	2.13	1.46	1.41
16	A	811	CLA	C4C-C3C	2.13	1.48	1.45
16	B	841	CLA	C1B-NB	-2.13	1.33	1.35
16	A	825	CLA	C1C-NC	-2.13	1.34	1.37
19	1	517	BCR	C12-C13	-2.13	1.41	1.45
16	B	840	CLA	C1B-CHB	2.13	1.46	1.41
16	A	811	CLA	C4B-CHC	2.12	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	201	CLA	C4B-CHC	2.12	1.46	1.41
16	B	810	CLA	C4D-CHA	2.12	1.46	1.38
16	A	843	CLA	C4B-CHC	2.12	1.46	1.41
16	5	413	CLA	C1D-C2D	2.12	1.49	1.45
19	I	102	BCR	C23-C22	-2.12	1.41	1.45
16	A	802	CLA	C4B-CHC	2.12	1.46	1.41
16	A	812	CLA	C1C-NC	-2.12	1.34	1.37
19	B	853	BCR	C15-C14	-2.12	1.36	1.43
16	A	816	CLA	C4B-CHC	2.12	1.46	1.41
16	A	803	CLA	C3D-C4D	-2.12	1.39	1.44
16	A	814	CLA	C1B-NB	-2.12	1.33	1.35
16	A	826	CLA	C4B-NB	-2.12	1.33	1.35
16	B	838	CLA	C1C-C2C	2.12	1.48	1.44
16	B	826	CLA	C1C-NC	-2.12	1.34	1.37
16	B	823	CLA	C4B-CHC	2.12	1.46	1.41
16	B	833	CLA	C1B-CHB	2.12	1.46	1.41
16	5	416	CLA	C1D-C2D	2.12	1.49	1.45
19	A	850	BCR	C11-C10	-2.12	1.36	1.43
19	1	518	BCR	C19-C18	-2.12	1.41	1.45
16	A	824	CLA	C1B-CHB	2.11	1.46	1.41
16	4	410	CLA	C1D-C2D	2.11	1.49	1.45
16	B	829	CLA	C4B-CHC	2.11	1.46	1.41
16	K	101	CLA	C1C-C2C	2.11	1.48	1.44
16	B	813	CLA	C1C-NC	-2.11	1.34	1.37
16	A	840	CLA	C1C-C2C	2.11	1.48	1.44
16	1	508	CLA	C1C-NC	-2.11	1.34	1.37
19	J	103	BCR	C12-C13	-2.11	1.41	1.45
16	A	806	CLA	C4D-CHA	2.11	1.45	1.38
16	A	838	CLA	C1C-NC	-2.11	1.34	1.37
16	A	833	CLA	C1C-C2C	2.10	1.48	1.44
16	B	817	CLA	C4D-CHA	2.10	1.45	1.38
16	A	836	CLA	C4B-CHC	2.10	1.46	1.41
16	B	836	CLA	C1B-CHB	2.10	1.46	1.41
16	5	406	CLA	C1D-C2D	2.10	1.49	1.45
16	B	811	CLA	C4C-C3C	2.10	1.48	1.45
19	B	848	BCR	C20-C21	-2.10	1.36	1.43
16	A	821	CLA	C1B-NB	-2.10	1.33	1.35
16	6	403	CLA	C1D-C2D	2.10	1.49	1.45
16	A	803	CLA	C1C-C2C	2.10	1.48	1.44
16	A	838	CLA	C1B-CHB	2.10	1.46	1.41
16	B	830	CLA	C4B-CHC	2.10	1.46	1.41
16	6	407	CLA	C1D-C2D	2.10	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	411	CLA	C1B-CHB	2.10	1.46	1.41
16	6	409	CLA	C1D-C2D	2.10	1.49	1.45
16	1	501	CLA	C1C-NC	-2.10	1.34	1.37
19	1	523	BCR	C20-C21	-2.09	1.37	1.43
16	4	409	CLA	C1D-C2D	2.09	1.49	1.45
16	4	406	CLA	C1B-CHB	2.09	1.46	1.41
16	A	820	CLA	C1C-C2C	2.09	1.48	1.44
16	A	828	CLA	C1B-NB	-2.09	1.33	1.35
16	A	833	CLA	C4D-CHA	2.09	1.45	1.38
16	5	414	CLA	C1C-NC	-2.09	1.34	1.37
16	A	820	CLA	C4D-CHA	2.09	1.45	1.38
19	B	848	BCR	C16-C17	-2.09	1.37	1.43
16	B	820	CLA	C1C-NC	-2.09	1.34	1.37
19	A	850	BCR	C16-C17	-2.09	1.37	1.43
16	B	823	CLA	C1B-CHB	2.09	1.46	1.41
16	J	102	CLA	C1B-CHB	2.09	1.46	1.41
16	5	408	CLA	C1D-C2D	2.09	1.49	1.45
16	A	842	CLA	C1B-NB	-2.09	1.33	1.35
16	B	825	CLA	C1C-NC	-2.09	1.34	1.37
16	A	807	CLA	C4B-CHC	2.09	1.46	1.41
16	A	840	CLA	C4C-C3C	2.09	1.48	1.45
16	A	812	CLA	C1C-C2C	2.09	1.48	1.44
16	B	834	CLA	C1B-CHB	2.08	1.46	1.41
16	B	831	CLA	C4B-CHC	2.08	1.46	1.41
16	A	831	CLA	C4B-CHC	2.08	1.46	1.41
16	2	402	CLA	C1D-C2D	2.08	1.49	1.45
16	B	841	CLA	C4B-CHC	2.08	1.46	1.41
16	6	402	CLA	C1D-C2D	2.08	1.49	1.45
16	B	814	CLA	C1B-CHB	2.08	1.46	1.41
16	A	831	CLA	C1C-NC	-2.08	1.34	1.37
16	B	830	CLA	C1C-C2C	2.08	1.48	1.44
16	A	812	CLA	C4D-CHA	2.08	1.45	1.38
16	B	831	CLA	C4C-C3C	2.07	1.48	1.45
16	2	404	CLA	C1D-C2D	2.07	1.49	1.45
16	A	833	CLA	C1B-CHB	2.07	1.46	1.41
16	4	402	CLA	C1D-C2D	2.07	1.49	1.45
15	A	801	CL0	C4B-CHC	2.07	1.46	1.41
16	1	501	CLA	C1B-CHB	2.07	1.46	1.41
19	A	848	BCR	C16-C17	-2.07	1.37	1.43
19	I	101	BCR	C16-C17	-2.07	1.37	1.43
16	B	824	CLA	C1B-CHB	2.07	1.46	1.41
16	A	817	CLA	C1C-NC	-2.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	410	CLA	C1B-NB	-2.06	1.33	1.35
16	1	509	CLA	C1B-CHB	2.06	1.46	1.41
15	A	801	CL0	C1B-CHB	2.06	1.46	1.41
16	B	801	CLA	C1B-CHB	2.06	1.46	1.41
16	A	806	CLA	C4B-CHC	2.06	1.46	1.41
16	A	836	CLA	C1B-CHB	2.06	1.46	1.41
16	B	839	CLA	C1C-C2C	2.06	1.48	1.44
16	4	411	CLA	C1D-C2D	2.06	1.49	1.45
16	A	841	CLA	C1B-CHB	2.05	1.46	1.41
16	A	841	CLA	C4B-NB	-2.05	1.33	1.35
16	A	823	CLA	C1C-NC	-2.05	1.34	1.37
16	B	814	CLA	C1B-NB	-2.05	1.33	1.35
16	X	101	CLA	C1B-NB	-2.05	1.33	1.35
16	A	826	CLA	C4C-C3C	2.05	1.48	1.45
16	B	830	CLA	C4C-C3C	2.05	1.48	1.45
16	B	818	CLA	C1C-C2C	2.05	1.48	1.44
16	5	417	CLA	C1D-C2D	2.05	1.49	1.45
16	B	806	CLA	C1B-CHB	2.05	1.46	1.41
19	A	846	BCR	C16-C17	-2.05	1.37	1.43
16	F	204	CLA	C4C-C3C	2.04	1.48	1.45
16	A	826	CLA	C1C-NC	-2.04	1.34	1.37
19	F	202	BCR	C20-C21	-2.04	1.37	1.43
19	1	522	BCR	C15-C14	-2.04	1.37	1.43
16	5	415	CLA	C1D-C2D	2.04	1.49	1.45
16	A	840	CLA	C1B-CHB	2.04	1.46	1.41
16	B	834	CLA	C4C-C3C	2.04	1.48	1.45
16	B	839	CLA	C1B-NB	-2.04	1.33	1.35
16	J	102	CLA	C4C-C3C	2.04	1.48	1.45
16	1	514	CLA	C1D-C2D	2.04	1.49	1.45
16	3	401	CLA	C1D-C2D	2.04	1.49	1.45
16	5	404	CLA	C4B-CHC	2.04	1.46	1.41
16	B	808	CLA	C1C-C2C	2.03	1.48	1.44
16	4	404	CLA	C1D-C2D	2.03	1.49	1.45
16	F	201	CLA	C1C-NC	-2.03	1.34	1.37
16	4	405	CLA	C1D-C2D	2.03	1.49	1.45
16	A	810	CLA	C1B-CHB	2.03	1.46	1.41
16	2	403	CLA	C1D-C2D	2.03	1.49	1.45
21	1	524	LMT	O1'-C1'	2.03	1.43	1.40
19	K	102	BCR	C19-C18	-2.03	1.41	1.45
16	A	837	CLA	C1C-NC	-2.03	1.34	1.37
16	B	836	CLA	C4C-C3C	2.03	1.48	1.45
16	5	421	CLA	C1D-C2D	2.03	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	402	BCR	C19-C18	-2.03	1.41	1.45
19	B	848	BCR	C15-C14	-2.03	1.37	1.43
19	A	850	BCR	C20-C21	-2.02	1.37	1.43
16	5	419	CLA	C1D-C2D	2.02	1.49	1.45
16	A	836	CLA	C1C-NC	-2.02	1.34	1.37
16	A	839	CLA	C1B-NB	-2.02	1.33	1.35
16	5	405	CLA	C1D-C2D	2.02	1.49	1.45
16	X	101	CLA	C1C-NC	-2.02	1.34	1.37
16	A	811	CLA	C1C-C2C	2.02	1.48	1.44
19	F	202	BCR	C16-C17	-2.02	1.37	1.43
16	B	835	CLA	C1B-CHB	2.02	1.46	1.41
16	6	405	CLA	C1D-C2D	2.02	1.49	1.45
16	6	404	CLA	C1D-C2D	2.01	1.49	1.45
16	B	838	CLA	C1B-CHB	2.01	1.46	1.41
16	A	837	CLA	C1B-NB	-2.01	1.33	1.35
16	1	526	CLA	C1D-C2D	2.01	1.49	1.45
16	B	801	CLA	C4B-CHC	2.01	1.46	1.41
16	1	505	CLA	C1D-C2D	2.01	1.49	1.45
19	1	517	BCR	C19-C18	-2.01	1.41	1.45
16	6	406	CLA	C1D-C2D	2.01	1.49	1.45
16	5	418	CLA	C1D-C2D	2.01	1.49	1.45
16	6	401	CLA	C1D-C2D	2.01	1.49	1.45
16	4	408	CLA	C1D-C2D	2.01	1.49	1.45
19	B	844	BCR	C16-C17	-2.01	1.37	1.43
16	1	504	CLA	C1D-C2D	2.01	1.49	1.45
16	5	409	CLA	C1D-C2D	2.00	1.49	1.45
16	B	839	CLA	C4C-C3C	2.00	1.48	1.45
21	B	851	LMT	O1'-C1'	2.00	1.43	1.40
16	5	416	CLA	C1C-NC	-2.00	1.34	1.37

All (4163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	816	CLA	C1D-ND-C4D	-11.19	98.39	106.33
16	A	823	CLA	C1D-ND-C4D	-11.09	98.46	106.33
16	1	520	CLA	C1D-ND-C4D	-11.05	98.48	106.33
16	B	841	CLA	C1D-ND-C4D	-10.97	98.54	106.33
16	B	832	CLA	C1D-ND-C4D	-10.81	98.66	106.33
16	A	818	CLA	C1D-ND-C4D	-10.81	98.66	106.33
16	B	826	CLA	C1D-ND-C4D	-10.74	98.71	106.33
16	1	504	CLA	C1D-ND-C4D	-10.71	98.72	106.33
16	5	415	CLA	C1D-ND-C4D	-10.67	98.75	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	812	CLA	C1D-ND-C4D	-10.50	98.87	106.33
16	B	813	CLA	C1D-ND-C4D	-10.50	98.88	106.33
16	A	806	CLA	C1D-ND-C4D	-10.49	98.88	106.33
16	5	405	CLA	C1D-ND-C4D	-10.44	98.92	106.33
16	B	810	CLA	C1D-ND-C4D	-10.39	98.95	106.33
16	A	824	CLA	C1D-ND-C4D	-10.30	99.02	106.33
16	B	808	CLA	C1D-ND-C4D	-10.28	99.03	106.33
16	A	840	CLA	C1D-ND-C4D	-10.24	99.06	106.33
16	4	403	CLA	C1D-ND-C4D	-10.21	99.08	106.33
16	5	403	CLA	C1D-ND-C4D	-10.15	99.13	106.33
16	A	843	CLA	C1D-ND-C4D	-10.15	99.13	106.33
16	4	402	CLA	C1D-ND-C4D	-10.15	99.13	106.33
16	B	833	CLA	C1D-ND-C4D	-10.10	99.16	106.33
16	1	502	CLA	C1D-ND-C4D	-10.09	99.16	106.33
16	1	519	CLA	C1D-ND-C4D	-10.09	99.17	106.33
15	A	801	CL0	C1D-ND-C4D	-10.07	99.18	106.33
16	5	408	CLA	C1D-ND-C4D	-10.03	99.21	106.33
16	2	401	CLA	C1D-ND-C4D	-10.02	99.21	106.33
16	B	814	CLA	C1D-ND-C4D	-10.01	99.22	106.33
16	A	827	CLA	C1D-ND-C4D	-10.01	99.22	106.33
16	A	838	CLA	C1D-ND-C4D	-10.01	99.22	106.33
16	A	816	CLA	C1D-ND-C4D	-10.01	99.22	106.33
16	A	828	CLA	C1D-ND-C4D	-10.00	99.23	106.33
16	A	823	CLA	C2D-C1D-ND	9.96	117.45	110.10
16	5	410	CLA	C1D-ND-C4D	-9.93	99.28	106.33
16	B	832	CLA	C2D-C1D-ND	9.93	117.42	110.10
16	5	416	CLA	C1D-ND-C4D	-9.91	99.29	106.33
16	A	804	CLA	C1D-ND-C4D	-9.91	99.30	106.33
16	4	407	CLA	C1D-ND-C4D	-9.90	99.31	106.33
16	B	827	CLA	C1D-ND-C4D	-9.89	99.31	106.33
16	K	103	CLA	C1D-ND-C4D	-9.89	99.31	106.33
16	4	409	CLA	C1D-ND-C4D	-9.87	99.32	106.33
16	A	811	CLA	C1D-ND-C4D	-9.87	99.32	106.33
16	A	810	CLA	C1D-ND-C4D	-9.87	99.32	106.33
16	1	505	CLA	C1D-ND-C4D	-9.86	99.33	106.33
16	A	833	CLA	C1D-ND-C4D	-9.85	99.34	106.33
16	B	817	CLA	C1D-ND-C4D	-9.84	99.34	106.33
16	B	829	CLA	C1D-ND-C4D	-9.84	99.35	106.33
16	B	801	CLA	C1D-ND-C4D	-9.83	99.35	106.33
16	5	421	CLA	C1D-ND-C4D	-9.82	99.36	106.33
16	A	839	CLA	C1D-ND-C4D	-9.82	99.36	106.33
16	A	803	CLA	C1D-ND-C4D	-9.81	99.37	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	831	CLA	C1D-ND-C4D	-9.80	99.37	106.33
16	2	404	CLA	C1D-ND-C4D	-9.79	99.38	106.33
16	A	807	CLA	C1D-ND-C4D	-9.79	99.38	106.33
16	B	823	CLA	C1D-ND-C4D	-9.76	99.40	106.33
16	1	506	CLA	C1D-ND-C4D	-9.76	99.40	106.33
16	4	411	CLA	C1D-ND-C4D	-9.74	99.41	106.33
16	6	404	CLA	C1D-ND-C4D	-9.74	99.42	106.33
16	B	820	CLA	C1D-ND-C4D	-9.73	99.42	106.33
16	A	821	CLA	C1D-ND-C4D	-9.72	99.43	106.33
16	A	835	CLA	C1D-ND-C4D	-9.72	99.43	106.33
16	A	842	CLA	C1D-ND-C4D	-9.72	99.43	106.33
16	6	407	CLA	C1D-ND-C4D	-9.71	99.44	106.33
16	B	837	CLA	C1D-ND-C4D	-9.70	99.44	106.33
16	B	841	CLA	C2D-C1D-ND	9.70	117.25	110.10
16	B	808	CLA	C2D-C1D-ND	9.69	117.25	110.10
16	1	514	CLA	C1D-ND-C4D	-9.69	99.45	106.33
16	5	406	CLA	C1D-ND-C4D	-9.69	99.45	106.33
16	B	810	CLA	C2D-C1D-ND	9.68	117.24	110.10
16	B	836	CLA	C1D-ND-C4D	-9.68	99.46	106.33
16	5	417	CLA	C1D-ND-C4D	-9.68	99.46	106.33
16	B	838	CLA	C1D-ND-C4D	-9.67	99.46	106.33
16	3	401	CLA	C1D-ND-C4D	-9.67	99.47	106.33
16	B	818	CLA	C1D-ND-C4D	-9.66	99.48	106.33
16	B	839	CLA	C1D-ND-C4D	-9.65	99.48	106.33
16	X	101	CLA	C1D-ND-C4D	-9.63	99.49	106.33
16	1	512	CLA	C1D-ND-C4D	-9.62	99.50	106.33
16	A	841	CLA	C1D-ND-C4D	-9.61	99.51	106.33
16	6	401	CLA	C1D-ND-C4D	-9.61	99.51	106.33
16	A	818	CLA	C2D-C1D-ND	9.60	117.18	110.10
16	6	408	CLA	C1D-ND-C4D	-9.59	99.52	106.33
16	5	413	CLA	C1D-ND-C4D	-9.59	99.52	106.33
16	B	840	CLA	C1D-ND-C4D	-9.58	99.53	106.33
16	A	836	CLA	C1D-ND-C4D	-9.58	99.53	106.33
16	A	832	CLA	C1D-ND-C4D	-9.58	99.53	106.33
16	1	509	CLA	C1D-ND-C4D	-9.57	99.54	106.33
16	A	822	CLA	C1D-ND-C4D	-9.57	99.54	106.33
16	4	410	CLA	C1D-ND-C4D	-9.55	99.55	106.33
16	4	404	CLA	C1D-ND-C4D	-9.55	99.55	106.33
16	A	831	CLA	C2D-C1D-ND	9.55	117.14	110.10
16	2	402	CLA	C1D-ND-C4D	-9.53	99.56	106.33
16	B	811	CLA	C1D-ND-C4D	-9.52	99.58	106.33
16	B	815	CLA	C1D-ND-C4D	-9.51	99.58	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	406	CLA	C1D-ND-C4D	-9.50	99.58	106.33
16	1	525	CLA	C1D-ND-C4D	-9.50	99.59	106.33
16	4	408	CLA	C1D-ND-C4D	-9.49	99.59	106.33
16	5	418	CLA	C1D-ND-C4D	-9.49	99.60	106.33
16	1	526	CLA	C1D-ND-C4D	-9.49	99.60	106.33
16	6	402	CLA	C1D-ND-C4D	-9.49	99.60	106.33
16	B	833	CLA	C2D-C1D-ND	9.48	117.09	110.10
16	1	515	CLA	C1D-ND-C4D	-9.46	99.61	106.33
16	B	835	CLA	C1D-ND-C4D	-9.45	99.62	106.33
16	A	805	CLA	C1D-ND-C4D	-9.45	99.62	106.33
16	5	422	CLA	C1D-ND-C4D	-9.45	99.62	106.33
16	5	419	CLA	C1D-ND-C4D	-9.45	99.62	106.33
16	6	409	CLA	C1D-ND-C4D	-9.44	99.63	106.33
16	B	825	CLA	C1D-ND-C4D	-9.44	99.63	106.33
16	5	412	CLA	C1D-ND-C4D	-9.43	99.63	106.33
16	B	826	CLA	C2D-C1D-ND	9.43	117.05	110.10
16	A	820	CLA	C1D-ND-C4D	-9.43	99.64	106.33
16	B	816	CLA	C2D-C1D-ND	9.42	117.04	110.10
16	B	821	CLA	C1D-ND-C4D	-9.41	99.65	106.33
16	5	409	CLA	C1D-ND-C4D	-9.41	99.65	106.33
16	A	825	CLA	C1D-ND-C4D	-9.41	99.65	106.33
16	6	405	CLA	C1D-ND-C4D	-9.40	99.66	106.33
16	1	520	CLA	C2D-C1D-ND	9.39	117.02	110.10
16	B	819	CLA	C1D-ND-C4D	-9.38	99.67	106.33
16	4	405	CLA	C1D-ND-C4D	-9.38	99.67	106.33
16	B	823	CLA	C2D-C1D-ND	9.37	117.01	110.10
16	6	406	CLA	C1D-ND-C4D	-9.36	99.68	106.33
16	F	204	CLA	C1D-ND-C4D	-9.36	99.69	106.33
16	A	802	CLA	C1D-ND-C4D	-9.36	99.69	106.33
16	B	804	CLA	C1D-ND-C4D	-9.36	99.69	106.33
16	A	808	CLA	C1D-ND-C4D	-9.35	99.69	106.33
16	A	814	CLA	C1D-ND-C4D	-9.35	99.69	106.33
16	B	806	CLA	C1D-ND-C4D	-9.32	99.71	106.33
16	J	102	CLA	C1D-ND-C4D	-9.31	99.72	106.33
16	1	513	CLA	C1D-ND-C4D	-9.30	99.73	106.33
16	2	405	CLA	C1D-ND-C4D	-9.30	99.73	106.33
16	K	101	CLA	C1D-ND-C4D	-9.29	99.73	106.33
16	A	837	CLA	C1D-ND-C4D	-9.28	99.74	106.33
16	B	822	CLA	C1D-ND-C4D	-9.27	99.75	106.33
16	A	809	CLA	C1D-ND-C4D	-9.26	99.76	106.33
16	1	521	CLA	C1D-ND-C4D	-9.25	99.76	106.33
16	4	406	CLA	C1D-ND-C4D	-9.25	99.77	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	403	CLA	C1D-ND-C4D	-9.25	99.77	106.33
16	A	806	CLA	C2D-C1D-ND	9.24	116.91	110.10
16	5	404	CLA	C1D-ND-C4D	-9.24	99.77	106.33
16	1	510	CLA	C1D-ND-C4D	-9.23	99.78	106.33
16	5	407	CLA	C1D-ND-C4D	-9.23	99.78	106.33
16	B	812	CLA	C1D-ND-C4D	-9.19	99.80	106.33
16	A	841	CLA	C2D-C1D-ND	9.19	116.88	110.10
16	A	827	CLA	C2D-C1D-ND	9.18	116.87	110.10
16	A	819	CLA	C1D-ND-C4D	-9.16	99.82	106.33
16	A	830	CLA	C1D-ND-C4D	-9.16	99.83	106.33
16	1	511	CLA	C1D-ND-C4D	-9.15	99.83	106.33
16	B	834	CLA	C1D-ND-C4D	-9.15	99.83	106.33
16	1	507	CLA	C1D-ND-C4D	-9.14	99.85	106.33
16	B	813	CLA	C2D-C1D-ND	9.12	116.83	110.10
16	6	403	CLA	C1D-ND-C4D	-9.12	99.86	106.33
16	B	827	CLA	C2D-C1D-ND	9.11	116.82	110.10
16	1	503	CLA	C1D-ND-C4D	-9.09	99.88	106.33
16	5	411	CLA	C1D-ND-C4D	-9.08	99.88	106.33
16	B	831	CLA	C1D-ND-C4D	-9.07	99.89	106.33
16	A	828	CLA	C2D-C1D-ND	9.06	116.78	110.10
16	1	508	CLA	C1D-ND-C4D	-9.03	99.92	106.33
16	B	824	CLA	C1D-ND-C4D	-9.03	99.92	106.33
16	A	817	CLA	C1D-ND-C4D	-9.02	99.93	106.33
16	5	414	CLA	C1D-ND-C4D	-9.00	99.94	106.33
16	A	840	CLA	C2D-C1D-ND	8.96	116.71	110.10
16	A	812	CLA	C2D-C1D-ND	8.95	116.70	110.10
16	A	813	CLA	C1D-ND-C4D	-8.91	100.00	106.33
16	K	103	CLA	C2D-C1D-ND	8.89	116.66	110.10
16	J	101	CLA	C1D-ND-C4D	-8.88	100.03	106.33
16	B	809	CLA	C1D-ND-C4D	-8.86	100.04	106.33
16	A	829	CLA	C1D-ND-C4D	-8.86	100.04	106.33
16	B	803	CLA	C1D-ND-C4D	-8.85	100.05	106.33
16	1	501	CLA	C1D-ND-C4D	-8.84	100.05	106.33
16	B	828	CLA	C1D-ND-C4D	-8.81	100.08	106.33
16	A	815	CLA	C1D-ND-C4D	-8.80	100.08	106.33
16	B	805	CLA	C1D-ND-C4D	-8.79	100.09	106.33
16	F	201	CLA	C1D-ND-C4D	-8.78	100.10	106.33
16	A	834	CLA	C1D-ND-C4D	-8.77	100.10	106.33
16	A	832	CLA	C2D-C1D-ND	8.73	116.54	110.10
16	B	807	CLA	C1D-ND-C4D	-8.71	100.15	106.33
16	A	835	CLA	C2D-C1D-ND	8.69	116.51	110.10
15	A	801	CL0	C2D-C1D-ND	8.69	116.50	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	825	CLA	C2D-C1D-ND	8.68	116.50	110.10
16	A	805	CLA	C2D-C1D-ND	8.63	116.46	110.10
16	A	842	CLA	C2D-C1D-ND	8.63	116.46	110.10
16	5	415	CLA	C2D-C1D-ND	8.61	116.45	110.10
16	B	802	CLA	C1D-ND-C4D	-8.61	100.22	106.33
16	B	814	CLA	C2D-C1D-ND	8.61	116.45	110.10
16	A	807	CLA	C2D-C1D-ND	8.60	116.44	110.10
16	1	504	CLA	C2D-C1D-ND	8.60	116.44	110.10
16	B	803	CLA	C2D-C1D-ND	8.59	116.44	110.10
16	A	803	CLA	C2D-C1D-ND	8.58	116.43	110.10
16	1	502	CLA	C2D-C1D-ND	8.57	116.42	110.10
16	B	829	CLA	C2D-C1D-ND	8.55	116.41	110.10
16	B	825	CLA	C2D-C1D-ND	8.54	116.40	110.10
16	1	519	CLA	C2D-C1D-ND	8.51	116.38	110.10
16	A	808	CLA	C2D-C1D-ND	8.50	116.37	110.10
16	B	817	CLA	C2D-C1D-ND	8.50	116.37	110.10
16	A	804	CLA	C2D-C1D-ND	8.49	116.36	110.10
16	B	835	CLA	C2D-C1D-ND	8.47	116.35	110.10
16	B	820	CLA	C2D-C1D-ND	8.45	116.33	110.10
16	5	405	CLA	C2D-C1D-ND	8.45	116.33	110.10
16	4	402	CLA	C2D-C1D-ND	8.43	116.32	110.10
16	5	403	CLA	C2D-C1D-ND	8.43	116.32	110.10
16	A	824	CLA	C2D-C1D-ND	8.43	116.32	110.10
16	A	836	CLA	C2D-C1D-ND	8.42	116.31	110.10
16	B	818	CLA	C2D-C1D-ND	8.41	116.31	110.10
16	B	821	CLA	C2D-C1D-ND	8.40	116.30	110.10
16	4	403	CLA	C2D-C1D-ND	8.37	116.27	110.10
16	B	812	CLA	C2D-C1D-ND	8.36	116.26	110.10
16	B	809	CLA	C2D-C1D-ND	8.35	116.26	110.10
16	B	839	CLA	C2D-C1D-ND	8.35	116.26	110.10
16	B	840	CLA	C2D-C1D-ND	8.32	116.24	110.10
16	B	802	CLA	C2D-C1D-ND	8.31	116.22	110.10
16	A	843	CLA	C2D-C1D-ND	8.30	116.22	110.10
16	1	509	CLA	C2D-C1D-ND	8.28	116.21	110.10
16	A	821	CLA	C2D-C1D-ND	8.26	116.19	110.10
16	B	830	CLA	C1D-ND-C4D	-8.24	100.48	106.33
16	A	813	CLA	C2D-C1D-ND	8.23	116.17	110.10
16	X	101	CLA	C2D-C1D-ND	8.22	116.17	110.10
16	4	407	CLA	C2D-C1D-ND	8.22	116.16	110.10
16	B	806	CLA	C2D-C1D-ND	8.20	116.15	110.10
16	K	101	CLA	C2D-C1D-ND	8.19	116.14	110.10
16	A	810	CLA	C2D-C1D-ND	8.18	116.13	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	410	CLA	C2D-C1D-ND	8.17	116.13	110.10
16	2	401	CLA	C2D-C1D-ND	8.17	116.12	110.10
16	A	811	CLA	C2D-C1D-ND	8.14	116.10	110.10
16	A	820	CLA	C2D-C1D-ND	8.13	116.09	110.10
16	1	505	CLA	C2D-C1D-ND	8.09	116.07	110.10
16	5	408	CLA	C2D-C1D-ND	8.09	116.07	110.10
16	B	805	CLA	C2D-C1D-ND	8.06	116.04	110.10
16	A	838	CLA	C2D-C1D-ND	8.05	116.04	110.10
16	B	801	CLA	C2D-C1D-ND	8.05	116.03	110.10
16	A	833	CLA	C2D-C1D-ND	8.05	116.03	110.10
16	A	837	CLA	C2D-C1D-ND	8.04	116.03	110.10
16	4	409	CLA	C2D-C1D-ND	8.04	116.03	110.10
16	A	819	CLA	C2D-C1D-ND	8.04	116.03	110.10
16	F	204	CLA	C2D-C1D-ND	8.03	116.02	110.10
16	B	834	CLA	C2D-C1D-ND	8.02	116.02	110.10
16	5	416	CLA	C2D-C1D-ND	8.01	116.01	110.10
16	B	804	CLA	C2D-C1D-ND	8.00	116.00	110.10
16	1	508	CLA	C2D-C1D-ND	7.98	115.98	110.10
16	5	412	CLA	C2D-C1D-ND	7.97	115.97	110.10
16	A	802	CLA	C2D-C1D-ND	7.96	115.97	110.10
16	B	815	CLA	C2D-C1D-ND	7.94	115.96	110.10
16	A	816	CLA	C2D-C1D-ND	7.94	115.96	110.10
16	A	809	CLA	C2D-C1D-ND	7.94	115.95	110.10
16	B	838	CLA	C2D-C1D-ND	7.93	115.95	110.10
16	3	401	CLA	C2D-C1D-ND	7.93	115.95	110.10
16	A	814	CLA	C2D-C1D-ND	7.93	115.95	110.10
16	4	406	CLA	C2D-C1D-ND	7.92	115.94	110.10
16	B	822	CLA	C2D-C1D-ND	7.91	115.93	110.10
16	2	404	CLA	C2D-C1D-ND	7.90	115.93	110.10
16	B	811	CLA	C2D-C1D-ND	7.89	115.92	110.10
16	6	404	CLA	C2D-C1D-ND	7.88	115.91	110.10
16	A	826	CLA	C1D-ND-C4D	-7.87	100.74	106.33
16	4	411	CLA	C2D-C1D-ND	7.87	115.90	110.10
16	5	418	CLA	C2D-C1D-ND	7.85	115.89	110.10
16	B	836	CLA	C2D-C1D-ND	7.83	115.88	110.10
16	5	409	CLA	C2D-C1D-ND	7.83	115.87	110.10
16	6	407	CLA	C2D-C1D-ND	7.82	115.87	110.10
16	5	406	CLA	C2D-C1D-ND	7.82	115.87	110.10
16	5	414	CLA	C2D-C1D-ND	7.82	115.87	110.10
16	2	402	CLA	C2D-C1D-ND	7.81	115.86	110.10
16	1	515	CLA	C2D-C1D-ND	7.80	115.85	110.10
16	1	513	CLA	C2D-C1D-ND	7.77	115.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	6	406	CLA	C2D-C1D-ND	7.76	115.83	110.10
16	1	511	CLA	C2D-C1D-ND	7.76	115.82	110.10
16	2	406	CLA	C2D-C1D-ND	7.76	115.82	110.10
16	6	402	CLA	C2D-C1D-ND	7.74	115.81	110.10
16	2	405	CLA	C2D-C1D-ND	7.74	115.81	110.10
16	1	510	CLA	C2D-C1D-ND	7.73	115.80	110.10
16	1	514	CLA	C2D-C1D-ND	7.73	115.80	110.10
16	J	102	CLA	C2D-C1D-ND	7.73	115.80	110.10
16	6	408	CLA	C2D-C1D-ND	7.73	115.80	110.10
16	A	839	CLA	C2D-C1D-ND	7.70	115.78	110.10
16	4	404	CLA	C2D-C1D-ND	7.70	115.78	110.10
16	A	815	CLA	C2D-C1D-ND	7.69	115.77	110.10
16	5	419	CLA	C2D-C1D-ND	7.69	115.77	110.10
16	B	831	CLA	C2D-C1D-ND	7.69	115.77	110.10
16	4	405	CLA	C2D-C1D-ND	7.68	115.77	110.10
16	2	403	CLA	C2D-C1D-ND	7.66	115.75	110.10
16	6	405	CLA	C2D-C1D-ND	7.66	115.75	110.10
16	A	817	CLA	C2D-C1D-ND	7.64	115.74	110.10
16	5	417	CLA	C2D-C1D-ND	7.62	115.72	110.10
16	A	829	CLA	C4A-NA-C1A	-7.61	103.28	106.71
16	6	401	CLA	C2D-C1D-ND	7.60	115.70	110.10
16	6	409	CLA	C2D-C1D-ND	7.59	115.69	110.10
16	1	504	CLA	CMD-C2D-C1D	7.59	138.08	124.71
16	1	506	CLA	C2D-C1D-ND	7.58	115.69	110.10
16	B	824	CLA	C4A-NA-C1A	-7.58	103.30	106.71
16	1	507	CLA	C2D-C1D-ND	7.57	115.68	110.10
16	B	837	CLA	C2D-C1D-ND	7.57	115.68	110.10
16	1	526	CLA	C2D-C1D-ND	7.56	115.67	110.10
16	B	824	CLA	C2D-C1D-ND	7.51	115.64	110.10
16	A	807	CLA	CMD-C2D-C1D	7.51	137.95	124.71
16	5	411	CLA	C2D-C1D-ND	7.51	115.64	110.10
16	6	403	CLA	C2D-C1D-ND	7.50	115.63	110.10
16	A	826	CLA	C2D-C1D-ND	7.50	115.63	110.10
16	5	422	CLA	C2D-C1D-ND	7.50	115.63	110.10
16	A	830	CLA	C2D-C1D-ND	7.49	115.62	110.10
16	1	503	CLA	C2D-C1D-ND	7.49	115.62	110.10
16	F	201	CLA	C2D-C1D-ND	7.48	115.62	110.10
16	A	822	CLA	C2D-C1D-ND	7.48	115.61	110.10
16	4	408	CLA	C2D-C1D-ND	7.47	115.61	110.10
16	5	413	CLA	C2D-C1D-ND	7.46	115.60	110.10
16	4	410	CLA	C2D-C1D-ND	7.43	115.58	110.10
16	1	512	CLA	C2D-C1D-ND	7.40	115.56	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	101	CLA	C2D-C1D-ND	7.40	115.56	110.10
16	1	521	CLA	C2D-C1D-ND	7.39	115.55	110.10
16	A	829	CLA	C2D-C1D-ND	7.35	115.52	110.10
16	5	404	CLA	C2D-C1D-ND	7.30	115.49	110.10
16	5	421	CLA	C2D-C1D-ND	7.30	115.48	110.10
16	B	819	CLA	CMD-C2D-C1D	7.29	137.56	124.71
16	1	501	CLA	C2D-C1D-ND	7.28	115.47	110.10
16	A	835	CLA	O2D-CGD-CBD	7.26	124.17	111.27
16	B	807	CLA	C2D-C1D-ND	7.24	115.44	110.10
16	B	818	CLA	CMD-C2D-C1D	7.20	137.41	124.71
16	1	525	CLA	C2D-C1D-ND	7.18	115.40	110.10
16	B	828	CLA	C4A-NA-C1A	-7.17	103.48	106.71
16	4	410	CLA	CMD-C2D-C1D	7.15	137.31	124.71
16	B	813	CLA	C4A-NA-C1A	-7.15	103.49	106.71
16	5	422	CLA	CMD-C2D-C1D	7.14	137.30	124.71
16	B	819	CLA	C2D-C1D-ND	7.12	115.35	110.10
16	B	819	CLA	CHD-C1D-ND	-7.12	117.91	124.45
16	A	834	CLA	C2D-C1D-ND	7.11	115.34	110.10
16	5	421	CLA	CMD-C2D-C1D	7.09	137.21	124.71
16	1	526	CLA	CMD-C2D-C1D	7.07	137.17	124.71
16	A	839	CLA	CMD-C2D-C1D	7.06	137.15	124.71
16	F	204	CLA	CMD-C2D-C1D	7.05	137.15	124.71
16	A	818	CLA	C4A-NA-C1A	-7.04	103.54	106.71
16	5	417	CLA	CMD-C2D-C1D	7.03	137.11	124.71
16	4	403	CLA	CMD-C2D-C1D	6.99	137.04	124.71
16	A	820	CLA	C4A-NA-C1A	-6.99	103.56	106.71
16	A	823	CLA	CHD-C1D-ND	-6.99	118.03	124.45
16	1	521	CLA	CMD-C2D-C1D	6.98	137.01	124.71
16	1	512	CLA	CMD-C2D-C1D	6.97	137.00	124.71
16	A	806	CLA	CMD-C2D-C1D	6.97	136.99	124.71
16	B	827	CLA	CMD-C2D-C1D	6.96	136.97	124.71
16	5	413	CLA	CMD-C2D-C1D	6.95	136.97	124.71
16	B	828	CLA	C2D-C1D-ND	6.94	115.22	110.10
16	5	405	CLA	CMD-C2D-C1D	6.94	136.94	124.71
16	A	839	CLA	O2D-CGD-CBD	6.93	123.59	111.27
16	A	829	CLA	CMD-C2D-C1D	6.93	136.92	124.71
16	B	825	CLA	O2D-CGD-CBD	6.92	123.57	111.27
16	5	409	CLA	CMD-C2D-C1D	6.91	136.90	124.71
16	4	408	CLA	CMD-C2D-C1D	6.91	136.90	124.71
16	B	830	CLA	C2D-C1D-ND	6.91	115.20	110.10
16	5	416	CLA	CMD-C2D-C1D	6.91	136.89	124.71
16	5	415	CLA	CMD-C2D-C1D	6.91	136.88	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	843	CLA	CHD-C1D-ND	-6.90	118.11	124.45
16	5	407	CLA	CMD-C2D-C1D	6.89	136.86	124.71
16	B	809	CLA	CMD-C2D-C1D	6.88	136.85	124.71
16	A	820	CLA	CMD-C2D-C1D	6.88	136.84	124.71
16	6	407	CLA	CMD-C2D-C1D	6.83	136.76	124.71
16	A	840	CLA	C4A-NA-C1A	-6.82	103.64	106.71
16	A	809	CLA	O2D-CGD-CBD	6.82	123.38	111.27
16	5	412	CLA	CMD-C2D-C1D	6.80	136.70	124.71
16	5	408	CLA	CMD-C2D-C1D	6.80	136.70	124.71
16	6	401	CLA	CMD-C2D-C1D	6.80	136.69	124.71
16	B	816	CLA	CMD-C2D-C1D	6.80	136.69	124.71
16	A	829	CLA	CHD-C1D-ND	-6.79	118.21	124.45
16	J	101	CLA	CMD-C2D-C1D	6.78	136.67	124.71
16	4	409	CLA	CMD-C2D-C1D	6.78	136.66	124.71
16	1	514	CLA	CMD-C2D-C1D	6.78	136.66	124.71
16	6	405	CLA	CMD-C2D-C1D	6.78	136.66	124.71
16	5	404	CLA	CMD-C2D-C1D	6.78	136.66	124.71
16	A	843	CLA	CMD-C2D-C1D	6.78	136.65	124.71
16	3	401	CLA	CMD-C2D-C1D	6.77	136.64	124.71
16	4	407	CLA	CMD-C2D-C1D	6.76	136.63	124.71
16	5	419	CLA	CMD-C2D-C1D	6.76	136.63	124.71
16	6	406	CLA	CMD-C2D-C1D	6.76	136.63	124.71
16	6	408	CLA	CMD-C2D-C1D	6.75	136.61	124.71
16	2	405	CLA	CMD-C2D-C1D	6.75	136.60	124.71
16	2	403	CLA	CMD-C2D-C1D	6.75	136.60	124.71
16	1	506	CLA	CMD-C2D-C1D	6.74	136.60	124.71
16	4	402	CLA	CMD-C2D-C1D	6.74	136.60	124.71
16	B	806	CLA	CMD-C2D-C1D	6.74	136.59	124.71
16	B	818	CLA	CHD-C1D-ND	-6.74	118.26	124.45
16	5	406	CLA	CMD-C2D-C1D	6.74	136.59	124.71
16	2	402	CLA	CMD-C2D-C1D	6.73	136.58	124.71
16	2	404	CLA	CMD-C2D-C1D	6.73	136.57	124.71
16	6	403	CLA	CMD-C2D-C1D	6.73	136.57	124.71
16	2	406	CLA	CMD-C2D-C1D	6.72	136.56	124.71
16	6	404	CLA	CMD-C2D-C1D	6.72	136.55	124.71
16	6	402	CLA	CMD-C2D-C1D	6.71	136.54	124.71
16	A	838	CLA	C4A-NA-C1A	-6.71	103.69	106.71
16	B	831	CLA	CMD-C2D-C1D	6.71	136.54	124.71
16	1	525	CLA	CMD-C2D-C1D	6.71	136.53	124.71
16	4	411	CLA	CMD-C2D-C1D	6.71	136.53	124.71
16	X	101	CLA	CMD-C2D-C1D	6.70	136.53	124.71
16	5	418	CLA	CMD-C2D-C1D	6.70	136.53	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	805	CLA	C2C-C1C-NC	6.70	116.25	109.97
16	2	401	CLA	CMD-C2D-C1D	6.70	136.51	124.71
16	4	406	CLA	CMD-C2D-C1D	6.69	136.51	124.71
16	1	501	CLA	CMD-C2D-C1D	6.69	136.50	124.71
16	B	827	CLA	CHD-C4C-C3C	-6.68	115.02	124.84
16	B	839	CLA	CMD-C2D-C1D	6.68	136.48	124.71
16	5	407	CLA	C2D-C1D-ND	6.67	115.02	110.10
16	4	405	CLA	CMD-C2D-C1D	6.67	136.47	124.71
16	1	515	CLA	CMD-C2D-C1D	6.67	136.47	124.71
16	1	510	CLA	CMD-C2D-C1D	6.66	136.46	124.71
16	1	505	CLA	CMD-C2D-C1D	6.66	136.46	124.71
16	6	409	CLA	CMD-C2D-C1D	6.66	136.45	124.71
16	1	504	CLA	CHD-C1D-ND	-6.65	118.34	124.45
16	A	837	CLA	CMD-C2D-C1D	6.64	136.42	124.71
16	1	511	CLA	CMD-C2D-C1D	6.64	136.42	124.71
16	5	403	CLA	CMD-C2D-C1D	6.64	136.41	124.71
16	B	836	CLA	CMD-C2D-C1D	6.63	136.40	124.71
16	4	404	CLA	CMD-C2D-C1D	6.61	136.37	124.71
16	A	822	CLA	C4A-NA-C1A	-6.61	103.73	106.71
16	A	828	CLA	CMD-C2D-C1D	6.60	136.35	124.71
16	A	811	CLA	CMD-C2D-C1D	6.60	136.34	124.71
16	5	413	CLA	CHD-C1D-ND	-6.59	118.40	124.45
16	A	832	CLA	CMD-C2D-C1D	6.56	136.28	124.71
16	5	403	CLA	CHD-C1D-ND	-6.56	118.43	124.45
16	B	829	CLA	C4A-NA-C1A	-6.56	103.76	106.71
16	5	410	CLA	CMD-C2D-C1D	6.54	136.25	124.71
16	4	402	CLA	CHD-C1D-ND	-6.54	118.45	124.45
16	A	807	CLA	CHD-C1D-ND	-6.53	118.45	124.45
16	B	812	CLA	CMD-C2D-C1D	6.53	136.22	124.71
16	5	405	CLA	CHD-C1D-ND	-6.52	118.46	124.45
16	1	507	CLA	CMD-C2D-C1D	6.51	136.18	124.71
16	J	102	CLA	CMD-C2D-C1D	6.49	136.15	124.71
16	4	409	CLA	CHD-C1D-ND	-6.49	118.49	124.45
16	A	814	CLA	CMD-C2D-C1D	6.49	136.15	124.71
16	A	842	CLA	O2D-CGD-CBD	6.49	122.79	111.27
16	A	828	CLA	C4A-NA-C1A	-6.48	103.79	106.71
16	B	801	CLA	CMD-C2D-C1D	6.48	136.13	124.71
16	A	813	CLA	CMD-C2D-C1D	6.48	136.13	124.71
16	A	820	CLA	CHD-C1D-ND	-6.47	118.50	124.45
16	5	411	CLA	CMD-C2D-C1D	6.47	136.12	124.71
16	A	804	CLA	CMD-C2D-C1D	6.46	136.09	124.71
16	2	401	CLA	CHD-C1D-ND	-6.45	118.53	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	824	CLA	CHD-C1D-ND	-6.44	118.53	124.45
16	1	520	CLA	CHD-C1D-ND	-6.44	118.53	124.45
16	A	802	CLA	CHD-C1D-ND	-6.44	118.54	124.45
16	A	831	CLA	O2D-CGD-CBD	6.43	122.70	111.27
16	B	832	CLA	O2D-CGD-CBD	6.42	122.68	111.27
16	5	416	CLA	CHD-C1D-ND	-6.42	118.55	124.45
16	B	805	CLA	CMD-C2D-C1D	6.42	136.02	124.71
16	1	502	CLA	CMD-C2D-C1D	6.41	136.02	124.71
16	A	833	CLA	CHD-C1D-ND	-6.41	118.56	124.45
16	5	408	CLA	CHD-C1D-ND	-6.41	118.56	124.45
16	1	519	CLA	CMD-C2D-C1D	6.40	136.00	124.71
16	1	508	CLA	CMD-C2D-C1D	6.39	135.97	124.71
16	5	409	CLA	CHD-C1D-ND	-6.37	118.60	124.45
16	A	834	CLA	CMD-C2D-C1D	6.37	135.94	124.71
16	A	818	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
16	B	826	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
16	B	808	CLA	CMD-C2D-C1D	6.35	135.90	124.71
16	A	838	CLA	CMD-C2D-C1D	6.35	135.90	124.71
16	6	404	CLA	CHD-C1D-ND	-6.34	118.63	124.45
16	2	404	CLA	CHD-C1D-ND	-6.34	118.63	124.45
16	6	407	CLA	CHD-C1D-ND	-6.33	118.63	124.45
16	A	806	CLA	CHD-C1D-ND	-6.33	118.64	124.45
16	5	419	CLA	CHD-C1D-ND	-6.33	118.64	124.45
16	4	410	CLA	CHD-C1D-ND	-6.32	118.64	124.45
16	1	505	CLA	CHD-C1D-ND	-6.32	118.64	124.45
16	5	406	CLA	CHD-C1D-ND	-6.32	118.65	124.45
16	B	804	CLA	CMD-C2D-C1D	6.31	135.84	124.71
16	5	415	CLA	CHD-C1D-ND	-6.31	118.66	124.45
16	B	830	CLA	CMD-C2D-C1D	6.30	135.82	124.71
16	B	820	CLA	O2D-CGD-CBD	6.30	122.46	111.27
16	1	519	CLA	CHD-C1D-ND	-6.29	118.67	124.45
16	B	826	CLA	CMD-C2D-C1D	6.29	135.80	124.71
16	A	821	CLA	CMD-C2D-C1D	6.29	135.79	124.71
16	5	417	CLA	CHD-C1D-ND	-6.29	118.68	124.45
16	1	502	CLA	CHD-C1D-ND	-6.28	118.69	124.45
16	B	802	CLA	O2D-CGD-CBD	6.27	122.42	111.27
16	6	408	CLA	CHD-C1D-ND	-6.27	118.69	124.45
16	5	404	CLA	C2C-C1C-NC	6.26	115.83	109.97
16	3	401	CLA	CHD-C1D-ND	-6.25	118.71	124.45
16	4	404	CLA	CHD-C1D-ND	-6.25	118.71	124.45
16	A	819	CLA	CMD-C2D-C1D	6.25	135.73	124.71
16	1	526	CLA	CHD-C1D-ND	-6.25	118.71	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	514	CLA	CHD-C1D-ND	-6.24	118.72	124.45
16	B	807	CLA	CMD-C2D-C1D	6.24	135.71	124.71
16	A	804	CLA	O2D-CGD-CBD	6.23	122.34	111.27
16	A	823	CLA	CMD-C2D-C1D	6.23	135.68	124.71
16	5	410	CLA	CHD-C1D-ND	-6.22	118.73	124.45
16	4	411	CLA	CHD-C1D-ND	-6.22	118.74	124.45
16	B	815	CLA	C4A-NA-C1A	-6.22	103.91	106.71
16	B	832	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
16	4	403	CLA	CHD-C1D-ND	-6.21	118.74	124.45
16	A	830	CLA	C4A-NA-C1A	-6.21	103.92	106.71
16	B	838	CLA	CHD-C1D-ND	-6.21	118.75	124.45
16	B	837	CLA	C4A-NA-C1A	-6.20	103.92	106.71
16	A	822	CLA	CHD-C1D-ND	-6.20	118.76	124.45
16	B	820	CLA	CMD-C2D-C1D	6.20	135.63	124.71
16	A	814	CLA	C4A-NA-C1A	-6.19	103.92	106.71
16	B	827	CLA	CHD-C1D-ND	-6.19	118.77	124.45
16	4	406	CLA	CHD-C1D-ND	-6.19	118.77	124.45
16	6	402	CLA	CHD-C1D-ND	-6.18	118.77	124.45
16	4	405	CLA	CHD-C1D-ND	-6.16	118.79	124.45
16	A	833	CLA	CMD-C2D-C1D	6.16	135.57	124.71
16	1	513	CLA	CMD-C2D-C1D	6.16	135.56	124.71
16	1	512	CLA	CHD-C1D-ND	-6.16	118.80	124.45
16	B	827	CLA	C4A-NA-C1A	-6.15	103.94	106.71
16	1	515	CLA	CHD-C1D-ND	-6.14	118.81	124.45
16	B	814	CLA	O2D-CGD-CBD	6.14	122.19	111.27
16	2	402	CLA	CHD-C1D-ND	-6.13	118.82	124.45
16	5	422	CLA	CHD-C1D-ND	-6.13	118.82	124.45
16	5	418	CLA	CHD-C1D-ND	-6.13	118.82	124.45
16	B	841	CLA	C2C-C1C-NC	6.13	115.71	109.97
16	5	421	CLA	CHD-C1D-ND	-6.12	118.83	124.45
16	A	810	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
16	6	406	CLA	CHD-C1D-ND	-6.11	118.83	124.45
16	B	839	CLA	C2C-C1C-NC	6.11	115.70	109.97
16	A	816	CLA	CMD-C2D-C1D	6.11	135.48	124.71
15	A	801	CL0	C2C-C1C-NC	6.11	115.69	109.97
16	4	408	CLA	CHD-C1D-ND	-6.11	118.84	124.45
16	6	405	CLA	CHD-C1D-ND	-6.11	118.84	124.45
16	J	102	CLA	CHD-C1D-ND	-6.10	118.84	124.45
16	1	520	CLA	CMD-C2D-C1D	6.10	135.47	124.71
16	A	822	CLA	CMD-C2D-C1D	6.10	135.46	124.71
16	B	815	CLA	CMD-C2D-C1D	6.10	135.46	124.71
16	4	407	CLA	CHD-C1D-ND	-6.09	118.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	841	CLA	C2C-C1C-NC	6.09	115.68	109.97
16	B	808	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
16	B	829	CLA	O2D-CGD-CBD	6.09	122.09	111.27
16	6	409	CLA	CHD-C1D-ND	-6.09	118.86	124.45
16	1	511	CLA	CHD-C1D-ND	-6.09	118.86	124.45
16	A	839	CLA	CHD-C1D-ND	-6.08	118.86	124.45
16	A	817	CLA	CMD-C2D-C1D	6.07	135.41	124.71
16	A	824	CLA	CMD-C2D-C1D	6.07	135.41	124.71
16	B	832	CLA	CMD-C2D-C1D	6.07	135.40	124.71
16	1	507	CLA	CHD-C1D-ND	-6.06	118.89	124.45
16	2	403	CLA	CHD-C1D-ND	-6.06	118.89	124.45
16	A	827	CLA	CHD-C1D-ND	-6.06	118.89	124.45
16	A	840	CLA	O2D-CGD-CBD	6.05	122.02	111.27
16	6	403	CLA	CHD-C1D-ND	-6.05	118.90	124.45
16	2	405	CLA	CHD-C1D-ND	-6.04	118.90	124.45
16	5	413	CLA	C4A-NA-C1A	-6.04	103.99	106.71
16	B	837	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
16	6	401	CLA	CHD-C1D-ND	-6.04	118.90	124.45
16	2	406	CLA	CHD-C1D-ND	-6.04	118.90	124.45
16	A	831	CLA	C2C-C1C-NC	6.04	115.63	109.97
16	5	408	CLA	C4A-NA-C1A	-6.03	103.99	106.71
16	B	815	CLA	O2D-CGD-CBD	6.02	121.97	111.27
16	X	101	CLA	CHD-C1D-ND	-6.02	118.92	124.45
16	1	509	CLA	C4A-NA-C1A	-6.01	104.00	106.71
16	A	827	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
16	F	201	CLA	CMD-C2D-C1D	6.01	135.31	124.71
16	B	832	CLA	CHD-C1D-ND	-6.01	118.93	124.45
16	B	825	CLA	CMD-C2D-C1D	6.00	135.29	124.71
16	B	807	CLA	CHD-C1D-ND	-5.99	118.95	124.45
16	B	801	CLA	CHD-C1D-ND	-5.99	118.95	124.45
16	1	506	CLA	CHD-C1D-ND	-5.98	118.95	124.45
16	B	824	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
16	B	840	CLA	CMD-C2D-C1D	5.98	135.25	124.71
16	A	828	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
16	B	805	CLA	O2D-CGD-CBD	5.97	121.88	111.27
16	A	825	CLA	CMD-C2D-C1D	5.97	135.24	124.71
16	B	801	CLA	C2C-C1C-NC	5.97	115.56	109.97
16	A	827	CLA	CMD-C2D-C1D	5.97	135.23	124.71
16	B	836	CLA	CHD-C1D-ND	-5.96	118.98	124.45
15	A	801	CL0	CHD-C4C-C3C	-5.95	116.09	124.84
16	A	811	CLA	CHD-C1D-ND	-5.95	118.98	124.45
16	A	841	CLA	CHD-C4C-C3C	-5.95	116.09	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	807	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
16	A	832	CLA	CHD-C1D-ND	-5.94	118.99	124.45
16	5	404	CLA	CHD-C1D-ND	-5.94	118.99	124.45
16	5	412	CLA	CHD-C1D-ND	-5.94	118.99	124.45
16	A	821	CLA	CHD-C1D-ND	-5.94	119.00	124.45
16	A	838	CLA	CHD-C1D-ND	-5.94	119.00	124.45
16	A	808	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
16	F	204	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
16	K	103	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
16	A	826	CLA	C2C-C1C-NC	5.93	115.52	109.97
16	B	819	CLA	C4A-NA-C1A	-5.92	104.04	106.71
16	B	835	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
16	B	816	CLA	CHD-C1D-ND	-5.92	119.02	124.45
16	B	810	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
16	B	808	CLA	O2D-CGD-CBD	5.92	121.78	111.27
16	A	836	CLA	CMD-C2D-C1D	5.91	135.13	124.71
16	B	817	CLA	CMD-C2D-C1D	5.91	135.12	124.71
16	5	411	CLA	CHD-C1D-ND	-5.91	119.03	124.45
16	1	521	CLA	CHD-C1D-ND	-5.89	119.04	124.45
16	K	103	CLA	CMD-C2D-C1D	5.89	135.09	124.71
16	B	827	CLA	O2D-CGD-CBD	5.88	121.72	111.27
16	A	840	CLA	CMD-C2D-C1D	5.88	135.08	124.71
16	B	806	CLA	C4A-NA-C1A	-5.88	104.06	106.71
16	A	829	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
16	A	813	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
16	A	817	CLA	C2C-C1C-NC	5.87	115.47	109.97
16	4	407	CLA	C4A-NA-C1A	-5.87	104.07	106.71
16	B	809	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
16	A	831	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
16	B	821	CLA	CMD-C2D-C1D	5.86	135.04	124.71
16	5	407	CLA	C2C-C1C-NC	5.85	115.45	109.97
16	B	841	CLA	CMD-C2D-C1D	5.85	135.02	124.71
16	B	831	CLA	CHD-C1D-ND	-5.85	119.08	124.45
16	A	819	CLA	C4A-NA-C1A	-5.85	104.08	106.71
16	A	840	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
16	B	826	CLA	CHD-C1D-ND	-5.84	119.09	124.45
16	A	805	CLA	CHD-C1D-ND	-5.84	119.09	124.45
16	1	525	CLA	CHD-C1D-ND	-5.83	119.09	124.45
16	1	503	CLA	CMD-C2D-C1D	5.83	134.99	124.71
16	1	507	CLA	C2C-C1C-NC	5.83	115.43	109.97
16	5	414	CLA	C2C-C1C-NC	5.83	115.43	109.97
16	F	204	CLA	CHD-C1D-ND	-5.83	119.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	823	CLA	C2C-C1C-NC	5.83	115.43	109.97
16	A	818	CLA	CMD-C2D-C1D	5.82	134.98	124.71
16	A	837	CLA	CHD-C1D-ND	-5.82	119.10	124.45
16	A	802	CLA	C2C-C1C-NC	5.82	115.42	109.97
16	A	802	CLA	CMD-C2D-C1D	5.82	134.96	124.71
16	A	832	CLA	CHD-C4C-C3C	-5.81	116.29	124.84
16	A	816	CLA	CHD-C1D-ND	-5.80	119.12	124.45
16	B	834	CLA	CMD-C2D-C1D	5.80	134.93	124.71
16	B	835	CLA	CHD-C1D-ND	-5.80	119.13	124.45
16	B	813	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
15	A	801	CL0	O2D-CGD-CBD	5.79	121.56	111.27
16	B	801	CLA	O2D-CGD-CBD	5.79	121.56	111.27
16	A	805	CLA	CMD-C2D-C1D	5.79	134.91	124.71
16	A	830	CLA	CMD-C2D-C1D	5.78	134.90	124.71
16	1	509	CLA	CMD-C2D-C1D	5.78	134.90	124.71
16	B	837	CLA	CMD-C2D-C1D	5.78	134.90	124.71
16	A	838	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
16	A	842	CLA	CMD-C2D-C1D	5.78	134.89	124.71
16	A	822	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
16	B	838	CLA	CMD-C2D-C1D	5.77	134.88	124.71
16	B	835	CLA	CMD-C2D-C1D	5.77	134.88	124.71
16	1	503	CLA	CHD-C1D-ND	-5.76	119.16	124.45
16	B	810	CLA	CMD-C2D-C1D	5.76	134.86	124.71
16	B	821	CLA	O2D-CGD-CBD	5.76	121.50	111.27
16	A	805	CLA	O2D-CGD-CBD	5.75	121.49	111.27
16	B	802	CLA	CMD-C2D-C1D	5.75	134.84	124.71
16	B	813	CLA	CHD-C1D-ND	-5.74	119.18	124.45
16	A	823	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
16	B	839	CLA	CHD-C1D-ND	-5.74	119.18	124.45
16	A	802	CLA	O2D-CGD-CBD	5.74	121.47	111.27
16	B	812	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
16	A	808	CLA	CHD-C1D-ND	-5.73	119.19	124.45
16	A	825	CLA	CHD-C1D-ND	-5.73	119.19	124.45
16	B	802	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
16	1	509	CLA	CHD-C1D-ND	-5.72	119.20	124.45
16	B	832	CLA	C4A-NA-C1A	-5.72	104.14	106.71
16	B	805	CLA	CHD-C1D-ND	-5.70	119.21	124.45
16	B	838	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
16	B	809	CLA	CHD-C1D-ND	-5.70	119.22	124.45
16	A	833	CLA	C2C-C1C-NC	5.70	115.31	109.97
16	B	811	CLA	CMD-C2D-C1D	5.69	134.75	124.71
16	B	833	CLA	CHD-C4C-C3C	-5.69	116.47	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	520	CLA	O2D-CGD-CBD	5.69	121.38	111.27
16	A	802	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
16	B	816	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
16	B	820	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
16	1	510	CLA	CHD-C1D-ND	-5.67	119.24	124.45
16	A	812	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
16	4	405	CLA	C4A-NA-C1A	-5.66	104.16	106.71
16	B	813	CLA	CMD-C2D-C1D	5.66	134.68	124.71
16	A	834	CLA	C4A-NA-C1A	-5.66	104.16	106.71
16	A	841	CLA	CMD-C2D-C1D	5.66	134.68	124.71
16	B	823	CLA	O2D-CGD-CBD	5.66	121.32	111.27
16	B	811	CLA	C4A-NA-C1A	-5.65	104.16	106.71
16	1	511	CLA	C2C-C1C-NC	5.65	115.27	109.97
16	B	821	CLA	CHD-C1D-ND	-5.65	119.26	124.45
16	A	804	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
16	B	802	CLA	C4A-NA-C1A	-5.65	104.17	106.71
16	1	509	CLA	O2D-CGD-CBD	5.64	121.30	111.27
16	B	834	CLA	CHD-C1D-ND	-5.64	119.27	124.45
16	B	811	CLA	C2C-C1C-NC	5.63	115.25	109.97
16	B	830	CLA	C4A-NA-C1A	-5.62	104.18	106.71
16	5	415	CLA	C4A-NA-C1A	-5.62	104.18	106.71
16	B	814	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
16	B	816	CLA	C4A-NA-C1A	-5.62	104.18	106.71
16	A	810	CLA	CMD-C2D-C1D	5.60	134.59	124.71
16	J	102	CLA	C4A-NA-C1A	-5.60	104.19	106.71
16	B	828	CLA	CHD-C1D-ND	-5.60	119.31	124.45
16	5	408	CLA	C2C-C1C-NC	5.60	115.22	109.97
16	1	521	CLA	C4A-NA-C1A	-5.60	104.19	106.71
16	A	824	CLA	O2D-CGD-CBD	5.60	121.21	111.27
16	A	826	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
16	B	814	CLA	CMD-C2D-C1D	5.59	134.56	124.71
16	B	818	CLA	O2D-CGD-CBD	5.59	121.20	111.27
16	A	815	CLA	C2C-C1C-NC	5.59	115.21	109.97
16	1	513	CLA	C2C-C1C-NC	5.58	115.20	109.97
16	B	828	CLA	CMD-C2D-C1D	5.58	134.55	124.71
16	1	508	CLA	CHD-C1D-ND	-5.58	119.33	124.45
16	A	830	CLA	CHD-C1D-ND	-5.58	119.33	124.45
16	B	830	CLA	CHD-C1D-ND	-5.58	119.33	124.45
16	A	836	CLA	CHD-C1D-ND	-5.57	119.33	124.45
16	A	808	CLA	CMD-C2D-C1D	5.57	134.53	124.71
16	B	812	CLA	CHD-C1D-ND	-5.57	119.34	124.45
16	A	816	CLA	C4A-NA-C1A	-5.57	104.20	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	411	CLA	C4A-NA-C1A	-5.56	104.21	106.71
16	A	804	CLA	CHD-C1D-ND	-5.56	119.35	124.45
16	B	806	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
16	B	817	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
16	B	817	CLA	C4A-NA-C1A	-5.54	104.21	106.71
16	1	519	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
16	6	403	CLA	C2C-C1C-NC	5.54	115.16	109.97
16	A	808	CLA	C4A-NA-C1A	-5.54	104.22	106.71
16	A	834	CLA	CHD-C1D-ND	-5.54	119.36	124.45
16	B	822	CLA	C2C-C1C-NC	5.53	115.16	109.97
16	B	825	CLA	CHD-C1D-ND	-5.53	119.38	124.45
16	A	805	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
16	B	829	CLA	CMD-C2D-C1D	5.52	134.45	124.71
16	5	407	CLA	CHD-C1D-ND	-5.52	119.38	124.45
16	B	840	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
16	B	817	CLA	CHD-C1D-ND	-5.52	119.38	124.45
16	5	407	CLA	O2D-CGD-CBD	5.52	121.08	111.27
16	A	816	CLA	CHD-C4C-C3C	-5.51	116.73	124.84
16	B	824	CLA	C4-C3-C5	5.51	124.54	115.27
16	B	809	CLA	C4A-NA-C1A	-5.51	104.23	106.71
16	B	815	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
16	B	833	CLA	O2D-CGD-CBD	5.51	121.06	111.27
16	A	823	CLA	O2D-CGD-CBD	5.51	121.05	111.27
16	A	823	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
16	B	826	CLA	C4A-NA-C1A	-5.49	104.24	106.71
16	B	820	CLA	CHD-C1D-ND	-5.49	119.41	124.45
16	B	818	CLA	C4A-NA-C1A	-5.49	104.24	106.71
16	B	811	CLA	CHD-C1D-ND	-5.49	119.41	124.45
16	1	520	CLA	C4A-NA-C1A	-5.49	104.24	106.71
16	B	802	CLA	C2C-C1C-NC	5.49	115.11	109.97
16	A	842	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
16	A	810	CLA	C4A-NA-C1A	-5.49	104.24	106.71
16	K	103	CLA	CHD-C1D-ND	-5.48	119.42	124.45
16	1	501	CLA	C4A-NA-C1A	-5.48	104.24	106.71
16	A	814	CLA	CHD-C1D-ND	-5.48	119.42	124.45
16	B	815	CLA	CHD-C1D-ND	-5.48	119.42	124.45
16	1	514	CLA	C4A-NA-C1A	-5.48	104.24	106.71
16	A	837	CLA	C2C-C1C-NC	5.47	115.10	109.97
16	B	823	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
16	1	502	CLA	O2D-CGD-CBD	5.47	120.98	111.27
16	B	821	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
16	5	409	CLA	O2D-CGD-CBD	5.46	120.97	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	803	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
16	A	831	CLA	CMD-C2D-C1D	5.46	134.34	124.71
16	B	824	CLA	O2D-CGD-CBD	5.46	120.96	111.27
16	B	841	CLA	O2D-CGD-CBD	5.45	120.96	111.27
16	A	824	CLA	C4A-NA-C1A	-5.45	104.26	106.71
16	A	814	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
16	B	839	CLA	O2D-CGD-CBD	5.45	120.95	111.27
16	4	406	CLA	CHD-C4C-C3C	-5.45	116.84	124.84
16	1	501	CLA	CHD-C1D-ND	-5.44	119.45	124.45
16	A	807	CLA	C4A-NA-C1A	-5.44	104.26	106.71
16	5	406	CLA	O2D-CGD-CBD	5.44	120.93	111.27
16	1	520	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
16	1	504	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
16	B	804	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
16	1	512	CLA	O2D-CGD-CBD	5.43	120.92	111.27
16	A	820	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
16	6	409	CLA	O2D-CGD-CBD	5.43	120.91	111.27
16	2	401	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
16	1	521	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
16	F	201	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
16	A	828	CLA	CHD-C1D-ND	-5.41	119.48	124.45
16	B	819	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
16	B	831	CLA	C2C-C1C-NC	5.41	115.04	109.97
16	B	823	CLA	CHD-C1D-ND	-5.40	119.49	124.45
16	A	839	CLA	C4A-NA-C1A	-5.40	104.28	106.71
16	1	514	CLA	C2C-C1C-NC	5.40	115.03	109.97
16	J	101	CLA	CHD-C1D-ND	-5.40	119.49	124.45
16	B	802	CLA	CHD-C1D-ND	-5.40	119.50	124.45
16	K	101	CLA	CMD-C2D-C1D	5.38	134.20	124.71
16	1	513	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
16	A	817	CLA	CHD-C1D-ND	-5.38	119.51	124.45
16	A	811	CLA	C2C-C1C-NC	5.38	115.01	109.97
16	A	815	CLA	CHD-C4C-C3C	-5.38	116.94	124.84
16	4	403	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
16	A	809	CLA	CHD-C1D-ND	-5.37	119.52	124.45
16	B	829	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
16	A	819	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
16	1	503	CLA	O2D-CGD-CBD	5.36	120.79	111.27
16	A	813	CLA	C2C-C1C-NC	5.36	114.99	109.97
16	B	806	CLA	CHD-C1D-ND	-5.36	119.53	124.45
16	B	840	CLA	CHD-C1D-ND	-5.36	119.53	124.45
16	A	826	CLA	O2D-CGD-CBD	5.35	120.78	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	812	CLA	CMD-C2D-C1D	5.35	134.14	124.71
16	J	102	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
16	A	835	CLA	CHD-C1D-ND	-5.34	119.54	124.45
16	5	403	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
16	A	834	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
16	5	405	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
16	B	839	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
16	1	504	CLA	C4A-NA-C1A	-5.33	104.31	106.71
16	A	809	CLA	CMD-C2D-C1D	5.33	134.11	124.71
16	B	803	CLA	CHD-C1D-ND	-5.33	119.56	124.45
16	4	409	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
16	5	415	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
16	1	506	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
16	1	505	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
16	A	826	CLA	CMD-C2D-C1D	5.32	134.10	124.71
16	A	821	CLA	O2D-CGD-CBD	5.32	120.73	111.27
16	1	509	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
16	A	830	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
16	B	814	CLA	CHD-C1D-ND	-5.31	119.57	124.45
16	1	504	CLA	C2C-C1C-NC	5.31	114.95	109.97
16	J	101	CLA	O2D-CGD-CBD	5.31	120.70	111.27
16	A	807	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
16	B	832	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
16	A	831	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
16	B	807	CLA	O2D-CGD-CBD	5.31	120.70	111.27
16	B	827	CLA	C3D-C2D-C1D	-5.30	98.59	105.83
16	B	829	CLA	CHD-C1D-ND	-5.30	119.58	124.45
16	A	803	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
16	B	827	CLA	C3C-C4C-NC	5.30	116.51	110.57
16	B	841	CLA	CHD-C1D-ND	-5.29	119.59	124.45
16	5	410	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
16	A	818	CLA	C3C-C4C-NC	5.29	116.50	110.57
16	B	822	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
16	B	807	CLA	C2C-C1C-NC	5.28	114.92	109.97
16	5	411	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
16	B	804	CLA	CHD-C1D-ND	-5.28	119.60	124.45
19	4	401	BCR	C15-C16-C17	5.28	134.29	123.47
16	A	837	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
16	A	841	CLA	CHD-C1D-ND	-5.28	119.60	124.45
16	1	501	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
16	B	831	CLA	O2D-CGD-CBD	5.28	120.65	111.27
16	5	408	CLA	CHD-C4C-C3C	-5.28	117.08	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	817	CLA	O2D-CGD-CBD	5.28	120.64	111.27
16	J	101	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
16	6	402	CLA	C2C-C1C-NC	5.27	114.91	109.97
16	1	513	CLA	CHD-C1D-ND	-5.27	119.61	124.45
16	A	803	CLA	CHD-C1D-ND	-5.27	119.61	124.45
16	1	521	CLA	O2D-CGD-CBD	5.27	120.63	111.27
16	A	821	CLA	C2C-C1C-NC	5.27	114.91	109.97
16	B	811	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
16	A	815	CLA	CHD-C1D-ND	-5.27	119.61	124.45
16	1	511	CLA	O2D-CGD-CBD	5.27	120.62	111.27
16	2	405	CLA	C2C-C1C-NC	5.26	114.90	109.97
16	4	407	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
16	B	831	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
16	A	812	CLA	C4A-NA-C1A	-5.25	104.34	106.71
16	1	502	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
16	4	411	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
16	4	402	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
16	A	811	CLA	C4A-NA-C1A	-5.24	104.35	106.71
16	A	821	CLA	C4A-NA-C1A	-5.24	104.35	106.71
16	A	835	CLA	CMD-C2D-C1D	5.23	133.94	124.71
16	B	836	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
16	A	835	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
16	5	412	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
16	B	828	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
16	B	801	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
16	A	809	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
16	A	812	CLA	CHD-C1D-ND	-5.23	119.65	124.45
16	B	809	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
16	5	415	CLA	O2D-CGD-CBD	5.22	120.55	111.27
16	B	810	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
16	2	404	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
16	A	833	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
16	1	508	CLA	C2C-C1C-NC	5.22	114.86	109.97
16	A	818	CLA	CHD-C1D-ND	-5.22	119.66	124.45
16	A	841	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
16	5	403	CLA	O2D-CGD-CBD	5.21	120.53	111.27
16	B	837	CLA	CHD-C1D-ND	-5.21	119.67	124.45
16	A	842	CLA	CHD-C1D-ND	-5.21	119.67	124.45
16	A	825	CLA	C4A-NA-C1A	-5.20	104.37	106.71
16	1	507	CLA	O2D-CGD-CBD	5.20	120.50	111.27
16	B	833	CLA	CHD-C1D-ND	-5.20	119.68	124.45
16	5	409	CLA	C2C-C1C-NC	5.19	114.84	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	405	CLA	C2C-C1C-NC	5.19	114.83	109.97
16	B	841	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
16	5	416	CLA	C2C-C1C-NC	5.19	114.83	109.97
16	A	806	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
16	A	836	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
16	A	839	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
16	4	402	CLA	O2D-CGD-CBD	5.18	120.47	111.27
16	5	415	CLA	C2C-C1C-NC	5.18	114.82	109.97
16	2	401	CLA	O2D-CGD-CBD	5.18	120.47	111.27
16	5	407	CLA	C4A-NA-C1A	-5.17	104.38	106.71
16	2	402	CLA	C2C-C1C-NC	5.17	114.82	109.97
16	2	403	CLA	C2C-C1C-NC	5.17	114.82	109.97
16	1	504	CLA	O2D-CGD-CBD	5.17	120.45	111.27
16	1	510	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
16	6	404	CLA	CHD-C4C-C3C	-5.17	117.25	124.84
16	A	806	CLA	O2D-CGD-CBD	5.17	120.45	111.27
16	1	525	CLA	O2D-CGD-CBD	5.17	120.45	111.27
16	5	414	CLA	O2D-CGD-CBD	5.16	120.44	111.27
16	B	824	CLA	CHD-C1D-ND	-5.16	119.71	124.45
16	K	103	CLA	C4A-NA-C1A	-5.16	104.39	106.71
16	B	818	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
16	B	818	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
16	A	813	CLA	C3D-C2D-C1D	-5.16	98.80	105.83
16	A	837	CLA	O2D-CGD-CBD	5.15	120.43	111.27
16	1	512	CLA	CHD-C4C-C3C	-5.15	117.26	124.84
16	4	408	CLA	C2C-C1C-NC	5.15	114.80	109.97
16	B	810	CLA	CMC-C2C-C1C	5.15	132.88	125.04
16	1	508	CLA	O2D-CGD-CBD	5.15	120.42	111.27
16	5	421	CLA	O2D-CGD-CBD	5.15	120.42	111.27
16	A	828	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
16	B	834	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
16	A	832	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
16	B	807	CLA	C4A-NA-C1A	-5.14	104.39	106.71
16	F	204	CLA	C4A-NA-C1A	-5.14	104.39	106.71
16	5	409	CLA	C4A-NA-C1A	-5.14	104.40	106.71
16	3	401	CLA	C2C-C1C-NC	5.14	114.78	109.97
16	A	821	CLA	CHD-C4C-C3C	-5.13	117.29	124.84
16	2	406	CLA	C2C-C1C-NC	5.13	114.78	109.97
16	B	824	CLA	CMD-C2D-C1D	5.13	133.76	124.71
16	A	832	CLA	O2D-CGD-CBD	5.13	120.39	111.27
16	K	101	CLA	C2C-C1C-NC	5.13	114.78	109.97
16	B	826	CLA	C3D-C2D-C1D	-5.13	98.83	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	820	CLA	O2D-CGD-CBD	5.12	120.36	111.27
16	B	823	CLA	CMD-C2D-C1D	5.12	133.73	124.71
16	B	813	CLA	CAC-C3C-C4C	5.11	131.45	124.81
16	B	812	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
16	6	409	CLA	C2C-C1C-NC	5.11	114.76	109.97
16	1	508	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
16	4	404	CLA	O2D-CGD-CBD	5.11	120.35	111.27
16	6	406	CLA	C2C-C1C-NC	5.11	114.76	109.97
16	5	412	CLA	O2D-CGD-CBD	5.11	120.34	111.27
16	2	406	CLA	O2D-CGD-CBD	5.10	120.33	111.27
16	A	824	CLA	CHD-C4C-C3C	-5.10	117.35	124.84
16	5	418	CLA	CHD-C4C-C3C	-5.10	117.35	124.84
16	B	810	CLA	CAC-C3C-C4C	5.10	131.42	124.81
16	A	836	CLA	C2C-C1C-NC	5.09	114.75	109.97
16	A	815	CLA	C4A-NA-C1A	-5.09	104.42	106.71
16	A	833	CLA	O2D-CGD-CBD	5.09	120.32	111.27
16	4	407	CLA	O2D-CGD-CBD	5.09	120.31	111.27
16	1	503	CLA	C2C-C1C-NC	5.09	114.74	109.97
16	4	409	CLA	C2C-C1C-NC	5.09	114.74	109.97
16	B	810	CLA	C4A-NA-C1A	-5.08	104.42	106.71
16	6	402	CLA	O2D-CGD-CBD	5.08	120.30	111.27
16	6	405	CLA	C2C-C1C-NC	5.08	114.73	109.97
16	A	811	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
16	6	407	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
16	A	842	CLA	C2C-C1C-NC	5.08	114.73	109.97
16	B	805	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
16	B	826	CLA	O2D-CGD-CBD	5.08	120.30	111.27
16	4	402	CLA	C2C-C1C-NC	5.08	114.73	109.97
16	A	819	CLA	CHD-C1D-ND	-5.08	119.79	124.45
16	4	405	CLA	C2C-C1C-NC	5.07	114.72	109.97
16	B	808	CLA	CHD-C1D-ND	-5.07	119.79	124.45
16	A	817	CLA	CAC-C3C-C4C	5.07	131.39	124.81
16	5	416	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
16	B	808	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
16	4	404	CLA	C2C-C1C-NC	5.06	114.72	109.97
16	B	823	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
16	1	520	CLA	C3D-C4D-ND	5.05	118.41	110.24
16	A	843	CLA	C3D-C4D-ND	5.05	118.41	110.24
16	5	406	CLA	C2C-C1C-NC	5.05	114.70	109.97
16	2	402	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
16	B	818	CLA	C2C-C1C-NC	5.05	114.70	109.97
16	4	409	CLA	C4A-NA-C1A	-5.04	104.44	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	6	401	CLA	C2C-C1C-NC	5.04	114.69	109.97
16	6	407	CLA	C2C-C1C-NC	5.04	114.69	109.97
16	4	404	CLA	CHD-C4C-C3C	-5.03	117.44	124.84
16	6	409	CLA	CHD-C4C-C3C	-5.03	117.44	124.84
16	B	830	CLA	CHD-C4C-C3C	-5.03	117.44	124.84
16	5	410	CLA	C4A-NA-C1A	-5.03	104.44	106.71
16	A	842	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
16	A	832	CLA	C2C-C1C-NC	5.03	114.69	109.97
16	B	802	CLA	C4-C3-C5	5.03	123.72	115.27
16	A	813	CLA	CHD-C1D-ND	-5.02	119.84	124.45
16	B	834	CLA	O2D-CGD-CBD	5.02	120.19	111.27
16	1	526	CLA	O2D-CGD-CBD	5.02	120.19	111.27
16	4	406	CLA	C4A-NA-C1A	-5.02	104.45	106.71
16	5	414	CLA	CAC-C3C-C4C	5.02	131.32	124.81
16	A	820	CLA	C2C-C1C-NC	5.02	114.67	109.97
16	X	101	CLA	C2C-C1C-NC	5.02	114.67	109.97
16	B	812	CLA	C4A-NA-C1A	-5.02	104.45	106.71
16	A	823	CLA	C3D-C4D-ND	5.02	118.35	110.24
16	4	408	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
16	3	401	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
16	J	101	CLA	C2C-C1C-NC	5.01	114.66	109.97
16	1	502	CLA	C2C-C1C-NC	5.01	114.66	109.97
16	5	419	CLA	C4A-NA-C1A	-5.00	104.46	106.71
16	A	840	CLA	CHD-C1D-ND	-5.00	119.86	124.45
16	B	807	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
16	1	507	CLA	CHD-C4C-C3C	-5.00	117.50	124.84
16	A	816	CLA	O2D-CGD-CBD	4.99	120.14	111.27
16	B	837	CLA	O2D-CGD-CBD	4.99	120.14	111.27
16	A	806	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
16	5	418	CLA	C2C-C1C-NC	4.99	114.65	109.97
16	5	419	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
16	A	820	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
16	B	808	CLA	C2C-C1C-NC	4.99	114.64	109.97
16	1	509	CLA	C2C-C1C-NC	4.98	114.64	109.97
16	4	403	CLA	C4A-NA-C1A	-4.98	104.47	106.71
16	5	417	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
16	2	406	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
16	A	818	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
16	B	804	CLA	C2C-C1C-NC	4.98	114.64	109.97
16	B	822	CLA	CHD-C1D-ND	-4.97	119.89	124.45
16	B	825	CLA	C2C-C1C-NC	4.97	114.62	109.97
16	B	802	CLA	C3C-C4C-NC	4.97	116.14	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	422	CLA	C2C-C1C-NC	4.96	114.62	109.97
16	1	512	CLA	C4A-NA-C1A	-4.96	104.47	106.71
16	B	813	CLA	C3D-C4D-ND	4.96	118.27	110.24
16	1	510	CLA	C2C-C1C-NC	4.96	114.62	109.97
16	1	526	CLA	C2C-C1C-NC	4.96	114.62	109.97
16	1	501	CLA	O2D-CGD-CBD	4.96	120.09	111.27
16	A	831	CLA	CHD-C1D-ND	-4.96	119.89	124.45
16	1	514	CLA	O2D-CGD-CBD	4.96	120.08	111.27
19	A	849	BCR	C8-C9-C10	4.96	126.55	118.94
16	6	408	CLA	C2C-C1C-NC	4.96	114.62	109.97
16	4	410	CLA	O2D-CGD-CBD	4.96	120.08	111.27
16	1	525	CLA	C2C-C1C-NC	4.96	114.61	109.97
16	2	403	CLA	CAC-C3C-C4C	4.95	131.24	124.81
16	5	422	CLA	O2D-CGD-CBD	4.95	120.07	111.27
16	A	843	CLA	C4A-NA-C1A	-4.95	104.48	106.71
16	5	422	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
16	B	825	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
16	X	101	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
16	A	813	CLA	C4A-NA-C1A	-4.95	104.48	106.71
16	5	415	CLA	C3D-C4D-ND	4.95	118.24	110.24
16	5	414	CLA	CMD-C2D-C1D	4.95	133.44	124.71
16	4	403	CLA	C2C-C1C-NC	4.95	114.61	109.97
16	A	827	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
16	4	405	CLA	CHD-C4C-C3C	-4.95	117.57	124.84
16	B	841	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
16	1	525	CLA	CHD-C4C-C3C	-4.95	117.57	124.84
16	A	824	CLA	C2C-C1C-NC	4.94	114.60	109.97
16	B	812	CLA	C2C-C1C-NC	4.94	114.60	109.97
16	A	805	CLA	C2C-C1C-NC	4.94	114.60	109.97
16	6	402	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
15	A	801	CL0	CMD-C2D-C1D	4.94	133.41	124.71
16	1	515	CLA	C4A-NA-C1A	-4.94	104.49	106.71
16	6	408	CLA	CHD-C4C-C3C	-4.93	117.59	124.84
16	2	405	CLA	CHD-C4C-C3C	-4.93	117.59	124.84
16	4	411	CLA	O2D-CGD-CBD	4.93	120.03	111.27
16	5	414	CLA	CHD-C4C-C3C	-4.93	117.60	124.84
16	B	821	CLA	C2C-C1C-NC	4.93	114.59	109.97
16	F	201	CLA	C2C-C1C-NC	4.93	114.59	109.97
16	B	839	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
16	6	401	CLA	O2D-CGD-CBD	4.92	120.02	111.27
16	3	401	CLA	O2D-CGD-CBD	4.92	120.02	111.27
16	5	403	CLA	C2C-C1C-NC	4.92	114.58	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	825	CLA	CAC-C3C-C4C	4.92	131.19	124.81
16	5	407	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
16	A	824	CLA	C3D-C4D-ND	4.91	118.19	110.24
16	6	406	CLA	O2D-CGD-CBD	4.91	120.00	111.27
16	A	833	CLA	C3D-C4D-ND	4.91	118.19	110.24
16	K	101	CLA	C4A-NA-C1A	-4.91	104.50	106.71
16	5	412	CLA	C2C-C1C-NC	4.91	114.57	109.97
16	1	526	CLA	CHD-C4C-C3C	-4.91	117.63	124.84
16	B	806	CLA	C2C-C1C-NC	4.90	114.57	109.97
16	A	803	CLA	C3D-C4D-ND	4.90	118.17	110.24
16	4	409	CLA	O2D-CGD-CBD	4.90	119.97	111.27
16	B	812	CLA	O2D-CGD-CBD	4.90	119.97	111.27
16	5	410	CLA	C2C-C1C-NC	4.90	114.56	109.97
19	I	102	BCR	C37-C22-C21	-4.89	116.08	122.92
16	4	402	CLA	C4A-NA-C1A	-4.88	104.51	106.71
16	5	406	CLA	CHD-C4C-C3C	-4.88	117.66	124.84
16	1	506	CLA	O2D-CGD-CBD	4.88	119.94	111.27
16	5	421	CLA	C3D-C4D-ND	4.88	118.14	110.24
16	B	833	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
16	B	814	CLA	C2C-C1C-NC	4.88	114.54	109.97
16	A	812	CLA	C3D-C4D-ND	4.88	118.13	110.24
16	6	406	CLA	CHD-C4C-C3C	-4.88	117.67	124.84
16	B	835	CLA	C4A-NA-C1A	-4.88	104.51	106.71
16	B	825	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
16	5	421	CLA	C2C-C1C-NC	4.88	114.54	109.97
16	5	405	CLA	C3D-C4D-ND	4.87	118.12	110.24
16	K	103	CLA	O2D-CGD-CBD	4.87	119.92	111.27
16	1	520	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
16	1	515	CLA	CAC-C3C-C4C	4.87	131.12	124.81
16	A	834	CLA	C2C-C1C-NC	4.87	114.53	109.97
19	I	102	BCR	C8-C9-C10	4.86	126.41	118.94
16	A	835	CLA	C4A-NA-C1A	-4.86	104.52	106.71
16	A	816	CLA	C3D-C4D-ND	4.86	118.11	110.24
16	B	838	CLA	C2C-C1C-NC	4.86	114.53	109.97
16	6	407	CLA	O2D-CGD-CBD	4.86	119.91	111.27
16	5	417	CLA	O2D-CGD-CBD	4.86	119.91	111.27
16	1	511	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
16	5	419	CLA	C2C-C1C-NC	4.86	114.53	109.97
16	A	835	CLA	C2C-C1C-NC	4.86	114.52	109.97
16	1	505	CLA	C4A-NA-C1A	-4.86	104.52	106.71
16	6	405	CLA	O2D-CGD-CBD	4.85	119.89	111.27
16	A	831	CLA	C4A-NA-C1A	-4.85	104.52	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	825	CLA	C2C-C1C-NC	4.85	114.52	109.97
16	B	830	CLA	C2C-C1C-NC	4.85	114.52	109.97
16	B	819	CLA	C3D-C4D-ND	4.85	118.08	110.24
16	B	822	CLA	O2D-CGD-CBD	4.85	119.88	111.27
16	A	839	CLA	C2C-C1C-NC	4.85	114.51	109.97
16	1	504	CLA	C3D-C4D-ND	4.84	118.07	110.24
16	B	803	CLA	C2C-C1C-NC	4.84	114.51	109.97
16	1	526	CLA	C4A-NA-C1A	-4.84	104.53	106.71
16	B	810	CLA	CHD-C1D-ND	-4.83	120.01	124.45
16	B	816	CLA	C3D-C4D-ND	4.83	118.06	110.24
16	A	810	CLA	CHD-C1D-ND	-4.83	120.01	124.45
16	2	401	CLA	C2C-C1C-NC	4.83	114.50	109.97
16	B	811	CLA	O2D-CGD-CBD	4.83	119.85	111.27
16	1	505	CLA	O2D-CGD-CBD	4.83	119.85	111.27
16	5	408	CLA	C3D-C4D-ND	4.83	118.05	110.24
16	4	403	CLA	O2D-CGD-CBD	4.83	119.84	111.27
16	6	408	CLA	O2D-CGD-CBD	4.83	119.84	111.27
16	1	525	CLA	C3D-C4D-ND	4.82	118.04	110.24
16	1	514	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
16	6	401	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
16	1	512	CLA	C2C-C1C-NC	4.82	114.49	109.97
16	A	819	CLA	CAC-C3C-C4C	4.82	131.07	124.81
16	B	831	CLA	C4A-NA-C1A	-4.82	104.54	106.71
16	5	413	CLA	C3D-C4D-ND	4.82	118.03	110.24
16	5	405	CLA	O2D-CGD-CBD	4.82	119.83	111.27
16	A	834	CLA	O2D-CGD-CBD	4.82	119.83	111.27
16	6	405	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
15	A	801	CL0	C3C-C4C-NC	4.81	115.97	110.57
16	A	825	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
16	6	408	CLA	C4A-NA-C1A	-4.81	104.54	106.71
16	B	836	CLA	C4A-NA-C1A	-4.81	104.55	106.71
16	1	515	CLA	C2C-C1C-NC	4.81	114.47	109.97
16	4	410	CLA	C2C-C1C-NC	4.81	114.47	109.97
16	1	504	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
16	B	805	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
16	B	822	CLA	CMD-C2D-C1D	4.80	133.18	124.71
16	2	405	CLA	O2D-CGD-CBD	4.80	119.79	111.27
16	B	821	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
16	A	802	CLA	C4A-NA-C1A	-4.79	104.55	106.71
16	A	805	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
16	K	103	CLA	C2C-C1C-NC	4.79	114.46	109.97
16	B	805	CLA	C3D-C2D-C1D	-4.79	99.29	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	409	CLA	C3D-C4D-ND	4.79	117.99	110.24
16	K	103	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
16	A	843	CLA	CHD-C4C-C3C	-4.79	117.80	124.84
16	4	410	CLA	CHD-C4C-C3C	-4.79	117.80	124.84
16	B	832	CLA	C3D-C4D-ND	4.78	117.98	110.24
16	2	404	CLA	C2C-C1C-NC	4.78	114.45	109.97
16	4	402	CLA	C3D-C4D-ND	4.78	117.98	110.24
16	5	403	CLA	C3D-C4D-ND	4.78	117.97	110.24
16	B	841	CLA	C3D-C4D-ND	4.78	117.97	110.24
16	A	813	CLA	C3C-C4C-NC	4.78	115.93	110.57
16	B	837	CLA	C3D-C4D-ND	4.78	117.97	110.24
16	5	409	CLA	CAC-C3C-C4C	4.78	131.01	124.81
16	1	502	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
16	B	801	CLA	CMC-C2C-C1C	4.78	132.31	125.04
16	1	506	CLA	C3D-C4D-ND	4.78	117.96	110.24
16	B	835	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
16	4	404	CLA	C4A-NA-C1A	-4.77	104.56	106.71
16	A	804	CLA	C2C-C1C-NC	4.77	114.44	109.97
16	5	416	CLA	C3D-C4D-ND	4.77	117.96	110.24
16	5	411	CLA	O2D-CGD-CBD	4.77	119.75	111.27
16	B	820	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
16	5	421	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
16	A	808	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
16	5	403	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
16	A	825	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
16	A	840	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
16	4	402	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
16	B	820	CLA	C2C-C1C-NC	4.76	114.43	109.97
16	1	509	CLA	C3D-C4D-ND	4.76	117.94	110.24
16	6	404	CLA	C2C-C1C-NC	4.76	114.43	109.97
16	B	802	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
16	2	403	CLA	O2D-CGD-CBD	4.76	119.72	111.27
16	A	822	CLA	C3D-C4D-ND	4.76	117.93	110.24
16	2	401	CLA	C3D-C4D-ND	4.76	117.93	110.24
16	5	417	CLA	C2C-C1C-NC	4.76	114.43	109.97
16	5	404	CLA	C1C-C2C-C3C	-4.76	101.96	106.96
16	4	403	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
16	4	405	CLA	O2D-CGD-CBD	4.75	119.71	111.27
16	B	834	CLA	C2C-C1C-NC	4.75	114.42	109.97
16	1	506	CLA	C2C-C1C-NC	4.75	114.42	109.97
16	B	838	CLA	C3D-C4D-ND	4.75	117.92	110.24
16	1	502	CLA	C3D-C4D-ND	4.75	117.92	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	409	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
16	1	514	CLA	C3D-C4D-ND	4.75	117.91	110.24
16	A	843	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
16	1	515	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
16	4	408	CLA	O2D-CGD-CBD	4.74	119.69	111.27
16	5	416	CLA	O2D-CGD-CBD	4.74	119.69	111.27
16	A	804	CLA	CMC-C2C-C1C	4.74	132.26	125.04
16	6	404	CLA	O2D-CGD-CBD	4.74	119.69	111.27
16	A	814	CLA	CAC-C3C-C4C	4.74	130.96	124.81
16	A	804	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
16	A	835	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
16	2	404	CLA	O2D-CGD-CBD	4.73	119.67	111.27
16	F	204	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
16	B	814	CLA	C4A-NA-C1A	-4.73	104.58	106.71
16	2	403	CLA	C4A-NA-C1A	-4.73	104.58	106.71
16	5	412	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
16	4	408	CLA	C3D-C4D-ND	4.72	117.88	110.24
16	B	816	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
16	1	505	CLA	C3D-C4D-ND	4.72	117.88	110.24
16	A	815	CLA	CMC-C2C-C1C	4.72	132.23	125.04
16	5	415	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
16	6	403	CLA	CAC-C3C-C4C	4.72	130.93	124.81
16	B	814	CLA	C3D-C4D-ND	4.72	117.87	110.24
16	5	406	CLA	C3D-C4D-ND	4.71	117.86	110.24
16	A	802	CLA	C3C-C4C-NC	4.71	115.86	110.57
16	B	806	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
16	4	403	CLA	C3D-C4D-ND	4.71	117.86	110.24
16	A	841	CLA	CMC-C2C-C1C	4.71	132.21	125.04
16	6	408	CLA	C3D-C4D-ND	4.71	117.86	110.24
16	5	405	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
16	4	407	CLA	C2C-C1C-NC	4.71	114.38	109.97
16	B	817	CLA	C3D-C4D-ND	4.70	117.85	110.24
16	1	512	CLA	C3D-C4D-ND	4.70	117.85	110.24
16	5	406	CLA	C4A-NA-C1A	-4.70	104.59	106.71
16	5	417	CLA	C3D-C4D-ND	4.70	117.85	110.24
16	5	410	CLA	C3D-C4D-ND	4.70	117.85	110.24
16	6	404	CLA	C3D-C4D-ND	4.70	117.85	110.24
16	2	404	CLA	C3D-C4D-ND	4.70	117.84	110.24
16	A	802	CLA	C3D-C4D-ND	4.70	117.84	110.24
16	A	839	CLA	C3D-C4D-ND	4.70	117.84	110.24
16	5	422	CLA	C4A-NA-C1A	-4.70	104.59	106.71
16	1	503	CLA	CAC-C3C-C4C	4.70	130.91	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	833	CLA	CMD-C2D-C1D	4.70	132.99	124.71
16	A	819	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
16	2	403	CLA	CHD-C4C-C3C	-4.69	117.94	124.84
16	A	830	CLA	C2C-C1C-NC	4.69	114.37	109.97
16	6	401	CLA	C3D-C4D-ND	4.69	117.83	110.24
16	A	815	CLA	CMD-C2D-C1D	4.69	132.98	124.71
16	1	519	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
16	A	821	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
16	A	831	CLA	C3C-C4C-NC	4.68	115.81	110.57
16	5	405	CLA	C4A-NA-C1A	-4.68	104.60	106.71
16	5	418	CLA	O2D-CGD-CBD	4.68	119.58	111.27
16	A	818	CLA	C3D-C4D-ND	4.67	117.80	110.24
16	4	406	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
16	A	836	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
16	B	808	CLA	C3C-C4C-NC	4.67	115.81	110.57
16	K	103	CLA	C3C-C4C-NC	4.67	115.81	110.57
16	6	407	CLA	C3D-C4D-ND	4.67	117.79	110.24
16	1	503	CLA	CHD-C4C-C3C	-4.67	117.98	124.84
16	5	407	CLA	C3D-C4D-ND	4.67	117.79	110.24
16	A	815	CLA	O2D-CGD-CBD	4.67	119.56	111.27
16	4	410	CLA	C4A-NA-C1A	-4.66	104.61	106.71
16	4	404	CLA	C3D-C4D-ND	4.66	117.78	110.24
16	4	406	CLA	C2C-C1C-NC	4.66	114.34	109.97
16	B	824	CLA	C3C-C4C-NC	4.66	115.80	110.57
16	5	409	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
16	6	402	CLA	C4A-NA-C1A	-4.66	104.61	106.71
16	6	403	CLA	O2D-CGD-CBD	4.66	119.55	111.27
16	A	817	CLA	CHD-C4C-C3C	-4.66	117.99	124.84
16	4	411	CLA	C3D-C4D-ND	4.66	117.77	110.24
16	4	408	CLA	C4A-NA-C1A	-4.65	104.61	106.71
16	5	416	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
16	A	829	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
16	B	829	CLA	C3D-C4D-ND	4.65	117.76	110.24
16	A	808	CLA	CMC-C2C-C1C	4.65	132.12	125.04
16	A	821	CLA	C3D-C4D-ND	4.64	117.75	110.24
16	A	817	CLA	C4A-NA-C1A	-4.64	104.62	106.71
16	A	814	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
16	5	419	CLA	C3D-C4D-ND	4.64	117.74	110.24
16	A	812	CLA	C2C-C1C-NC	4.64	114.32	109.97
16	4	407	CLA	C3D-C2D-C1D	-4.64	99.51	105.83
16	B	811	CLA	C3D-C4D-ND	4.63	117.73	110.24
16	1	519	CLA	C3D-C4D-ND	4.63	117.73	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	833	CLA	C1C-C2C-C3C	-4.63	102.09	106.96
16	B	801	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
16	6	407	CLA	C4A-NA-C1A	-4.63	104.63	106.71
16	4	411	CLA	C4A-NA-C1A	-4.62	104.63	106.71
16	A	838	CLA	C3D-C4D-ND	4.62	117.72	110.24
16	6	409	CLA	C3D-C4D-ND	4.62	117.72	110.24
16	A	805	CLA	C4A-NA-C1A	-4.62	104.63	106.71
16	2	405	CLA	C4A-NA-C1A	-4.62	104.63	106.71
16	3	401	CLA	C3D-C4D-ND	4.62	117.72	110.24
16	B	836	CLA	C3D-C4D-ND	4.62	117.71	110.24
16	1	503	CLA	C4A-NA-C1A	-4.62	104.63	106.71
16	B	841	CLA	C3C-C4C-NC	4.62	115.75	110.57
16	X	101	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
16	1	511	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
16	A	832	CLA	C3C-C4C-NC	4.61	115.75	110.57
16	4	410	CLA	C3D-C4D-ND	4.61	117.70	110.24
16	2	406	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
16	K	101	CLA	CHD-C1D-ND	-4.61	120.22	124.45
16	1	509	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
16	A	810	CLA	CMC-C2C-C1C	4.61	132.06	125.04
16	6	401	CLA	C4A-NA-C1A	-4.61	104.63	106.71
16	B	810	CLA	C2C-C1C-NC	4.61	114.29	109.97
16	1	519	CLA	O2D-CGD-CBD	4.61	119.45	111.27
16	B	840	CLA	C4A-NA-C1A	-4.61	104.64	106.71
16	2	402	CLA	O2D-CGD-CBD	4.61	119.45	111.27
16	1	526	CLA	C3D-C4D-ND	4.61	117.69	110.24
16	6	402	CLA	C3D-C4D-ND	4.61	117.69	110.24
16	A	827	CLA	O2D-CGD-CBD	4.61	119.45	111.27
16	5	413	CLA	O2D-CGD-CBD	4.60	119.45	111.27
16	5	408	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
16	6	403	CLA	C4A-NA-C1A	-4.60	104.64	106.71
16	4	409	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
16	B	813	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
16	B	813	CLA	C3C-C4C-NC	4.60	115.73	110.57
16	5	419	CLA	O2D-CGD-CBD	4.60	119.44	111.27
19	1	523	BCR	C37-C22-C21	-4.60	116.48	122.92
16	2	406	CLA	C3D-C4D-ND	4.60	117.67	110.24
16	1	510	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
16	K	101	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
15	A	801	CL0	C3D-C4D-ND	4.59	117.67	110.24
16	B	815	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
16	2	402	CLA	C3D-C4D-ND	4.59	117.67	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	505	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
16	6	403	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
16	5	418	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
16	A	836	CLA	C3D-C4D-ND	4.59	117.66	110.24
16	1	503	CLA	C3D-C4D-ND	4.59	117.66	110.24
16	1	508	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
16	A	830	CLA	C3D-C4D-ND	4.58	117.65	110.24
16	5	410	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
16	A	827	CLA	C4A-NA-C1A	-4.58	104.65	106.71
16	2	401	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
16	B	822	CLA	C3D-C4D-ND	4.58	117.64	110.24
16	A	835	CLA	C3D-C4D-ND	4.58	117.64	110.24
16	J	102	CLA	C2C-C1C-NC	4.57	114.26	109.97
16	5	404	CLA	CHD-C4C-C3C	-4.57	118.12	124.84
16	A	840	CLA	C3D-C4D-ND	4.57	117.63	110.24
16	B	831	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
16	A	837	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
16	2	405	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
16	3	401	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
19	1	518	BCR	C37-C22-C21	-4.57	116.53	122.92
16	J	102	CLA	C3D-C4D-ND	4.57	117.62	110.24
16	5	404	CLA	C3D-C4D-ND	4.57	117.62	110.24
16	2	404	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
16	J	102	CLA	O2D-CGD-CBD	4.56	119.38	111.27
16	A	811	CLA	C3D-C4D-ND	4.56	117.62	110.24
16	5	409	CLA	C3D-C4D-ND	4.56	117.62	110.24
16	B	826	CLA	C3D-C4D-ND	4.56	117.61	110.24
16	5	416	CLA	C4A-NA-C1A	-4.56	104.66	106.71
16	A	806	CLA	C3D-C4D-ND	4.56	117.61	110.24
16	B	833	CLA	C3D-C4D-ND	4.56	117.61	110.24
15	A	801	CL0	CHD-C1D-ND	-4.56	120.27	124.45
16	A	826	CLA	CHD-C1D-ND	-4.56	120.27	124.45
16	B	804	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
16	5	417	CLA	C4A-NA-C1A	-4.55	104.66	106.71
16	6	404	CLA	C4A-NA-C1A	-4.55	104.66	106.71
16	B	829	CLA	C2C-C1C-NC	4.55	114.23	109.97
16	B	810	CLA	C3C-C4C-NC	4.55	115.67	110.57
16	6	406	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
16	A	840	CLA	C3C-C4C-NC	4.55	115.67	110.57
16	F	204	CLA	C2C-C1C-NC	4.55	114.23	109.97
16	1	515	CLA	C3D-C4D-ND	4.54	117.59	110.24
16	A	843	CLA	C2C-C1C-NC	4.54	114.23	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	102	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
16	6	407	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
16	A	840	CLA	C2C-C1C-NC	4.54	114.22	109.97
16	1	506	CLA	C4A-NA-C1A	-4.54	104.67	106.71
16	B	828	CLA	C3D-C4D-ND	4.53	117.57	110.24
16	B	817	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
16	4	406	CLA	O2D-CGD-CBD	4.53	119.32	111.27
16	5	403	CLA	C4A-NA-C1A	-4.53	104.67	106.71
16	2	402	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
16	B	816	CLA	O2D-CGD-CBD	4.53	119.32	111.27
16	6	402	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
16	A	810	CLA	C3D-C4D-ND	4.53	117.57	110.24
16	2	403	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
16	F	201	CLA	CHD-C1D-ND	-4.53	120.29	124.45
16	4	407	CLA	C3D-C4D-ND	4.53	117.56	110.24
16	4	411	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
16	1	515	CLA	C3D-C2D-C1D	-4.53	99.66	105.83
16	B	824	CLA	C3D-C4D-ND	4.52	117.56	110.24
16	B	838	CLA	C4A-NA-C1A	-4.52	104.67	106.71
16	4	405	CLA	C3D-C4D-ND	4.52	117.55	110.24
16	6	404	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
16	6	408	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
16	5	422	CLA	C3D-C4D-ND	4.52	117.55	110.24
16	A	840	CLA	CAC-C3C-C4C	4.52	130.67	124.81
16	1	521	CLA	C3D-C4D-ND	4.51	117.54	110.24
16	5	413	CLA	CHD-C4C-C3C	-4.51	118.21	124.84
16	A	833	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
16	K	101	CLA	CHD-C4C-C3C	-4.51	118.21	124.84
16	A	832	CLA	C4A-NA-C1A	-4.51	104.68	106.71
16	A	824	CLA	CAC-C3C-C4C	4.51	130.66	124.81
16	A	834	CLA	CMC-C2C-C1C	4.51	131.91	125.04
16	5	406	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
16	B	840	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
16	1	521	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
16	6	405	CLA	C4A-NA-C1A	-4.51	104.68	106.71
16	J	102	CLA	CMC-C2C-C1C	4.51	131.90	125.04
16	B	816	CLA	C3C-C4C-NC	4.51	115.62	110.57
16	B	841	CLA	CAC-C3C-C4C	4.50	130.65	124.81
16	1	507	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
16	4	410	CLA	CAC-C3C-C4C	4.50	130.65	124.81
19	A	849	BCR	C37-C22-C21	-4.50	116.62	122.92
16	4	405	CLA	C3D-C2D-C1D	-4.50	99.69	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	419	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
16	B	810	CLA	O2D-CGD-CBD	4.50	119.26	111.27
16	B	823	CLA	C3D-C4D-ND	4.50	117.51	110.24
16	B	804	CLA	C3D-C4D-ND	4.49	117.50	110.24
16	5	418	CLA	C3D-C4D-ND	4.49	117.50	110.24
16	6	405	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
16	B	823	CLA	C3C-C4C-NC	4.49	115.61	110.57
16	A	838	CLA	O2D-CGD-CBD	4.49	119.24	111.27
16	A	808	CLA	C3D-C4D-ND	4.49	117.50	110.24
16	B	834	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
16	4	404	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
16	B	820	CLA	C3D-C4D-ND	4.48	117.48	110.24
16	A	825	CLA	O2D-CGD-CBD	4.48	119.22	111.27
16	6	403	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
16	A	817	CLA	C3D-C4D-ND	4.48	117.48	110.24
16	B	840	CLA	C3D-C4D-ND	4.47	117.48	110.24
16	1	515	CLA	O2D-CGD-CBD	4.47	119.22	111.27
16	6	405	CLA	C3D-C4D-ND	4.47	117.47	110.24
16	B	835	CLA	C3D-C4D-ND	4.47	117.47	110.24
16	B	836	CLA	O2D-CGD-CBD	4.47	119.21	111.27
16	1	507	CLA	C4A-NA-C1A	-4.47	104.70	106.71
16	5	422	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
16	A	820	CLA	C3D-C4D-ND	4.47	117.46	110.24
16	6	406	CLA	C4A-NA-C1A	-4.46	104.70	106.71
16	1	513	CLA	C3D-C4D-ND	4.46	117.46	110.24
16	6	409	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
16	A	817	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
16	B	809	CLA	O2D-CGD-CBD	4.46	119.19	111.27
16	A	841	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
16	B	815	CLA	C3D-C4D-ND	4.46	117.45	110.24
16	2	403	CLA	C3D-C4D-ND	4.45	117.44	110.24
16	1	526	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
16	5	411	CLA	C3D-C4D-ND	4.45	117.43	110.24
16	A	826	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
16	X	101	CLA	C3D-C4D-ND	4.44	117.43	110.24
16	6	406	CLA	C3D-C4D-ND	4.44	117.43	110.24
16	B	807	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
16	K	103	CLA	C3D-C4D-ND	4.44	117.43	110.24
16	A	842	CLA	C3D-C4D-ND	4.44	117.42	110.24
16	B	829	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
16	K	101	CLA	C3D-C4D-ND	4.44	117.42	110.24
16	B	839	CLA	C3D-C4D-ND	4.44	117.42	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	814	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
16	A	811	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
16	A	819	CLA	O2D-CGD-CBD	4.43	119.14	111.27
16	B	801	CLA	C4A-NA-C1A	-4.43	104.71	106.71
16	F	201	CLA	C4A-NA-C1A	-4.43	104.71	106.71
16	A	838	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
16	6	403	CLA	C3D-C4D-ND	4.43	117.40	110.24
16	A	809	CLA	C2C-C1C-NC	4.43	114.12	109.97
16	B	801	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
16	1	502	CLA	C4A-NA-C1A	-4.42	104.72	106.71
16	5	412	CLA	C4A-NA-C1A	-4.42	104.72	106.71
16	4	411	CLA	CMC-C2C-C1C	4.42	131.78	125.04
16	1	510	CLA	CAC-C3C-C4C	4.42	130.55	124.81
16	B	816	CLA	C2C-C1C-NC	4.42	114.11	109.97
16	1	514	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
16	B	830	CLA	O2D-CGD-CBD	4.42	119.11	111.27
16	A	827	CLA	C3D-C4D-ND	4.41	117.38	110.24
16	B	812	CLA	CMC-C2C-C1C	4.41	131.76	125.04
16	A	812	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
16	A	807	CLA	C3D-C4D-ND	4.41	117.36	110.24
16	A	810	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
16	5	413	CLA	C2C-C1C-NC	4.40	114.10	109.97
16	5	419	CLA	CAC-C3C-C4C	4.40	130.52	124.81
16	B	813	CLA	CMC-C2C-C1C	4.40	131.74	125.04
16	B	840	CLA	CAC-C3C-C4C	4.40	130.52	124.81
16	2	402	CLA	C4A-NA-C1A	-4.40	104.73	106.71
16	2	404	CLA	C4A-NA-C1A	-4.40	104.73	106.71
16	B	815	CLA	C2C-C1C-NC	4.40	114.09	109.97
16	5	414	CLA	CHD-C1D-ND	-4.40	120.41	124.45
16	A	828	CLA	C3C-C4C-NC	4.39	115.50	110.57
16	B	838	CLA	C3D-C2D-C1D	-4.39	99.83	105.83
16	4	411	CLA	C2C-C1C-NC	4.39	114.09	109.97
16	2	405	CLA	C3D-C4D-ND	4.39	117.34	110.24
16	B	826	CLA	C3C-C4C-NC	4.39	115.49	110.57
16	5	417	CLA	C3D-C2D-C1D	-4.39	99.85	105.83
16	A	843	CLA	O2D-CGD-CBD	4.38	119.06	111.27
16	B	809	CLA	CMC-C2C-C1C	4.38	131.72	125.04
16	J	101	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
16	A	819	CLA	C2C-C1C-NC	4.38	114.08	109.97
16	A	802	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
16	B	810	CLA	C3D-C4D-ND	4.38	117.33	110.24
16	1	507	CLA	C3D-C4D-ND	4.38	117.33	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	6	401	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
16	A	805	CLA	C3D-C4D-ND	4.37	117.31	110.24
16	B	806	CLA	CMC-C2C-C1C	4.37	131.70	125.04
16	B	803	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
16	6	409	CLA	C4A-NA-C1A	-4.37	104.74	106.71
16	B	801	CLA	C3D-C4D-ND	4.37	117.30	110.24
16	A	808	CLA	O2D-CGD-CBD	4.36	119.02	111.27
16	A	831	CLA	C3D-C4D-ND	4.36	117.30	110.24
16	4	406	CLA	C3D-C4D-ND	4.36	117.30	110.24
19	1	517	BCR	C34-C9-C10	-4.36	116.81	122.92
16	B	836	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
16	B	839	CLA	C4A-NA-C1A	-4.36	104.75	106.71
16	1	513	CLA	C4A-NA-C1A	-4.36	104.75	106.71
16	1	510	CLA	C3D-C4D-ND	4.36	117.29	110.24
19	K	102	BCR	C37-C22-C21	-4.36	116.82	122.92
16	5	414	CLA	C3C-C4C-NC	4.35	115.45	110.57
16	1	519	CLA	C2C-C1C-NC	4.35	114.05	109.97
16	A	814	CLA	C3D-C4D-ND	4.35	117.27	110.24
16	4	410	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
16	5	412	CLA	C3D-C4D-ND	4.35	117.27	110.24
16	1	525	CLA	C4A-NA-C1A	-4.35	104.75	106.71
16	B	821	CLA	C3D-C4D-ND	4.34	117.27	110.24
16	B	827	CLA	C2C-C1C-NC	4.34	114.04	109.97
16	1	505	CLA	C2C-C1C-NC	4.34	114.04	109.97
16	A	825	CLA	C3D-C4D-ND	4.34	117.26	110.24
16	B	807	CLA	CAC-C3C-C4C	4.34	130.44	124.81
16	B	828	CLA	C2C-C1C-NC	4.34	114.04	109.97
16	A	816	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
16	5	414	CLA	C3D-C4D-ND	4.34	117.25	110.24
16	5	411	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
16	5	418	CLA	C4A-NA-C1A	-4.34	104.76	106.71
16	B	833	CLA	C3C-C4C-NC	4.33	115.43	110.57
16	A	824	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
16	5	411	CLA	C2C-C1C-NC	4.33	114.03	109.97
16	B	834	CLA	C3D-C4D-ND	4.33	117.25	110.24
16	B	805	CLA	C3B-C4B-NB	4.33	114.81	109.21
16	A	837	CLA	CMC-C2C-C1C	4.33	131.63	125.04
16	B	803	CLA	O2D-CGD-CBD	4.33	118.96	111.27
16	A	838	CLA	C2C-C1C-NC	4.33	114.03	109.97
16	X	101	CLA	O2D-CGD-CBD	4.33	118.96	111.27
16	A	804	CLA	C3D-C4D-ND	4.32	117.23	110.24
15	A	801	CL0	C3D-C2D-C1D	-4.32	99.93	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	826	CLA	CAC-C3C-C4C	4.32	130.41	124.81
19	B	845	BCR	C37-C22-C21	-4.32	116.87	122.92
16	5	413	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
16	5	409	CLA	CMC-C2C-C1C	4.31	131.61	125.04
16	2	406	CLA	C4A-NA-C1A	-4.31	104.77	106.71
16	A	834	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
16	1	511	CLA	C4A-NA-C1A	-4.30	104.77	106.71
16	A	815	CLA	C3D-C4D-ND	4.30	117.20	110.24
16	B	811	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
16	4	408	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
16	B	830	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
16	B	805	CLA	CMC-C2C-C1C	4.30	131.59	125.04
16	B	831	CLA	C3D-C4D-ND	4.30	117.19	110.24
16	A	819	CLA	C3C-C4C-NC	4.30	115.39	110.57
16	A	826	CLA	C3C-C4C-NC	4.30	115.39	110.57
16	1	513	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
16	B	840	CLA	C3C-C4C-NC	4.29	115.39	110.57
16	B	813	CLA	O2D-CGD-CBD	4.29	118.89	111.27
16	A	808	CLA	C3C-C4C-NC	4.29	115.38	110.57
16	2	401	CLA	C4A-NA-C1A	-4.29	104.78	106.71
16	A	809	CLA	C3D-C4D-ND	4.29	117.17	110.24
16	5	404	CLA	CMC-C2C-C1C	4.29	131.57	125.04
19	5	402	BCR	C37-C22-C21	-4.29	116.92	122.92
16	A	835	CLA	CAC-C3C-C4C	4.29	130.37	124.81
16	A	808	CLA	C2C-C1C-NC	4.28	113.99	109.97
16	B	835	CLA	C2C-C1C-NC	4.28	113.98	109.97
16	A	825	CLA	C3C-C4C-NC	4.28	115.38	110.57
16	A	841	CLA	C3C-C4C-NC	4.28	115.38	110.57
16	B	835	CLA	O2D-CGD-CBD	4.28	118.87	111.27
16	B	812	CLA	C3C-C4C-NC	4.28	115.37	110.57
16	J	101	CLA	C3D-C4D-ND	4.28	117.16	110.24
16	B	807	CLA	CMC-C2C-C1C	4.27	131.55	125.04
16	A	828	CLA	C3D-C4D-ND	4.27	117.15	110.24
16	B	837	CLA	CAC-C3C-C4C	4.27	130.35	124.81
16	A	806	CLA	C2C-C1C-NC	4.27	113.97	109.97
16	A	809	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
16	A	823	CLA	C2C-C1C-NC	4.27	113.97	109.97
16	A	817	CLA	O2D-CGD-CBD	4.27	118.85	111.27
16	A	829	CLA	C3C-C4C-NC	4.27	115.36	110.57
16	1	513	CLA	O2D-CGD-CBD	4.26	118.84	111.27
16	5	414	CLA	C4A-NA-C1A	-4.26	104.79	106.71
16	A	826	CLA	CMC-C2C-C1C	4.26	131.52	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	414	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
16	F	204	CLA	C3C-C4C-NC	4.25	115.34	110.57
16	B	837	CLA	C3C-C4C-NC	4.25	115.34	110.57
16	A	812	CLA	O2D-CGD-CBD	4.25	118.82	111.27
16	1	503	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
16	B	836	CLA	CAC-C3C-C4C	4.25	130.32	124.81
16	B	817	CLA	C3C-C4C-NC	4.25	115.33	110.57
16	A	839	CLA	C3D-C2D-C1D	-4.25	100.04	105.83
16	B	819	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
16	1	511	CLA	C3D-C4D-ND	4.24	117.10	110.24
16	A	837	CLA	C3D-C4D-ND	4.24	117.10	110.24
16	A	814	CLA	O2D-CGD-CBD	4.24	118.80	111.27
16	5	419	CLA	CMC-C2C-C1C	4.24	131.49	125.04
16	B	832	CLA	C3C-C4C-NC	4.24	115.32	110.57
16	3	401	CLA	C4A-NA-C1A	-4.24	104.80	106.71
16	A	830	CLA	CMC-C2C-C1C	4.23	131.49	125.04
16	5	413	CLA	CAC-C3C-C4C	4.23	130.30	124.81
16	B	822	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
16	F	201	CLA	C3D-C4D-ND	4.23	117.08	110.24
16	A	830	CLA	O2D-CGD-CBD	4.23	118.78	111.27
16	A	803	CLA	C1-O2A-CGA	4.23	127.53	116.44
16	A	810	CLA	C1D-CHD-C4C	-4.22	116.94	126.06
16	B	839	CLA	C3C-C4C-NC	4.22	115.31	110.57
16	1	512	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
16	A	814	CLA	C3C-C4C-NC	4.22	115.30	110.57
16	B	836	CLA	C2C-C1C-NC	4.22	113.92	109.97
16	B	840	CLA	C2C-C1C-NC	4.22	113.92	109.97
16	2	401	CLA	CMC-C2C-C1C	4.22	131.46	125.04
16	A	816	CLA	C2C-C1C-NC	4.22	113.92	109.97
16	A	833	CLA	CMC-C2C-C1C	4.22	131.46	125.04
19	1	517	BCR	C16-C15-C14	4.22	132.11	123.47
16	B	807	CLA	C3D-C4D-ND	4.22	117.06	110.24
16	5	421	CLA	C4A-NA-C1A	-4.22	104.81	106.71
16	A	815	CLA	CAC-C3C-C4C	4.21	130.28	124.81
16	B	825	CLA	CMC-C2C-C1C	4.21	131.45	125.04
16	F	201	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
16	6	405	CLA	CAC-C3C-C4C	4.21	130.27	124.81
16	1	510	CLA	O2D-CGD-CBD	4.20	118.73	111.27
16	B	805	CLA	CAC-C3C-C4C	4.20	130.26	124.81
16	A	806	CLA	CMC-C2C-C1C	4.20	131.44	125.04
16	A	829	CLA	C3D-C4D-ND	4.20	117.03	110.24
16	5	412	CLA	CAC-C3C-C4C	4.20	130.26	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	822	CLA	C4A-NA-C1A	-4.20	104.82	106.71
16	B	825	CLA	C3D-C4D-ND	4.20	117.03	110.24
16	1	502	CLA	CMC-C2C-C1C	4.19	131.43	125.04
16	1	501	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
16	A	838	CLA	C3C-C4C-NC	4.19	115.27	110.57
16	5	408	CLA	C3C-C4C-NC	4.19	115.27	110.57
16	2	406	CLA	CAC-C3C-C4C	4.18	130.23	124.81
16	5	404	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
16	A	835	CLA	C3C-C4C-NC	4.18	115.26	110.57
16	F	201	CLA	CMC-C2C-C1C	4.18	131.40	125.04
16	B	824	CLA	CAC-C3C-C4C	4.18	130.23	124.81
16	A	815	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
16	1	501	CLA	C2C-C1C-NC	4.17	113.88	109.97
16	F	204	CLA	C3D-C4D-ND	4.17	116.99	110.24
16	1	506	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
16	4	405	CLA	CAC-C3C-C4C	4.17	130.22	124.81
16	B	805	CLA	C3D-C4D-ND	4.17	116.98	110.24
16	B	818	CLA	C3D-C4D-ND	4.17	116.98	110.24
16	A	807	CLA	CMC-C2C-C1C	4.17	131.39	125.04
16	A	829	CLA	CMC-C2C-C1C	4.17	131.39	125.04
16	A	834	CLA	C3D-C4D-ND	4.17	116.98	110.24
16	1	510	CLA	CMC-C2C-C1C	4.17	131.38	125.04
16	A	832	CLA	C3D-C4D-ND	4.17	116.98	110.24
16	B	814	CLA	CMC-C2C-C1C	4.17	131.38	125.04
16	A	806	CLA	C1-O2A-CGA	4.17	127.37	116.44
16	A	809	CLA	CMC-C2C-C1C	4.16	131.38	125.04
16	B	838	CLA	C3C-C4C-NC	4.16	115.24	110.57
16	B	838	CLA	O2D-CGD-CBD	4.16	118.66	111.27
16	J	101	CLA	CAC-C3C-C4C	4.16	130.21	124.81
16	5	412	CLA	CMC-C2C-C1C	4.15	131.36	125.04
16	1	511	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
16	B	812	CLA	C3D-C4D-ND	4.15	116.95	110.24
16	B	814	CLA	C3C-C4C-NC	4.15	115.22	110.57
16	A	841	CLA	C3D-C4D-ND	4.15	116.94	110.24
16	B	808	CLA	C3D-C4D-ND	4.13	116.93	110.24
16	A	829	CLA	C2C-C1C-NC	4.13	113.84	109.97
16	B	827	CLA	C3D-C4D-ND	4.13	116.92	110.24
16	A	812	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
16	1	508	CLA	C3D-C4D-ND	4.13	116.92	110.24
19	A	851	BCR	C15-C16-C17	4.13	131.93	123.47
16	1	507	CLA	C3B-C4B-NB	4.13	114.54	109.21
16	A	827	CLA	CMC-C2C-C1C	4.12	131.32	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	6	401	CLA	CAC-C3C-C4C	4.12	130.15	124.81
16	1	513	CLA	C3C-C4C-NC	4.12	115.19	110.57
19	A	851	BCR	C34-C9-C10	-4.12	117.16	122.92
16	A	824	CLA	C3C-C4C-NC	4.11	115.19	110.57
16	B	806	CLA	C3D-C4D-ND	4.11	116.89	110.24
19	B	847	BCR	C37-C22-C21	-4.11	117.16	122.92
16	A	813	CLA	O2D-CGD-CBD	4.11	118.57	111.27
16	A	809	CLA	CAC-C3C-C4C	4.11	130.14	124.81
16	1	511	CLA	CAC-C3C-C4C	4.10	130.13	124.81
16	A	802	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
16	A	814	CLA	C2C-C1C-NC	4.10	113.81	109.97
16	5	421	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
16	A	812	CLA	CMC-C2C-C1C	4.09	131.27	125.04
16	A	815	CLA	C3C-C4C-NC	4.09	115.16	110.57
16	A	819	CLA	C3D-C4D-ND	4.09	116.85	110.24
16	B	823	CLA	C4-C3-C5	4.09	122.15	115.27
19	1	516	BCR	C16-C15-C14	4.09	131.85	123.47
16	B	822	CLA	C3C-C4C-NC	4.09	115.15	110.57
16	A	810	CLA	C2C-C1C-NC	4.08	113.80	109.97
16	B	808	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
16	A	826	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
16	5	404	CLA	O2D-CGD-CBD	4.08	118.52	111.27
16	B	820	CLA	C4A-NA-C1A	-4.08	104.87	106.71
16	X	101	CLA	C4A-NA-C1A	-4.08	104.87	106.71
16	B	837	CLA	CMC-C2C-C1C	4.08	131.25	125.04
16	A	803	CLA	O2A-CGA-CBA	4.08	124.70	111.91
16	B	833	CLA	C2C-C1C-NC	4.08	113.79	109.97
16	4	410	CLA	CMC-C2C-C1C	4.07	131.24	125.04
16	B	804	CLA	C4A-NA-C1A	-4.07	104.88	106.71
19	A	846	BCR	C37-C22-C21	-4.07	117.22	122.92
16	1	508	CLA	CAC-C3C-C4C	4.07	130.09	124.81
16	A	826	CLA	C4A-NA-C1A	-4.07	104.88	106.71
19	J	104	BCR	C37-C22-C21	-4.07	117.22	122.92
16	B	804	CLA	O2D-CGD-CBD	4.07	118.49	111.27
16	B	818	CLA	C1C-C2C-C3C	-4.06	102.68	106.96
16	1	514	CLA	CAC-C3C-C4C	4.06	130.08	124.81
16	B	823	CLA	CAC-C3C-C4C	4.06	130.08	124.81
16	J	101	CLA	C3C-C4C-NC	4.06	115.12	110.57
16	B	803	CLA	C3C-C4C-NC	4.06	115.12	110.57
16	A	843	CLA	CAC-C3C-C4C	4.05	130.07	124.81
19	B	846	BCR	C37-C22-C21	-4.05	117.25	122.92
16	A	839	CLA	CMC-C2C-C1C	4.05	131.21	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	837	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
16	B	803	CLA	C3D-C4D-ND	4.05	116.79	110.24
16	6	408	CLA	CAC-C3C-C4C	4.05	130.06	124.81
16	J	101	CLA	C4A-NA-C1A	-4.05	104.89	106.71
19	B	853	BCR	C37-C22-C21	-4.04	117.26	122.92
16	B	837	CLA	C3D-C2D-C1D	-4.04	100.31	105.83
16	1	507	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
16	4	411	CLA	CAC-C3C-C4C	4.04	130.05	124.81
16	B	830	CLA	C3D-C4D-ND	4.04	116.77	110.24
16	A	822	CLA	CMC-C2C-C1C	4.04	131.19	125.04
16	A	818	CLA	CAC-C3C-C4C	4.04	130.05	124.81
16	A	842	CLA	C3C-C4C-NC	4.04	115.10	110.57
16	A	842	CLA	O2A-CGA-CBA	4.04	124.57	111.91
16	F	201	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
16	B	839	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
16	A	803	CLA	CMD-C2D-C1D	4.03	131.81	124.71
16	A	842	CLA	CAC-C3C-C4C	4.03	130.04	124.81
15	A	801	CL0	C1C-C2C-C3C	-4.03	102.72	106.96
16	B	825	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
16	B	809	CLA	C2C-C1C-NC	4.02	113.74	109.97
16	B	803	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
19	B	848	BCR	C37-C22-C23	4.02	124.41	118.08
16	1	521	CLA	CAC-C3C-C4C	4.02	130.03	124.81
16	1	525	CLA	C3D-C2D-C1D	-4.02	100.35	105.83
19	1	516	BCR	C37-C22-C21	-4.01	117.30	122.92
16	B	827	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
16	A	803	CLA	CMC-C2C-C1C	4.01	131.15	125.04
16	A	837	CLA	CAC-C3C-C4C	4.01	130.01	124.81
19	M	102	BCR	C37-C22-C21	-4.01	117.31	122.92
16	B	804	CLA	C3C-C4C-NC	4.00	115.06	110.57
16	A	803	CLA	C2C-C1C-NC	4.00	113.72	109.97
16	A	803	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
16	A	820	CLA	C3C-C4C-NC	4.00	115.05	110.57
16	1	507	CLA	CMC-C2C-C1C	4.00	131.12	125.04
16	1	507	CLA	CAC-C3C-C4C	3.99	129.99	124.81
19	A	848	BCR	C37-C22-C23	3.99	124.36	118.08
19	4	401	BCR	C37-C22-C21	-3.99	117.34	122.92
16	2	404	CLA	CMC-C2C-C1C	3.99	131.11	125.04
16	5	408	CLA	O2D-CGD-CBD	3.99	118.35	111.27
16	B	808	CLA	C4A-NA-C1A	-3.99	104.91	106.71
16	4	402	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
16	B	832	CLA	C2C-C1C-NC	3.98	113.70	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	837	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
16	B	819	CLA	CMC-C2C-C1C	3.98	131.09	125.04
16	A	826	CLA	C1C-C2C-C3C	-3.98	102.78	106.96
16	A	828	CLA	CMC-C2C-C1C	3.97	131.09	125.04
16	B	819	CLA	O2D-CGD-CBD	3.97	118.33	111.27
16	1	509	CLA	C3C-C4C-NC	3.97	115.03	110.57
16	B	808	CLA	CAC-C3C-C4C	3.97	129.96	124.81
16	B	833	CLA	C4A-NA-C1A	-3.97	104.92	106.71
19	B	844	BCR	C34-C9-C10	-3.96	117.37	122.92
16	A	807	CLA	C2C-C1C-NC	3.96	113.69	109.97
16	5	406	CLA	CAC-C3C-C4C	3.96	129.95	124.81
16	B	831	CLA	C3B-C4B-NB	3.96	114.33	109.21
16	A	805	CLA	C3C-C4C-NC	3.96	115.01	110.57
16	B	820	CLA	C3C-C4C-NC	3.96	115.01	110.57
19	5	420	BCR	C37-C22-C21	-3.96	117.38	122.92
16	1	510	CLA	C4A-NA-C1A	-3.96	104.93	106.71
16	B	824	CLA	C3D-C2D-C1D	-3.96	100.43	105.83
16	J	101	CLA	CMC-C2C-C1C	3.95	131.06	125.04
16	B	817	CLA	C2C-C1C-NC	3.95	113.67	109.97
16	B	810	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
16	B	827	CLA	C4C-C3C-C2C	-3.94	101.16	106.90
16	A	813	CLA	C3D-C4D-ND	3.94	116.61	110.24
16	6	406	CLA	CAC-C3C-C4C	3.94	129.92	124.81
16	B	803	CLA	CMD-C2D-C1D	3.93	131.65	124.71
16	5	405	CLA	C3C-C4C-NC	3.93	114.98	110.57
16	A	805	CLA	CAC-C3C-C4C	3.93	129.91	124.81
16	A	810	CLA	C3C-C4C-NC	3.93	114.98	110.57
16	K	101	CLA	C3C-C4C-NC	3.93	114.98	110.57
19	I	101	BCR	C37-C22-C21	-3.93	117.42	122.92
16	B	815	CLA	C3C-C4C-NC	3.93	114.97	110.57
16	1	519	CLA	C4A-NA-C1A	-3.93	104.94	106.71
15	A	801	CL0	C3B-C4B-NB	3.92	114.28	109.21
16	B	802	CLA	C3D-C4D-ND	3.92	116.58	110.24
16	5	404	CLA	C3B-C4B-NB	3.92	114.28	109.21
16	A	839	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
16	4	406	CLA	C3C-C4C-NC	3.92	114.97	110.57
16	B	814	CLA	CAC-C3C-C4C	3.92	129.89	124.81
15	A	801	CL0	C1D-CHD-C4C	-3.92	117.61	126.06
16	A	840	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
16	F	204	CLA	O2D-CGD-CBD	3.91	118.22	111.27
16	A	818	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
16	A	842	CLA	C4A-NA-C1A	-3.91	104.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	405	CLA	CMC-C2C-C1C	3.90	130.99	125.04
16	1	504	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
16	5	422	CLA	CAC-C3C-C4C	3.90	129.87	124.81
16	1	501	CLA	C3D-C4D-ND	3.90	116.55	110.24
16	A	811	CLA	CAC-C3C-C4C	3.90	129.87	124.81
16	B	805	CLA	C3C-C4C-NC	3.89	114.94	110.57
16	B	828	CLA	C3C-C4C-NC	3.89	114.94	110.57
16	B	836	CLA	CMC-C2C-C1C	3.89	130.96	125.04
16	A	830	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
16	B	829	CLA	C4-C3-C5	3.89	121.81	115.27
16	A	822	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
19	A	847	BCR	C37-C22-C21	-3.88	117.48	122.92
16	B	815	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
16	B	809	CLA	C3C-C4C-NC	3.88	114.92	110.57
16	1	504	CLA	C3C-C4C-NC	3.88	114.92	110.57
16	5	407	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
19	I	101	BCR	C37-C22-C23	3.88	124.19	118.08
16	B	835	CLA	C3C-C4C-NC	3.87	114.92	110.57
16	A	823	CLA	C3C-C4C-NC	3.87	114.91	110.57
16	4	409	CLA	C3C-C4C-NC	3.87	114.91	110.57
16	A	831	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
16	B	802	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
16	1	508	CLA	C4A-NA-C1A	-3.87	104.97	106.71
16	A	836	CLA	C4A-NA-C1A	-3.87	104.97	106.71
16	B	818	CLA	O2D-CGD-O1D	-3.86	116.28	123.84
16	1	502	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
16	2	401	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
16	A	813	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
16	B	835	CLA	CMC-C2C-C1C	3.86	130.91	125.04
16	1	508	CLA	C1D-CHD-C4C	-3.85	117.74	126.06
16	A	830	CLA	C1C-C2C-C3C	-3.85	102.90	106.96
16	B	832	CLA	O2A-CGA-CBA	3.85	124.00	111.91
19	B	846	BCR	C37-C22-C23	3.85	124.15	118.08
16	5	404	CLA	C4A-NA-C1A	-3.85	104.97	106.71
16	A	828	CLA	CAC-C3C-C4C	3.85	129.81	124.81
16	B	811	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
16	A	843	CLA	CMC-C2C-C1C	3.85	130.90	125.04
16	A	818	CLA	CMC-C2C-C1C	3.85	130.90	125.04
19	1	517	BCR	C37-C22-C21	-3.85	117.54	122.92
16	A	836	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
16	F	201	CLA	C3C-C4C-NC	3.84	114.88	110.57
16	B	841	CLA	C4A-NA-C1A	-3.84	104.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	834	CLA	C3C-C4C-NC	3.84	114.88	110.57
16	A	829	CLA	O2D-CGD-CBD	3.84	118.08	111.27
16	B	806	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
16	A	836	CLA	CMC-C2C-C1C	3.83	130.88	125.04
16	B	828	CLA	C3D-C2D-C1D	-3.83	100.60	105.83
16	B	806	CLA	O2D-CGD-CBD	3.83	118.07	111.27
16	A	830	CLA	C3C-C4C-NC	3.83	114.86	110.57
16	F	204	CLA	CAC-C3C-C4C	3.83	129.77	124.81
16	B	809	CLA	C3D-C4D-ND	3.82	116.42	110.24
16	5	407	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
16	J	102	CLA	C3C-C4C-NC	3.82	114.86	110.57
16	4	405	CLA	C3B-C4B-NB	3.82	114.15	109.21
16	A	831	CLA	C3B-C4B-NB	3.82	114.15	109.21
16	A	840	CLA	C4C-C3C-C2C	-3.82	101.33	106.90
16	A	804	CLA	CAC-C3C-C4C	3.82	129.77	124.81
16	B	824	CLA	CMC-C2C-C1C	3.82	130.86	125.04
16	5	415	CLA	C3C-C4C-NC	3.82	114.86	110.57
16	5	403	CLA	CMC-C2C-C1C	3.82	130.85	125.04
16	A	818	CLA	C4C-C3C-C2C	-3.82	101.33	106.90
16	1	526	CLA	CAC-C3C-C4C	3.82	129.76	124.81
16	A	834	CLA	C3C-C4C-NC	3.81	114.85	110.57
19	F	202	BCR	C37-C22-C21	-3.81	117.59	122.92
16	1	501	CLA	CAC-C3C-C4C	3.81	129.75	124.81
16	A	804	CLA	C3C-C4C-NC	3.81	114.84	110.57
16	B	831	CLA	C3C-C4C-NC	3.81	114.84	110.57
16	1	519	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
16	B	811	CLA	C3C-C4C-NC	3.80	114.84	110.57
19	A	850	BCR	C37-C22-C23	3.80	124.07	118.08
16	F	204	CLA	CMC-C2C-C1C	3.80	130.83	125.04
16	6	404	CLA	CMC-C2C-C1C	3.80	130.83	125.04
16	B	813	CLA	C4C-C3C-C2C	-3.80	101.36	106.90
16	5	412	CLA	C3C-C4C-NC	3.80	114.83	110.57
16	A	837	CLA	C3B-C4B-NB	3.80	114.12	109.21
16	B	835	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
16	5	407	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
16	4	403	CLA	C3C-C4C-NC	3.79	114.83	110.57
16	2	405	CLA	CAC-C3C-C4C	3.79	129.73	124.81
16	A	837	CLA	C3C-C4C-NC	3.79	114.83	110.57
16	5	410	CLA	C3C-C4C-NC	3.79	114.83	110.57
21	A	854	LMT	O1B-C4'-C3'	3.79	117.37	107.28
16	1	504	CLA	CMC-C2C-C1C	3.79	130.81	125.04
16	A	843	CLA	C1C-C2C-C3C	-3.79	102.97	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	845	BCR	C34-C9-C10	-3.79	117.61	122.92
16	A	842	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
16	A	828	CLA	O2D-CGD-CBD	3.79	118.00	111.27
16	B	801	CLA	C3C-C4C-NC	3.79	114.82	110.57
16	A	831	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
16	B	839	CLA	CAC-C3C-C4C	3.79	129.73	124.81
16	A	821	CLA	C3C-C4C-NC	3.79	114.82	110.57
16	B	822	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
16	1	521	CLA	C3C-C4C-NC	3.79	114.82	110.57
16	A	833	CLA	C4A-NA-C1A	-3.79	105.00	106.71
16	F	201	CLA	O2D-CGD-CBD	3.78	117.99	111.27
16	B	805	CLA	C4A-NA-C1A	-3.78	105.00	106.71
16	A	802	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
16	B	837	CLA	C2C-C1C-NC	3.78	113.52	109.97
16	B	835	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
16	A	833	CLA	C3B-C4B-NB	3.78	114.09	109.21
16	B	807	CLA	C3C-C4C-NC	3.78	114.81	110.57
16	A	806	CLA	C3B-C4B-NB	3.78	114.09	109.21
16	X	101	CLA	C3C-C4C-NC	3.78	114.81	110.57
19	1	517	BCR	C8-C9-C10	3.78	124.73	118.94
16	1	513	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
16	A	839	CLA	CAC-C3C-C4C	3.76	129.69	124.81
16	B	814	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
16	B	816	CLA	CAC-C3C-C4C	3.76	129.69	124.81
16	A	838	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
16	A	814	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
16	B	836	CLA	C3C-C4C-NC	3.76	114.78	110.57
16	A	808	CLA	CAC-C3C-C4C	3.75	129.68	124.81
16	B	831	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
16	B	803	CLA	C3B-C4B-NB	3.75	114.06	109.21
16	B	822	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
16	B	814	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
16	A	826	CLA	C3B-C4B-NB	3.74	114.05	109.21
16	1	508	CLA	C3C-C4C-NC	3.74	114.77	110.57
16	A	811	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
16	1	507	CLA	C3C-C4C-NC	3.74	114.76	110.57
16	B	821	CLA	CAC-C3C-C4C	3.73	129.66	124.81
16	5	403	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
16	A	837	CLA	C4A-NA-C1A	-3.73	105.03	106.71
16	B	806	CLA	C3C-C4C-NC	3.73	114.76	110.57
16	1	521	CLA	C2C-C1C-NC	3.73	113.47	109.97
16	B	817	CLA	CMB-C2B-C3B	3.73	131.66	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	101	CLA	CAC-C3C-C4C	3.73	129.65	124.81
16	F	204	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
16	B	821	CLA	C3C-C4C-NC	3.73	114.75	110.57
16	K	101	CLA	OBD-CAD-C3D	-3.73	122.57	128.74
16	A	816	CLA	C3C-C4C-NC	3.73	114.75	110.57
16	1	506	CLA	C3C-C4C-NC	3.73	114.75	110.57
16	A	839	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
19	I	101	BCR	C15-C16-C17	3.72	131.10	123.47
16	B	825	CLA	CAC-C3C-C4C	3.72	129.64	124.81
16	B	826	CLA	CMC-C2C-C1C	3.72	130.70	125.04
16	5	414	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
16	B	804	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
16	4	404	CLA	C3C-C4C-NC	3.71	114.73	110.57
19	B	848	BCR	C37-C22-C21	-3.71	117.73	122.92
16	A	818	CLA	C2C-C1C-NC	3.71	113.45	109.97
16	B	829	CLA	C3C-C4C-NC	3.71	114.73	110.57
16	A	803	CLA	C3C-C4C-NC	3.71	114.73	110.57
16	B	834	CLA	CMC-C2C-C1C	3.71	130.68	125.04
16	A	841	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
16	B	830	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
16	5	409	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
16	6	403	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
16	A	823	CLA	C4A-NA-C1A	-3.70	105.04	106.71
16	2	404	CLA	C3C-C4C-NC	3.70	114.72	110.57
16	B	834	CLA	C4A-NA-C1A	-3.70	105.04	106.71
16	A	827	CLA	C3C-C4C-NC	3.70	114.72	110.57
19	5	420	BCR	C16-C15-C14	3.69	131.04	123.47
16	B	834	CLA	C4-C3-C5	3.69	121.48	115.27
16	1	505	CLA	C3C-C4C-NC	3.69	114.71	110.57
19	J	103	BCR	C37-C22-C21	-3.69	117.76	122.92
16	2	406	CLA	C3C-C4C-NC	3.69	114.71	110.57
16	2	405	CLA	C3C-C4C-NC	3.69	114.70	110.57
16	A	802	CLA	CMC-C2C-C1C	3.68	130.64	125.04
16	6	409	CLA	C3C-C4C-NC	3.68	114.70	110.57
16	A	816	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
16	6	404	CLA	CAC-C3C-C4C	3.68	129.58	124.81
16	B	816	CLA	CMC-C2C-C1C	3.68	130.64	125.04
16	B	826	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
16	A	817	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
16	A	829	CLA	C4-C3-C5	3.68	121.45	115.27
16	B	838	CLA	CAC-C3C-C4C	3.67	129.58	124.81
19	J	103	BCR	C8-C9-C10	3.67	124.58	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	525	CLA	CAC-C3C-C4C	3.67	129.58	124.81
16	B	820	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
16	B	829	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
16	1	519	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
16	4	409	CLA	CMC-C2C-C1C	3.67	130.63	125.04
16	5	417	CLA	CMC-C2C-C1C	3.67	130.63	125.04
16	B	827	CLA	O2A-CGA-CBA	3.67	123.42	111.91
16	1	513	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
16	A	838	CLA	CAC-C3C-C4C	3.67	129.57	124.81
16	A	806	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
16	5	418	CLA	C3C-C4C-NC	3.66	114.68	110.57
16	1	515	CLA	CMC-C2C-C1C	3.66	130.62	125.04
16	A	828	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
16	B	833	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
16	5	410	CLA	O2D-CGD-CBD	3.66	117.77	111.27
16	1	510	CLA	C3C-C4C-NC	3.66	114.67	110.57
16	1	525	CLA	C3C-C4C-NC	3.66	114.67	110.57
16	5	411	CLA	C3C-C4C-NC	3.66	114.67	110.57
16	B	818	CLA	C4-C3-C5	3.66	121.42	115.27
16	6	407	CLA	C3C-C4C-NC	3.65	114.67	110.57
16	A	815	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
16	4	408	CLA	C3C-C4C-NC	3.65	114.67	110.57
16	4	409	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
16	B	812	CLA	CAC-C3C-C4C	3.65	129.55	124.81
16	1	514	CLA	C3C-C4C-NC	3.65	114.67	110.57
16	2	402	CLA	C3C-C4C-NC	3.65	114.67	110.57
16	1	501	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
16	B	802	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
16	2	404	CLA	CAC-C3C-C4C	3.65	129.54	124.81
16	5	418	CLA	CAC-C3C-C4C	3.64	129.54	124.81
16	A	831	CLA	CAC-C3C-C4C	3.64	129.54	124.81
16	B	807	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
16	A	819	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
16	A	802	CLA	CAC-C3C-C4C	3.64	129.53	124.81
16	2	402	CLA	CAC-C3C-C4C	3.64	129.53	124.81
16	1	501	CLA	CMC-C2C-C1C	3.64	130.58	125.04
16	B	839	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
16	6	409	CLA	CAC-C3C-C4C	3.64	129.53	124.81
16	B	814	CLA	C3B-C4B-NB	3.64	113.91	109.21
16	A	807	CLA	C3C-C4C-NC	3.64	114.65	110.57
16	A	821	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
16	A	822	CLA	C3C-C4C-NC	3.63	114.65	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	811	CLA	O2D-CGD-CBD	3.63	117.72	111.27
16	A	811	CLA	C3C-C4C-NC	3.63	114.65	110.57
16	A	814	CLA	C4C-C3C-C2C	-3.63	101.60	106.90
16	B	831	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
16	B	808	CLA	CMC-C2C-C1C	3.63	130.57	125.04
16	A	804	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
16	1	501	CLA	C3C-C4C-NC	3.63	114.64	110.57
16	A	834	CLA	CAC-C3C-C4C	3.63	129.52	124.81
16	A	812	CLA	C3C-C4C-NC	3.63	114.64	110.57
16	4	406	CLA	CAC-C3C-C4C	3.63	129.52	124.81
19	J	104	BCR	C34-C9-C10	-3.63	117.84	122.92
16	A	820	CLA	CAC-C3C-C4C	3.63	129.52	124.81
16	J	102	CLA	CAC-C3C-C4C	3.63	129.52	124.81
16	A	809	CLA	C3C-C4C-NC	3.63	114.64	110.57
16	A	807	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
16	B	832	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
16	3	401	CLA	C3C-C4C-NC	3.62	114.64	110.57
16	5	417	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
19	A	846	BCR	C34-C9-C10	-3.62	117.85	122.92
16	A	811	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
16	A	813	CLA	C4-C3-C5	3.62	121.36	115.27
16	B	831	CLA	CMB-C2B-C3B	3.62	131.45	124.68
16	K	103	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
16	A	828	CLA	C4C-C3C-C2C	-3.62	101.63	106.90
16	A	831	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
16	B	830	CLA	C3C-C4C-NC	3.62	114.63	110.57
16	6	402	CLA	C3C-C4C-NC	3.61	114.62	110.57
16	B	841	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
16	A	839	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
16	B	805	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
16	B	802	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
16	F	201	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
16	B	811	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
19	J	104	BCR	C8-C9-C10	3.61	124.48	118.94
16	B	834	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
16	A	826	CLA	C3D-C4D-ND	3.61	116.08	110.24
16	B	838	CLA	CMC-C2C-C1C	3.61	130.54	125.04
16	B	812	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
16	4	407	CLA	C3C-C4C-NC	3.61	114.62	110.57
16	5	408	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
16	6	407	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
16	A	836	CLA	C3C-C4C-NC	3.60	114.61	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	821	CLA	C1D-CHD-C4C	-3.60	118.28	126.06
16	5	407	CLA	C3C-C4C-NC	3.60	114.61	110.57
19	1	522	BCR	C37-C22-C21	-3.60	117.88	122.92
16	B	824	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
16	A	834	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
16	1	512	CLA	C3C-C4C-NC	3.60	114.61	110.57
16	1	509	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
16	A	835	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
16	B	801	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
16	2	403	CLA	C3C-C4C-NC	3.59	114.60	110.57
16	A	820	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
16	6	402	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
16	6	401	CLA	C3C-C4C-NC	3.59	114.60	110.57
16	B	824	CLA	C4C-C3C-C2C	-3.59	101.67	106.90
19	B	847	BCR	C16-C15-C14	3.59	130.82	123.47
16	A	836	CLA	CAC-C3C-C4C	3.59	129.46	124.81
16	B	806	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
16	B	819	CLA	C2C-C1C-NC	3.59	113.33	109.97
16	X	101	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
19	M	102	BCR	C37-C22-C23	3.58	123.72	118.08
16	1	519	CLA	CMC-C2C-C1C	3.58	130.50	125.04
16	B	825	CLA	C3C-C4C-NC	3.58	114.59	110.57
16	B	801	CLA	CAC-C3C-C4C	3.58	129.46	124.81
16	3	401	CLA	CAC-C3C-C4C	3.58	129.46	124.81
16	A	822	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
16	A	841	CLA	O2A-CGA-CBA	3.58	123.15	111.91
16	B	839	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
16	B	805	CLA	CHC-C1C-C2C	-3.58	116.82	126.72
16	B	827	CLA	CAC-C3C-C4C	3.58	129.46	124.81
16	6	409	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
16	A	807	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
16	B	803	CLA	CAC-C3C-C4C	3.58	129.45	124.81
16	5	422	CLA	C3C-C4C-NC	3.57	114.58	110.57
16	1	506	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
19	A	850	BCR	C34-C9-C8	3.57	123.71	118.08
16	F	201	CLA	CAC-C3C-C4C	3.57	129.45	124.81
16	6	406	CLA	C3C-C4C-NC	3.57	114.58	110.57
16	5	416	CLA	C3C-C4C-NC	3.57	114.58	110.57
16	5	406	CLA	C3C-C4C-NC	3.57	114.58	110.57
16	B	817	CLA	CAC-C3C-C4C	3.57	129.44	124.81
16	1	510	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
16	A	805	CLA	C1D-CHD-C4C	-3.57	118.36	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	806	CLA	CAC-C3C-C4C	3.57	129.44	124.81
16	A	812	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
16	6	404	CLA	C3C-C4C-NC	3.57	114.57	110.57
16	1	512	CLA	CAC-C3C-C4C	3.57	129.44	124.81
16	5	421	CLA	CAC-C3C-C4C	3.56	129.43	124.81
16	5	415	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
16	4	408	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
19	B	847	BCR	C37-C22-C23	3.56	123.68	118.08
16	B	821	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
16	B	838	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
16	5	407	CLA	C3B-C4B-NB	3.55	113.81	109.21
16	3	401	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
19	B	843	BCR	C34-C9-C10	-3.55	117.94	122.92
16	A	835	CLA	C4C-C3C-C2C	-3.55	101.72	106.90
16	A	809	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
16	A	815	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
16	5	406	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
16	A	804	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
16	B	812	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
16	2	405	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
16	1	503	CLA	C3C-C4C-NC	3.54	114.55	110.57
16	6	408	CLA	C3C-C4C-NC	3.54	114.55	110.57
16	A	808	CLA	C4-C3-C5	3.54	120.03	115.98
16	A	817	CLA	C3C-C4C-NC	3.54	114.55	110.57
16	B	822	CLA	C3B-C4B-NB	3.54	113.79	109.21
16	1	509	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
16	A	837	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
16	5	405	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
16	B	813	CLA	C2C-C1C-NC	3.54	113.29	109.97
16	A	834	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
16	4	411	CLA	C3C-C4C-NC	3.54	114.54	110.57
16	B	823	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
16	K	103	CLA	C4C-C3C-C2C	-3.54	101.74	106.90
16	B	809	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
19	B	843	BCR	C37-C22-C21	-3.53	117.97	122.92
16	A	828	CLA	C2C-C1C-NC	3.53	113.28	109.97
16	A	814	CLA	CMC-C2C-C1C	3.53	130.42	125.04
16	A	817	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
16	1	514	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
16	5	404	CLA	CHC-C1C-C2C	-3.53	116.96	126.72
16	B	822	CLA	CAC-C3C-C4C	3.53	129.39	124.81
16	A	815	CLA	C3B-C4B-NB	3.53	113.77	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	404	CLA	CAC-C3C-C4C	3.53	129.39	124.81
16	B	801	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
16	4	407	CLA	CMC-C2C-C1C	3.53	130.41	125.04
16	6	405	CLA	C3C-C4C-NC	3.53	114.53	110.57
16	A	803	CLA	O2D-CGD-CBD	3.53	117.53	111.27
16	A	836	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
16	1	511	CLA	C3B-C4B-NB	3.52	113.76	109.21
16	B	823	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
16	5	406	CLA	CMC-C2C-C1C	3.52	130.40	125.04
16	B	824	CLA	C2C-C1C-NC	3.52	113.27	109.97
16	B	827	CLA	CMC-C2C-C1C	3.52	130.40	125.04
16	A	829	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
16	B	837	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
16	2	401	CLA	C3C-C4C-NC	3.52	114.52	110.57
16	1	521	CLA	CMC-C2C-C1C	3.52	130.39	125.04
16	1	525	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
16	2	402	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
16	5	410	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
16	B	808	CLA	CBC-CAC-C3C	-3.51	102.74	112.43
16	A	832	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
16	5	407	CLA	CHC-C1C-C2C	-3.51	117.01	126.72
16	B	828	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
16	A	803	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
16	B	821	CLA	C3B-C4B-NB	3.51	113.74	109.21
16	B	807	CLA	C1D-CHD-C4C	-3.51	118.50	126.06
16	5	403	CLA	C3C-C4C-NC	3.51	114.50	110.57
16	5	419	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
16	B	811	CLA	CHC-C1C-C2C	-3.50	117.03	126.72
16	B	816	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
16	6	402	CLA	CAC-C3C-C4C	3.50	129.36	124.81
16	1	505	CLA	CMC-C2C-C1C	3.50	130.37	125.04
16	B	828	CLA	CMC-C2C-C1C	3.50	130.37	125.04
16	1	515	CLA	C3C-C4C-NC	3.50	114.50	110.57
16	B	840	CLA	O2D-CGD-CBD	3.50	117.49	111.27
19	A	850	BCR	C37-C22-C21	-3.50	118.02	122.92
16	1	502	CLA	C3C-C4C-NC	3.50	114.50	110.57
16	B	826	CLA	C4C-C3C-C2C	-3.50	101.80	106.90
16	5	415	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
16	1	521	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
16	B	836	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
16	A	827	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
16	A	822	CLA	O2D-CGD-CBD	3.49	117.47	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	101	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
16	1	520	CLA	C3C-C4C-NC	3.49	114.48	110.57
16	B	840	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
16	4	403	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
16	4	402	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
16	B	802	CLA	C5-C3-C2	-3.49	114.06	121.12
16	5	408	CLA	CED-O2D-CGD	3.49	123.82	115.94
16	B	820	CLA	CMC-C2C-C1C	3.49	130.35	125.04
16	5	416	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
16	4	410	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
19	B	853	BCR	C34-C9-C10	-3.48	118.05	122.92
16	A	829	CLA	C5-C3-C2	-3.47	114.08	121.12
16	4	411	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
16	5	409	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
16	1	512	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
16	4	407	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
16	1	502	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
19	B	844	BCR	C37-C22-C21	-3.47	118.06	122.92
16	2	404	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
19	F	202	BCR	C34-C9-C10	-3.47	118.07	122.92
16	4	405	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
16	A	808	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
16	B	820	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
16	1	526	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
16	4	405	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
16	5	403	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
16	A	833	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
16	2	401	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
16	B	829	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
16	5	411	CLA	CAC-C3C-C4C	3.45	129.29	124.81
16	5	422	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
16	6	404	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
16	2	406	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
16	1	526	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
16	A	819	CLA	O2A-CGA-CBA	3.45	122.73	111.91
15	A	801	CL0	CHB-C4A-NA	3.44	129.27	124.51
16	A	839	CLA	C3C-C4C-NC	3.44	114.43	110.57
19	5	402	BCR	C34-C9-C10	-3.44	118.10	122.92
16	6	406	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
16	4	405	CLA	C3C-C4C-NC	3.44	114.43	110.57
16	B	833	CLA	O2A-CGA-CBA	3.44	122.70	111.91
16	4	406	CLA	C1D-CHD-C4C	-3.44	118.64	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	419	CLA	C3C-C4C-NC	3.44	114.43	110.57
16	4	403	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
16	6	405	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
16	1	526	CLA	C3C-C4C-NC	3.43	114.42	110.57
19	I	102	BCR	C36-C18-C17	-3.43	118.11	122.92
16	B	817	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
16	A	821	CLA	CAC-C3C-C4C	3.43	129.26	124.81
16	5	417	CLA	CAC-C3C-C4C	3.43	129.26	124.81
16	B	823	CLA	C5-C3-C2	-3.43	114.18	121.12
16	5	416	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
16	1	506	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
16	5	418	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
16	5	412	CLA	C1C-C2C-C3C	-3.43	103.36	106.96
16	B	815	CLA	CAC-C3C-C4C	3.42	129.25	124.81
16	4	409	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
16	J	102	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
16	A	842	CLA	CMC-C2C-C1C	3.42	130.25	125.04
16	1	512	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
16	B	803	CLA	CMC-C2C-C1C	3.42	130.24	125.04
16	J	102	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
16	4	410	CLA	C3C-C4C-NC	3.42	114.40	110.57
16	B	819	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
16	A	822	CLA	C2C-C1C-NC	3.41	113.17	109.97
19	A	851	BCR	C37-C22-C21	-3.41	118.14	122.92
19	A	846	BCR	C23-C22-C21	3.41	124.18	118.94
16	4	407	CLA	CAC-C3C-C4C	3.41	129.24	124.81
16	5	422	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
16	B	817	CLA	C4C-C3C-C2C	-3.41	101.92	106.90
16	5	421	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
16	4	408	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
16	A	810	CLA	O2D-CGD-CBD	3.41	117.33	111.27
16	A	818	CLA	O2D-CGD-CBD	3.41	117.33	111.27
16	5	404	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
16	B	802	CLA	CMC-C2C-C1C	3.41	130.23	125.04
16	5	421	CLA	C3C-C4C-NC	3.41	114.39	110.57
16	A	831	CLA	CHC-C1C-C2C	-3.41	117.30	126.72
16	5	408	CLA	C1D-CHD-C4C	-3.40	118.71	126.06
16	1	514	CLA	C1D-CHD-C4C	-3.40	118.71	126.06
16	5	408	CLA	C3B-C4B-NB	3.40	113.61	109.21
16	B	808	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
16	1	511	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
16	A	835	CLA	O2D-CGD-O1D	-3.40	117.19	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	419	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
16	A	808	CLA	O2A-CGA-CBA	3.40	122.58	111.91
16	A	813	CLA	CAC-C3C-C4C	3.40	129.22	124.81
16	4	407	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
16	A	824	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
16	6	404	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
16	5	411	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
16	5	412	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
16	6	408	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
19	I	102	BCR	C15-C16-C17	3.40	130.43	123.47
16	4	408	CLA	CAC-C3C-C4C	3.40	129.22	124.81
16	A	825	CLA	CMC-C2C-C1C	3.39	130.21	125.04
16	1	526	CLA	C1D-CHD-C4C	-3.39	118.73	126.06
16	A	803	CLA	CAC-C3C-C4C	3.39	129.21	124.81
16	2	404	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
16	B	813	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
16	B	823	CLA	C4A-NA-C1A	-3.39	105.18	106.71
16	5	403	CLA	CAC-C3C-C4C	3.39	129.21	124.81
15	A	801	CL0	CAA-C2A-C3A	-3.39	103.49	112.78
16	K	101	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
16	2	402	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
16	B	841	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
16	1	505	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
16	K	103	CLA	CAC-C3C-C4C	3.38	129.20	124.81
16	1	505	CLA	CAC-C3C-C4C	3.38	129.20	124.81
16	1	511	CLA	CHC-C1C-C2C	-3.38	117.36	126.72
16	A	820	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
16	A	832	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
16	J	101	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
16	B	817	CLA	O2A-CGA-CBA	3.38	122.53	111.91
16	B	811	CLA	CAC-C3C-C4C	3.38	129.20	124.81
16	A	838	CLA	CMC-C2C-C1C	3.38	130.19	125.04
16	1	525	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
16	B	823	CLA	C3B-C4B-NB	3.38	113.58	109.21
16	5	413	CLA	CED-O2D-CGD	3.38	123.58	115.94
16	6	409	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
16	6	401	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
16	A	840	CLA	O2D-CGD-O1D	-3.38	117.24	123.84
16	5	417	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
16	6	403	CLA	C3C-C4C-NC	3.38	114.36	110.57
16	B	818	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
16	6	403	CLA	C1D-CHD-C4C	-3.37	118.78	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	801	CL0	CMC-C2C-C1C	3.37	130.18	125.04
16	J	101	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
16	A	804	CLA	C4A-NA-C1A	-3.37	105.19	106.71
15	A	801	CL0	O2D-CGD-O1D	-3.37	117.26	123.84
16	A	841	CLA	CED-O2D-CGD	3.37	123.55	115.94
16	1	503	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
16	B	831	CLA	CMC-C2C-C1C	3.36	130.16	125.04
16	2	406	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
16	6	402	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
16	4	404	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
19	1	518	BCR	C37-C22-C23	3.36	123.37	118.08
16	1	504	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
16	6	407	CLA	CAC-C3C-C4C	3.36	129.17	124.81
16	6	405	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
16	B	830	CLA	C4-C3-C5	3.36	120.92	115.27
16	A	823	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
16	5	415	CLA	CAC-C3C-C4C	3.36	129.16	124.81
16	2	405	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
19	A	848	BCR	C37-C22-C21	-3.35	118.22	122.92
16	3	401	CLA	C1D-CHD-C4C	-3.35	118.82	126.06
16	6	401	CLA	C1D-CHD-C4C	-3.35	118.82	126.06
16	B	841	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
16	5	414	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
16	1	510	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
16	6	408	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
16	5	413	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
16	2	403	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
16	B	825	CLA	CAA-C2A-C3A	-3.35	103.61	112.78
16	B	823	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
16	B	825	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
16	5	417	CLA	C3C-C4C-NC	3.35	114.33	110.57
16	1	503	CLA	CMC-C2C-C1C	3.35	130.14	125.04
16	A	813	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
16	A	819	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
16	2	403	CLA	CMC-C2C-C1C	3.34	130.13	125.04
16	B	830	CLA	CAC-C3C-C4C	3.34	129.14	124.81
16	B	804	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
16	B	806	CLA	CAC-C3C-C4C	3.34	129.14	124.81
16	2	403	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
16	B	825	CLA	C3B-C4B-NB	3.34	113.52	109.21
16	1	507	CLA	C1D-CHD-C4C	-3.33	118.86	126.06
16	4	404	CLA	C1D-CHD-C4C	-3.33	118.87	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	205	BCR	C37-C22-C21	-3.33	118.26	122.92
16	B	801	CLA	CMB-C2B-C1B	3.33	133.58	128.46
16	5	418	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
16	A	809	CLA	O2A-CGA-CBA	3.33	122.36	111.91
16	1	525	CLA	CMC-C2C-C1C	3.33	130.11	125.04
16	A	817	CLA	CHC-C1C-C2C	-3.33	117.51	126.72
16	A	829	CLA	CAC-C3C-C4C	3.33	129.13	124.81
16	B	809	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
16	1	506	CLA	CMC-C2C-C1C	3.33	130.11	125.04
16	1	509	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
16	6	403	CLA	CHC-C1C-C2C	-3.33	117.52	126.72
16	B	821	CLA	CMC-C2C-C1C	3.33	130.10	125.04
16	B	802	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
16	6	407	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
16	B	830	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
16	A	809	CLA	C3B-C4B-NB	3.32	113.51	109.21
16	6	406	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
16	A	825	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
16	1	504	CLA	C3B-C4B-NB	3.32	113.50	109.21
16	B	819	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
16	1	511	CLA	C3C-C4C-NC	3.32	114.30	110.57
16	B	840	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
16	1	511	CLA	CMC-C2C-C1C	3.32	130.09	125.04
16	B	832	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
16	A	805	CLA	C3B-C4B-NB	3.32	113.50	109.21
16	5	405	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
16	5	408	CLA	CAC-C3C-C4C	3.32	129.11	124.81
16	A	820	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
19	B	843	BCR	C16-C15-C14	3.31	130.26	123.47
16	A	813	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
16	A	803	CLA	CMB-C2B-C3B	3.31	130.88	124.68
16	5	405	CLA	CAC-C3C-C4C	3.31	129.11	124.81
19	A	849	BCR	C34-C9-C10	-3.31	118.28	122.92
16	1	520	CLA	C2C-C1C-NC	3.31	113.08	109.97
16	A	823	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
16	A	821	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
16	B	826	CLA	C2C-C1C-NC	3.31	113.07	109.97
16	A	831	CLA	CMC-C2C-C1C	3.31	130.07	125.04
16	5	414	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
16	4	409	CLA	CAC-C3C-C4C	3.30	129.10	124.81
16	1	515	CLA	C1D-CHD-C4C	-3.30	118.93	126.06
19	I	102	BCR	C34-C9-C10	-3.30	118.30	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	410	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
16	B	825	CLA	CHB-C4A-NA	3.30	129.07	124.51
16	A	810	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
16	B	802	CLA	CAC-C3C-C4C	3.29	129.08	124.81
16	A	836	CLA	O2D-CGD-CBD	3.29	117.12	111.27
16	5	409	CLA	C3C-C4C-NC	3.29	114.26	110.57
16	1	520	CLA	CMC-C2C-C1C	3.29	130.05	125.04
16	4	402	CLA	C3C-C4C-NC	3.29	114.26	110.57
16	1	520	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
16	A	843	CLA	C2A-C1A-CHA	-3.29	118.10	123.86
16	B	829	CLA	CMC-C2C-C1C	3.29	130.05	125.04
16	5	421	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
16	A	833	CLA	C3C-C4C-NC	3.29	114.26	110.57
16	B	818	CLA	CMC-C2C-C1C	3.29	130.04	125.04
16	B	833	CLA	CAC-C3C-C4C	3.29	129.07	124.81
16	1	521	CLA	C4-C3-C5	3.28	120.80	115.27
15	A	801	CL0	CAC-C3C-C4C	3.28	129.07	124.81
16	1	502	CLA	CAC-C3C-C4C	3.28	129.07	124.81
16	B	826	CLA	C2A-C1A-CHA	-3.28	118.12	123.86
19	B	853	BCR	C37-C22-C23	3.28	123.25	118.08
16	A	819	CLA	CMB-C2B-C3B	3.28	130.82	124.68
16	A	810	CLA	O2A-CGA-CBA	3.28	122.20	111.91
16	1	504	CLA	CAC-C3C-C4C	3.28	129.06	124.81
16	1	508	CLA	CHC-C1C-C2C	-3.28	117.65	126.72
16	B	804	CLA	CAC-C3C-C4C	3.27	129.06	124.81
16	A	834	CLA	C1-C2-C3	-3.27	120.38	126.04
19	1	523	BCR	C36-C18-C17	-3.27	118.34	122.92
16	A	825	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
19	A	850	BCR	C34-C9-C10	-3.27	118.34	122.92
19	1	523	BCR	C34-C9-C10	-3.27	118.34	122.92
16	A	809	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
16	A	809	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
16	A	806	CLA	O2A-CGA-CBA	3.27	122.16	111.91
16	A	811	CLA	CHC-C1C-C2C	-3.27	117.69	126.72
16	5	417	CLA	O2D-CGD-O1D	-3.26	117.45	123.84
16	B	839	CLA	CHC-C1C-C2C	-3.26	117.69	126.72
16	1	506	CLA	CAC-C3C-C4C	3.26	129.04	124.81
16	B	834	CLA	CAC-C3C-C4C	3.26	129.04	124.81
16	B	831	CLA	CAC-C3C-C4C	3.26	129.04	124.81
16	4	406	CLA	CMC-C2C-C1C	3.26	130.00	125.04
16	1	508	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
16	A	806	CLA	C1D-CHD-C4C	-3.26	119.03	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	818	CLA	C3C-C4C-NC	3.26	114.22	110.57
16	B	824	CLA	C1-C2-C3	-3.26	120.41	126.04
19	F	205	BCR	C36-C18-C17	-3.25	118.36	122.92
16	1	513	CLA	CMC-C2C-C1C	3.25	129.99	125.04
16	5	410	CLA	CHC-C1C-C2C	-3.24	117.75	126.72
16	A	826	CLA	CHC-C1C-C2C	-3.24	117.75	126.72
16	A	805	CLA	CMC-C2C-C1C	3.24	129.98	125.04
16	A	803	CLA	C4A-NA-C1A	-3.24	105.25	106.71
16	A	807	CLA	CAC-C3C-C4C	3.24	129.01	124.81
19	A	848	BCR	C36-C18-C17	-3.24	118.39	122.92
19	1	516	BCR	C34-C9-C10	-3.24	118.39	122.92
16	A	830	CLA	C1D-CHD-C4C	-3.24	119.08	126.06
16	A	809	CLA	O2A-CGA-O1A	-3.24	115.42	123.59
16	A	816	CLA	CMC-C2C-C1C	3.24	129.97	125.04
19	1	518	BCR	C16-C15-C14	3.24	130.10	123.47
16	B	833	CLA	C4C-C3C-C2C	-3.23	102.18	106.90
16	1	519	CLA	C3C-C4C-NC	3.23	114.20	110.57
16	B	828	CLA	C1-O2A-CGA	3.23	124.92	116.44
19	K	102	BCR	C15-C16-C17	3.23	130.09	123.47
16	B	803	CLA	CHC-C1C-C2C	-3.23	117.79	126.72
16	4	411	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
16	A	811	CLA	CMC-C2C-C1C	3.23	129.95	125.04
16	A	817	CLA	C3B-C4B-NB	3.23	113.38	109.21
19	B	844	BCR	C37-C22-C23	3.23	123.16	118.08
16	A	835	CLA	CHC-C1C-C2C	-3.22	117.80	126.72
16	1	513	CLA	CAC-C3C-C4C	3.22	128.99	124.81
16	B	838	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
16	B	823	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
16	A	842	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
16	1	512	CLA	CED-O2D-CGD	3.22	123.22	115.94
19	A	849	BCR	C16-C15-C14	3.22	130.07	123.47
16	A	821	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
16	B	810	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
16	B	818	CLA	CAC-C3C-C4C	3.22	128.99	124.81
16	5	406	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
19	A	847	BCR	C15-C16-C17	3.22	130.06	123.47
16	5	416	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
16	J	101	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
16	B	828	CLA	C1D-CHD-C4C	-3.21	119.13	126.06
19	F	202	BCR	C37-C22-C23	3.21	123.14	118.08
16	A	807	CLA	CHD-C4C-NC	3.21	129.26	124.20
16	B	807	CLA	C3B-C4B-NB	3.21	113.36	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	808	CLA	O2A-CGA-CBA	3.21	121.97	111.91
16	B	841	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
16	B	832	CLA	C1C-C2C-C3C	-3.21	103.59	106.96
16	6	402	CLA	CHC-C1C-C2C	-3.21	117.86	126.72
21	B	851	LMT	O1B-C4'-C3'	3.20	115.81	107.28
16	5	416	CLA	C3B-C4B-NB	3.20	113.35	109.21
16	A	819	CLA	CMC-C2C-C1C	3.20	129.92	125.04
16	A	810	CLA	CED-O2D-CGD	3.20	123.18	115.94
16	B	832	CLA	CMC-C2C-C1C	3.20	129.92	125.04
19	B	843	BCR	C34-C9-C8	3.20	123.12	118.08
16	B	808	CLA	CAA-C2A-C3A	-3.20	104.01	112.78
16	B	829	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
16	A	829	CLA	C1C-C2C-C3C	-3.20	103.60	106.96
16	B	839	CLA	C3B-C4B-NB	3.20	113.34	109.21
16	B	821	CLA	C4A-NA-C1A	-3.19	105.27	106.71
16	A	823	CLA	O2A-CGA-CBA	3.19	121.93	111.91
16	A	813	CLA	CMC-C2C-C1C	3.19	129.90	125.04
16	5	410	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
16	A	843	CLA	CBC-CAC-C3C	-3.19	103.63	112.43
16	A	803	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
19	I	101	BCR	C34-C9-C10	-3.19	118.45	122.92
16	A	823	CLA	CMC-C2C-C1C	3.19	129.90	125.04
16	1	503	CLA	C3B-C4B-NB	3.19	113.33	109.21
16	1	515	CLA	C1C-C2C-C3C	-3.19	103.61	106.96
16	1	509	CLA	CAC-C3C-C4C	3.19	128.94	124.81
16	F	204	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
16	B	841	CLA	C3B-C4B-NB	3.18	113.33	109.21
16	B	801	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
16	4	409	CLA	C3B-C4B-NB	3.18	113.33	109.21
16	A	824	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
16	A	827	CLA	CHD-C4C-NC	3.18	129.21	124.20
16	A	809	CLA	C4A-NA-C1A	-3.18	105.28	106.71
16	B	804	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
16	B	818	CLA	CHC-C1C-C2C	-3.18	117.94	126.72
19	J	103	BCR	C37-C22-C23	3.17	123.08	118.08
15	A	801	CL0	CHC-C1C-C2C	-3.17	117.94	126.72
19	J	103	BCR	C34-C9-C10	-3.17	118.48	122.92
19	5	402	BCR	C15-C16-C17	3.17	129.97	123.47
16	1	510	CLA	C3B-C4B-NB	3.17	113.31	109.21
16	6	403	CLA	CMC-C2C-C1C	3.17	129.87	125.04
19	A	846	BCR	C36-C18-C17	-3.17	118.48	122.92
16	5	413	CLA	C1D-CHD-C4C	-3.17	119.22	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	503	CLA	C1C-C2C-C3C	-3.17	103.63	106.96
16	5	410	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
16	A	803	CLA	CHB-C4A-NA	3.16	128.88	124.51
16	6	407	CLA	CMC-C2C-C1C	3.16	129.85	125.04
16	A	820	CLA	CHC-C1C-C2C	-3.16	117.99	126.72
16	B	803	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
19	F	202	BCR	C15-C16-C17	3.16	129.94	123.47
16	1	514	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
16	A	809	CLA	C1-C2-C3	-3.15	120.59	126.04
16	B	816	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
16	5	404	CLA	CAC-C3C-C4C	3.15	128.90	124.81
16	A	839	CLA	C3B-C4B-NB	3.15	113.28	109.21
16	5	414	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
16	A	842	CLA	C1C-C2C-C3C	-3.15	103.65	106.96
16	5	404	CLA	CED-O2D-CGD	3.15	123.05	115.94
16	B	825	CLA	O1D-CGD-CBD	-3.15	118.05	124.48
16	B	833	CLA	CMC-C2C-C1C	3.14	129.83	125.04
16	A	841	CLA	CAC-C3C-C4C	3.14	128.89	124.81
16	B	834	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
16	6	403	CLA	C3B-C4B-NB	3.14	113.27	109.21
16	6	405	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
16	2	406	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
16	A	843	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
16	A	810	CLA	CHD-C4C-NC	3.14	129.15	124.20
16	A	840	CLA	CMC-C2C-C1C	3.14	129.82	125.04
16	B	822	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
16	1	526	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
15	A	801	CL0	C4C-C3C-C2C	-3.14	102.33	106.90
16	5	410	CLA	C3B-C4B-NB	3.14	113.26	109.21
16	5	421	CLA	CHC-C1C-C2C	-3.13	118.05	126.72
16	1	503	CLA	CHC-C1C-C2C	-3.13	118.05	126.72
16	A	837	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
16	B	835	CLA	CAC-C3C-C4C	3.13	128.88	124.81
16	2	402	CLA	CHC-C1C-C2C	-3.13	118.05	126.72
16	2	405	CLA	CHC-C1C-C2C	-3.13	118.06	126.72
16	6	406	CLA	CHC-C1C-C2C	-3.13	118.06	126.72
16	A	832	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
19	B	845	BCR	C15-C16-C17	3.13	129.89	123.47
16	1	505	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
16	A	841	CLA	O2D-CGD-CBD	3.13	116.83	111.27
16	6	408	CLA	CMC-C2C-C1C	3.13	129.80	125.04
16	X	101	CLA	C1D-CHD-C4C	-3.13	119.31	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	847	BCR	C37-C22-C23	3.12	123.00	118.08
16	A	827	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
19	B	846	BCR	C34-C9-C10	-3.12	118.55	122.92
16	X	101	CLA	CAC-C3C-C4C	3.12	128.86	124.81
16	5	410	CLA	CED-O2D-CGD	3.12	123.00	115.94
16	1	521	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
16	A	806	CLA	C3C-C4C-NC	3.12	114.07	110.57
16	B	819	CLA	C3C-C4C-NC	3.12	114.07	110.57
16	A	806	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
16	A	834	CLA	CED-O2D-CGD	3.12	122.99	115.94
16	5	418	CLA	CHC-C1C-C2C	-3.12	118.10	126.72
16	1	508	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
16	5	414	CLA	CMC-C2C-C1C	3.12	129.78	125.04
16	A	838	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
16	B	814	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
16	B	820	CLA	CAC-C3C-C4C	3.11	128.85	124.81
16	3	401	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
16	A	812	CLA	C1-O2A-CGA	3.11	124.60	116.44
16	2	403	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
19	1	518	BCR	C34-C9-C10	-3.11	118.57	122.92
19	4	401	BCR	C37-C22-C23	3.11	122.97	118.08
19	1	518	BCR	C15-C16-C17	3.11	129.84	123.47
16	4	408	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
16	A	824	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
16	4	406	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
16	A	805	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
16	5	416	CLA	CAC-C3C-C4C	3.10	128.83	124.81
16	A	831	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
16	1	519	CLA	CHD-C4C-NC	3.10	129.09	124.20
16	1	513	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
16	1	514	CLA	C3B-C4B-NB	3.10	113.21	109.21
16	A	842	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
19	1	516	BCR	C1-C6-C5	-3.09	118.25	122.61
17	A	844	PQN	C2M-C2-C3	-3.09	119.35	124.40
16	1	504	CLA	C2A-C1A-CHA	-3.09	118.45	123.86
16	6	409	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
16	B	830	CLA	CED-O2D-CGD	3.09	122.93	115.94
16	6	402	CLA	C3B-C4B-NB	3.09	113.21	109.21
16	B	815	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
16	A	837	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
19	K	102	BCR	C34-C9-C10	-3.09	118.60	122.92
16	B	830	CLA	CHC-C1C-C2C	-3.09	118.19	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	507	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
16	B	815	CLA	CMC-C2C-C1C	3.08	129.73	125.04
16	A	808	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
16	6	409	CLA	CMC-C2C-C1C	3.08	129.73	125.04
16	B	811	CLA	C3B-C4B-NB	3.08	113.19	109.21
16	1	512	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
16	A	812	CLA	C2A-C1A-CHA	-3.07	118.49	123.86
16	B	819	CLA	CHD-C4C-NC	3.07	129.04	124.20
16	A	843	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
16	B	818	CLA	O2A-CGA-CBA	3.07	121.54	111.91
16	4	403	CLA	CAC-C3C-C4C	3.07	128.79	124.81
16	5	409	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
16	A	810	CLA	CAC-C3C-C4C	3.06	128.79	124.81
16	A	843	CLA	O2A-CGA-CBA	3.06	121.52	111.91
16	K	103	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
16	B	816	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
16	4	402	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
19	A	849	BCR	C35-C13-C14	-3.06	118.64	122.92
16	B	820	CLA	O2A-CGA-CBA	3.06	121.50	111.91
16	B	808	CLA	O1D-CGD-CBD	-3.06	118.23	124.48
16	A	820	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
16	A	842	CLA	C3B-C4B-NB	3.06	113.16	109.21
16	B	804	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
16	A	808	CLA	CED-O2D-CGD	3.05	122.84	115.94
16	6	408	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
16	K	101	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
16	A	827	CLA	C2C-C1C-NC	3.05	112.83	109.97
16	A	816	CLA	CAC-C3C-C4C	3.05	128.76	124.81
16	K	103	CLA	CMC-C2C-C1C	3.05	129.68	125.04
16	B	831	CLA	CHC-C1C-C2C	-3.05	118.30	126.72
16	A	822	CLA	CHD-C4C-NC	3.04	129.00	124.20
16	A	839	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
16	2	401	CLA	CAC-C3C-C4C	3.04	128.76	124.81
16	4	402	CLA	C3B-C4B-NB	3.04	113.14	109.21
16	B	826	CLA	CHD-C4C-NC	3.04	128.99	124.20
16	B	825	CLA	C4A-NA-C1A	-3.04	105.34	106.71
21	5	401	LMT	O1B-C4'-C3'	3.04	115.36	107.28
16	5	422	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
16	4	404	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
16	A	821	CLA	C1-C2-C3	-3.03	121.84	126.75
16	B	803	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
16	5	415	CLA	CHC-C1C-C2C	-3.03	118.33	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	406	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
16	5	408	CLA	CMC-C2C-C1C	3.03	129.66	125.04
16	6	401	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
16	A	823	CLA	CAC-C3C-C4C	3.03	128.74	124.81
19	B	846	BCR	C36-C18-C17	-3.03	118.68	122.92
16	X	101	CLA	CMC-C2C-C1C	3.03	129.65	125.04
16	B	818	CLA	C4-C3-C2	-3.03	115.91	123.68
16	5	404	CLA	C3C-C4C-NC	3.03	113.97	110.57
16	5	405	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
16	A	843	CLA	C3C-C4C-NC	3.02	113.96	110.57
16	A	808	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
19	1	523	BCR	C15-C16-C17	3.02	129.66	123.47
16	1	502	CLA	C3B-C4B-NB	3.02	113.12	109.21
16	B	828	CLA	CBA-CAA-C2A	3.02	122.78	113.86
16	4	402	CLA	CMC-C2C-C1C	3.02	129.64	125.04
16	B	838	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
16	A	833	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
16	B	840	CLA	CMC-C2C-C1C	3.02	129.64	125.04
16	5	403	CLA	C3B-C4B-NB	3.02	113.11	109.21
19	1	518	BCR	C35-C13-C14	-3.02	118.69	122.92
16	B	828	CLA	O2D-CGD-CBD	3.02	116.63	111.27
16	6	401	CLA	CMC-C2C-C1C	3.02	129.63	125.04
19	B	848	BCR	C15-C16-C17	3.02	129.65	123.47
16	A	817	CLA	CMC-C2C-C1C	3.02	129.63	125.04
16	A	836	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
16	4	404	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
16	A	816	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
16	5	419	CLA	CED-O2D-CGD	3.01	122.75	115.94
16	4	404	CLA	C3B-C4B-NB	3.01	113.10	109.21
16	A	824	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
16	2	405	CLA	CED-O2D-CGD	3.01	122.75	115.94
16	A	838	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
16	B	822	CLA	CMC-C2C-C1C	3.01	129.62	125.04
16	B	808	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
16	A	842	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
16	B	821	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
16	B	841	CLA	CMC-C2C-C1C	3.01	129.62	125.04
16	A	825	CLA	C1D-CHD-C4C	-3.01	119.57	126.06
16	2	403	CLA	C3B-C4B-NB	3.01	113.10	109.21
16	B	804	CLA	C3B-C4B-NB	3.01	113.10	109.21
19	F	205	BCR	C35-C13-C14	-3.01	118.71	122.92
16	B	838	CLA	CHC-C1C-C2C	-3.01	118.41	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	405	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
19	M	102	BCR	C34-C9-C8	3.00	122.81	118.08
16	A	836	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
16	1	509	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
16	B	829	CLA	C5-C3-C2	-3.00	115.04	121.12
16	1	504	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
19	K	102	BCR	C36-C18-C17	-3.00	118.72	122.92
16	A	822	CLA	CAC-C3C-C4C	3.00	128.70	124.81
16	B	805	CLA	CHB-C4A-NA	3.00	128.66	124.51
16	A	829	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
16	B	807	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
19	4	401	BCR	C34-C9-C8	3.00	122.80	118.08
16	J	101	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
16	A	839	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
19	B	843	BCR	C37-C22-C23	2.99	122.79	118.08
16	2	406	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
16	B	832	CLA	CHD-C4C-NC	2.99	128.92	124.20
16	B	810	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
19	A	847	BCR	C36-C18-C17	-2.99	118.73	122.92
16	B	832	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
16	5	418	CLA	C3B-C4B-NB	2.99	113.08	109.21
16	A	821	CLA	CMC-C2C-C1C	2.99	129.59	125.04
16	5	405	CLA	C3B-C4B-NB	2.99	113.07	109.21
16	A	836	CLA	C4-C3-C5	2.99	119.40	115.98
16	A	813	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
16	B	834	CLA	CHB-C4A-NA	2.98	128.64	124.51
16	1	515	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
16	A	822	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
16	5	411	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
16	1	501	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
16	5	406	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
16	5	413	CLA	C3C-C4C-NC	2.98	113.92	110.57
16	F	204	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
16	B	801	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
19	5	402	BCR	C36-C18-C17	-2.98	118.75	122.92
16	5	408	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
16	5	419	CLA	C3B-C4B-NB	2.98	113.06	109.21
16	6	407	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
16	5	416	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
16	B	835	CLA	CHD-C4C-NC	2.98	128.90	124.20
16	A	816	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
19	I	102	BCR	C37-C22-C23	2.98	122.77	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	512	CLA	O1D-CGD-CBD	-2.98	118.40	124.48
16	5	413	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
16	A	836	CLA	C3B-C4B-NB	2.97	113.06	109.21
16	1	503	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
16	5	408	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
16	X	101	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
16	1	506	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
16	5	405	CLA	CMC-C2C-C1C	2.97	129.56	125.04
16	A	843	CLA	C3B-C4B-NB	2.97	113.05	109.21
16	3	401	CLA	C3B-C4B-NB	2.97	113.05	109.21
16	5	406	CLA	C3B-C4B-NB	2.97	113.05	109.21
16	5	411	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
16	6	404	CLA	CED-O2D-CGD	2.97	122.65	115.94
16	5	422	CLA	CMC-C2C-C1C	2.97	129.56	125.04
16	K	101	CLA	C2A-C1A-CHA	-2.97	118.67	123.86
16	A	841	CLA	C3B-C4B-NB	2.96	113.04	109.21
16	F	204	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
16	B	811	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
16	A	825	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
16	1	512	CLA	CMC-C2C-C1C	2.96	129.55	125.04
19	F	202	BCR	C34-C9-C8	2.96	122.75	118.08
19	A	848	BCR	C16-C15-C14	2.96	129.54	123.47
16	B	815	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
19	1	517	BCR	C35-C13-C14	-2.96	118.77	122.92
16	B	832	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
16	5	415	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
19	F	205	BCR	C34-C9-C10	-2.96	118.78	122.92
16	1	526	CLA	C3B-C4B-NB	2.96	113.04	109.21
19	M	102	BCR	C34-C9-C10	-2.96	118.78	122.92
16	2	402	CLA	C3B-C4B-NB	2.96	113.03	109.21
16	5	418	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
16	B	836	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
16	4	403	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
16	A	805	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
16	2	405	CLA	C3B-C4B-NB	2.96	113.03	109.21
16	4	403	CLA	CMC-C2C-C1C	2.95	129.54	125.04
16	A	814	CLA	O2A-CGA-CBA	2.95	121.18	111.91
16	4	405	CLA	CMB-C2B-C3B	2.95	130.21	124.68
17	A	844	PQN	C2M-C2-C1	2.95	121.17	116.27
16	2	401	CLA	C3B-C4B-NB	2.95	113.03	109.21
19	1	522	BCR	C16-C15-C14	2.95	129.52	123.47
19	4	401	BCR	C34-C9-C10	-2.95	118.79	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	809	CLA	CHD-C4C-NC	2.95	128.85	124.20
16	B	839	CLA	CBC-CAC-C3C	-2.95	104.30	112.43
19	5	402	BCR	C37-C22-C23	2.95	122.72	118.08
19	B	853	BCR	C16-C15-C14	2.95	129.51	123.47
16	B	828	CLA	CAC-C3C-C4C	2.95	128.63	124.81
16	6	405	CLA	C3B-C4B-NB	2.95	113.02	109.21
16	B	815	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
16	B	808	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
16	B	805	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
16	B	817	CLA	CMC-C2C-C1C	2.94	129.52	125.04
16	A	809	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
16	1	509	CLA	CMC-C2C-C1C	2.94	129.52	125.04
16	5	419	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
16	5	411	CLA	CMC-C2C-C1C	2.94	129.52	125.04
16	4	404	CLA	CMC-C2C-C1C	2.94	129.51	125.04
16	5	405	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
16	1	501	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
16	A	802	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
16	5	421	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
16	2	406	CLA	C3B-C4B-NB	2.94	113.00	109.21
16	1	514	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
16	1	505	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
16	5	421	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
16	6	404	CLA	C3B-C4B-NB	2.93	113.00	109.21
16	6	405	CLA	CED-O2D-CGD	2.93	122.57	115.94
19	B	847	BCR	C34-C9-C10	-2.93	118.81	122.92
16	3	401	CLA	CMC-C2C-C1C	2.93	129.50	125.04
16	A	841	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
16	X	101	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
16	5	415	CLA	CMC-C2C-C1C	2.93	129.50	125.04
16	6	405	CLA	CMC-C2C-C1C	2.93	129.50	125.04
16	2	403	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
16	A	841	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
16	A	832	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
16	5	413	CLA	CMC-C2C-C1C	2.93	129.50	125.04
16	A	805	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
16	B	822	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
16	B	829	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
16	5	407	CLA	CAC-C3C-C4C	2.92	128.60	124.81
16	1	515	CLA	CED-O2D-CGD	2.92	122.55	115.94
16	B	811	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
16	1	525	CLA	C2A-C1A-CHA	-2.92	118.75	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	525	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
16	5	422	CLA	C3B-C4B-NB	2.92	112.99	109.21
16	4	403	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
21	B	852	LMT	O1B-C4'-C3'	2.92	115.05	107.28
16	A	806	CLA	CHB-C4A-NA	2.92	128.55	124.51
16	A	806	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
16	6	401	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
16	B	839	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
16	B	840	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
16	A	804	CLA	C3B-C4B-NB	2.92	112.98	109.21
16	B	828	CLA	CED-O2D-CGD	2.92	122.54	115.94
16	4	405	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	F	205	BCR	C16-C15-C14	2.92	129.45	123.47
16	4	403	CLA	CED-O2D-CGD	2.92	122.53	115.94
16	B	812	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
16	1	515	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
16	B	805	CLA	O2A-CGA-CBA	2.91	121.05	111.91
16	A	815	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
16	A	803	CLA	C11-C10-C8	-2.91	106.51	115.92
16	A	825	CLA	O2A-CGA-CBA	2.91	121.04	111.91
16	5	417	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
16	B	825	CLA	CMB-C2B-C3B	2.91	130.12	124.68
16	2	402	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
19	K	102	BCR	C23-C22-C21	2.91	123.40	118.94
16	6	408	CLA	C3B-C4B-NB	2.91	112.97	109.21
16	A	830	CLA	CAC-C3C-C4C	2.91	128.58	124.81
16	B	812	CLA	C3B-C4B-NB	2.91	112.97	109.21
16	6	406	CLA	C3B-C4B-NB	2.90	112.97	109.21
16	B	827	CLA	CMB-C2B-C3B	2.90	130.11	124.68
16	A	840	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
16	4	407	CLA	C3B-C4B-NB	2.90	112.96	109.21
16	A	838	CLA	C2A-C1A-CHA	-2.90	118.78	123.86
16	1	513	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
16	1	526	CLA	CMC-C2C-C1C	2.90	129.46	125.04
16	6	406	CLA	CMC-C2C-C1C	2.90	129.46	125.04
16	A	816	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
16	A	832	CLA	CMC-C2C-C1C	2.90	129.45	125.04
16	2	405	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
16	6	401	CLA	C3B-C4B-NB	2.90	112.95	109.21
16	B	829	CLA	C2A-C1A-CHA	-2.90	118.79	123.86
16	A	824	CLA	C2A-C1A-CHA	-2.90	118.80	123.86
16	5	407	CLA	C4C-C3C-C2C	-2.89	102.68	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	849	BCR	C15-C16-C17	2.89	129.40	123.47
16	A	815	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
16	4	410	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
16	A	834	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
16	4	406	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
16	1	501	CLA	CED-O2D-CGD	2.89	122.48	115.94
19	1	518	BCR	C12-C13-C14	2.89	123.38	118.94
16	1	513	CLA	C3B-C4B-NB	2.89	112.95	109.21
16	A	812	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
16	4	409	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
16	B	806	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
16	5	422	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
19	A	846	BCR	C16-C15-C14	2.89	129.39	123.47
19	A	851	BCR	C36-C18-C17	-2.88	118.88	122.92
16	5	421	CLA	C3B-C4B-NB	2.88	112.94	109.21
16	B	820	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
16	5	403	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
16	A	824	CLA	CMC-C2C-C1C	2.88	129.42	125.04
16	4	408	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
16	6	402	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
16	6	408	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
16	A	803	CLA	C1C-C2C-C3C	-2.87	103.93	106.96
16	B	835	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
16	1	502	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
16	A	818	CLA	C1-O2A-CGA	2.87	123.98	116.44
16	6	406	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
16	B	836	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
16	5	409	CLA	C3B-C4B-NB	2.87	112.92	109.21
16	A	838	CLA	O2A-CGA-CBA	2.87	120.91	111.91
16	A	812	CLA	CHD-C4C-NC	2.87	128.72	124.20
15	A	801	CL0	CMA-C3A-C4A	-2.87	104.06	111.77
16	4	403	CLA	C3B-C4B-NB	2.87	112.92	109.21
16	B	829	CLA	CAC-C3C-C4C	2.87	128.53	124.81
16	1	511	CLA	C4-C3-C5	2.87	119.26	115.98
16	A	802	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
16	6	407	CLA	C3B-C4B-NB	2.87	112.92	109.21
16	B	807	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
16	A	833	CLA	C2A-C1A-CHA	-2.87	118.85	123.86
16	2	404	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
19	5	402	BCR	C16-C15-C14	2.86	129.34	123.47
16	J	101	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
16	B	823	CLA	CMC-C2C-C1C	2.86	129.40	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	809	CLA	CMB-C2B-C3B	2.86	130.03	124.68
16	A	823	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
16	6	404	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
16	6	409	CLA	C3B-C4B-NB	2.86	112.91	109.21
16	B	835	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
16	B	840	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
19	1	517	BCR	C15-C16-C17	2.86	129.33	123.47
16	A	835	CLA	O1D-CGD-CBD	-2.86	118.64	124.48
16	1	515	CLA	C3B-C4B-NB	2.86	112.90	109.21
16	B	839	CLA	CMC-C2C-C1C	2.86	129.39	125.04
16	4	409	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
16	X	101	CLA	C3B-C4B-NB	2.85	112.90	109.21
16	1	506	CLA	C3B-C4B-NB	2.85	112.90	109.21
16	A	810	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
16	1	525	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
16	5	407	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
16	A	832	CLA	CMB-C2B-C1B	2.85	132.84	128.46
16	A	804	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
16	2	402	CLA	CMC-C2C-C1C	2.85	129.38	125.04
16	B	838	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
16	1	501	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
16	1	509	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
16	B	829	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
16	F	201	CLA	C1-O2A-CGA	2.85	123.92	116.44
16	B	830	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
16	A	806	CLA	CHD-C4C-NC	2.85	128.69	124.20
16	B	825	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
16	B	820	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
16	6	405	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
16	B	815	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
16	4	411	CLA	C3B-C4B-NB	2.84	112.89	109.21
16	A	823	CLA	CHD-C4C-NC	2.84	128.68	124.20
19	1	518	BCR	C36-C18-C17	-2.84	118.94	122.92
16	A	827	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
16	4	407	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
16	1	514	CLA	CMC-C2C-C1C	2.84	129.37	125.04
16	B	838	CLA	C3B-C4B-NB	2.84	112.88	109.21
16	2	404	CLA	C3B-C4B-NB	2.84	112.88	109.21
16	B	830	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
16	1	501	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	F	205	BCR	C15-C16-C17	2.84	129.29	123.47
16	5	415	CLA	C2A-C1A-CHA	-2.84	118.90	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	401	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
16	B	831	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
16	1	506	CLA	C2A-C1A-CHA	-2.84	118.90	123.86
16	4	408	CLA	C2A-C1A-CHA	-2.84	118.90	123.86
16	2	405	CLA	CMC-C2C-C1C	2.84	129.36	125.04
16	B	834	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
16	5	411	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
16	A	823	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
16	6	409	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
16	B	819	CLA	CMB-C2B-C3B	2.83	129.98	124.68
16	5	412	CLA	C3B-C4B-NB	2.83	112.87	109.21
16	B	837	CLA	CHD-C4C-NC	2.83	128.66	124.20
16	B	826	CLA	CAC-C3C-C4C	2.83	128.48	124.81
16	5	412	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
16	A	834	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
15	A	801	CL0	CMB-C2B-C3B	2.82	129.95	124.68
16	K	101	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
16	1	512	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
16	B	825	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
16	A	822	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
16	B	831	CLA	CED-O2D-CGD	2.82	122.31	115.94
19	M	102	BCR	C15-C16-C17	2.81	129.24	123.47
19	A	848	BCR	C34-C9-C10	-2.81	118.98	122.92
16	B	814	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
16	A	831	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
16	1	506	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
16	1	508	CLA	C3B-C4B-NB	2.81	112.84	109.21
16	B	831	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
16	1	520	CLA	CHD-C4C-NC	2.81	128.63	124.20
16	5	409	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
16	5	413	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
16	6	407	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
19	A	849	BCR	C36-C18-C17	-2.81	118.99	122.92
16	1	510	CLA	CED-O2D-CGD	2.81	122.29	115.94
16	A	804	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
16	6	408	CLA	C2A-C1A-CHA	-2.81	118.95	123.85
16	5	412	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
16	5	415	CLA	C3B-C4B-NB	2.81	112.84	109.21
16	A	804	CLA	CHB-C4A-NA	2.81	128.39	124.51
19	1	522	BCR	C34-C9-C10	-2.81	118.99	122.92
16	A	802	CLA	C3B-C4B-NB	2.81	112.84	109.21
16	B	802	CLA	C3B-C4B-NB	2.81	112.84	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	514	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
16	A	826	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
16	A	820	CLA	CMC-C2C-C1C	2.80	129.31	125.04
16	1	505	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
16	2	401	CLA	CHD-C4C-NC	2.80	128.62	124.20
16	5	414	CLA	C3B-C4B-NB	2.80	112.83	109.21
16	A	817	CLA	CBC-CAC-C3C	-2.80	104.72	112.43
16	B	833	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
16	1	503	CLA	C4-C3-C5	2.80	119.18	115.98
16	B	809	CLA	CAC-C3C-C4C	2.80	128.44	124.81
16	A	819	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
16	A	838	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
16	A	827	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
16	4	410	CLA	C3B-C4B-NB	2.79	112.82	109.21
16	A	821	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
16	A	812	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
16	A	804	CLA	CHD-C4C-NC	2.79	128.60	124.20
16	B	831	CLA	O2A-CGA-CBA	2.79	120.66	111.91
16	1	526	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
16	A	815	CLA	CBC-CAC-C3C	-2.79	104.75	112.43
16	K	103	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
16	A	833	CLA	CAC-C3C-C4C	2.79	128.43	124.81
16	B	834	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
16	2	404	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
16	A	821	CLA	O2A-CGA-CBA	2.79	120.65	111.91
16	A	835	CLA	C2A-C1A-CHA	-2.79	118.99	123.86
16	1	510	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
16	B	838	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
16	1	525	CLA	C3B-C4B-NB	2.78	112.81	109.21
16	4	411	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
16	4	402	CLA	CHD-C4C-NC	2.78	128.59	124.20
16	A	803	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
16	B	804	CLA	C4-C3-C5	2.78	119.95	115.27
16	B	810	CLA	C3B-C4B-NB	2.78	112.80	109.21
16	B	828	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
16	5	406	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
19	1	517	BCR	C12-C13-C14	2.78	123.20	118.94
16	B	816	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
16	4	407	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
19	J	103	BCR	C16-C15-C14	2.78	129.16	123.47
19	1	517	BCR	C36-C18-C17	-2.78	119.03	122.92
16	2	406	CLA	CMC-C2C-C1C	2.78	129.27	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	102	BCR	C16-C15-C14	2.78	129.16	123.47
19	M	102	BCR	C36-C18-C17	-2.77	119.04	122.92
16	5	419	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
16	F	201	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
16	A	833	CLA	CHD-C4C-NC	2.77	128.57	124.20
16	A	817	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
16	2	401	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
16	1	520	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
16	1	520	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
19	B	846	BCR	C15-C16-C17	2.77	129.15	123.47
16	4	408	CLA	C3B-C4B-NB	2.77	112.79	109.21
19	B	845	BCR	C35-C13-C14	-2.77	119.04	122.92
16	1	521	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
16	A	812	CLA	C3B-C4B-NB	2.77	112.79	109.21
19	B	847	BCR	C36-C18-C17	-2.77	119.04	122.92
16	B	806	CLA	CHD-C4C-NC	2.77	128.57	124.20
19	4	401	BCR	C35-C13-C14	-2.77	119.04	122.92
16	B	834	CLA	C4-C3-C2	-2.77	116.58	123.68
16	A	832	CLA	CAC-C3C-C4C	2.77	128.40	124.81
16	A	836	CLA	O2A-CGA-CBA	2.77	120.59	111.91
16	1	510	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
16	A	824	CLA	C3B-C4B-NB	2.77	112.78	109.21
16	B	841	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
16	B	834	CLA	CMA-C3A-C4A	-2.76	104.34	111.77
16	1	511	CLA	C1-O2A-CGA	2.76	123.68	116.44
16	B	819	CLA	C4-C3-C5	2.76	119.91	115.27
19	B	848	BCR	C34-C9-C8	2.76	122.42	118.08
16	A	822	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
16	A	825	CLA	CED-O2D-CGD	2.76	122.17	115.94
16	A	803	CLA	C3B-C4B-NB	2.76	112.77	109.21
16	A	823	CLA	C3B-C4B-NB	2.76	112.77	109.21
16	6	404	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
16	B	801	CLA	CHB-C4A-NA	2.75	128.32	124.51
16	A	811	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
19	J	104	BCR	C37-C22-C23	2.75	122.41	118.08
19	B	845	BCR	C37-C22-C23	2.75	122.41	118.08
16	B	830	CLA	CMC-C2C-C1C	2.75	129.23	125.04
16	A	835	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
16	B	801	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
16	1	512	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
16	A	841	CLA	C4A-NA-C1A	-2.75	105.47	106.71
16	A	823	CLA	C2A-C1A-CHA	-2.75	119.06	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	841	CLA	CHD-C4C-NC	2.75	128.53	124.20
16	5	410	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
16	F	204	CLA	CHD-C4C-NC	2.74	128.53	124.20
16	2	406	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
16	B	810	CLA	CED-O2D-CGD	2.74	122.14	115.94
16	B	818	CLA	CHD-C4C-NC	2.74	128.52	124.20
19	I	101	BCR	C34-C9-C8	2.74	122.39	118.08
16	A	813	CLA	OBD-CAD-C3D	-2.74	121.94	128.52
19	1	518	BCR	C34-C9-C8	2.73	122.39	118.08
16	B	807	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
16	X	101	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
16	B	825	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
16	5	405	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
16	5	403	CLA	CHD-C4C-NC	2.73	128.51	124.20
16	1	502	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
16	A	840	CLA	C4-C3-C5	2.73	119.86	115.27
16	5	406	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
19	F	205	BCR	C37-C22-C23	2.73	122.38	118.08
16	A	803	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
16	B	820	CLA	O1D-CGD-CBD	-2.73	118.91	124.48
16	A	830	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
16	A	829	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
19	A	847	BCR	C34-C9-C10	-2.72	119.11	122.92
16	A	806	CLA	C4-C3-C5	2.72	119.85	115.27
16	B	812	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
16	B	829	CLA	CBC-CAC-C3C	-2.72	104.92	112.43
16	A	820	CLA	C1-O2A-CGA	2.72	123.59	116.44
16	B	839	CLA	O2A-CGA-CBA	2.72	120.45	111.91
16	A	808	CLA	CHD-C4C-NC	2.72	128.49	124.20
16	B	810	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
16	F	201	CLA	O2A-CGA-CBA	2.72	120.45	111.91
16	B	840	CLA	CED-O2D-CGD	2.72	122.09	115.94
16	B	809	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
16	A	816	CLA	CHD-C4C-NC	2.72	128.49	124.20
16	B	820	CLA	CHD-C4C-NC	2.72	128.49	124.20
19	5	420	BCR	C34-C9-C10	-2.72	119.11	122.92
16	B	836	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
16	A	807	CLA	C3B-C4B-NB	2.72	112.72	109.21
16	A	809	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
16	B	833	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
19	A	851	BCR	C19-C18-C17	2.71	123.10	118.94
16	A	802	CLA	C1B-CHB-C4A	-2.71	124.74	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	102	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
16	5	418	CLA	CMC-C2C-C1C	2.71	129.17	125.04
16	A	814	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
16	B	812	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
16	A	802	CLA	CAA-C2A-C3A	-2.71	105.37	112.78
16	B	812	CLA	CHC-C1C-C2C	-2.71	119.24	126.72
16	4	408	CLA	CED-O2D-CGD	2.70	122.05	115.94
16	4	410	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
19	A	851	BCR	C37-C22-C23	2.70	122.33	118.08
16	B	814	CLA	CMB-C2B-C3B	2.70	129.73	124.68
16	B	816	CLA	CBA-CAA-C2A	2.70	121.84	113.86
16	B	817	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
16	4	405	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
16	A	841	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
16	4	408	CLA	CMC-C2C-C1C	2.70	129.15	125.04
16	1	519	CLA	CHC-C1C-C2C	-2.70	119.27	126.72
16	A	828	CLA	CHD-C4C-NC	2.69	128.45	124.20
19	B	843	BCR	C36-C18-C17	-2.69	119.15	122.92
16	6	403	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
16	4	411	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
16	5	416	CLA	C2A-C1A-CHA	-2.69	119.15	123.85
16	2	402	CLA	CED-O2D-CGD	2.69	122.03	115.94
16	B	828	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
16	A	803	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
16	B	827	CLA	CHD-C4C-NC	2.69	128.44	124.20
16	A	839	CLA	C1-O2A-CGA	2.69	123.50	116.44
16	A	818	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
16	B	821	CLA	CHD-C4C-NC	2.69	128.44	124.20
16	A	821	CLA	C3B-C4B-NB	2.69	112.68	109.21
16	A	829	CLA	CHD-C4C-NC	2.69	128.44	124.20
16	A	834	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
16	B	809	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
16	1	501	CLA	C3B-C4B-NB	2.68	112.68	109.21
16	A	829	CLA	CMB-C2B-C1B	2.68	132.59	128.46
16	B	814	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
16	1	504	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
16	4	409	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
16	B	802	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
16	A	805	CLA	CMB-C2B-C3B	2.68	129.69	124.68
16	B	824	CLA	C5-C3-C2	-2.68	115.70	121.12
16	J	102	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
19	5	420	BCR	C36-C18-C17	-2.67	119.18	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	831	CLA	C2A-C1A-CHA	-2.67	119.18	123.86
16	1	521	CLA	C5-C3-C2	-2.67	115.71	121.12
16	F	204	CLA	C3B-C4B-NB	2.67	112.66	109.21
16	B	837	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
16	A	811	CLA	C3B-C4B-NB	2.67	112.66	109.21
16	B	813	CLA	O2A-CGA-CBA	2.67	120.28	111.91
16	1	521	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
16	B	818	CLA	C3B-C4B-NB	2.66	112.65	109.21
16	B	820	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
16	B	817	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
16	B	827	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
16	B	838	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	A	801	CL0	CMA-C3A-C2A	-2.66	103.09	113.83
16	B	809	CLA	C1-O2A-CGA	2.66	123.42	116.44
16	5	404	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
16	B	833	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
16	5	417	CLA	C3B-C4B-NB	2.66	112.64	109.21
16	A	833	CLA	CMB-C2B-C3B	2.66	129.65	124.68
16	4	405	CLA	CED-O2D-CGD	2.66	121.94	115.94
16	B	811	CLA	CMC-C2C-C1C	2.66	129.08	125.04
16	F	201	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
16	A	820	CLA	C2A-C1A-CHA	-2.66	119.22	123.86
19	I	101	BCR	C36-C18-C17	-2.66	119.20	122.92
16	A	807	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
16	5	422	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
16	B	834	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
16	1	512	CLA	C3B-C4B-NB	2.65	112.64	109.21
16	B	834	CLA	C3B-C4B-NB	2.65	112.64	109.21
16	A	838	CLA	CHD-C4C-NC	2.65	128.38	124.20
16	B	827	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
16	1	521	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
16	B	822	CLA	CMB-C2B-C3B	2.65	129.63	124.68
19	F	202	BCR	C36-C18-C17	-2.64	119.22	122.92
19	B	844	BCR	C15-C14-C13	2.64	131.08	127.31
21	B	852	LMT	C1'-C2'-C3'	2.64	115.50	110.00
16	B	804	CLA	CMC-C2C-C1C	2.64	129.06	125.04
16	1	502	CLA	CHD-C4C-NC	2.64	128.37	124.20
16	B	827	CLA	CHC-C1C-C2C	-2.64	119.41	126.72
16	B	823	CLA	O2A-CGA-CBA	2.64	120.19	111.91
16	6	407	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
16	B	830	CLA	CMB-C2B-C1B	2.64	132.52	128.46
16	A	808	CLA	O2D-CGD-O1D	-2.64	118.69	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	819	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
16	2	404	CLA	C2A-C1A-CHA	-2.63	119.25	123.86
16	B	821	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
16	A	834	CLA	C1-O2A-CGA	2.63	123.35	116.44
16	B	841	CLA	O2A-CGA-CBA	2.63	120.17	111.91
16	A	816	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
16	A	815	CLA	CMB-C2B-C3B	2.63	129.60	124.68
16	B	837	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
16	A	837	CLA	CMB-C2B-C3B	2.63	129.60	124.68
16	5	419	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
16	4	403	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
16	6	409	CLA	CED-O2D-CGD	2.63	121.88	115.94
16	A	806	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
16	B	832	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
16	A	835	CLA	CED-O2D-CGD	2.63	121.88	115.94
16	A	839	CLA	CHD-C4C-NC	2.63	128.34	124.20
16	A	833	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
16	A	813	CLA	O2A-CGA-CBA	2.63	120.15	111.91
16	B	839	CLA	CMB-C2B-C3B	2.63	129.59	124.68
16	B	812	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
16	B	823	CLA	CHB-C4A-NA	2.63	128.14	124.51
16	B	817	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
19	B	848	BCR	C34-C9-C10	-2.62	119.25	122.92
19	J	103	BCR	C36-C18-C17	-2.62	119.25	122.92
16	A	841	CLA	CHB-C4A-NA	2.62	128.14	124.51
16	1	526	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
16	B	819	CLA	C5-C3-C2	-2.62	115.82	121.12
16	B	819	CLA	CAC-C3C-C4C	2.62	128.21	124.81
16	A	812	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
19	1	516	BCR	C36-C18-C17	-2.62	119.26	122.92
16	A	818	CLA	C2A-C3A-C4A	-2.62	97.64	101.87
16	A	817	CLA	CMB-C2B-C3B	2.62	129.57	124.68
16	5	408	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
16	B	818	CLA	CBC-CAC-C3C	-2.61	105.22	112.43
16	A	805	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
16	5	408	CLA	CMB-C2B-C3B	2.61	129.57	124.68
16	A	838	CLA	C4-C3-C5	2.61	118.97	115.98
16	1	507	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
16	1	521	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
16	A	813	CLA	C3B-C4B-NB	2.61	112.59	109.21
16	A	802	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
16	B	812	CLA	CED-O2D-CGD	2.61	121.84	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	504	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
16	B	814	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
16	B	828	CLA	C3B-C4B-NB	2.61	112.58	109.21
16	4	411	CLA	CHD-C4C-NC	2.61	128.31	124.20
16	A	810	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
16	A	828	CLA	O2A-CGA-CBA	2.61	120.09	111.91
19	1	523	BCR	C37-C22-C23	2.61	122.19	118.08
16	B	826	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	B	844	BCR	C15-C16-C17	2.60	128.81	123.47
16	1	521	CLA	CHD-C4C-NC	2.60	128.31	124.20
19	B	846	BCR	C34-C9-C8	2.60	122.18	118.08
16	B	820	CLA	C3B-C4B-NB	2.60	112.57	109.21
16	5	413	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
16	5	403	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
16	2	401	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
16	B	808	CLA	CHD-C4C-NC	2.60	128.30	124.20
16	A	809	CLA	O1D-CGD-CBD	-2.60	119.17	124.48
16	B	829	CLA	C3B-C4B-NB	2.60	112.57	109.21
16	X	101	CLA	CHB-C4A-NA	2.60	128.10	124.51
16	B	838	CLA	CHD-C4C-NC	2.60	128.29	124.20
16	B	835	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
16	5	403	CLA	C2A-C1A-CHA	-2.59	119.32	123.86
16	A	808	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
16	B	817	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
16	A	837	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
16	4	402	CLA	CAC-C3C-C4C	2.59	128.17	124.81
16	6	406	CLA	CED-O2D-CGD	2.59	121.79	115.94
16	B	808	CLA	C2A-C3A-C4A	-2.59	97.69	101.87
16	5	417	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
16	A	817	CLA	C1-O2A-CGA	2.59	123.23	116.44
16	A	803	CLA	C6-C7-C8	-2.58	107.57	115.92
16	4	402	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
16	A	805	CLA	CHD-C4C-NC	2.58	128.27	124.20
16	A	807	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
16	A	829	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
16	A	836	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
16	B	837	CLA	CMB-C2B-C1B	2.58	132.43	128.46
16	K	101	CLA	C3B-C4B-NB	2.58	112.54	109.21
16	B	807	CLA	CMB-C2B-C1B	2.58	132.43	128.46
16	1	505	CLA	CHD-C4C-NC	2.58	128.26	124.20
16	1	507	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
16	5	414	CLA	O2D-CGD-O1D	-2.58	118.80	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	501	CLA	CHD-C4C-NC	2.58	128.26	124.20
16	A	834	CLA	CHB-C4A-NA	2.58	128.07	124.51
16	4	411	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
16	1	520	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
16	2	406	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
16	B	808	CLA	C3B-C4B-NB	2.57	112.54	109.21
16	A	812	CLA	CAC-C3C-C4C	2.57	128.15	124.81
16	A	835	CLA	C4-C3-C5	2.57	119.59	115.27
16	4	407	CLA	CHD-C4C-NC	2.57	128.25	124.20
16	5	411	CLA	CHD-C4C-NC	2.57	128.25	124.20
16	A	833	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
16	B	819	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
16	5	403	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
16	B	825	CLA	O2A-CGA-CBA	2.57	119.96	111.91
16	A	841	CLA	C4C-C3C-C2C	-2.57	103.16	106.90
16	B	826	CLA	C3B-C4B-NB	2.57	112.53	109.21
19	B	848	BCR	C24-C23-C22	2.57	130.11	126.23
16	B	823	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
16	B	819	CLA	CED-O2D-CGD	2.57	121.74	115.94
16	4	404	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
19	B	848	BCR	C36-C18-C17	-2.56	119.33	122.92
16	B	829	CLA	O2A-CGA-CBA	2.56	119.95	111.91
16	A	834	CLA	C4-C3-C5	2.56	119.58	115.27
16	1	506	CLA	CHD-C4C-NC	2.56	128.24	124.20
16	1	505	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
16	A	818	CLA	C3B-C4B-NB	2.56	112.52	109.21
16	A	843	CLA	CHD-C4C-NC	2.56	128.23	124.20
16	4	403	CLA	CHD-C4C-NC	2.56	128.23	124.20
16	B	820	CLA	CBA-CAA-C2A	2.55	121.40	113.86
16	B	815	CLA	CHD-C4C-NC	2.55	128.23	124.20
16	4	409	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
16	B	829	CLA	CHD-C4C-NC	2.55	128.23	124.20
16	B	805	CLA	CMB-C2B-C3B	2.55	129.45	124.68
16	6	409	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
16	1	508	CLA	CMC-C2C-C1C	2.55	128.93	125.04
19	1	522	BCR	C36-C18-C17	-2.55	119.35	122.92
16	A	826	CLA	CED-O2D-CGD	2.55	121.71	115.94
16	6	404	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
16	A	810	CLA	CMB-C2B-C3B	2.55	129.45	124.68
16	6	401	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
16	A	841	CLA	CMB-C2B-C3B	2.55	129.44	124.68
16	B	801	CLA	CBC-CAC-C3C	-2.55	105.41	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	812	CLA	CHD-C4C-NC	2.55	128.22	124.20
16	B	837	CLA	CED-O2D-CGD	2.55	121.69	115.94
16	A	825	CLA	C3B-C4B-NB	2.54	112.50	109.21
16	1	521	CLA	O2A-CGA-CBA	2.54	119.88	111.91
16	A	804	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
16	B	801	CLA	CMA-C3A-C2A	-2.54	103.59	113.83
16	A	804	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
16	A	807	CLA	O2A-CGA-CBA	2.54	119.87	111.91
16	4	410	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
16	A	828	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
16	4	406	CLA	CHD-C4C-NC	2.53	128.20	124.20
16	B	803	CLA	O2A-CGA-CBA	2.53	119.86	111.91
16	B	821	CLA	CMB-C2B-C3B	2.53	129.42	124.68
16	B	836	CLA	CED-O2D-CGD	2.53	121.66	115.94
16	F	201	CLA	CHD-C4C-NC	2.53	128.19	124.20
16	1	504	CLA	CHD-C4C-NC	2.53	128.19	124.20
16	A	822	CLA	C4-C3-C5	2.53	119.52	115.27
19	I	102	BCR	C16-C15-C14	2.53	128.65	123.47
16	5	417	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
19	5	420	BCR	C11-C10-C9	2.53	130.92	127.31
16	F	204	CLA	CED-O2D-CGD	2.53	121.65	115.94
16	A	803	CLA	CHD-C4C-NC	2.53	128.19	124.20
16	6	404	CLA	CHD-C4C-NC	2.53	128.19	124.20
16	B	812	CLA	O2A-CGA-CBA	2.52	122.14	114.03
16	A	818	CLA	CHC-C1C-C2C	-2.52	119.74	126.72
16	1	519	CLA	CBA-CAA-C2A	2.52	121.31	113.86
19	A	850	BCR	C16-C15-C14	2.52	128.64	123.47
16	A	805	CLA	C4-C3-C5	2.52	119.51	115.27
16	B	810	CLA	CHB-C4A-NA	2.52	128.00	124.51
16	1	505	CLA	C3B-C4B-NB	2.52	112.47	109.21
16	A	802	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
19	I	102	BCR	C15-C14-C13	2.52	130.91	127.31
16	B	808	CLA	CMB-C2B-C1B	2.52	132.34	128.46
16	B	806	CLA	C11-C12-C13	-2.52	107.78	115.92
15	A	801	CL0	C2A-C1A-CHA	-2.52	119.46	123.86
16	A	820	CLA	C1-C2-C3	-2.52	121.69	126.04
16	A	809	CLA	CHD-C4C-NC	2.52	128.17	124.20
16	A	813	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
16	1	502	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
16	1	502	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
16	B	807	CLA	O2A-CGA-CBA	2.52	119.80	111.91
16	1	519	CLA	O2A-CGA-CBA	2.52	119.80	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	401	BCR	C36-C18-C17	-2.51	119.40	122.92
16	B	839	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
16	B	810	CLA	CHD-C4C-NC	2.51	128.16	124.20
16	A	813	CLA	CED-O2D-CGD	2.51	121.62	115.94
16	A	812	CLA	O2A-CGA-CBA	2.51	119.79	111.91
16	A	822	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
16	A	836	CLA	CHD-C4C-NC	2.51	128.16	124.20
16	B	822	CLA	O2A-CGA-CBA	2.51	119.79	111.91
16	B	816	CLA	O2A-CGA-CBA	2.51	119.78	111.91
16	B	813	CLA	CMB-C2B-C1B	2.51	132.32	128.46
16	J	102	CLA	CHD-C4C-NC	2.51	128.16	124.20
16	5	409	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
15	A	801	CL0	C1-O2A-CGA	2.51	123.02	116.44
16	5	417	CLA	CHD-C4C-NC	2.51	128.16	124.20
16	B	814	CLA	CHD-C4C-NC	2.51	128.15	124.20
16	2	401	CLA	C2A-C1A-CHA	-2.51	119.48	123.86
16	A	820	CLA	C3B-C4B-NB	2.51	112.45	109.21
16	1	501	CLA	O2A-CGA-CBA	2.51	122.08	114.03
16	B	824	CLA	CHD-C4C-NC	2.51	128.15	124.20
19	B	847	BCR	C34-C9-C8	2.50	122.02	118.08
16	J	102	CLA	C3B-C4B-NB	2.50	112.45	109.21
16	A	819	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
16	A	823	CLA	O1D-CGD-CBD	-2.50	119.36	124.48
16	B	838	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
16	B	836	CLA	C3B-C4B-NB	2.50	112.44	109.21
16	B	824	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
16	B	827	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
16	A	830	CLA	C3B-C4B-NB	2.50	112.44	109.21
19	A	846	BCR	C15-C16-C17	2.50	128.59	123.47
16	B	805	CLA	C1-O2A-CGA	2.50	122.99	116.44
16	A	834	CLA	CHD-C4C-NC	2.49	128.13	124.20
16	B	840	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
16	B	803	CLA	CHB-C4A-NA	2.49	127.96	124.51
16	5	411	CLA	CED-O2D-CGD	2.49	121.57	115.94
16	A	830	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
16	A	842	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
16	1	512	CLA	CHD-C4C-NC	2.49	128.12	124.20
16	2	401	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
16	6	402	CLA	CMC-C2C-C1C	2.49	128.83	125.04
16	6	402	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
16	B	833	CLA	C3B-C4B-NB	2.48	112.42	109.21
16	A	832	CLA	O1D-CGD-CBD	-2.48	119.40	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	831	CLA	CBC-CAC-C3C	-2.48	105.58	112.43
16	5	415	CLA	CHD-C4C-NC	2.48	128.12	124.20
16	B	801	CLA	C4-C3-C5	2.48	119.45	115.27
16	B	802	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
16	A	830	CLA	CHD-C4C-NC	2.48	128.11	124.20
16	2	404	CLA	CHD-C4C-NC	2.48	128.11	124.20
16	B	821	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
16	A	803	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
15	A	801	CL0	CGD-CBD-CAD	-2.48	102.70	110.73
19	1	516	BCR	C37-C22-C23	2.48	121.98	118.08
19	I	101	BCR	C15-C14-C13	2.48	130.85	127.31
16	A	829	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
16	B	819	CLA	C4C-C3C-C2C	-2.48	103.29	106.90
16	1	509	CLA	C3B-C4B-NB	2.48	112.41	109.21
19	I	101	BCR	C24-C23-C22	2.47	129.97	126.23
16	A	816	CLA	C3B-C4B-NB	2.47	112.41	109.21
16	A	837	CLA	CHD-C4C-NC	2.47	128.10	124.20
16	A	806	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
16	A	840	CLA	CMB-C2B-C1B	2.47	132.26	128.46
21	A	854	LMT	O5'-C1'-C2'	-2.47	105.13	110.35
16	B	817	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
16	A	827	CLA	CMB-C2B-C1B	2.46	132.25	128.46
16	4	406	CLA	C3B-C4B-NB	2.46	112.40	109.21
16	A	811	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
16	B	810	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
16	B	812	CLA	CMB-C2B-C3B	2.46	129.29	124.68
16	B	817	CLA	CAA-C2A-C3A	-2.46	106.03	112.78
16	A	810	CLA	CAA-C2A-C1A	-2.46	103.91	111.97
16	5	409	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
16	A	820	CLA	CHD-C4C-NC	2.46	128.08	124.20
16	5	413	CLA	C3B-C4B-NB	2.46	112.39	109.21
16	A	809	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
16	1	510	CLA	CHD-C4C-NC	2.46	128.08	124.20
16	4	409	CLA	CHD-C4C-NC	2.46	128.08	124.20
16	A	824	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
16	6	402	CLA	CED-O2D-CGD	2.46	121.49	115.94
16	5	410	CLA	CHD-C4C-NC	2.45	128.07	124.20
16	5	422	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
16	1	503	CLA	C1-O2A-CGA	2.45	122.88	116.44
16	A	840	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
16	A	826	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
16	B	803	CLA	C4A-NA-C1A	-2.45	105.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	836	CLA	CHD-C4C-NC	2.45	128.07	124.20
16	5	419	CLA	CHD-C4C-NC	2.45	128.06	124.20
16	B	801	CLA	C11-C10-C8	-2.45	108.00	115.92
16	1	509	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
16	1	509	CLA	O2A-CGA-O1A	-2.45	117.19	123.30
19	1	523	BCR	C34-C9-C8	2.45	121.94	118.08
16	K	103	CLA	CHD-C4C-NC	2.45	128.06	124.20
16	B	801	CLA	C3B-C4B-NB	2.45	112.37	109.21
16	5	407	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
16	A	811	CLA	CMB-C2B-C1B	2.45	132.22	128.46
16	A	840	CLA	CHD-C4C-NC	2.45	128.06	124.20
16	5	415	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
16	B	833	CLA	CHD-C4C-NC	2.44	128.06	124.20
16	A	833	CLA	CAA-C2A-C1A	-2.44	103.97	111.97
16	A	810	CLA	C2A-C3A-C4A	-2.44	97.92	101.87
16	A	827	CLA	CHB-C4A-NA	2.44	127.89	124.51
16	4	410	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
16	B	831	CLA	CHD-C4C-NC	2.44	128.05	124.20
16	A	843	CLA	CED-O2D-CGD	2.44	121.45	115.94
16	A	810	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
16	B	803	CLA	CHD-C4C-NC	2.44	128.04	124.20
16	5	415	CLA	CED-O2D-CGD	2.44	121.45	115.94
16	A	828	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
16	B	838	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
16	A	827	CLA	O2A-CGA-CBA	2.44	119.55	111.91
16	1	501	CLA	O2A-CGA-O1A	-2.44	117.23	123.30
16	B	824	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
19	B	853	BCR	C15-C16-C17	2.43	128.46	123.47
16	B	831	CLA	C1-O2A-CGA	2.43	122.83	116.44
16	4	404	CLA	CED-O2D-CGD	2.43	121.44	115.94
19	A	850	BCR	C15-C16-C17	2.43	128.46	123.47
16	B	802	CLA	CHA-C1A-NA	-2.43	120.83	126.40
16	A	806	CLA	CMB-C2B-C3B	2.43	129.23	124.68
16	A	836	CLA	CHB-C4A-NA	2.43	127.87	124.51
16	B	821	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
16	B	819	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
16	A	838	CLA	CED-O2D-CGD	2.43	121.43	115.94
16	B	838	CLA	O2A-CGA-CBA	2.43	119.53	111.91
16	B	811	CLA	CHD-C4C-NC	2.43	128.03	124.20
16	1	514	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
16	B	803	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
16	B	823	CLA	C1B-CHB-C4A	-2.43	125.31	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	202	BCR	C15-C14-C13	2.43	130.77	127.31
16	B	813	CLA	C2A-C1A-CHA	-2.43	119.62	123.86
16	5	416	CLA	CHD-C4C-NC	2.42	128.02	124.20
16	B	830	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
16	B	802	CLA	CMB-C2B-C3B	2.42	129.21	124.68
19	A	849	BCR	C7-C8-C9	2.42	129.90	126.23
16	B	830	CLA	C4-C3-C2	-2.42	117.46	123.68
16	B	803	CLA	CMB-C2B-C3B	2.42	129.21	124.68
16	B	836	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
19	B	845	BCR	C36-C18-C17	-2.42	119.53	122.92
16	3	401	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
16	A	821	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
16	B	838	CLA	CED-O2D-CGD	2.42	121.41	115.94
16	B	824	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
16	5	410	CLA	CAC-C3C-C4C	2.42	127.95	124.81
16	5	405	CLA	CHD-C4C-NC	2.42	128.01	124.20
16	A	828	CLA	C3B-C4B-NB	2.42	112.33	109.21
16	A	842	CLA	CHD-C4C-NC	2.42	128.01	124.20
16	4	404	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
16	1	511	CLA	CHD-C4C-NC	2.42	128.01	124.20
16	5	412	CLA	CHD-C4C-NC	2.42	128.01	124.20
16	X	101	CLA	C2A-C1A-CHA	-2.42	119.64	123.86
16	1	501	CLA	CHB-C4A-NA	2.41	127.85	124.51
16	J	102	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
16	B	839	CLA	C4-C3-C2	-2.41	117.48	123.68
16	1	507	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
16	B	823	CLA	CAA-CBA-CGA	-2.41	106.20	113.25
19	B	853	BCR	C36-C18-C17	-2.41	119.55	122.92
16	A	828	CLA	C4-C3-C5	2.41	119.33	115.27
16	4	402	CLA	C4C-C3C-C2C	-2.41	103.38	106.90
16	A	804	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
16	A	805	CLA	O2A-CGA-CBA	2.41	119.47	111.91
16	B	801	CLA	C1-O2A-CGA	2.41	122.76	116.44
16	A	818	CLA	CHD-C4C-NC	2.41	128.00	124.20
16	B	817	CLA	CHB-C4A-NA	2.40	127.84	124.51
19	J	104	BCR	C16-C15-C14	2.40	128.40	123.47
16	A	826	CLA	O2A-CGA-CBA	2.40	119.45	111.91
19	A	846	BCR	C34-C9-C8	2.40	121.86	118.08
16	B	806	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
16	B	824	CLA	CMA-C3A-C4A	2.40	118.23	111.77
16	1	526	CLA	O2A-CGA-CBA	2.40	121.74	114.03
16	B	806	CLA	C1-O2A-CGA	2.40	122.74	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	839	CLA	C5-C3-C2	-2.40	116.26	121.12
16	K	101	CLA	O2A-CGA-CBA	2.40	121.74	114.03
16	B	816	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
16	A	821	CLA	CED-O2D-CGD	2.40	121.36	115.94
16	A	827	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
16	A	832	CLA	C3B-C4B-NB	2.40	112.31	109.21
16	A	833	CLA	CHB-C4A-NA	2.39	127.82	124.51
16	B	802	CLA	C1-O2A-CGA	2.39	122.72	116.44
16	4	405	CLA	CHD-C4C-NC	2.39	127.97	124.20
16	A	807	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
16	B	806	CLA	O2A-CGA-CBA	2.39	119.41	111.91
16	6	401	CLA	CED-O2D-CGD	2.39	121.34	115.94
16	5	418	CLA	CHD-C4C-NC	2.39	127.97	124.20
19	J	104	BCR	C10-C11-C12	2.39	130.67	123.22
16	B	817	CLA	CAA-C2A-C1A	-2.39	104.15	111.97
16	1	503	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
16	A	802	CLA	O1D-CGD-CBD	-2.39	119.60	124.48
16	B	820	CLA	CED-O2D-CGD	2.39	121.33	115.94
16	A	807	CLA	CHB-C4A-NA	2.39	127.81	124.51
16	6	407	CLA	CHD-C4C-NC	2.38	127.96	124.20
16	J	102	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
19	B	845	BCR	C16-C15-C14	2.38	128.35	123.47
16	B	826	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
16	1	513	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
19	A	851	BCR	C8-C9-C10	2.38	122.59	118.94
16	B	827	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
16	B	825	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
16	B	820	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	I	102	BCR	C24-C23-C22	2.38	129.83	126.23
16	1	526	CLA	CHD-C4C-NC	2.38	127.95	124.20
16	B	816	CLA	C3B-C4B-NB	2.38	112.28	109.21
16	B	813	CLA	CHD-C4C-NC	2.38	127.95	124.20
16	B	801	CLA	C4C-C3C-C2C	-2.37	103.44	106.90
19	5	420	BCR	C37-C22-C23	2.37	121.82	118.08
16	1	519	CLA	C4C-C3C-C2C	-2.37	103.44	106.90
19	A	847	BCR	C35-C13-C14	-2.37	119.60	122.92
16	J	101	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
16	B	823	CLA	CMB-C2B-C3B	2.37	129.12	124.68
16	B	823	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
16	B	801	CLA	CHD-C4C-NC	2.37	127.94	124.20
16	B	831	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
16	2	402	CLA	C2A-C1A-CHA	-2.37	119.71	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	832	CLA	CHD-C4C-NC	2.37	127.94	124.20
16	B	811	CLA	O2A-CGA-CBA	2.37	119.34	111.91
19	B	843	BCR	C35-C13-C14	-2.37	119.60	122.92
16	A	836	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
16	1	511	CLA	C4C-C3C-C2C	-2.37	103.44	106.90
19	B	844	BCR	C16-C17-C18	2.37	130.69	127.31
16	B	833	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
16	1	508	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
16	1	503	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
16	A	826	CLA	CHD-C4C-NC	2.37	127.93	124.20
16	5	406	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
16	A	817	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
15	A	801	CL0	CHD-C4C-NC	2.36	127.93	124.20
16	A	831	CLA	CHD-C4C-NC	2.36	127.93	124.20
16	B	817	CLA	CHD-C4C-NC	2.36	127.93	124.20
16	1	519	CLA	CHB-C4A-NA	2.36	127.78	124.51
16	1	520	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
16	B	828	CLA	O2A-CGA-CBA	2.36	119.32	111.91
16	4	405	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
16	A	828	CLA	OBD-CAD-C3D	-2.36	122.84	128.52
16	B	804	CLA	CHD-C4C-NC	2.36	127.92	124.20
16	2	403	CLA	CED-O2D-CGD	2.36	121.27	115.94
16	A	834	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
16	A	822	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
16	A	809	CLA	CHB-C4A-NA	2.36	127.77	124.51
16	1	519	CLA	C3B-C4B-NB	2.36	112.26	109.21
19	I	102	BCR	C2-C1-C6	2.36	114.11	110.48
16	A	805	CLA	CHB-C4A-NA	2.36	127.77	124.51
16	B	830	CLA	CHD-C4C-NC	2.36	127.92	124.20
17	A	844	PQN	C14-C13-C15	2.36	119.23	115.27
16	B	806	CLA	CHB-C4A-NA	2.36	127.77	124.51
16	2	402	CLA	CHD-C4C-NC	2.36	127.92	124.20
16	B	834	CLA	C2A-C1A-CHA	-2.35	119.74	123.86
16	A	842	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
16	B	841	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
16	A	820	CLA	O2A-CGA-CBA	2.35	119.29	111.91
16	A	808	CLA	C3B-C4B-NB	2.35	112.25	109.21
16	4	404	CLA	CMB-C2B-C3B	2.35	129.07	124.68
16	A	815	CLA	CHD-C4C-NC	2.35	127.90	124.20
16	A	812	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
16	J	101	CLA	CHB-C4A-NA	2.35	127.76	124.51
16	A	830	CLA	C2A-C1A-CHA	-2.35	119.76	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	828	CLA	CHD-C4C-NC	2.35	127.90	124.20
16	A	828	CLA	CED-O2D-CGD	2.34	121.24	115.94
16	B	809	CLA	O2A-CGA-CBA	2.34	119.26	111.91
16	A	835	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	B	848	BCR	C11-C10-C9	2.34	130.65	127.31
16	B	804	CLA	CMB-C2B-C3B	2.34	129.06	124.68
16	B	816	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
16	5	406	CLA	CED-O2D-CGD	2.34	121.23	115.94
16	1	509	CLA	CHD-C4C-NC	2.34	127.89	124.20
16	B	826	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
16	A	824	CLA	O2A-CGA-CBA	2.34	119.25	111.91
16	B	808	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	K	102	BCR	C35-C13-C14	-2.34	119.65	122.92
16	A	843	CLA	C4C-C3C-C2C	-2.34	103.49	106.90
16	5	416	CLA	CED-O2D-CGD	2.34	121.23	115.94
16	B	827	CLA	OBD-CAD-C3D	-2.34	122.89	128.52
16	A	821	CLA	CHD-C4C-NC	2.34	127.89	124.20
16	3	401	CLA	CHD-C4C-NC	2.34	127.89	124.20
16	B	822	CLA	C2A-C1A-CHA	-2.34	119.78	123.86
16	5	404	CLA	CHD-C4C-NC	2.33	127.88	124.20
19	J	103	BCR	C15-C14-C13	2.33	130.64	127.31
16	B	825	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
16	A	805	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
16	A	802	CLA	CMB-C2B-C3B	2.33	129.04	124.68
16	6	409	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
16	1	513	CLA	CHD-C4C-NC	2.33	127.88	124.20
16	5	413	CLA	CHD-C4C-NC	2.33	127.88	124.20
16	B	813	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
16	5	412	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
16	B	815	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
16	B	804	CLA	CHB-C4A-NA	2.33	127.74	124.51
16	A	826	CLA	CMA-C3A-C4A	2.33	118.04	111.77
16	B	806	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
16	B	837	CLA	O2A-CGA-CBA	2.33	119.22	111.91
16	B	831	CLA	CHB-C4A-NA	2.33	127.73	124.51
16	6	403	CLA	CED-O2D-CGD	2.33	121.20	115.94
16	B	814	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	5	420	BCR	C15-C16-C17	2.33	128.24	123.47
16	5	421	CLA	CMC-C2C-C1C	2.33	128.58	125.04
16	B	818	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
19	J	104	BCR	C35-C13-C14	-2.33	119.67	122.92
19	J	104	BCR	C36-C18-C17	-2.33	119.67	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	833	CLA	C1-O2A-CGA	2.33	122.55	116.44
16	B	833	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
16	6	408	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
16	A	829	CLA	C16-C15-C13	-2.32	108.41	115.92
16	6	407	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
16	A	814	CLA	CHD-C4C-NC	2.32	127.86	124.20
16	4	408	CLA	CHD-C4C-NC	2.32	127.86	124.20
16	6	408	CLA	CHD-C4C-NC	2.32	127.86	124.20
16	B	807	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
16	B	809	CLA	OBD-CAD-C3D	-2.32	122.93	128.52
16	A	832	CLA	CED-O2D-CGD	2.32	121.19	115.94
16	K	101	CLA	O2A-CGA-O1A	-2.32	117.51	123.30
16	1	506	CLA	CED-O2D-CGD	2.32	121.19	115.94
16	A	811	CLA	CHD-C4C-NC	2.32	127.86	124.20
19	A	846	BCR	C21-C20-C19	2.32	130.46	123.22
16	6	409	CLA	CHD-C4C-NC	2.32	127.86	124.20
16	3	401	CLA	CED-O2D-CGD	2.32	121.18	115.94
16	5	422	CLA	CHD-C4C-NC	2.32	127.86	124.20
16	3	401	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
16	B	840	CLA	CHD-C4C-NC	2.32	127.86	124.20
16	5	409	CLA	CHD-C4C-NC	2.32	127.86	124.20
16	J	102	CLA	CED-O2D-CGD	2.32	121.18	115.94
16	B	816	CLA	CHD-C4C-NC	2.32	127.85	124.20
16	B	815	CLA	O1D-CGD-CBD	-2.32	119.75	124.48
19	1	523	BCR	C15-C14-C13	2.31	130.61	127.31
16	A	839	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
16	6	405	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
16	A	813	CLA	CHD-C4C-NC	2.31	127.85	124.20
16	1	508	CLA	CHD-C4C-NC	2.31	127.85	124.20
16	A	829	CLA	C3B-C4B-NB	2.31	112.20	109.21
16	B	815	CLA	C3B-C4B-NB	2.31	112.20	109.21
16	A	835	CLA	CHB-C4A-NA	2.31	127.71	124.51
16	B	816	CLA	CED-O2D-CGD	2.31	121.17	115.94
16	B	803	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
16	A	824	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
16	B	809	CLA	C5-C3-C2	-2.31	116.44	121.12
16	1	515	CLA	CHB-C4A-NA	2.31	127.71	124.51
16	B	811	CLA	CHC-C1C-NC	2.31	127.71	124.20
16	1	503	CLA	CMB-C2B-C3B	2.31	129.00	124.68
16	2	404	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
15	A	801	CL0	C4A-NA-C1A	-2.31	105.67	106.71
16	B	810	CLA	O1D-CGD-CBD	-2.31	119.77	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	411	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
16	1	511	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
16	5	417	CLA	O2A-CGA-CBA	2.30	121.43	114.03
16	1	519	CLA	CED-O2D-CGD	2.30	121.14	115.94
16	B	840	CLA	C1-O2A-CGA	2.30	122.48	116.44
16	K	103	CLA	C3B-C4B-NB	2.30	112.19	109.21
16	B	818	CLA	OBD-CAD-C3D	-2.30	122.98	128.52
16	A	813	CLA	C5-C3-C2	-2.30	116.47	121.12
16	5	421	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
16	A	812	CLA	C4-C3-C5	2.30	119.14	115.27
16	4	404	CLA	CHD-C4C-NC	2.30	127.83	124.20
16	1	510	CLA	CMB-C2B-C3B	2.30	128.98	124.68
19	5	402	BCR	C34-C9-C8	2.30	121.70	118.08
16	B	825	CLA	CHD-C4C-NC	2.30	127.82	124.20
16	1	515	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
16	A	833	CLA	CED-O2D-CGD	2.30	121.13	115.94
16	A	809	CLA	CAA-C2A-C3A	-2.29	106.49	112.78
16	1	520	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
16	1	520	CLA	CAC-C3C-C4C	2.29	127.78	124.81
16	4	402	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
16	B	832	CLA	C3B-C4B-NB	2.29	112.17	109.21
16	1	519	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
16	A	825	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
16	A	826	CLA	CMB-C2B-C3B	2.29	128.96	124.68
16	1	520	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
16	5	410	CLA	CHC-C1C-NC	2.29	127.68	124.20
16	1	520	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
16	A	831	CLA	CMB-C2B-C3B	2.29	128.96	124.68
16	A	805	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
16	A	828	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
16	6	404	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
16	B	820	CLA	C1-O2A-CGA	2.29	123.37	116.73
16	A	837	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
16	B	801	CLA	CMA-C3A-C4A	-2.28	105.63	111.77
16	A	840	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
16	1	505	CLA	CMB-C2B-C3B	2.28	128.95	124.68
16	B	817	CLA	CED-O2D-CGD	2.28	121.10	115.94
16	6	409	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
16	B	821	CLA	O2A-CGA-CBA	2.28	121.36	114.03
16	B	805	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
16	B	810	CLA	C1-C2-C3	-2.28	122.10	126.04
16	B	830	CLA	CHB-C4A-NA	2.28	127.66	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	802	CLA	CHB-C4A-NA	2.28	127.66	124.51
16	6	402	CLA	CHD-C4C-NC	2.28	127.79	124.20
16	B	803	CLA	CHC-C1C-NC	2.28	127.66	124.20
16	B	804	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
16	4	410	CLA	CHD-C4C-NC	2.28	127.79	124.20
19	4	401	BCR	C16-C15-C14	2.28	128.14	123.47
19	A	850	BCR	C36-C18-C17	-2.28	119.73	122.92
16	1	513	CLA	CBA-CAA-C2A	2.28	120.58	113.86
19	4	401	BCR	C12-C13-C14	2.28	122.43	118.94
16	5	405	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
16	1	508	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
16	J	101	CLA	CHD-C4C-NC	2.28	127.79	124.20
19	1	516	BCR	C35-C13-C14	-2.28	119.74	122.92
16	4	407	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
16	1	520	CLA	CMB-C2B-C1B	2.27	131.96	128.46
16	B	807	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
16	B	834	CLA	CHD-C4C-NC	2.27	127.78	124.20
16	A	829	CLA	C1-O2A-CGA	2.27	122.41	116.44
16	1	506	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
16	A	835	CLA	CHC-C1C-NC	2.27	127.65	124.20
16	5	414	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
16	A	835	CLA	CMB-C2B-C1B	2.27	131.95	128.46
16	A	832	CLA	CHB-C4A-NA	2.27	127.65	124.51
16	B	810	CLA	O2A-CGA-CBA	2.27	119.03	111.91
16	5	418	CLA	CED-O2D-CGD	2.27	121.06	115.94
16	B	804	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
16	A	832	CLA	C2A-C1A-CHA	-2.27	119.90	123.86
16	B	819	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
16	B	834	CLA	CMA-C3A-C2A	-2.27	104.69	113.83
16	5	421	CLA	CHD-C4C-NC	2.26	127.77	124.20
16	F	201	CLA	C3B-C4B-NB	2.26	112.14	109.21
16	2	406	CLA	CHD-C4C-NC	2.26	127.77	124.20
16	4	407	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
16	5	418	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
16	1	503	CLA	CED-O2D-CGD	2.26	121.05	115.94
16	B	827	CLA	C5-C3-C2	-2.26	116.54	121.12
16	A	839	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
19	K	102	BCR	C15-C14-C13	2.26	130.54	127.31
16	A	805	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
16	A	822	CLA	O2A-CGA-CBA	2.26	119.00	111.91
19	1	516	BCR	C2-C1-C6	2.26	113.96	110.48
16	B	836	CLA	CHB-C4A-NA	2.26	127.64	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	409	CLA	CED-O2D-CGD	2.26	121.05	115.94
16	5	406	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
16	B	806	CLA	C3B-C4B-NB	2.26	112.13	109.21
21	B	852	LMT	C1-O1'-C1'	2.26	117.58	113.84
16	B	822	CLA	CHD-C4C-NC	2.26	127.76	124.20
16	A	802	CLA	CHA-C1A-NA	-2.26	121.23	126.40
16	B	837	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
16	5	406	CLA	CHD-C4C-NC	2.26	127.76	124.20
16	1	525	CLA	CHD-C4C-NC	2.26	127.76	124.20
16	A	827	CLA	CAC-C3C-C4C	2.26	127.74	124.81
16	1	519	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
16	6	406	CLA	CHD-C4C-NC	2.25	127.75	124.20
16	B	827	CLA	C3B-C4B-NB	2.25	112.12	109.21
19	5	402	BCR	C35-C13-C14	-2.25	119.77	122.92
16	B	825	CLA	C4-C3-C5	2.25	119.06	115.27
16	1	507	CLA	CED-O2D-CGD	2.25	121.02	115.94
16	5	407	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
16	K	103	CLA	O2A-CGA-O1A	-2.25	117.69	123.30
16	A	833	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
16	1	525	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
16	6	408	CLA	CED-O2D-CGD	2.25	121.02	115.94
16	B	839	CLA	CHB-C4A-NA	2.25	127.62	124.51
16	A	832	CLA	O2A-CGA-CBA	2.25	118.95	111.91
16	A	815	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
16	B	823	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
16	B	818	CLA	C4C-C3C-C2C	-2.24	103.63	106.90
16	5	416	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
16	2	403	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
16	1	507	CLA	CHD-C4C-NC	2.24	127.73	124.20
16	B	804	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
16	6	402	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
16	2	403	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
16	6	407	CLA	CED-O2D-CGD	2.23	120.99	115.94
19	A	849	BCR	C19-C18-C17	2.23	122.37	118.94
19	B	847	BCR	C35-C13-C14	-2.23	119.80	122.92
16	5	418	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
16	B	813	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
16	1	520	CLA	C2A-C3A-C4A	-2.23	98.27	101.87
16	B	812	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
16	5	405	CLA	CED-O2D-CGD	2.23	120.98	115.94
19	1	522	BCR	C24-C23-C22	-2.23	122.87	126.23
16	A	826	CLA	C1-C2-C3	-2.23	122.19	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	803	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
16	6	405	CLA	CHD-C4C-NC	2.22	127.71	124.20
16	2	405	CLA	CHD-C4C-NC	2.22	127.70	124.20
16	A	803	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
16	A	802	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
16	A	826	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
16	B	807	CLA	CHD-C4C-NC	2.22	127.70	124.20
16	5	412	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
16	B	837	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
16	5	407	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
16	1	510	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
16	B	839	CLA	CHD-C4C-NC	2.21	127.69	124.20
16	A	839	CLA	C4-C3-C5	2.21	119.00	115.27
16	5	405	CLA	O2A-CGA-O1A	-2.21	117.78	123.30
16	B	804	CLA	CED-O2D-CGD	2.21	120.94	115.94
16	A	823	CLA	CHB-C4A-NA	2.21	127.57	124.51
16	B	832	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
16	1	509	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
16	B	816	CLA	CMB-C2B-C1B	2.21	131.86	128.46
19	1	517	BCR	C37-C22-C23	2.21	121.56	118.08
16	A	829	CLA	CED-O2D-CGD	2.21	120.93	115.94
16	A	829	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
16	A	811	CLA	CED-O2D-CGD	2.21	120.93	115.94
16	5	407	CLA	CHD-C4C-NC	2.21	127.68	124.20
16	1	503	CLA	O2A-CGA-CBA	2.21	118.83	111.91
16	B	822	CLA	CED-O2D-CGD	2.20	120.92	115.94
16	A	826	CLA	C6-C5-C3	2.20	119.23	113.45
16	B	809	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
16	1	520	CLA	O2A-CGA-CBA	2.20	118.82	111.91
16	5	421	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
19	A	851	BCR	C15-C14-C13	2.20	130.45	127.31
19	I	102	BCR	C10-C11-C12	2.20	130.08	123.22
16	A	814	CLA	CMB-C2B-C1B	2.20	131.84	128.46
16	B	822	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
16	A	812	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
16	A	820	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
16	A	841	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
16	A	843	CLA	CHC-C1C-NC	2.20	127.53	124.20
19	B	844	BCR	C20-C21-C22	2.20	130.44	127.31
16	5	410	CLA	O2A-CGA-O1A	-2.20	117.83	123.30
16	A	813	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
16	A	807	CLA	OBD-CAD-C3D	-2.20	123.24	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	503	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
16	B	835	CLA	C3B-C4B-NB	2.19	112.05	109.21
19	B	843	BCR	C15-C16-C17	2.19	127.97	123.47
16	1	521	CLA	C1-O2A-CGA	2.19	122.20	116.44
16	A	819	CLA	CHD-C4C-NC	2.19	127.66	124.20
16	A	804	CLA	O2A-CGA-CBA	2.19	118.79	111.91
16	5	407	CLA	CED-O2D-CGD	2.19	120.90	115.94
19	A	848	BCR	C11-C10-C9	2.19	130.44	127.31
16	A	837	CLA	CED-O2D-CGD	2.19	120.89	115.94
16	A	802	CLA	CHD-C4C-NC	2.19	127.66	124.20
16	6	406	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
16	A	819	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
16	A	834	CLA	C3B-C4B-NB	2.19	112.04	109.21
16	2	405	CLA	CHB-C4A-NA	2.19	127.54	124.51
19	1	522	BCR	C34-C9-C8	2.19	121.53	118.08
16	6	403	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
16	6	401	CLA	CHD-C4C-NC	2.19	127.65	124.20
19	A	848	BCR	C35-C13-C14	-2.19	119.86	122.92
19	A	851	BCR	C16-C15-C14	2.19	127.96	123.47
16	B	825	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
16	B	823	CLA	CED-O2D-CGD	2.19	120.89	115.94
16	6	403	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
16	5	417	CLA	CMB-C2B-C3B	2.19	128.77	124.68
16	A	830	CLA	O2A-CGA-CBA	2.19	118.77	111.91
16	1	510	CLA	CHB-C4A-NA	2.19	127.54	124.51
16	4	406	CLA	CED-O2D-CGD	2.19	120.88	115.94
16	B	828	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
16	1	501	CLA	CHC-C1C-NC	2.19	127.52	124.20
16	5	408	CLA	CHD-C4C-NC	2.19	127.65	124.20
16	B	836	CLA	O2A-CGA-CBA	2.19	121.05	114.03
16	A	806	CLA	C4C-C3C-C2C	-2.19	103.71	106.90
16	B	805	CLA	CHD-C4C-NC	2.18	127.64	124.20
19	A	848	BCR	C34-C9-C8	2.18	121.52	118.08
16	B	825	CLA	CAA-C2A-C1A	-2.18	104.82	111.97
16	B	827	CLA	CHB-C4A-NA	2.18	127.53	124.51
16	A	840	CLA	C1-O2A-CGA	2.18	122.17	116.44
16	4	403	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
16	A	823	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
16	5	411	CLA	C3B-C4B-NB	2.18	112.03	109.21
16	B	829	CLA	C16-C15-C13	-2.18	108.87	115.92
16	A	809	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
16	A	823	CLA	C1B-CHB-C4A	-2.18	125.80	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	405	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
16	B	804	CLA	O2A-CGA-CBA	2.18	118.74	111.91
16	B	805	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
16	1	515	CLA	CHD-C4C-NC	2.18	127.63	124.20
16	K	103	CLA	O2A-CGA-CBA	2.18	121.02	114.03
19	A	849	BCR	C10-C11-C12	2.17	130.00	123.22
16	6	406	CLA	CHB-C4A-NA	2.17	127.52	124.51
16	5	417	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
16	5	418	CLA	CHB-C4A-NA	2.17	127.52	124.51
16	A	832	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
16	B	837	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
16	B	824	CLA	C1C-C2C-C3C	-2.17	104.67	106.96
16	A	811	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
16	B	822	CLA	C1-O2A-CGA	2.17	122.14	116.44
16	A	805	CLA	C1-O2A-CGA	2.17	122.14	116.44
16	A	833	CLA	C1-O2A-CGA	2.17	122.14	116.44
17	A	844	PQN	C15-C13-C12	-2.17	116.73	121.12
19	B	853	BCR	C35-C13-C14	-2.17	119.89	122.92
16	B	802	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
16	X	101	CLA	CHD-C4C-NC	2.17	127.62	124.20
16	A	803	CLA	CMA-C3A-C2A	-2.17	105.08	113.83
16	A	843	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
16	4	406	CLA	CHB-C4A-NA	2.17	127.51	124.51
16	B	805	CLA	C4C-C3C-C2C	-2.17	103.74	106.90
16	5	407	CLA	CHC-C1C-NC	2.17	127.49	124.20
16	A	835	CLA	O2A-CGA-CBA	2.17	118.70	111.91
16	B	814	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
16	1	511	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
16	B	830	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
16	1	508	CLA	CHC-C1C-NC	2.16	127.48	124.20
16	B	819	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
16	B	825	CLA	C6-C7-C8	-2.16	108.94	115.92
16	A	824	CLA	CHC-C1C-NC	2.16	127.48	124.20
16	1	504	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
19	K	102	BCR	C16-C15-C14	2.16	127.90	123.47
16	A	808	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
19	1	522	BCR	C11-C10-C9	2.16	130.39	127.31
16	A	826	CLA	CHA-C1A-NA	-2.16	121.45	126.40
16	A	812	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
19	B	848	BCR	C15-C14-C13	2.16	130.39	127.31
16	K	101	CLA	CHB-C4A-NA	2.16	127.50	124.51
16	A	837	CLA	CBC-CAC-C3C	-2.16	106.48	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	519	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
16	A	807	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
19	A	846	BCR	C35-C13-C14	-2.15	119.91	122.92
16	A	839	CLA	C6-C7-C8	-2.15	108.96	115.92
16	A	814	CLA	C1C-C2C-C3C	-2.15	104.69	106.96
16	B	825	CLA	OBD-CAD-C3D	-2.15	123.34	128.52
21	A	854	LMT	O1B-C4'-C5'	-2.15	103.55	109.45
16	B	824	CLA	C2A-C3A-C4A	-2.15	98.39	101.87
16	6	404	CLA	CMB-C2B-C3B	2.15	128.70	124.68
16	B	816	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
16	B	824	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
16	B	816	CLA	CHB-C4A-NA	2.15	127.48	124.51
16	1	506	CLA	CHB-C4A-NA	2.15	127.48	124.51
16	5	413	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
16	B	819	CLA	C3B-C4B-NB	2.15	111.99	109.21
16	B	815	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
16	A	817	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
16	B	809	CLA	CED-O2D-CGD	2.15	120.79	115.94
16	1	508	CLA	CED-O2D-CGD	2.15	120.79	115.94
16	4	405	CLA	C1B-CHB-C4A	-2.15	125.87	130.12
19	A	849	BCR	C23-C22-C21	2.15	122.23	118.94
16	5	411	CLA	C2A-C1A-CHA	-2.15	120.11	123.86
16	4	408	CLA	O2D-CGD-O1D	-2.14	119.64	123.84
16	B	808	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
16	B	821	CLA	CHB-C4A-NA	2.14	127.47	124.51
16	4	411	CLA	CMB-C2B-C3B	2.14	128.68	124.68
16	5	406	CLA	CMB-C2B-C3B	2.14	128.68	124.68
16	B	820	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
16	6	406	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
16	1	511	CLA	O2A-CGA-CBA	2.14	118.62	111.91
16	1	514	CLA	CHD-C4C-NC	2.14	127.57	124.20
16	A	822	CLA	CED-O2D-CGD	2.14	120.77	115.94
16	6	403	CLA	CHB-C4A-NA	2.14	127.47	124.51
16	1	525	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
16	4	402	CLA	CED-O2D-CGD	2.14	120.77	115.94
16	B	841	CLA	CHB-C4A-NA	2.14	127.47	124.51
16	B	823	CLA	CHD-C4C-NC	2.13	127.57	124.20
16	B	819	CLA	O2A-CGA-CBA	2.13	118.60	111.91
16	A	827	CLA	CHC-C1C-C2C	-2.13	120.82	126.72
16	A	820	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
16	5	414	CLA	CED-O2D-CGD	2.13	120.76	115.94
16	A	813	CLA	CMB-C2B-C3B	2.13	128.67	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	802	CLA	C4-C3-C5	2.13	118.86	115.27
16	B	832	CLA	C6-C7-C8	-2.13	109.03	115.92
16	B	808	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
16	B	821	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
16	B	814	CLA	O2A-CGA-CBA	2.13	118.59	111.91
16	A	822	CLA	C5-C3-C2	-2.13	116.81	121.12
19	A	851	BCR	C35-C13-C14	-2.13	119.94	122.92
16	B	822	CLA	C4-C3-C5	2.13	118.85	115.27
16	B	809	CLA	CHB-C4A-NA	2.13	127.46	124.51
16	A	816	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
16	1	501	CLA	OBD-CAD-C3D	-2.13	123.40	128.52
16	A	826	CLA	C1-O2A-CGA	2.13	122.03	116.44
16	A	835	CLA	CHD-C4C-NC	2.13	127.56	124.20
16	5	411	CLA	CMB-C2B-C1B	2.13	131.73	128.46
15	A	801	CL0	C1B-CHB-C4A	-2.13	125.90	130.12
16	6	405	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
16	A	842	CLA	CHB-C4A-NA	2.13	127.45	124.51
19	J	104	BCR	C15-C16-C17	2.13	127.83	123.47
16	1	515	CLA	CMB-C2B-C3B	2.13	128.66	124.68
16	B	827	CLA	CHA-C1A-NA	-2.13	121.53	126.40
16	A	810	CLA	CAA-CBA-CGA	-2.12	107.04	113.25
19	M	102	BCR	C35-C13-C14	-2.12	119.95	122.92
16	6	403	CLA	CHD-C4C-NC	2.12	127.55	124.20
16	A	834	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
16	B	834	CLA	CED-O2D-CGD	2.12	120.73	115.94
16	B	824	CLA	O2A-CGA-CBA	2.12	118.56	111.91
16	A	814	CLA	CHB-C4A-NA	2.12	127.44	124.51
16	1	508	CLA	CHB-C4A-NA	2.12	127.44	124.51
16	F	201	CLA	CHB-C4A-NA	2.12	127.44	124.51
16	1	525	CLA	CHB-C4A-NA	2.12	127.44	124.51
16	B	813	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
16	6	401	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
16	5	412	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
16	A	821	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
16	A	811	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
16	A	815	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
16	5	413	CLA	CHC-C1C-NC	2.11	127.41	124.20
16	A	836	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
16	B	803	CLA	C1-O2A-CGA	2.11	121.99	116.44
16	4	407	CLA	CMB-C2B-C3B	2.11	128.63	124.68
16	5	421	CLA	CHC-C1C-NC	2.11	127.41	124.20
16	A	838	CLA	C3B-C4B-NB	2.11	111.94	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	402	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
16	A	840	CLA	C3B-C4B-NB	2.11	111.94	109.21
16	A	816	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
16	1	511	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
16	A	826	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
16	1	520	CLA	CHB-C4A-NA	2.11	127.43	124.51
16	B	823	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
16	A	841	CLA	C1-C2-C3	-2.11	122.40	126.04
16	F	204	CLA	CHA-C1A-NA	-2.11	121.57	126.40
16	B	804	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
16	A	805	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
16	2	404	CLA	CED-O2D-CGD	2.11	120.70	115.94
16	B	836	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
16	5	416	CLA	CMC-C2C-C1C	2.11	128.25	125.04
16	B	809	CLA	CHA-C1A-NA	-2.11	121.58	126.40
21	1	524	LMT	O1B-C4'-C3'	2.10	112.88	107.28
16	B	805	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
16	B	815	CLA	O2A-CGA-O1A	-2.10	118.06	123.30
16	2	405	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
19	B	845	BCR	C34-C9-C8	2.10	121.39	118.08
16	A	804	CLA	CED-O2D-CGD	2.10	120.69	115.94
16	B	811	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
16	A	828	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
16	A	819	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
16	4	409	CLA	CED-O2D-CGD	2.10	120.69	115.94
19	5	420	BCR	C35-C13-C14	-2.10	119.98	122.92
16	4	410	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
16	A	804	CLA	C4-C3-C5	2.10	118.80	115.27
16	B	823	CLA	C1-O2A-CGA	2.10	121.95	116.44
16	B	837	CLA	C3B-C4B-NB	2.10	111.92	109.21
16	K	103	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
16	B	809	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
16	A	821	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
16	B	829	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
16	A	835	CLA	C3B-C4B-NB	2.09	111.92	109.21
16	2	403	CLA	CHB-C4A-NA	2.09	127.41	124.51
16	B	840	CLA	C3B-C4B-NB	2.09	111.91	109.21
16	B	811	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
16	1	521	CLA	C3B-C4B-NB	2.09	111.91	109.21
16	A	841	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
19	I	101	BCR	C11-C10-C9	2.09	130.29	127.31
16	B	840	CLA	CHB-C4A-NA	2.09	127.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	839	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
16	B	805	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
16	A	815	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
16	A	843	CLA	C4-C3-C5	2.09	118.78	115.27
16	B	802	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
16	A	816	CLA	CHC-C1C-NC	2.09	127.37	124.20
16	B	823	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
16	1	511	CLA	CHC-C1C-NC	2.09	127.37	124.20
16	1	511	CLA	CMB-C2B-C1B	2.09	131.67	128.46
15	A	801	CL0	O2A-CGA-CBA	2.09	118.45	111.91
16	5	414	CLA	CHB-C4A-NA	2.08	127.39	124.51
16	F	204	CLA	O2A-CGA-O1A	-2.08	118.11	123.30
21	A	854	LMT	O1'-C1'-C2'	2.08	111.56	108.30
16	B	818	CLA	CHB-C4A-NA	2.08	127.39	124.51
19	F	205	BCR	C12-C13-C14	2.08	122.14	118.94
16	4	405	CLA	CHB-C4A-NA	2.08	127.39	124.51
16	B	818	CLA	CHC-C1C-NC	2.08	127.36	124.20
16	A	814	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
16	1	512	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
16	B	824	CLA	CMB-C2B-C1B	2.08	131.66	128.46
16	A	819	CLA	CED-O2D-CGD	2.08	120.64	115.94
16	B	806	CLA	C4-C3-C5	2.08	118.77	115.27
16	B	833	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
16	4	407	CLA	CHB-C4A-NA	2.08	127.38	124.51
16	6	402	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
16	A	820	CLA	C11-C12-C13	-2.08	109.21	115.92
16	1	520	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
16	5	421	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
16	J	102	CLA	CHB-C4A-NA	2.07	127.38	124.51
16	A	838	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
16	J	101	CLA	O2A-CGA-CBA	2.07	120.69	114.03
16	B	804	CLA	C1-O2A-CGA	2.07	121.89	116.44
16	A	807	CLA	C4-C3-C5	2.07	118.76	115.27
16	1	503	CLA	CHD-C4C-NC	2.07	127.47	124.20
19	1	522	BCR	C35-C13-C14	-2.07	120.02	122.92
16	1	505	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
16	B	831	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
19	I	102	BCR	C35-C13-C14	-2.07	120.02	122.92
16	A	838	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
16	A	836	CLA	CED-O2D-CGD	2.07	120.62	115.94
16	A	834	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
16	B	822	CLA	CHB-C4A-NA	2.07	127.37	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	806	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
16	A	807	CLA	CED-O2D-CGD	2.07	120.62	115.94
16	A	817	CLA	CHD-C4C-NC	2.07	127.46	124.20
16	B	826	CLA	OBD-CAD-C3D	-2.07	123.55	128.52
16	5	416	CLA	CHC-C1C-NC	2.07	127.34	124.20
16	1	526	CLA	CHC-C1C-NC	2.07	127.34	124.20
16	B	811	CLA	CHB-C4A-NA	2.06	127.37	124.51
16	A	824	CLA	CHD-C4C-NC	2.06	127.46	124.20
16	A	820	CLA	CHC-C1C-NC	2.06	127.33	124.20
16	B	833	CLA	CHB-C4A-NA	2.06	127.36	124.51
16	2	403	CLA	CHD-C4C-NC	2.06	127.45	124.20
16	B	831	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
19	A	847	BCR	C16-C15-C14	2.06	127.70	123.47
16	5	422	CLA	CMB-C2B-C3B	2.06	128.53	124.68
16	1	502	CLA	CMB-C2B-C3B	2.06	128.53	124.68
16	A	822	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
16	1	512	CLA	O2A-CGA-CBA	2.06	120.65	114.03
16	A	833	CLA	O2A-CGA-CBA	2.06	118.37	111.91
16	4	407	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
16	K	103	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
19	1	516	BCR	C11-C10-C9	2.06	130.25	127.31
16	A	839	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
16	A	829	CLA	C2A-C3A-C4A	-2.06	98.55	101.87
16	A	812	CLA	CHB-C4A-NA	2.06	127.36	124.51
16	B	806	CLA	C2A-C1A-CHA	-2.06	120.27	123.86
16	6	405	CLA	CMB-C2B-C3B	2.06	128.52	124.68
16	B	812	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
16	6	403	CLA	CHC-C1C-NC	2.05	127.32	124.20
16	6	401	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
17	B	842	PQN	C14-C13-C15	2.05	118.72	115.27
16	A	833	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
16	B	803	CLA	CED-O2D-CGD	2.05	120.58	115.94
16	B	807	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
16	A	808	CLA	C2A-C3A-C4A	-2.05	98.56	101.87
16	B	815	CLA	CHC-C1C-NC	2.05	127.31	124.20
16	1	513	CLA	CED-O2D-CGD	2.05	120.56	115.94
16	B	833	CLA	CED-O2D-CGD	2.04	120.56	115.94
16	B	832	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
16	A	809	CLA	C11-C12-C13	-2.04	109.31	115.92
16	B	828	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
16	B	813	CLA	C1C-C2C-C3C	-2.04	104.81	106.96
16	A	804	CLA	C1-O2A-CGA	2.04	121.80	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	802	CLA	CHD-C4C-NC	2.04	127.42	124.20
16	A	816	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
16	B	841	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
19	A	848	BCR	C15-C16-C17	2.04	127.65	123.47
16	2	402	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
16	A	816	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
16	A	810	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
19	1	516	BCR	C34-C9-C8	2.04	121.29	118.08
16	B	805	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
16	6	405	CLA	CHB-C4A-NA	2.04	127.33	124.51
16	B	840	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
16	1	510	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
16	B	830	CLA	CHC-C1C-NC	2.04	127.29	124.20
16	1	512	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
16	A	809	CLA	CHC-C1C-NC	2.04	127.29	124.20
16	5	412	CLA	CHB-C4A-NA	2.03	127.33	124.51
16	5	411	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
19	K	102	BCR	C34-C9-C8	2.03	121.28	118.08
16	1	512	CLA	CHC-C1C-NC	2.03	127.29	124.20
16	B	834	CLA	O2A-CGA-CBA	2.03	118.29	111.91
16	1	525	CLA	CBA-CAA-C2A	2.03	119.86	113.86
16	B	819	CLA	CHB-C4A-NA	2.03	127.32	124.51
19	1	518	BCR	C11-C10-C9	2.03	130.21	127.31
16	B	838	CLA	CMB-C2B-C1B	2.03	131.59	128.46
19	F	202	BCR	C11-C10-C9	2.03	130.21	127.31
16	B	825	CLA	C5-C3-C2	-2.03	117.01	121.12
16	B	839	CLA	C4-C3-C5	2.03	118.69	115.27
16	B	808	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
16	4	411	CLA	CED-O2D-CGD	2.03	120.52	115.94
16	J	102	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
19	B	846	BCR	C35-C13-C14	-2.03	120.08	122.92
16	1	519	CLA	C1B-CHB-C4A	-2.03	126.11	130.12
16	A	834	CLA	CMB-C2B-C1B	2.03	131.58	128.46
16	B	826	CLA	CBA-CAA-C2A	-2.03	107.89	113.86
16	4	407	CLA	CED-O2D-CGD	2.02	120.52	115.94
16	F	201	CLA	C2A-C1A-CHA	-2.02	120.32	123.86
16	K	103	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
19	1	522	BCR	C15-C16-C17	2.02	127.62	123.47
16	B	829	CLA	C6-C5-C3	2.02	118.76	113.45
16	A	811	CLA	CHB-C4A-NA	2.02	127.31	124.51
16	A	812	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
16	1	513	CLA	CHB-C4A-NA	2.02	127.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	829	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
16	F	201	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
16	5	422	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
16	A	819	CLA	CHB-C4A-NA	2.02	127.30	124.51
16	5	419	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
16	A	814	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
16	B	804	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
19	5	420	BCR	C34-C9-C8	2.02	121.25	118.08
16	B	806	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
16	5	410	CLA	CMB-C2B-C3B	2.02	128.45	124.68
16	A	806	CLA	CHC-C1C-NC	2.01	127.26	124.20
16	A	843	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
16	1	505	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
16	B	819	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
16	A	824	CLA	C4-C3-C5	2.01	118.28	115.98
19	1	523	BCR	C16-C15-C14	2.01	127.60	123.47
19	A	846	BCR	C24-C23-C22	2.01	129.28	126.23
16	A	822	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
16	B	837	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
16	1	508	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
16	A	832	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
16	A	832	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
16	A	814	CLA	C1-C2-C3	-2.01	122.57	126.04
16	5	418	CLA	CHC-C1C-NC	2.01	127.25	124.20
16	A	818	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
16	A	814	CLA	CHA-C1A-NA	-2.01	121.80	126.40
19	B	844	BCR	C16-C15-C14	2.01	127.59	123.47
16	B	802	CLA	O2A-CGA-CBA	2.01	118.21	111.91
16	5	421	CLA	CED-O2D-CGD	2.01	120.47	115.94
16	1	509	CLA	O2A-CGA-CBA	2.00	120.47	114.03
16	J	101	CLA	CMB-C2B-C3B	2.00	128.43	124.68
16	1	514	CLA	CED-O2D-CGD	2.00	120.47	115.94
16	A	811	CLA	CHC-C1C-NC	2.00	127.24	124.20
16	J	101	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
16	5	412	CLA	CED-O2D-CGD	2.00	120.47	115.94
16	6	405	CLA	CHC-C1C-NC	2.00	127.24	124.20
16	F	204	CLA	CHC-C1C-NC	2.00	127.24	124.20
16	1	504	CLA	C1B-CHB-C4A	-2.00	126.16	130.12

All (141) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
15	A	801	CL0	NC
15	A	801	CL0	ND
16	A	802	CLA	ND
16	A	803	CLA	ND
16	A	804	CLA	ND
16	A	805	CLA	ND
16	A	806	CLA	ND
16	A	807	CLA	ND
16	A	808	CLA	ND
16	A	809	CLA	ND
16	A	811	CLA	ND
16	A	812	CLA	ND
16	A	813	CLA	ND
16	A	814	CLA	ND
16	A	815	CLA	ND
16	A	816	CLA	ND
16	A	819	CLA	ND
16	A	820	CLA	ND
16	A	822	CLA	ND
16	A	826	CLA	ND
16	A	827	CLA	ND
16	A	828	CLA	ND
16	A	829	CLA	ND
16	A	830	CLA	ND
16	A	831	CLA	ND
16	A	833	CLA	ND
16	A	834	CLA	ND
16	A	835	CLA	ND
16	A	836	CLA	ND
16	A	837	CLA	ND
16	A	838	CLA	ND
16	A	839	CLA	ND
16	A	840	CLA	ND
16	A	841	CLA	ND
16	A	842	CLA	ND
16	A	843	CLA	ND
16	B	801	CLA	ND
16	B	802	CLA	ND
16	B	803	CLA	ND
16	B	804	CLA	ND
16	B	805	CLA	ND

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Mol	Chain	Res	Type	Atom
16	B	806	CLA	ND
16	B	807	CLA	ND
16	B	808	CLA	ND
16	B	809	CLA	ND
16	B	810	CLA	ND
16	B	811	CLA	ND
16	B	812	CLA	ND
16	B	813	CLA	ND
16	B	814	CLA	ND
16	B	817	CLA	ND
16	B	818	CLA	ND
16	B	819	CLA	ND
16	B	822	CLA	ND
16	B	823	CLA	ND
16	B	824	CLA	ND
16	B	825	CLA	ND
16	B	826	CLA	ND
16	B	827	CLA	ND
16	B	828	CLA	ND
16	B	829	CLA	ND
16	B	830	CLA	ND
16	B	831	CLA	ND
16	B	832	CLA	ND
16	B	833	CLA	ND
16	B	834	CLA	ND
16	B	835	CLA	ND
16	B	836	CLA	ND
16	B	837	CLA	ND
16	B	838	CLA	ND
16	B	839	CLA	ND
16	B	840	CLA	ND
16	F	201	CLA	ND
16	F	204	CLA	ND
16	J	101	CLA	ND
16	J	102	CLA	ND
16	K	101	CLA	ND
16	K	103	CLA	ND
16	X	101	CLA	ND
16	1	501	CLA	ND
16	1	502	CLA	ND
16	1	503	CLA	ND
16	1	505	CLA	ND

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Mol	Chain	Res	Type	Atom
16	1	506	CLA	ND
16	1	507	CLA	ND
16	1	508	CLA	ND
16	1	509	CLA	ND
16	1	510	CLA	ND
16	1	511	CLA	ND
16	1	512	CLA	ND
16	1	513	CLA	ND
16	1	514	CLA	ND
16	1	515	CLA	ND
16	1	521	CLA	ND
16	1	525	CLA	ND
16	1	526	CLA	ND
16	2	401	CLA	ND
16	2	402	CLA	ND
16	2	403	CLA	ND
16	2	404	CLA	ND
16	2	405	CLA	ND
16	2	406	CLA	ND
16	3	401	CLA	ND
16	4	402	CLA	ND
16	4	403	CLA	ND
16	4	404	CLA	ND
16	4	405	CLA	ND
16	4	406	CLA	ND
16	4	407	CLA	ND
16	4	408	CLA	ND
16	4	409	CLA	ND
16	4	410	CLA	ND
16	4	411	CLA	ND
16	5	403	CLA	ND
16	5	404	CLA	ND
16	5	405	CLA	ND
16	5	406	CLA	ND
16	5	407	CLA	ND
16	5	408	CLA	ND
16	5	409	CLA	ND
16	5	410	CLA	ND
16	5	411	CLA	ND
16	5	412	CLA	ND
16	5	413	CLA	ND
16	5	414	CLA	ND

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Mol	Chain	Res	Type	Atom
16	5	415	CLA	ND
16	5	416	CLA	ND
16	5	417	CLA	ND
16	5	418	CLA	ND
16	5	419	CLA	ND
16	5	421	CLA	ND
16	5	422	CLA	ND
16	6	401	CLA	ND
16	6	402	CLA	ND
16	6	403	CLA	ND
16	6	404	CLA	ND
16	6	405	CLA	ND
16	6	406	CLA	ND
16	6	407	CLA	ND
16	6	408	CLA	ND
16	6	409	CLA	ND

All (1379) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	806	CLA	CBA-CGA-O2A-C1
16	A	806	CLA	O1A-CGA-O2A-C1
16	A	806	CLA	CHA-CBD-CGD-O1D
16	A	806	CLA	CHA-CBD-CGD-O2D
16	A	806	CLA	CAD-CBD-CGD-O1D
16	A	808	CLA	C4-C3-C5-C6
16	A	810	CLA	C1A-C2A-CAA-CBA
16	A	814	CLA	O2A-C1-C2-C3
16	A	819	CLA	C3A-C2A-CAA-CBA
16	A	820	CLA	C1A-C2A-CAA-CBA
16	A	820	CLA	C3A-C2A-CAA-CBA
16	A	823	CLA	C3A-C2A-CAA-CBA
16	A	825	CLA	CHA-CBD-CGD-O1D
16	A	829	CLA	C4-C3-C5-C6
16	A	831	CLA	CHA-CBD-CGD-O1D
16	A	831	CLA	CHA-CBD-CGD-O2D
16	A	832	CLA	C2A-CAA-CBA-CGA
16	A	835	CLA	CHA-CBD-CGD-O1D
16	A	835	CLA	CHA-CBD-CGD-O2D
16	A	836	CLA	C2-C3-C5-C6
16	A	836	CLA	C4-C3-C5-C6
16	A	838	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	A	838	CLA	C3A-C2A-CAA-CBA
16	A	838	CLA	C2-C3-C5-C6
16	A	838	CLA	C4-C3-C5-C6
16	A	841	CLA	CHA-CBD-CGD-O1D
16	A	841	CLA	CHA-CBD-CGD-O2D
16	A	843	CLA	C2-C3-C5-C6
16	A	843	CLA	C4-C3-C5-C6
16	B	801	CLA	CHA-CBD-CGD-O1D
16	B	801	CLA	CHA-CBD-CGD-O2D
16	B	801	CLA	CBD-CGD-O2D-CED
16	B	803	CLA	CBD-CGD-O2D-CED
16	B	805	CLA	C3A-C2A-CAA-CBA
16	B	815	CLA	CHA-CBD-CGD-O1D
16	B	815	CLA	CHA-CBD-CGD-O2D
16	B	816	CLA	C1A-C2A-CAA-CBA
16	B	816	CLA	C3A-C2A-CAA-CBA
16	B	818	CLA	C1A-C2A-CAA-CBA
16	B	818	CLA	C3A-C2A-CAA-CBA
16	B	818	CLA	C2-C3-C5-C6
16	B	818	CLA	C4-C3-C5-C6
16	B	819	CLA	C2-C3-C5-C6
16	B	819	CLA	C4-C3-C5-C6
16	B	820	CLA	C1A-C2A-CAA-CBA
16	B	820	CLA	C3A-C2A-CAA-CBA
16	B	824	CLA	C4-C3-C5-C6
16	B	827	CLA	C1A-C2A-CAA-CBA
16	B	827	CLA	C3A-C2A-CAA-CBA
16	B	828	CLA	C1A-C2A-CAA-CBA
16	B	828	CLA	C3A-C2A-CAA-CBA
16	B	829	CLA	CHA-CBD-CGD-O1D
16	B	829	CLA	CHA-CBD-CGD-O2D
16	B	829	CLA	C4-C3-C5-C6
16	B	830	CLA	C2-C3-C5-C6
16	B	830	CLA	C4-C3-C5-C6
16	B	834	CLA	C2-C3-C5-C6
16	B	834	CLA	C4-C3-C5-C6
16	B	835	CLA	C1A-C2A-CAA-CBA
16	B	835	CLA	C3A-C2A-CAA-CBA
16	B	838	CLA	CHA-CBD-CGD-O1D
16	B	841	CLA	CBD-CGD-O2D-CED
16	J	101	CLA	CHA-CBD-CGD-O1D
16	J	101	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	1	501	CLA	CHA-CBD-CGD-O1D
16	1	501	CLA	CHA-CBD-CGD-O2D
16	1	501	CLA	CAD-CBD-CGD-O1D
16	1	507	CLA	CBD-CGD-O2D-CED
16	1	508	CLA	CHA-CBD-CGD-O1D
16	1	508	CLA	CHA-CBD-CGD-O2D
16	1	511	CLA	CBD-CGD-O2D-CED
16	1	511	CLA	C4-C3-C5-C6
16	1	513	CLA	C1A-C2A-CAA-CBA
16	1	513	CLA	C3A-C2A-CAA-CBA
16	1	515	CLA	C1A-C2A-CAA-CBA
16	1	515	CLA	C3A-C2A-CAA-CBA
16	1	519	CLA	C1A-C2A-CAA-CBA
16	1	519	CLA	C3A-C2A-CAA-CBA
16	3	401	CLA	CBD-CGD-O2D-CED
16	4	403	CLA	CBD-CGD-O2D-CED
16	4	406	CLA	CBD-CGD-O2D-CED
16	5	413	CLA	C1A-C2A-CAA-CBA
16	5	414	CLA	CBD-CGD-O2D-CED
16	5	417	CLA	CBD-CGD-O2D-CED
16	6	402	CLA	CBD-CGD-O2D-CED
19	A	849	BCR	C6-C7-C8-C9
19	A	849	BCR	C7-C8-C9-C10
19	A	849	BCR	C7-C8-C9-C34
19	A	849	BCR	C17-C18-C19-C20
19	A	849	BCR	C36-C18-C19-C20
19	A	849	BCR	C18-C19-C20-C21
19	A	849	BCR	C20-C21-C22-C37
19	A	849	BCR	C21-C22-C23-C24
19	A	849	BCR	C37-C22-C23-C24
19	A	850	BCR	C21-C22-C23-C24
19	A	850	BCR	C37-C22-C23-C24
19	B	843	BCR	C21-C22-C23-C24
19	B	843	BCR	C37-C22-C23-C24
19	B	844	BCR	C7-C8-C9-C10
19	B	844	BCR	C7-C8-C9-C34
19	B	845	BCR	C21-C22-C23-C24
19	B	845	BCR	C37-C22-C23-C24
19	B	847	BCR	C23-C24-C25-C30
19	F	202	BCR	C37-C22-C23-C24
19	J	103	BCR	C7-C8-C9-C10
19	J	103	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
19	J	103	BCR	C11-C10-C9-C34
19	K	102	BCR	C1-C6-C7-C8
19	K	102	BCR	C5-C6-C7-C8
19	K	102	BCR	C22-C23-C24-C25
19	M	102	BCR	C7-C8-C9-C34
19	1	516	BCR	C6-C7-C8-C9
19	1	516	BCR	C16-C17-C18-C19
19	1	516	BCR	C16-C17-C18-C36
19	1	516	BCR	C23-C24-C25-C26
19	1	516	BCR	C23-C24-C25-C30
19	1	517	BCR	C1-C6-C7-C8
19	1	517	BCR	C5-C6-C7-C8
19	1	517	BCR	C6-C7-C8-C9
19	1	517	BCR	C11-C10-C9-C8
19	1	517	BCR	C11-C10-C9-C34
19	1	517	BCR	C10-C11-C12-C13
19	1	517	BCR	C22-C23-C24-C25
19	1	518	BCR	C6-C7-C8-C9
19	1	522	BCR	C37-C22-C23-C24
19	1	522	BCR	C23-C24-C25-C26
19	1	523	BCR	C22-C23-C24-C25
19	4	401	BCR	C7-C8-C9-C34
19	4	401	BCR	C11-C12-C13-C14
19	4	401	BCR	C11-C12-C13-C35
19	4	401	BCR	C16-C17-C18-C19
19	4	401	BCR	C16-C17-C18-C36
19	4	401	BCR	C22-C23-C24-C25
19	5	402	BCR	C6-C7-C8-C9
19	5	420	BCR	C22-C23-C24-C25
20	A	853	LHG	O1-C1-C2-C3
20	B	850	LHG	O1-C1-C2-C3
20	B	850	LHG	C3-O3-P-O5
20	F	203	LHG	O1-C1-C2-C3
20	F	203	LHG	C2-C3-O3-P
16	5	411	CLA	O1D-CGD-O2D-CED
21	A	854	LMT	C3'-C4'-O1B-C1B
16	4	406	CLA	O1D-CGD-O2D-CED
16	5	405	CLA	O1D-CGD-O2D-CED
16	A	824	CLA	CBD-CGD-O2D-CED
16	A	835	CLA	CBD-CGD-O2D-CED
16	B	814	CLA	CBD-CGD-O2D-CED
16	B	821	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	B	835	CLA	CBD-CGD-O2D-CED
16	F	201	CLA	CBD-CGD-O2D-CED
16	J	101	CLA	CBD-CGD-O2D-CED
16	X	101	CLA	CBD-CGD-O2D-CED
16	1	504	CLA	CBD-CGD-O2D-CED
16	1	509	CLA	CBD-CGD-O2D-CED
16	1	525	CLA	CBD-CGD-O2D-CED
16	1	526	CLA	CBD-CGD-O2D-CED
16	2	401	CLA	CBD-CGD-O2D-CED
16	4	402	CLA	CBD-CGD-O2D-CED
16	4	407	CLA	CBD-CGD-O2D-CED
16	4	410	CLA	CBD-CGD-O2D-CED
16	4	411	CLA	CBD-CGD-O2D-CED
16	5	405	CLA	CBD-CGD-O2D-CED
16	5	411	CLA	CBD-CGD-O2D-CED
16	5	412	CLA	CBD-CGD-O2D-CED
16	5	421	CLA	CBD-CGD-O2D-CED
16	6	409	CLA	CBD-CGD-O2D-CED
16	B	831	CLA	O1A-CGA-O2A-C1
21	B	852	LMT	C3'-C4'-O1B-C1B
16	B	801	CLA	O1D-CGD-O2D-CED
16	X	101	CLA	O1D-CGD-O2D-CED
16	1	504	CLA	O1D-CGD-O2D-CED
16	1	526	CLA	O1D-CGD-O2D-CED
16	5	414	CLA	O1D-CGD-O2D-CED
16	B	841	CLA	O1D-CGD-O2D-CED
16	1	507	CLA	O1D-CGD-O2D-CED
16	1	509	CLA	O1D-CGD-O2D-CED
16	1	511	CLA	O1D-CGD-O2D-CED
16	3	401	CLA	O1D-CGD-O2D-CED
16	4	403	CLA	O1D-CGD-O2D-CED
16	5	417	CLA	O1D-CGD-O2D-CED
16	B	831	CLA	CBA-CGA-O2A-C1
16	A	817	CLA	CBD-CGD-O2D-CED
16	B	806	CLA	CBD-CGD-O2D-CED
16	B	808	CLA	CBD-CGD-O2D-CED
16	B	815	CLA	CBD-CGD-O2D-CED
16	B	825	CLA	CBD-CGD-O2D-CED
16	B	829	CLA	CBD-CGD-O2D-CED
16	1	502	CLA	CBD-CGD-O2D-CED
16	1	503	CLA	CBD-CGD-O2D-CED
16	1	506	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	2	405	CLA	CBD-CGD-O2D-CED
16	4	409	CLA	CBD-CGD-O2D-CED
16	5	403	CLA	CBD-CGD-O2D-CED
16	5	409	CLA	CBD-CGD-O2D-CED
16	5	415	CLA	CBD-CGD-O2D-CED
16	5	422	CLA	CBD-CGD-O2D-CED
16	6	405	CLA	CBD-CGD-O2D-CED
16	A	803	CLA	O1A-CGA-O2A-C1
16	A	809	CLA	O1A-CGA-O2A-C1
16	A	822	CLA	O1A-CGA-O2A-C1
16	B	803	CLA	O1D-CGD-O2D-CED
21	B	851	LMT	C3'-C4'-O1B-C1B
16	B	811	CLA	CBD-CGD-O2D-CED
16	B	818	CLA	CBD-CGD-O2D-CED
16	B	833	CLA	CBD-CGD-O2D-CED
16	1	510	CLA	CBD-CGD-O2D-CED
16	1	521	CLA	CBD-CGD-O2D-CED
16	2	404	CLA	CBD-CGD-O2D-CED
16	5	419	CLA	CBD-CGD-O2D-CED
16	6	404	CLA	CBD-CGD-O2D-CED
16	6	402	CLA	O1D-CGD-O2D-CED
16	A	821	CLA	O1A-CGA-O2A-C1
16	A	814	CLA	C3-C5-C6-C7
16	A	827	CLA	C3-C5-C6-C7
16	B	808	CLA	C3-C5-C6-C7
16	B	825	CLA	C3-C5-C6-C7
16	B	834	CLA	C3-C5-C6-C7
16	A	803	CLA	CBA-CGA-O2A-C1
16	A	805	CLA	CBA-CGA-O2A-C1
16	A	809	CLA	CBA-CGA-O2A-C1
16	A	822	CLA	CBA-CGA-O2A-C1
16	B	810	CLA	CBA-CGA-O2A-C1
16	A	824	CLA	O1D-CGD-O2D-CED
16	A	831	CLA	CBD-CGD-O2D-CED
16	B	805	CLA	CBD-CGD-O2D-CED
16	1	519	CLA	O1A-CGA-O2A-C1
21	5	401	LMT	C3'-C4'-O1B-C1B
16	B	824	CLA	C2-C3-C5-C6
16	B	819	CLA	CBD-CGD-O2D-CED
16	1	508	CLA	CBD-CGD-O2D-CED
16	1	519	CLA	CBD-CGD-O2D-CED
16	A	809	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	A	838	CLA	C2A-CAA-CBA-CGA
16	B	810	CLA	C2A-CAA-CBA-CGA
16	J	102	CLA	C2A-CAA-CBA-CGA
16	4	410	CLA	C2A-CAA-CBA-CGA
16	5	418	CLA	C2A-CAA-CBA-CGA
16	B	816	CLA	O1A-CGA-O2A-C1
16	J	101	CLA	O1D-CGD-O2D-CED
16	6	409	CLA	O1D-CGD-O2D-CED
16	A	807	CLA	C3-C5-C6-C7
16	B	804	CLA	C3-C5-C6-C7
16	B	822	CLA	C3-C5-C6-C7
16	B	829	CLA	C3-C5-C6-C7
16	B	833	CLA	C3-C5-C6-C7
16	B	839	CLA	C3-C5-C6-C7
16	A	812	CLA	CBA-CGA-O2A-C1
16	A	820	CLA	CBA-CGA-O2A-C1
16	A	821	CLA	CBA-CGA-O2A-C1
16	B	811	CLA	CBA-CGA-O2A-C1
16	B	833	CLA	CBA-CGA-O2A-C1
16	B	839	CLA	CBA-CGA-O2A-C1
16	F	201	CLA	O1D-CGD-O2D-CED
16	4	411	CLA	O1D-CGD-O2D-CED
16	A	805	CLA	CBD-CGD-O2D-CED
16	A	823	CLA	CBD-CGD-O2D-CED
16	A	835	CLA	O1D-CGD-O2D-CED
16	B	821	CLA	O1D-CGD-O2D-CED
16	B	810	CLA	O1A-CGA-O2A-C1
16	B	835	CLA	O1D-CGD-O2D-CED
16	4	410	CLA	O1D-CGD-O2D-CED
19	4	401	BCR	C15-C16-C17-C18
16	A	814	CLA	CBD-CGD-O2D-CED
16	A	820	CLA	CBD-CGD-O2D-CED
16	A	825	CLA	CBD-CGD-O2D-CED
16	A	833	CLA	CBD-CGD-O2D-CED
16	A	840	CLA	CBD-CGD-O2D-CED
16	A	842	CLA	CBD-CGD-O2D-CED
16	B	831	CLA	CBD-CGD-O2D-CED
16	1	505	CLA	CBD-CGD-O2D-CED
16	2	406	CLA	CBD-CGD-O2D-CED
16	B	814	CLA	O1D-CGD-O2D-CED
16	4	402	CLA	O1D-CGD-O2D-CED
17	A	844	PQN	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	A	807	CLA	CBA-CGA-O2A-C1
16	A	838	CLA	CBA-CGA-O2A-C1
16	B	805	CLA	CBA-CGA-O2A-C1
16	B	816	CLA	CBA-CGA-O2A-C1
16	B	834	CLA	CBA-CGA-O2A-C1
16	1	519	CLA	CBA-CGA-O2A-C1
16	A	805	CLA	O1A-CGA-O2A-C1
16	A	820	CLA	O1A-CGA-O2A-C1
16	B	811	CLA	O1A-CGA-O2A-C1
22	B	849	LMG	O6-C5-C6-O5
16	1	525	CLA	O1D-CGD-O2D-CED
16	A	837	CLA	CBD-CGD-O2D-CED
16	B	809	CLA	CBD-CGD-O2D-CED
16	1	514	CLA	CBD-CGD-O2D-CED
16	5	412	CLA	O1D-CGD-O2D-CED
16	B	838	CLA	C3-C5-C6-C7
16	A	812	CLA	O1A-CGA-O2A-C1
16	B	833	CLA	O1A-CGA-O2A-C1
16	A	813	CLA	C4-C3-C5-C6
16	B	802	CLA	C4-C3-C5-C6
16	B	823	CLA	C4-C3-C5-C6
16	1	521	CLA	C4-C3-C5-C6
22	B	849	LMG	C4-C5-C6-O5
16	A	813	CLA	C2-C3-C5-C6
16	A	829	CLA	C2-C3-C5-C6
16	B	802	CLA	C2-C3-C5-C6
16	B	823	CLA	C2-C3-C5-C6
16	B	829	CLA	C2-C3-C5-C6
16	1	521	CLA	C2-C3-C5-C6
16	A	803	CLA	C2A-CAA-CBA-CGA
16	B	840	CLA	C2A-CAA-CBA-CGA
16	5	421	CLA	C2A-CAA-CBA-CGA
16	5	421	CLA	O1D-CGD-O2D-CED
16	B	805	CLA	O1A-CGA-O2A-C1
16	B	834	CLA	O1A-CGA-O2A-C1
16	B	839	CLA	O1A-CGA-O2A-C1
21	B	851	LMT	O5'-C1'-O1'-C1
16	A	806	CLA	C3-C5-C6-C7
16	A	824	CLA	CBA-CGA-O2A-C1
16	B	822	CLA	CBA-CGA-O2A-C1
16	A	817	CLA	O1D-CGD-O2D-CED
21	M	101	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
16	B	815	CLA	O1D-CGD-O2D-CED
16	1	506	CLA	O1D-CGD-O2D-CED
16	2	401	CLA	O1D-CGD-O2D-CED
16	4	407	CLA	O1D-CGD-O2D-CED
16	5	403	CLA	O1D-CGD-O2D-CED
16	5	409	CLA	O1D-CGD-O2D-CED
16	A	807	CLA	O1A-CGA-O2A-C1
16	B	806	CLA	O1D-CGD-O2D-CED
16	2	405	CLA	O1D-CGD-O2D-CED
16	4	409	CLA	O1D-CGD-O2D-CED
16	6	405	CLA	O1D-CGD-O2D-CED
16	B	824	CLA	CBD-CGD-O2D-CED
16	6	408	CLA	CBD-CGD-O2D-CED
16	A	824	CLA	O1A-CGA-O2A-C1
16	A	838	CLA	O1A-CGA-O2A-C1
16	B	822	CLA	O1A-CGA-O2A-C1
16	B	841	CLA	C3-C5-C6-C7
16	A	813	CLA	CBA-CGA-O2A-C1
16	A	832	CLA	CBA-CGA-O2A-C1
16	A	843	CLA	CBA-CGA-O2A-C1
16	B	841	CLA	CBA-CGA-O2A-C1
16	B	836	CLA	CBD-CGD-O2D-CED
16	5	416	CLA	CBD-CGD-O2D-CED
16	6	401	CLA	CBD-CGD-O2D-CED
16	B	825	CLA	O1D-CGD-O2D-CED
19	1	523	BCR	C19-C20-C21-C22
16	A	804	CLA	C5-C6-C7-C8
16	A	806	CLA	C10-C11-C12-C13
16	A	831	CLA	C13-C15-C16-C17
16	B	826	CLA	C10-C11-C12-C13
16	B	828	CLA	C15-C16-C17-C18
16	A	813	CLA	O1A-CGA-O2A-C1
16	A	832	CLA	O1A-CGA-O2A-C1
16	A	833	CLA	C4-C3-C5-C6
16	A	809	CLA	C6-C7-C8-C9
16	B	831	CLA	C11-C12-C13-C14
16	5	415	CLA	O1D-CGD-O2D-CED
16	B	803	CLA	C15-C16-C17-C18
16	A	843	CLA	C2A-CAA-CBA-CGA
19	A	846	BCR	C37-C22-C23-C24
19	A	847	BCR	C37-C22-C23-C24
19	A	851	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	B	848	BCR	C7-C8-C9-C34
19	I	102	BCR	C7-C8-C9-C34
19	J	103	BCR	C36-C18-C19-C20
19	1	516	BCR	C37-C22-C23-C24
19	1	517	BCR	C7-C8-C9-C34
19	1	523	BCR	C37-C22-C23-C24
19	5	420	BCR	C36-C18-C19-C20
19	5	420	BCR	C37-C22-C23-C24
19	A	851	BCR	C21-C22-C23-C24
19	I	102	BCR	C7-C8-C9-C10
19	K	102	BCR	C21-C22-C23-C24
19	M	102	BCR	C7-C8-C9-C10
19	1	517	BCR	C7-C8-C9-C10
19	1	522	BCR	C21-C22-C23-C24
19	1	523	BCR	C21-C22-C23-C24
16	A	843	CLA	O1A-CGA-O2A-C1
16	A	820	CLA	C13-C15-C16-C17
16	A	826	CLA	C15-C16-C17-C18
16	B	825	CLA	C8-C10-C11-C12
16	B	834	CLA	C8-C10-C11-C12
16	1	503	CLA	O1D-CGD-O2D-CED
16	A	804	CLA	CBA-CGA-O2A-C1
16	A	840	CLA	C15-C16-C17-C18
16	B	808	CLA	C13-C15-C16-C17
16	B	809	CLA	C5-C6-C7-C8
16	B	827	CLA	C8-C10-C11-C12
16	B	829	CLA	C10-C11-C12-C13
16	B	832	CLA	C15-C16-C17-C18
16	B	829	CLA	O1D-CGD-O2D-CED
16	5	422	CLA	O1D-CGD-O2D-CED
16	A	804	CLA	C13-C15-C16-C17
16	B	819	CLA	C10-C11-C12-C13
16	B	808	CLA	O1D-CGD-O2D-CED
16	A	809	CLA	CBD-CGD-O2D-CED
16	B	813	CLA	C5-C6-C7-C8
16	B	813	CLA	C10-C11-C12-C13
16	A	830	CLA	CBA-CGA-O2A-C1
16	A	809	CLA	C13-C15-C16-C17
16	A	822	CLA	C8-C10-C11-C12
16	B	839	CLA	C5-C6-C7-C8
16	1	520	CLA	C10-C11-C12-C13
17	B	842	PQN	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
16	B	811	CLA	O1D-CGD-O2D-CED
21	1	524	LMT	C3'-C4'-O1B-C1B
16	B	801	CLA	C10-C11-C12-C13
16	B	808	CLA	C5-C6-C7-C8
17	A	844	PQN	C15-C16-C17-C18
16	1	510	CLA	O1D-CGD-O2D-CED
16	B	826	CLA	C6-C7-C8-C10
16	A	804	CLA	O1A-CGA-O2A-C1
19	4	401	BCR	C9-C10-C11-C12
16	A	837	CLA	C2A-CAA-CBA-CGA
16	B	817	CLA	C2A-CAA-CBA-CGA
16	1	515	CLA	C2A-CAA-CBA-CGA
16	B	818	CLA	O1D-CGD-O2D-CED
16	1	502	CLA	O1D-CGD-O2D-CED
16	1	521	CLA	O1D-CGD-O2D-CED
16	2	404	CLA	O1D-CGD-O2D-CED
16	5	419	CLA	O1D-CGD-O2D-CED
16	6	404	CLA	O1D-CGD-O2D-CED
19	I	101	BCR	C6-C7-C8-C9
16	6	403	CLA	CBD-CGD-O2D-CED
16	B	832	CLA	C10-C11-C12-C13
16	A	831	CLA	O1D-CGD-O2D-CED
19	A	848	BCR	C10-C11-C12-C13
19	B	843	BCR	C18-C19-C20-C21
19	J	104	BCR	C18-C19-C20-C21
19	K	102	BCR	C18-C19-C20-C21
19	1	523	BCR	C18-C19-C20-C21
19	4	401	BCR	C10-C11-C12-C13
19	4	401	BCR	C18-C19-C20-C21
16	A	843	CLA	C10-C11-C12-C13
16	B	805	CLA	C13-C15-C16-C17
16	B	830	CLA	C10-C11-C12-C13
16	B	840	CLA	C8-C10-C11-C12
16	B	841	CLA	O1A-CGA-O2A-C1
16	A	803	CLA	C15-C16-C17-C18
16	B	828	CLA	C13-C15-C16-C17
16	A	830	CLA	O1A-CGA-O2A-C1
16	A	826	CLA	C8-C10-C11-C12
16	A	840	CLA	C8-C10-C11-C12
16	1	520	CLA	CBA-CGA-O2A-C1
16	B	822	CLA	CBD-CGD-O2D-CED
20	B	850	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	B	805	CLA	O1D-CGD-O2D-CED
16	B	833	CLA	O1D-CGD-O2D-CED
16	1	508	CLA	O1D-CGD-O2D-CED
16	A	805	CLA	C3-C5-C6-C7
16	A	805	CLA	O1D-CGD-O2D-CED
16	A	836	CLA	CBA-CGA-O2A-C1
16	A	814	CLA	O1D-CGD-O2D-CED
16	6	407	CLA	CBD-CGD-O2D-CED
19	A	849	BCR	C11-C10-C9-C34
19	B	843	BCR	C11-C10-C9-C34
19	B	846	BCR	C35-C13-C14-C15
19	B	847	BCR	C11-C10-C9-C34
19	B	847	BCR	C35-C13-C14-C15
19	F	202	BCR	C35-C13-C14-C15
19	F	205	BCR	C35-C13-C14-C15
19	I	102	BCR	C20-C21-C22-C37
19	M	102	BCR	C11-C10-C9-C34
19	M	102	BCR	C20-C21-C22-C37
19	1	517	BCR	C35-C13-C14-C15
19	4	401	BCR	C11-C10-C9-C34
20	F	203	LHG	C28-C29-C30-C31
16	1	519	CLA	O1D-CGD-O2D-CED
16	B	822	CLA	C6-C7-C8-C9
22	B	849	LMG	C11-C12-C13-C14
22	B	849	LMG	C34-C35-C36-C37
16	A	820	CLA	O1D-CGD-O2D-CED
16	B	819	CLA	O1D-CGD-O2D-CED
16	B	816	CLA	C2C-C3C-CAC-CBC
22	B	849	LMG	C17-C18-C19-C20
16	A	829	CLA	C3-C5-C6-C7
19	A	849	BCR	C11-C10-C9-C8
19	A	849	BCR	C20-C21-C22-C23
19	B	846	BCR	C12-C13-C14-C15
19	B	847	BCR	C11-C10-C9-C8
19	F	202	BCR	C12-C13-C14-C15
19	I	102	BCR	C20-C21-C22-C23
19	J	103	BCR	C11-C10-C9-C8
19	M	102	BCR	C11-C10-C9-C8
19	1	517	BCR	C12-C13-C14-C15
19	4	401	BCR	C11-C10-C9-C8
16	B	825	CLA	C6-C7-C8-C9
16	A	823	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	1	505	CLA	O1D-CGD-O2D-CED
20	A	852	LHG	C10-C11-C12-C13
21	A	854	LMT	C4-C5-C6-C7
22	B	849	LMG	C36-C37-C38-C39
16	B	808	CLA	C8-C10-C11-C12
16	B	841	CLA	C2A-CAA-CBA-CGA
16	2	401	CLA	C2A-CAA-CBA-CGA
16	2	402	CLA	C2A-CAA-CBA-CGA
16	A	825	CLA	O1D-CGD-O2D-CED
16	1	520	CLA	O1A-CGA-O2A-C1
19	K	102	BCR	C37-C22-C23-C24
19	A	846	BCR	C21-C22-C23-C24
19	J	104	BCR	C7-C8-C9-C10
16	A	842	CLA	O1D-CGD-O2D-CED
16	1	519	CLA	C10-C11-C12-C13
21	1	524	LMT	C6-C7-C8-C9
16	B	822	CLA	C6-C7-C8-C10
22	B	849	LMG	C21-C22-C23-C24
16	B	826	CLA	CBD-CGD-O2D-CED
16	2	406	CLA	O1D-CGD-O2D-CED
20	A	852	LHG	C24-C25-C26-C27
21	B	852	LMT	C5-C6-C7-C8
22	B	849	LMG	C29-C30-C31-C32
16	B	811	CLA	C5-C6-C7-C8
16	A	829	CLA	CBA-CGA-O2A-C1
16	A	833	CLA	O1D-CGD-O2D-CED
16	A	837	CLA	O1D-CGD-O2D-CED
16	A	807	CLA	C3A-C2A-CAA-CBA
16	A	810	CLA	C3A-C2A-CAA-CBA
16	1	512	CLA	C3A-C2A-CAA-CBA
16	4	408	CLA	C3A-C2A-CAA-CBA
16	5	413	CLA	C3A-C2A-CAA-CBA
16	A	834	CLA	C8-C10-C11-C12
16	A	840	CLA	C5-C6-C7-C8
21	A	854	LMT	C2-C1-O1'-C1'
20	A	852	LHG	C30-C31-C32-C33
16	B	840	CLA	CBD-CGD-O2D-CED
20	B	850	LHG	C25-C26-C27-C28
20	F	203	LHG	C11-C10-C9-C8
16	B	805	CLA	C10-C11-C12-C13
16	B	807	CLA	C4-C3-C5-C6
16	B	828	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	A	820	CLA	C2-C3-C5-C6
16	A	833	CLA	C2-C3-C5-C6
16	B	807	CLA	C2-C3-C5-C6
16	B	828	CLA	C2-C3-C5-C6
20	A	853	LHG	O1-C1-C2-O2
20	B	850	LHG	O1-C1-C2-O2
16	B	829	CLA	C5-C6-C7-C8
16	A	829	CLA	O1A-CGA-O2A-C1
16	A	836	CLA	O1A-CGA-O2A-C1
16	A	822	CLA	C10-C11-C12-C13
20	B	850	LHG	C26-C27-C28-C29
16	A	829	CLA	C2-C1-O2A-CGA
16	A	843	CLA	C2-C1-O2A-CGA
21	B	852	LMT	C4'-C5'-C6'-O6'
21	M	101	LMT	C4'-C5'-C6'-O6'
16	B	840	CLA	C10-C11-C12-C13
19	A	849	BCR	C23-C24-C25-C26
19	A	849	BCR	C23-C24-C25-C30
19	B	845	BCR	C23-C24-C25-C26
19	B	845	BCR	C23-C24-C25-C30
19	B	846	BCR	C23-C24-C25-C30
19	B	847	BCR	C23-C24-C25-C26
19	B	853	BCR	C23-C24-C25-C26
19	B	853	BCR	C23-C24-C25-C30
19	J	103	BCR	C1-C6-C7-C8
19	J	103	BCR	C5-C6-C7-C8
19	J	104	BCR	C23-C24-C25-C26
19	J	104	BCR	C23-C24-C25-C30
19	K	102	BCR	C23-C24-C25-C26
19	K	102	BCR	C23-C24-C25-C30
19	M	102	BCR	C23-C24-C25-C26
19	M	102	BCR	C23-C24-C25-C30
19	1	522	BCR	C23-C24-C25-C30
19	5	420	BCR	C23-C24-C25-C26
19	5	420	BCR	C23-C24-C25-C30
16	A	803	CLA	C10-C11-C12-C13
16	A	833	CLA	C5-C6-C7-C8
16	A	820	CLA	C4-C3-C5-C6
16	B	840	CLA	C4-C3-C5-C6
16	B	809	CLA	O1D-CGD-O2D-CED
16	A	843	CLA	C6-C7-C8-C10
16	B	803	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	B	810	CLA	C11-C10-C8-C7
16	B	818	CLA	C5-C6-C7-C8
16	A	840	CLA	O1D-CGD-O2D-CED
16	1	514	CLA	O1D-CGD-O2D-CED
16	B	804	CLA	CBA-CGA-O2A-C1
16	B	820	CLA	CBA-CGA-O2A-C1
16	A	802	CLA	C2A-CAA-CBA-CGA
16	3	401	CLA	C2A-CAA-CBA-CGA
16	4	402	CLA	C2A-CAA-CBA-CGA
16	A	828	CLA	C10-C11-C12-C13
16	A	830	CLA	C5-C6-C7-C8
16	B	806	CLA	C5-C6-C7-C8
21	B	852	LMT	O5'-C5'-C6'-O6'
20	B	850	LHG	C11-C10-C9-C8
22	B	849	LMG	C32-C33-C34-C35
16	B	831	CLA	O1D-CGD-O2D-CED
20	F	203	LHG	C30-C31-C32-C33
16	B	836	CLA	O1D-CGD-O2D-CED
19	A	851	BCR	C22-C23-C24-C25
19	5	402	BCR	C22-C23-C24-C25
16	A	817	CLA	CBA-CGA-O2A-C1
16	B	818	CLA	C13-C15-C16-C17
20	B	850	LHG	C32-C33-C34-C35
16	K	101	CLA	C2C-C3C-CAC-CBC
20	A	852	LHG	C32-C33-C34-C35
16	B	839	CLA	C10-C11-C12-C13
20	A	852	LHG	C11-C10-C9-C8
22	B	849	LMG	C37-C38-C39-C40
16	B	840	CLA	C2-C3-C5-C6
20	A	852	LHG	C28-C29-C30-C31
16	A	814	CLA	C11-C12-C13-C14
16	A	822	CLA	C11-C10-C8-C9
16	A	843	CLA	C6-C7-C8-C9
16	B	803	CLA	C11-C10-C8-C9
16	B	826	CLA	C6-C7-C8-C9
16	1	519	CLA	C11-C10-C8-C9
16	A	822	CLA	C2A-CAA-CBA-CGA
16	A	830	CLA	C2A-CAA-CBA-CGA
16	K	101	CLA	C2A-CAA-CBA-CGA
16	5	407	CLA	C2A-CAA-CBA-CGA
20	F	203	LHG	C24-C25-C26-C27
16	B	829	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	J	104	BCR	C7-C8-C9-C34
16	A	807	CLA	C1A-C2A-CAA-CBA
16	A	816	CLA	C1A-C2A-CAA-CBA
16	A	819	CLA	C1A-C2A-CAA-CBA
16	A	823	CLA	C1A-C2A-CAA-CBA
16	B	805	CLA	C1A-C2A-CAA-CBA
16	B	833	CLA	C1A-C2A-CAA-CBA
16	1	512	CLA	C1A-C2A-CAA-CBA
16	1	525	CLA	C1A-C2A-CAA-CBA
16	4	408	CLA	C1A-C2A-CAA-CBA
16	4	409	CLA	C1A-C2A-CAA-CBA
16	5	417	CLA	C1A-C2A-CAA-CBA
19	K	102	BCR	C19-C20-C21-C22
16	A	809	CLA	O1D-CGD-O2D-CED
16	6	401	CLA	O1D-CGD-O2D-CED
16	6	408	CLA	O1D-CGD-O2D-CED
21	1	524	LMT	C5'-C4'-O1B-C1B
16	B	829	CLA	C15-C16-C17-C18
16	A	827	CLA	CBA-CGA-O2A-C1
20	F	203	LHG	C1-C2-C3-O3
16	A	826	CLA	C4-C3-C5-C6
16	B	832	CLA	C4-C3-C5-C6
16	B	832	CLA	C2-C3-C5-C6
16	1	519	CLA	C2-C3-C5-C6
16	A	841	CLA	C8-C10-C11-C12
16	5	416	CLA	O1D-CGD-O2D-CED
16	B	833	CLA	C10-C11-C12-C13
16	A	816	CLA	CBD-CGD-O2D-CED
21	B	851	LMT	C6-C7-C8-C9
21	1	524	LMT	O5'-C5'-C6'-O6'
16	B	808	CLA	C10-C11-C12-C13
16	B	804	CLA	O1A-CGA-O2A-C1
16	B	816	CLA	C4C-C3C-CAC-CBC
21	1	524	LMT	C11-C10-C9-C8
20	F	203	LHG	O1-C1-C2-O2
16	A	817	CLA	O1A-CGA-O2A-C1
19	A	850	BCR	C20-C21-C22-C37
19	A	851	BCR	C20-C21-C22-C37
19	B	845	BCR	C11-C10-C9-C34
19	J	104	BCR	C11-C10-C9-C34
19	J	104	BCR	C35-C13-C14-C15
19	1	516	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
19	5	402	BCR	C35-C13-C14-C15
16	1	519	CLA	C4-C3-C5-C6
16	A	813	CLA	CBD-CGD-O2D-CED
16	1	506	CLA	C2A-CAA-CBA-CGA
16	A	835	CLA	C15-C16-C17-C18
16	A	821	CLA	C2-C1-O2A-CGA
16	B	818	CLA	C3-C5-C6-C7
16	B	822	CLA	O1D-CGD-O2D-CED
16	B	824	CLA	O1D-CGD-O2D-CED
16	6	403	CLA	O1D-CGD-O2D-CED
16	B	829	CLA	O1A-CGA-O2A-C1
16	B	823	CLA	C15-C16-C17-C18
19	B	843	BCR	C11-C10-C9-C8
19	M	102	BCR	C20-C21-C22-C23
16	B	820	CLA	O1A-CGA-O2A-C1
20	A	852	LHG	C26-C27-C28-C29
16	B	813	CLA	C4-C3-C5-C6
16	B	837	CLA	C4-C3-C5-C6
16	A	809	CLA	C6-C7-C8-C10
16	A	814	CLA	C11-C12-C13-C15
16	A	822	CLA	C11-C10-C8-C7
16	A	835	CLA	C12-C13-C15-C16
16	A	839	CLA	C11-C12-C13-C15
16	A	841	CLA	C11-C10-C8-C7
16	B	801	CLA	C11-C10-C8-C7
16	B	813	CLA	C2-C3-C5-C6
16	B	829	CLA	C11-C12-C13-C15
16	B	829	CLA	C12-C13-C15-C16
16	B	830	CLA	C11-C12-C13-C15
16	1	519	CLA	C11-C10-C8-C7
16	A	834	CLA	C3-C5-C6-C7
16	A	829	CLA	C11-C12-C13-C14
16	A	830	CLA	C14-C13-C15-C16
16	A	833	CLA	C11-C10-C8-C9
16	A	835	CLA	C14-C13-C15-C16
16	A	839	CLA	C11-C12-C13-C14
16	A	841	CLA	C11-C10-C8-C9
16	B	801	CLA	C11-C10-C8-C9
16	B	818	CLA	C6-C7-C8-C9
16	B	830	CLA	C11-C12-C13-C14
16	B	832	CLA	C11-C10-C8-C9
16	B	814	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	853	LHG	C24-C23-O8-C6
16	B	814	CLA	C5-C6-C7-C8
16	B	824	CLA	C13-C15-C16-C17
16	5	403	CLA	C2A-CAA-CBA-CGA
19	J	104	BCR	C37-C22-C23-C24
19	F	202	BCR	C21-C22-C23-C24
19	5	420	BCR	C21-C22-C23-C24
16	B	825	CLA	CBA-CGA-O2A-C1
16	A	826	CLA	C13-C15-C16-C17
16	B	824	CLA	C5-C6-C7-C8
19	4	401	BCR	C6-C7-C8-C9
16	A	827	CLA	O1A-CGA-O2A-C1
20	A	852	LHG	C16-C17-C18-C19
20	B	850	LHG	C29-C30-C31-C32
16	B	828	CLA	CBA-CGA-O2A-C1
16	B	826	CLA	O1D-CGD-O2D-CED
16	B	840	CLA	O1D-CGD-O2D-CED
16	6	407	CLA	O1D-CGD-O2D-CED
20	A	852	LHG	C27-C28-C29-C30
16	A	826	CLA	C2-C3-C5-C6
16	B	837	CLA	C2-C3-C5-C6
20	F	203	LHG	C23-C24-C25-C26
20	A	852	LHG	C25-C26-C27-C28
16	A	810	CLA	C10-C11-C12-C13
16	A	810	CLA	C2A-CAA-CBA-CGA
19	A	849	BCR	C19-C20-C21-C22
22	B	849	LMG	C33-C34-C35-C36
16	A	813	CLA	O1D-CGD-O2D-CED
16	A	818	CLA	C6-C7-C8-C9
16	B	824	CLA	O2A-C1-C2-C3
20	F	203	LHG	C3-O3-P-O6
20	A	852	LHG	C7-C8-C9-C10
20	A	853	LHG	O10-C23-O8-C6
20	F	203	LHG	C11-C12-C13-C14
16	A	809	CLA	C3-C5-C6-C7
16	6	409	CLA	C2A-CAA-CBA-CGA
16	1	503	CLA	CBA-CGA-O2A-C1
20	F	203	LHG	C32-C33-C34-C35
16	B	814	CLA	O1A-CGA-O2A-C1
16	A	829	CLA	C5-C6-C7-C8
16	A	813	CLA	C2-C1-O2A-CGA
20	B	850	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
16	A	823	CLA	CAA-CBA-CGA-O2A
16	B	806	CLA	C6-C7-C8-C9
16	B	809	CLA	C14-C13-C15-C16
16	B	829	CLA	C11-C12-C13-C14
16	B	839	CLA	C11-C10-C8-C9
21	B	851	LMT	C3-C4-C5-C6
16	A	835	CLA	C5-C6-C7-C8
16	B	825	CLA	C13-C15-C16-C17
16	B	828	CLA	O1A-CGA-O2A-C1
16	B	828	CLA	C2A-CAA-CBA-CGA
19	A	846	BCR	C23-C24-C25-C26
19	A	846	BCR	C23-C24-C25-C30
19	A	850	BCR	C23-C24-C25-C30
19	B	846	BCR	C23-C24-C25-C26
19	I	102	BCR	C23-C24-C25-C26
19	I	102	BCR	C23-C24-C25-C30
16	B	837	CLA	C10-C11-C12-C13
20	F	203	LHG	C27-C28-C29-C30
20	F	203	LHG	O7-C7-C8-C9
19	4	401	BCR	C37-C22-C23-C24
19	A	847	BCR	C21-C22-C23-C24
19	B	848	BCR	C7-C8-C9-C10
19	1	516	BCR	C21-C22-C23-C24
19	4	401	BCR	C7-C8-C9-C10
19	5	420	BCR	C17-C18-C19-C20
16	A	807	CLA	C5-C6-C7-C8
19	B	847	BCR	C14-C15-C16-C17
16	A	826	CLA	C3-C5-C6-C7
16	A	820	CLA	C11-C12-C13-C15
16	A	829	CLA	C11-C12-C13-C15
16	A	830	CLA	C12-C13-C15-C16
16	A	833	CLA	C11-C10-C8-C7
16	B	806	CLA	C6-C7-C8-C10
16	B	818	CLA	C6-C7-C8-C10
16	B	832	CLA	C11-C10-C8-C7
16	B	838	CLA	C11-C10-C8-C7
16	B	840	CLA	C11-C10-C8-C7
19	5	420	BCR	C19-C20-C21-C22
16	B	806	CLA	C8-C10-C11-C12
16	A	808	CLA	C2A-CAA-CBA-CGA
16	A	810	CLA	C8-C10-C11-C12
19	A	846	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
19	A	847	BCR	C35-C13-C14-C15
19	A	848	BCR	C20-C21-C22-C37
19	K	102	BCR	C11-C10-C9-C34
19	5	420	BCR	C35-C13-C14-C15
16	A	841	CLA	C5-C6-C7-C8
16	A	826	CLA	CBA-CGA-O2A-C1
16	A	803	CLA	C5-C6-C7-C8
16	A	829	CLA	C15-C16-C17-C18
16	A	806	CLA	CAD-CBD-CGD-O2D
16	A	808	CLA	CAD-CBD-CGD-O2D
16	A	820	CLA	CAD-CBD-CGD-O2D
16	B	804	CLA	CAD-CBD-CGD-O2D
16	B	821	CLA	CAD-CBD-CGD-O2D
16	1	501	CLA	CAD-CBD-CGD-O2D
16	1	510	CLA	CAD-CBD-CGD-O2D
16	1	511	CLA	CAD-CBD-CGD-O2D
16	1	526	CLA	CAD-CBD-CGD-O2D
16	2	402	CLA	CAD-CBD-CGD-O2D
16	4	407	CLA	CAD-CBD-CGD-O2D
16	4	411	CLA	CAD-CBD-CGD-O2D
16	5	404	CLA	CAD-CBD-CGD-O2D
16	5	412	CLA	CAD-CBD-CGD-O2D
16	B	830	CLA	C13-C15-C16-C17
20	B	850	LHG	C7-C8-C9-C10
19	B	846	BCR	C22-C23-C24-C25
19	B	853	BCR	C22-C23-C24-C25
19	1	516	BCR	C22-C23-C24-C25
16	A	833	CLA	CBA-CGA-O2A-C1
16	B	837	CLA	CBA-CGA-O2A-C1
16	B	827	CLA	C10-C11-C12-C13
20	A	853	LHG	C7-C8-C9-C10
16	5	418	CLA	CBD-CGD-O2D-CED
16	B	810	CLA	C15-C16-C17-C18
16	B	802	CLA	C3-C5-C6-C7
16	B	802	CLA	C2A-CAA-CBA-CGA
16	A	804	CLA	CHA-CBD-CGD-O1D
16	A	804	CLA	CHA-CBD-CGD-O2D
16	A	809	CLA	CHA-CBD-CGD-O1D
16	A	809	CLA	CHA-CBD-CGD-O2D
16	A	814	CLA	CHA-CBD-CGD-O1D
16	A	814	CLA	CHA-CBD-CGD-O2D
16	A	825	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	A	837	CLA	CHA-CBD-CGD-O1D
16	B	802	CLA	CHA-CBD-CGD-O1D
16	B	802	CLA	CHA-CBD-CGD-O2D
16	B	808	CLA	CHA-CBD-CGD-O1D
16	B	808	CLA	CHA-CBD-CGD-O2D
16	B	823	CLA	CHA-CBD-CGD-O1D
16	B	823	CLA	CHA-CBD-CGD-O2D
16	B	824	CLA	CHA-CBD-CGD-O1D
16	B	824	CLA	CHA-CBD-CGD-O2D
16	B	825	CLA	CHA-CBD-CGD-O1D
16	B	838	CLA	CHA-CBD-CGD-O2D
16	X	101	CLA	CHA-CBD-CGD-O1D
16	X	101	CLA	CHA-CBD-CGD-O2D
16	1	507	CLA	CHA-CBD-CGD-O1D
16	2	402	CLA	CHA-CBD-CGD-O1D
16	5	406	CLA	CHA-CBD-CGD-O1D
16	5	406	CLA	CHA-CBD-CGD-O2D
16	1	503	CLA	O1A-CGA-O2A-C1
19	A	850	BCR	C20-C21-C22-C23
19	F	205	BCR	C12-C13-C14-C15
19	J	104	BCR	C12-C13-C14-C15
19	1	516	BCR	C20-C21-C22-C23
16	B	825	CLA	O1A-CGA-O2A-C1
16	A	804	CLA	C3-C5-C6-C7
16	A	834	CLA	C4-C3-C5-C6
16	A	812	CLA	C11-C12-C13-C14
16	1	520	CLA	C14-C13-C15-C16
21	1	524	LMT	C4-C5-C6-C7
16	A	826	CLA	O1A-CGA-O2A-C1
16	A	833	CLA	O1A-CGA-O2A-C1
16	B	839	CLA	C16-C17-C18-C20
16	A	812	CLA	C15-C16-C17-C18
19	A	846	BCR	C36-C18-C19-C20
19	B	844	BCR	C37-C22-C23-C24
20	A	852	LHG	C17-C18-C19-C20
20	F	203	LHG	C15-C16-C17-C18
19	J	103	BCR	C17-C18-C19-C20
16	A	812	CLA	C1A-C2A-CAA-CBA
16	1	505	CLA	C1A-C2A-CAA-CBA
16	2	404	CLA	C1A-C2A-CAA-CBA
16	2	406	CLA	C1A-C2A-CAA-CBA
16	5	403	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	5	404	CLA	C1A-C2A-CAA-CBA
16	5	406	CLA	C1A-C2A-CAA-CBA
16	5	408	CLA	C1A-C2A-CAA-CBA
16	5	410	CLA	C1A-C2A-CAA-CBA
16	6	401	CLA	C1A-C2A-CAA-CBA
16	B	840	CLA	C5-C6-C7-C8
16	B	817	CLA	C10-C11-C12-C13
16	B	833	CLA	C2-C1-O2A-CGA
20	B	850	LHG	C3-O3-P-O6
20	A	853	LHG	O2-C2-C3-O3
22	B	849	LMG	C30-C31-C32-C33
16	A	828	CLA	C4-C3-C5-C6
16	B	838	CLA	C4-C3-C5-C6
16	B	802	CLA	C8-C10-C11-C12
20	B	850	LHG	C2-C3-O3-P
20	F	203	LHG	C33-C34-C35-C36
21	A	854	LMT	C5-C6-C7-C8
21	M	101	LMT	O5'-C1'-O1'-C1
16	5	422	CLA	C2A-CAA-CBA-CGA
16	A	808	CLA	C2-C3-C5-C6
16	A	814	CLA	CAD-CBD-CGD-O1D
16	B	802	CLA	CAD-CBD-CGD-O1D
16	B	823	CLA	CAD-CBD-CGD-O1D
16	F	201	CLA	C2-C3-C5-C6
16	J	101	CLA	CAD-CBD-CGD-O1D
16	1	503	CLA	C2-C3-C5-C6
16	1	507	CLA	CAD-CBD-CGD-O1D
16	1	511	CLA	C2-C3-C5-C6
16	4	406	CLA	CAD-CBD-CGD-O1D
16	5	414	CLA	CAD-CBD-CGD-O1D
21	B	852	LMT	C4-C5-C6-C7
20	A	852	LHG	C24-C23-O8-C6
16	A	839	CLA	C6-C7-C8-C10
16	B	806	CLA	C12-C13-C15-C16
16	1	520	CLA	C12-C13-C15-C16
16	B	837	CLA	O1A-CGA-O2A-C1
22	B	849	LMG	C41-C42-C43-C44
20	F	203	LHG	O2-C2-C3-O3
16	A	819	CLA	CAA-CBA-CGA-O2A
16	A	803	CLA	O2A-C1-C2-C3
16	B	832	CLA	CAA-CBA-CGA-O2A
16	A	843	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	A	852	LHG	O10-C23-O8-C6
17	A	844	PQN	C25-C26-C27-C28
16	B	810	CLA	C4-C3-C5-C6
16	A	842	CLA	CBA-CGA-O2A-C1
16	B	803	CLA	C8-C10-C11-C12
16	A	806	CLA	C11-C10-C8-C9
16	A	820	CLA	C11-C12-C13-C14
16	B	829	CLA	C6-C7-C8-C9
16	B	840	CLA	C11-C10-C8-C9
16	A	825	CLA	O1A-CGA-O2A-C1
16	B	804	CLA	C2A-CAA-CBA-CGA
16	J	101	CLA	C2A-CAA-CBA-CGA
19	A	848	BCR	C37-C22-C23-C24
16	5	418	CLA	O1D-CGD-O2D-CED
19	4	401	BCR	C21-C22-C23-C24
16	B	814	CLA	C4-C3-C5-C6
16	A	828	CLA	C2-C3-C5-C6
16	A	814	CLA	C10-C11-C12-C13
16	A	823	CLA	C1-C2-C3-C4
16	B	837	CLA	C5-C6-C7-C8
16	A	806	CLA	C2A-CAA-CBA-CGA
16	A	813	CLA	C2A-CAA-CBA-CGA
16	B	822	CLA	C2A-CAA-CBA-CGA
16	1	525	CLA	C2A-CAA-CBA-CGA
16	B	810	CLA	C13-C15-C16-C17
16	A	803	CLA	C2-C1-O2A-CGA
16	A	805	CLA	C2-C1-O2A-CGA
16	A	806	CLA	C2-C1-O2A-CGA
16	A	823	CLA	C2-C1-O2A-CGA
16	A	827	CLA	C2-C1-O2A-CGA
16	A	836	CLA	C2-C1-O2A-CGA
19	A	847	BCR	C23-C24-C25-C30
16	A	834	CLA	C2-C3-C5-C6
22	B	849	LMG	C31-C32-C33-C34
16	1	520	CLA	C16-C17-C18-C20
19	A	846	BCR	C20-C21-C22-C23
19	A	851	BCR	C16-C17-C18-C19
19	A	851	BCR	C20-C21-C22-C23
19	B	845	BCR	C11-C10-C9-C8
19	B	847	BCR	C12-C13-C14-C15
20	A	852	LHG	C12-C13-C14-C15
20	A	852	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
20	A	853	LHG	C3-O3-P-O6
16	A	821	CLA	O1D-CGD-O2D-CED
16	A	806	CLA	C4-C3-C5-C6
16	B	825	CLA	C4-C3-C5-C6
16	B	809	CLA	C12-C13-C15-C16
16	B	838	CLA	C2-C3-C5-C6
16	A	834	CLA	C11-C10-C8-C9
16	B	803	CLA	C14-C13-C15-C16
21	5	401	LMT	C5'-C4'-O1B-C1B
21	A	854	LMT	C1-C2-C3-C4
16	A	835	CLA	O1A-CGA-O2A-C1
16	B	839	CLA	C16-C17-C18-C19
16	A	819	CLA	CBA-CGA-O2A-C1
16	B	830	CLA	CBD-CGD-O2D-CED
16	A	816	CLA	O1D-CGD-O2D-CED
19	M	102	BCR	C22-C23-C24-C25
16	A	825	CLA	CBA-CGA-O2A-C1
20	B	850	LHG	C16-C17-C18-C19
21	A	854	LMT	C7-C8-C9-C10
16	A	814	CLA	C2A-CAA-CBA-CGA
16	X	101	CLA	C2A-CAA-CBA-CGA
16	1	512	CLA	C2A-CAA-CBA-CGA
19	I	102	BCR	C9-C10-C11-C12
20	A	852	LHG	O9-C7-O7-C5
19	B	853	BCR	C18-C19-C20-C21
16	A	841	CLA	C4-C3-C5-C6
16	B	827	CLA	C4-C3-C5-C6
16	A	842	CLA	O1A-CGA-O2A-C1
16	5	414	CLA	CAA-CBA-CGA-O1A
16	6	406	CLA	CAA-CBA-CGA-O1A
15	A	801	CL0	C2-C1-O2A-CGA
16	A	822	CLA	C2-C1-O2A-CGA
16	B	830	CLA	C2-C1-O2A-CGA
16	J	102	CLA	O1D-CGD-O2D-CED
16	A	823	CLA	C2A-CAA-CBA-CGA
16	A	829	CLA	C2A-CAA-CBA-CGA
16	1	502	CLA	C2A-CAA-CBA-CGA
16	A	835	CLA	CBA-CGA-O2A-C1
16	B	833	CLA	CAA-CBA-CGA-O2A
16	A	821	CLA	CBD-CGD-O2D-CED
16	5	422	CLA	CAA-CBA-CGA-O1A
16	B	805	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	2	403	CLA	CAA-CBA-CGA-O2A
16	2	406	CLA	CAA-CBA-CGA-O2A
16	B	817	CLA	CAA-CBA-CGA-O2A
16	B	819	CLA	C11-C12-C13-C14
16	6	406	CLA	CAA-CBA-CGA-O2A
19	A	846	BCR	C35-C13-C14-C15
19	A	851	BCR	C16-C17-C18-C36
19	B	844	BCR	C11-C10-C9-C34
19	B	845	BCR	C35-C13-C14-C15
19	B	845	BCR	C20-C21-C22-C37
19	B	853	BCR	C35-C13-C14-C15
19	B	853	BCR	C16-C17-C18-C36
19	M	102	BCR	C16-C17-C18-C36
19	1	516	BCR	C35-C13-C14-C15
16	6	405	CLA	CAA-CBA-CGA-O1A
16	6	407	CLA	CAA-CBA-CGA-O1A
16	B	809	CLA	C8-C10-C11-C12
20	B	850	LHG	C27-C28-C29-C30
16	A	804	CLA	O1D-CGD-O2D-CED
16	J	101	CLA	CAA-CBA-CGA-O1A
16	5	409	CLA	CAA-CBA-CGA-O1A
16	5	419	CLA	CAA-CBA-CGA-O2A
19	1	518	BCR	C11-C12-C13-C35
16	2	403	CLA	CAA-CBA-CGA-O1A
16	2	404	CLA	CAA-CBA-CGA-O1A
16	5	407	CLA	CAA-CBA-CGA-O2A
16	5	412	CLA	CAA-CBA-CGA-O1A
16	6	403	CLA	CAA-CBA-CGA-O1A
16	K	103	CLA	C1A-C2A-CAA-CBA
16	1	502	CLA	C1A-C2A-CAA-CBA
16	1	509	CLA	C1A-C2A-CAA-CBA
16	1	514	CLA	C1A-C2A-CAA-CBA
16	4	402	CLA	C1A-C2A-CAA-CBA
16	4	411	CLA	C1A-C2A-CAA-CBA
16	5	415	CLA	C1A-C2A-CAA-CBA
16	5	419	CLA	C1A-C2A-CAA-CBA
16	5	421	CLA	C1A-C2A-CAA-CBA
16	6	402	CLA	C1A-C2A-CAA-CBA
16	6	404	CLA	C1A-C2A-CAA-CBA
16	6	407	CLA	C1A-C2A-CAA-CBA
16	A	807	CLA	C12-C13-C15-C16
16	A	829	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
16	A	840	CLA	C12-C13-C15-C16
16	A	842	CLA	C6-C7-C8-C10
16	B	801	CLA	C12-C13-C15-C16
16	B	807	CLA	C12-C13-C15-C16
16	B	810	CLA	C2-C3-C5-C6
16	B	825	CLA	C6-C7-C8-C10
16	J	101	CLA	CAA-CBA-CGA-O2A
16	5	407	CLA	CAA-CBA-CGA-O1A
16	5	419	CLA	CAA-CBA-CGA-O1A
16	5	422	CLA	CAA-CBA-CGA-O2A
16	6	404	CLA	CAA-CBA-CGA-O1A
16	6	407	CLA	CAA-CBA-CGA-O2A
16	6	409	CLA	CAA-CBA-CGA-O1A
20	F	203	LHG	C29-C30-C31-C32
16	X	101	CLA	CAA-CBA-CGA-O1A
16	1	525	CLA	CAA-CBA-CGA-O2A
16	4	410	CLA	CAA-CBA-CGA-O1A
16	5	403	CLA	CAA-CBA-CGA-O2A
16	5	409	CLA	CAA-CBA-CGA-O2A
16	5	414	CLA	CAA-CBA-CGA-O2A
16	1	520	CLA	C2A-CAA-CBA-CGA
16	A	804	CLA	C10-C11-C12-C13
16	1	525	CLA	CAA-CBA-CGA-O1A
16	4	402	CLA	CAA-CBA-CGA-O1A
16	4	407	CLA	CAA-CBA-CGA-O1A
16	5	403	CLA	CAA-CBA-CGA-O1A
20	A	852	LHG	C29-C30-C31-C32
16	A	840	CLA	C4-C3-C5-C6
16	A	820	CLA	C8-C10-C11-C12
16	2	406	CLA	CAA-CBA-CGA-O1A
16	4	411	CLA	CAA-CBA-CGA-O1A
16	A	807	CLA	C10-C11-C12-C13
19	B	844	BCR	C11-C10-C9-C8
19	K	102	BCR	C11-C10-C9-C8
16	5	418	CLA	CAA-CBA-CGA-O2A
19	4	401	BCR	C19-C20-C21-C22
16	B	840	CLA	C3-C5-C6-C7
16	X	101	CLA	CAA-CBA-CGA-O2A
16	5	415	CLA	CAA-CBA-CGA-O1A
16	5	415	CLA	CAA-CBA-CGA-O2A
16	6	403	CLA	CAA-CBA-CGA-O2A
16	2	402	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
16	2	404	CLA	CAA-CBA-CGA-O2A
16	6	404	CLA	CAA-CBA-CGA-O2A
16	6	409	CLA	CAA-CBA-CGA-O2A
16	B	804	CLA	C4-C3-C5-C6
16	A	804	CLA	C2-C1-O2A-CGA
16	B	801	CLA	C2-C1-O2A-CGA
16	B	805	CLA	C2-C1-O2A-CGA
16	B	825	CLA	C2-C1-O2A-CGA
16	A	806	CLA	C2-C3-C5-C6
16	A	841	CLA	C2-C3-C5-C6
16	B	814	CLA	C2-C3-C5-C6
16	B	825	CLA	C2-C3-C5-C6
16	B	827	CLA	C2-C3-C5-C6
19	A	846	BCR	C10-C11-C12-C13
16	5	418	CLA	CAA-CBA-CGA-O1A
16	6	405	CLA	CAA-CBA-CGA-O2A
16	B	806	CLA	C11-C12-C13-C14
16	B	826	CLA	C11-C12-C13-C14
16	A	819	CLA	O1A-CGA-O2A-C1
16	2	402	CLA	CAA-CBA-CGA-O2A
16	4	410	CLA	CAA-CBA-CGA-O2A
16	5	408	CLA	CAA-CBA-CGA-O2A
16	5	412	CLA	CAA-CBA-CGA-O2A
21	B	851	LMT	C1-C2-C3-C4
16	B	819	CLA	C13-C15-C16-C17
16	F	201	CLA	C4-C3-C5-C6
16	1	503	CLA	C4-C3-C5-C6
16	1	502	CLA	CAA-CBA-CGA-O2A
16	B	819	CLA	O1A-CGA-O2A-C1
19	A	850	BCR	C23-C24-C25-C26
19	B	843	BCR	C23-C24-C25-C30
19	1	517	BCR	C23-C24-C25-C30
19	1	518	BCR	C23-C24-C25-C30
19	5	402	BCR	C23-C24-C25-C30
16	5	417	CLA	CAA-CBA-CGA-O1A
16	6	402	CLA	CAA-CBA-CGA-O2A
16	A	822	CLA	C4-C3-C5-C6
16	B	809	CLA	C4-C3-C5-C6
16	3	401	CLA	CAA-CBA-CGA-O2A
16	4	407	CLA	CAA-CBA-CGA-O2A
16	4	408	CLA	CAA-CBA-CGA-O2A
16	1	510	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	1	515	CLA	CAA-CBA-CGA-O2A
16	2	401	CLA	CAA-CBA-CGA-O2A
16	4	402	CLA	CAA-CBA-CGA-O2A
16	1	506	CLA	CAA-CBA-CGA-O2A
16	5	408	CLA	CAA-CBA-CGA-O1A
16	5	421	CLA	CAA-CBA-CGA-O2A
16	A	833	CLA	CAA-CBA-CGA-O2A
16	1	502	CLA	CAA-CBA-CGA-O1A
16	1	514	CLA	CAA-CBA-CGA-O2A
16	A	804	CLA	C4-C3-C5-C6
16	A	822	CLA	C2-C3-C5-C6
16	B	829	CLA	C6-C7-C8-C10
16	B	831	CLA	C8-C10-C11-C12
16	A	814	CLA	CAA-CBA-CGA-O2A
16	J	102	CLA	CAA-CBA-CGA-O1A
16	J	102	CLA	CAA-CBA-CGA-O2A
16	4	405	CLA	CAA-CBA-CGA-O2A
16	B	819	CLA	CBA-CGA-O2A-C1
16	B	830	CLA	CBA-CGA-O2A-C1
16	A	839	CLA	C5-C6-C7-C8
16	2	401	CLA	CAA-CBA-CGA-O1A
16	A	824	CLA	CAA-CBA-CGA-O2A
21	M	101	LMT	C1-C2-C3-C4
16	5	411	CLA	C2A-CAA-CBA-CGA
16	B	836	CLA	CAA-CBA-CGA-O2A
16	1	510	CLA	CAA-CBA-CGA-O1A
16	1	512	CLA	CAA-CBA-CGA-O2A
19	A	851	BCR	C11-C10-C9-C34
19	1	518	BCR	C35-C13-C14-C15
19	1	518	BCR	C20-C21-C22-C37
16	A	828	CLA	CAA-CBA-CGA-O2A
16	B	809	CLA	CAA-CBA-CGA-O2A
16	A	802	CLA	C4-C3-C5-C6
16	A	805	CLA	C4-C3-C5-C6
16	A	830	CLA	C4-C3-C5-C6
16	B	808	CLA	C4-C3-C5-C6
16	6	401	CLA	CAA-CBA-CGA-O2A
16	A	812	CLA	C14-C13-C15-C16
16	A	839	CLA	C6-C7-C8-C9
16	A	842	CLA	C11-C12-C13-C14
16	B	806	CLA	C14-C13-C15-C16
16	B	829	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
16	B	838	CLA	C11-C10-C8-C9
16	1	506	CLA	CAA-CBA-CGA-O1A
16	1	514	CLA	CAA-CBA-CGA-O1A
16	B	834	CLA	C3A-C2A-CAA-CBA
16	B	806	CLA	CAA-CBA-CGA-O2A
16	B	823	CLA	CAA-CBA-CGA-O2A
16	K	101	CLA	C4C-C3C-CAC-CBC
16	B	835	CLA	CAA-CBA-CGA-O2A
16	B	836	CLA	CAA-CBA-CGA-O1A
16	2	405	CLA	CAA-CBA-CGA-O2A
16	4	403	CLA	CAA-CBA-CGA-O2A
16	A	805	CLA	CAD-CBD-CGD-O2D
16	A	813	CLA	CAD-CBD-CGD-O2D
16	A	821	CLA	CAD-CBD-CGD-O2D
16	A	827	CLA	CAD-CBD-CGD-O2D
16	A	834	CLA	CAD-CBD-CGD-O2D
16	B	813	CLA	CAD-CBD-CGD-O2D
16	B	818	CLA	CAD-CBD-CGD-O2D
16	B	820	CLA	CAD-CBD-CGD-O2D
16	B	826	CLA	CAD-CBD-CGD-O2D
16	B	833	CLA	CAD-CBD-CGD-O2D
16	B	839	CLA	CAD-CBD-CGD-O2D
16	J	102	CLA	CAD-CBD-CGD-O2D
16	1	504	CLA	CAD-CBD-CGD-O2D
16	1	525	CLA	CAD-CBD-CGD-O2D
16	2	405	CLA	CAD-CBD-CGD-O2D
16	4	403	CLA	CAD-CBD-CGD-O2D
16	4	404	CLA	CAD-CBD-CGD-O2D
16	5	410	CLA	CAD-CBD-CGD-O2D
16	5	417	CLA	CAD-CBD-CGD-O2D
16	5	421	CLA	CAD-CBD-CGD-O2D
16	6	401	CLA	CAD-CBD-CGD-O2D
16	6	402	CLA	CAD-CBD-CGD-O2D
19	B	843	BCR	C15-C16-C17-C18
16	K	103	CLA	CAA-CBA-CGA-O2A
16	1	504	CLA	CAA-CBA-CGA-O2A
16	5	413	CLA	CAA-CBA-CGA-O2A
20	F	203	LHG	O9-C7-C8-C9
16	B	830	CLA	O1D-CGD-O2D-CED
16	A	810	CLA	C4-C3-C5-C6
16	4	406	CLA	CAA-CBA-CGA-O2A
16	6	402	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
16	A	840	CLA	C2-C3-C5-C6
16	B	809	CLA	C2-C3-C5-C6
16	1	511	CLA	CAA-CBA-CGA-O2A
16	B	830	CLA	O1A-CGA-O2A-C1
19	B	844	BCR	C21-C22-C23-C24
19	K	102	BCR	C7-C8-C9-C10
16	1	515	CLA	CAA-CBA-CGA-O1A
16	4	406	CLA	CAA-CBA-CGA-O1A
16	5	404	CLA	CAA-CBA-CGA-O2A
16	5	421	CLA	CAA-CBA-CGA-O1A
20	A	852	LHG	O6-C4-C5-O7
16	A	823	CLA	O2A-C1-C2-C3
16	1	512	CLA	CAA-CBA-CGA-O1A
16	3	401	CLA	CAA-CBA-CGA-O1A
16	5	411	CLA	CAA-CBA-CGA-O2A
16	B	832	CLA	C13-C15-C16-C17
16	A	826	CLA	O2A-C1-C2-C3
16	A	829	CLA	O2A-C1-C2-C3
16	B	817	CLA	O2A-C1-C2-C3
16	B	841	CLA	C4C-C3C-CAC-CBC
16	A	830	CLA	C13-C15-C16-C17
16	B	822	CLA	CAA-CBA-CGA-O2A
16	1	521	CLA	CAA-CBA-CGA-O2A
16	B	835	CLA	CAA-CBA-CGA-O1A
16	1	508	CLA	CAA-CBA-CGA-O2A
16	4	408	CLA	CAA-CBA-CGA-O1A
16	A	819	CLA	C5-C6-C7-C8
16	A	811	CLA	CHA-CBD-CGD-O1D
16	A	811	CLA	CHA-CBD-CGD-O2D
16	A	815	CLA	CHA-CBD-CGD-O1D
16	A	815	CLA	CHA-CBD-CGD-O2D
16	A	828	CLA	CHA-CBD-CGD-O2D
16	A	837	CLA	CHA-CBD-CGD-O2D
16	A	839	CLA	CHA-CBD-CGD-O1D
16	A	840	CLA	CHA-CBD-CGD-O1D
16	A	840	CLA	CHA-CBD-CGD-O2D
16	B	814	CLA	CHA-CBD-CGD-O1D
16	B	825	CLA	CHA-CBD-CGD-O2D
16	F	201	CLA	CHA-CBD-CGD-O1D
16	F	201	CLA	CHA-CBD-CGD-O2D
16	1	503	CLA	CHA-CBD-CGD-O1D
16	1	507	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	1	509	CLA	CHA-CBD-CGD-O1D
16	1	509	CLA	CHA-CBD-CGD-O2D
16	2	406	CLA	CHA-CBD-CGD-O1D
16	2	406	CLA	CHA-CBD-CGD-O2D
16	4	406	CLA	CHA-CBD-CGD-O1D
16	4	411	CLA	CHA-CBD-CGD-O1D
16	5	408	CLA	CHA-CBD-CGD-O2D
16	5	409	CLA	CHA-CBD-CGD-O1D
16	5	409	CLA	CHA-CBD-CGD-O2D
16	5	414	CLA	CHA-CBD-CGD-O1D
16	5	414	CLA	CHA-CBD-CGD-O2D
16	5	416	CLA	CHA-CBD-CGD-O1D
16	5	416	CLA	CHA-CBD-CGD-O2D
16	6	405	CLA	CHA-CBD-CGD-O2D
16	1	504	CLA	CAA-CBA-CGA-O1A
16	1	508	CLA	CAA-CBA-CGA-O1A
16	4	405	CLA	CAA-CBA-CGA-O1A
16	4	411	CLA	CAA-CBA-CGA-O2A
16	5	404	CLA	CAA-CBA-CGA-O1A
16	5	406	CLA	CAA-CBA-CGA-O2A
16	5	413	CLA	CAA-CBA-CGA-O1A
16	A	803	CLA	CAA-CBA-CGA-O2A
19	A	851	BCR	C11-C10-C9-C8
19	B	845	BCR	C20-C21-C22-C23
19	J	104	BCR	C11-C10-C9-C8
19	1	518	BCR	C12-C13-C14-C15
16	2	405	CLA	CAA-CBA-CGA-O1A
22	B	849	LMG	O7-C10-C11-C12
16	1	526	CLA	CAA-CBA-CGA-O1A
16	4	403	CLA	CAA-CBA-CGA-O1A
16	5	411	CLA	CAA-CBA-CGA-O1A
16	6	401	CLA	CAA-CBA-CGA-O1A
16	A	821	CLA	C2A-CAA-CBA-CGA
16	K	103	CLA	CAA-CBA-CGA-O1A
21	1	524	LMT	C1-C2-C3-C4
16	B	813	CLA	CAA-CBA-CGA-O2A
16	A	803	CLA	C11-C10-C8-C7
16	A	830	CLA	C2-C3-C5-C6
17	B	842	PQN	C26-C27-C28-C30
16	A	839	CLA	C10-C11-C12-C13
16	A	810	CLA	CAA-CBA-CGA-O2A
16	A	807	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
16	B	807	CLA	C14-C13-C15-C16
16	B	827	CLA	C6-C7-C8-C9
16	A	823	CLA	CAA-CBA-CGA-O1A
19	A	849	BCR	C9-C10-C11-C12
16	A	814	CLA	C15-C16-C17-C18
16	5	417	CLA	CAA-CBA-CGA-O2A
16	A	828	CLA	CAA-CBA-CGA-O1A
20	A	852	LHG	C8-C7-O7-C5
16	B	822	CLA	CAA-CBA-CGA-O1A
16	A	810	CLA	O1D-CGD-O2D-CED
21	B	851	LMT	C5'-C4'-O1B-C1B
19	B	846	BCR	C11-C12-C13-C35
16	A	839	CLA	C4-C3-C5-C6
16	A	802	CLA	C13-C15-C16-C17
16	A	810	CLA	CBD-CGD-O2D-CED
19	J	104	BCR	C21-C22-C23-C24
16	B	826	CLA	C13-C15-C16-C17
16	B	813	CLA	C1A-C2A-CAA-CBA
16	B	832	CLA	C1A-C2A-CAA-CBA
16	1	507	CLA	C1A-C2A-CAA-CBA
16	1	526	CLA	C1A-C2A-CAA-CBA
16	5	422	CLA	C1A-C2A-CAA-CBA
16	B	806	CLA	CAA-CBA-CGA-O1A
16	B	807	CLA	C15-C16-C17-C18
16	5	406	CLA	CAA-CBA-CGA-O1A
16	B	829	CLA	C2-C1-O2A-CGA
16	B	801	CLA	C5-C6-C7-C8
16	B	809	CLA	CAA-CBA-CGA-O1A
16	B	827	CLA	C3-C5-C6-C7
16	A	803	CLA	CAA-CBA-CGA-O1A
16	B	823	CLA	CAA-CBA-CGA-O1A
16	A	814	CLA	CAA-CBA-CGA-O1A
19	B	843	BCR	C22-C23-C24-C25
16	B	831	CLA	C15-C16-C17-C18
20	A	852	LHG	C3-O3-P-O5
20	A	853	LHG	C3-O3-P-O5
20	F	203	LHG	C3-O3-P-O5
16	B	841	CLA	C2C-C3C-CAC-CBC
16	A	810	CLA	CAA-CBA-CGA-O1A
16	A	824	CLA	CAA-CBA-CGA-O1A
16	1	511	CLA	CAA-CBA-CGA-O1A
22	B	849	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	4	401	BCR	C35-C13-C14-C15
19	A	847	BCR	C23-C24-C25-C26
16	A	814	CLA	C5-C6-C7-C8
16	1	521	CLA	CAA-CBA-CGA-O1A
16	A	839	CLA	CAA-CBA-CGA-O2A
16	A	810	CLA	CBA-CGA-O2A-C1
16	A	825	CLA	CAA-CBA-CGA-O2A
16	A	835	CLA	C4-C3-C5-C6
15	A	801	CL0	CAD-CBD-CGD-O1D
16	A	824	CLA	C2-C3-C5-C6
16	A	839	CLA	CAD-CBD-CGD-O1D
16	B	810	CLA	CAD-CBD-CGD-O1D
16	B	814	CLA	CAD-CBD-CGD-O1D
16	1	506	CLA	CAD-CBD-CGD-O1D
16	5	418	CLA	CAD-CBD-CGD-O1D
16	B	824	CLA	C15-C16-C17-C18
16	A	810	CLA	C14-C13-C15-C16
16	A	820	CLA	C11-C10-C8-C9
16	A	829	CLA	C14-C13-C15-C16
16	A	840	CLA	C14-C13-C15-C16
16	A	842	CLA	C6-C7-C8-C9
16	B	801	CLA	C14-C13-C15-C16
21	5	401	LMT	C6-C7-C8-C9
16	A	837	CLA	CAA-CBA-CGA-O2A
16	B	810	CLA	C5-C6-C7-C8
16	A	813	CLA	CAA-CBA-CGA-O2A
16	F	201	CLA	CAA-CBA-CGA-O2A
16	1	526	CLA	CAA-CBA-CGA-O2A
16	B	817	CLA	C11-C12-C13-C14
16	B	813	CLA	CAA-CBA-CGA-O1A
16	1	520	CLA	C8-C10-C11-C12
16	A	812	CLA	C11-C12-C13-C15
16	A	834	CLA	C11-C10-C8-C7
16	A	842	CLA	C12-C13-C15-C16
16	B	813	CLA	C3A-C2A-CAA-CBA
16	B	819	CLA	C11-C12-C13-C15
16	B	826	CLA	C11-C12-C13-C15
16	B	827	CLA	C6-C7-C8-C10
16	B	827	CLA	C11-C10-C8-C7
16	1	525	CLA	C3A-C2A-CAA-CBA
16	A	826	CLA	CAA-CBA-CGA-O2A
19	4	401	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
16	A	837	CLA	CAA-CBA-CGA-O1A
16	1	520	CLA	C16-C17-C18-C19
16	B	828	CLA	C10-C11-C12-C13
16	B	838	CLA	C5-C6-C7-C8
16	A	826	CLA	CAA-CBA-CGA-O1A
16	B	805	CLA	C3-C5-C6-C7
16	B	827	CLA	CAA-CBA-CGA-O2A
16	F	201	CLA	CAA-CBA-CGA-O1A
16	B	803	CLA	C2A-CAA-CBA-CGA
16	1	501	CLA	C2A-CAA-CBA-CGA
16	B	837	CLA	C8-C10-C11-C12
16	A	813	CLA	CAA-CBA-CGA-O1A
16	B	826	CLA	C2C-C3C-CAC-CBC

There are no ring outliers.

183 monomers are involved in 464 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	M	101	LMT	2	0
16	B	822	CLA	3	0
16	1	514	CLA	2	0
19	B	847	BCR	4	0
16	1	512	CLA	4	0
16	B	816	CLA	1	0
16	5	417	CLA	2	0
16	6	404	CLA	1	0
16	5	413	CLA	4	0
16	4	402	CLA	1	0
16	B	839	CLA	13	0
16	1	513	CLA	1	0
19	I	101	BCR	2	0
16	A	840	CLA	4	0
16	6	405	CLA	1	0
16	B	818	CLA	3	0
16	2	402	CLA	1	0
16	B	837	CLA	1	0
16	A	819	CLA	5	0
16	B	828	CLA	6	0
16	B	813	CLA	7	0
19	J	103	BCR	3	0
16	B	817	CLA	3	0
16	K	101	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	807	CLA	4	0
16	B	832	CLA	4	0
16	B	823	CLA	5	0
19	K	102	BCR	6	0
16	A	817	CLA	1	0
16	A	821	CLA	5	0
19	M	102	BCR	2	0
16	6	409	CLA	2	0
20	A	853	LHG	1	0
16	J	102	CLA	2	0
16	K	103	CLA	4	0
16	1	515	CLA	2	0
16	J	101	CLA	2	0
16	B	802	CLA	12	0
16	1	519	CLA	2	0
19	A	849	BCR	2	0
16	B	805	CLA	1	0
16	A	830	CLA	2	0
16	A	828	CLA	4	0
16	B	827	CLA	7	0
16	2	403	CLA	1	0
16	5	407	CLA	6	0
16	A	806	CLA	5	0
16	5	411	CLA	1	0
20	B	850	LHG	3	0
16	B	819	CLA	5	0
16	6	403	CLA	1	0
16	A	843	CLA	5	0
16	4	409	CLA	1	0
16	5	421	CLA	2	0
16	4	410	CLA	1	0
16	A	815	CLA	2	0
16	A	810	CLA	4	0
16	B	830	CLA	7	0
16	6	401	CLA	1	0
16	5	405	CLA	1	0
16	1	508	CLA	2	0
16	A	805	CLA	2	0
16	1	511	CLA	4	0
16	5	412	CLA	4	0
16	A	836	CLA	2	0
16	B	840	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	834	CLA	7	0
19	A	846	BCR	4	0
19	J	104	BCR	1	0
20	A	852	LHG	3	0
16	4	404	CLA	1	0
16	5	409	CLA	1	0
16	1	501	CLA	4	0
16	5	414	CLA	5	0
16	A	820	CLA	4	0
16	6	408	CLA	1	0
17	B	842	PQN	5	0
16	B	807	CLA	7	0
19	A	848	BCR	1	0
17	A	844	PQN	5	0
16	A	804	CLA	3	0
16	X	101	CLA	2	0
16	A	813	CLA	1	0
16	5	406	CLA	2	0
16	5	415	CLA	2	0
16	A	809	CLA	5	0
16	A	814	CLA	3	0
16	A	842	CLA	6	0
16	3	401	CLA	2	0
16	A	802	CLA	5	0
16	2	405	CLA	1	0
16	B	806	CLA	6	0
16	4	408	CLA	3	0
19	B	844	BCR	4	0
16	B	812	CLA	3	0
16	A	832	CLA	2	0
16	2	404	CLA	1	0
16	A	826	CLA	6	0
16	5	408	CLA	2	0
16	A	823	CLA	2	0
16	A	808	CLA	1	0
16	4	407	CLA	1	0
19	B	843	BCR	2	0
16	5	403	CLA	2	0
19	5	402	BCR	4	0
19	A	850	BCR	2	0
19	F	202	BCR	4	0
16	B	810	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	401	BCR	3	0
16	A	811	CLA	4	0
16	A	829	CLA	10	0
16	A	824	CLA	1	0
16	F	204	CLA	2	0
16	5	419	CLA	4	0
16	1	502	CLA	1	0
16	6	406	CLA	1	0
16	6	407	CLA	1	0
16	B	808	CLA	5	0
16	5	404	CLA	6	0
16	A	833	CLA	9	0
16	B	824	CLA	6	0
16	A	827	CLA	3	0
16	1	520	CLA	5	0
16	1	521	CLA	3	0
16	1	510	CLA	3	0
16	5	410	CLA	1	0
19	B	845	BCR	3	0
16	F	201	CLA	6	0
16	A	825	CLA	2	0
16	B	815	CLA	3	0
16	A	831	CLA	6	0
16	1	504	CLA	2	0
16	A	822	CLA	6	0
16	5	422	CLA	2	0
16	A	835	CLA	2	0
16	A	816	CLA	1	0
16	6	402	CLA	1	0
19	A	851	BCR	5	0
16	5	418	CLA	1	0
19	5	420	BCR	1	0
16	1	506	CLA	1	0
19	1	517	BCR	2	0
16	B	804	CLA	3	0
16	A	839	CLA	7	0
16	B	803	CLA	3	0
22	B	849	LMG	3	0
16	4	403	CLA	1	0
18	C	102	SF4	1	0
16	B	809	CLA	8	0
16	B	835	CLA	3	0

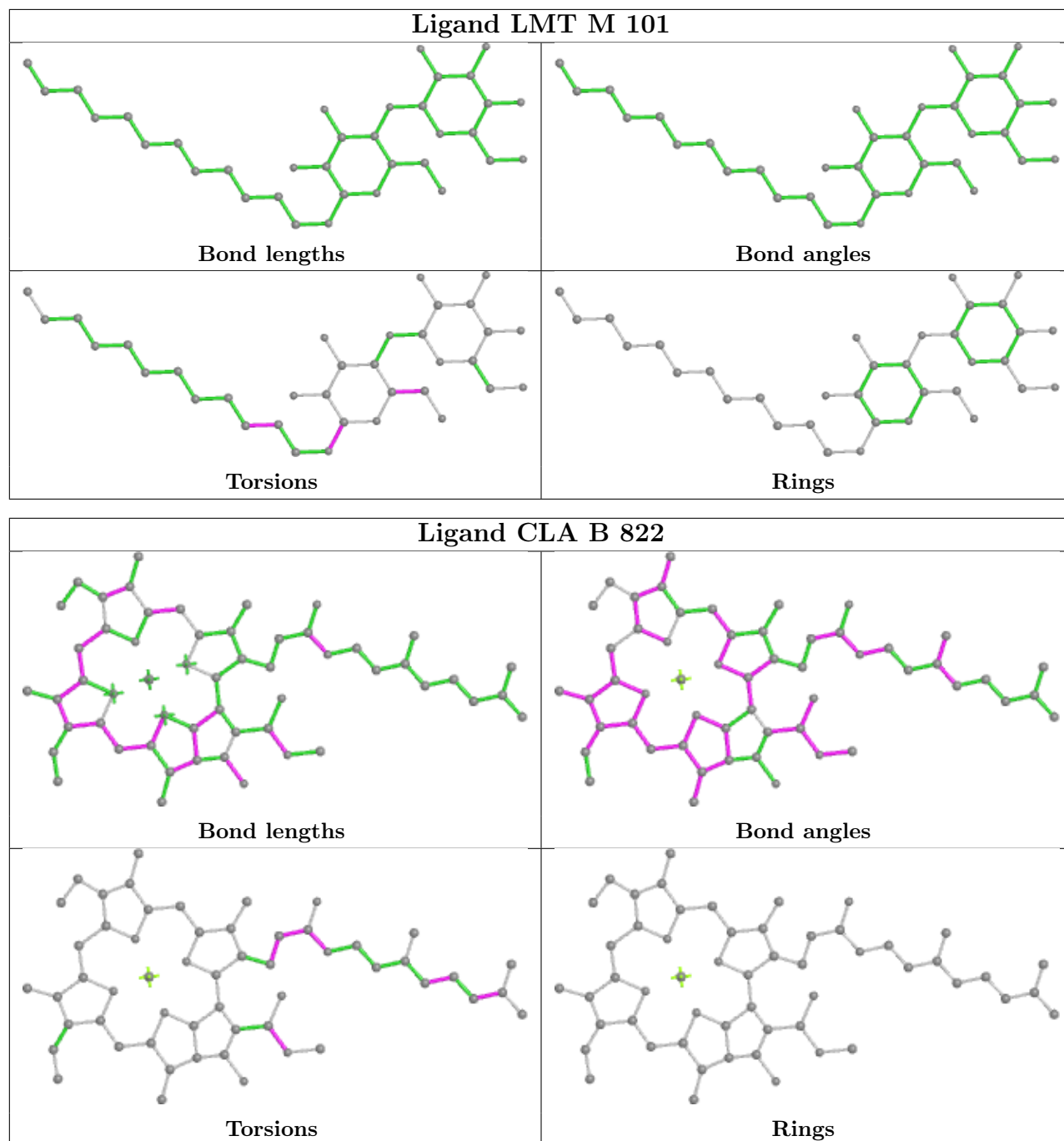
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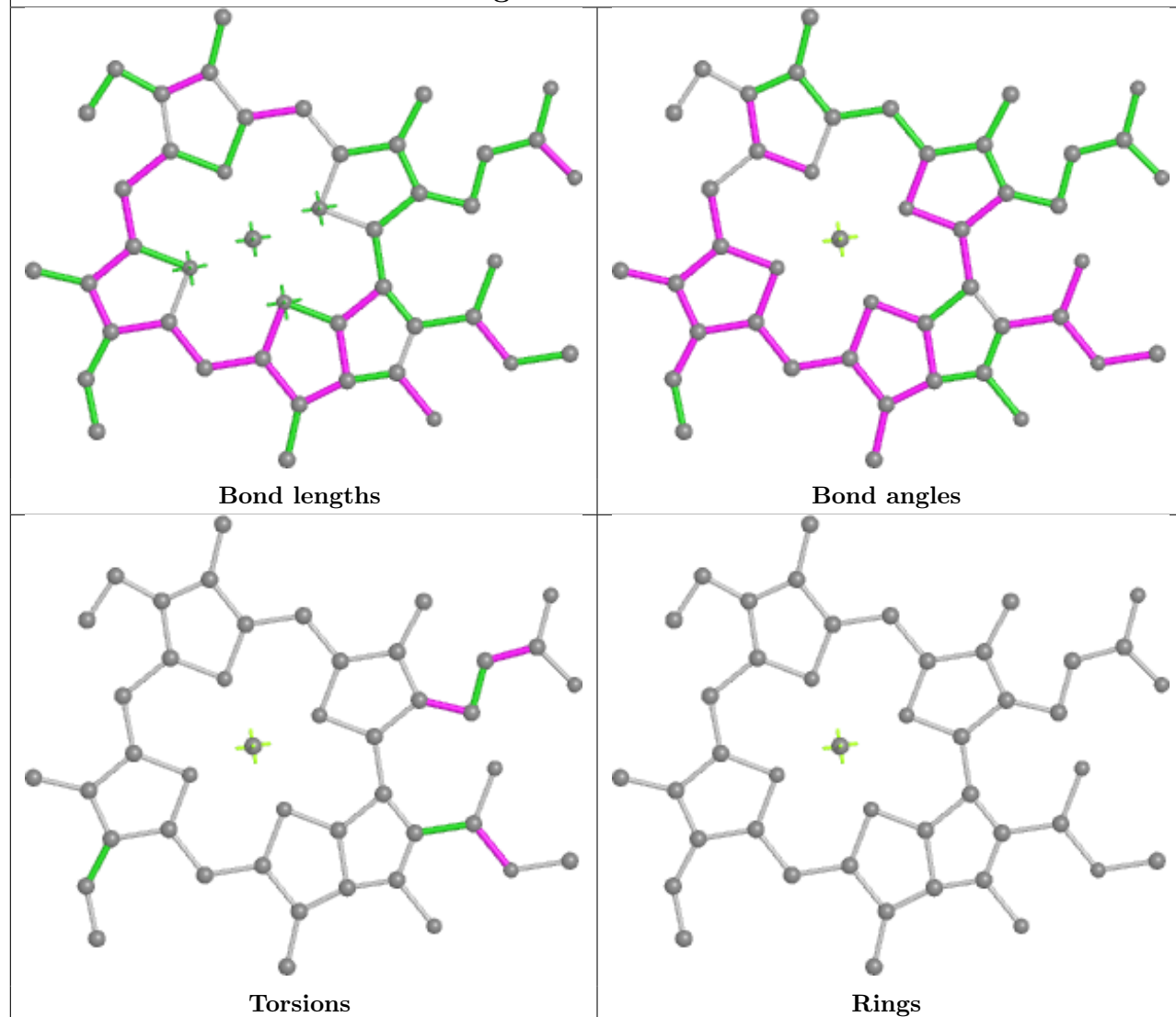
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	801	CL0	7	0
16	1	526	CLA	1	0
16	4	411	CLA	3	0
19	1	523	BCR	5	0
16	A	837	CLA	2	0
16	2	401	CLA	1	0
16	2	406	CLA	3	0
19	I	102	BCR	5	0
19	1	516	BCR	1	0
16	4	405	CLA	1	0
16	1	509	CLA	2	0
16	B	829	CLA	6	0
16	B	826	CLA	4	0
16	5	416	CLA	1	0
16	B	838	CLA	5	0
16	A	803	CLA	5	0
16	A	838	CLA	1	0
16	1	503	CLA	1	0
16	B	834	CLA	6	0
19	B	853	BCR	3	0
16	A	812	CLA	3	0
16	B	821	CLA	3	0
16	B	801	CLA	5	0
16	A	818	CLA	2	0
16	B	833	CLA	5	0
16	A	841	CLA	6	0
16	B	820	CLA	2	0
16	B	814	CLA	2	0
16	B	841	CLA	6	0
16	B	831	CLA	4	0
16	1	525	CLA	1	0
16	B	811	CLA	2	0
16	B	825	CLA	6	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

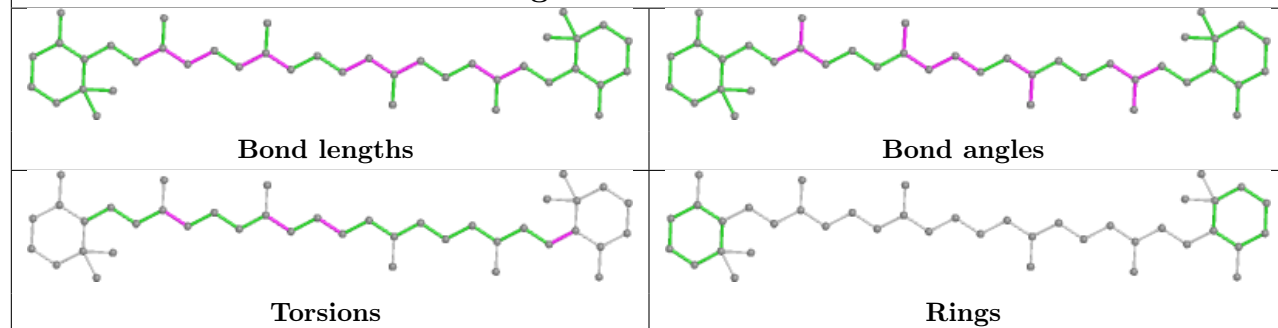
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



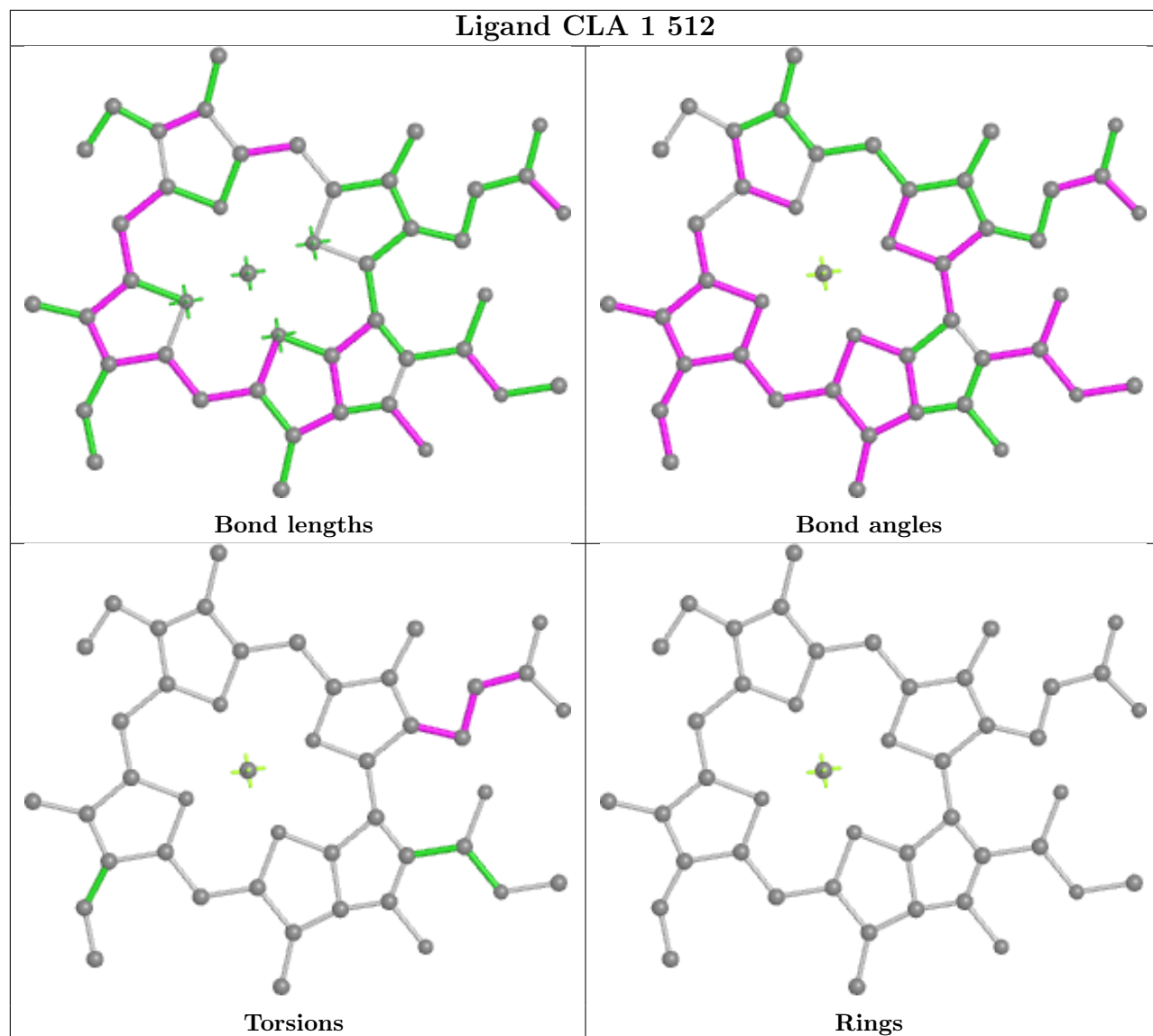
Ligand CLA 1 514

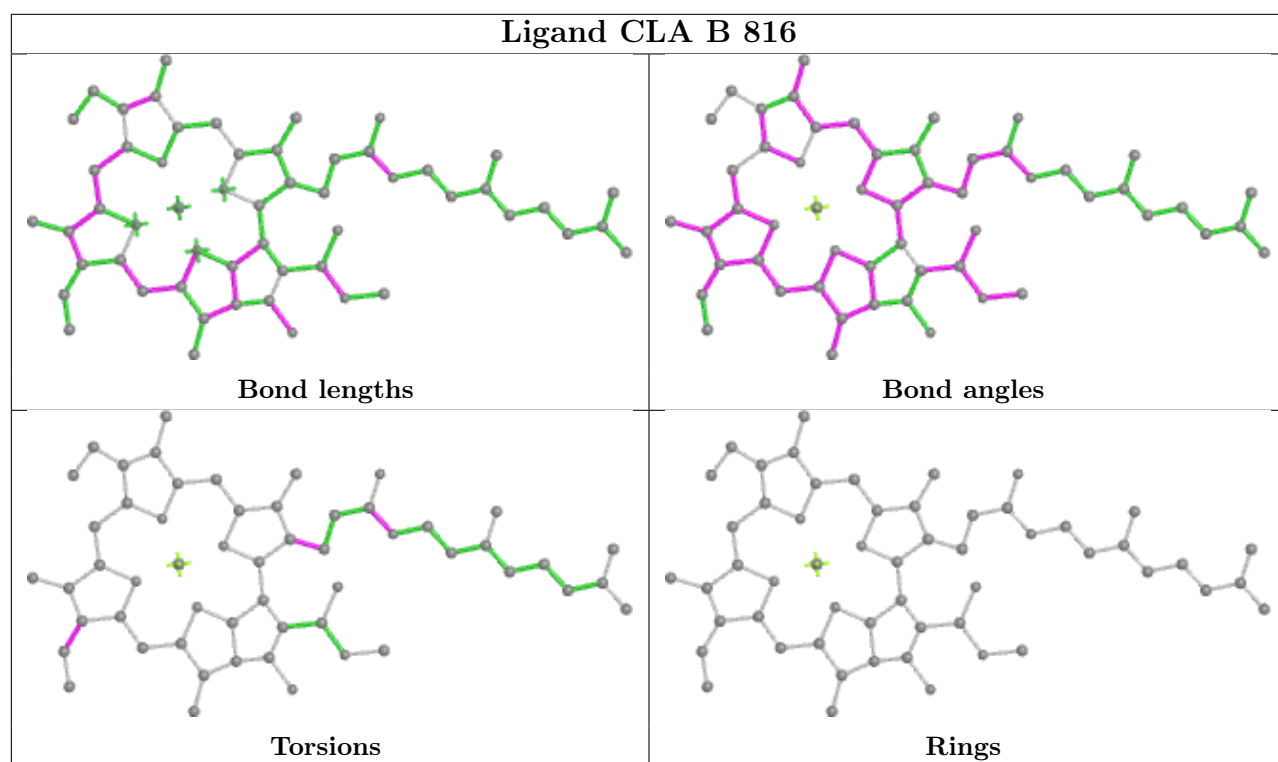


Ligand BCR B 847

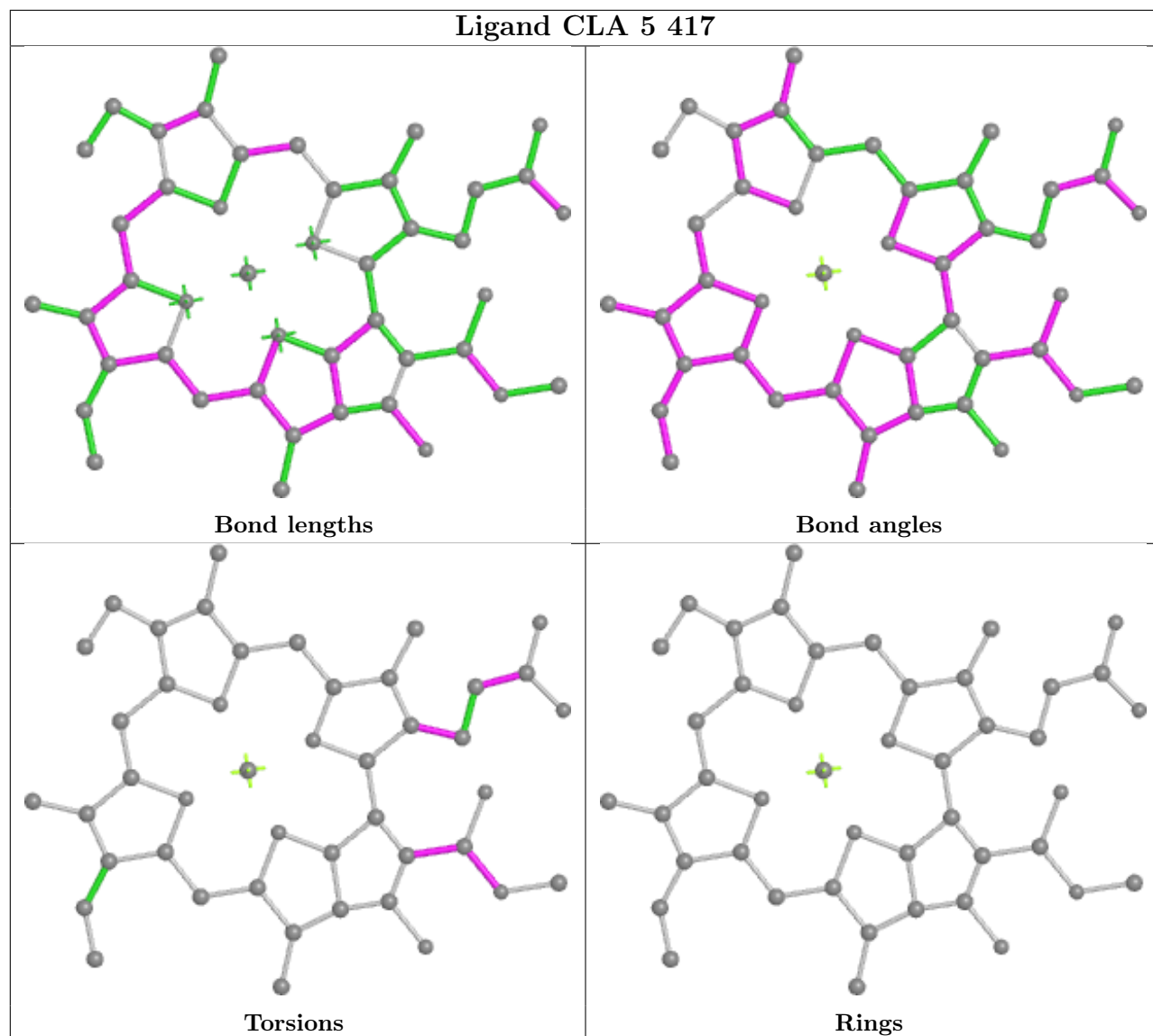


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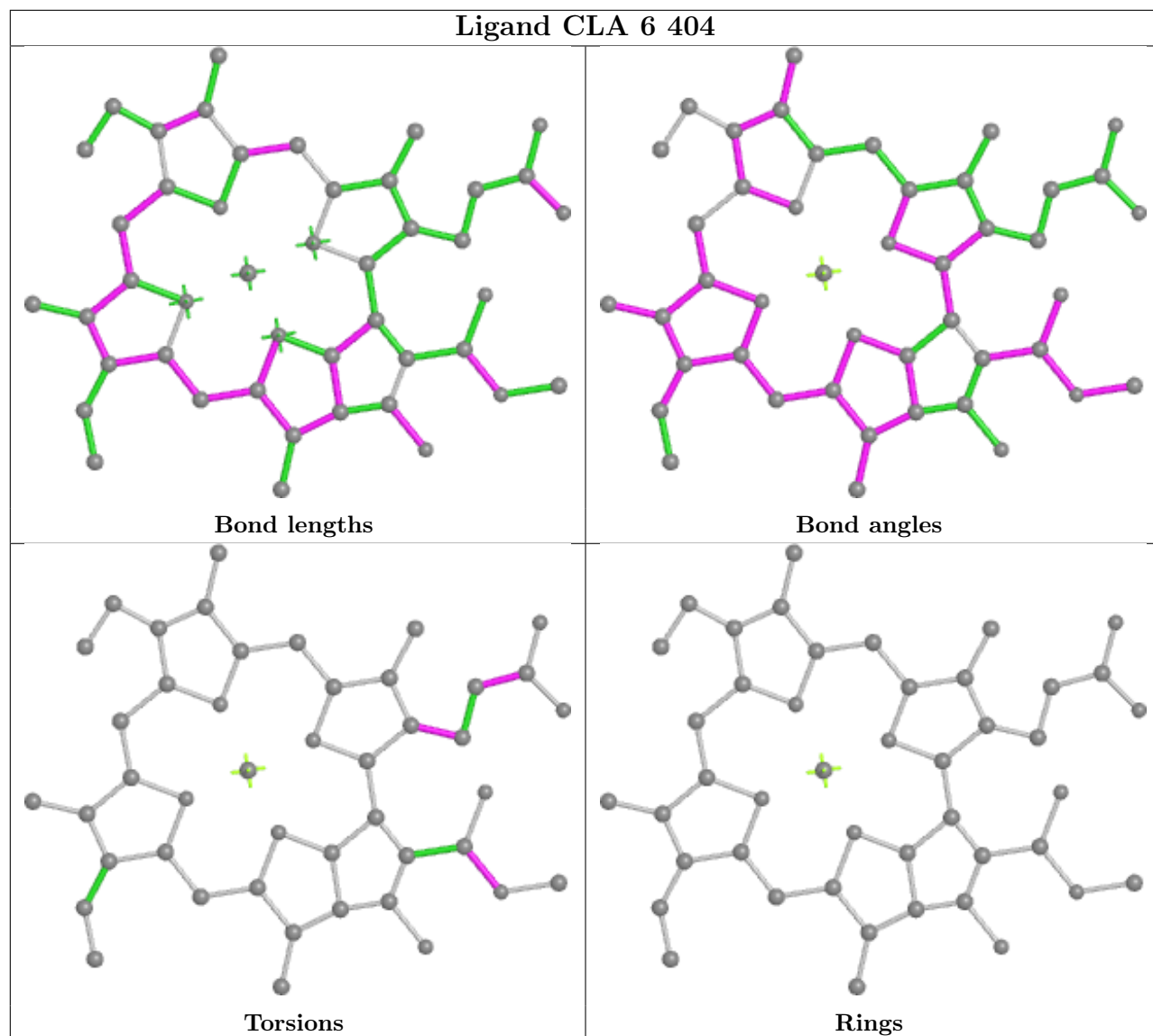




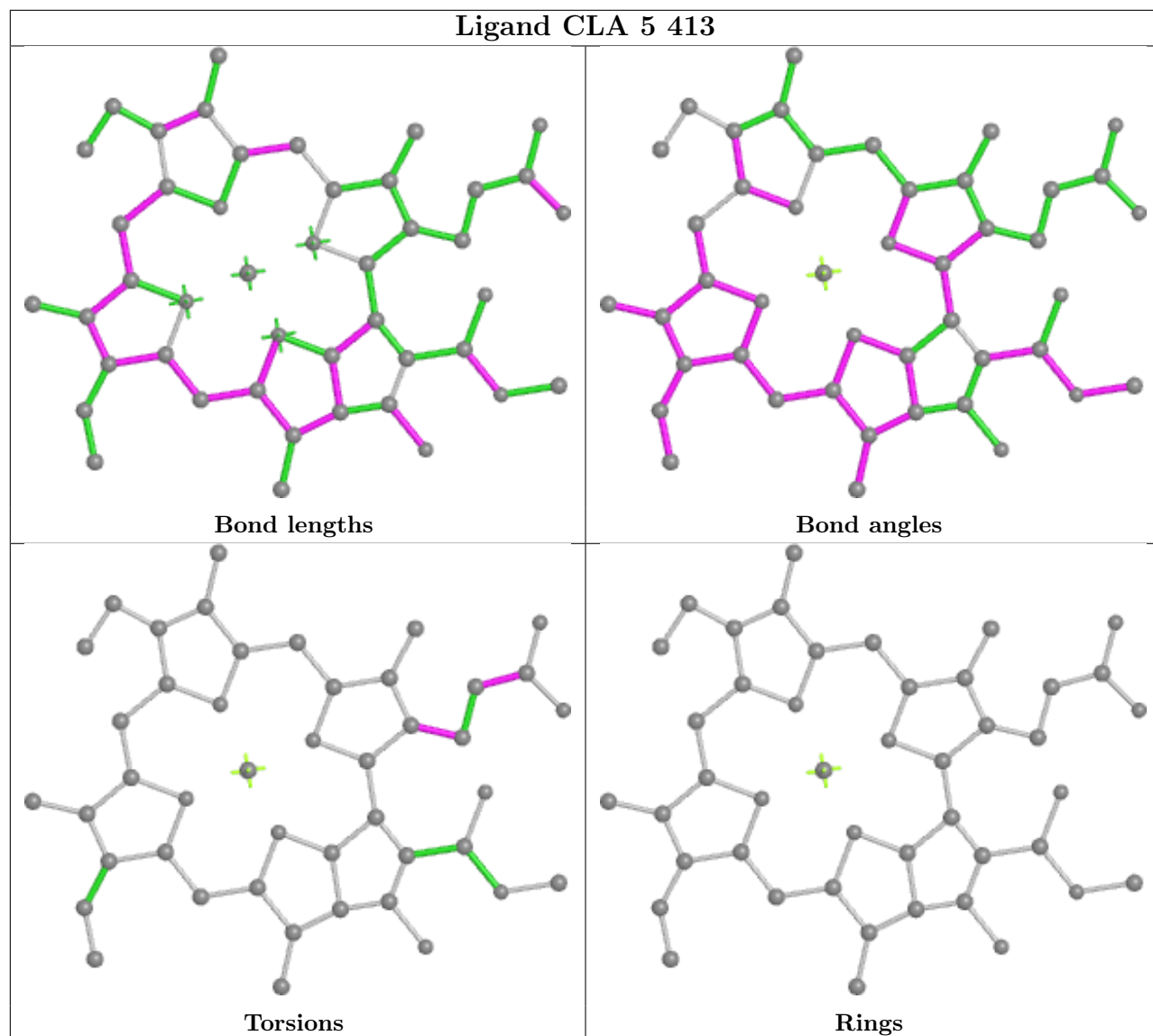
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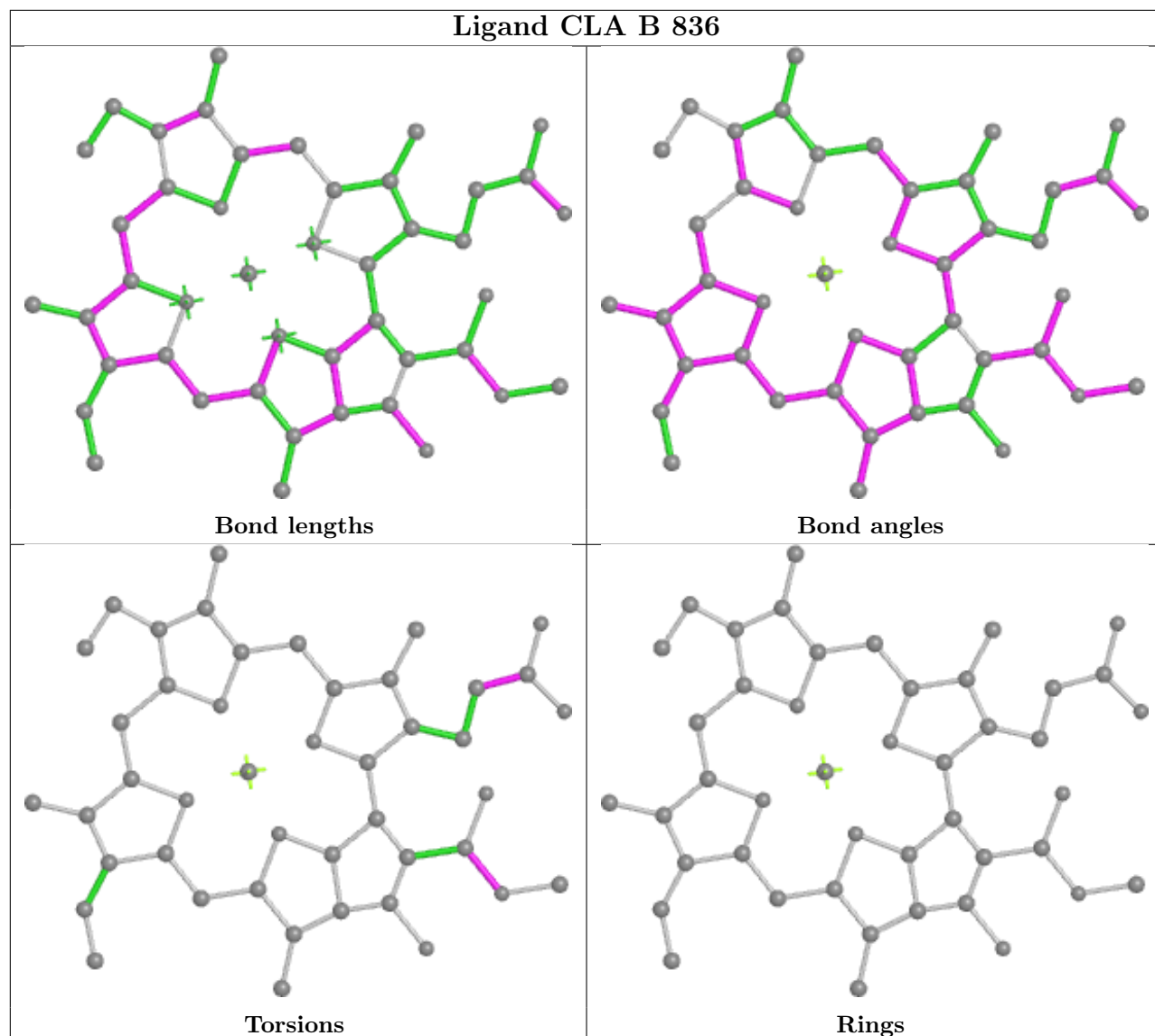
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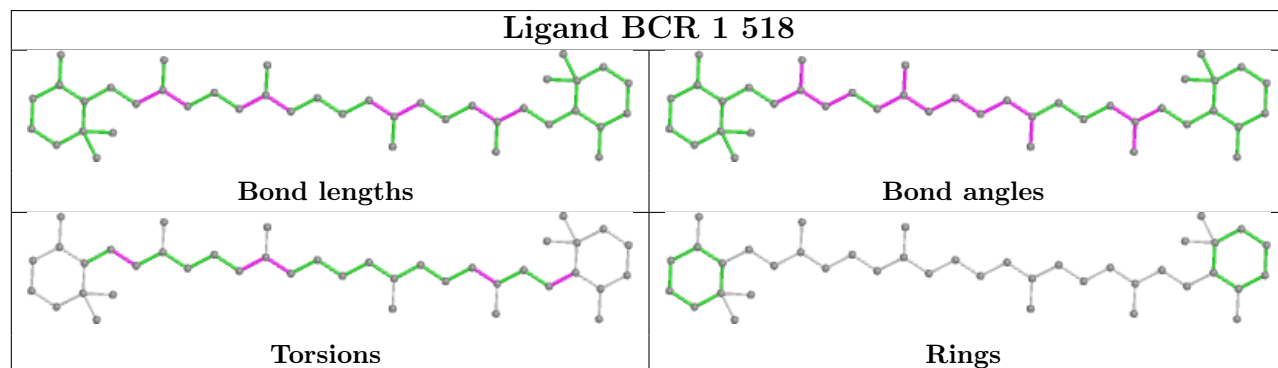
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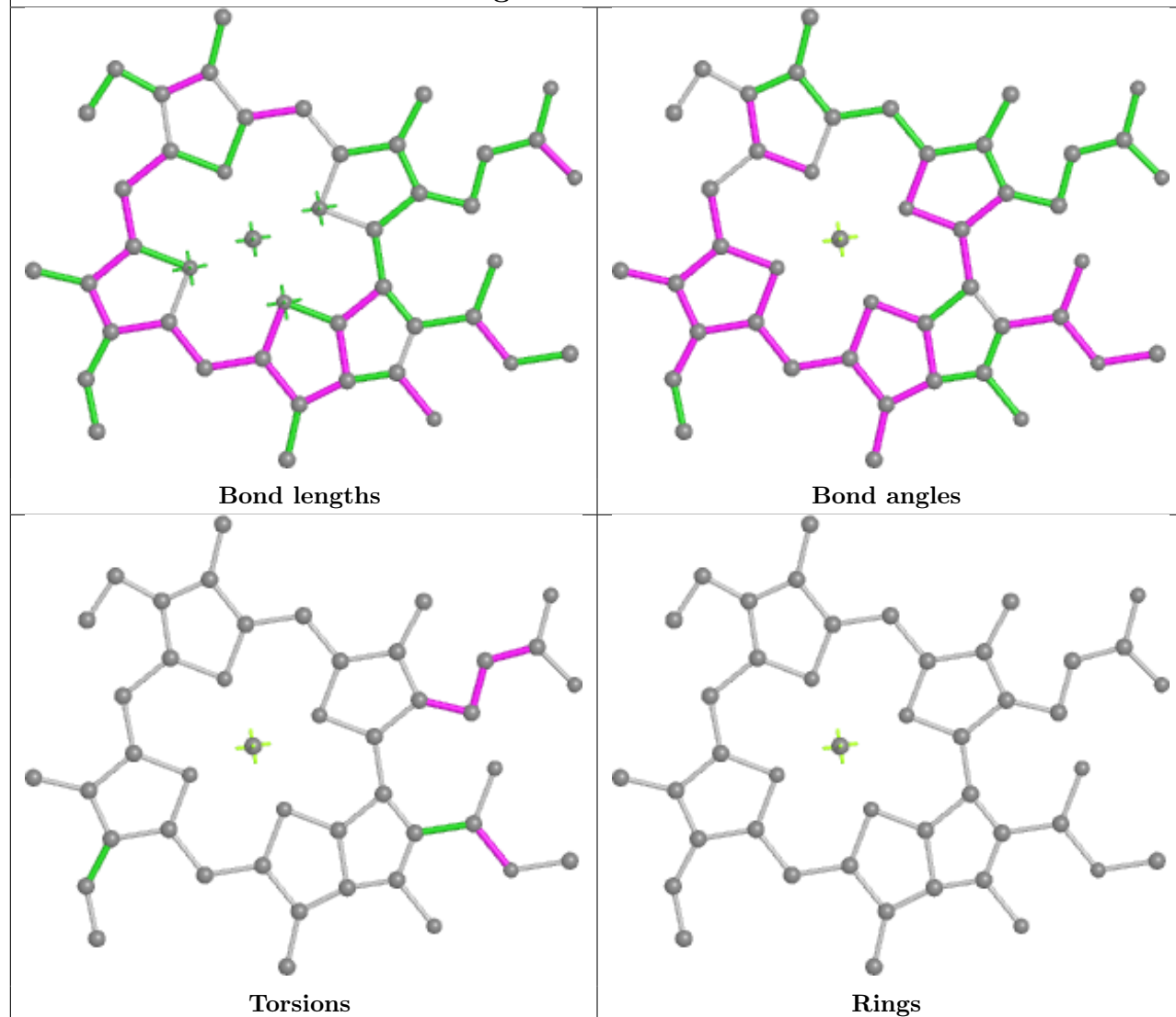
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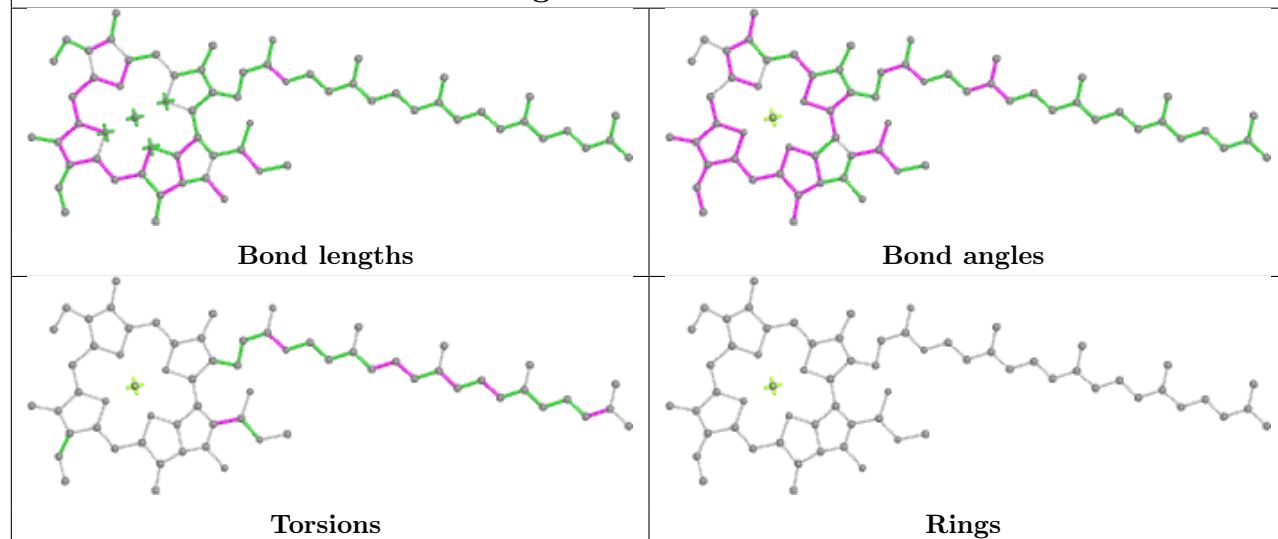
Ligand BCR 1 518



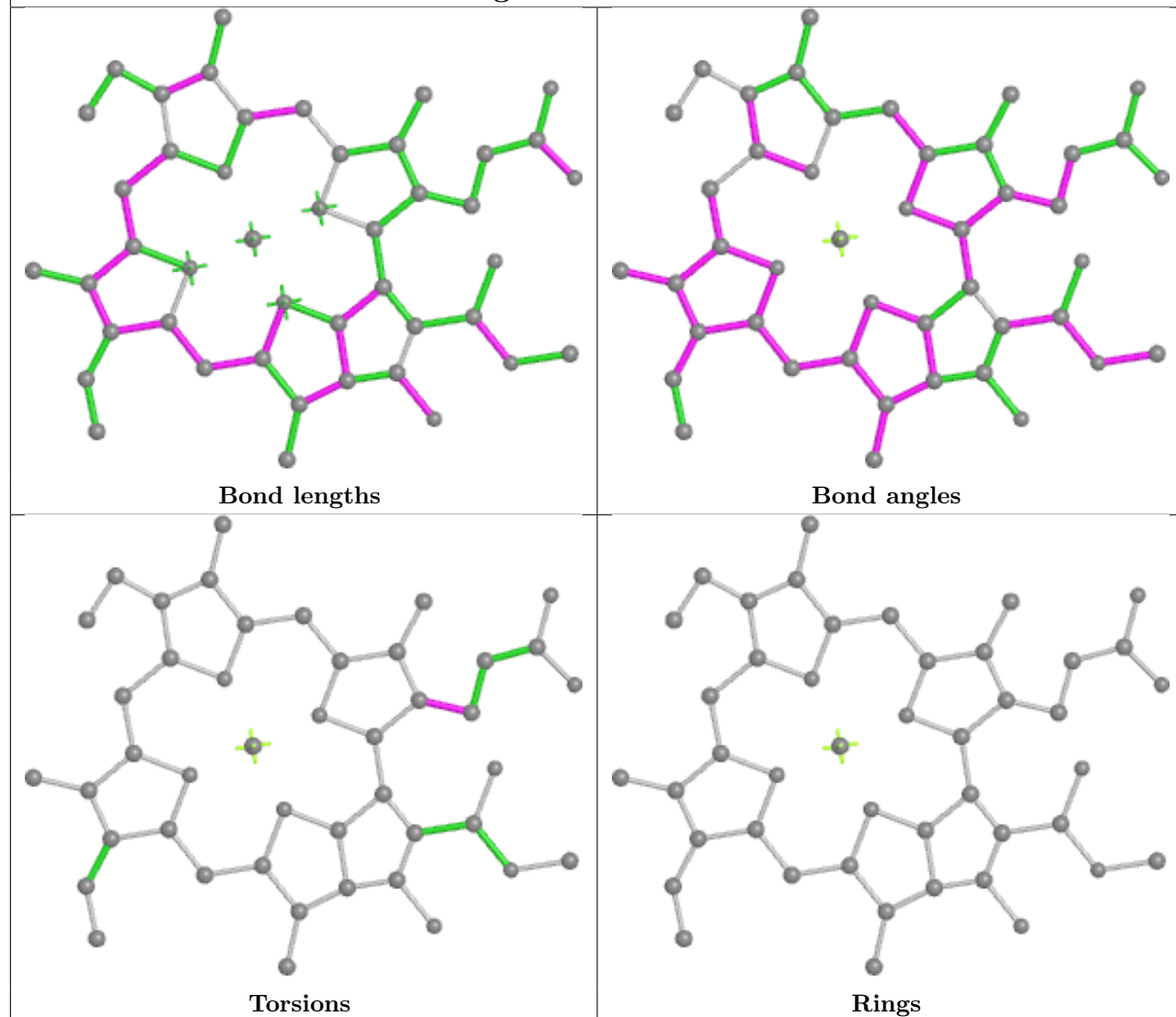
Ligand CLA 4 402



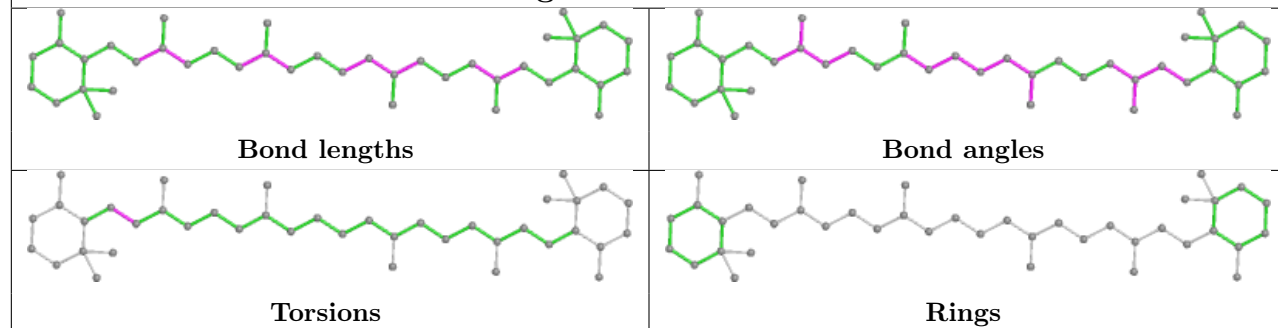
Ligand CLA B 839



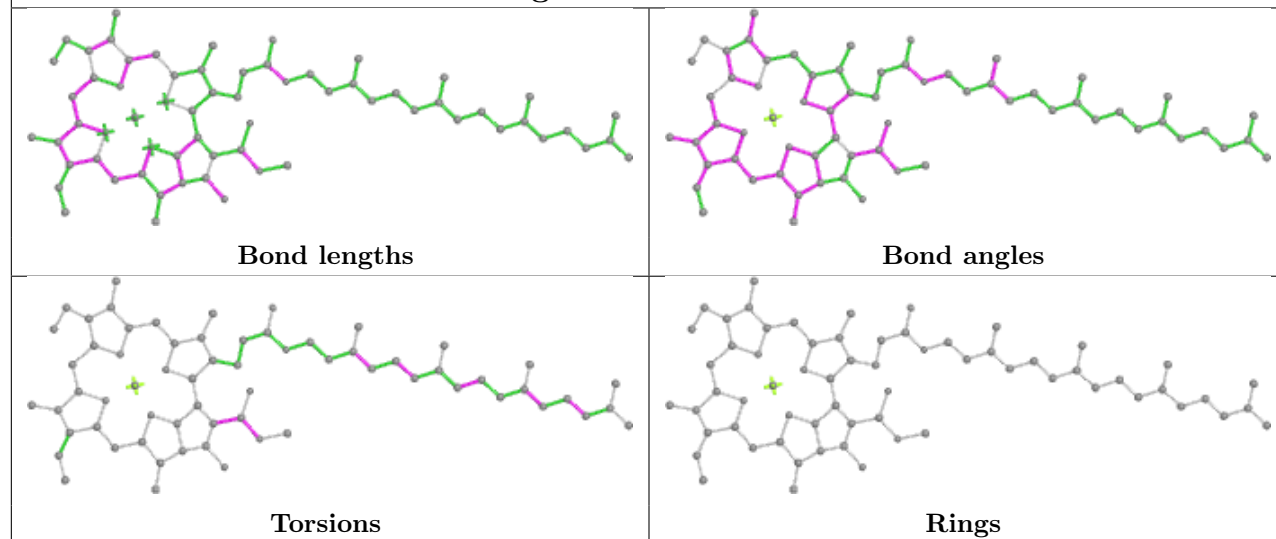
Ligand CLA 1 513



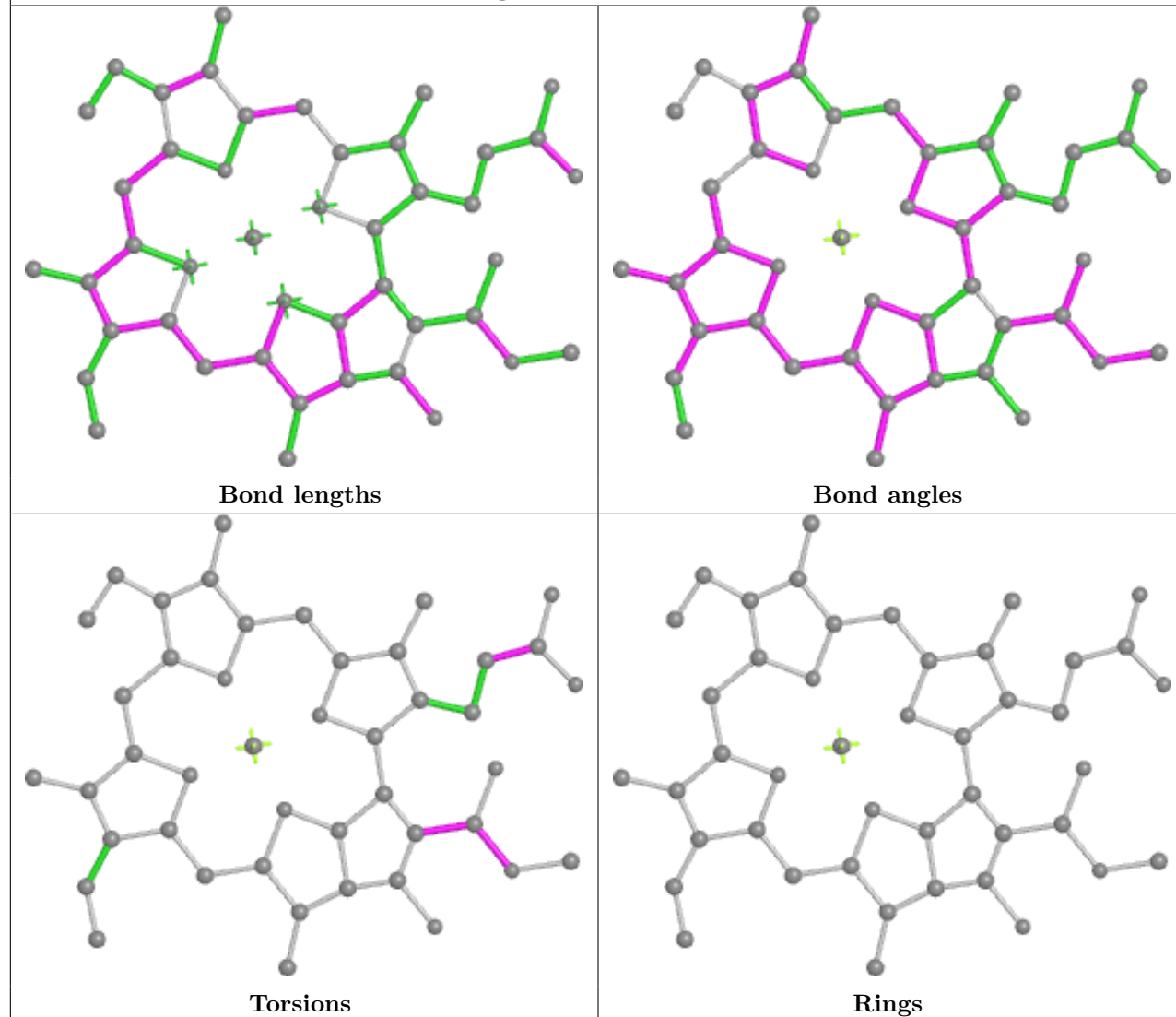
Ligand BCR I 101



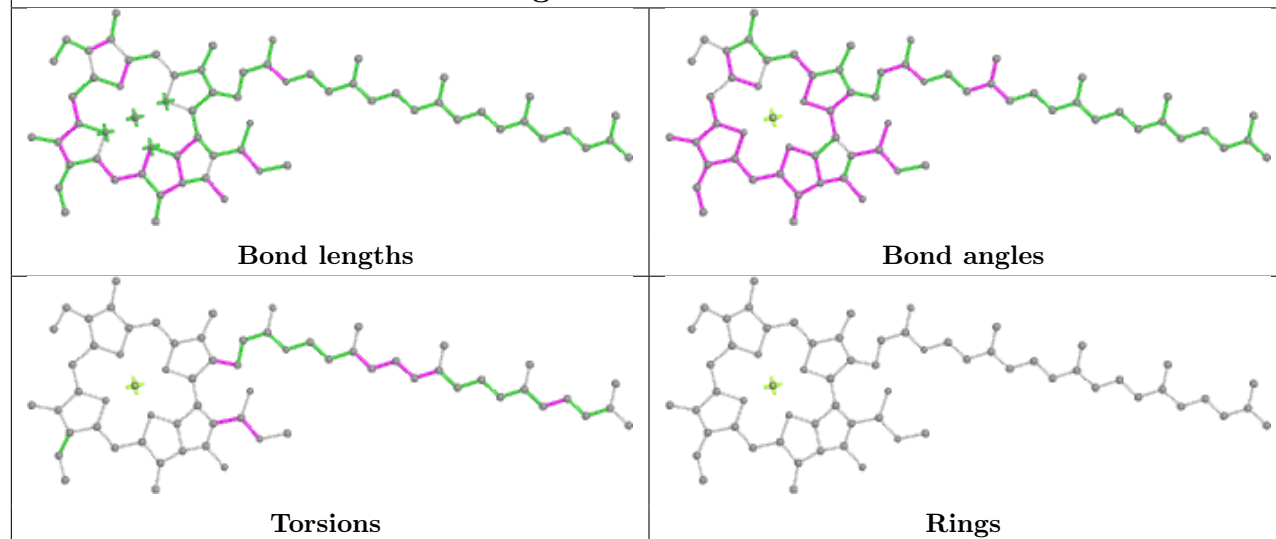
Ligand CLA A 840



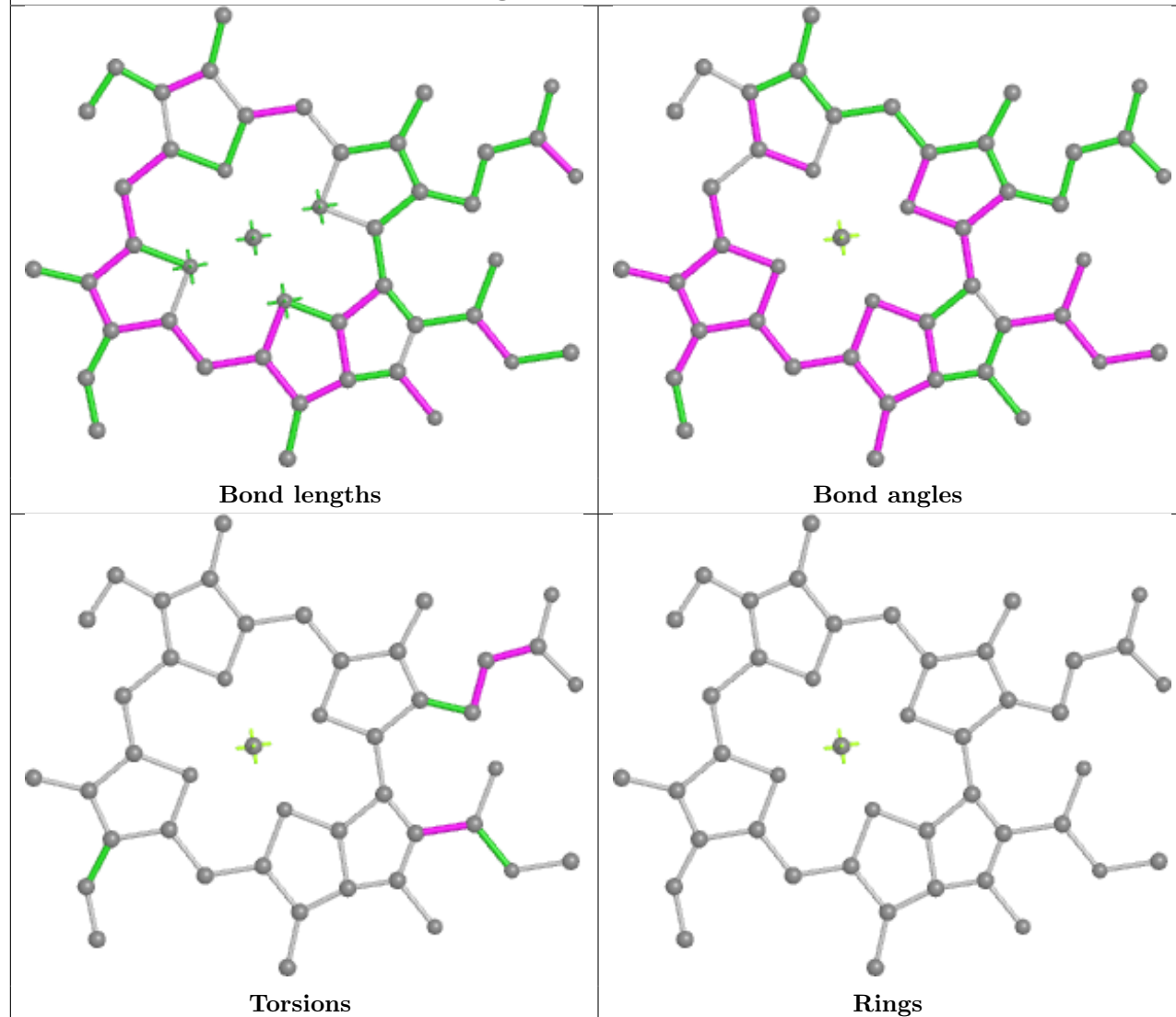
Ligand CLA 6 405



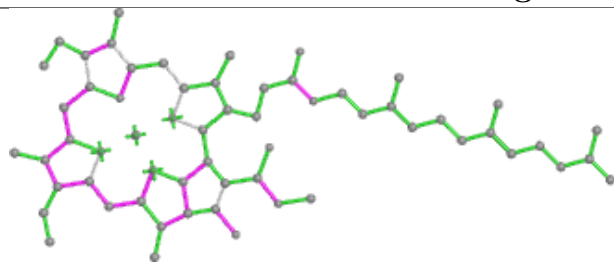
Ligand CLA B 818



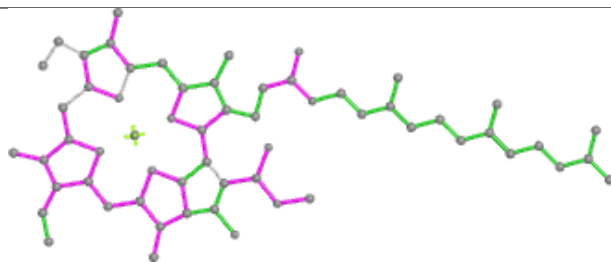
Ligand CLA 2 402



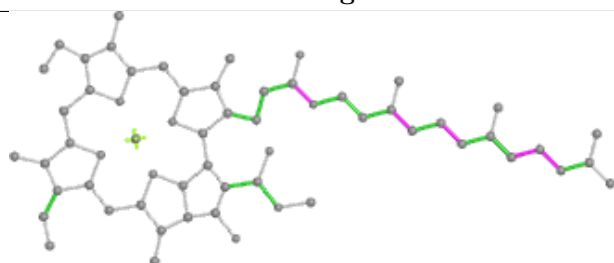
Ligand CLA B 837



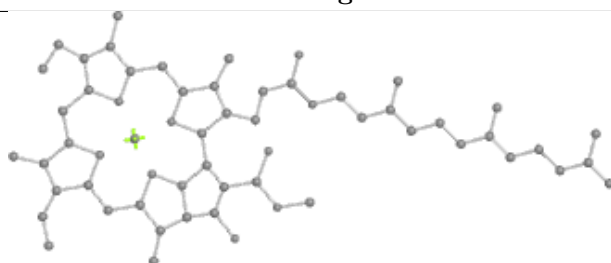
Bond lengths



Bond angles

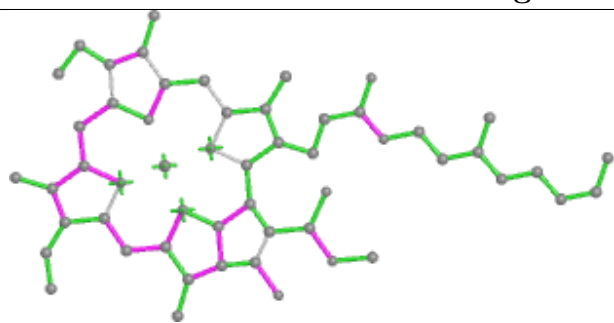


Torsions

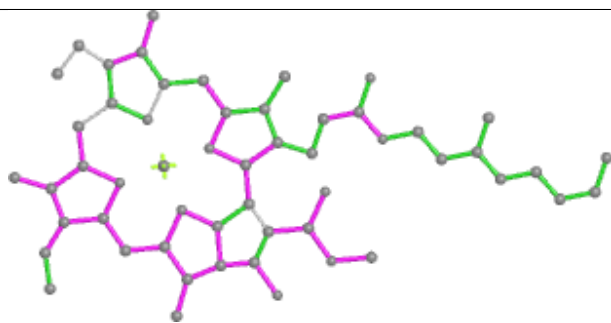


Rings

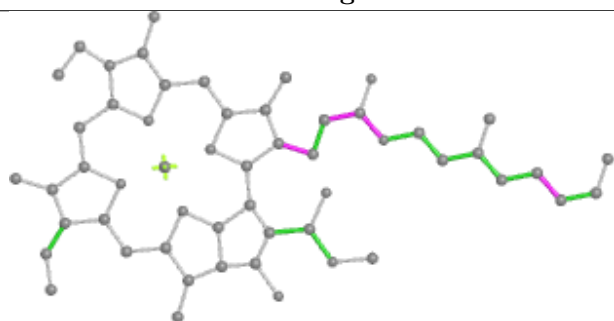
Ligand CLA A 819



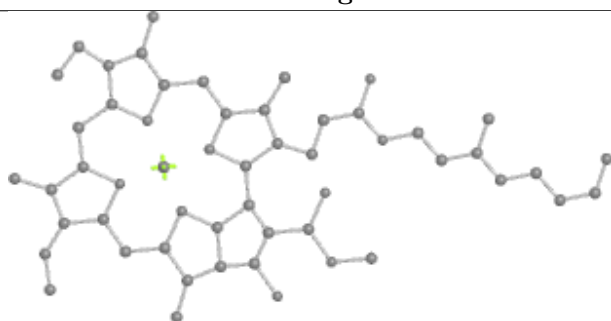
Bond lengths



Bond angles

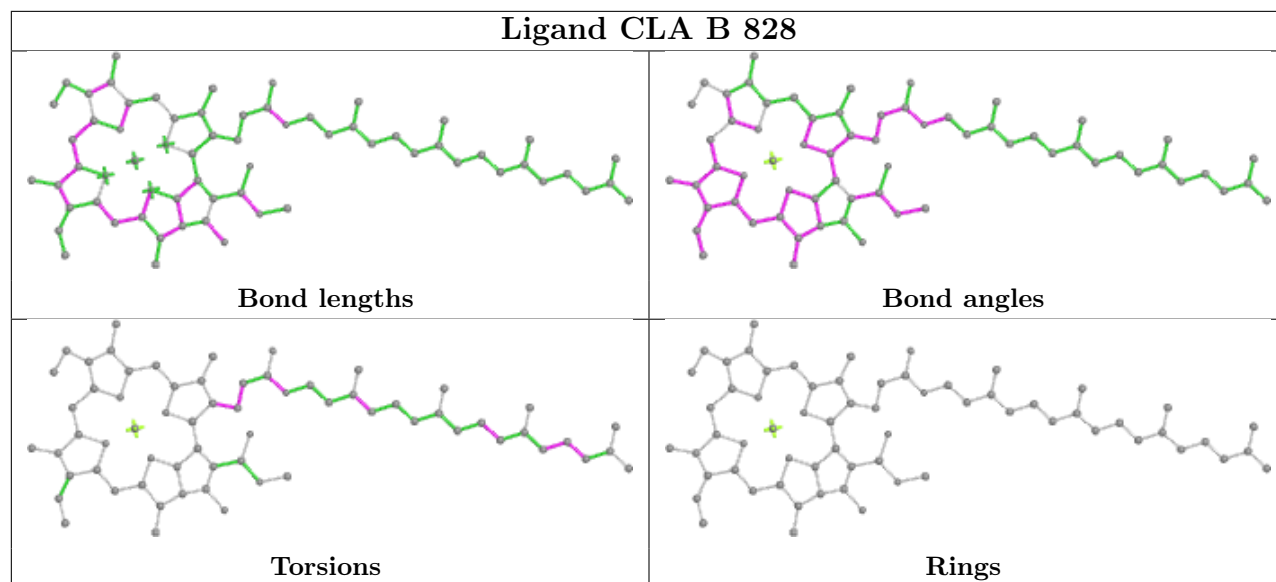


Torsions

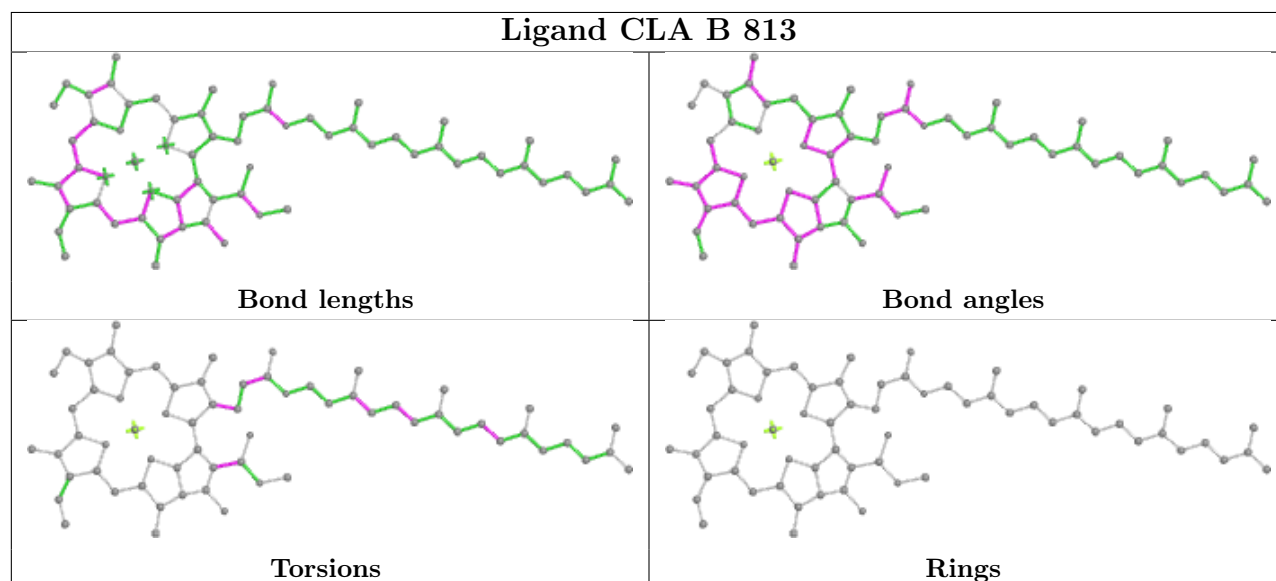


Rings

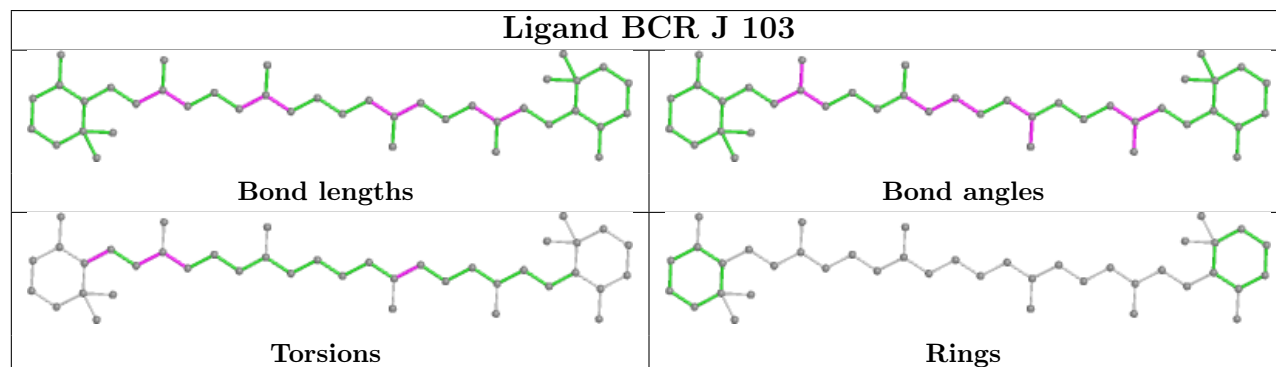
Ligand CLA B 828

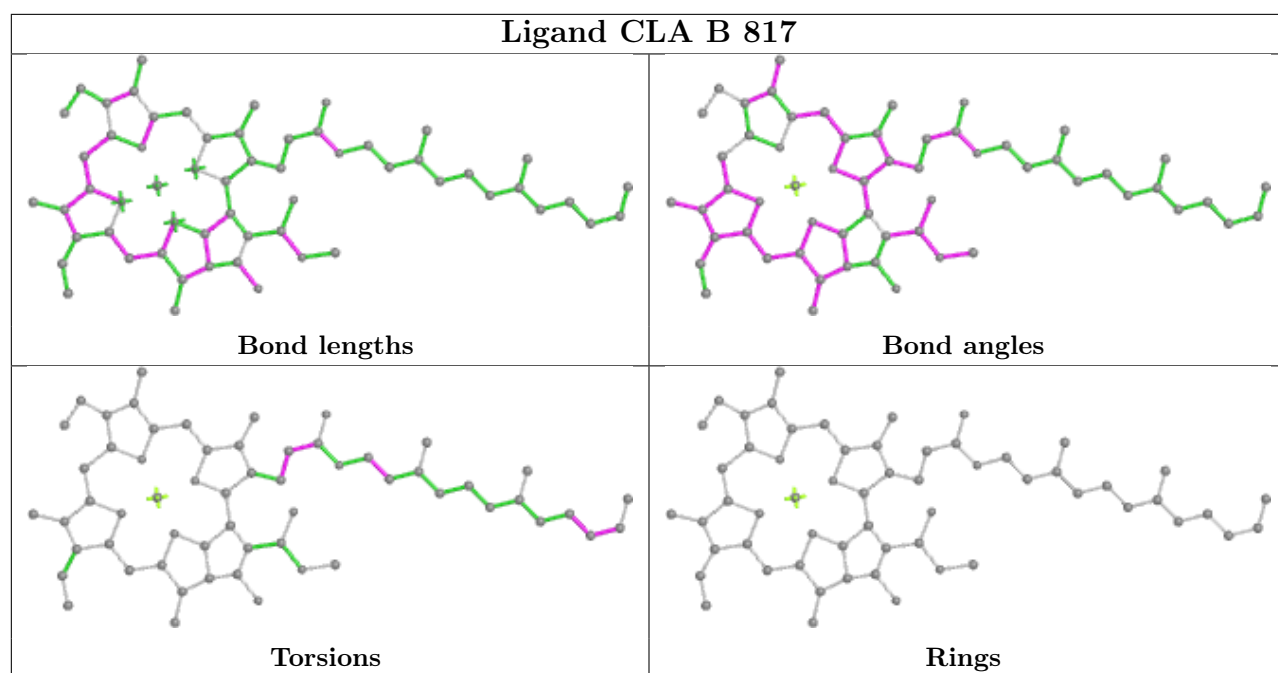


Ligand CLA B 813

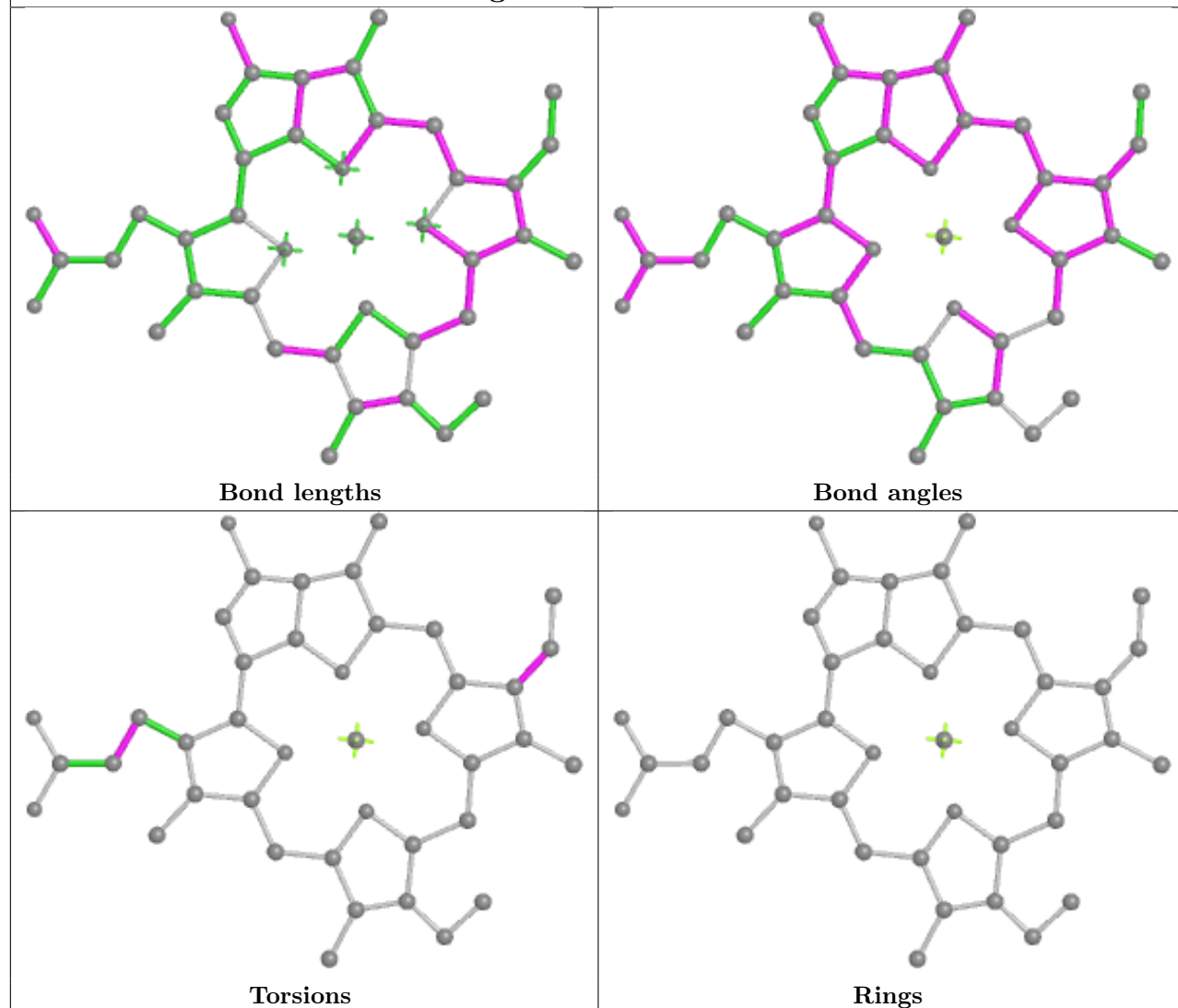


Ligand BCR J 103

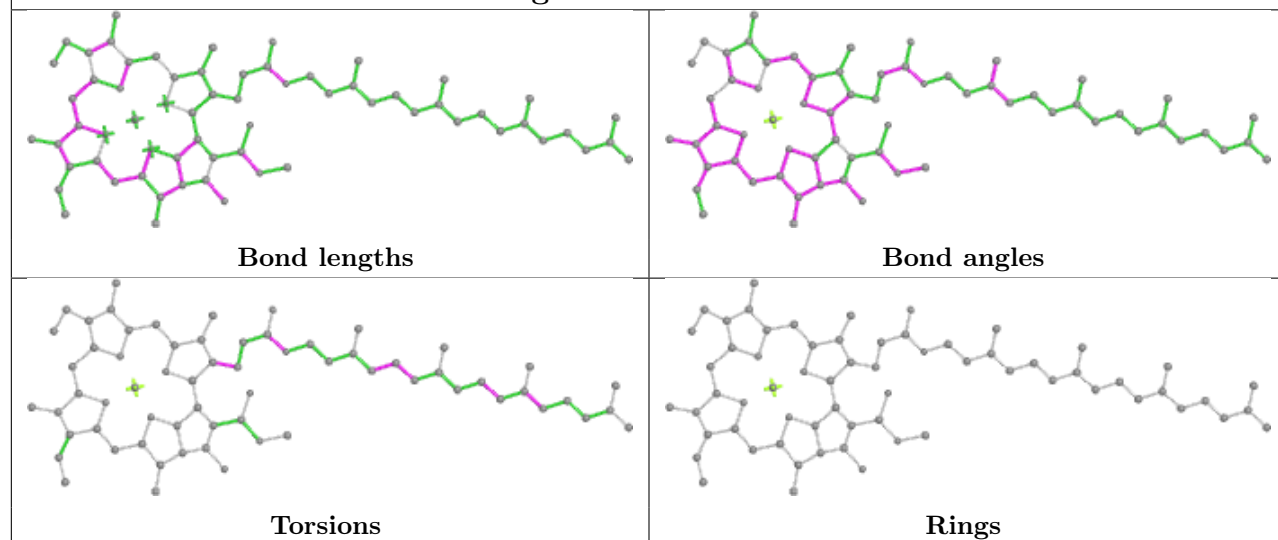


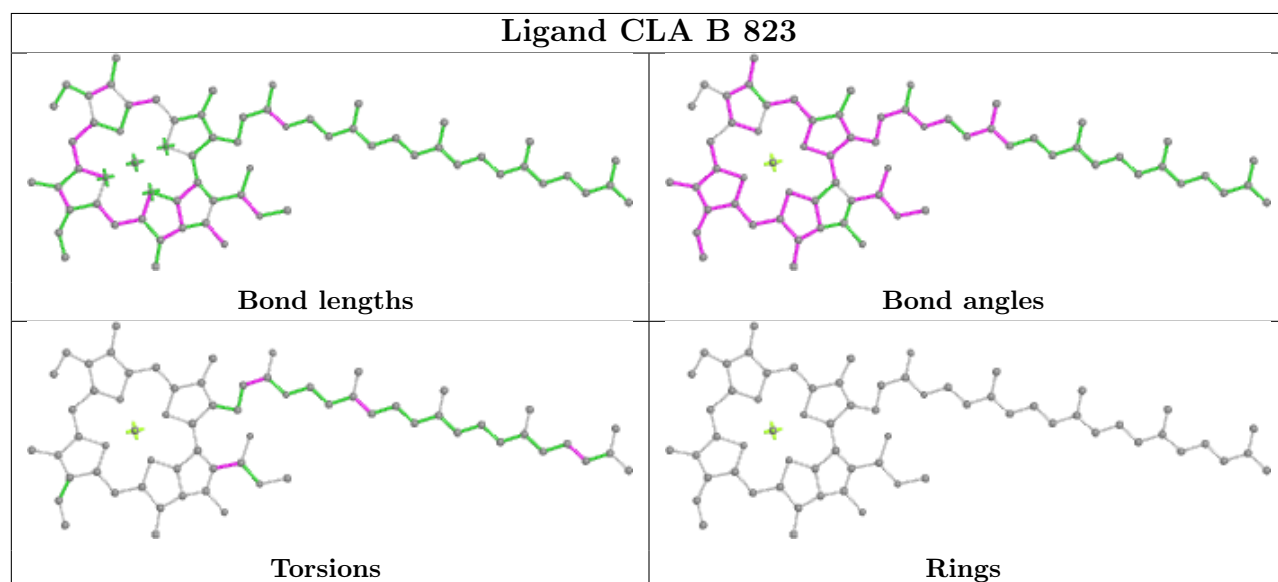
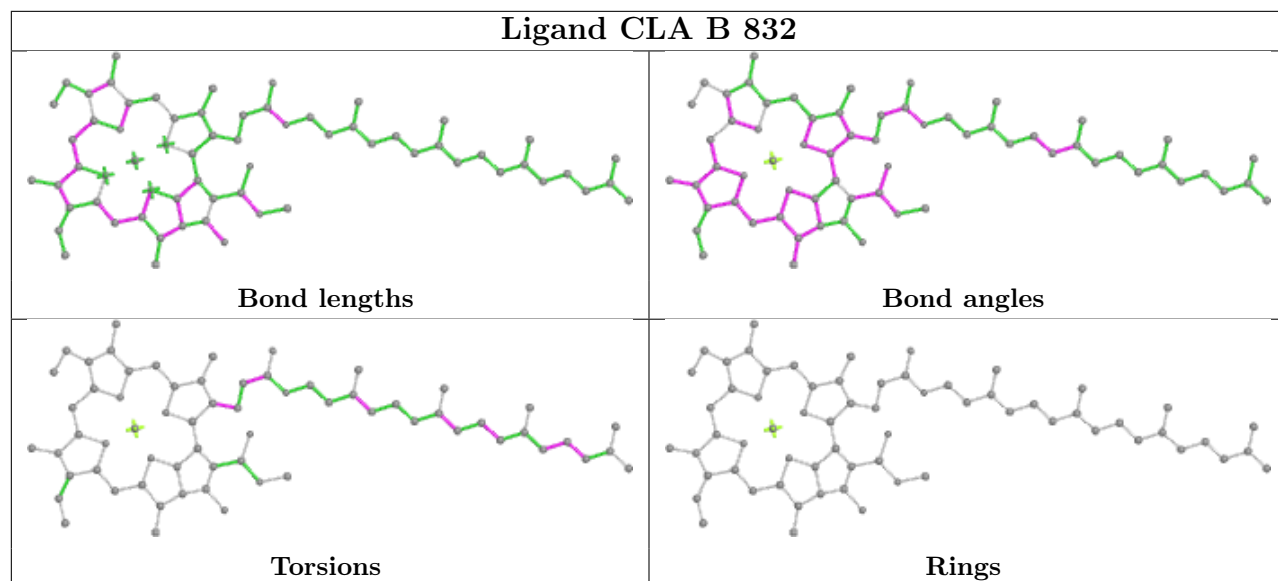
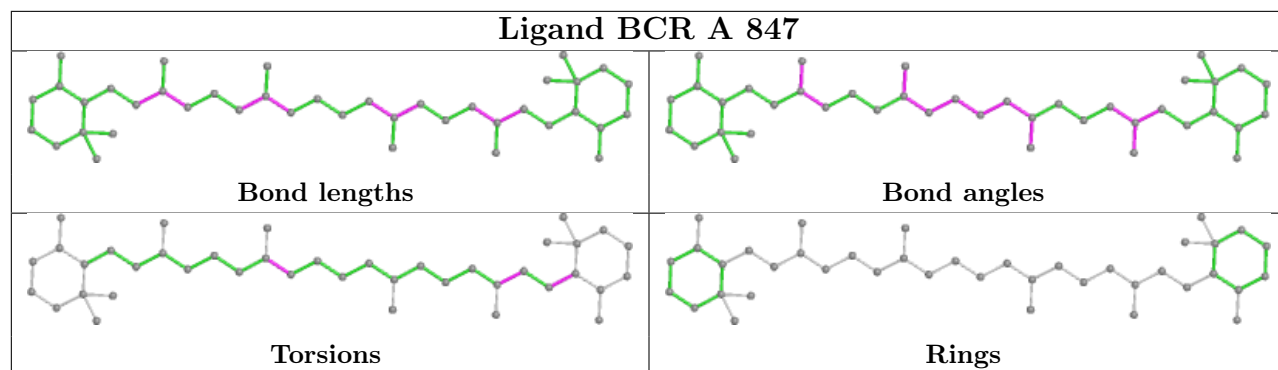


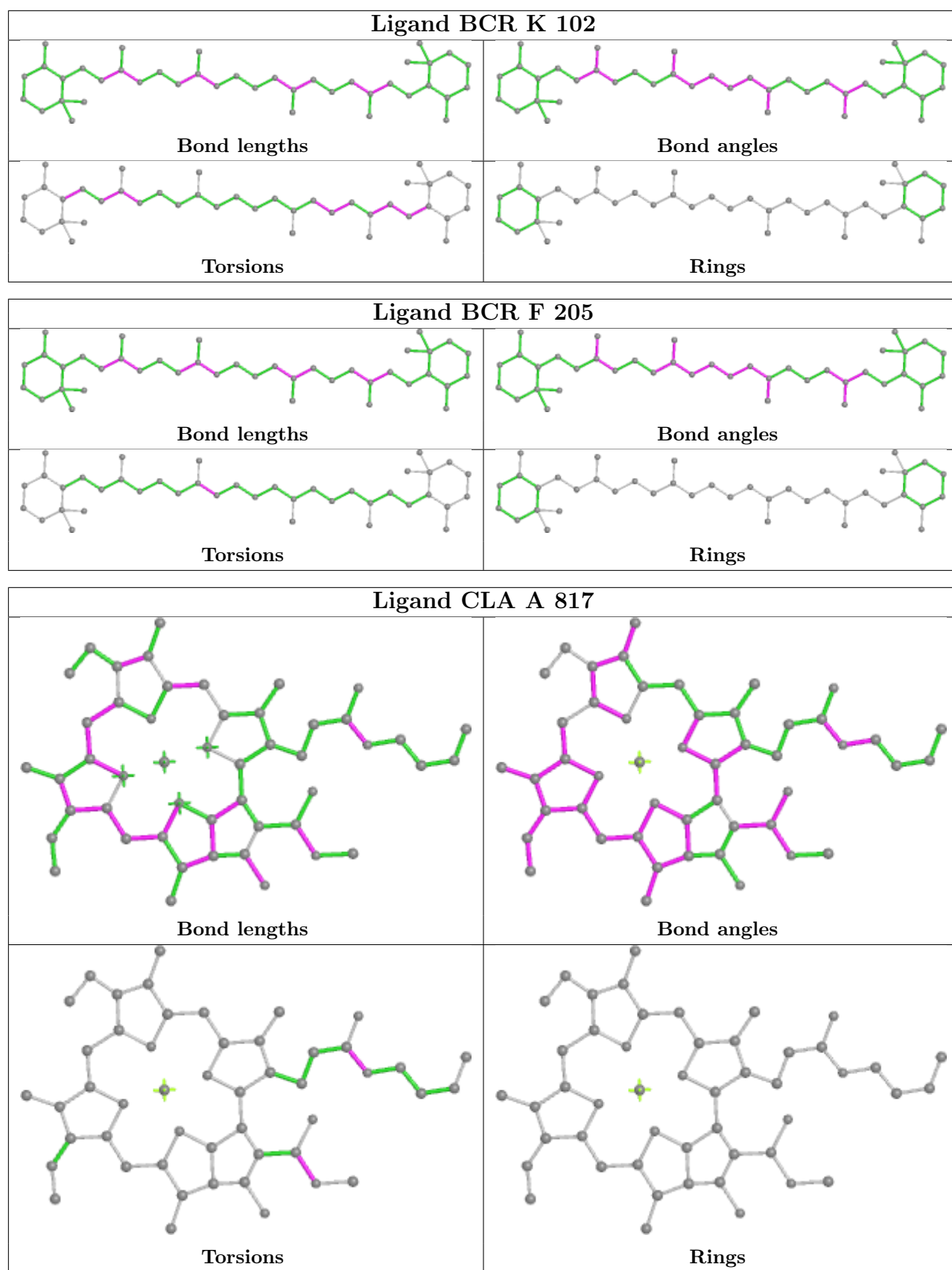
Ligand CLA K 101

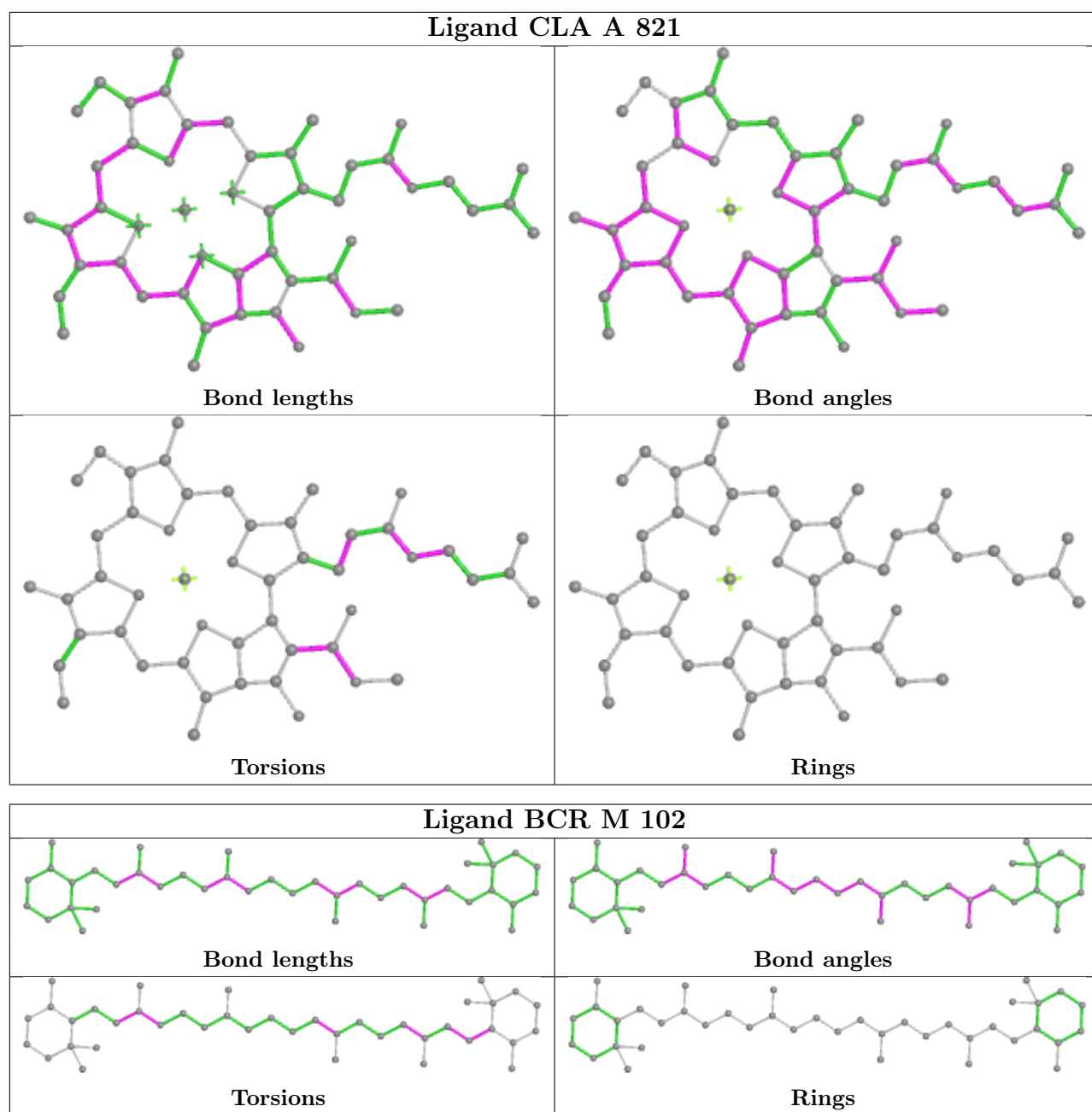


Ligand CLA A 807

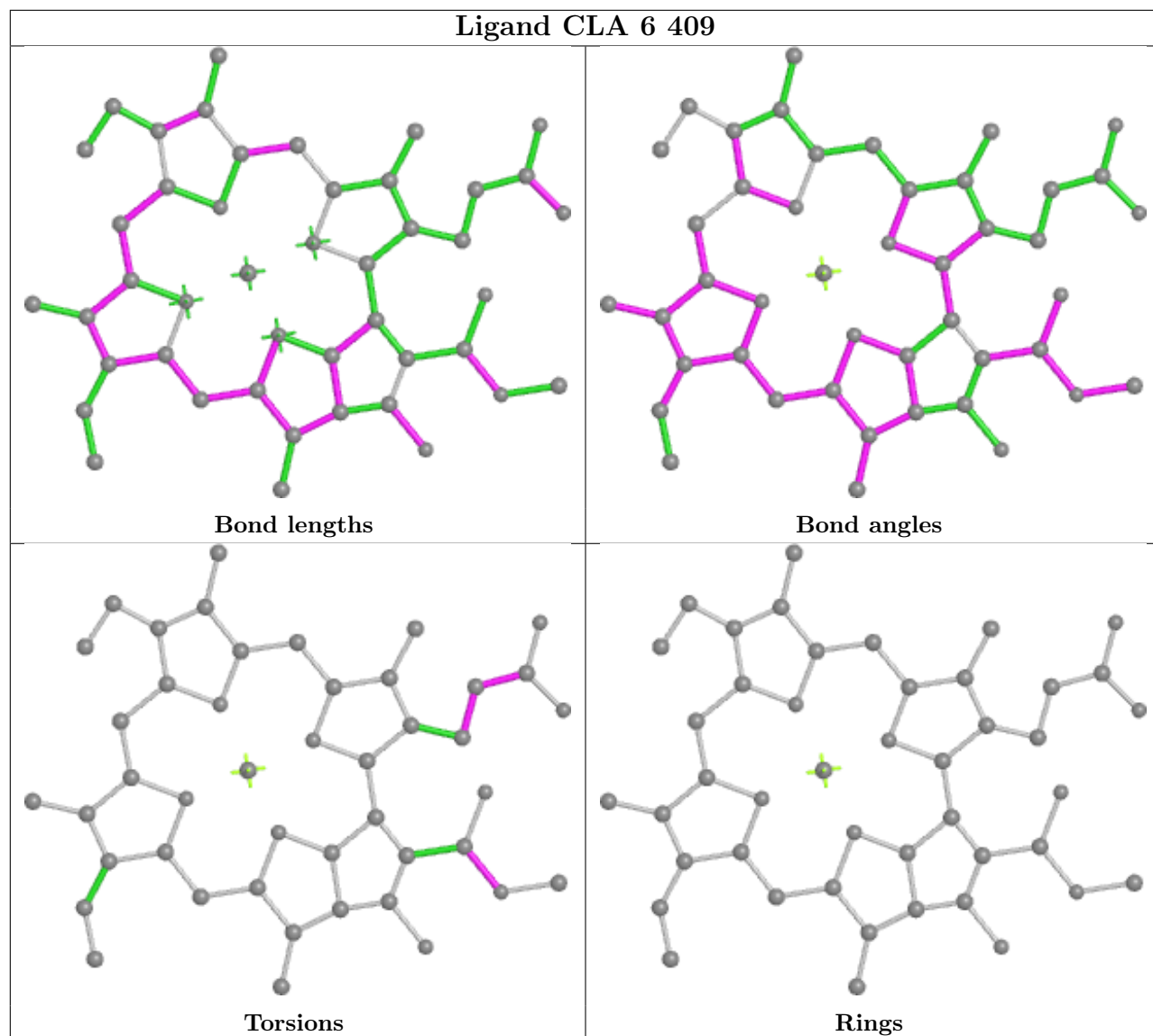


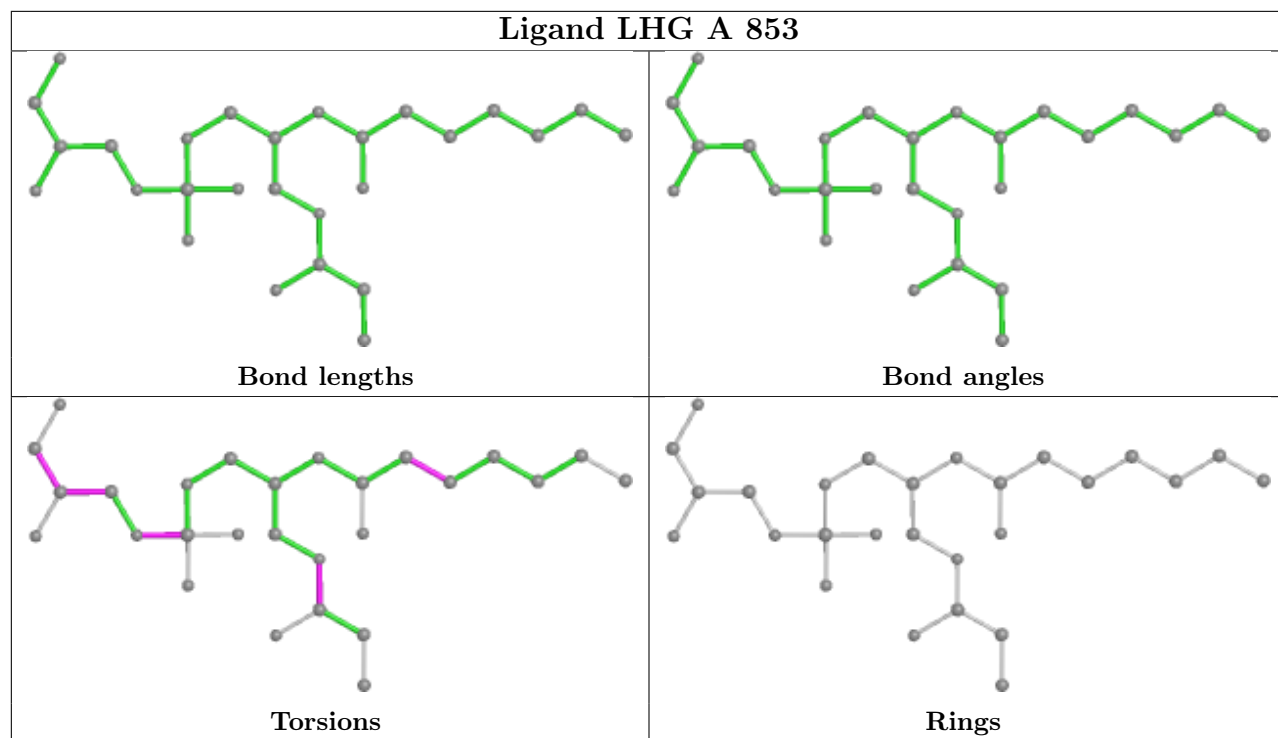




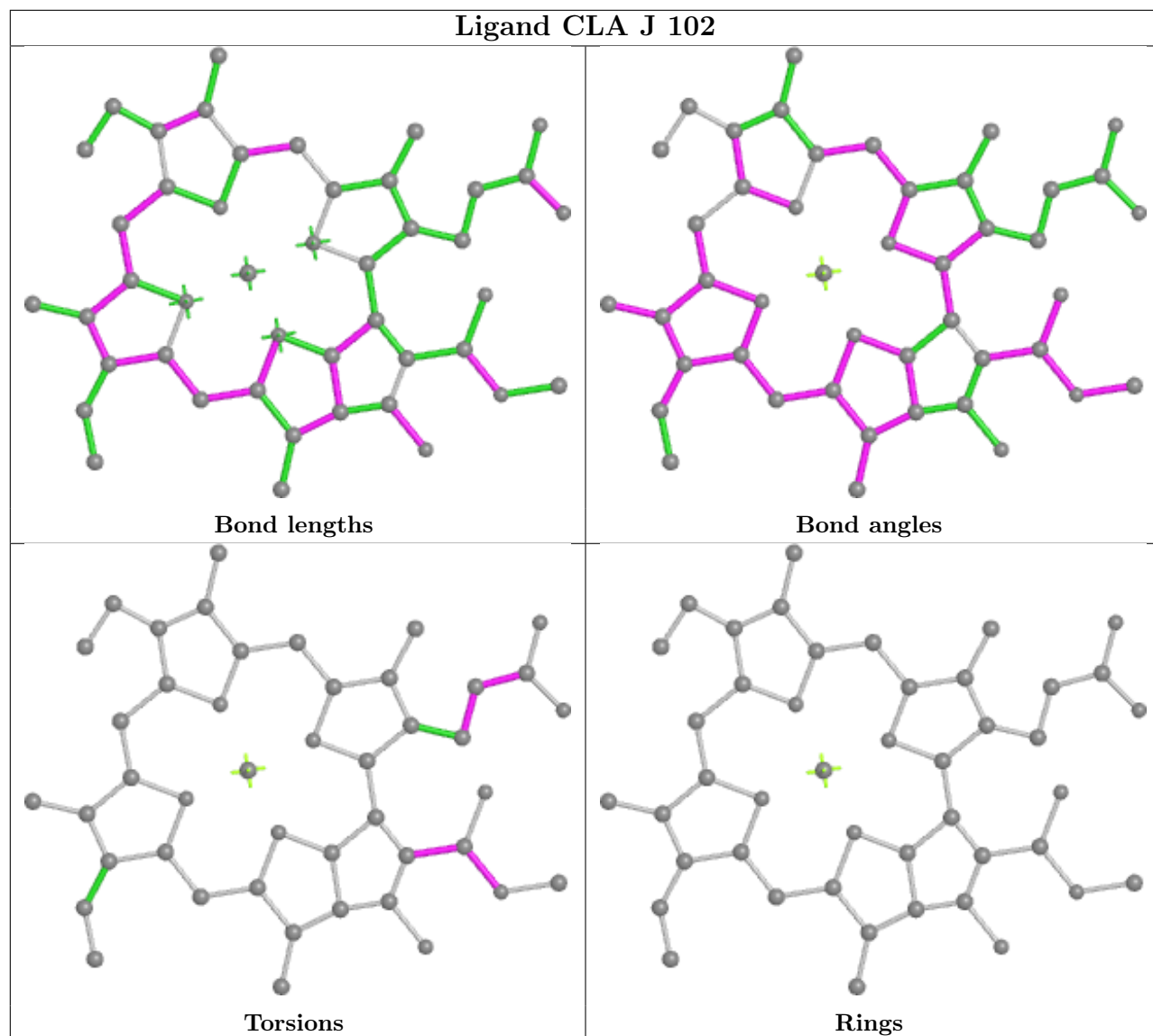


Ligand CLA 6 409

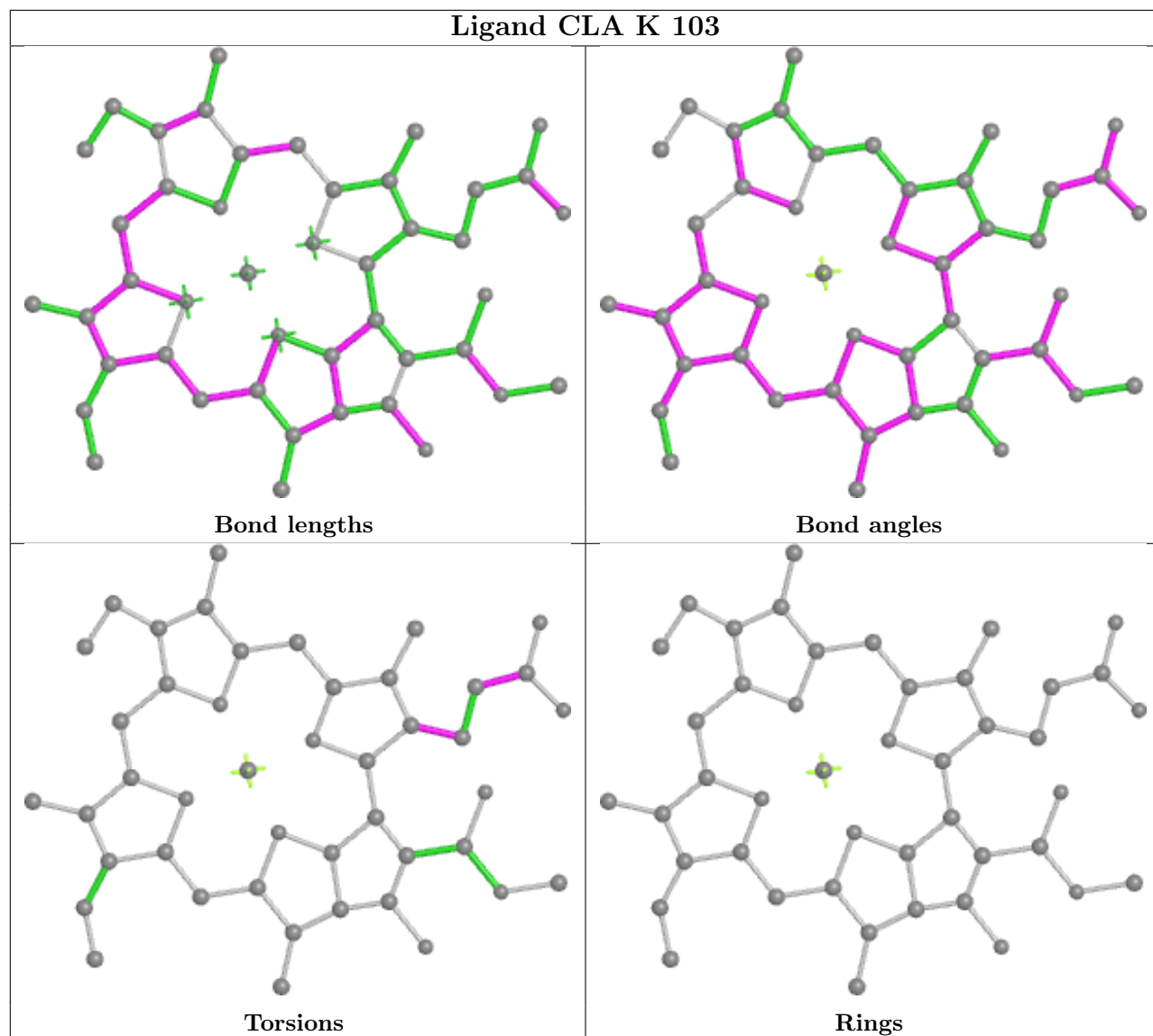




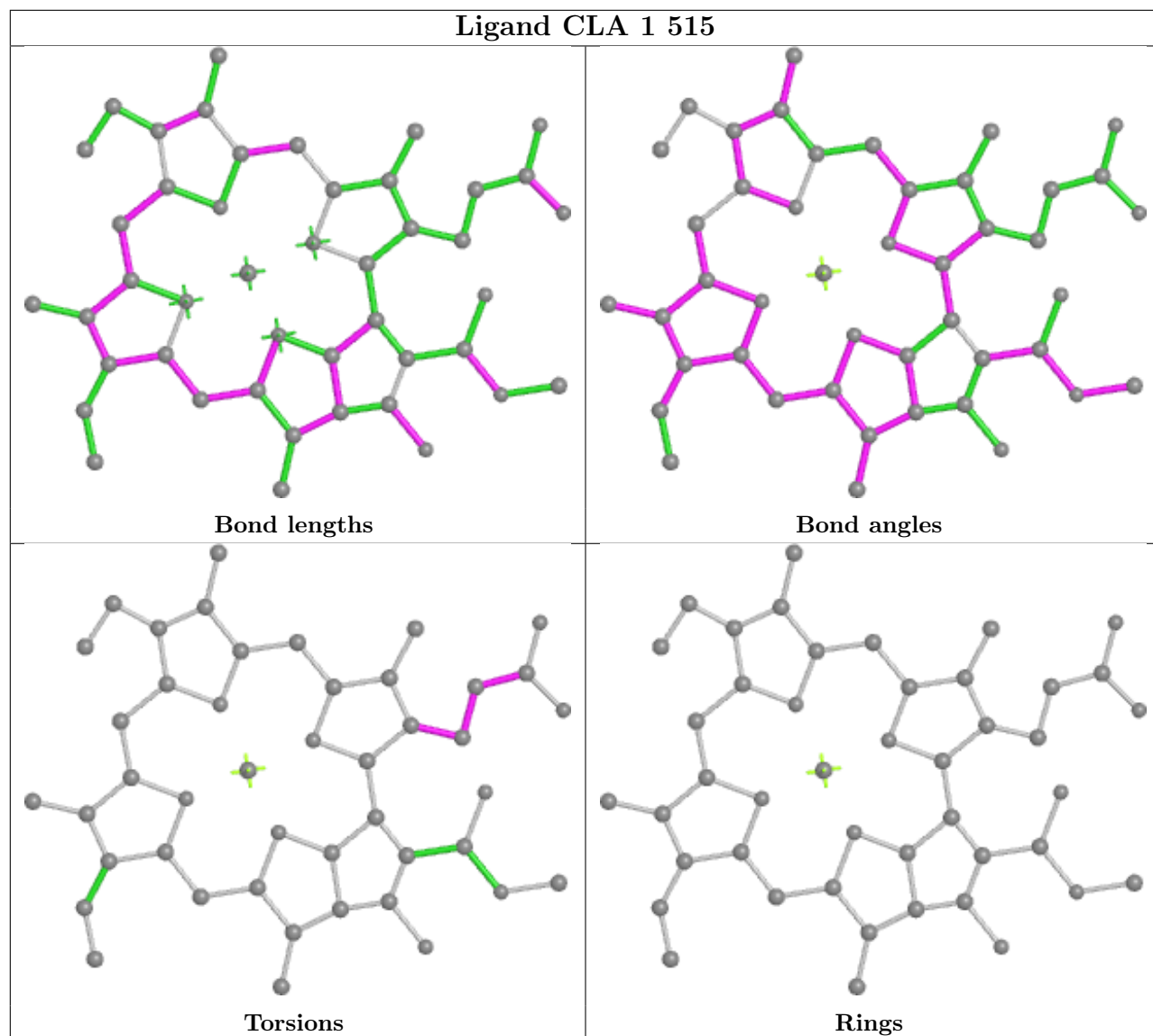
Ligand CLA J 102



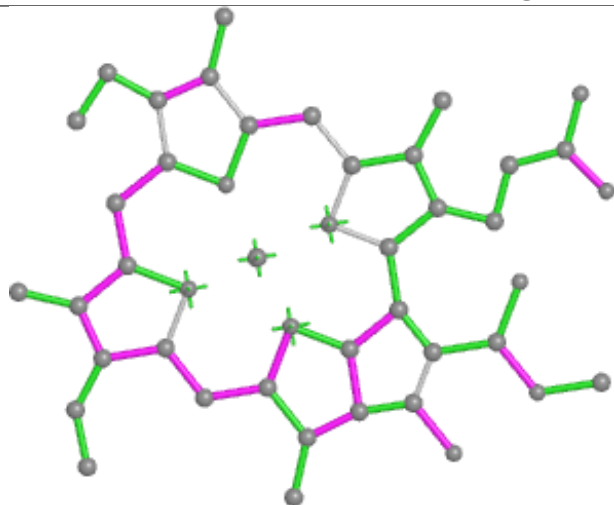
Ligand CLA K 103



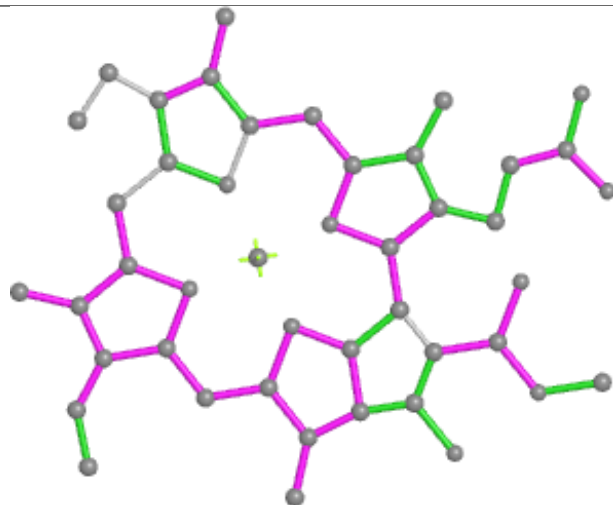
Ligand CLA 1 515



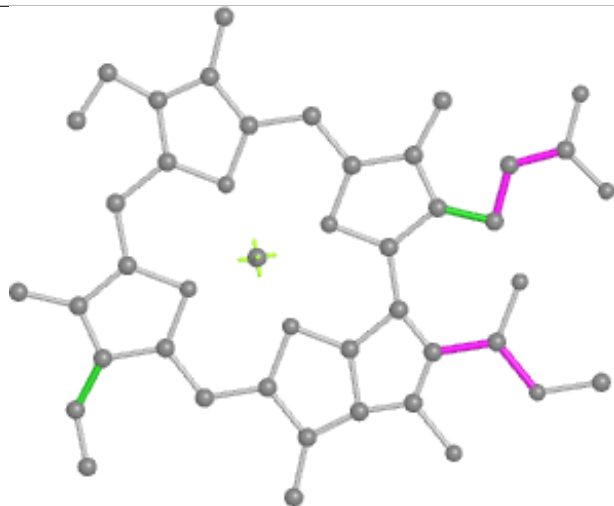
Ligand CLA J 101



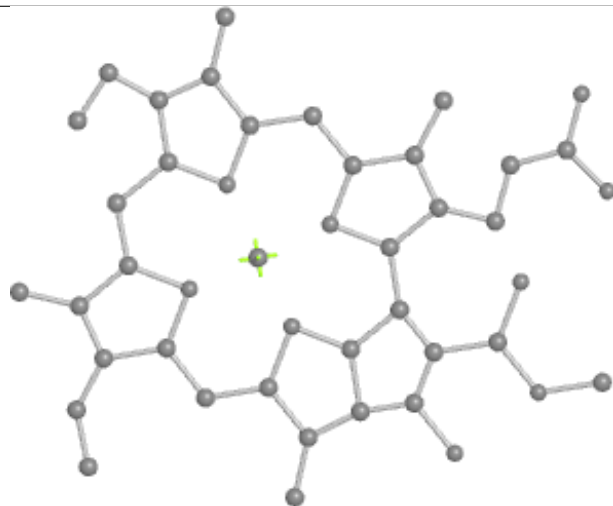
Bond lengths



Bond angles

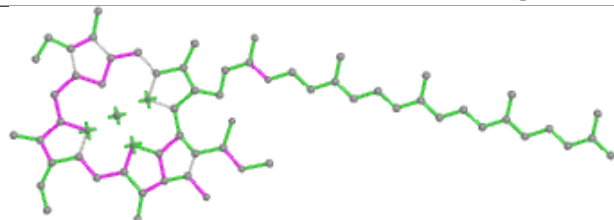


Torsions

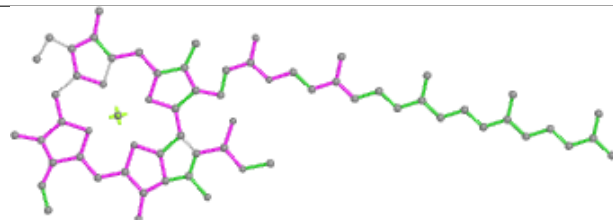


Rings

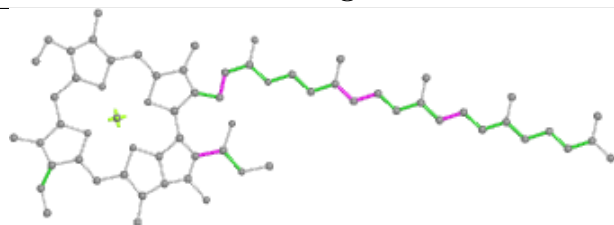
Ligand CLA B 802



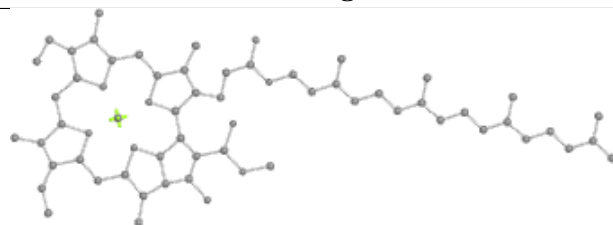
Bond lengths



Bond angles

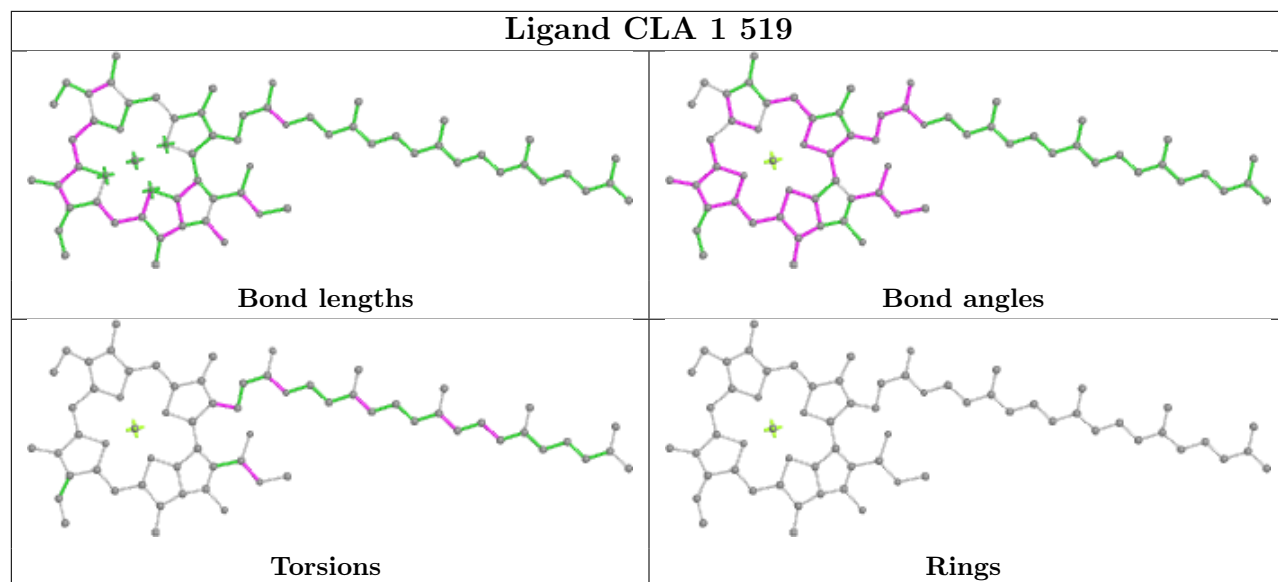


Torsions

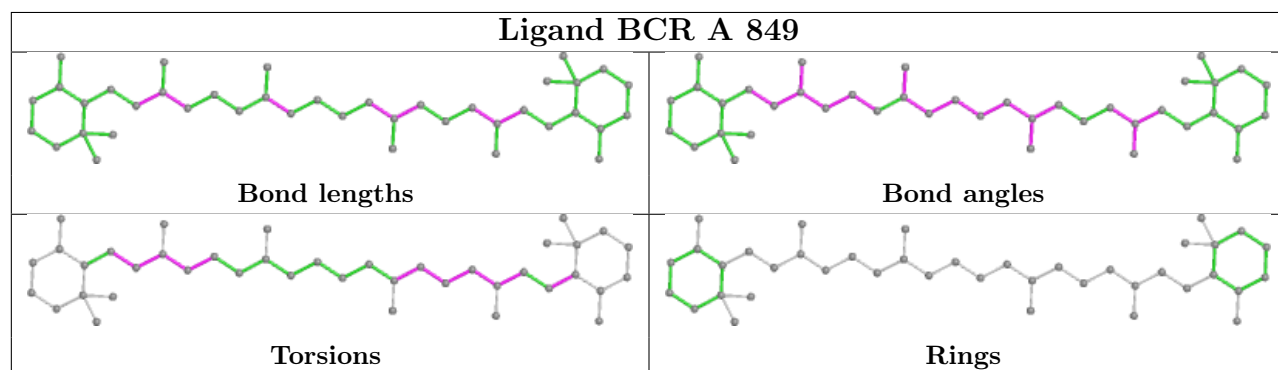


Rings

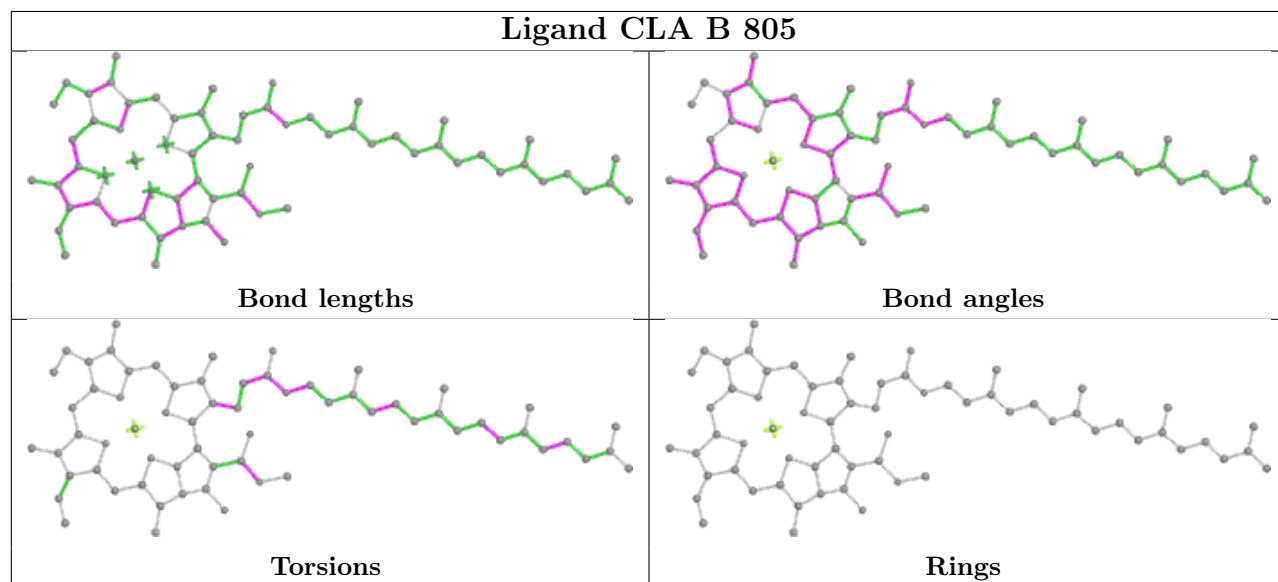
Ligand CLA 1 519



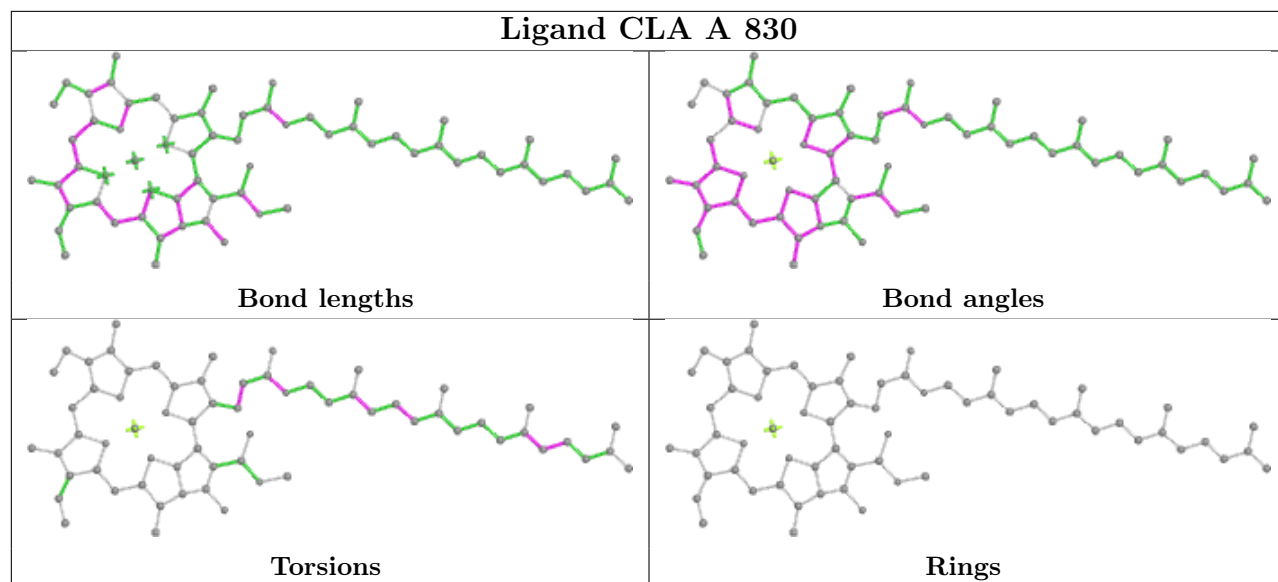
Ligand BCR A 849



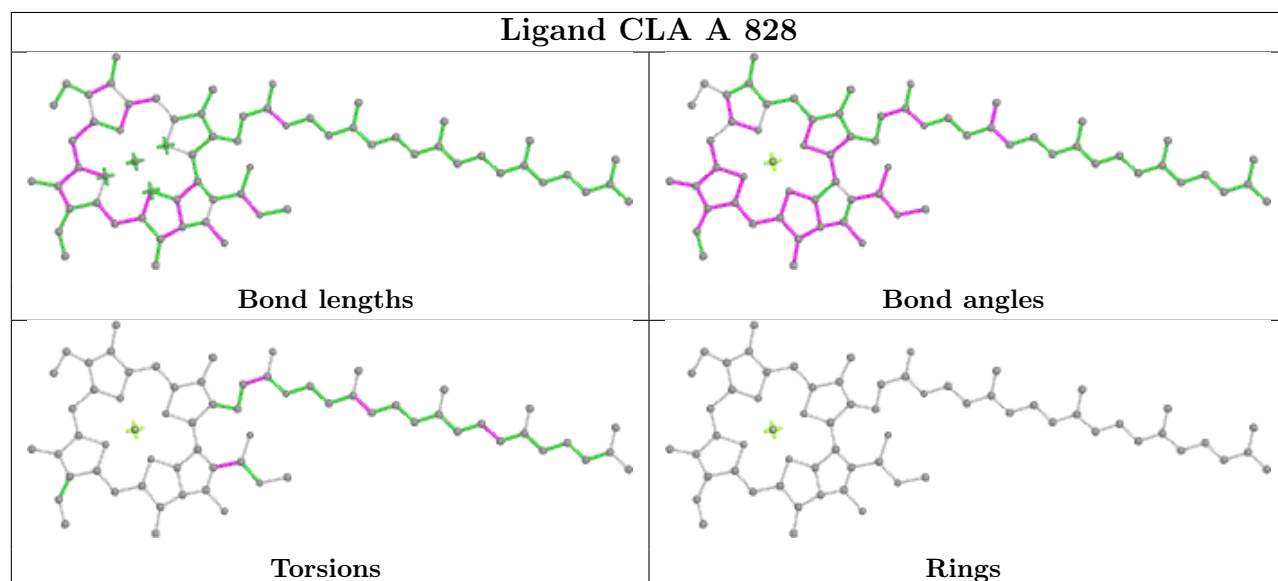
Ligand CLA B 805



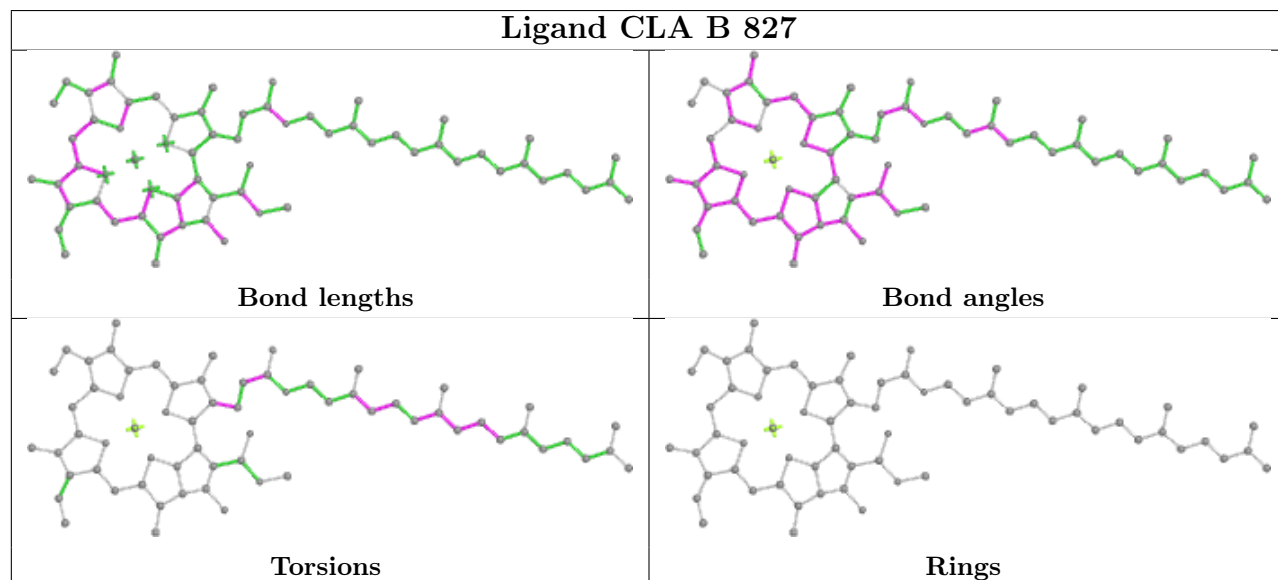
Ligand CLA A 830



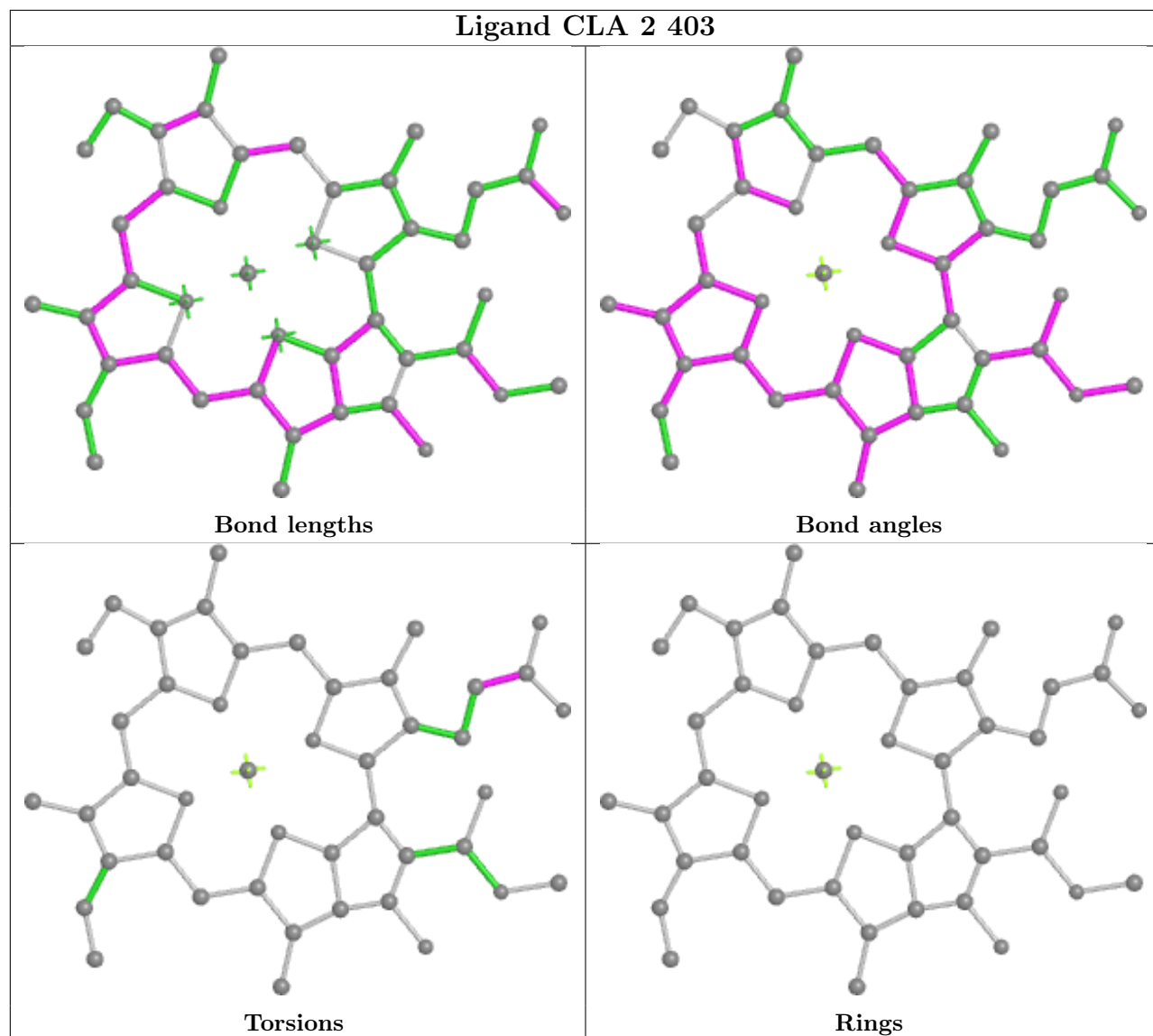
Ligand CLA A 828



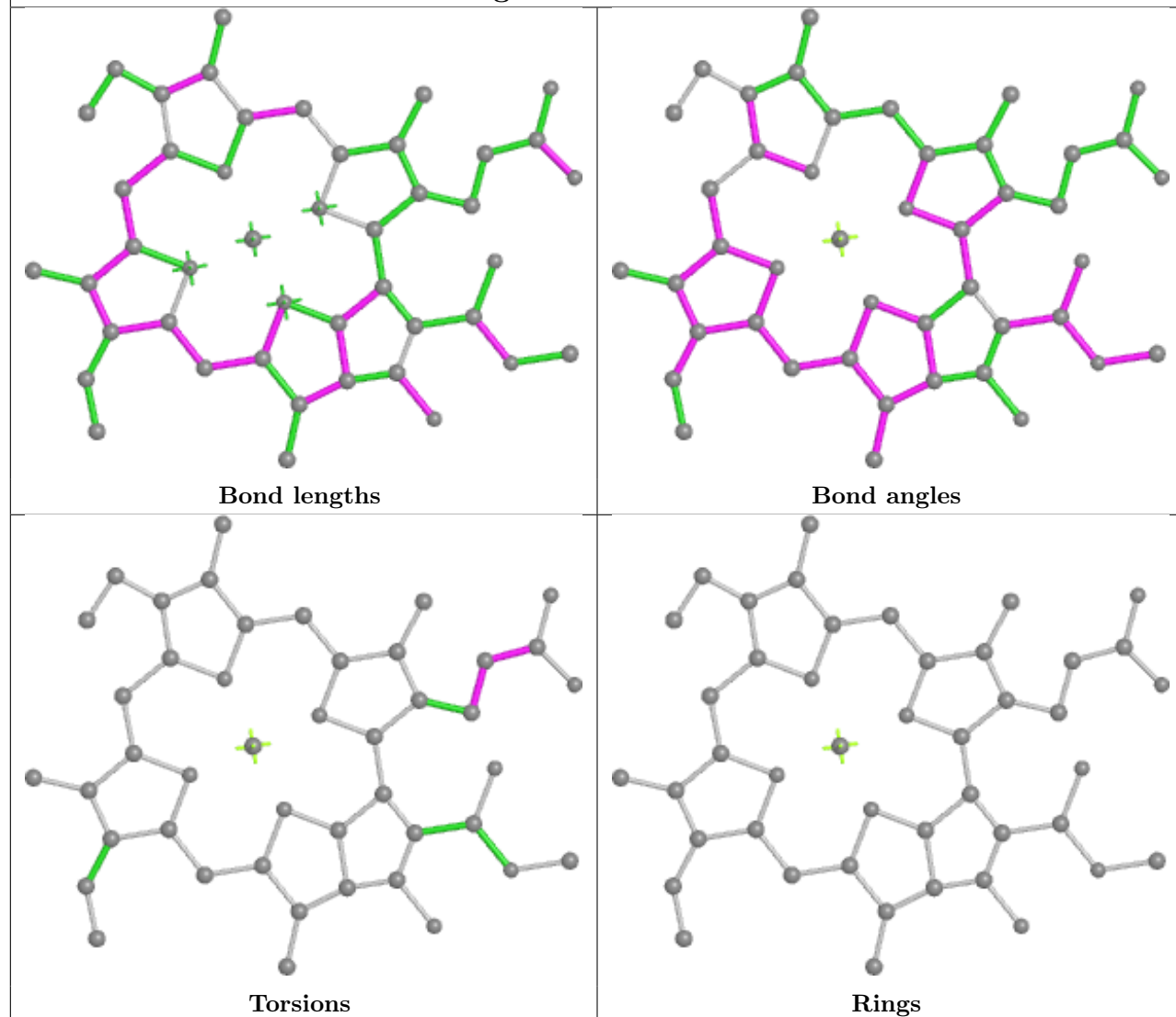
Ligand CLA B 827



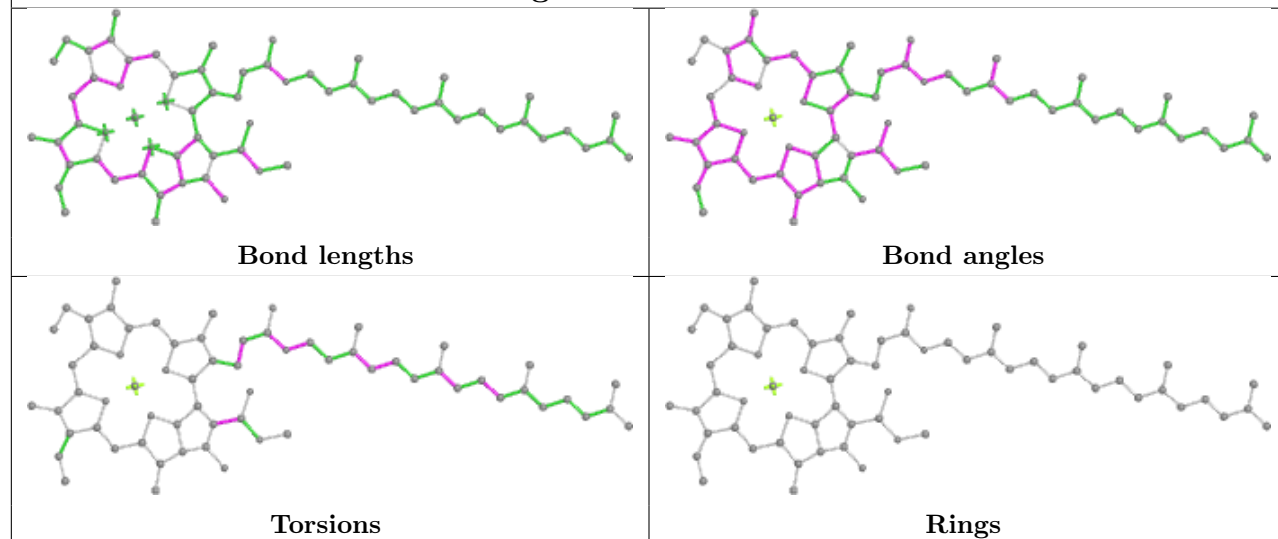
Ligand CLA 2 403



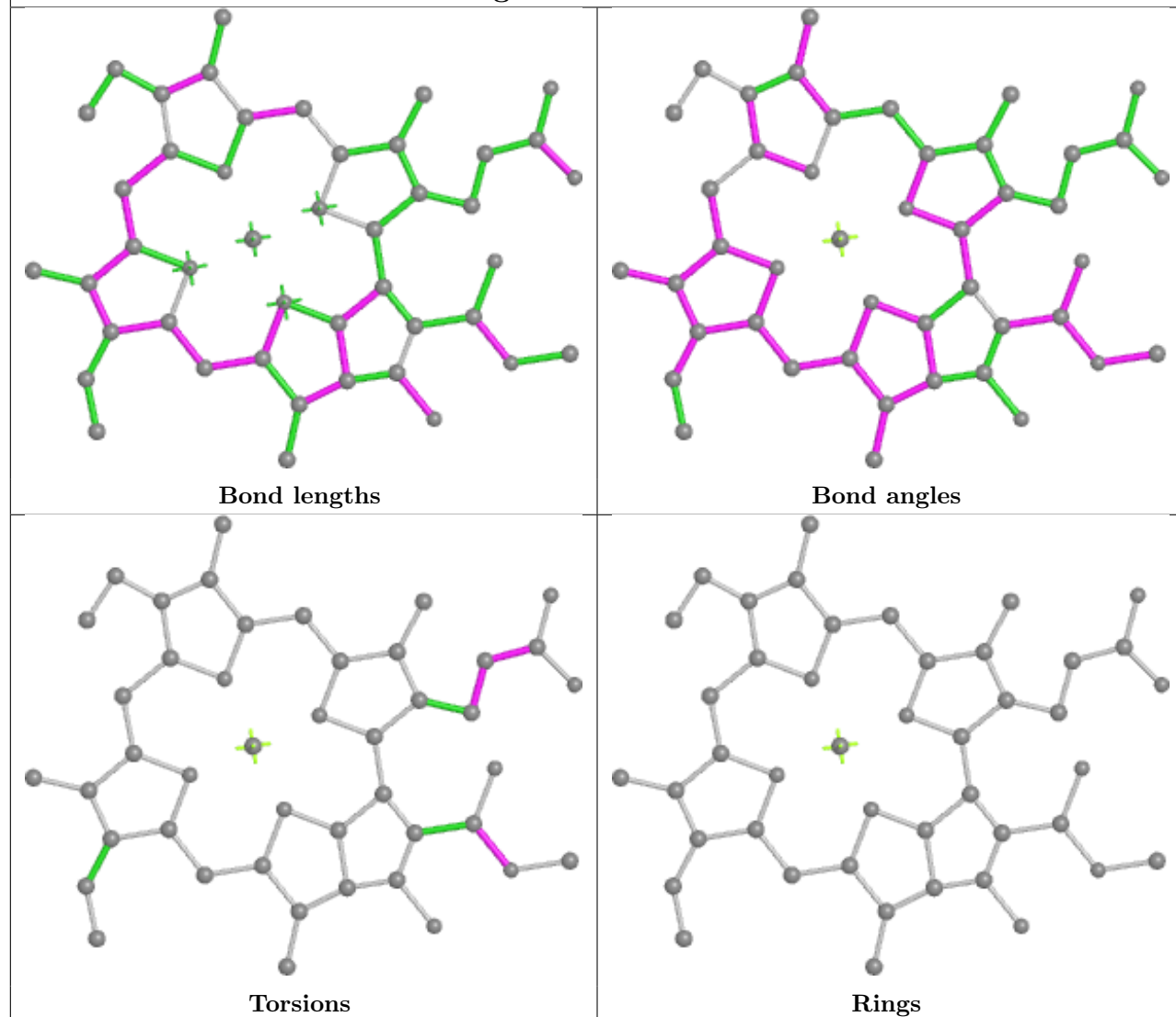
Ligand CLA 5 407



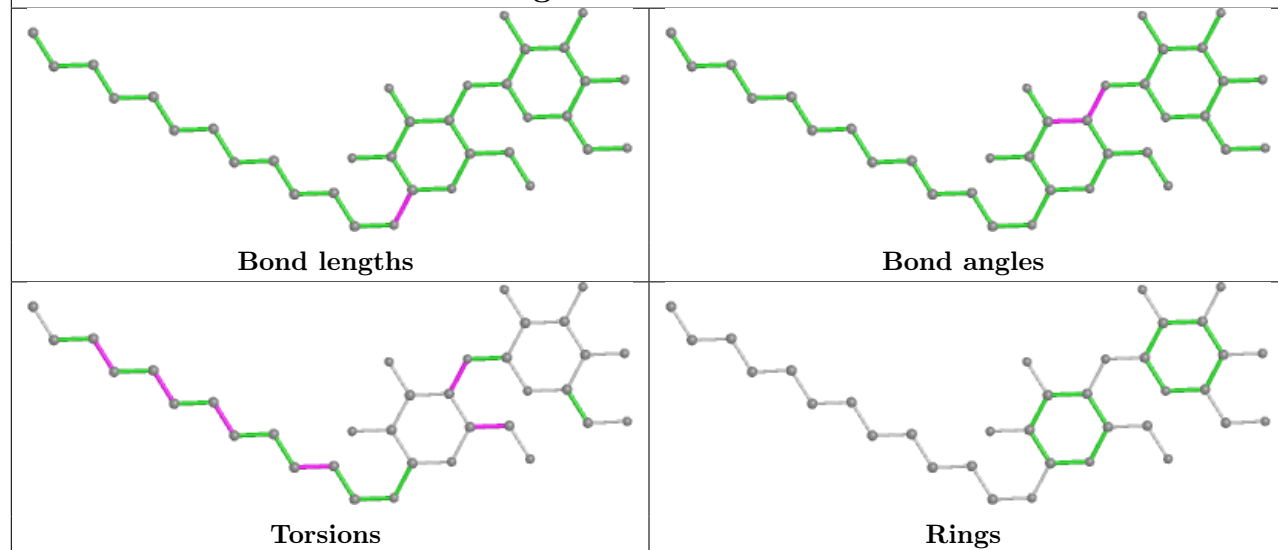
Ligand CLA A 806

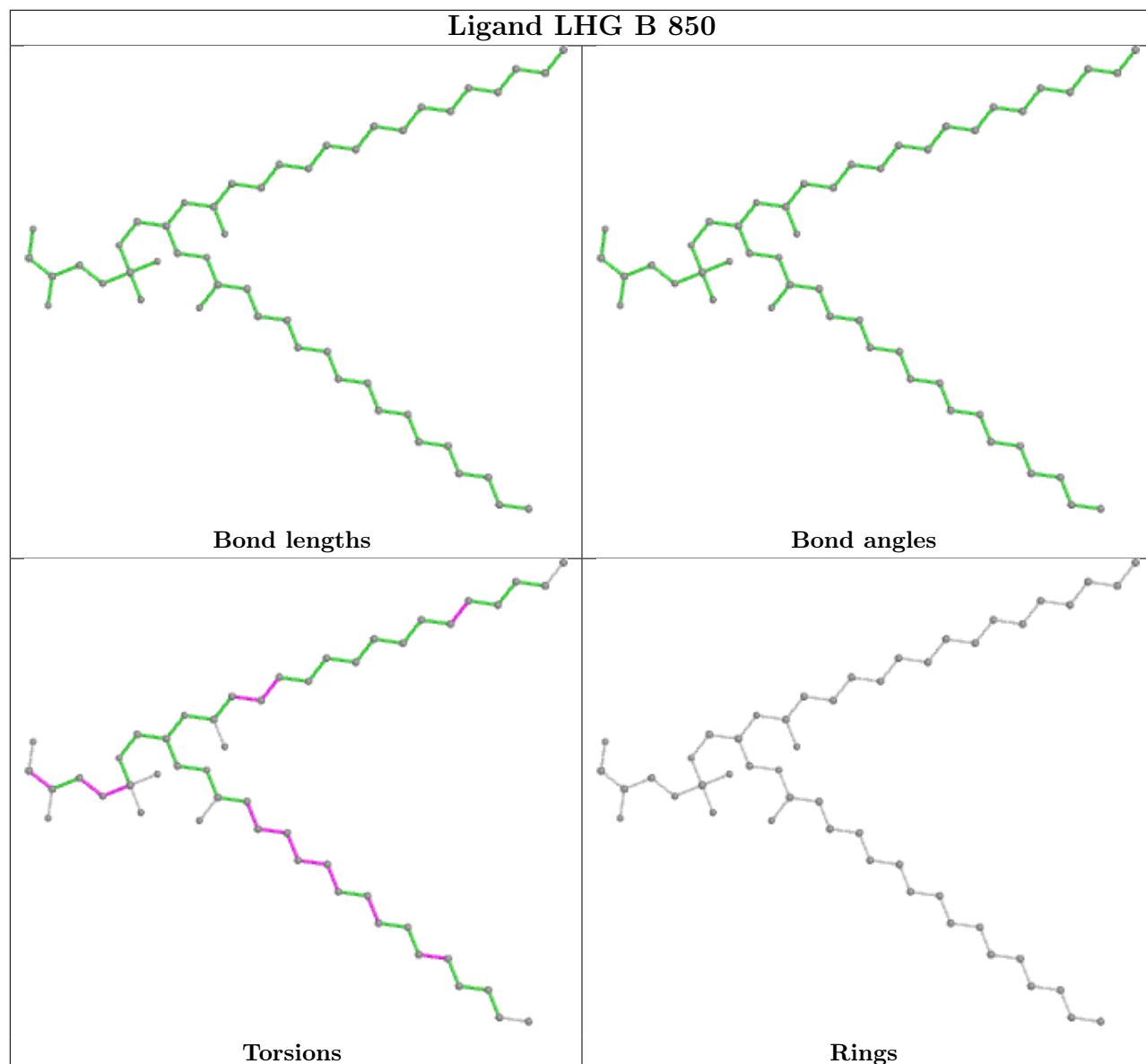
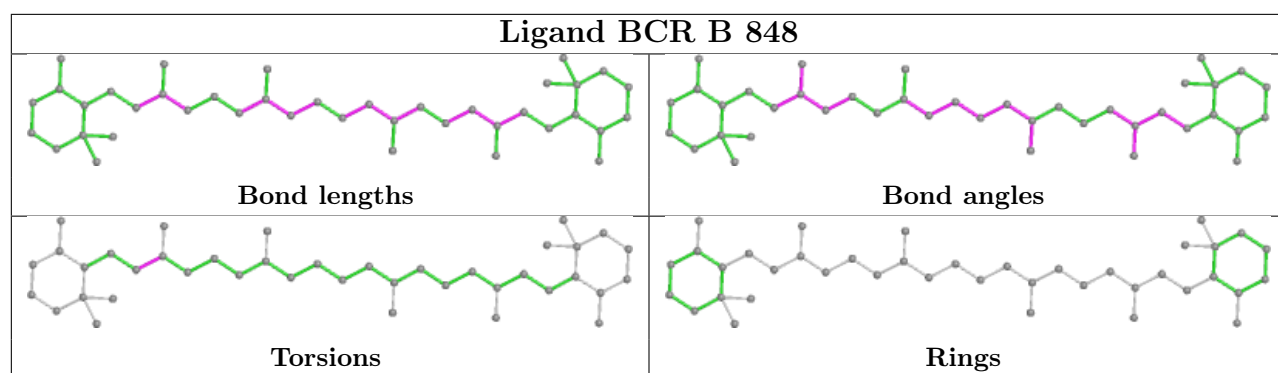


Ligand CLA 5 411

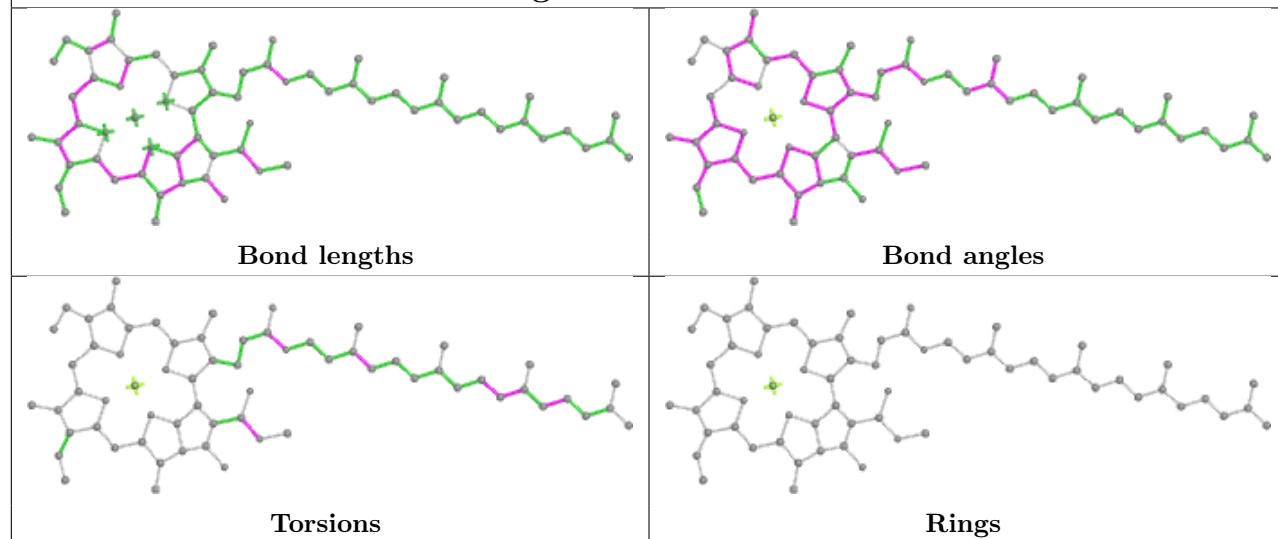


Ligand LMT 1 524

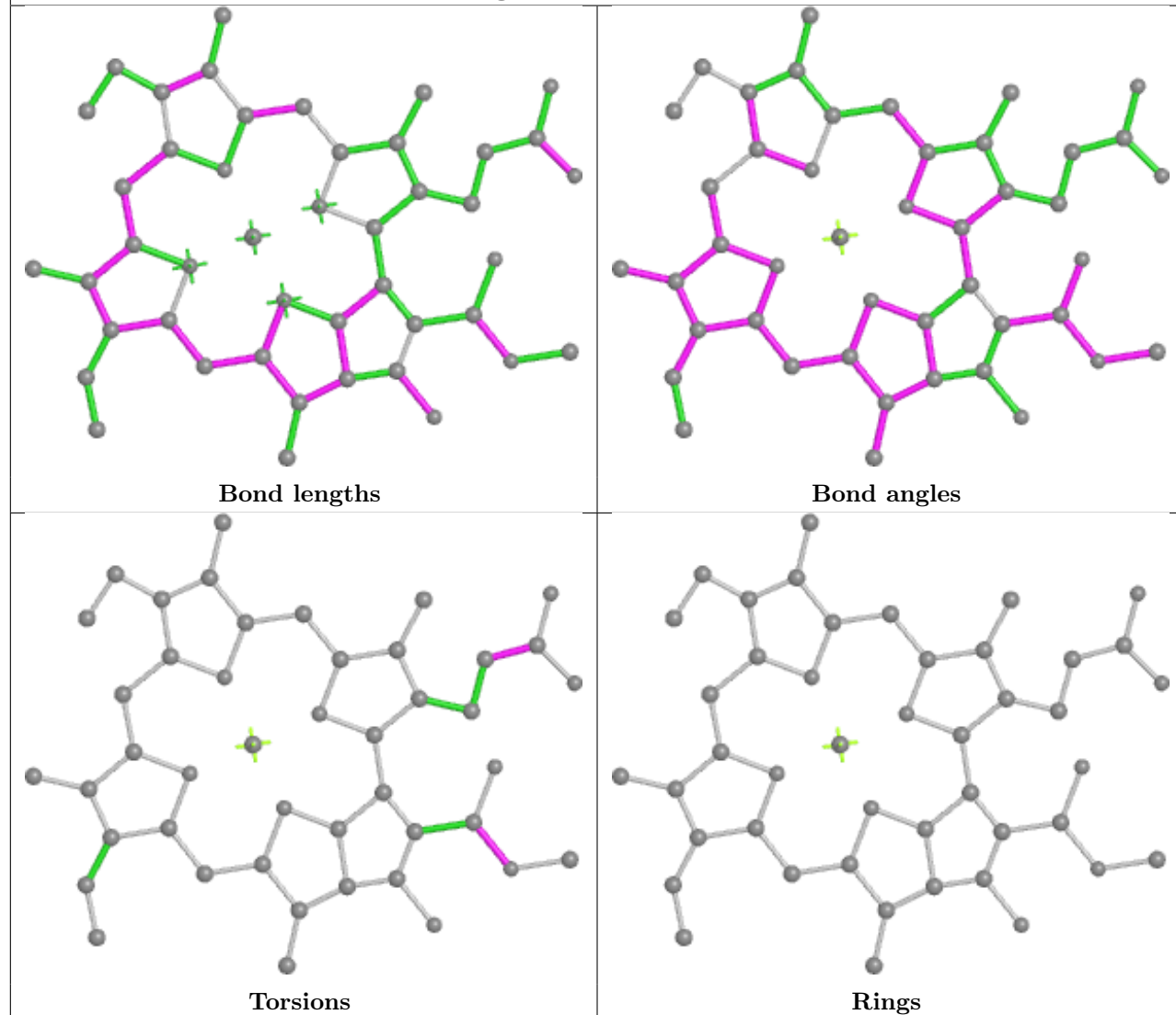




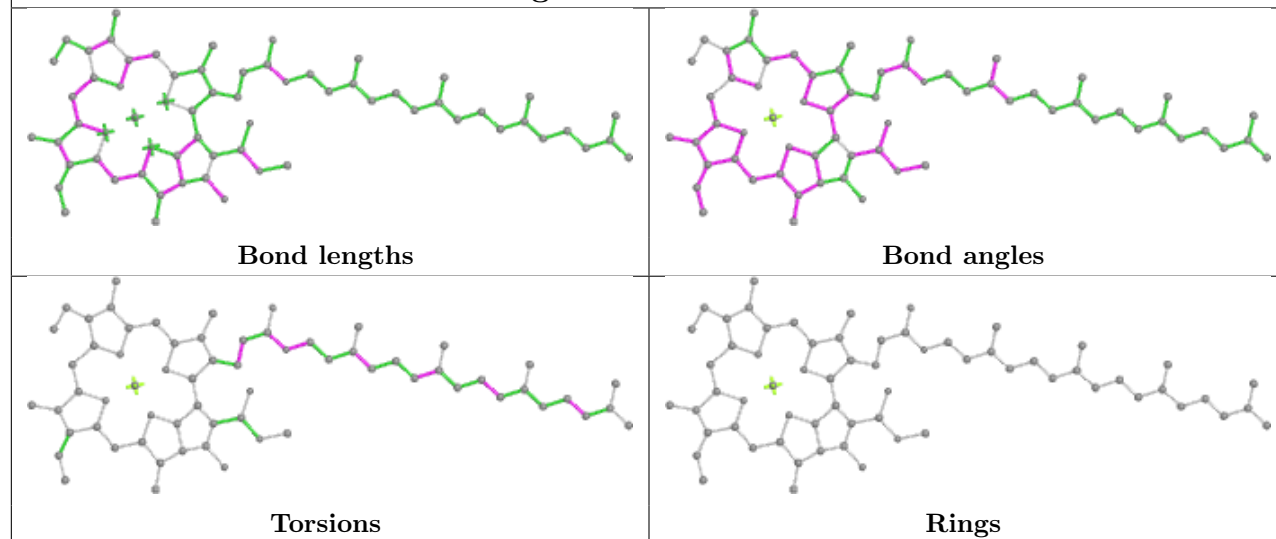
Ligand CLA B 819



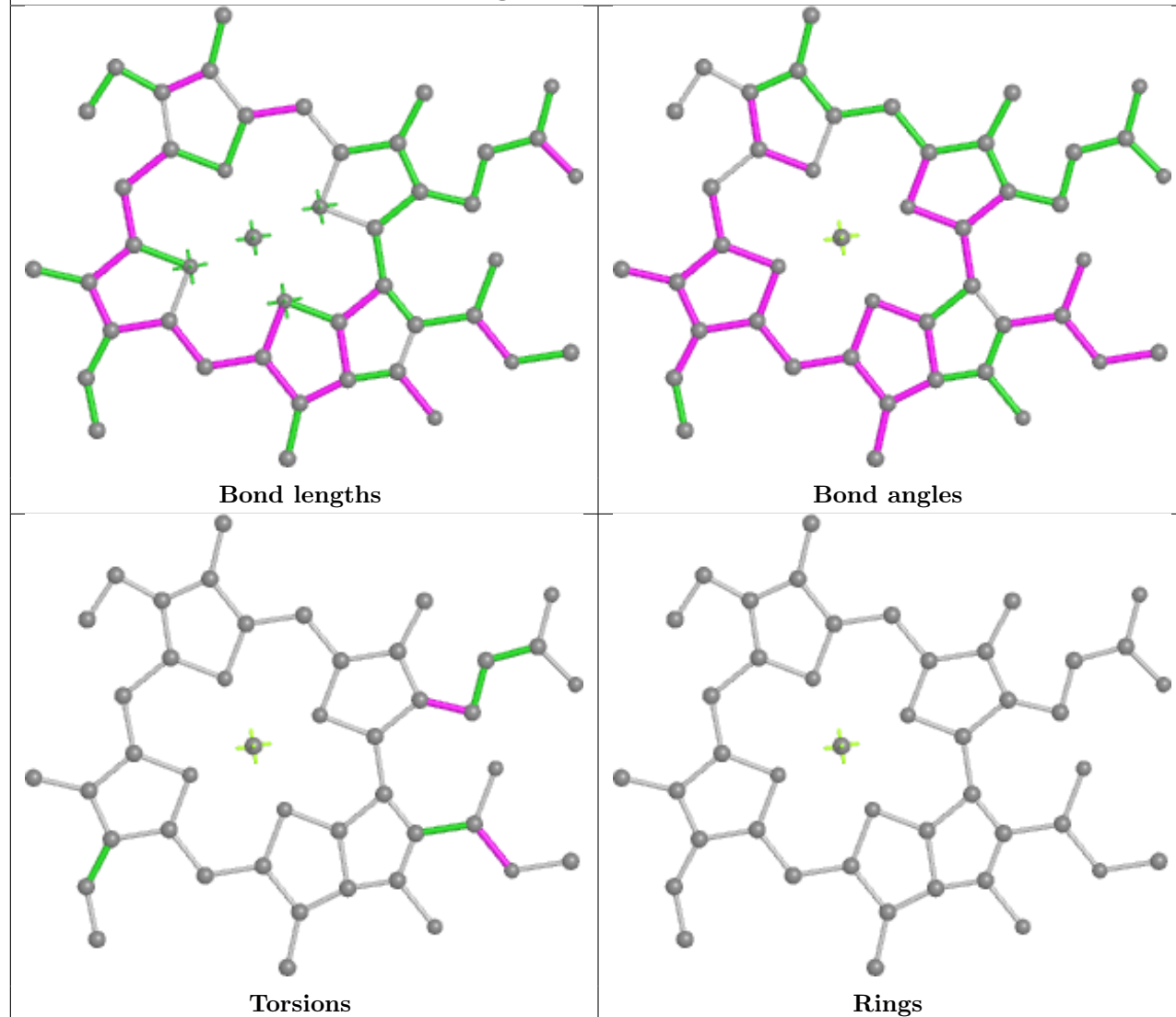
Ligand CLA 6 403



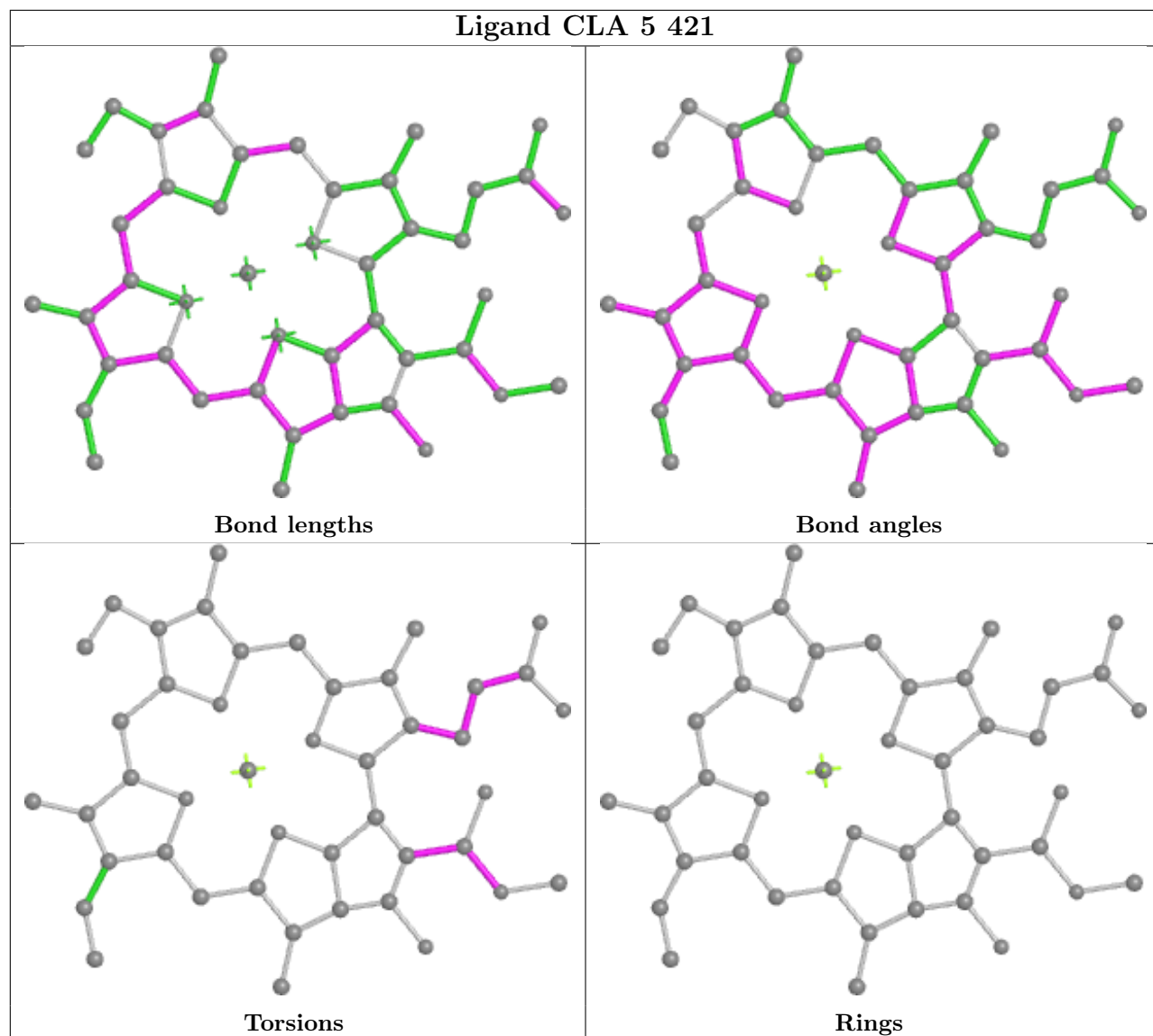
Ligand CLA A 843



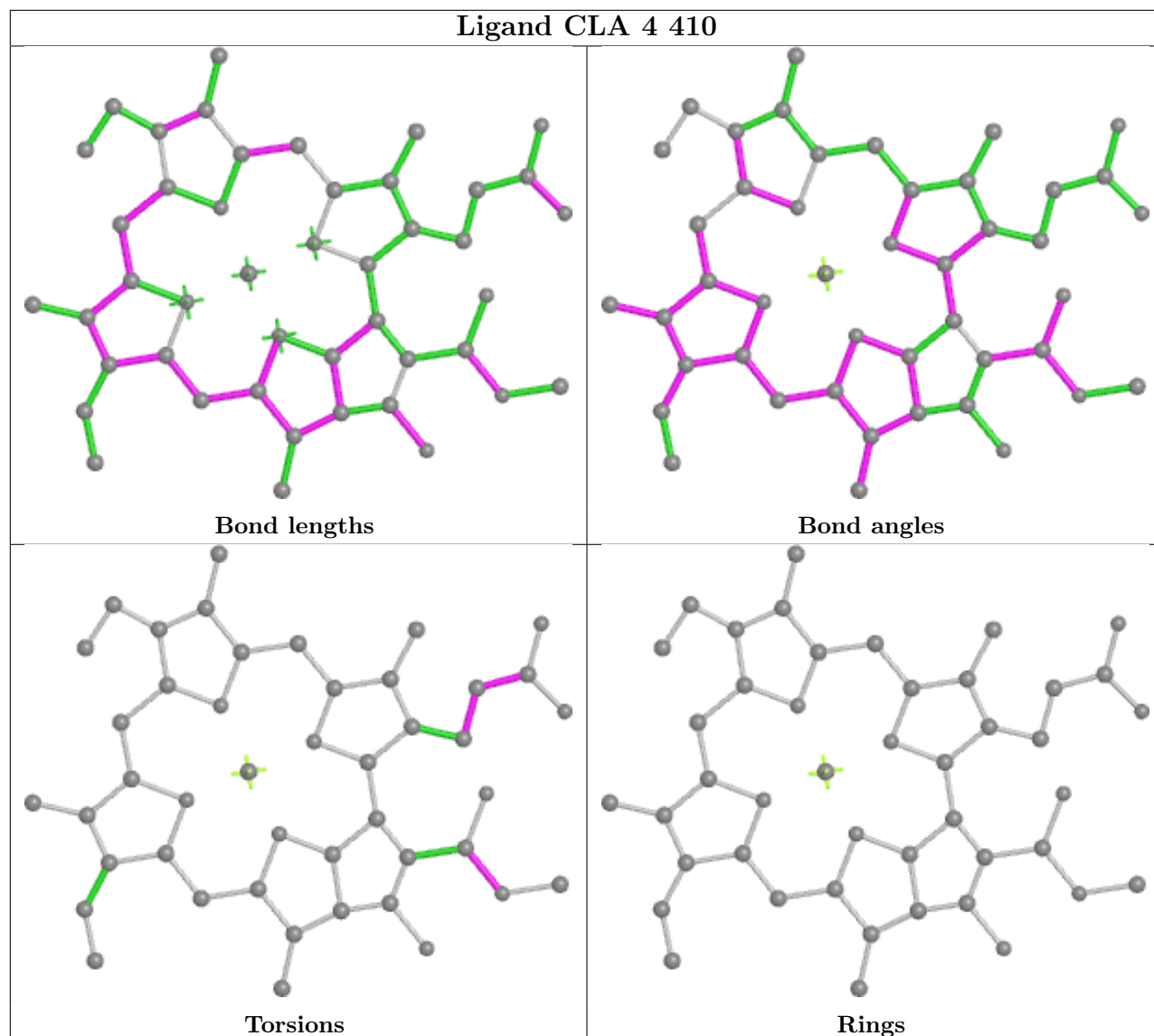
Ligand CLA 4 409



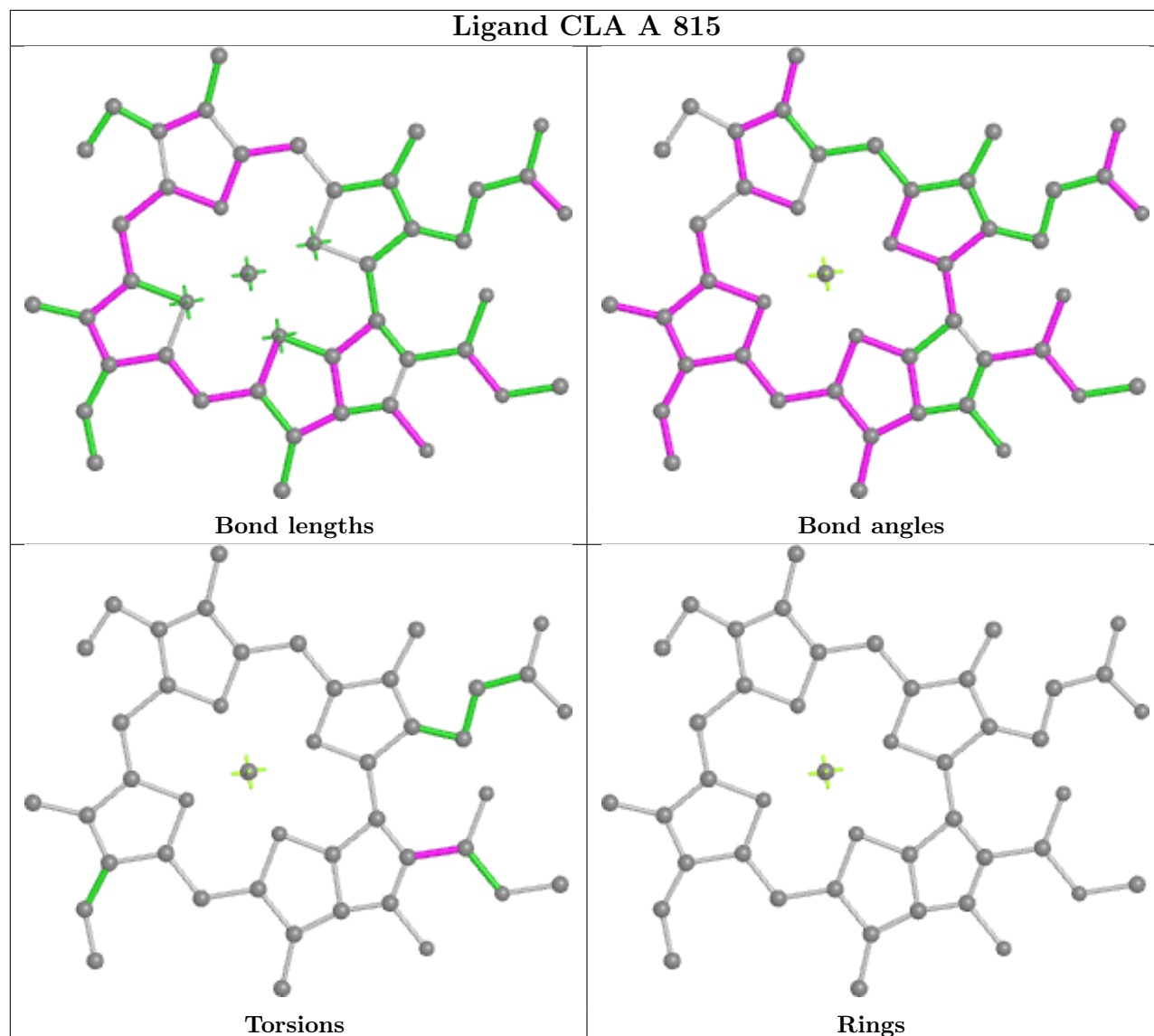
Ligand CLA 5 421



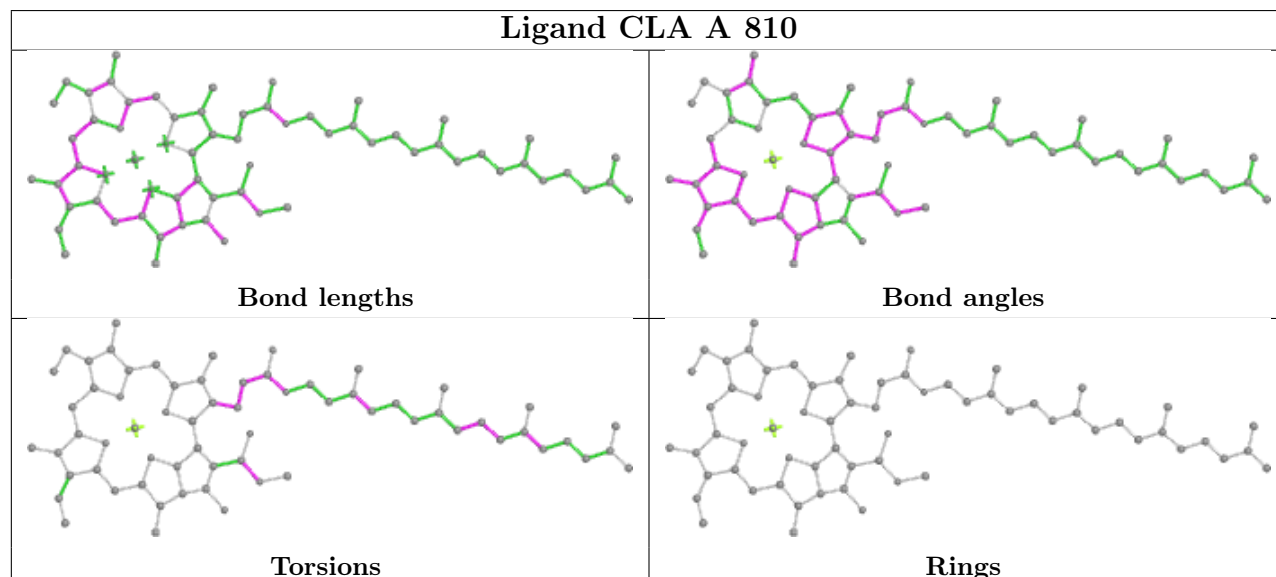
Ligand CLA 4 410



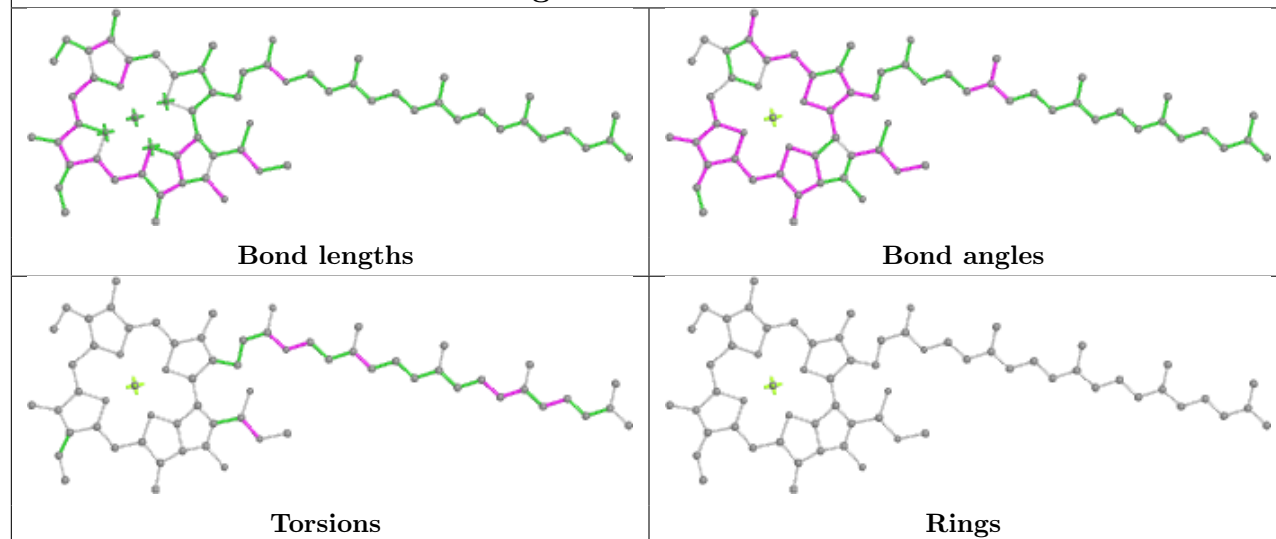
Ligand CLA A 815



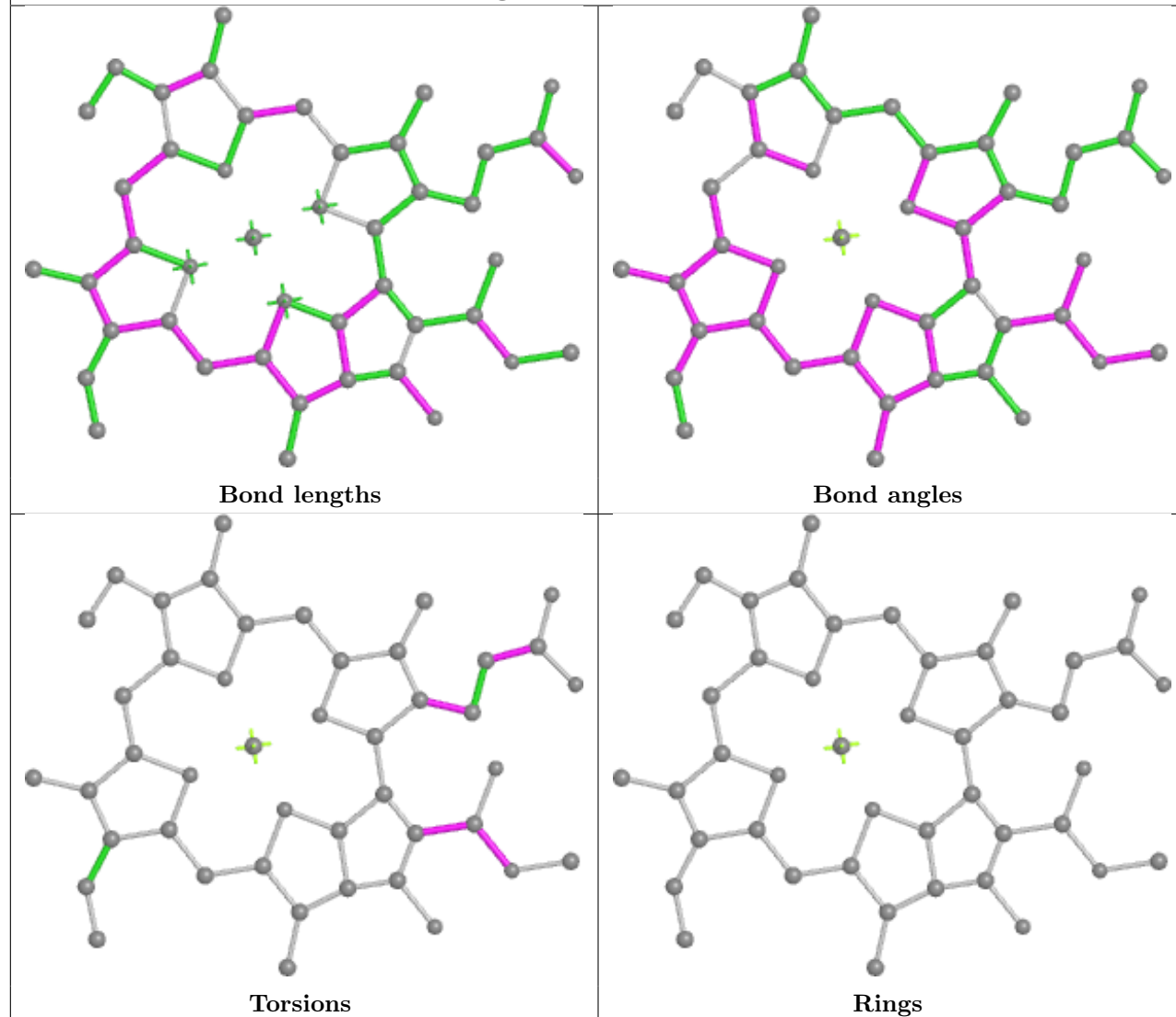
Ligand CLA A 810



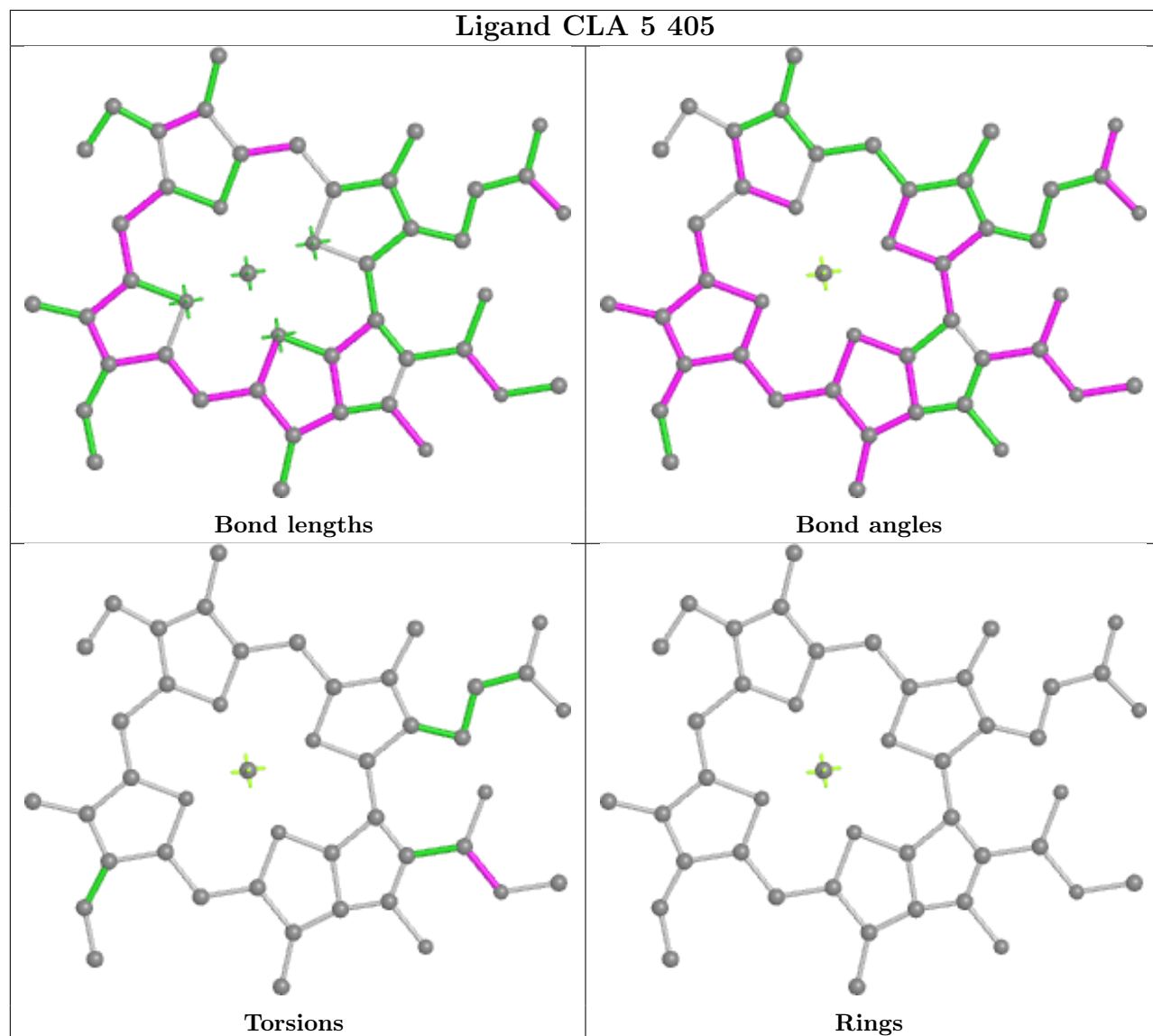
Ligand CLA B 830



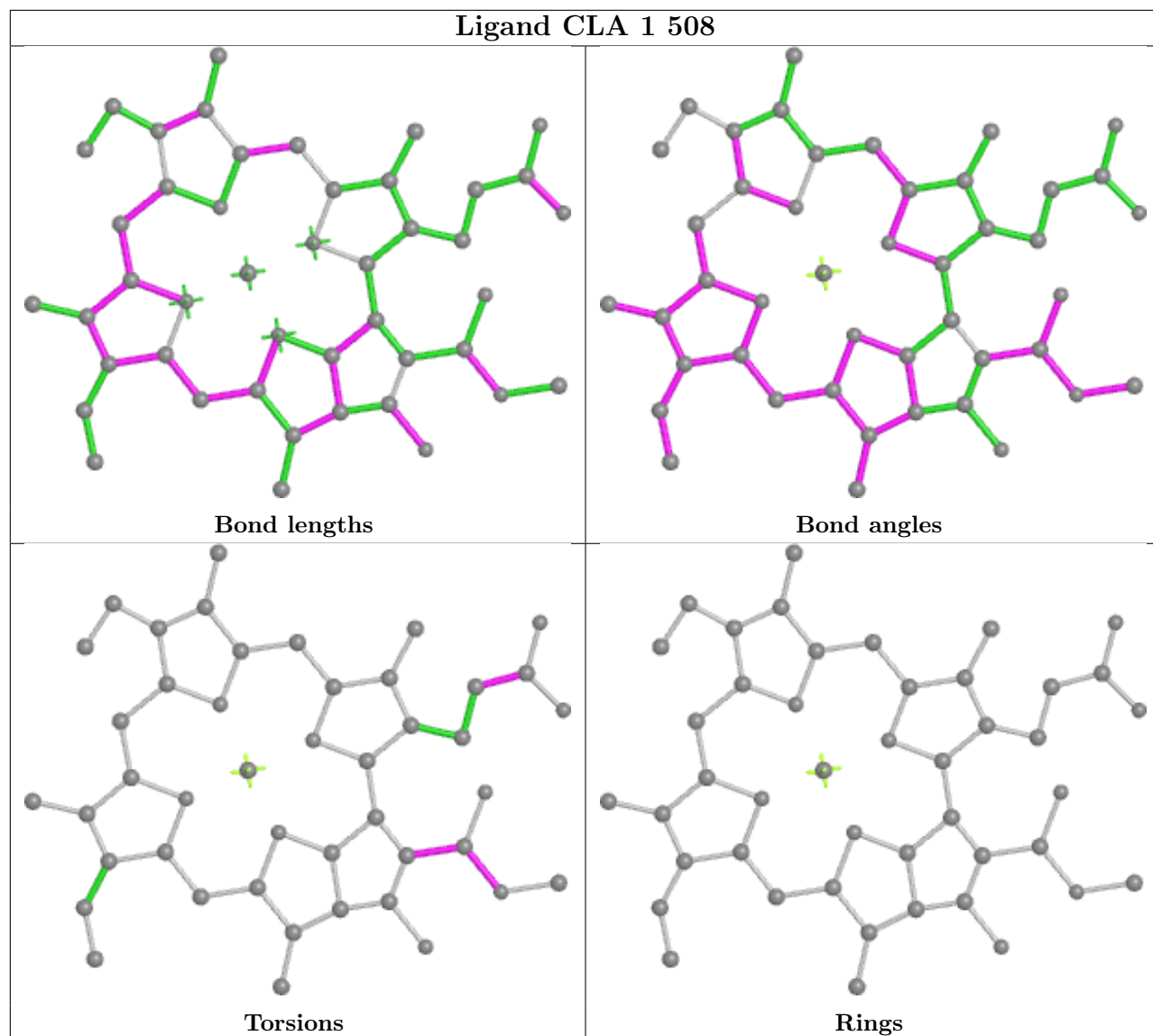
Ligand CLA 6 401



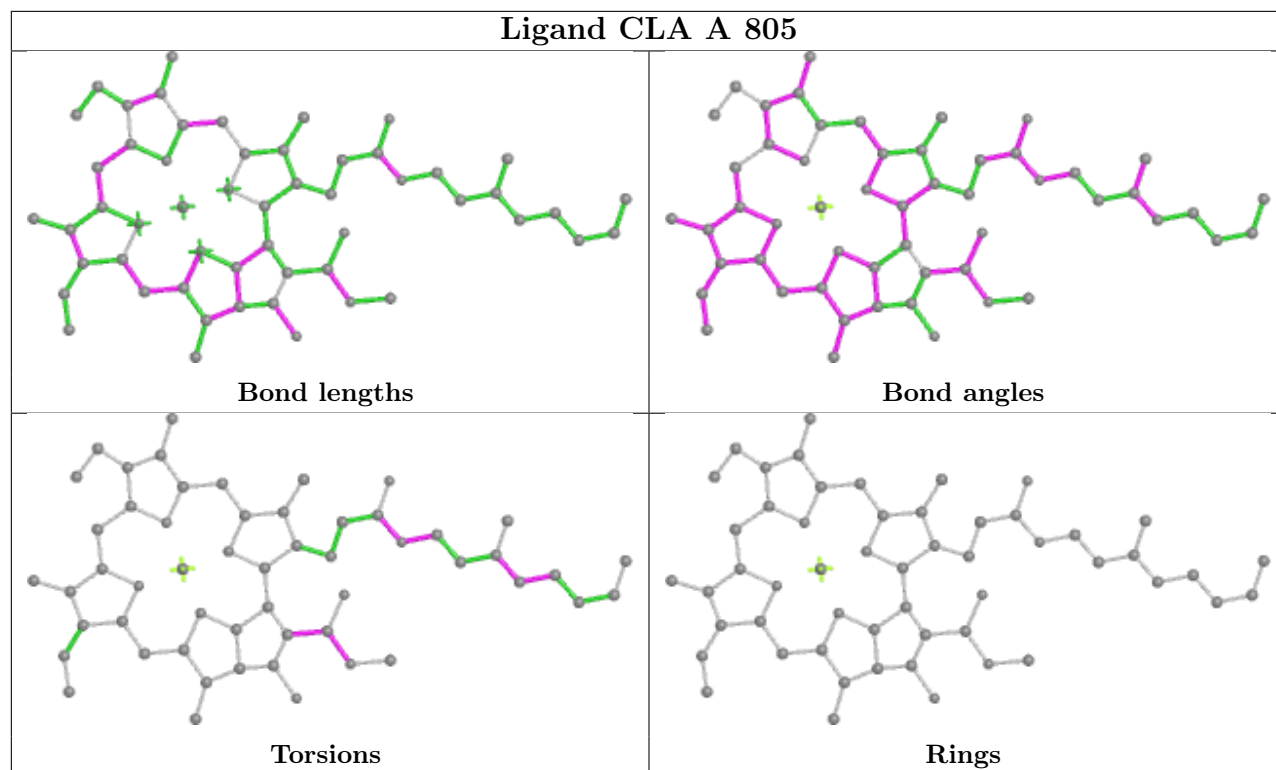
Ligand CLA 5 405



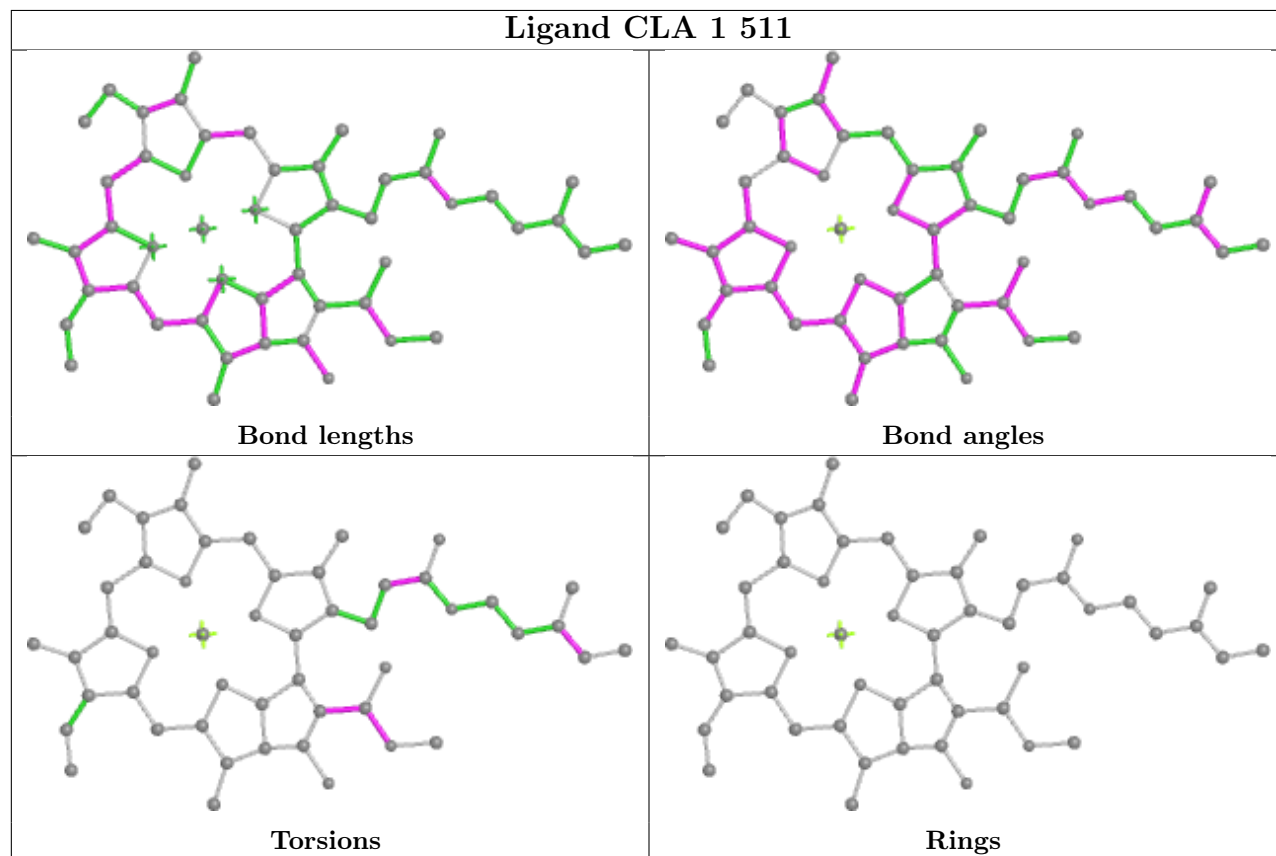
Ligand CLA 1 508



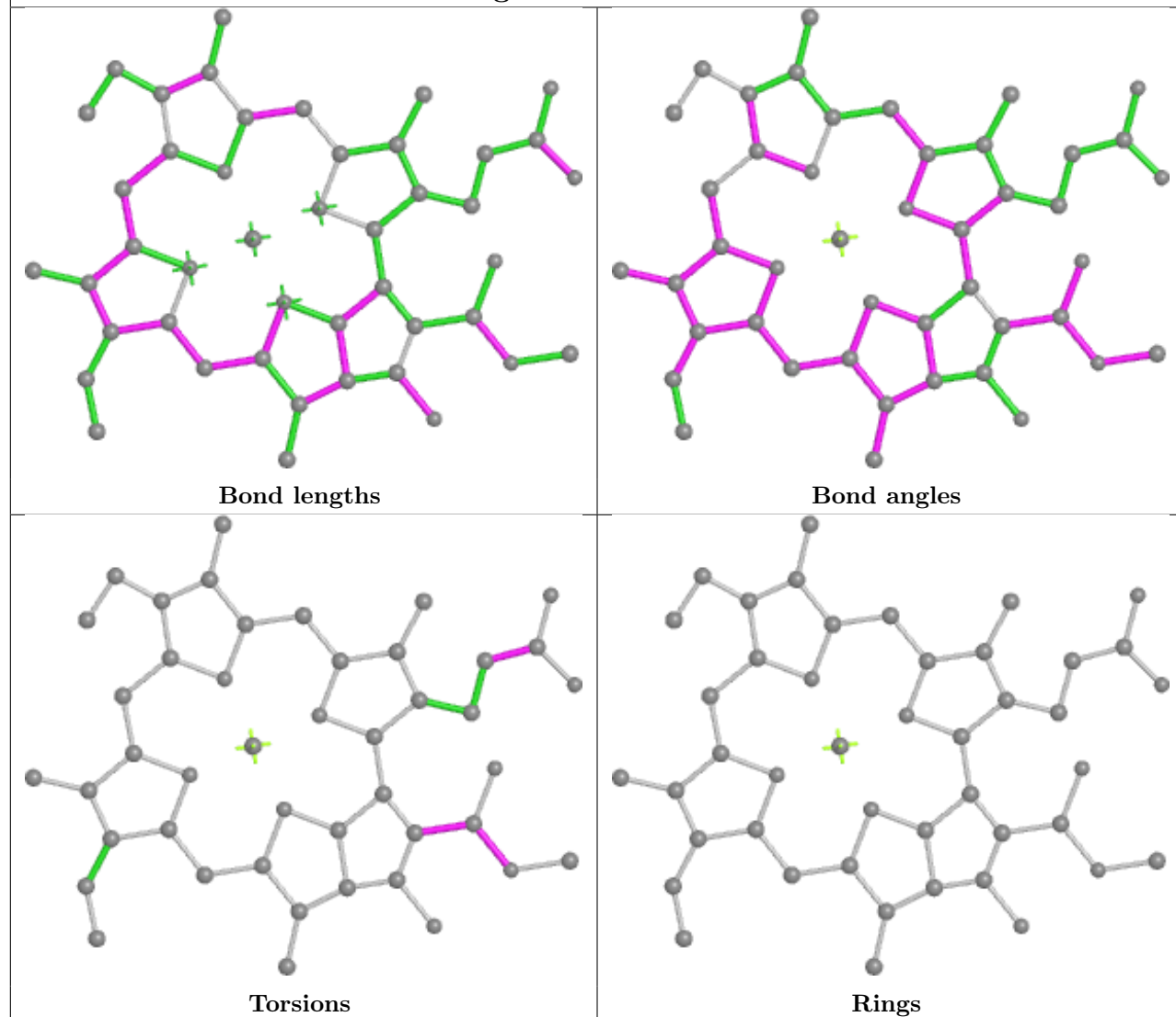
Ligand CLA A 805



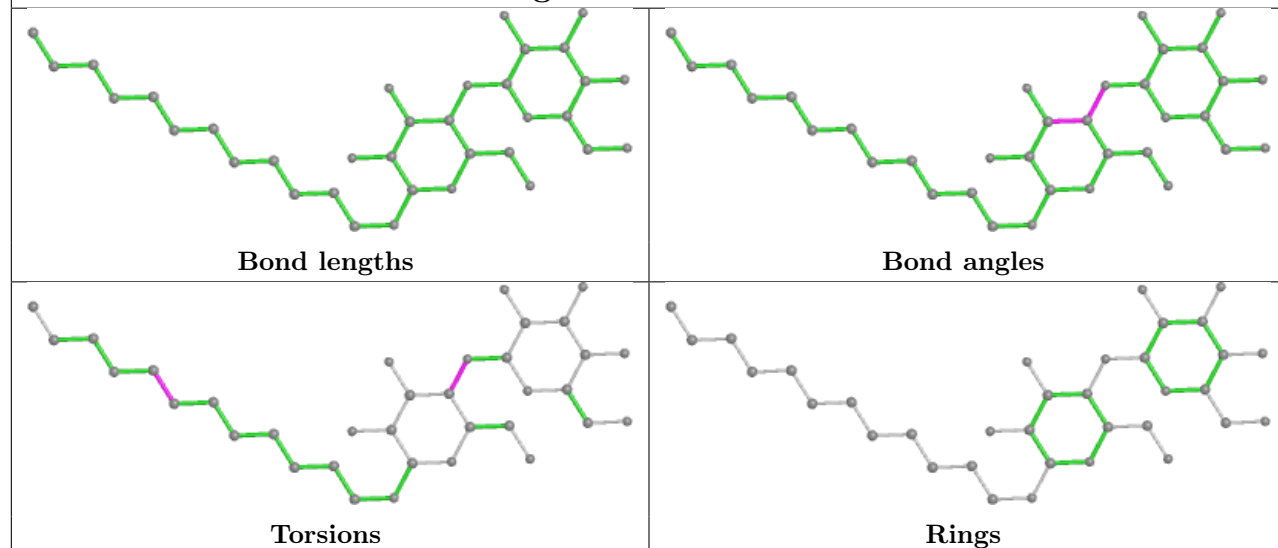
Ligand CLA 1 511



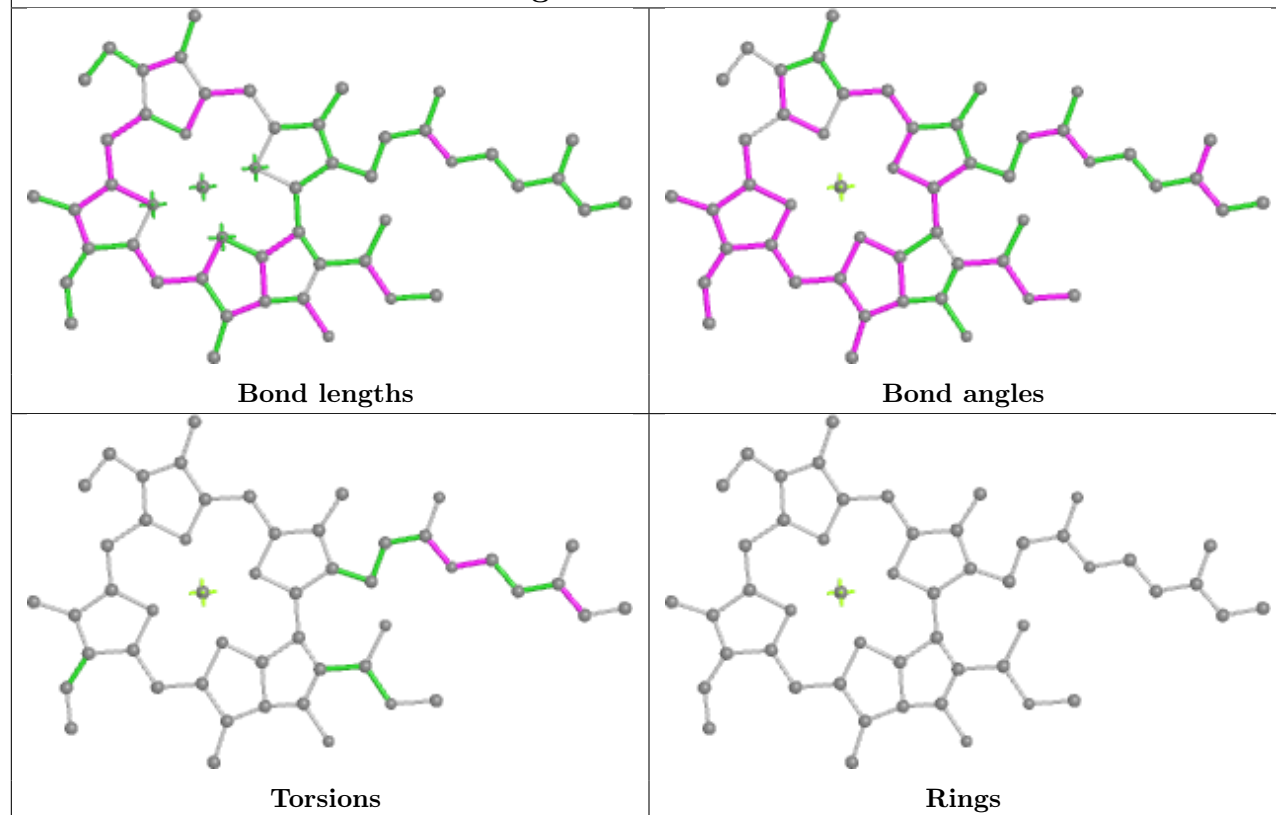
Ligand CLA 5 412



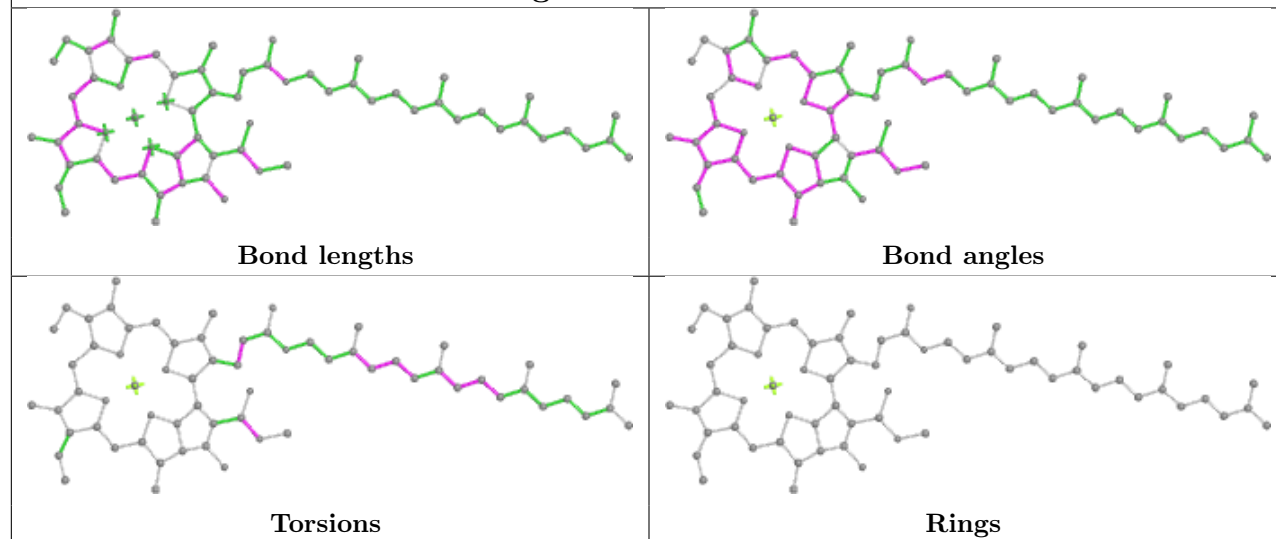
Ligand LMT 5 401

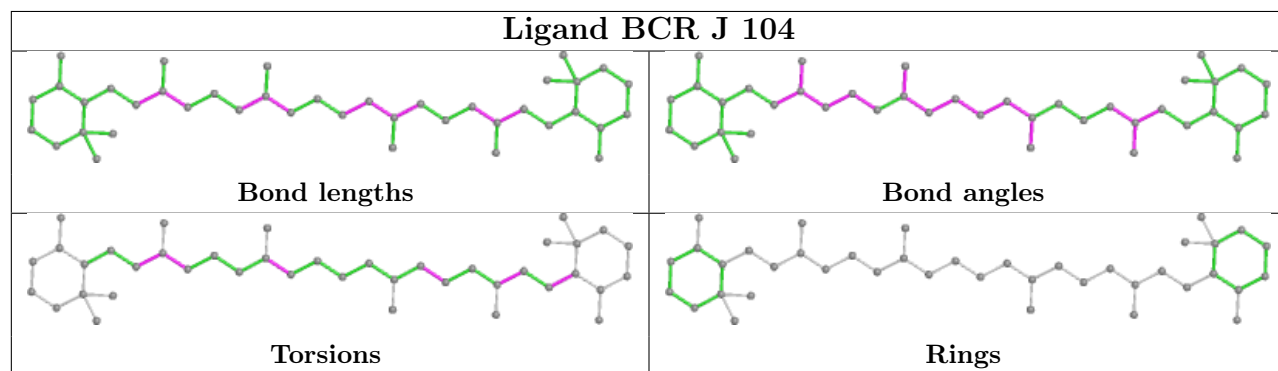
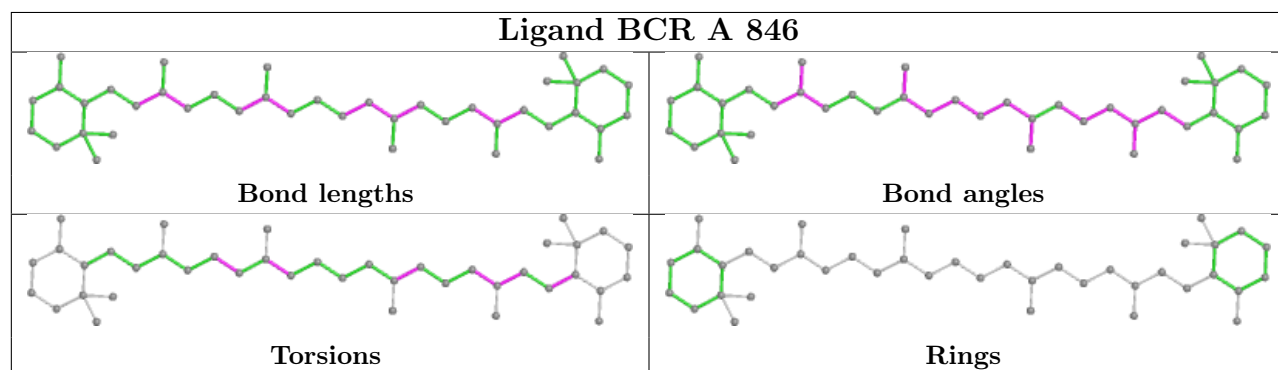
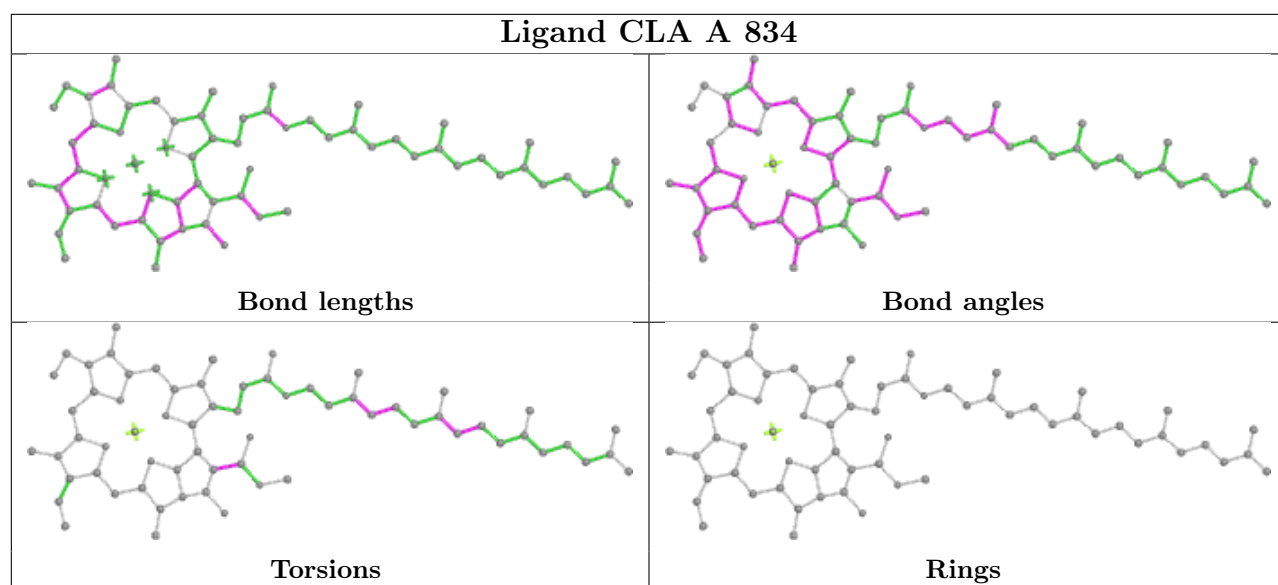


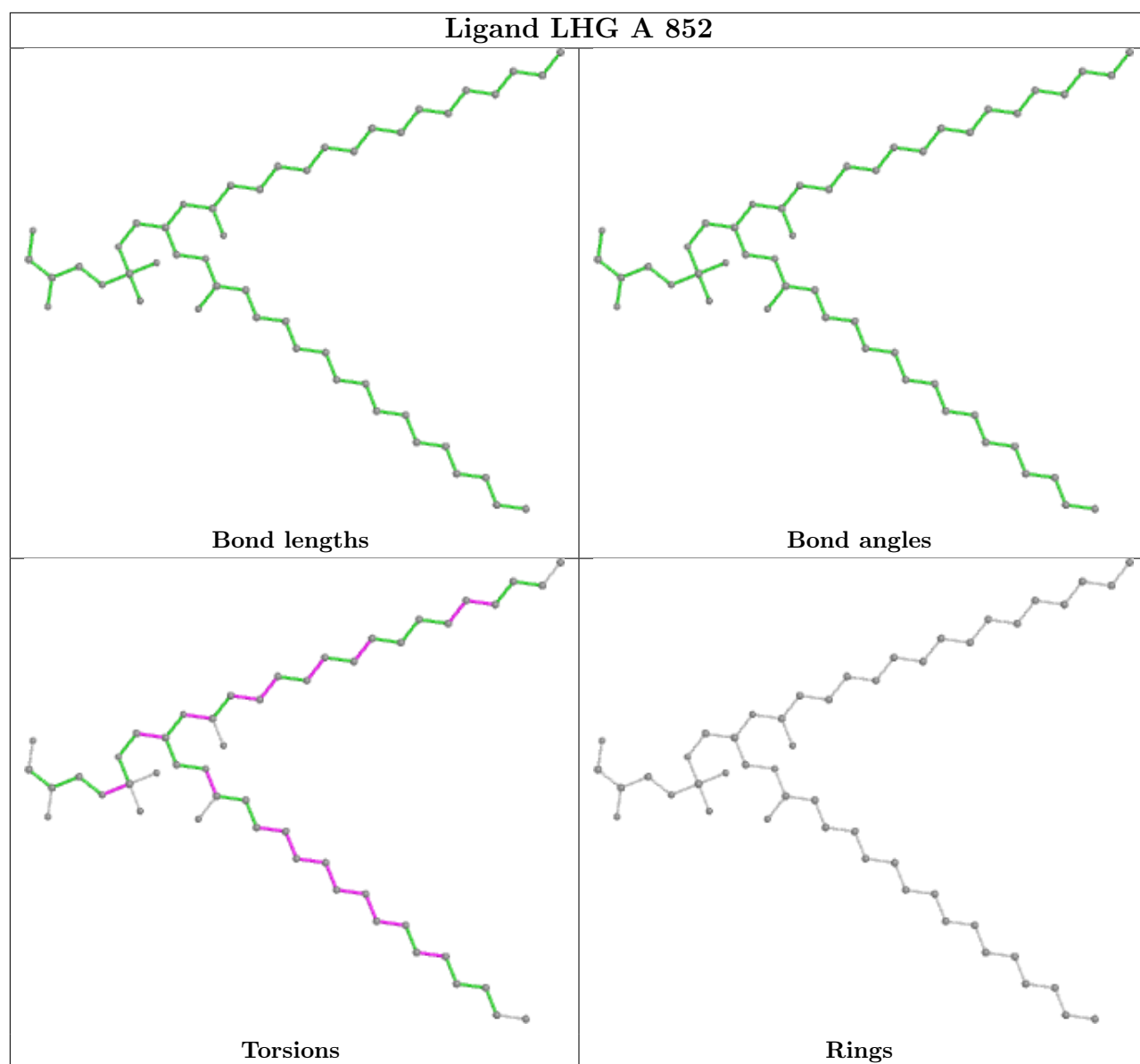
Ligand CLA A 836



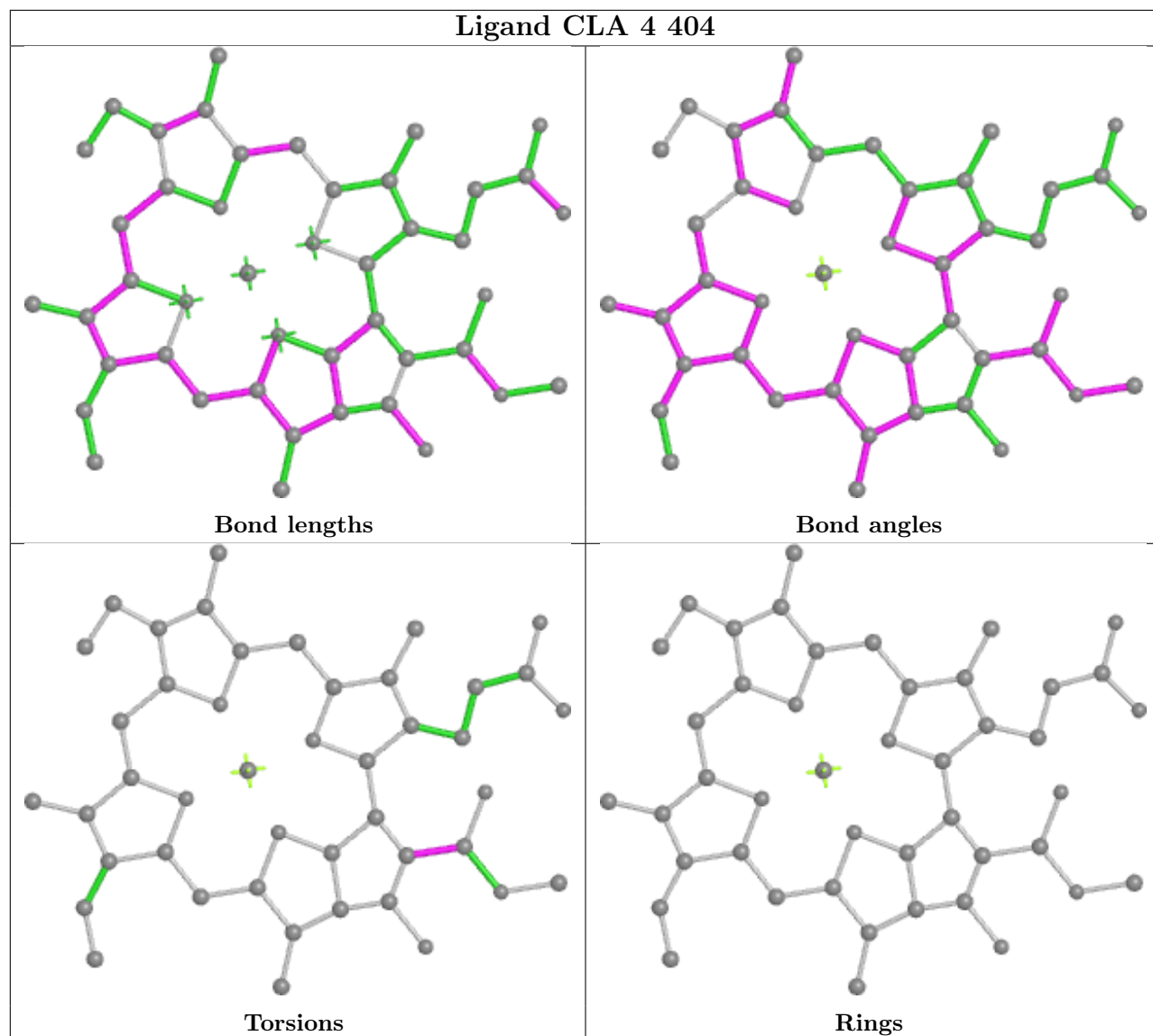
Ligand CLA B 840



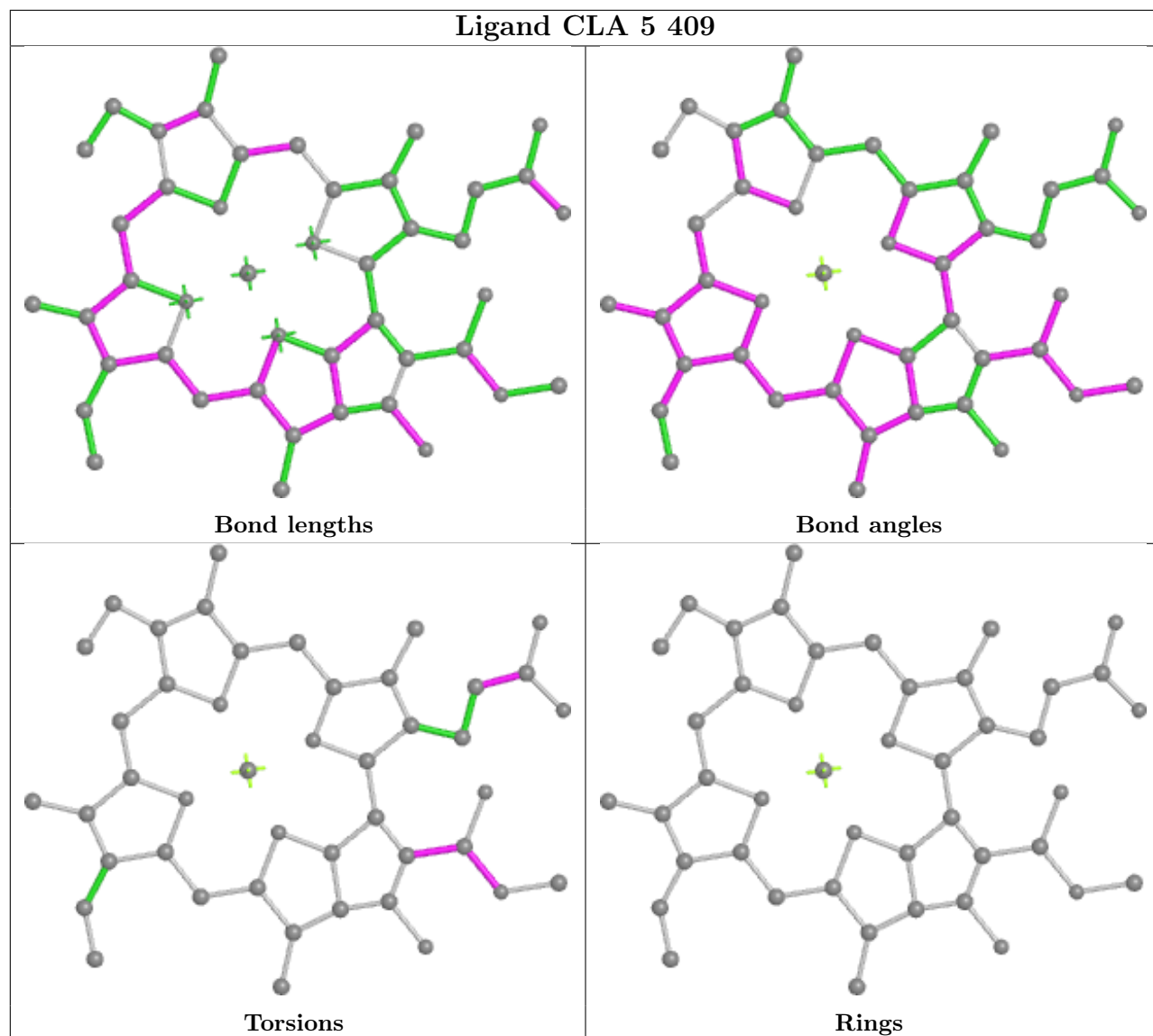




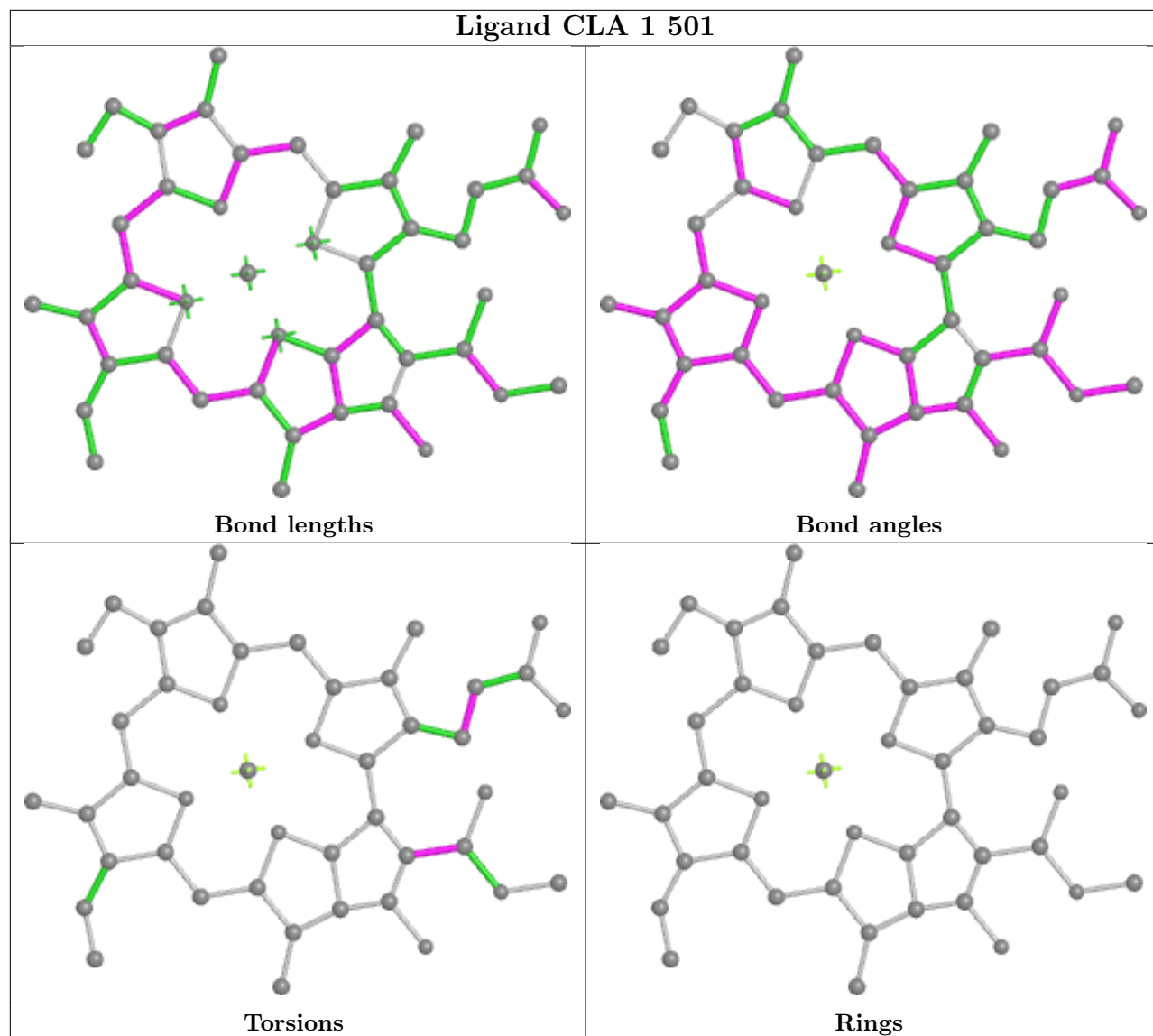
Ligand CLA 4 404



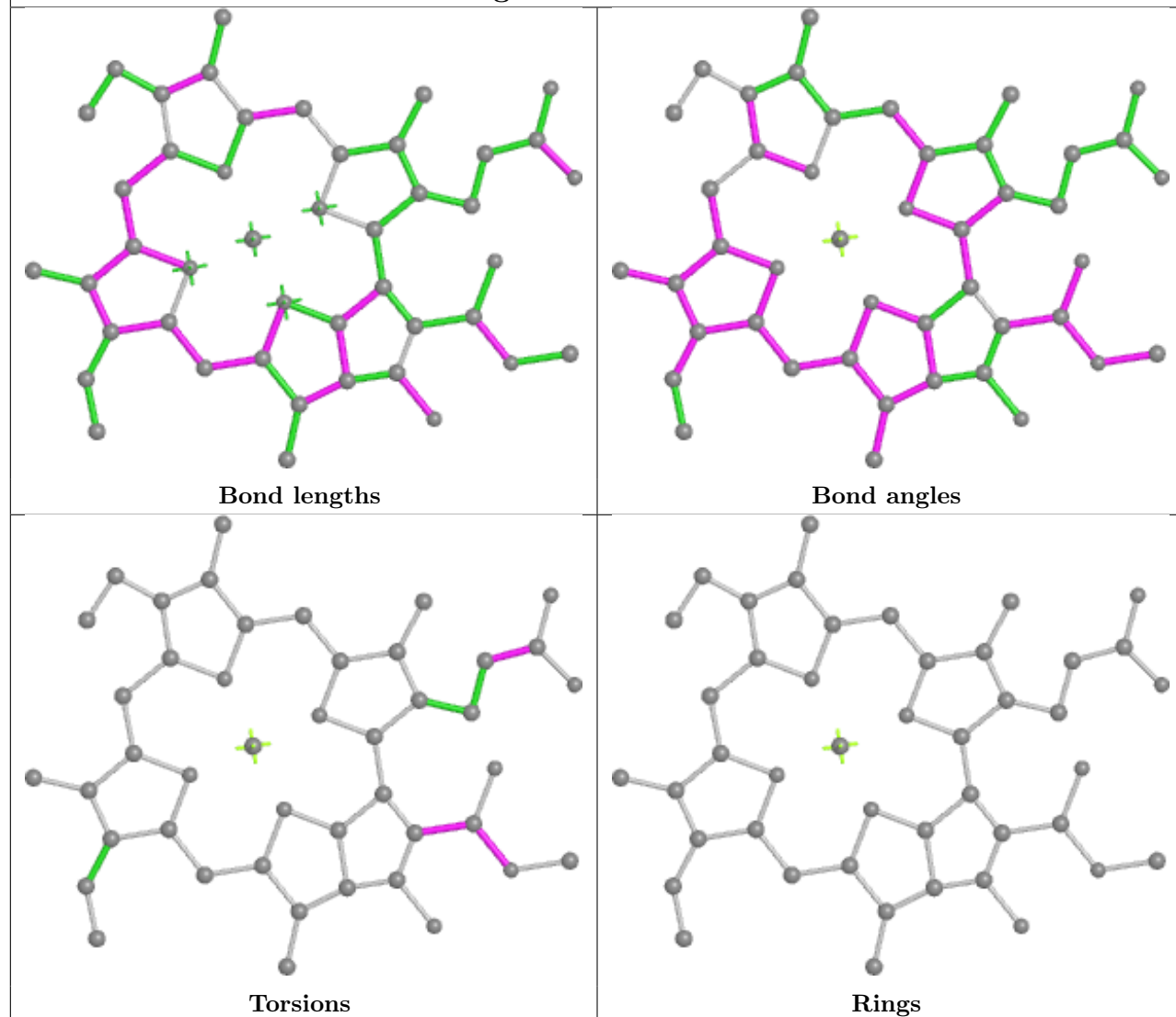
Ligand CLA 5 409



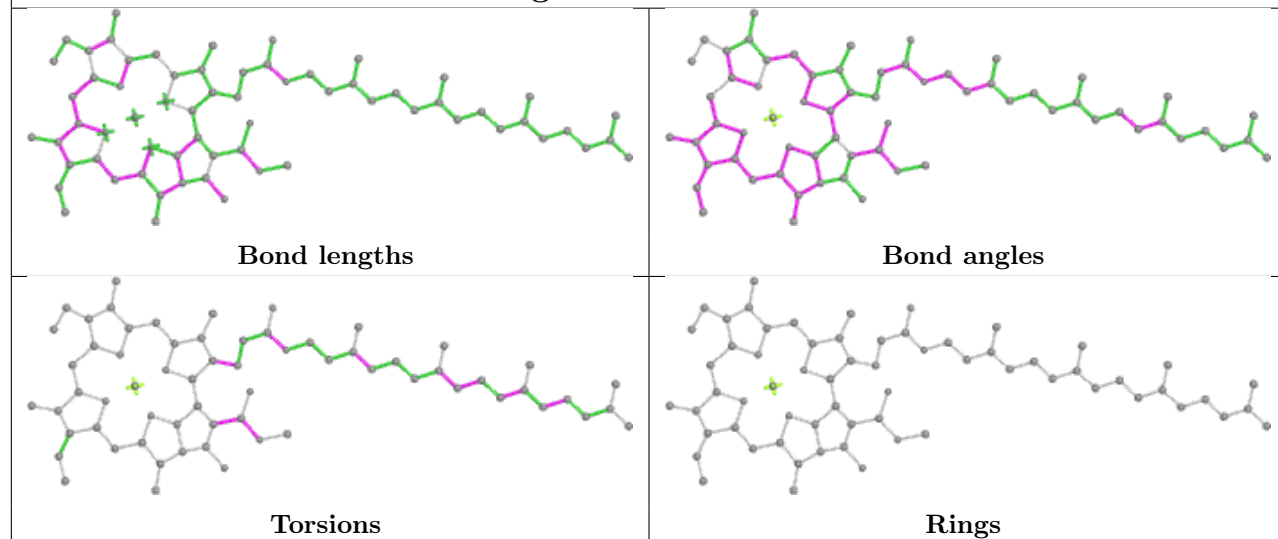
Ligand CLA 1 501



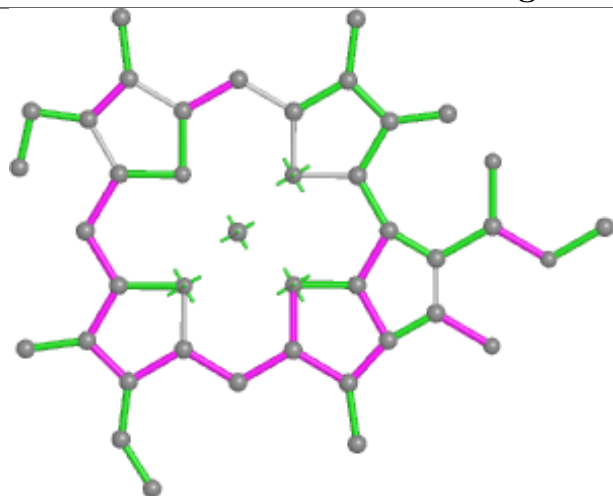
Ligand CLA 5 414



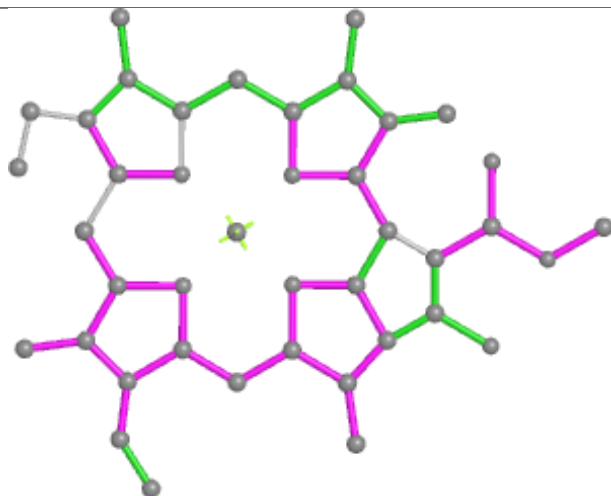
Ligand CLA A 820



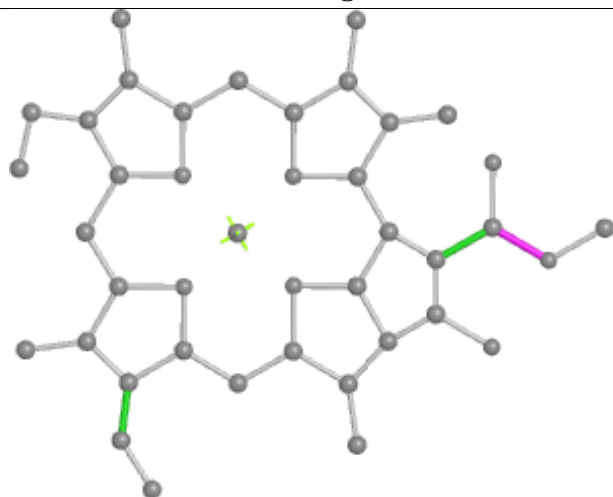
Ligand CLA 6 408



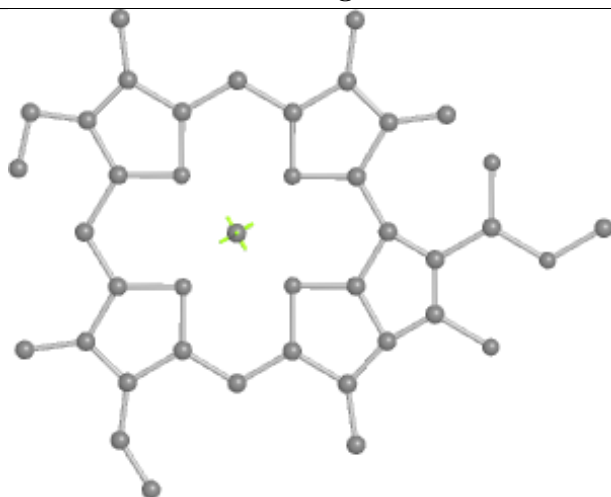
Bond lengths



Bond angles

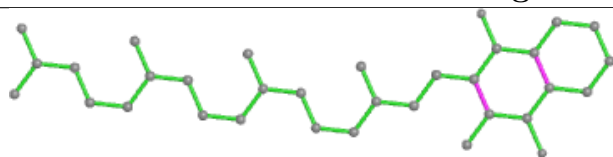


Torsions

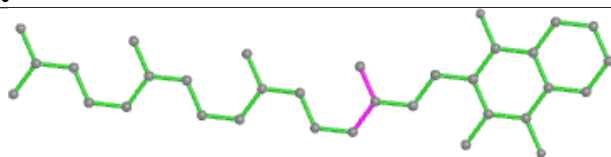


Rings

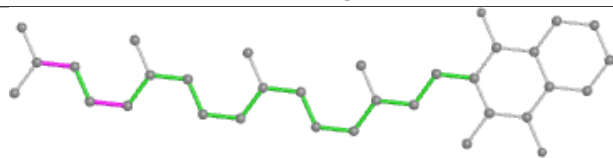
Ligand PQN B 842



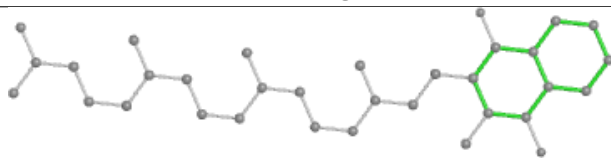
Bond lengths



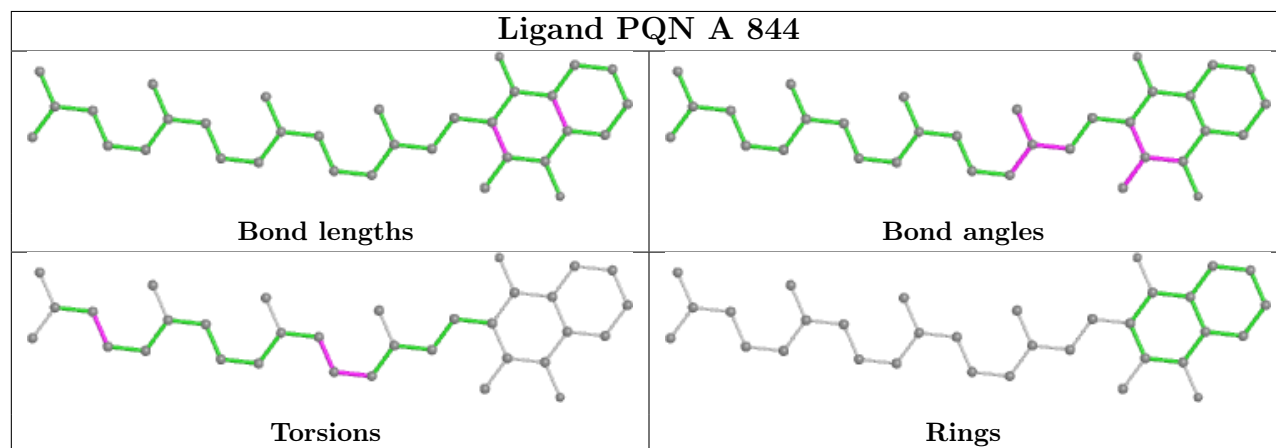
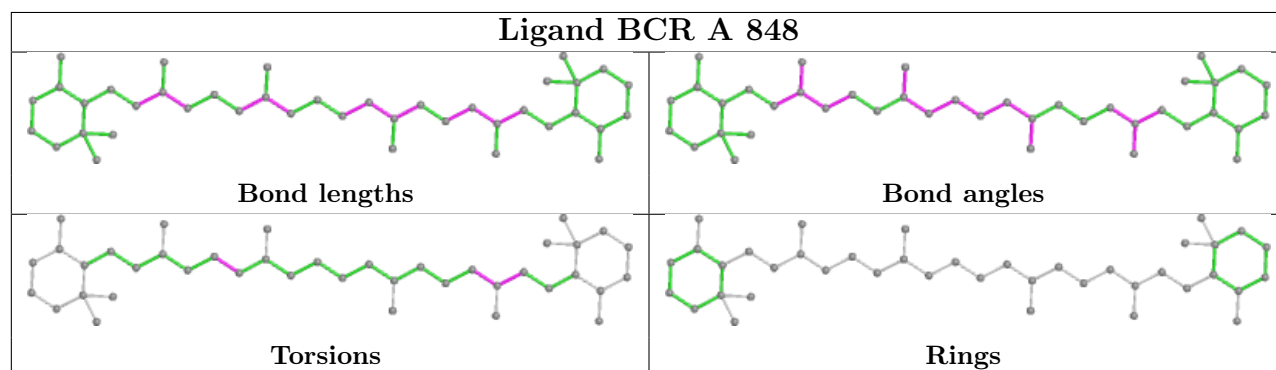
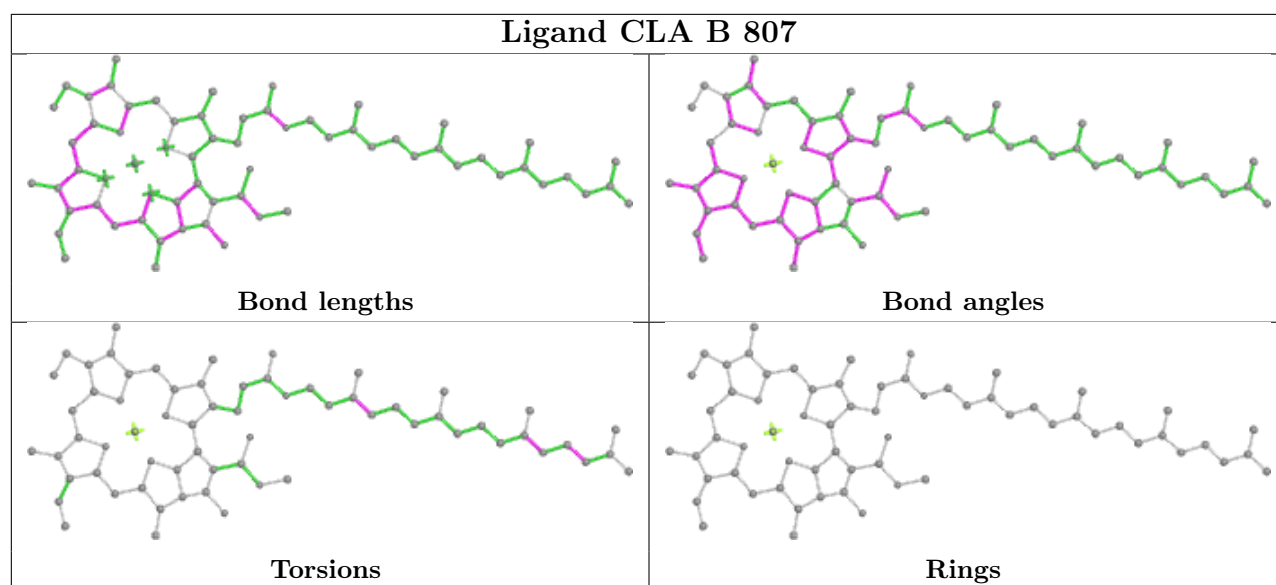
Bond angles



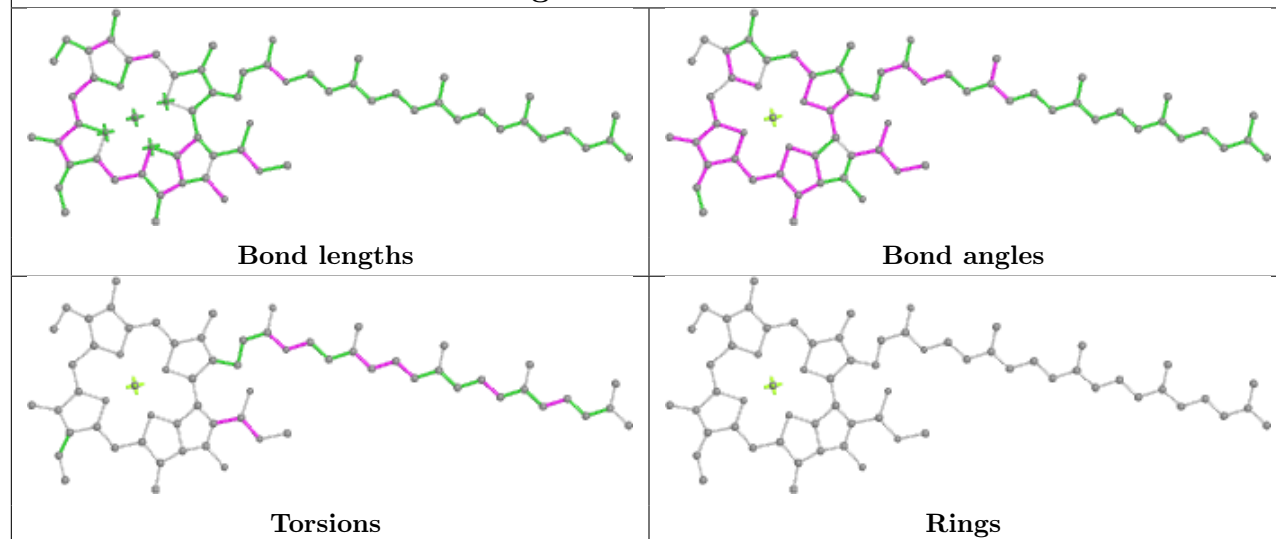
Torsions



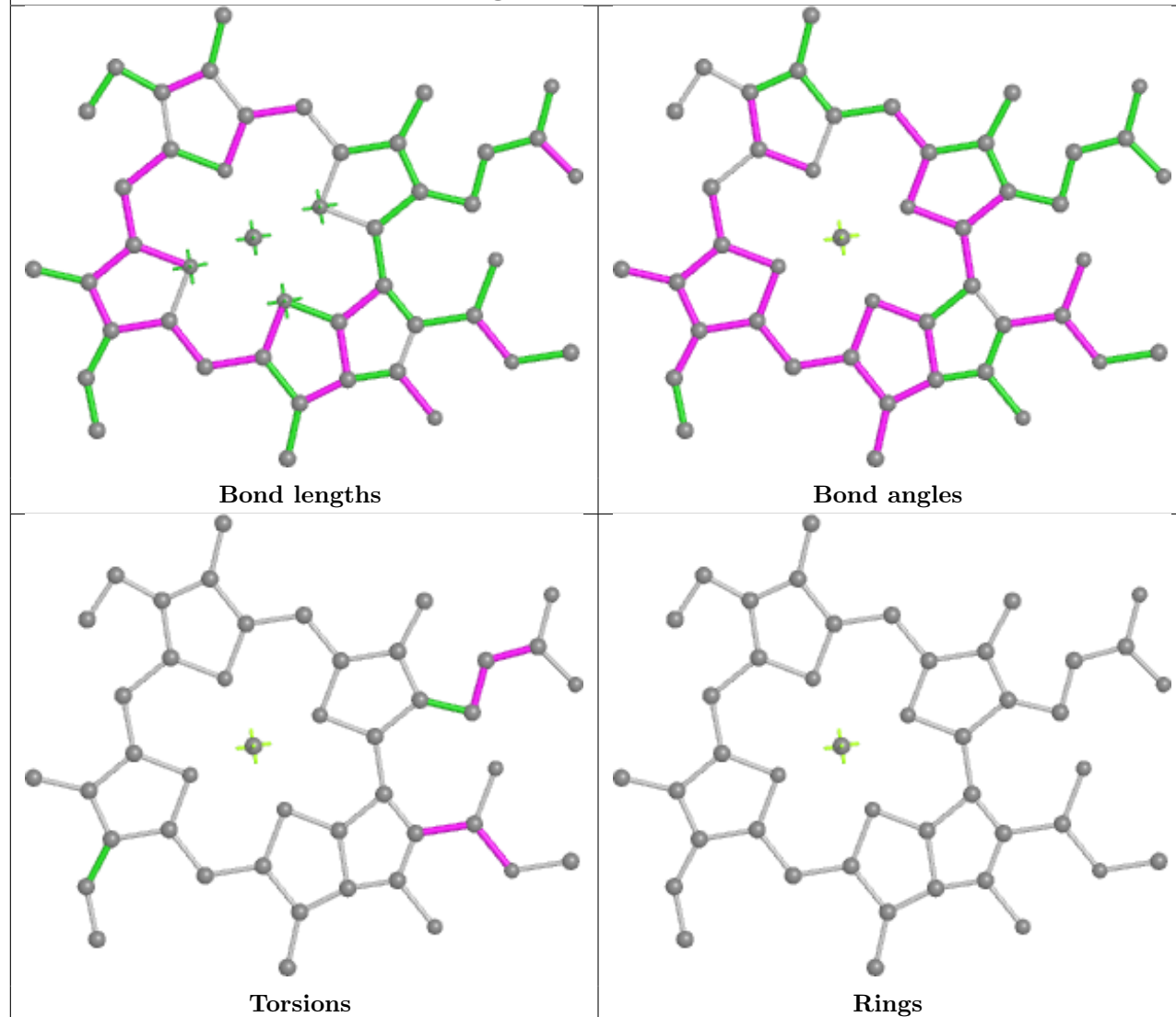
Rings

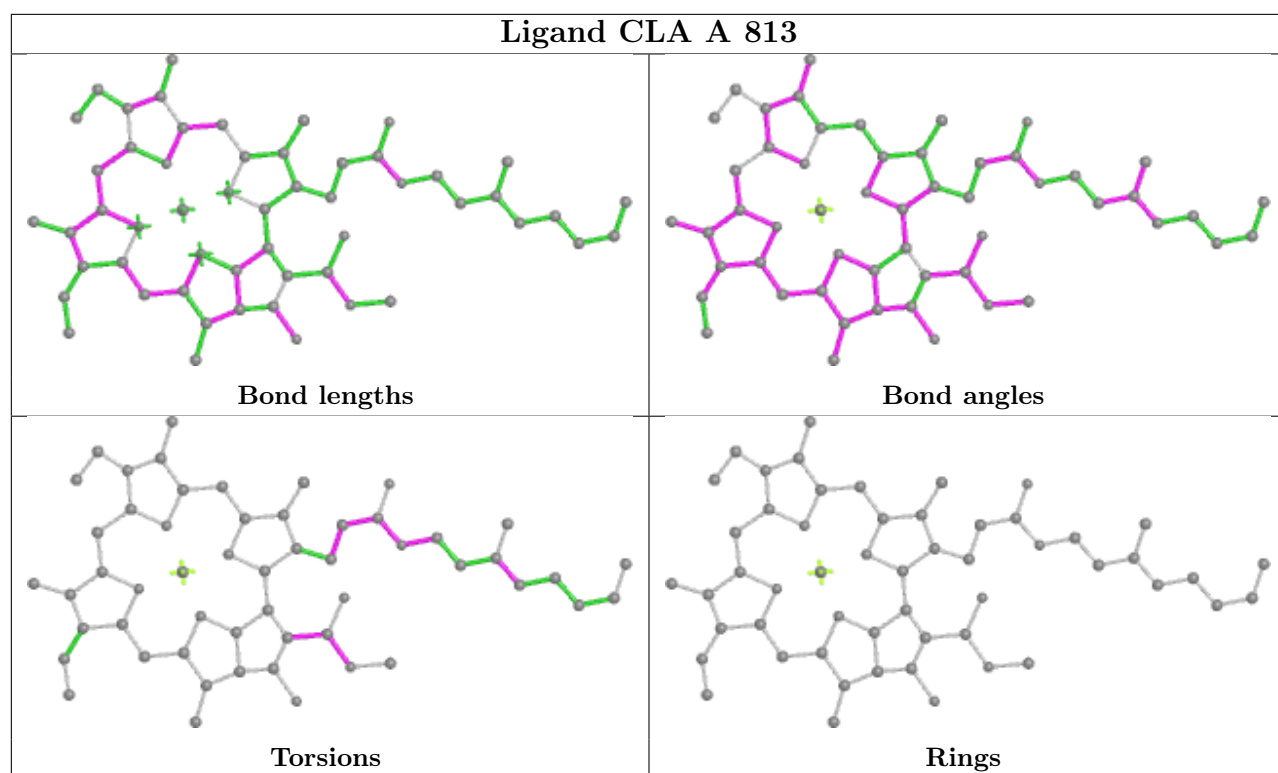


Ligand CLA A 804

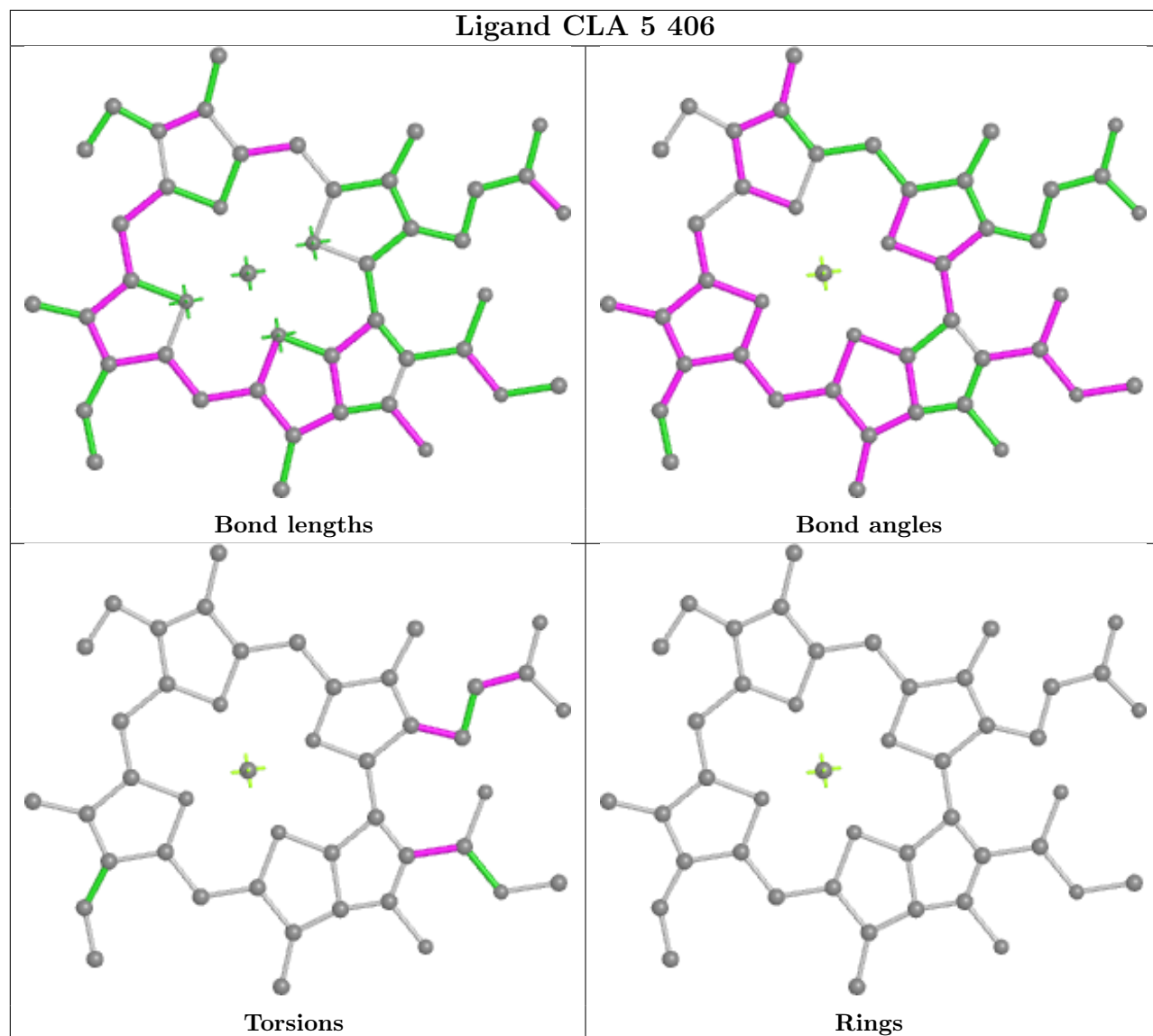


Ligand CLA X 101

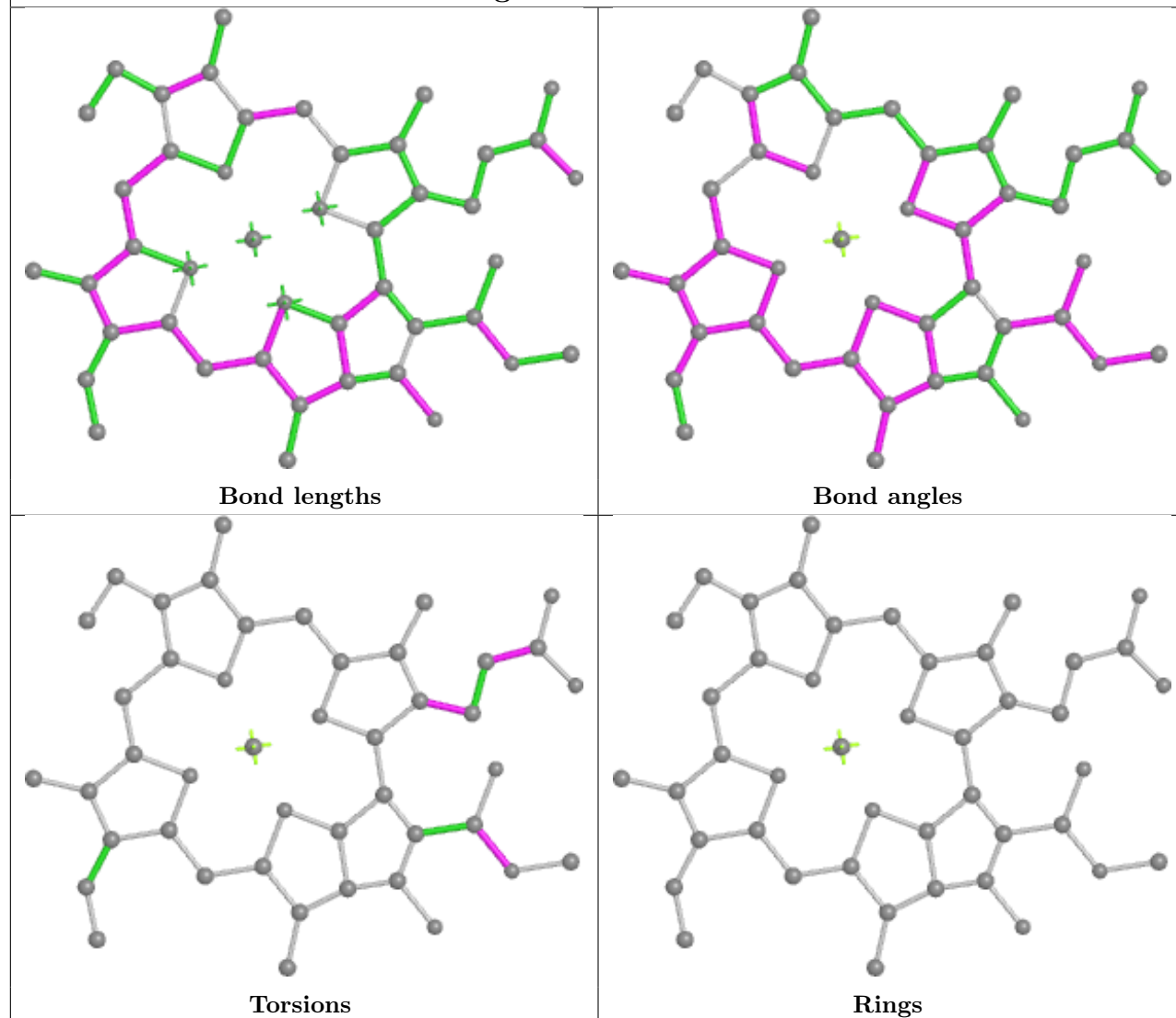




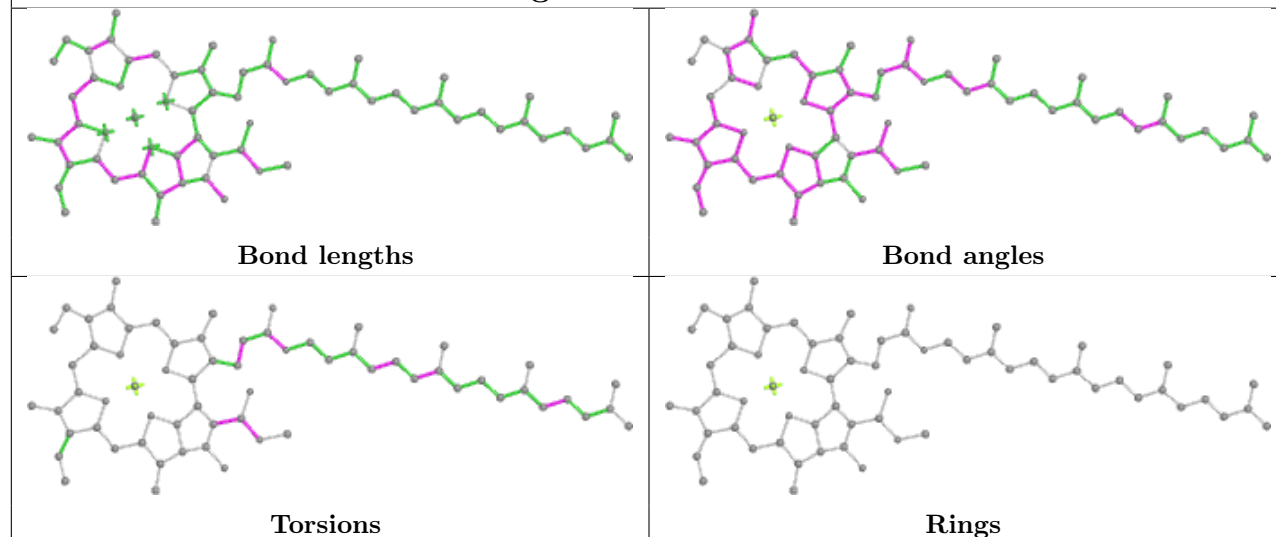
Ligand CLA 5 406



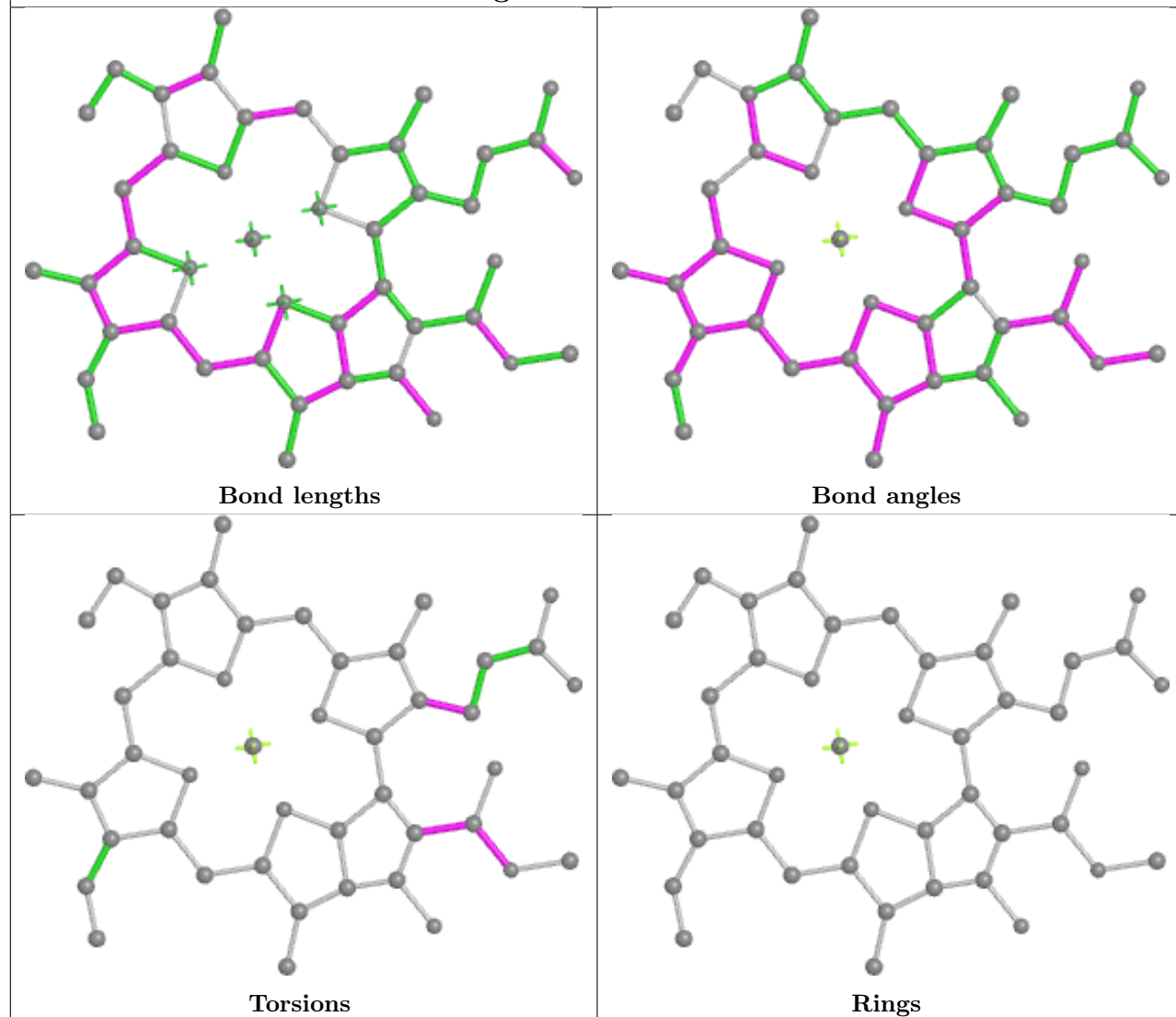
Ligand CLA 5 415



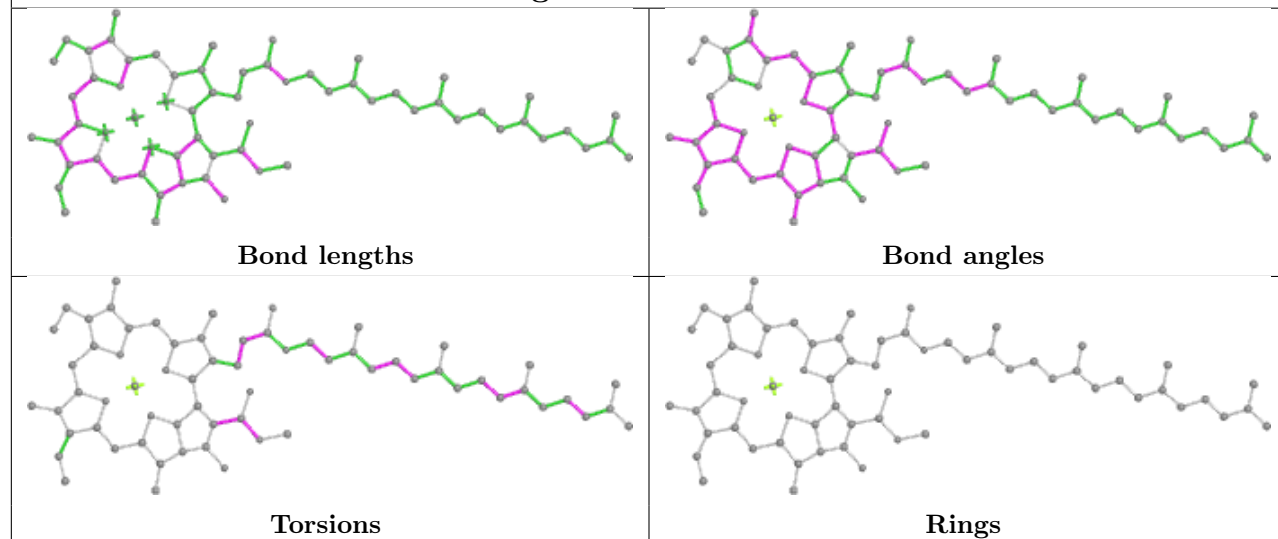
Ligand CLA A 809



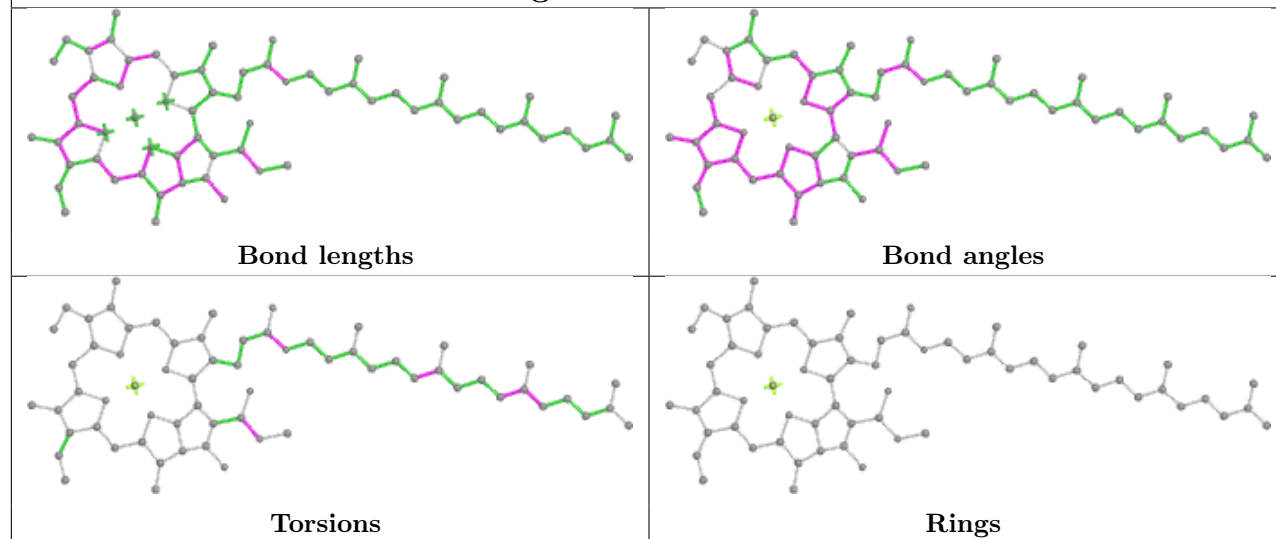
Ligand CLA 1 507



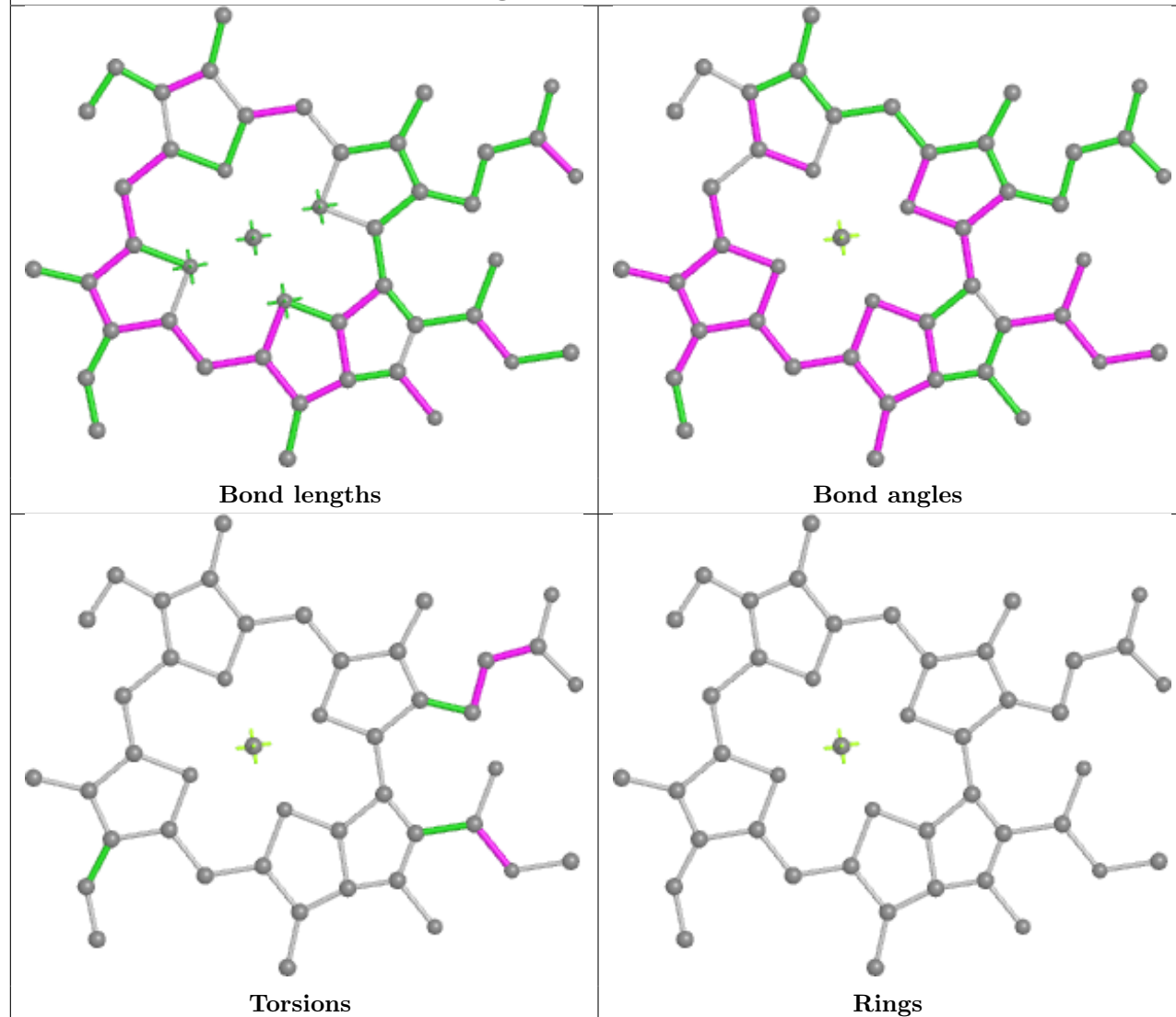
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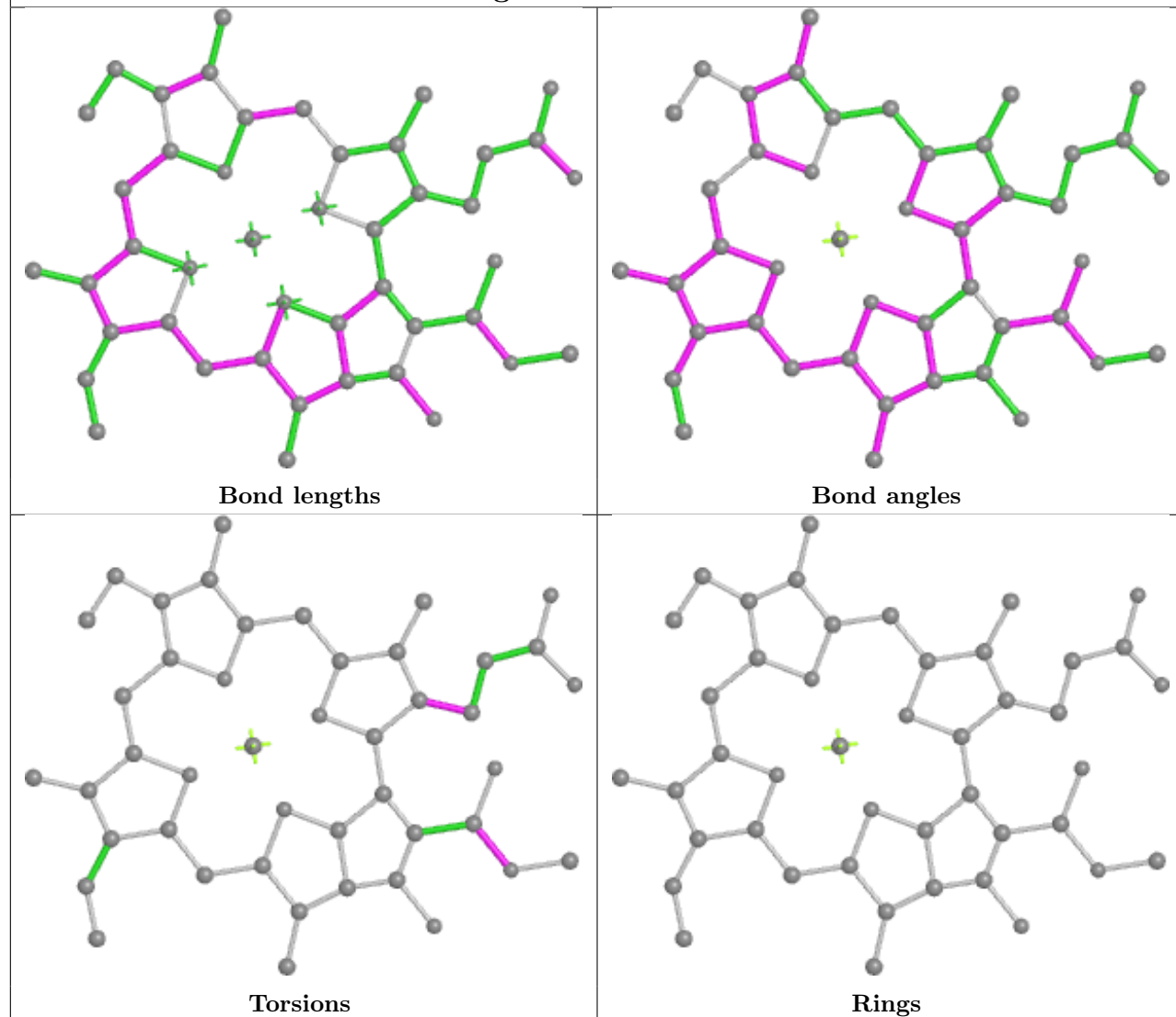
Ligand CLA A 842



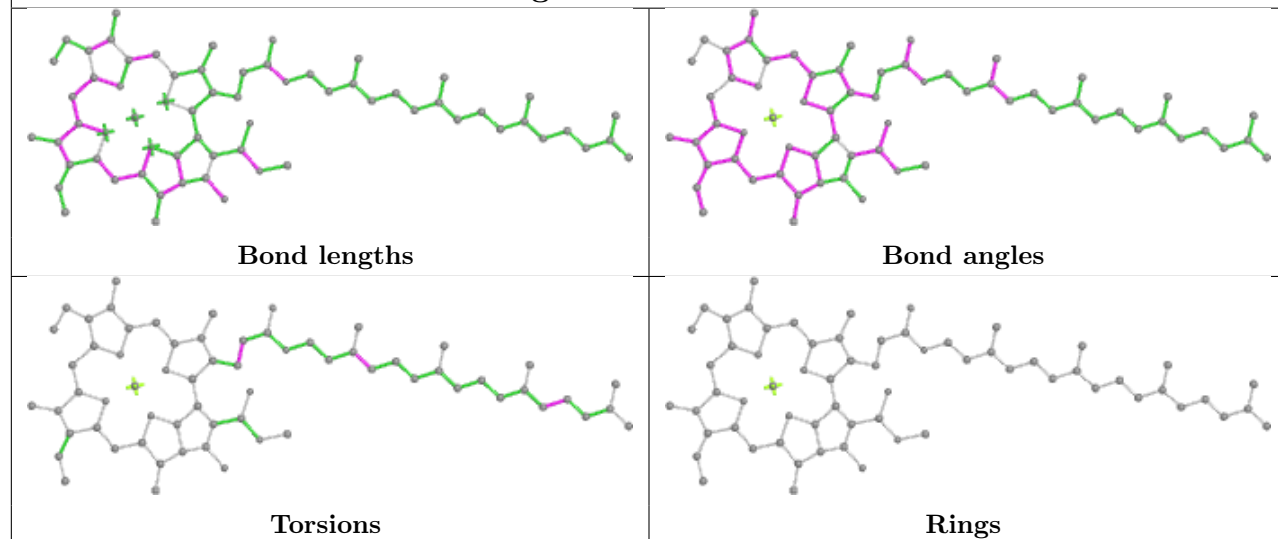
Ligand CLA 3 401



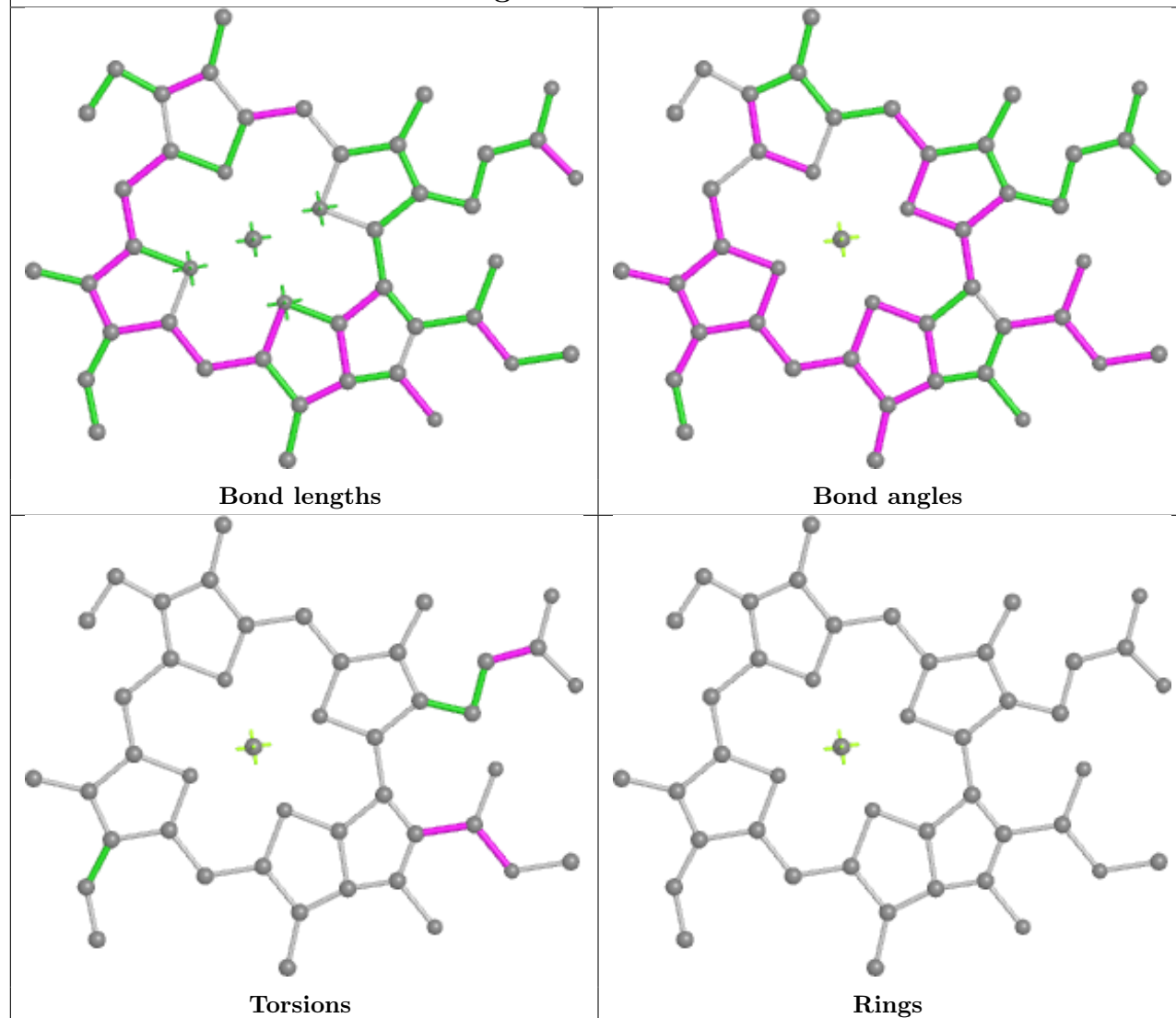
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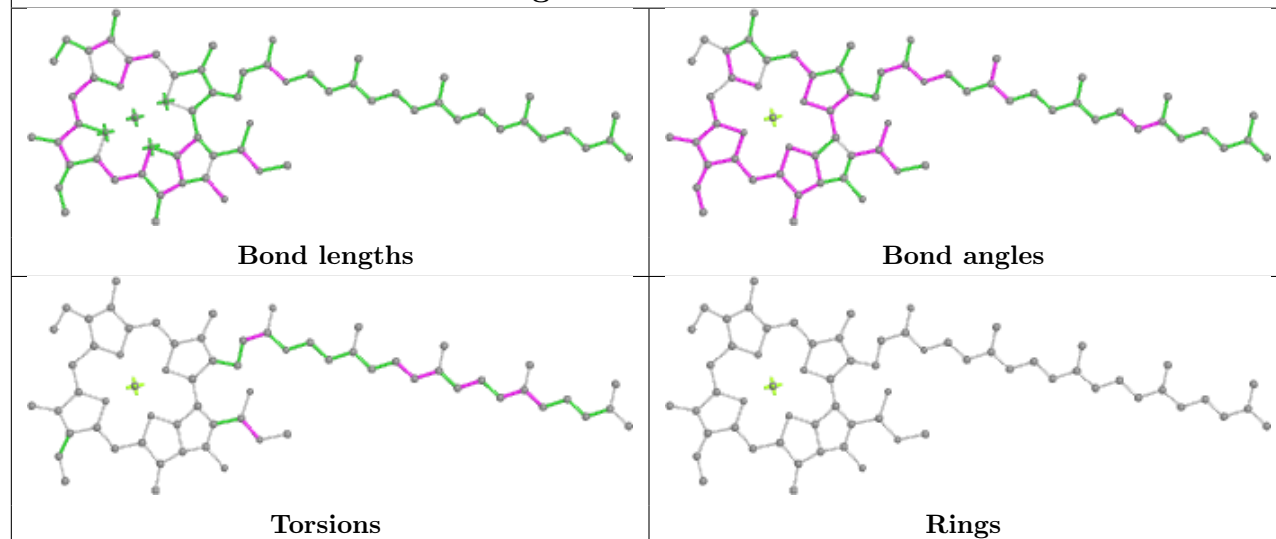
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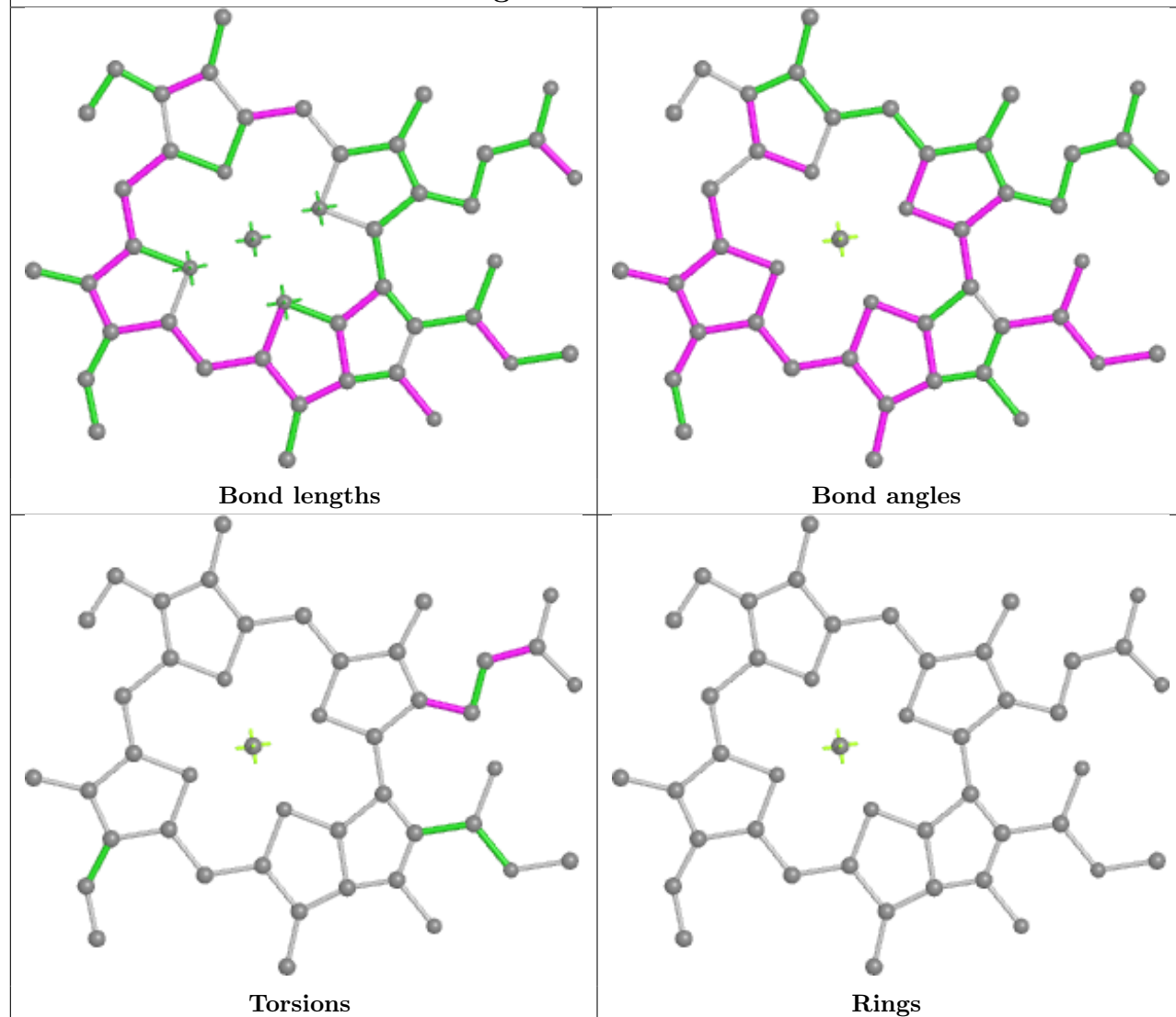
Ligand CLA 2 405



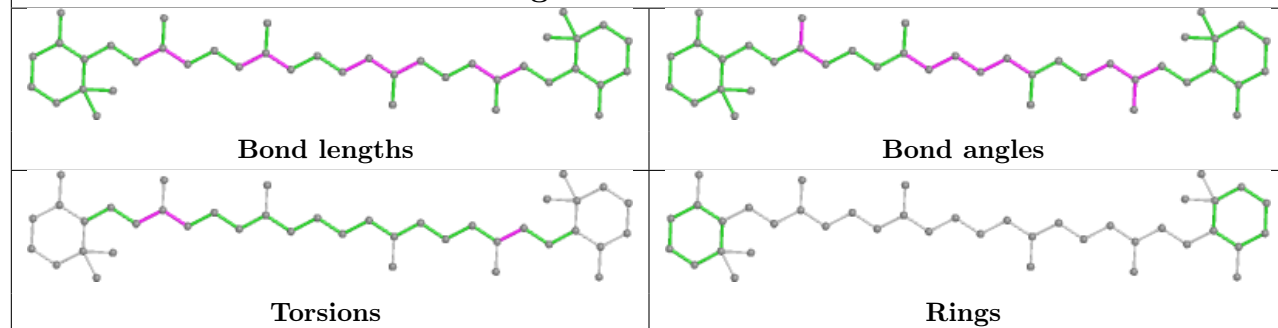
Ligand CLA B 806



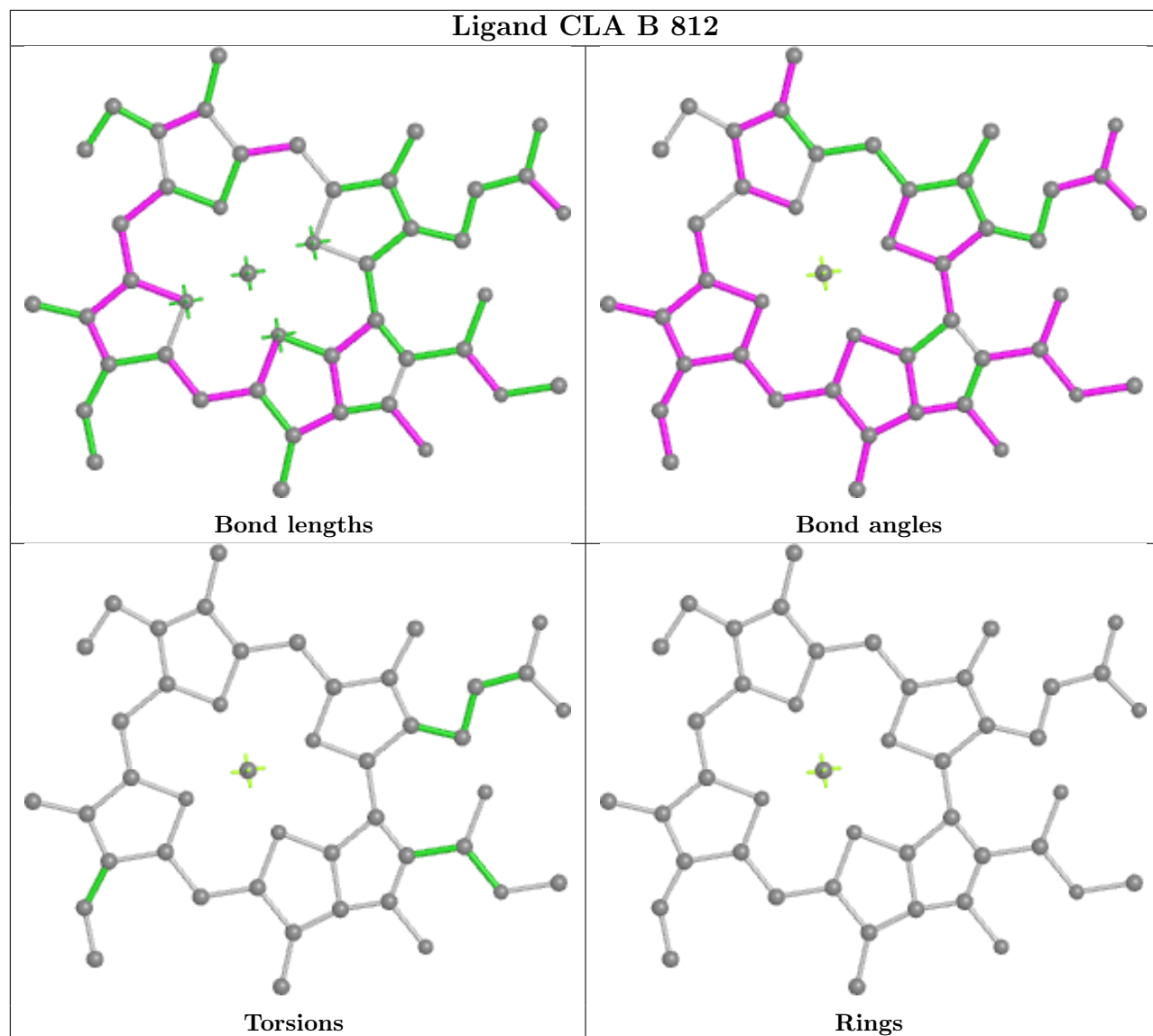
Ligand CLA 4 408

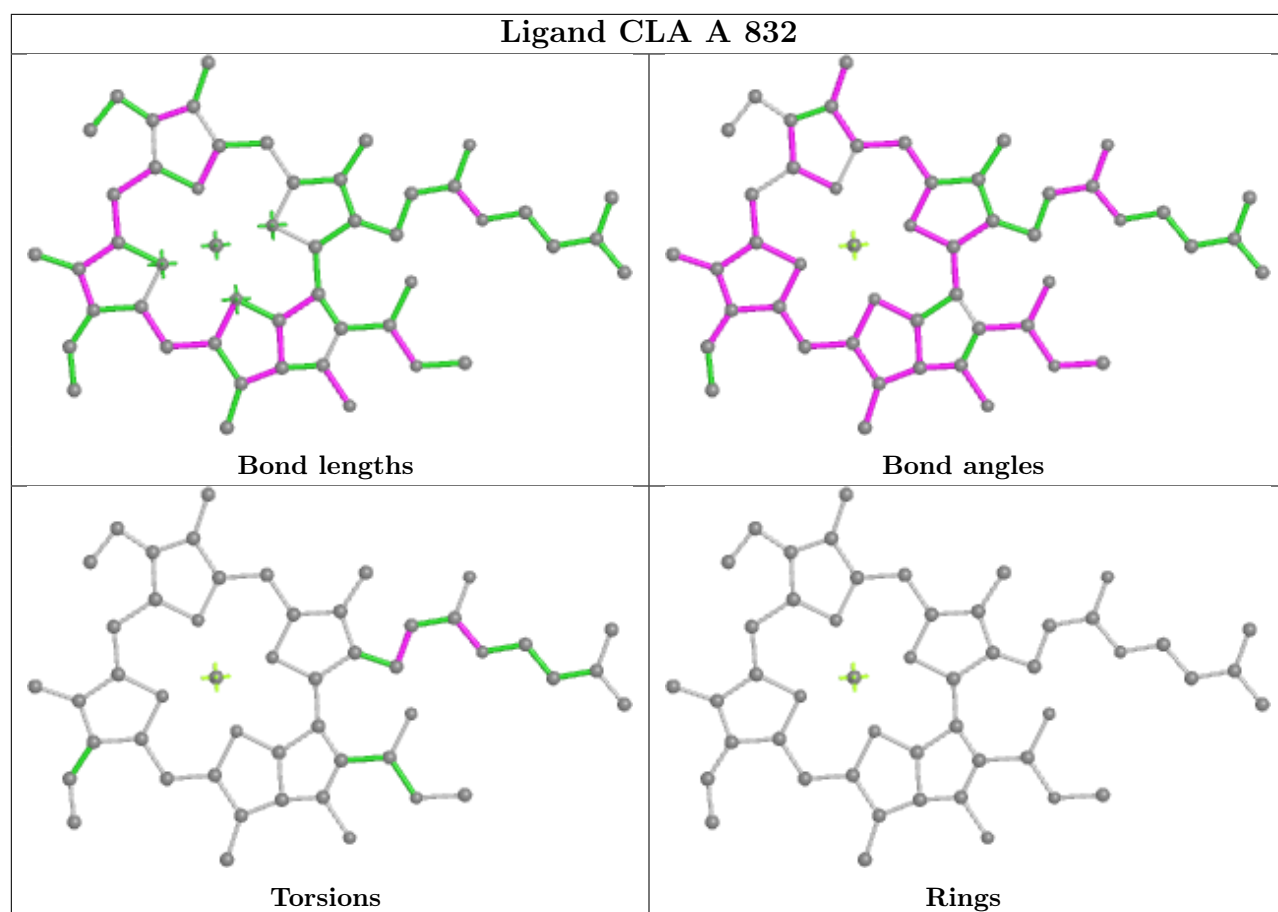


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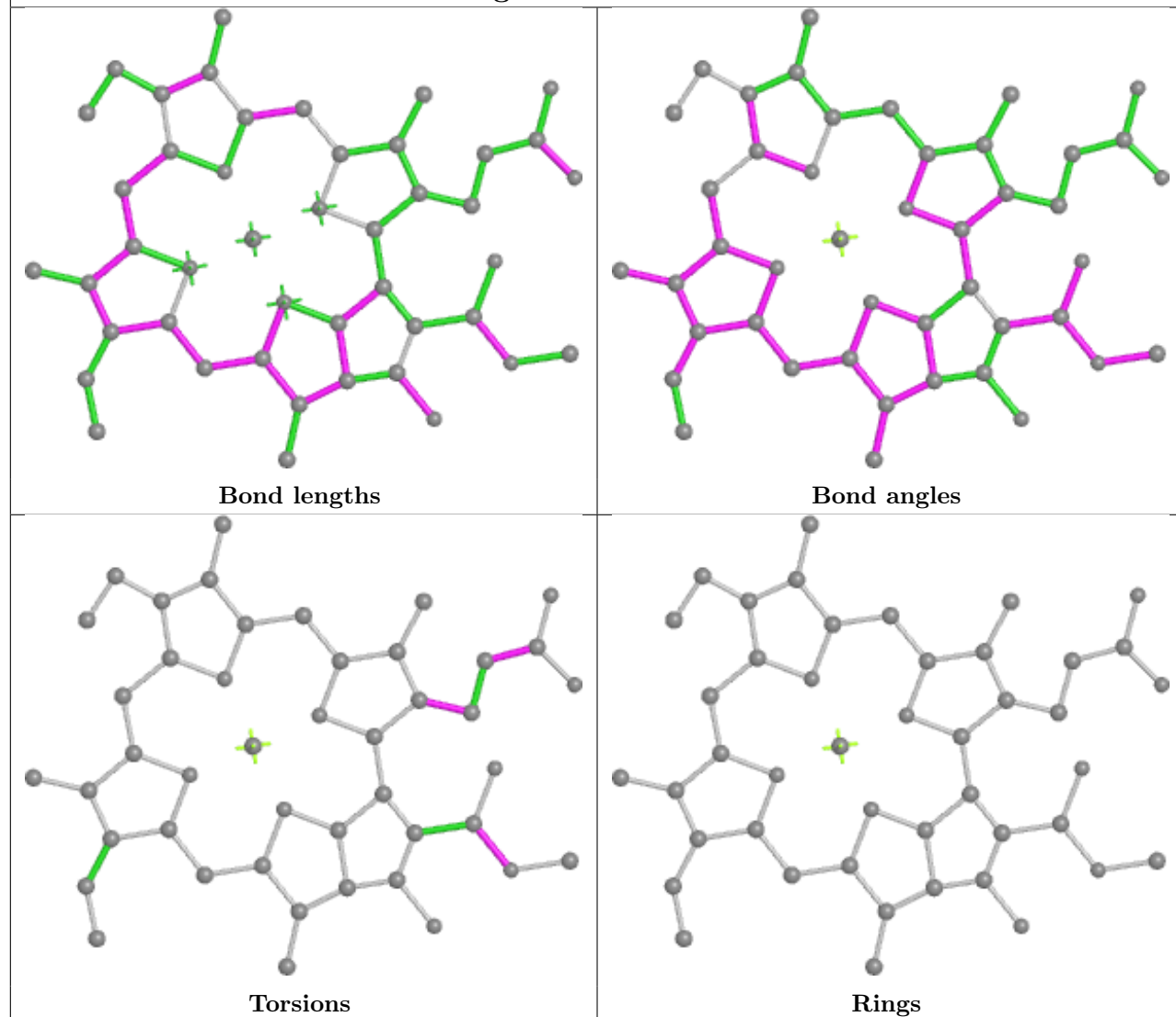


Ligand CLA B 812

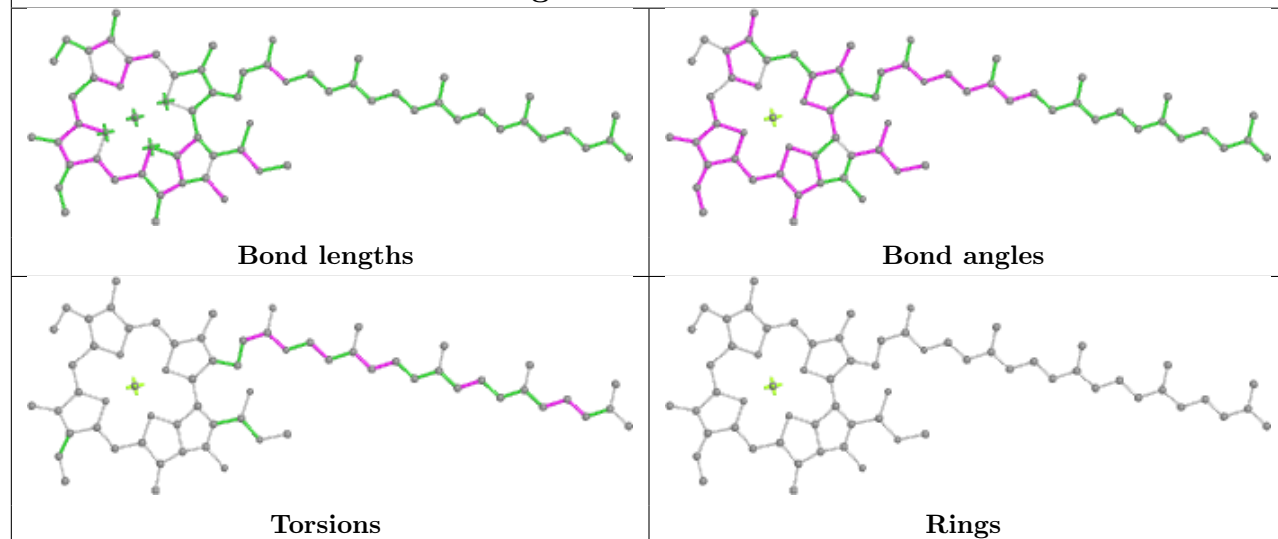




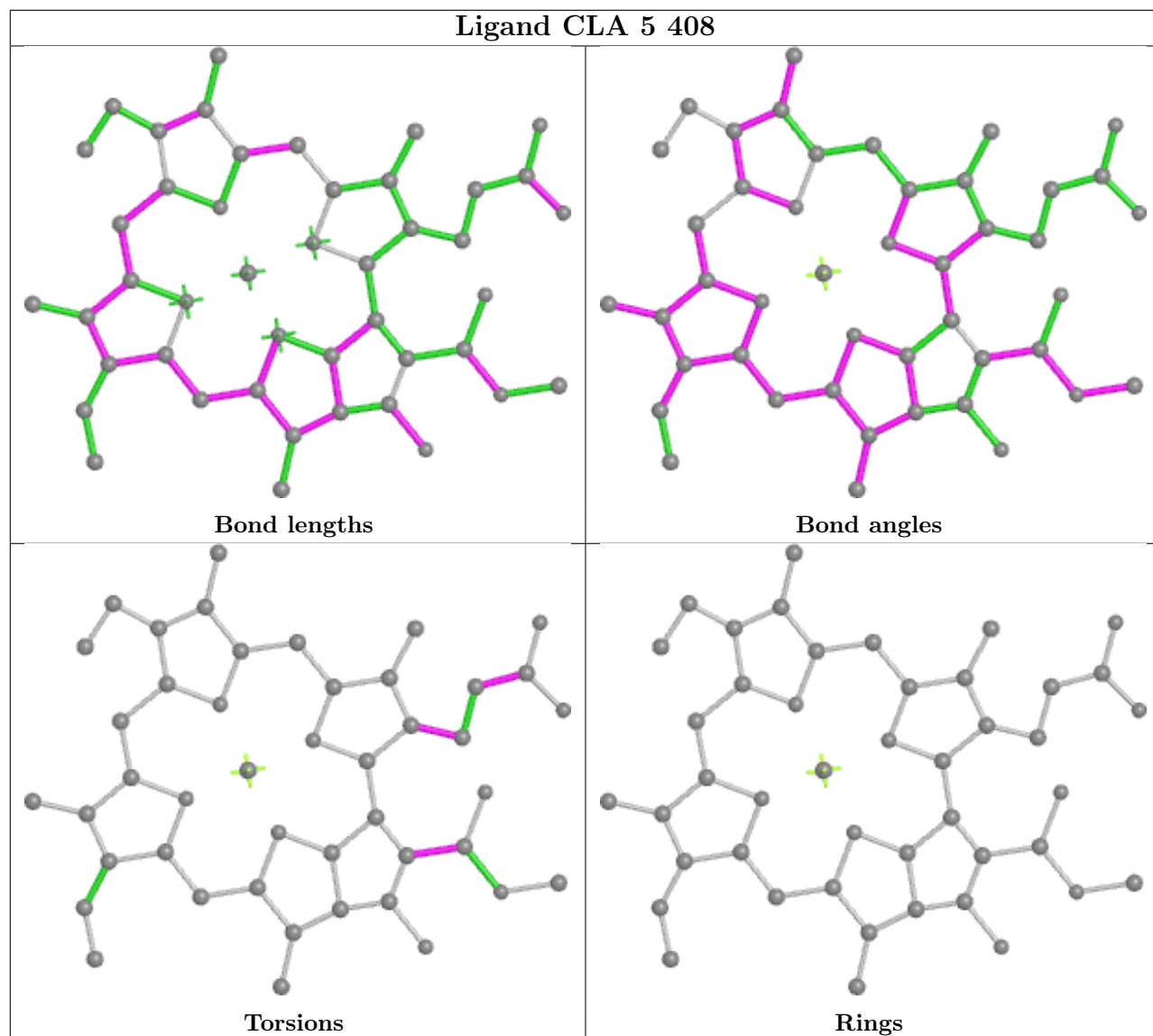
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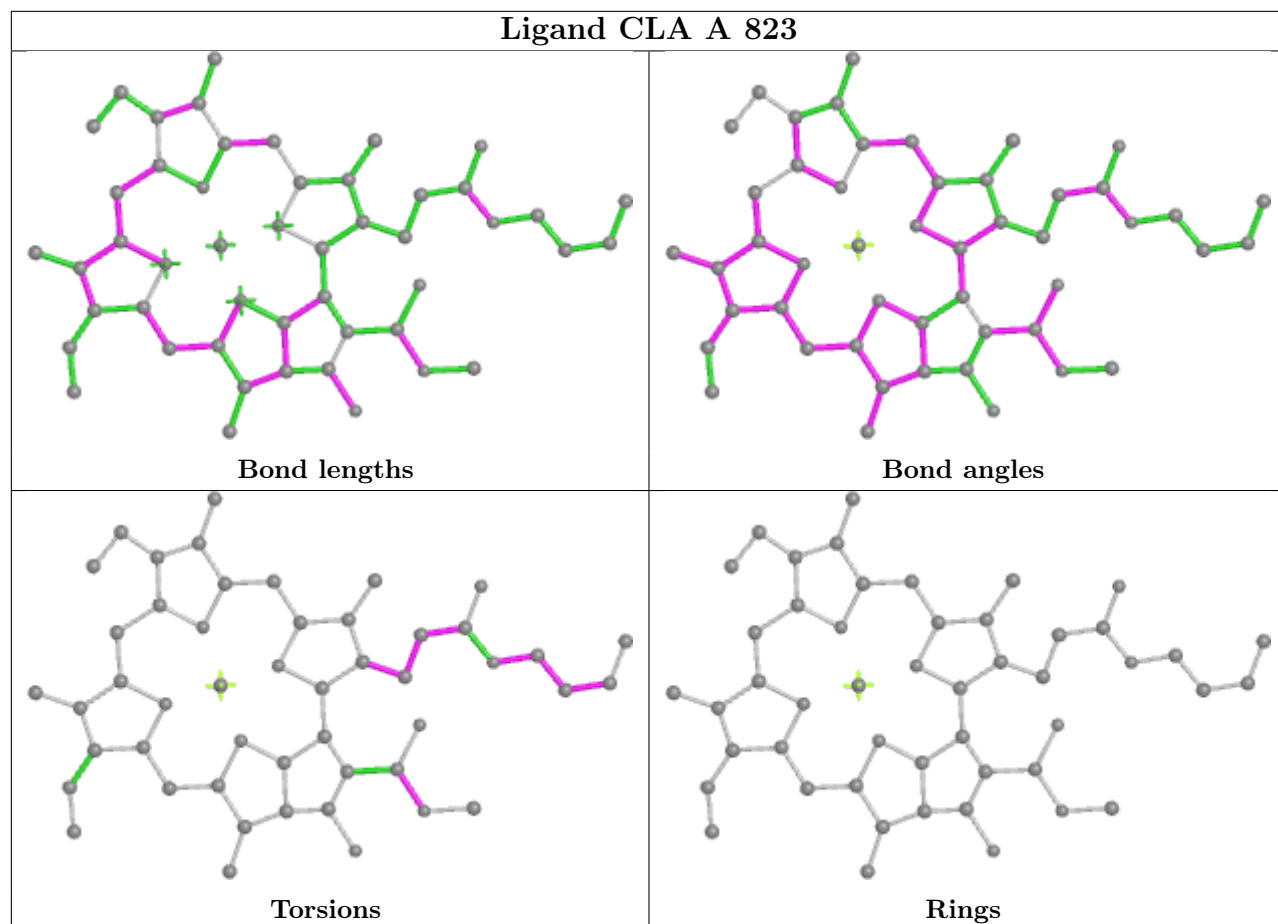
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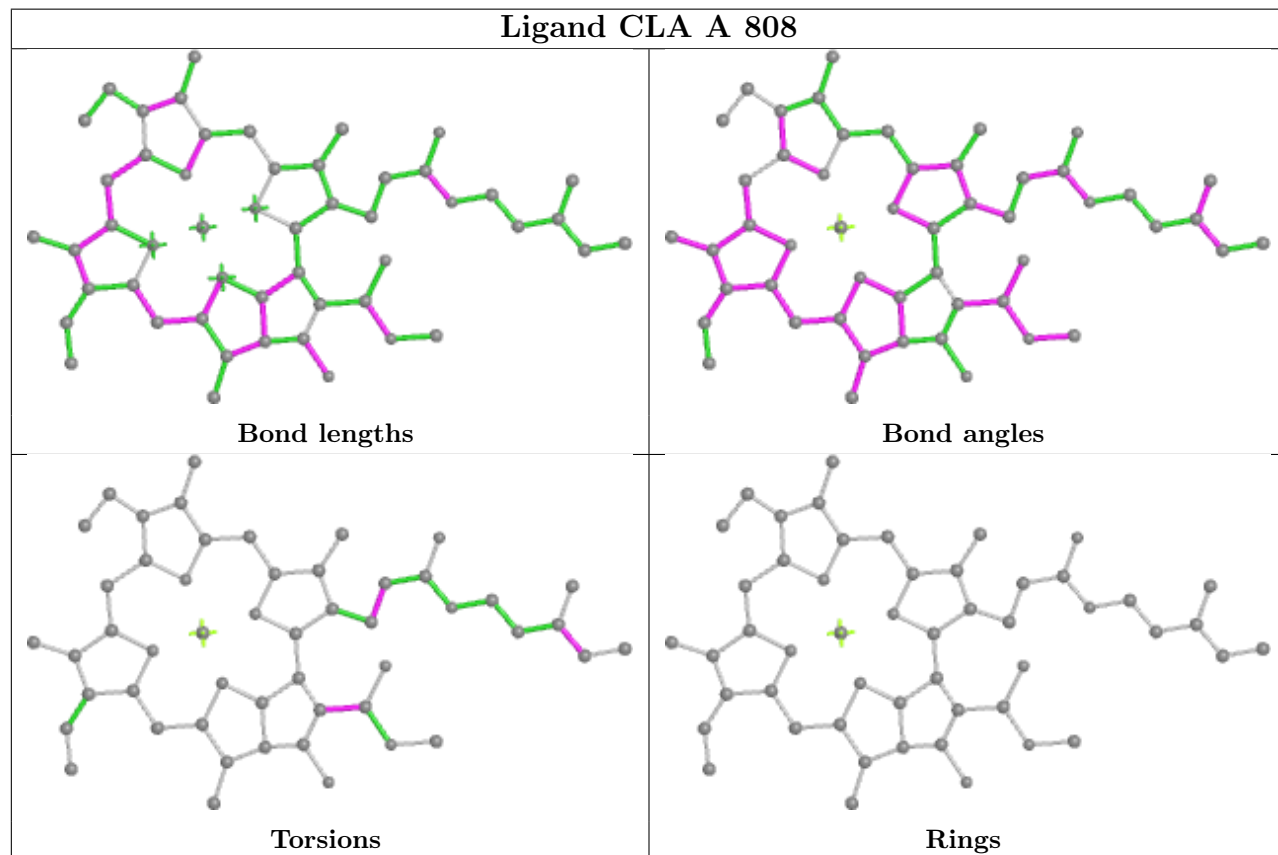
Ligand CLA 5 408



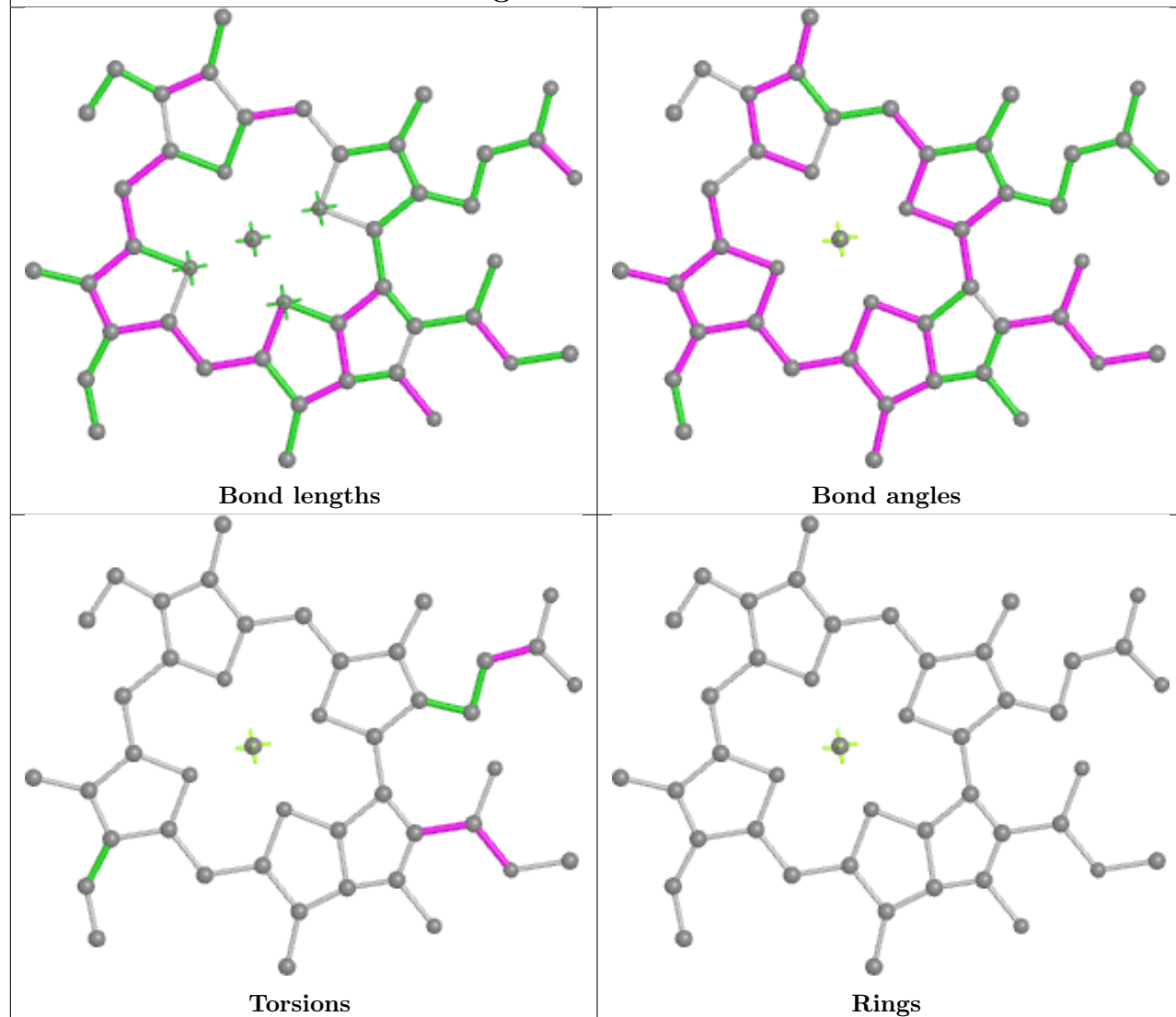
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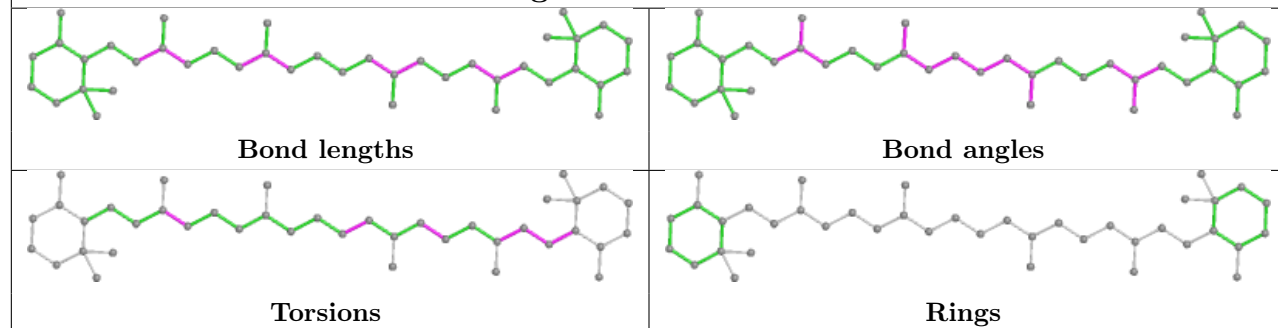
Ligand CLA A 808



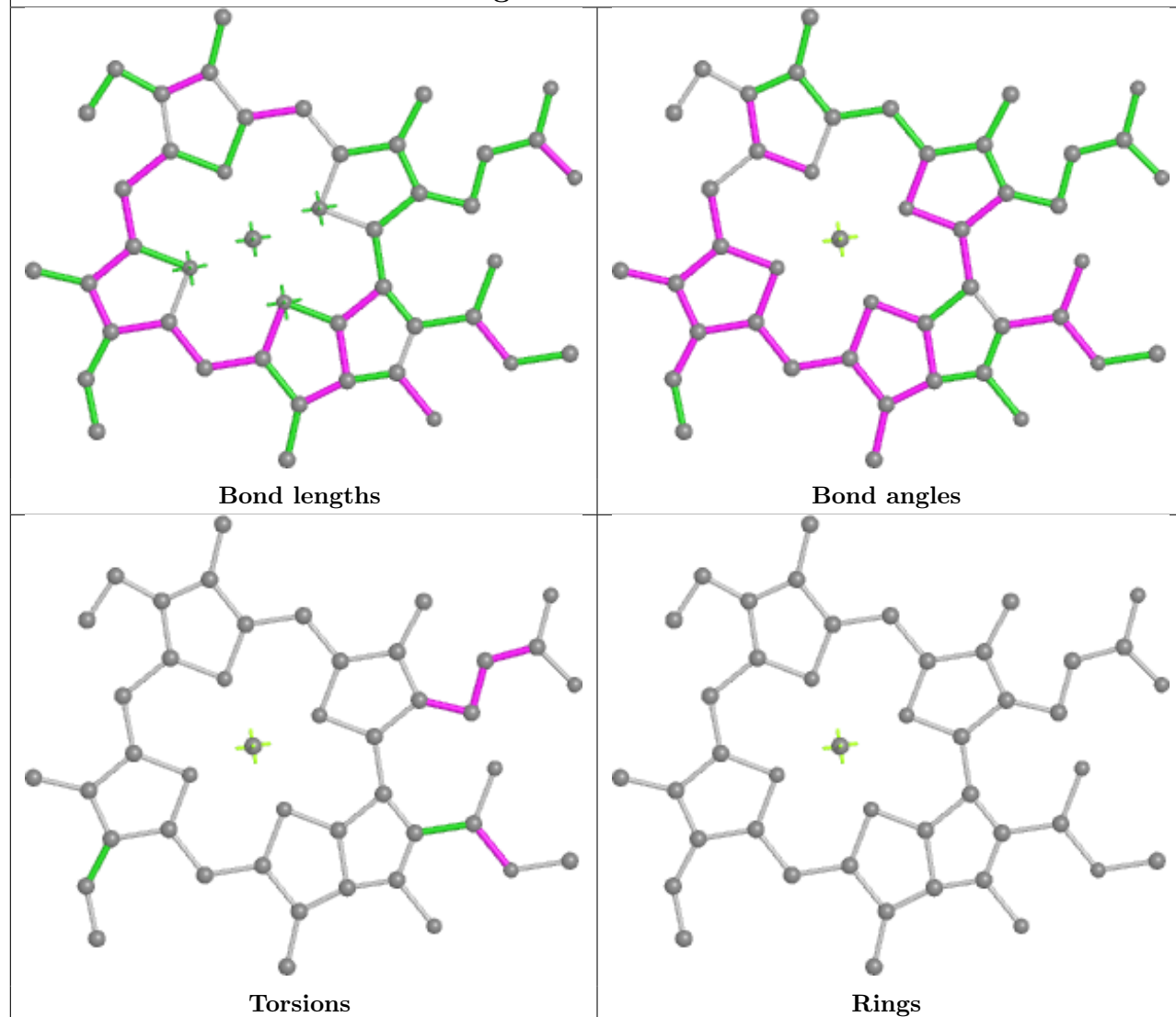
Ligand CLA 4 407



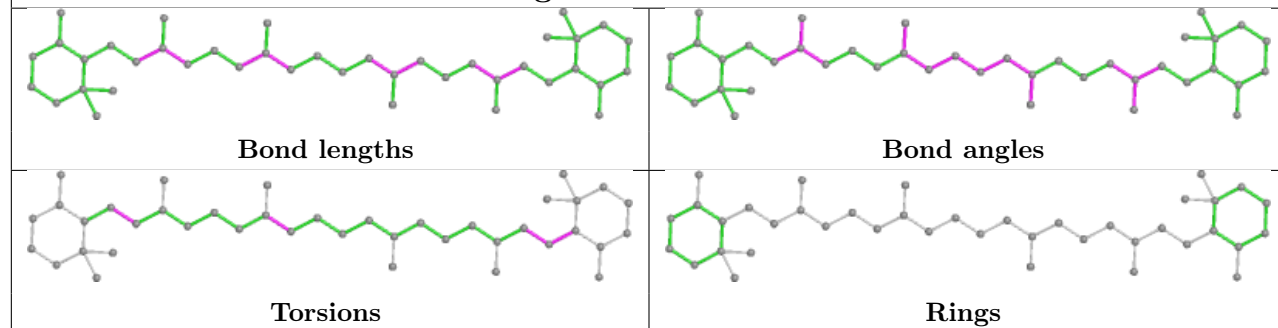
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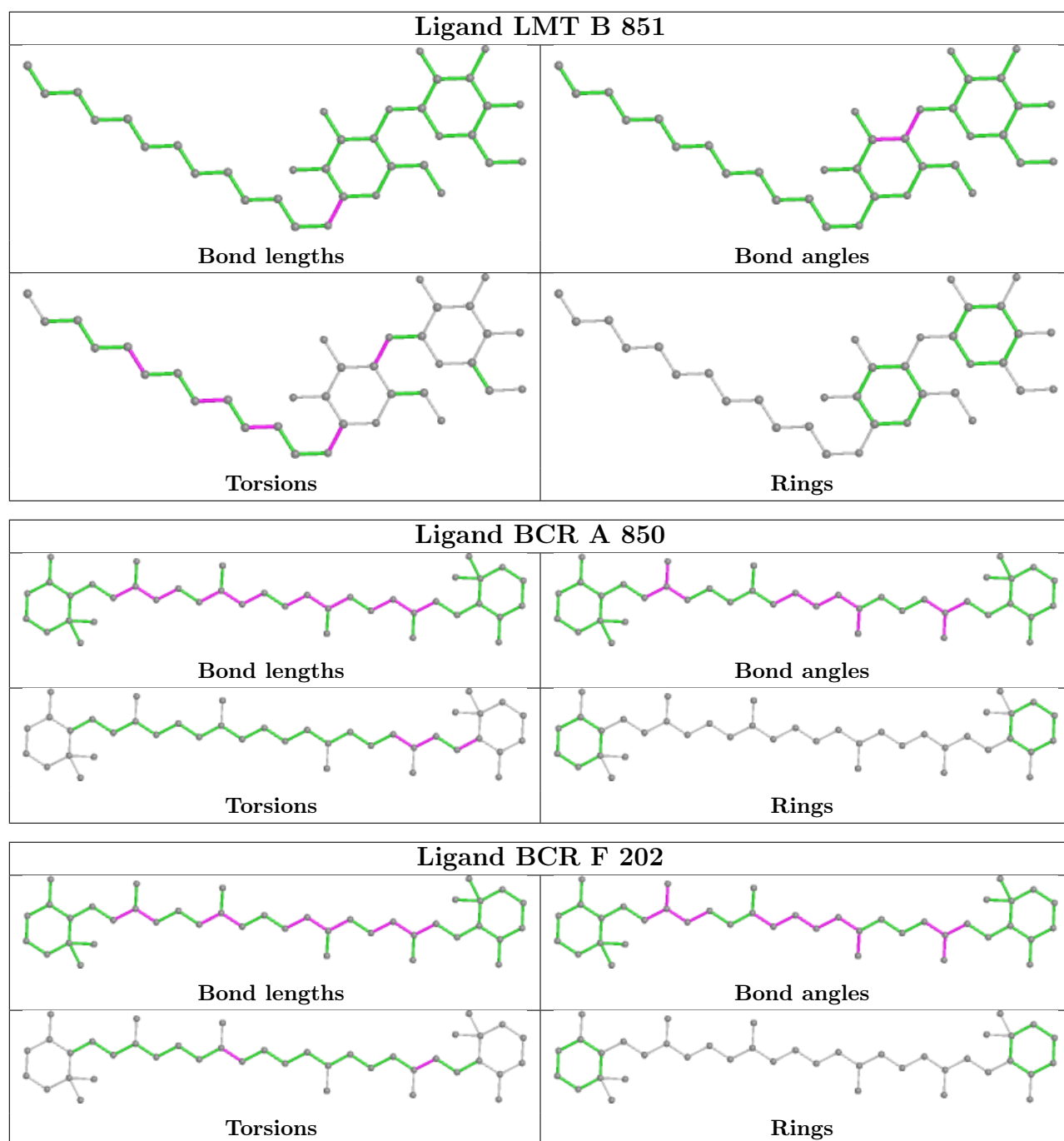


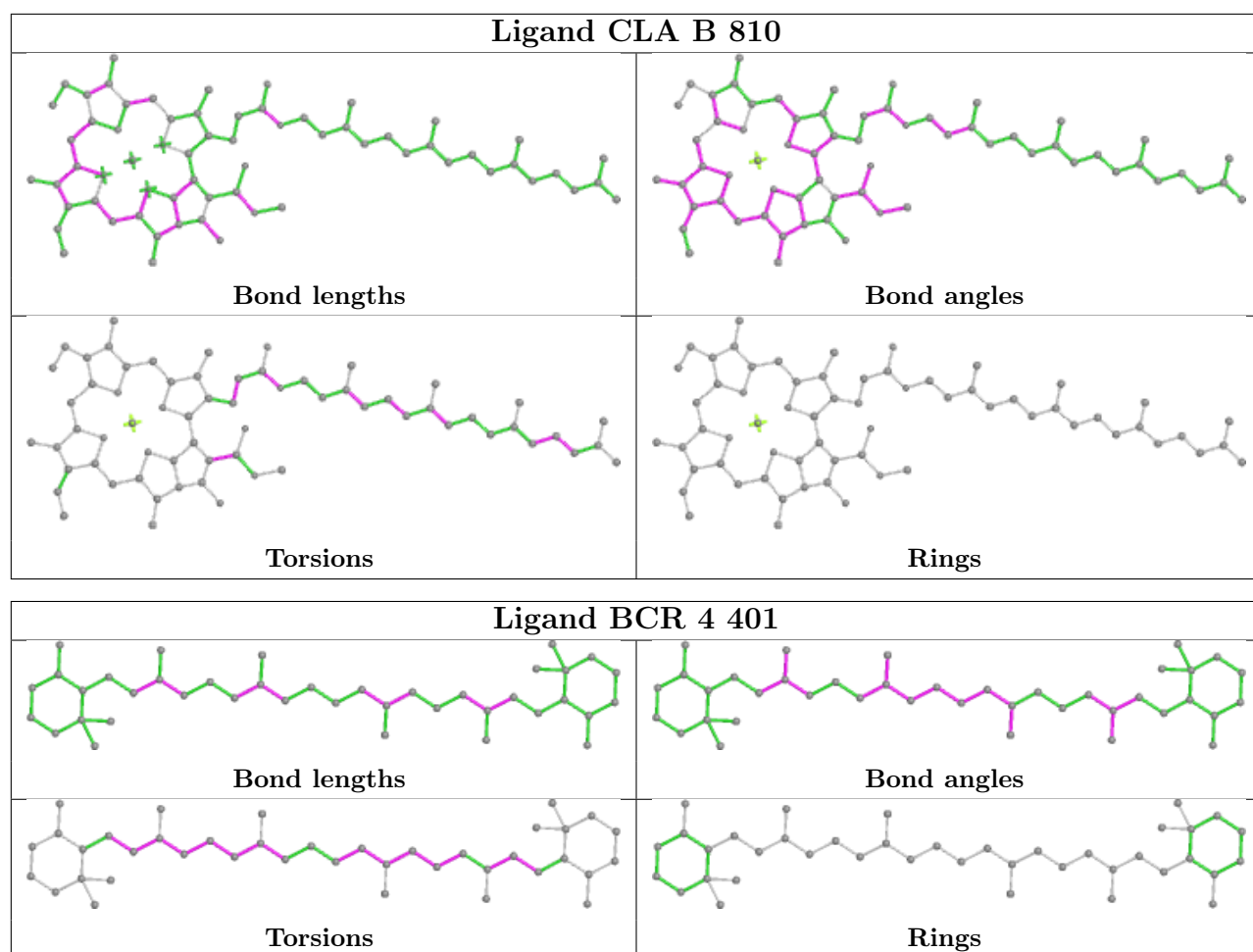
Ligand CLA 5 403



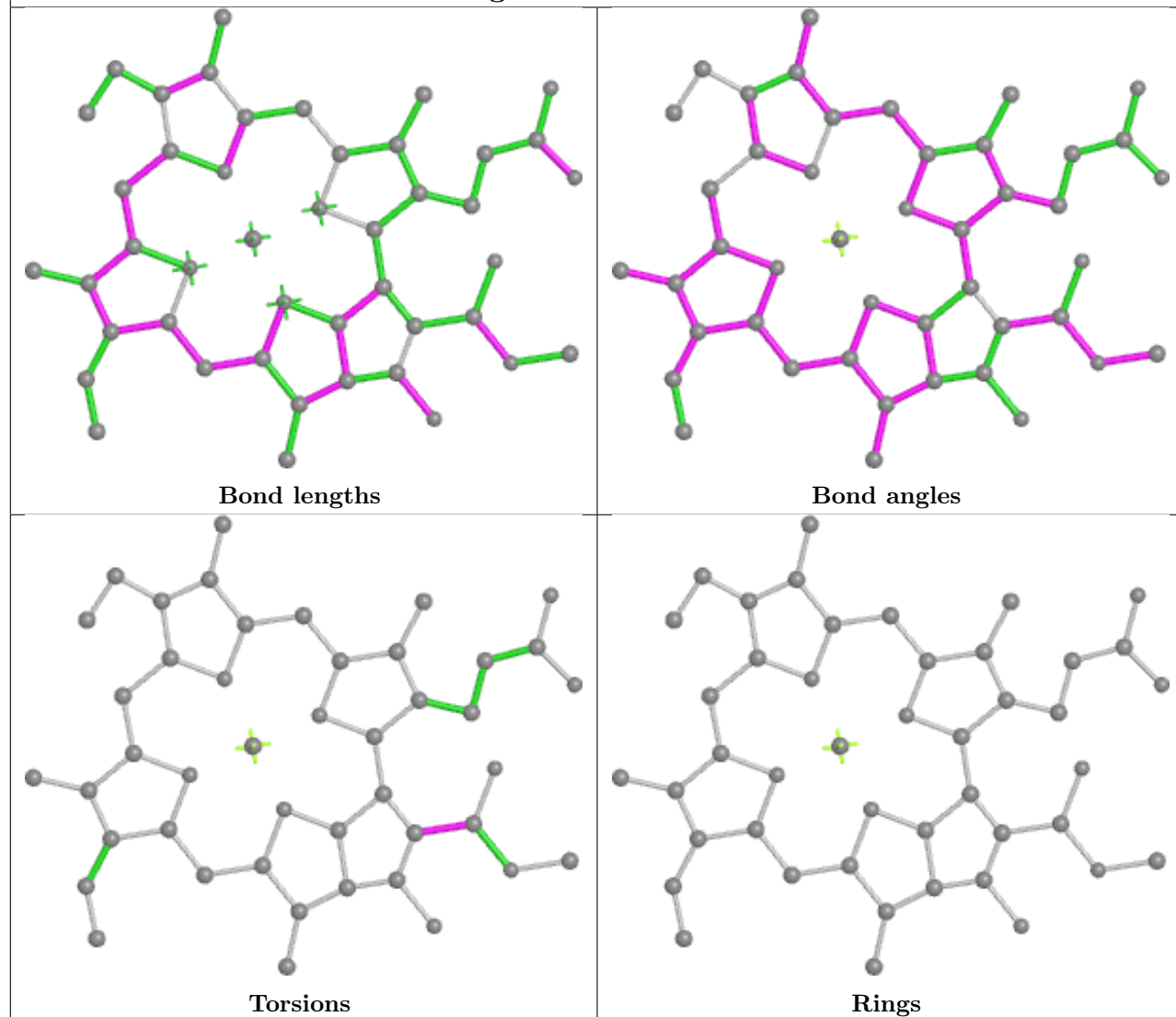
Ligand BCR 5 402



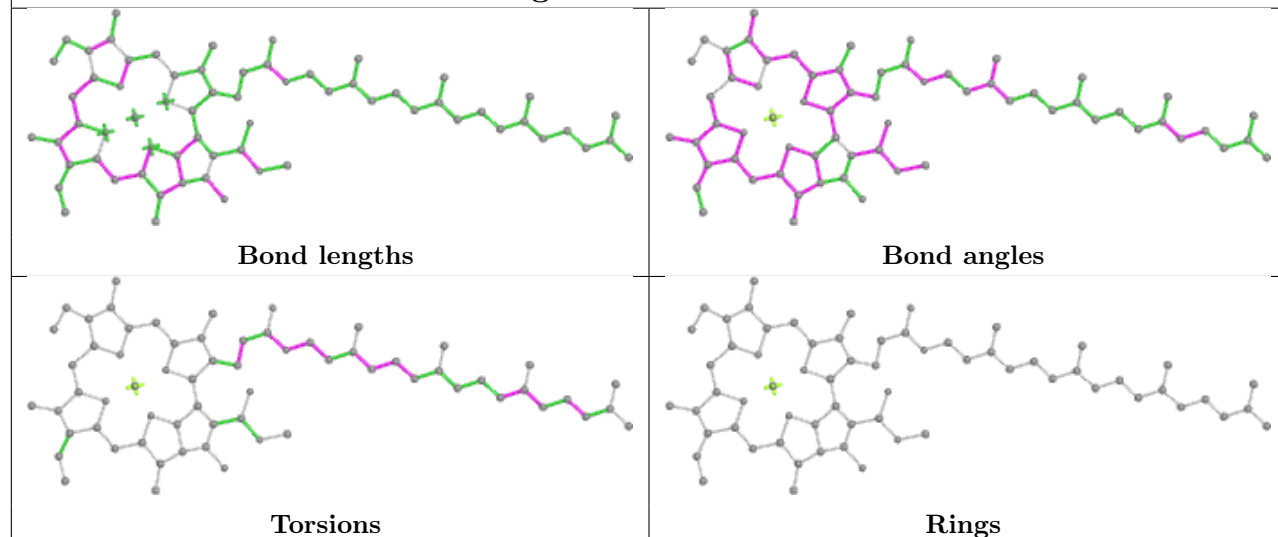


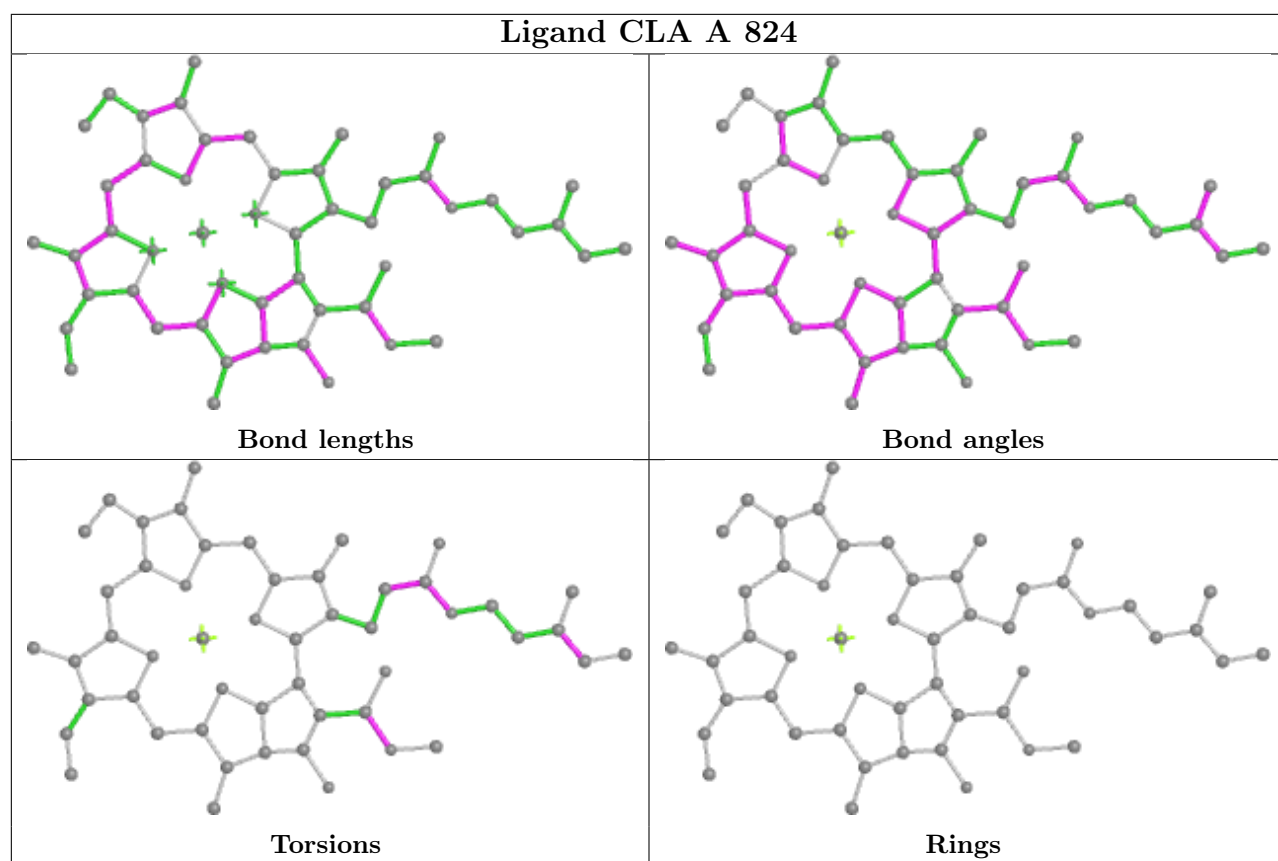


Ligand CLA A 811

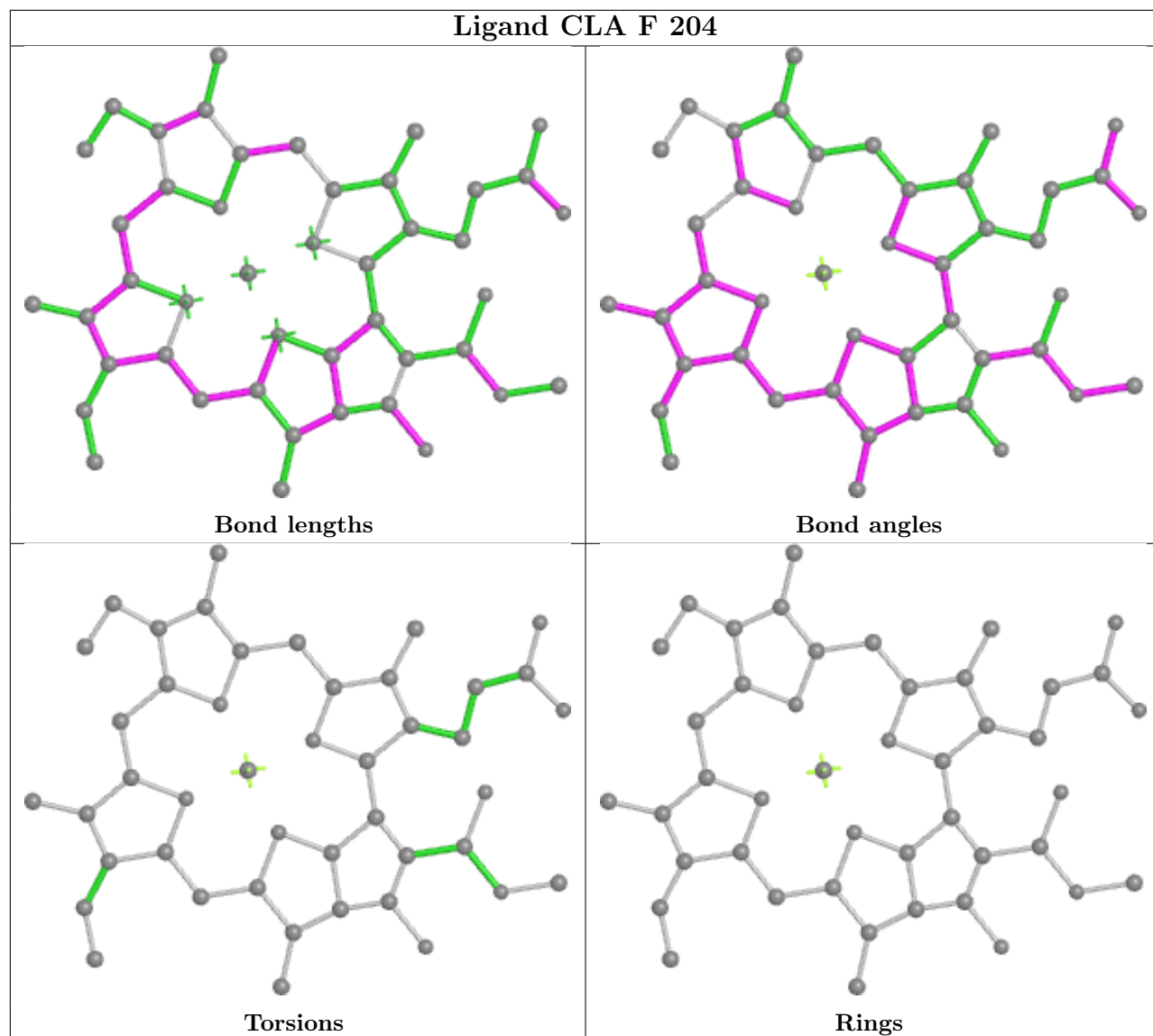


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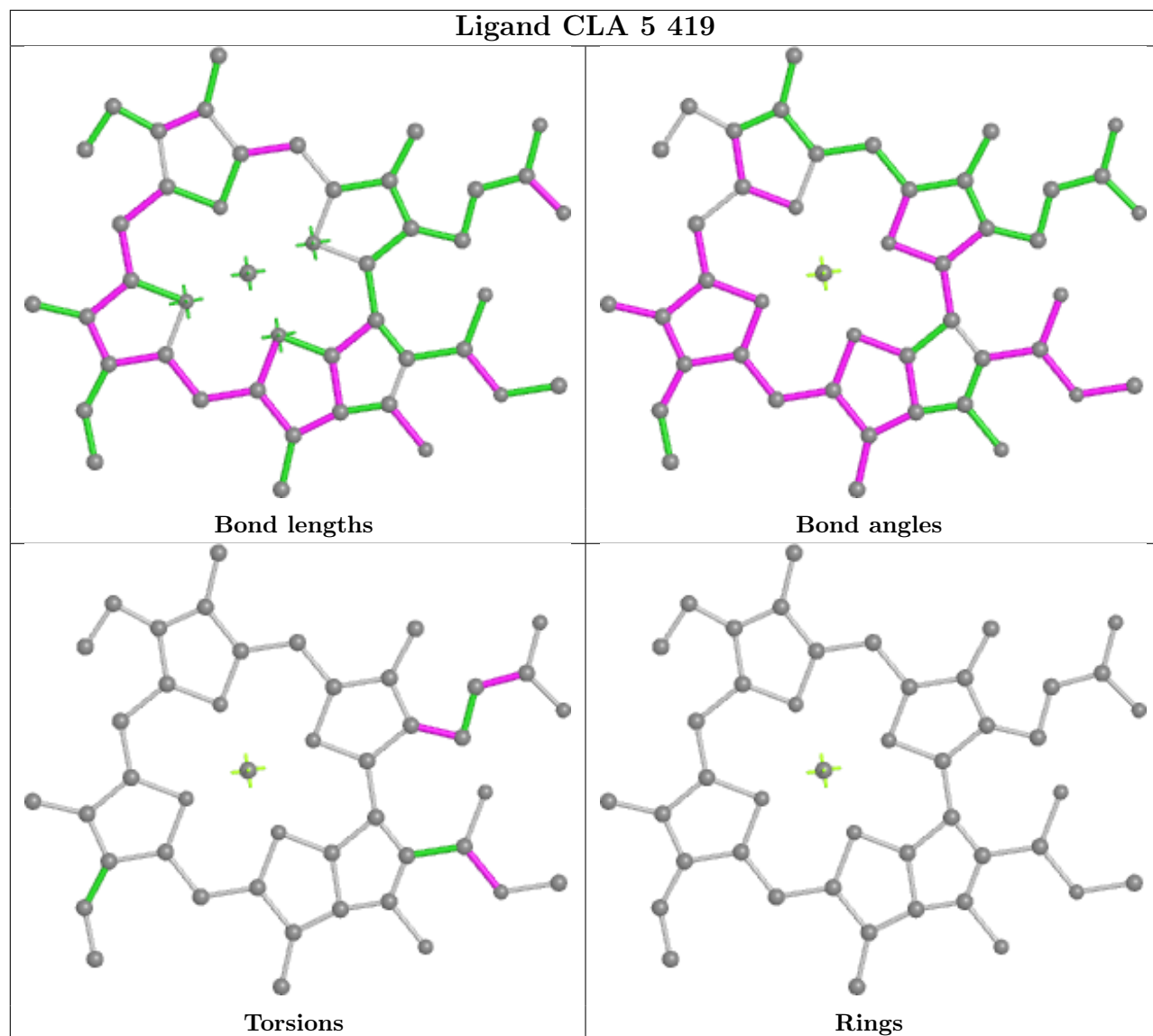




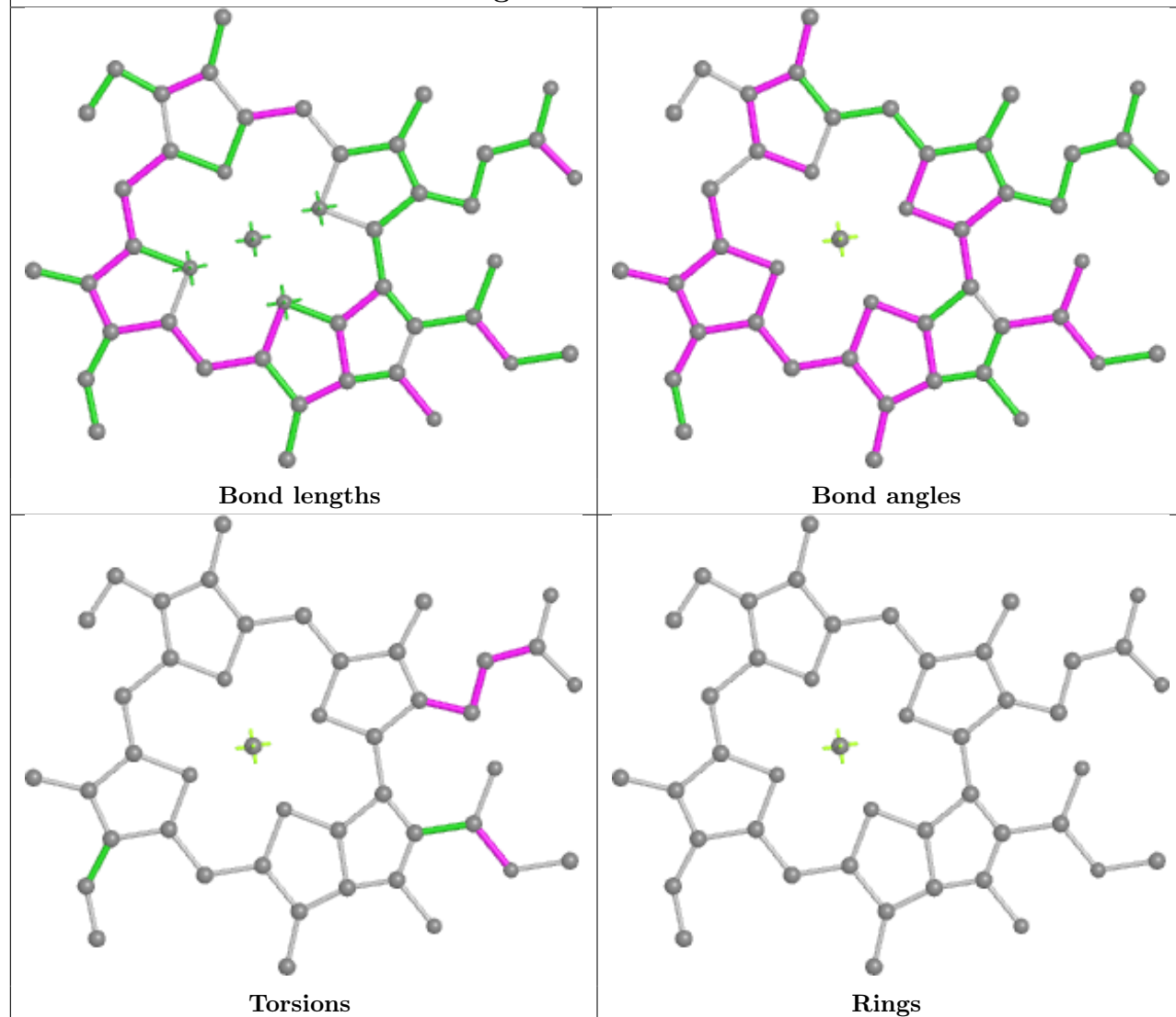
Ligand CLA F 204



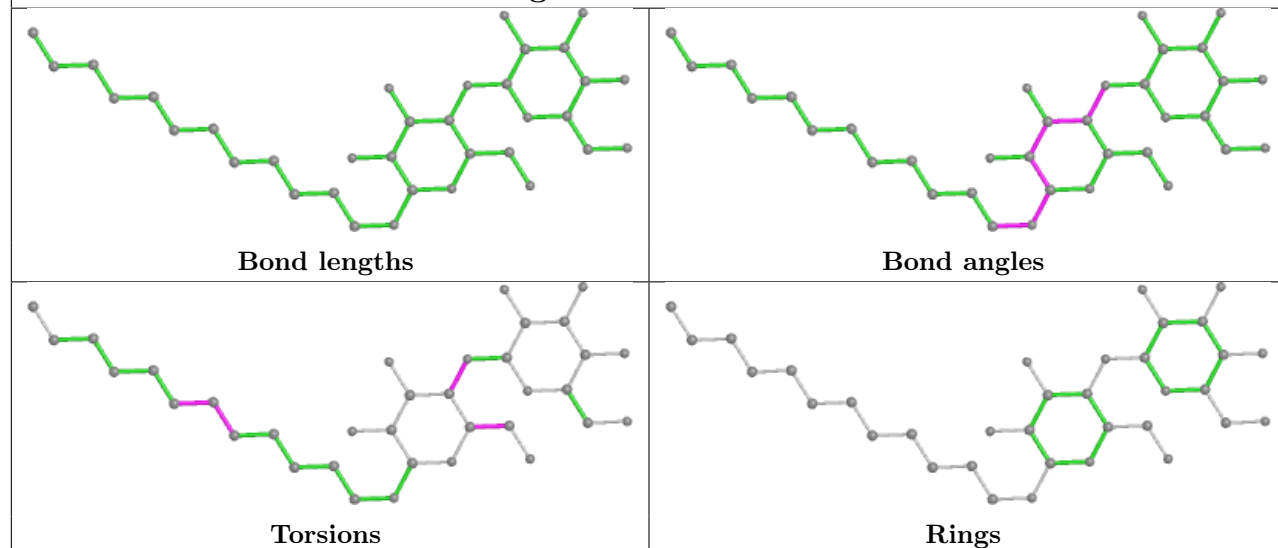
Ligand CLA 5 419



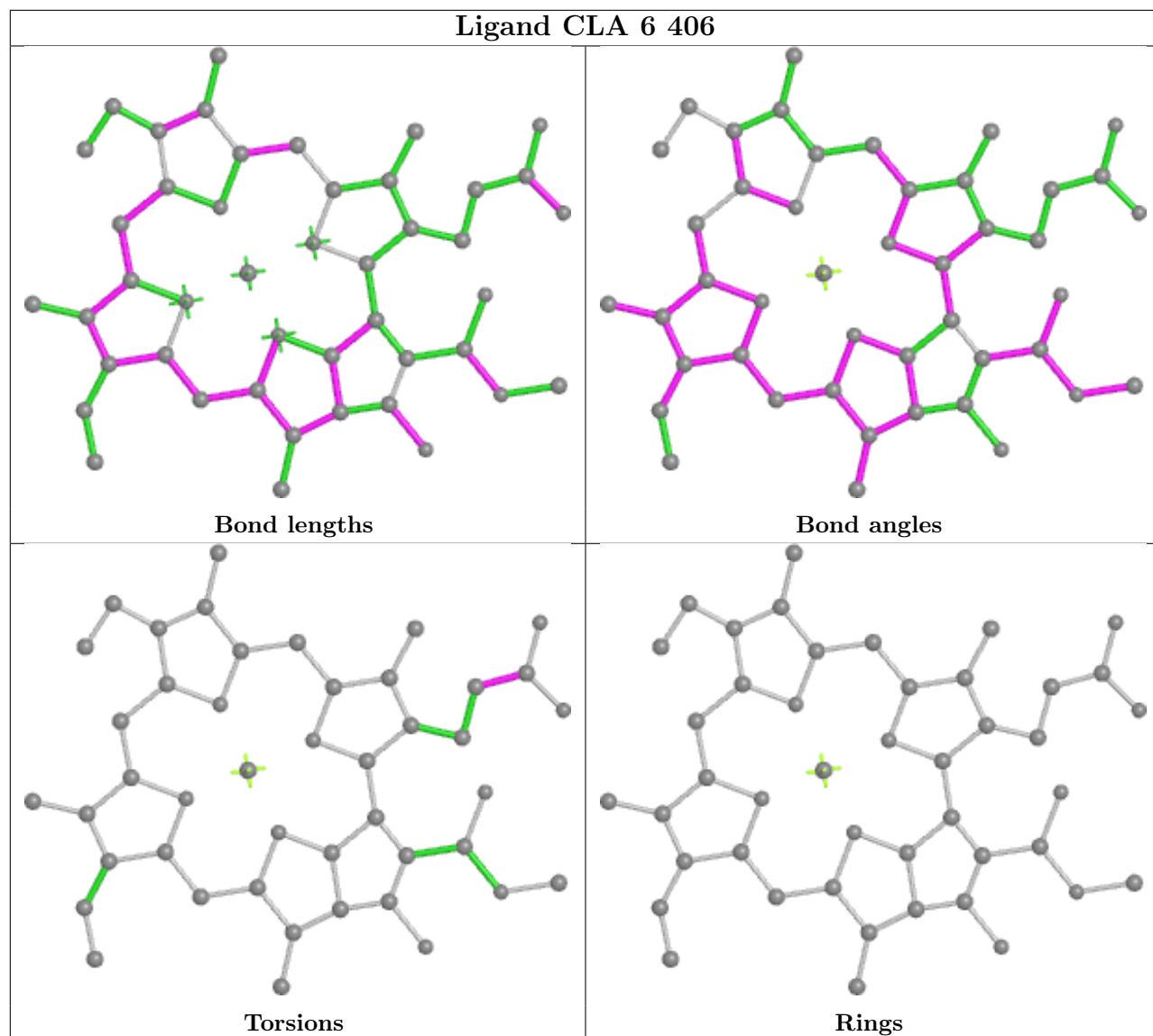
Ligand CLA 1 502



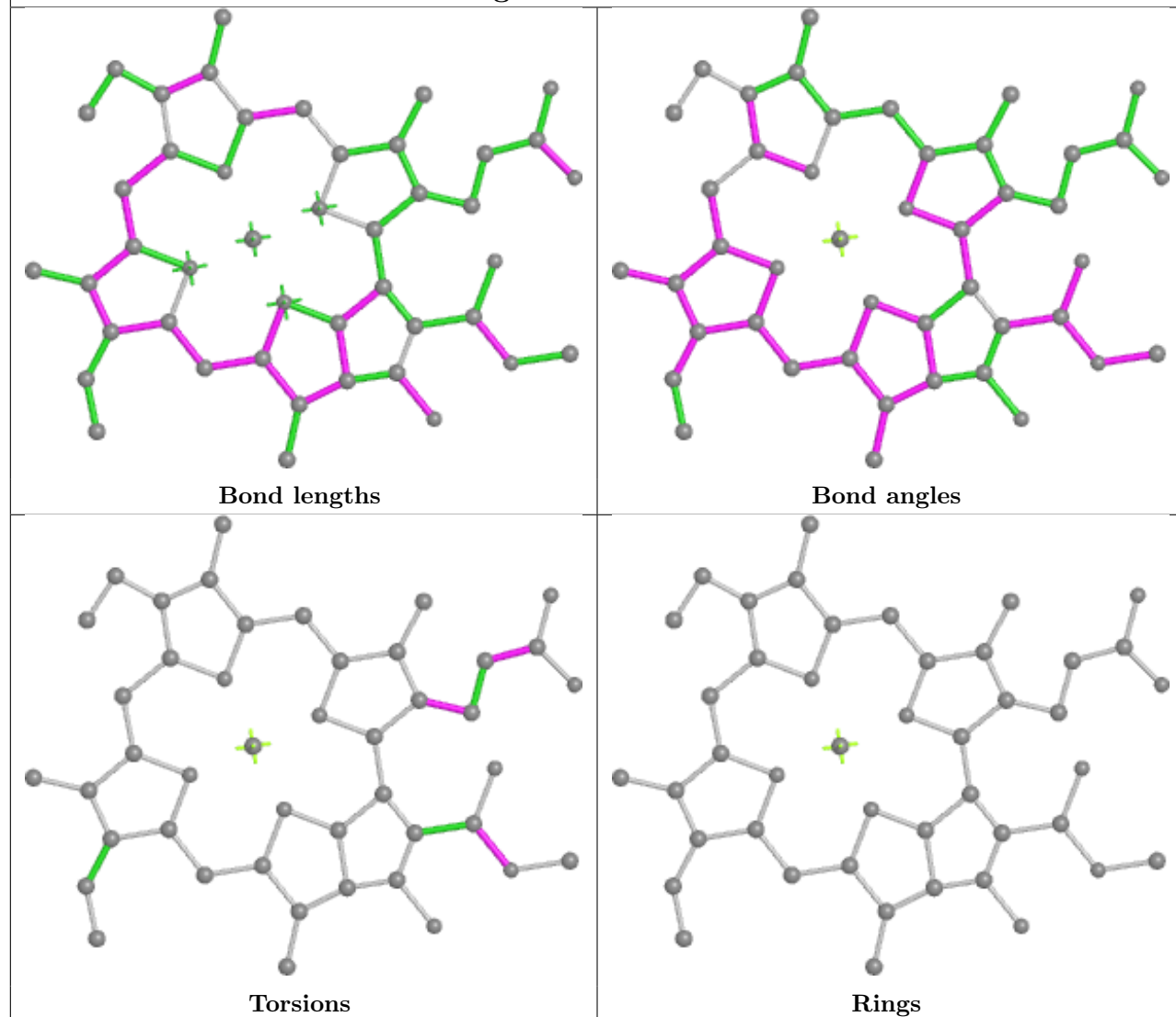
Ligand LMT B 852



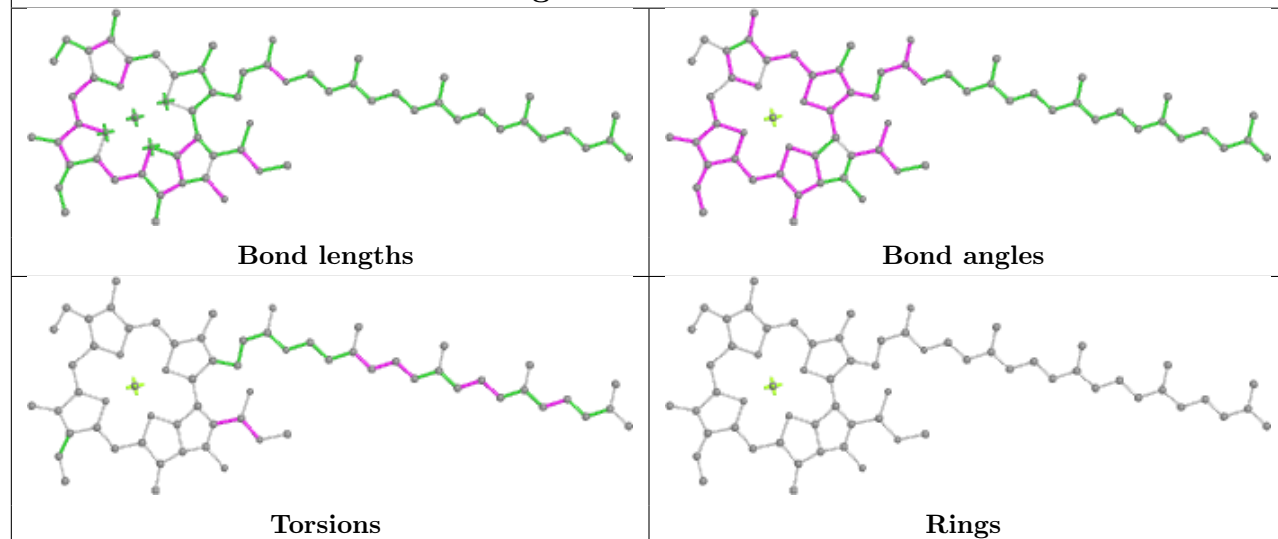
Ligand CLA 6 406



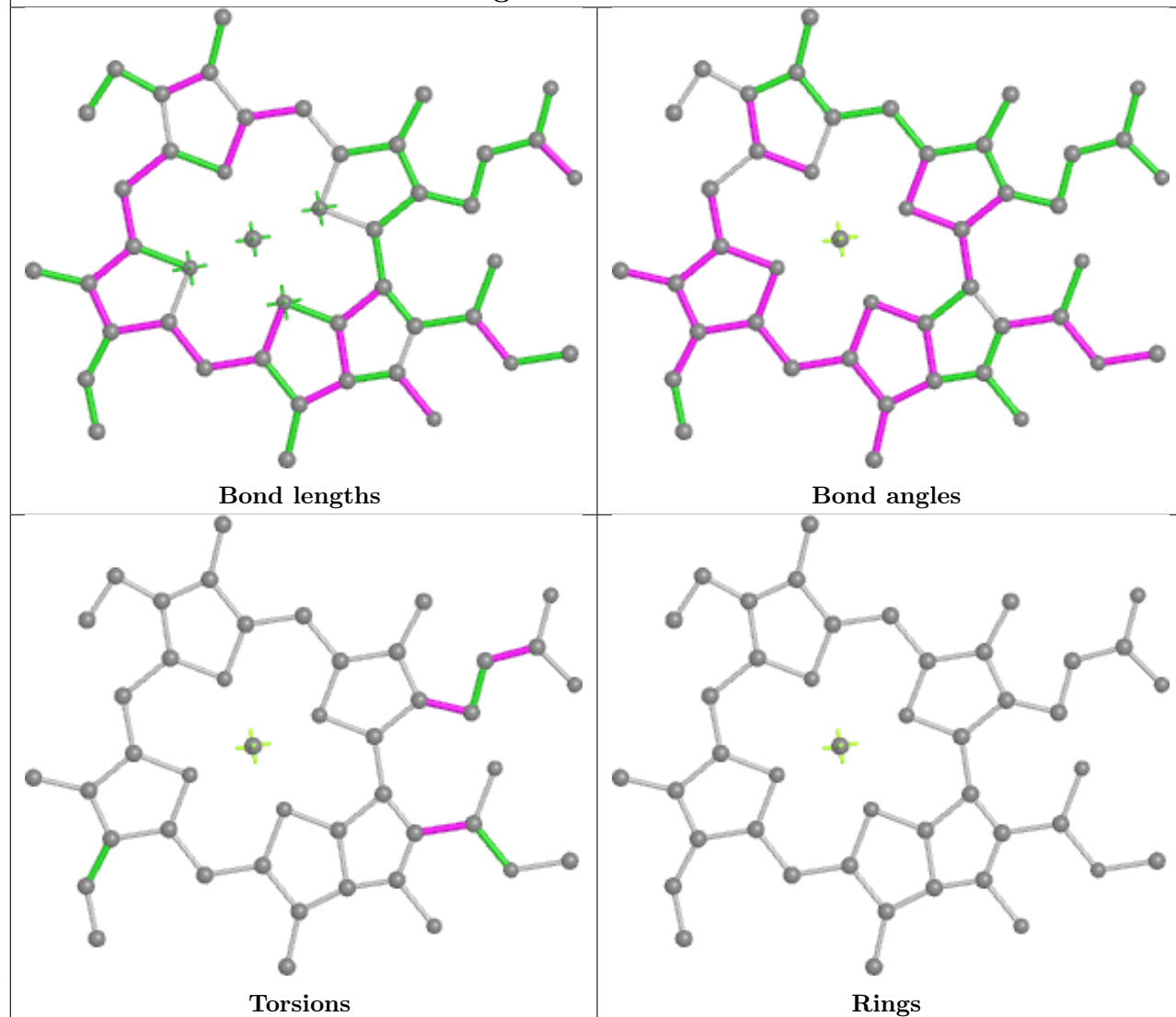
Ligand CLA 6 407



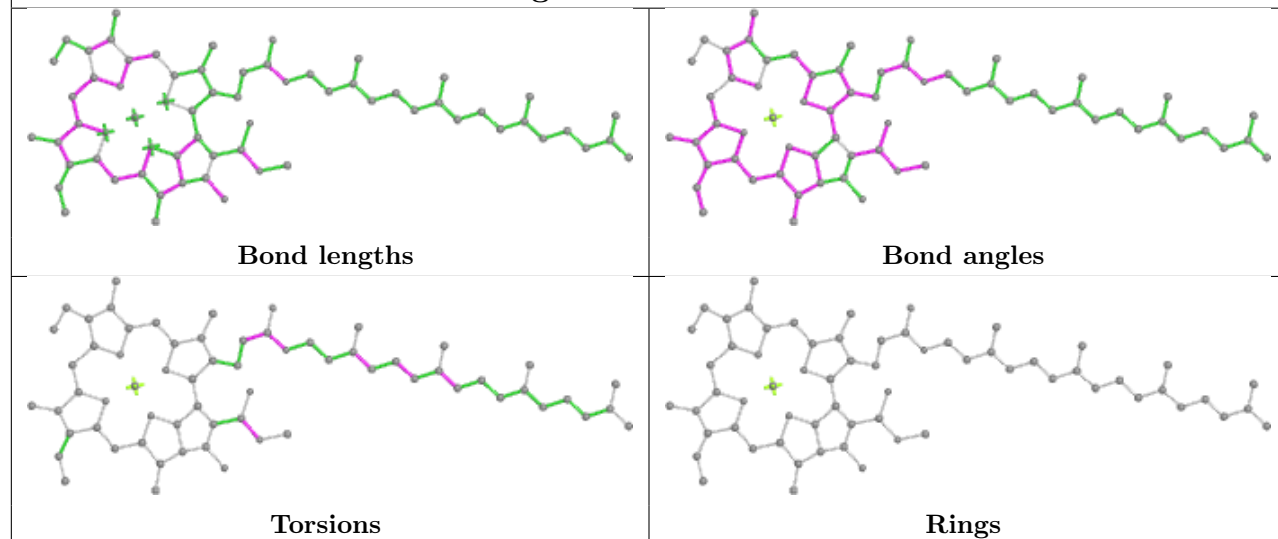
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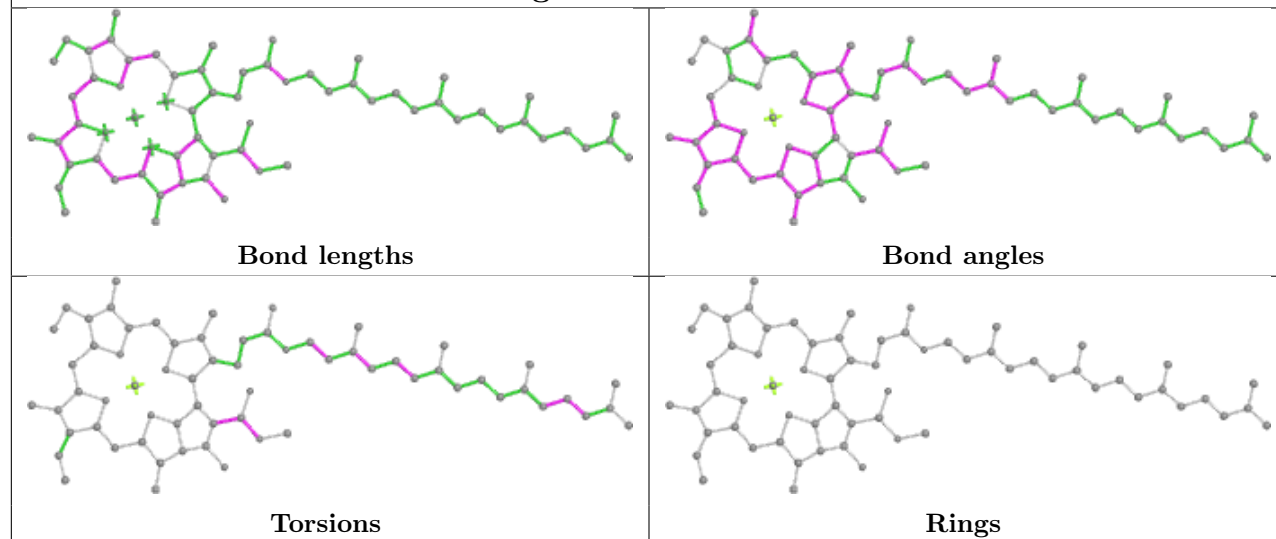
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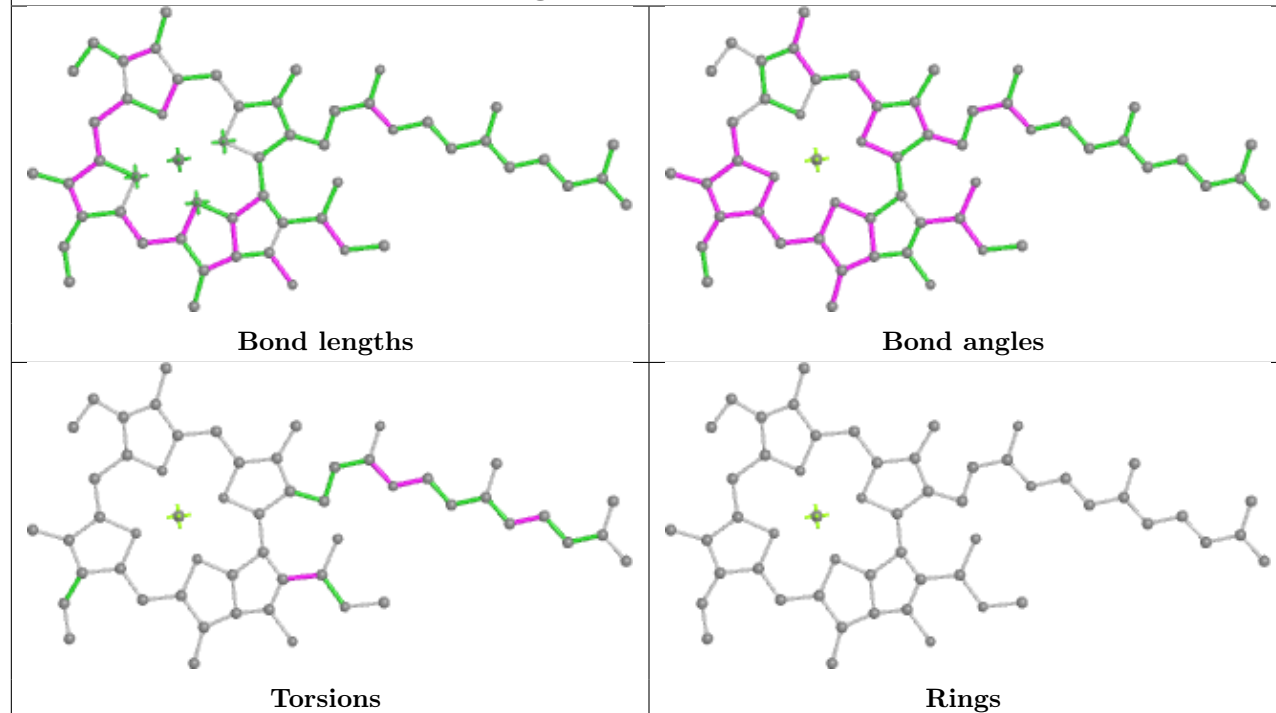
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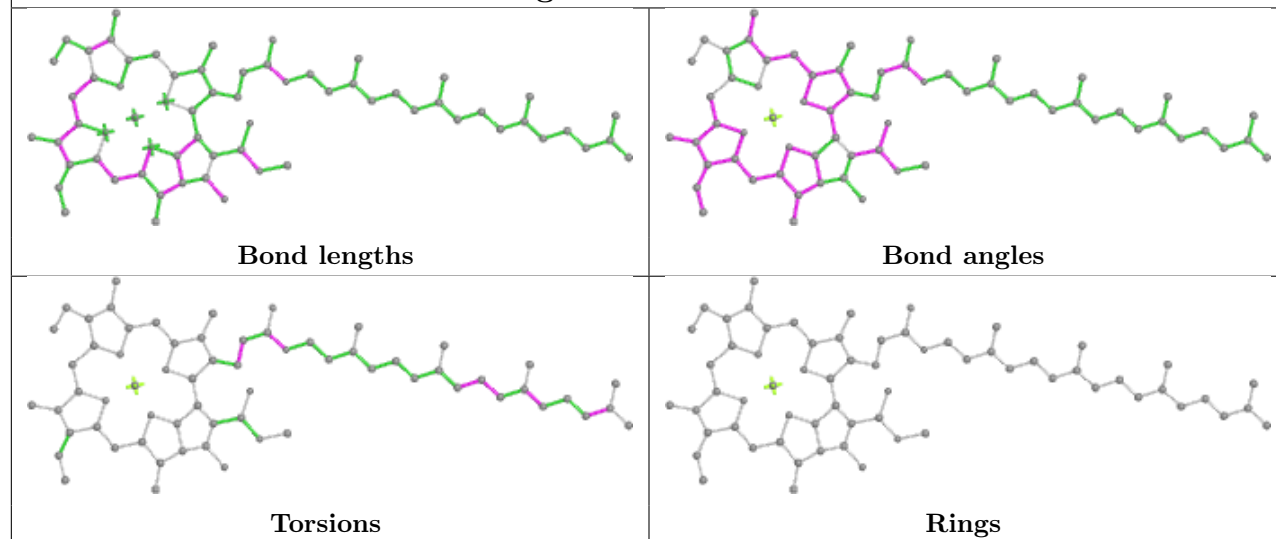
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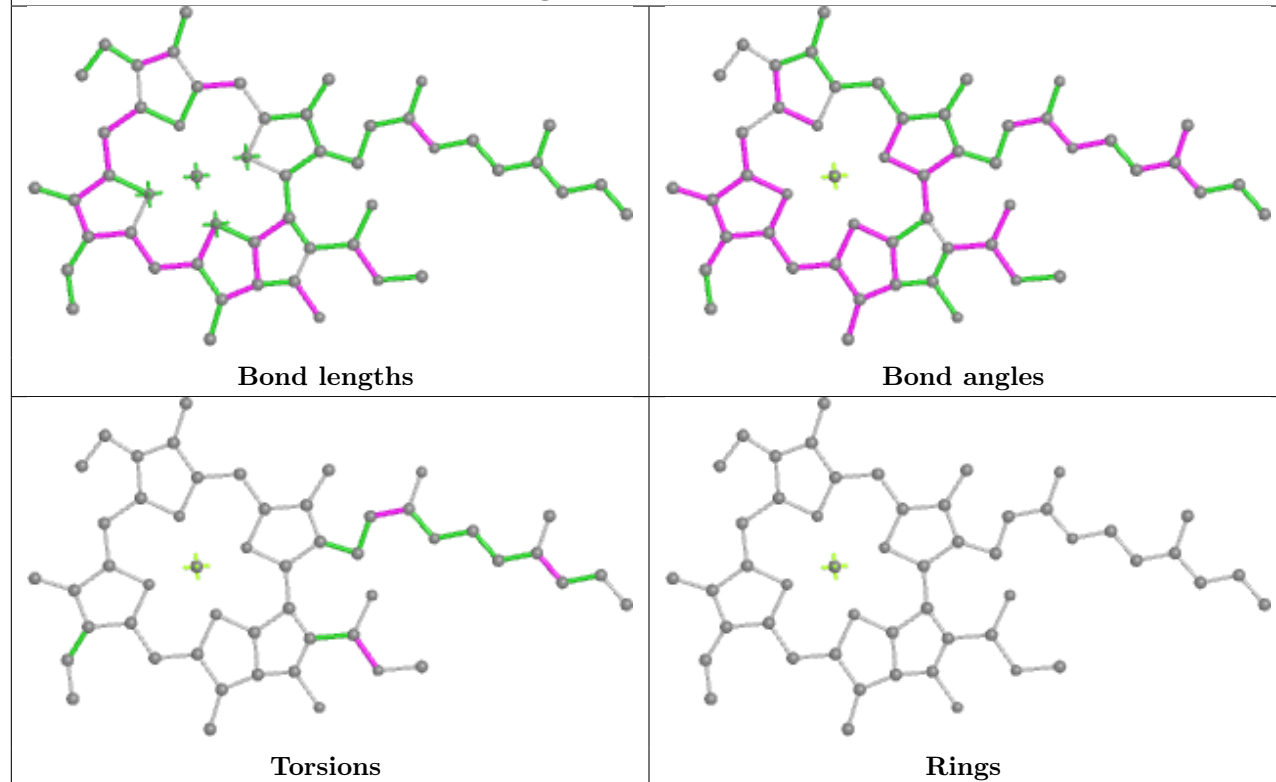
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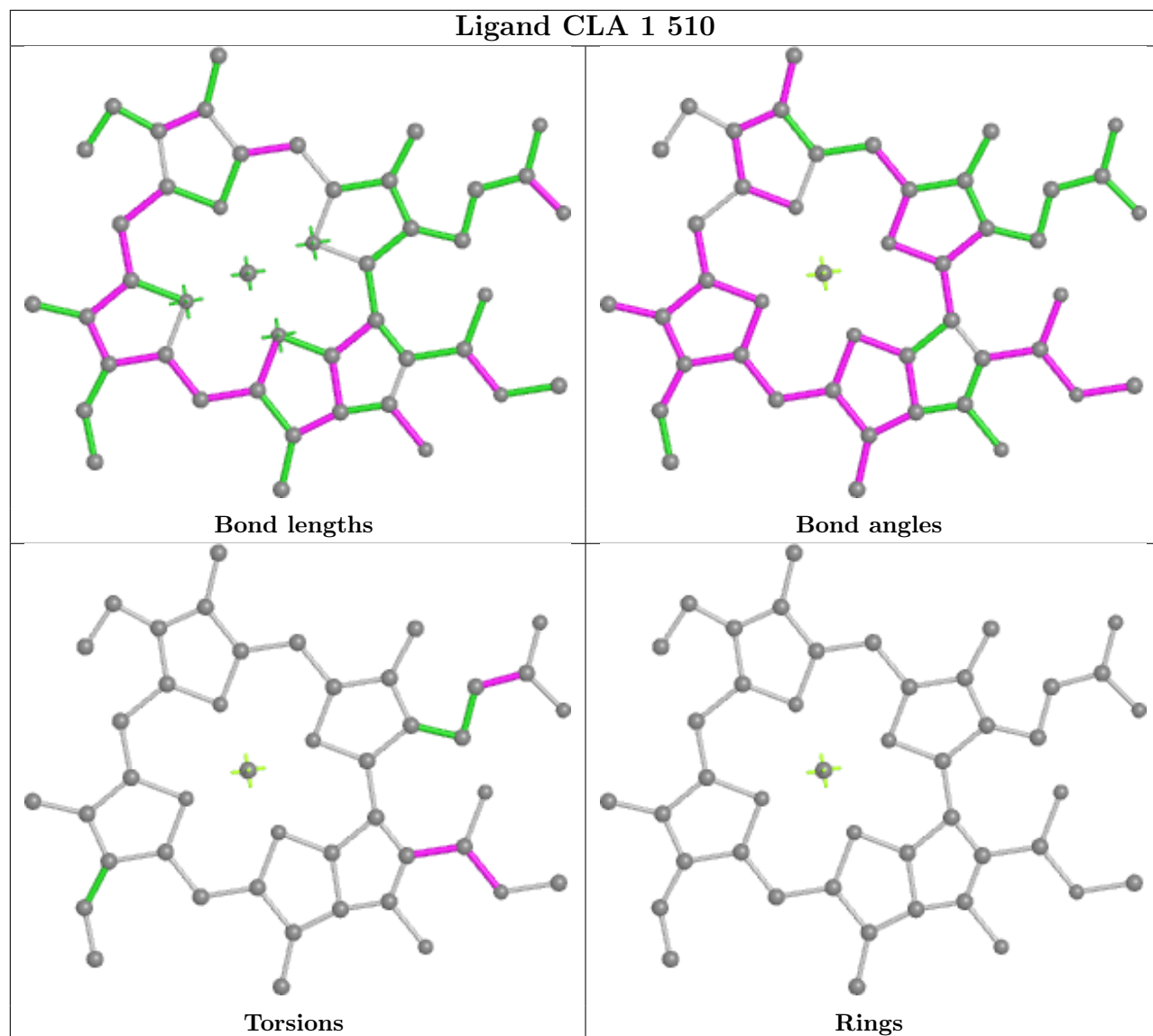
Ligand CLA 1 520



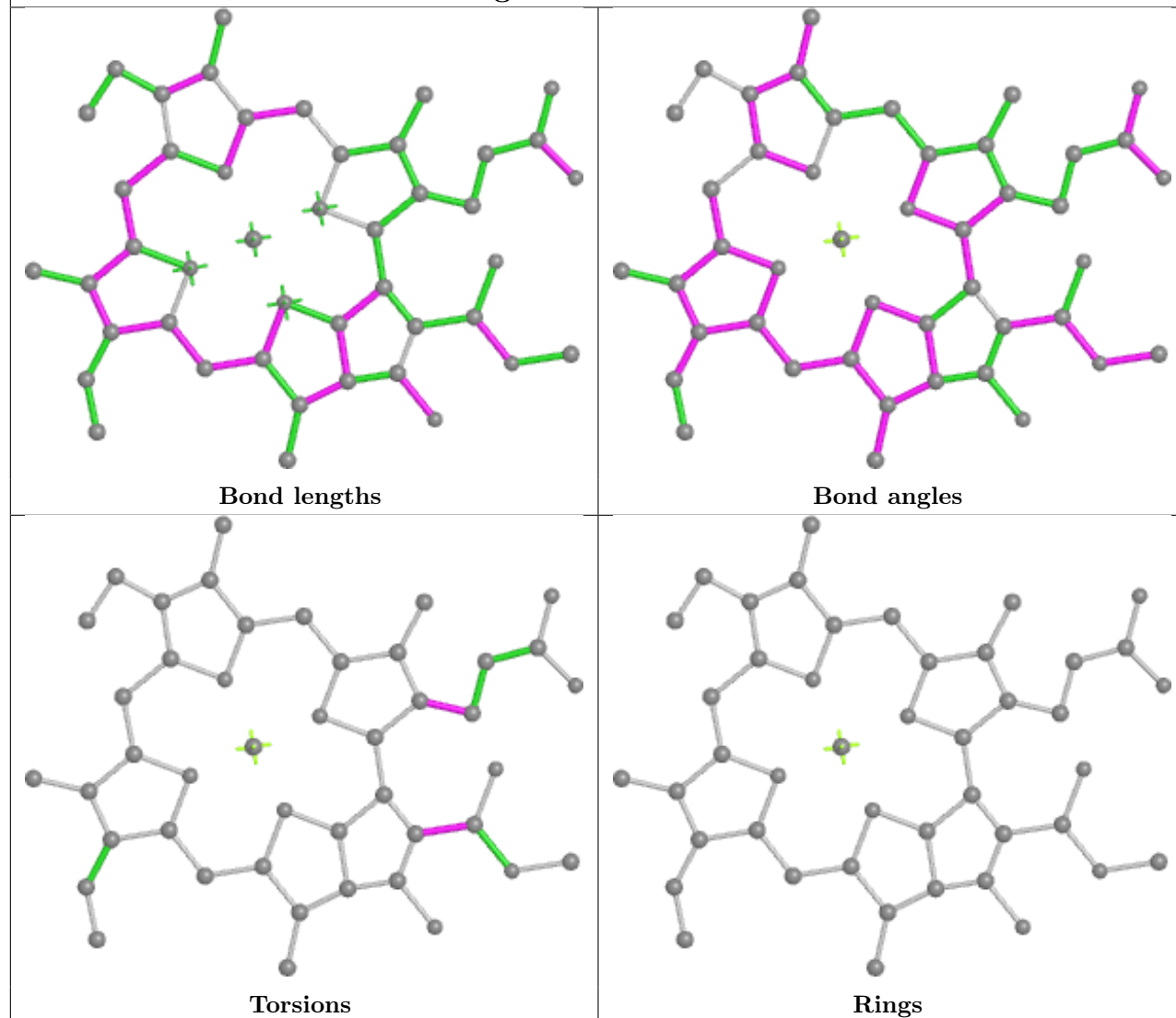
Ligand CLA 1 521



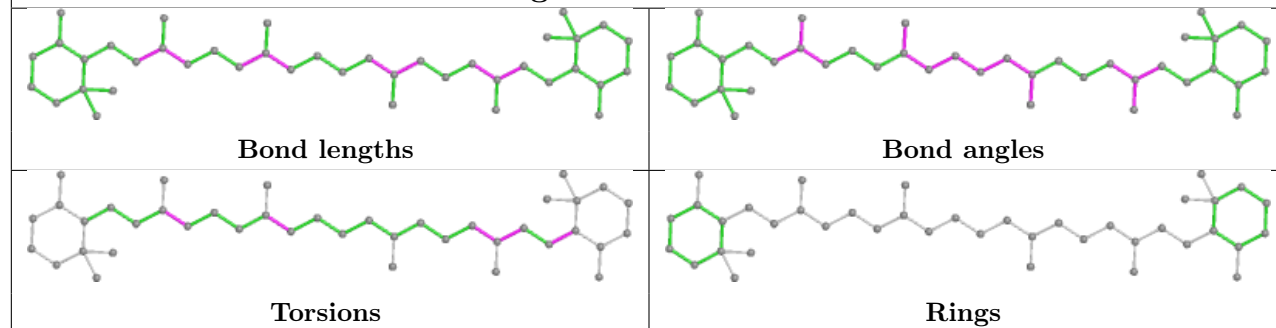
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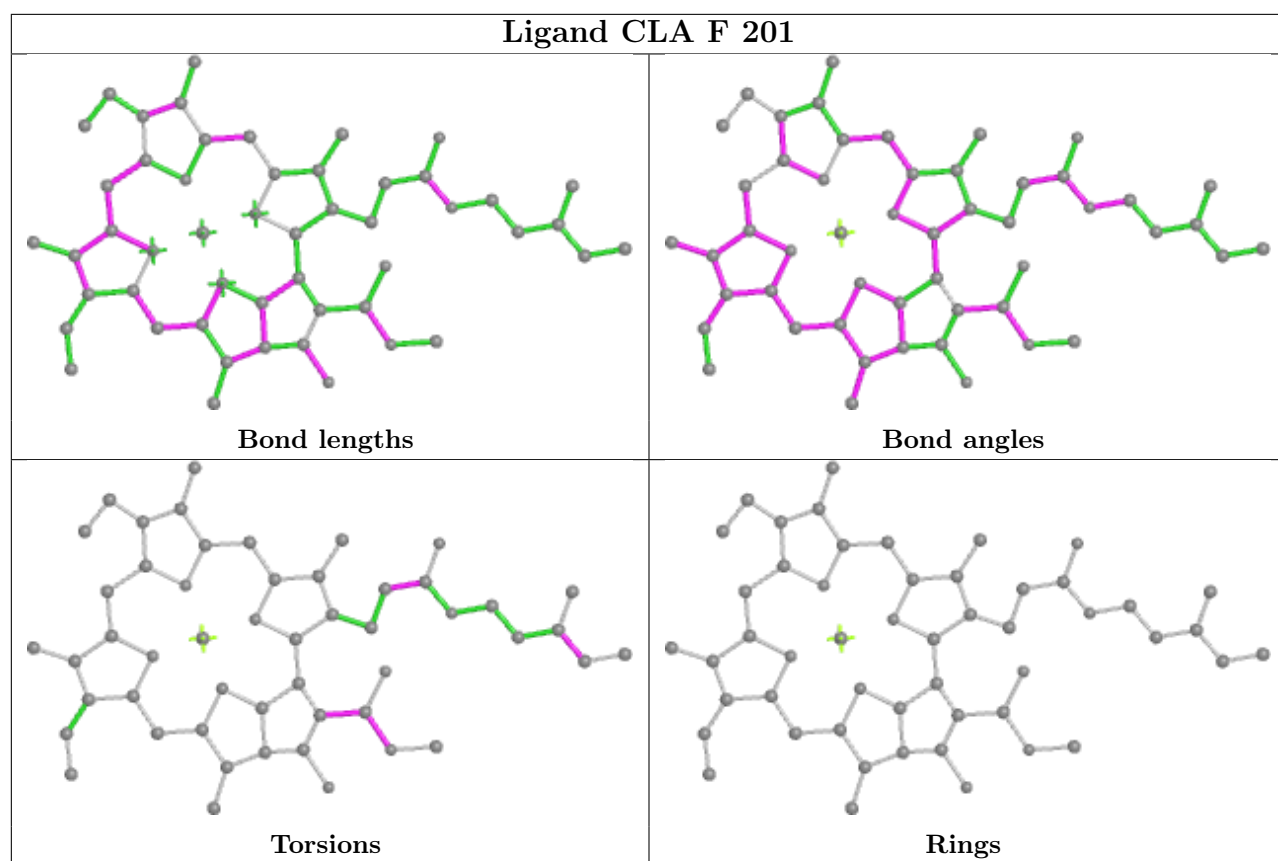


Ligand CLA 5 410

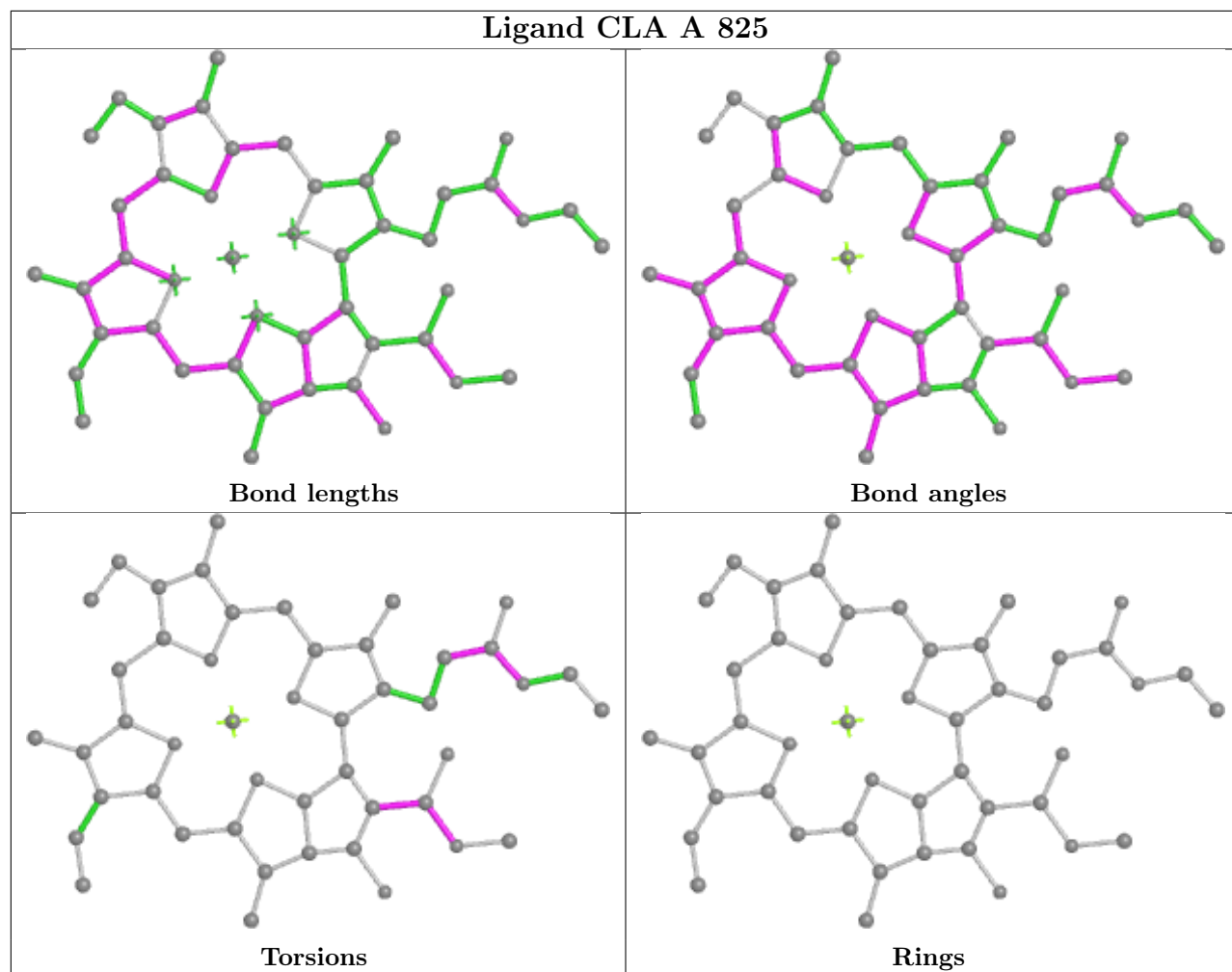


Ligand BCR B 845

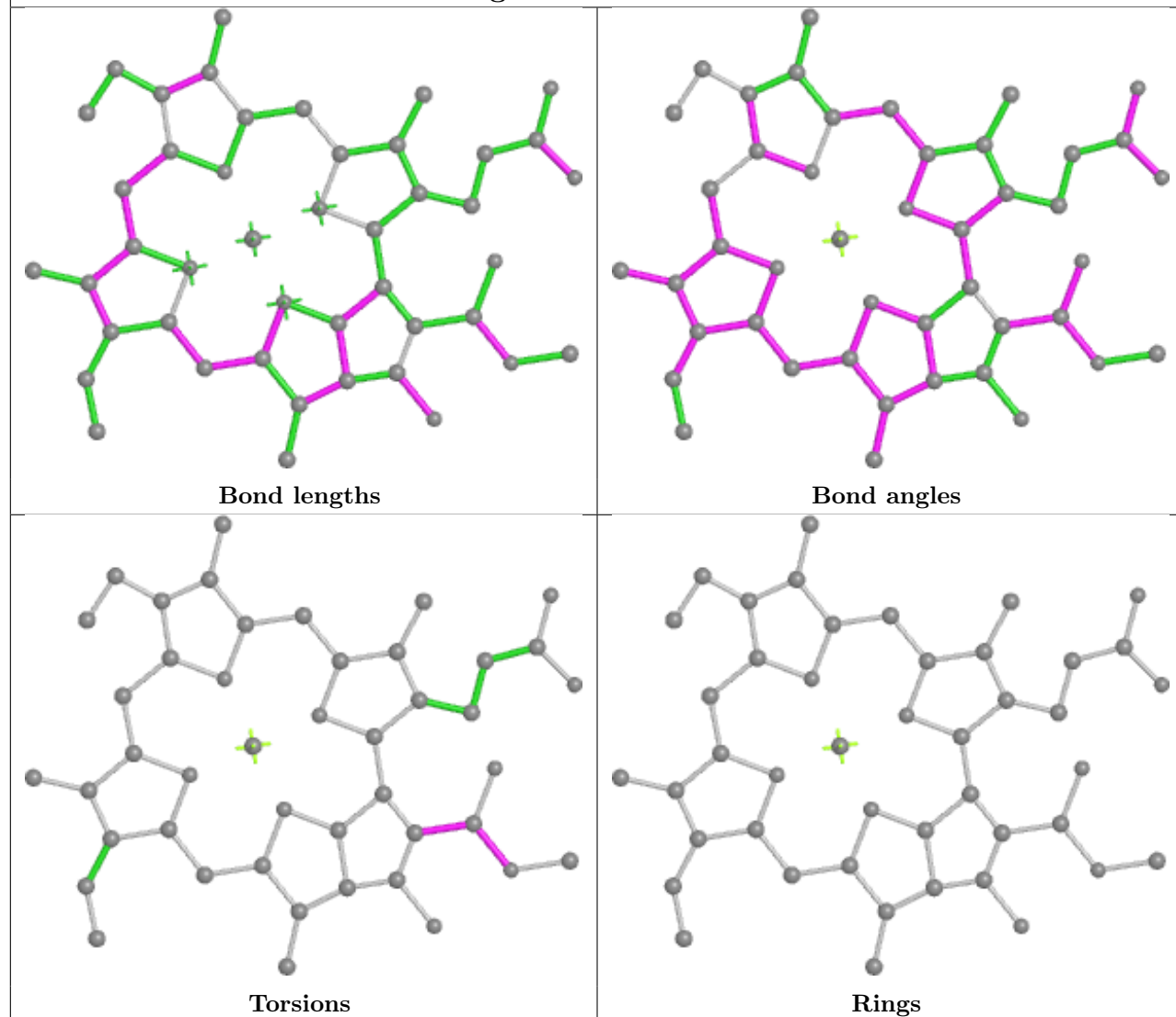




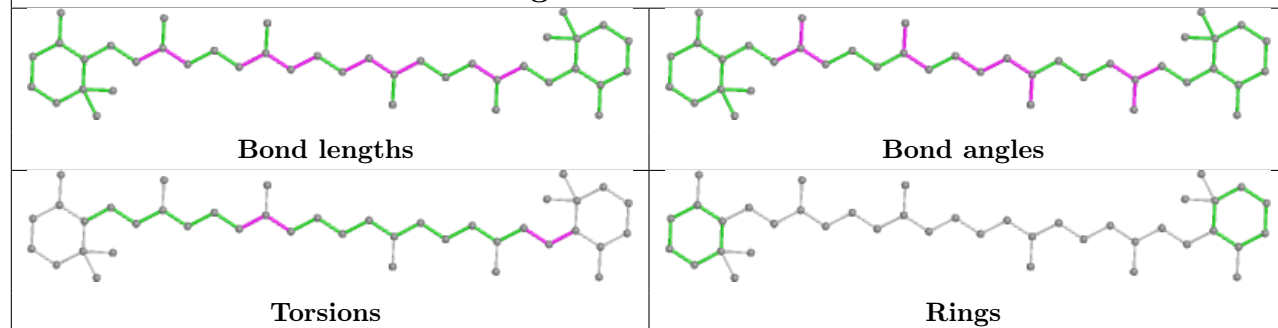
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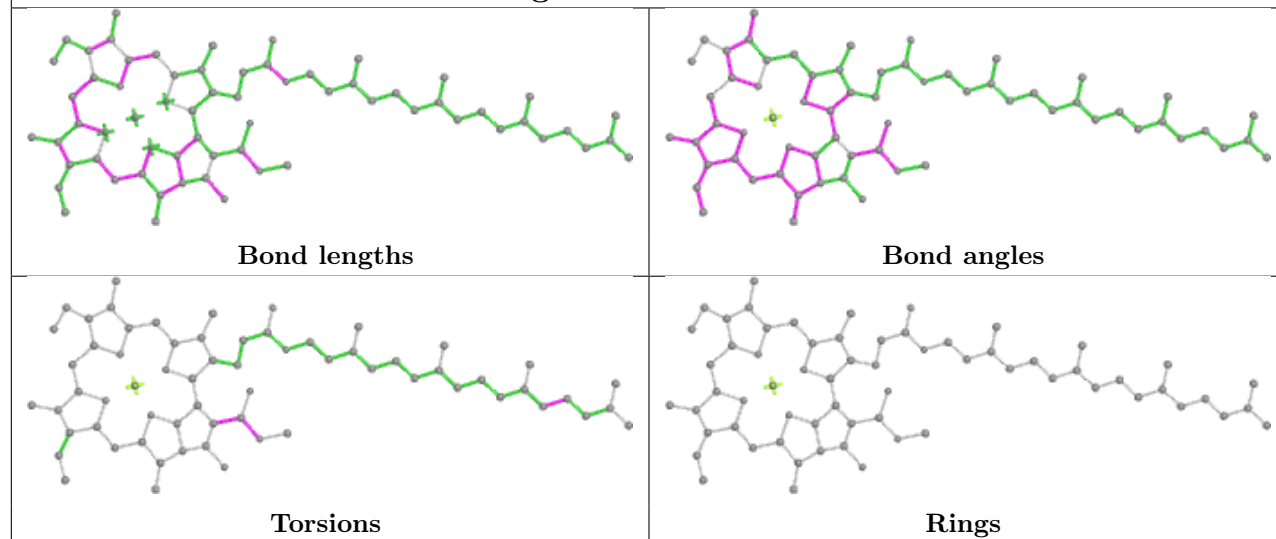
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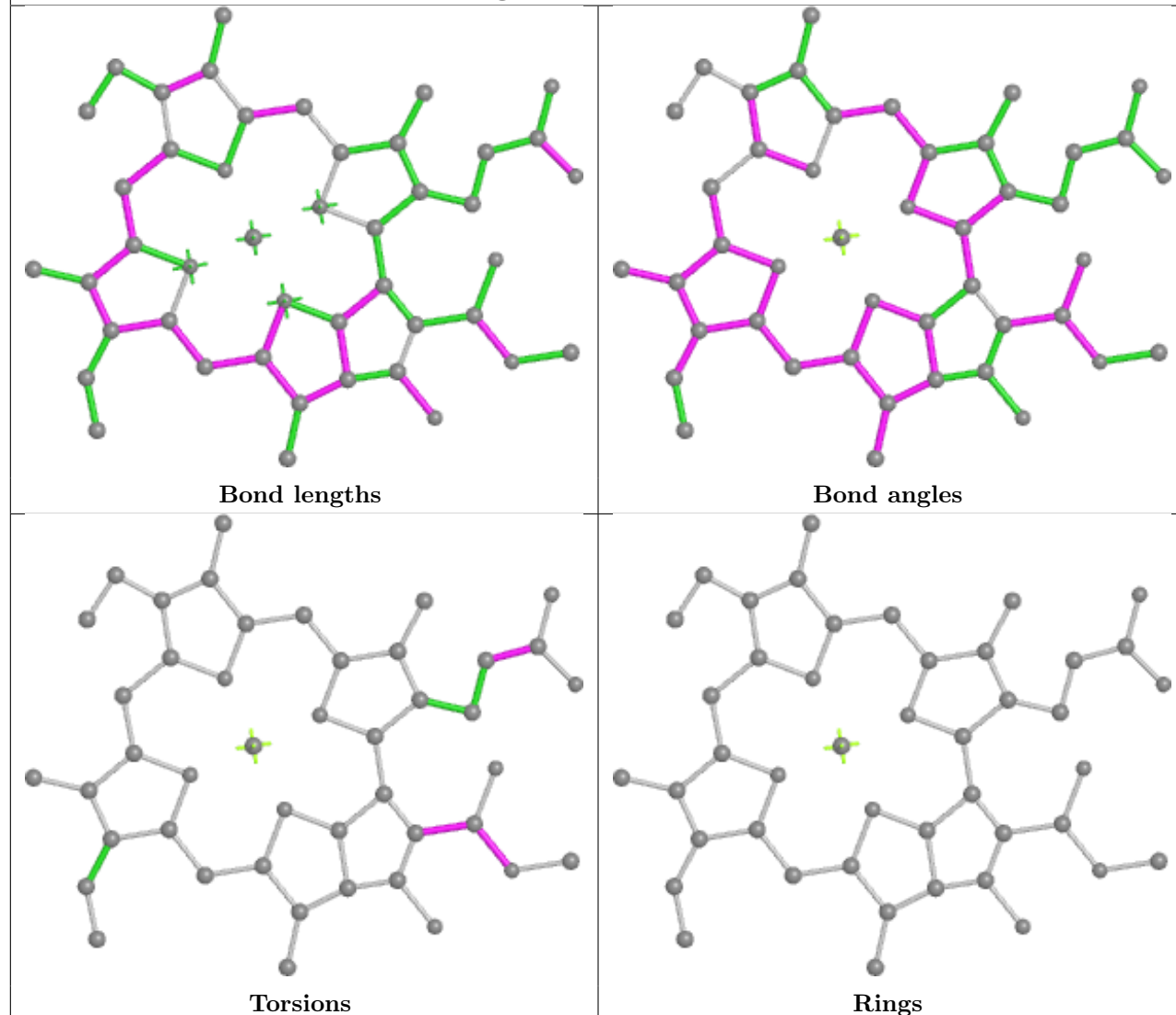
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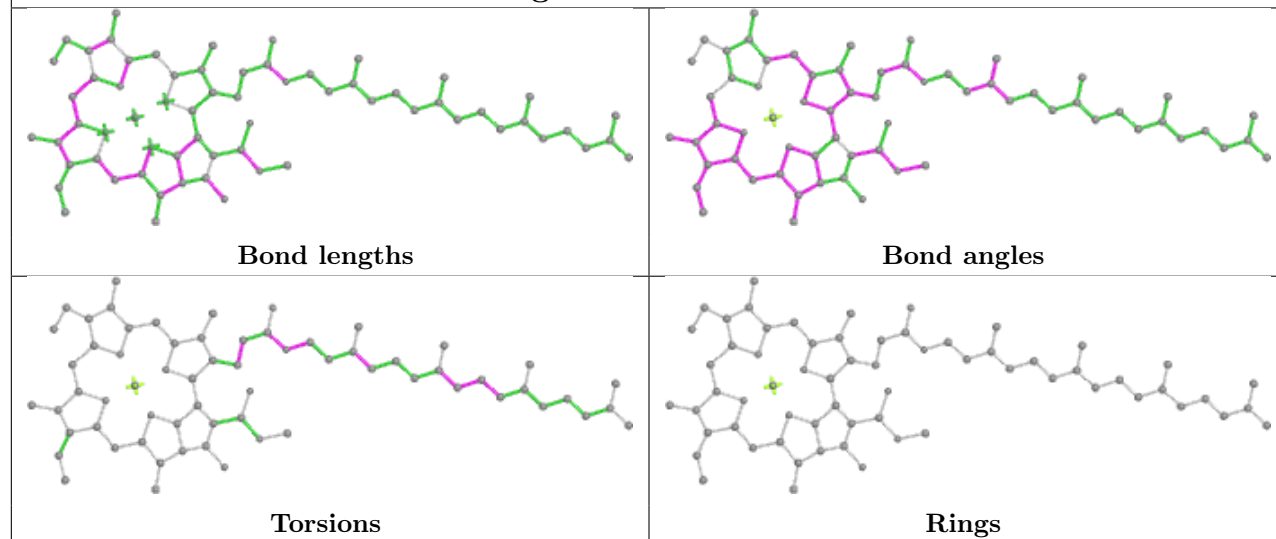
Ligand CLA A 831



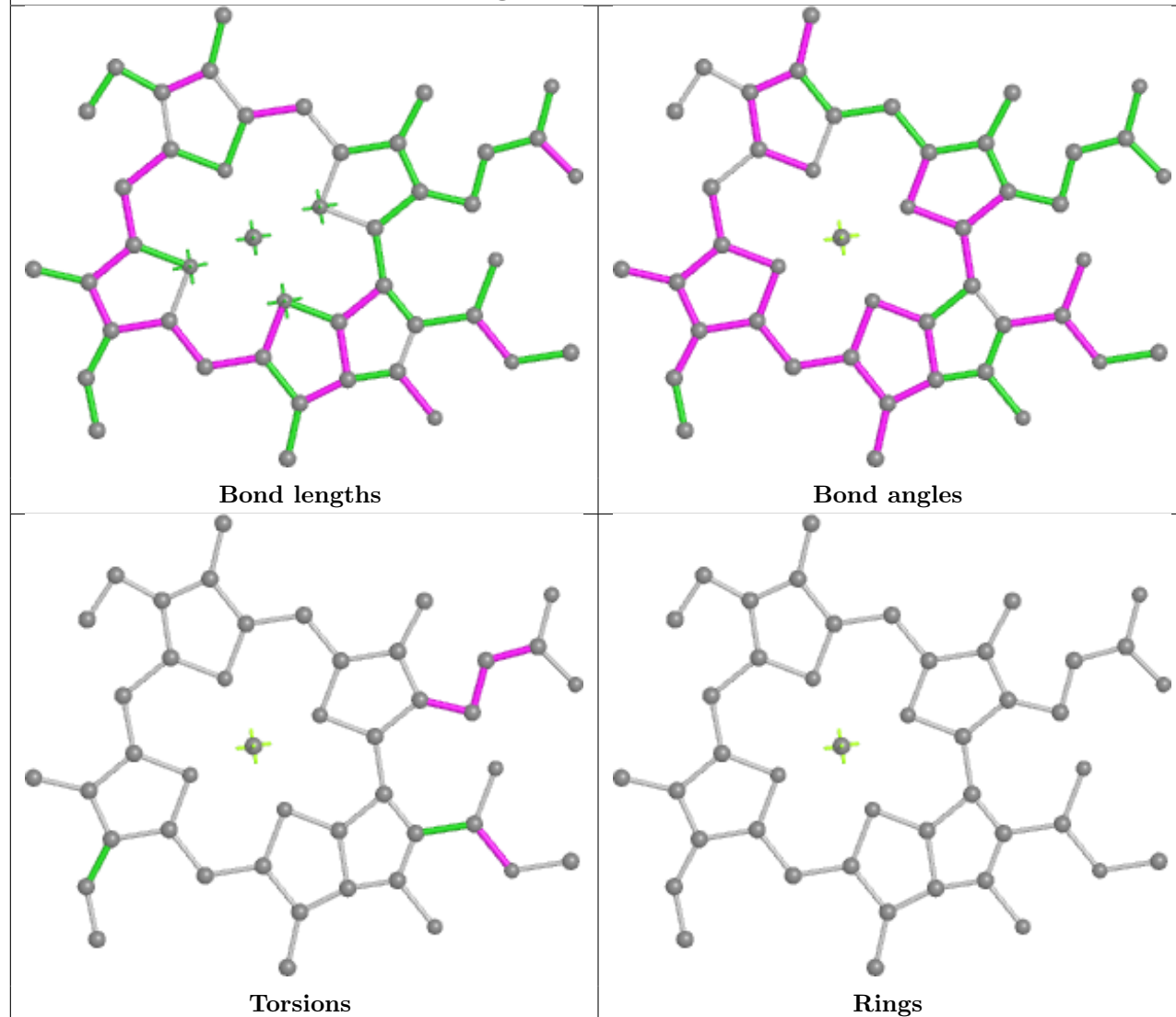
Ligand CLA 1 504



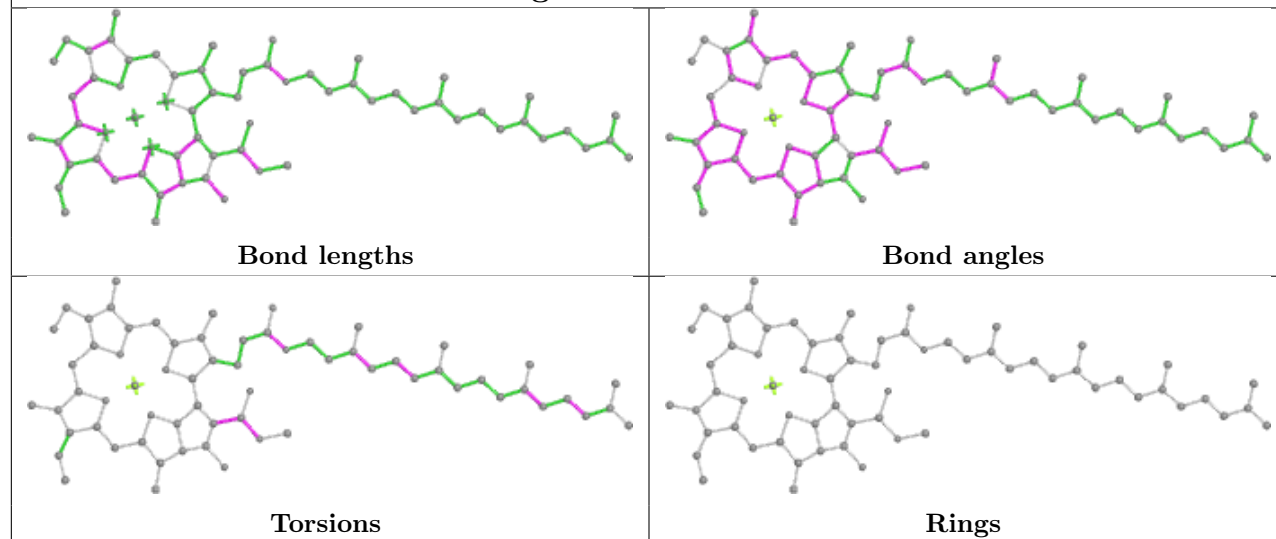
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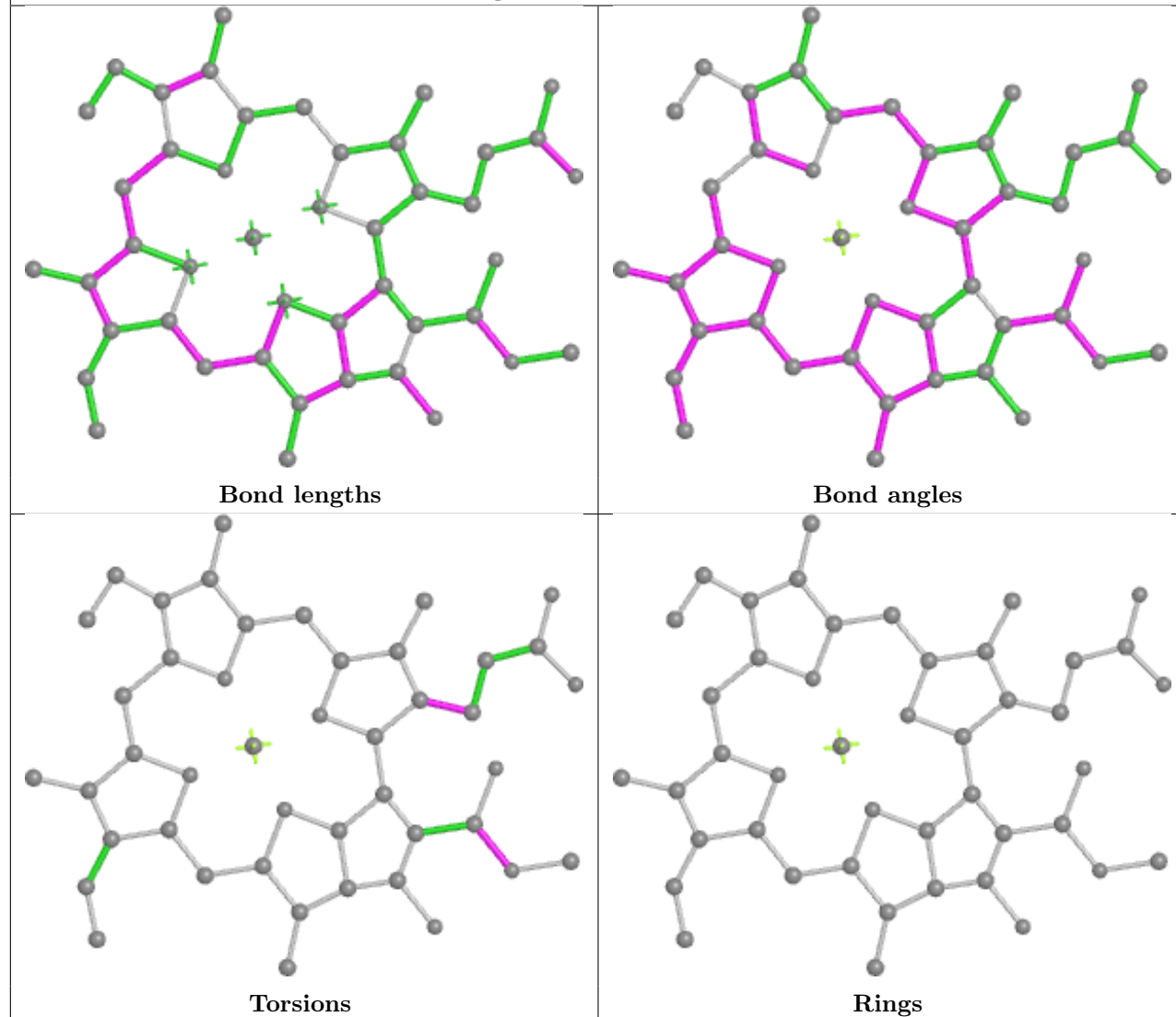
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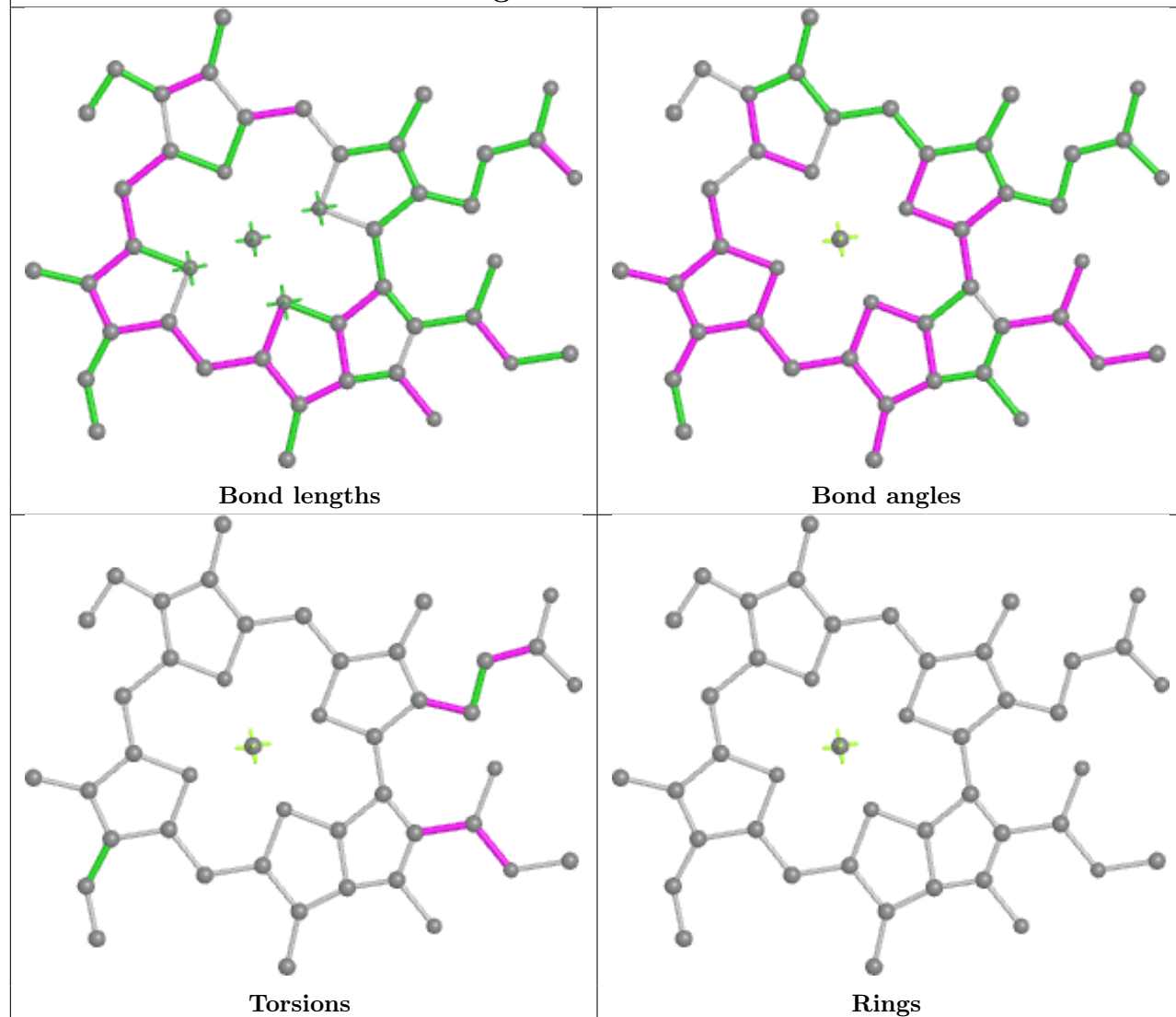
Ligand CLA A 835



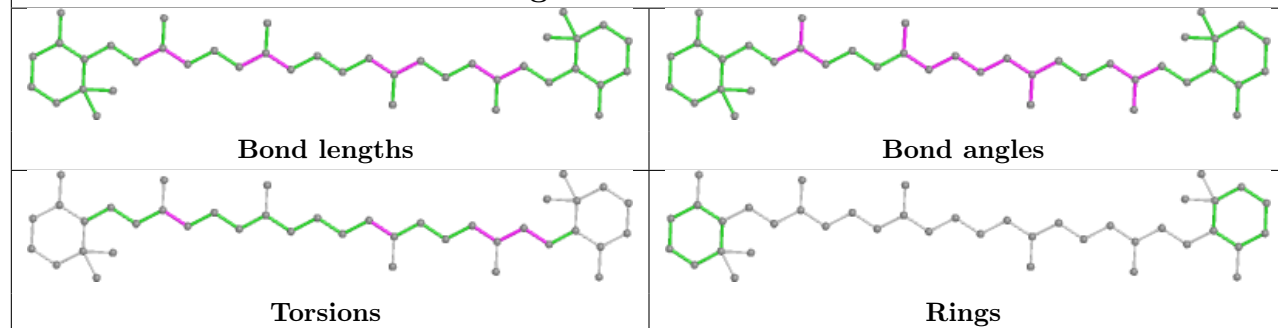
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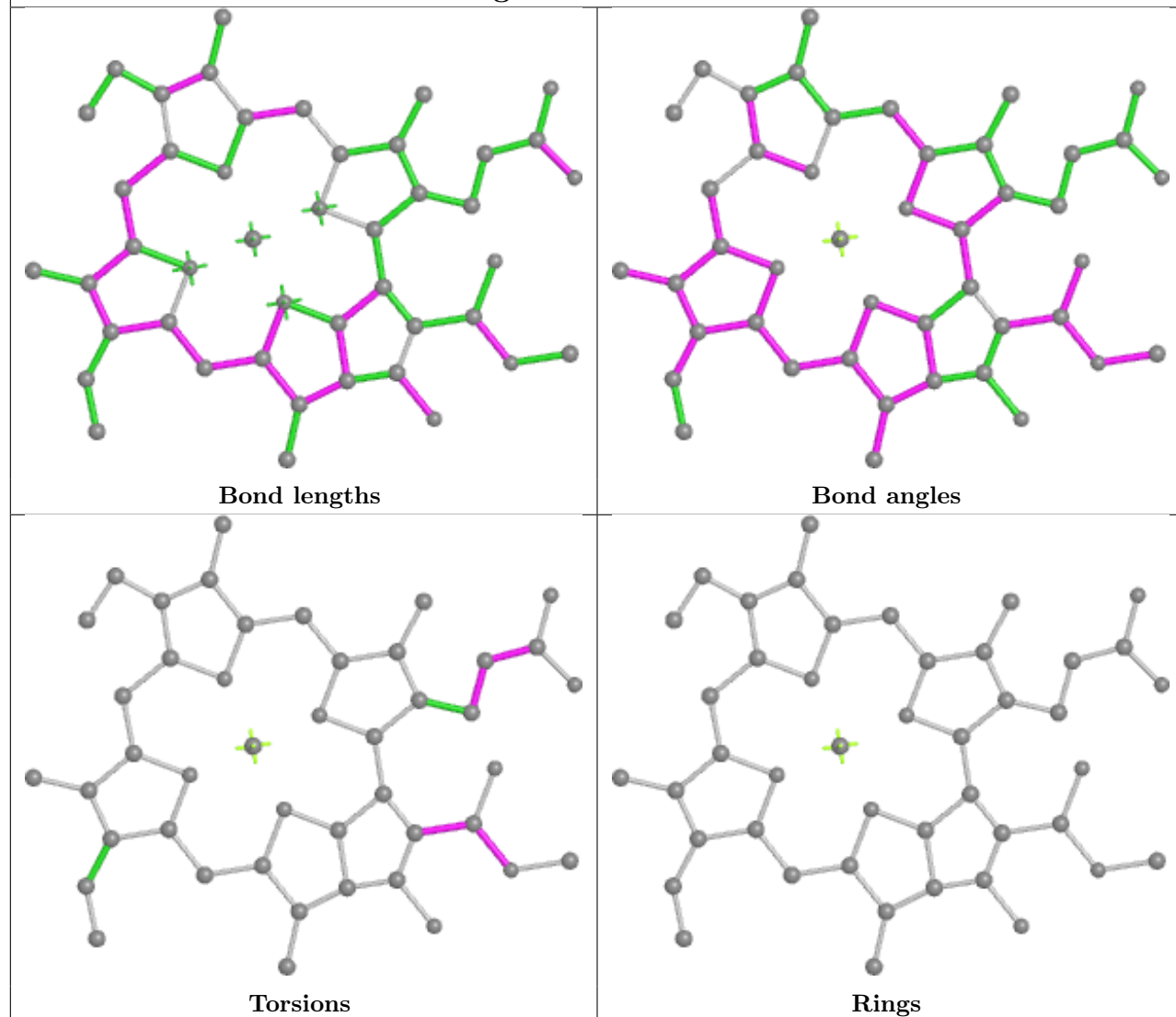
Ligand CLA 6 402



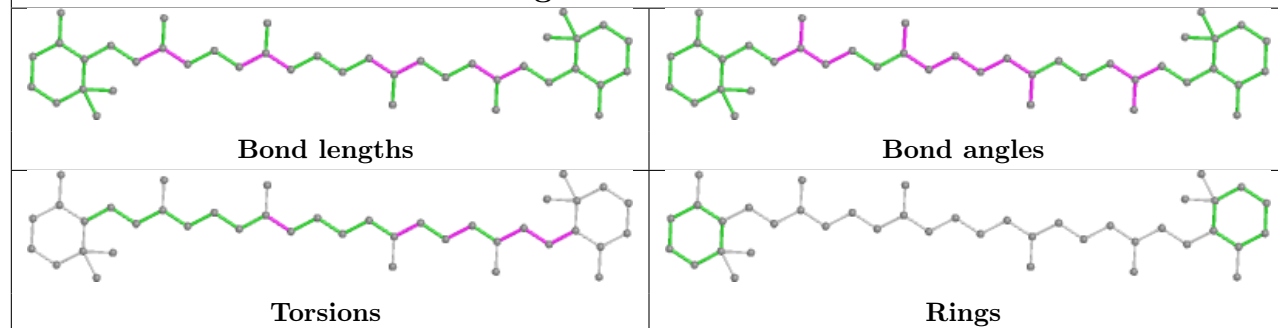
Ligand BCR A 851



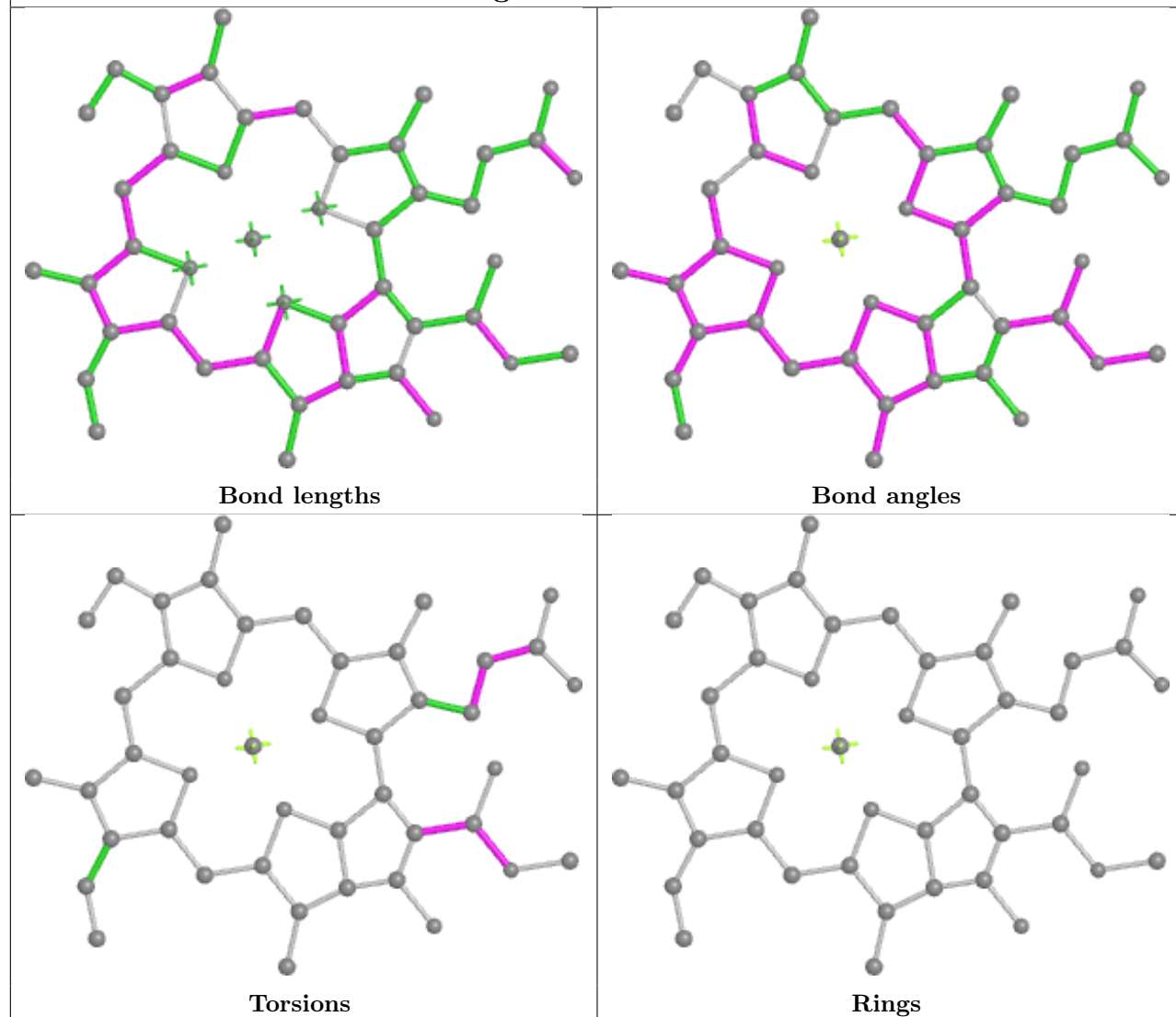
Ligand CLA 5 418



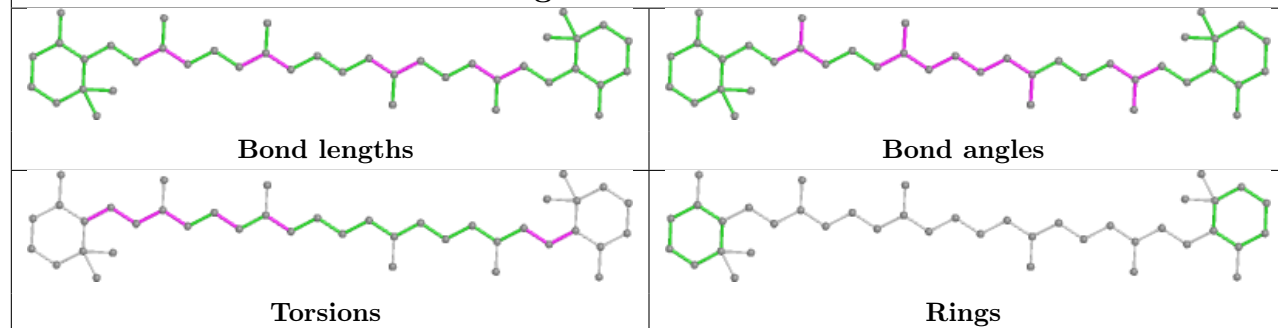
Ligand BCR 5 420



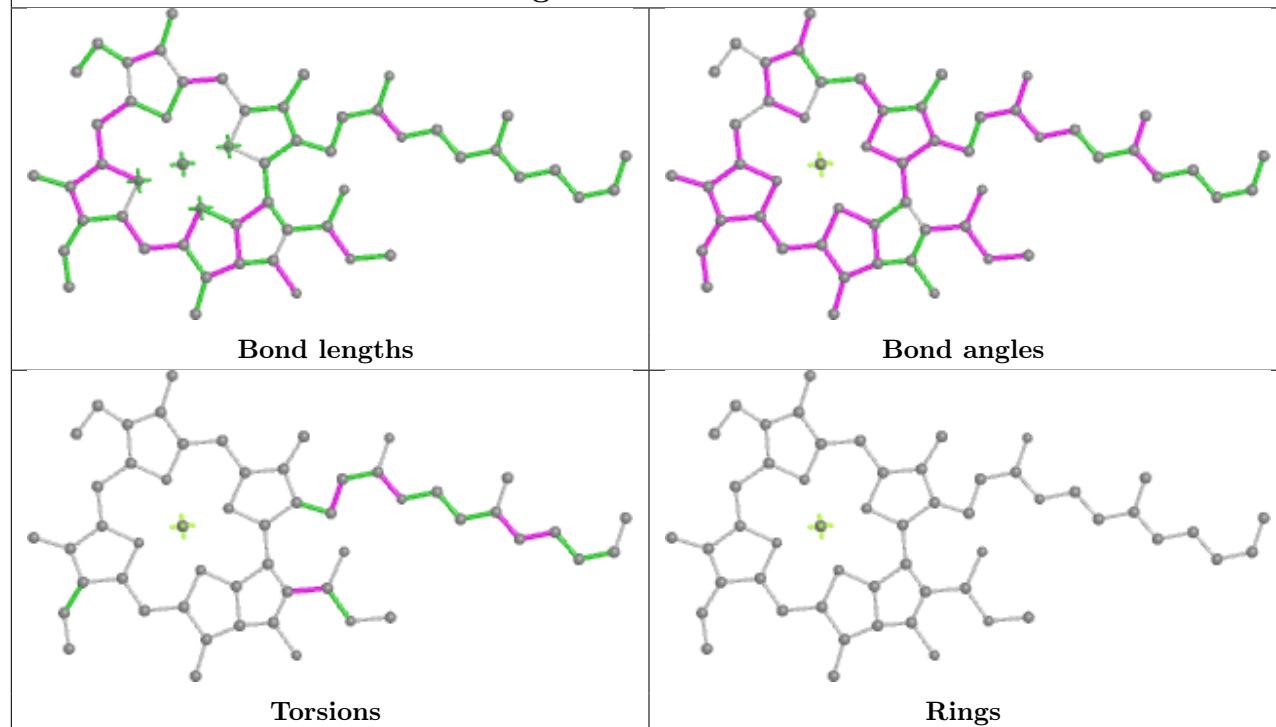
Ligand CLA 1 506



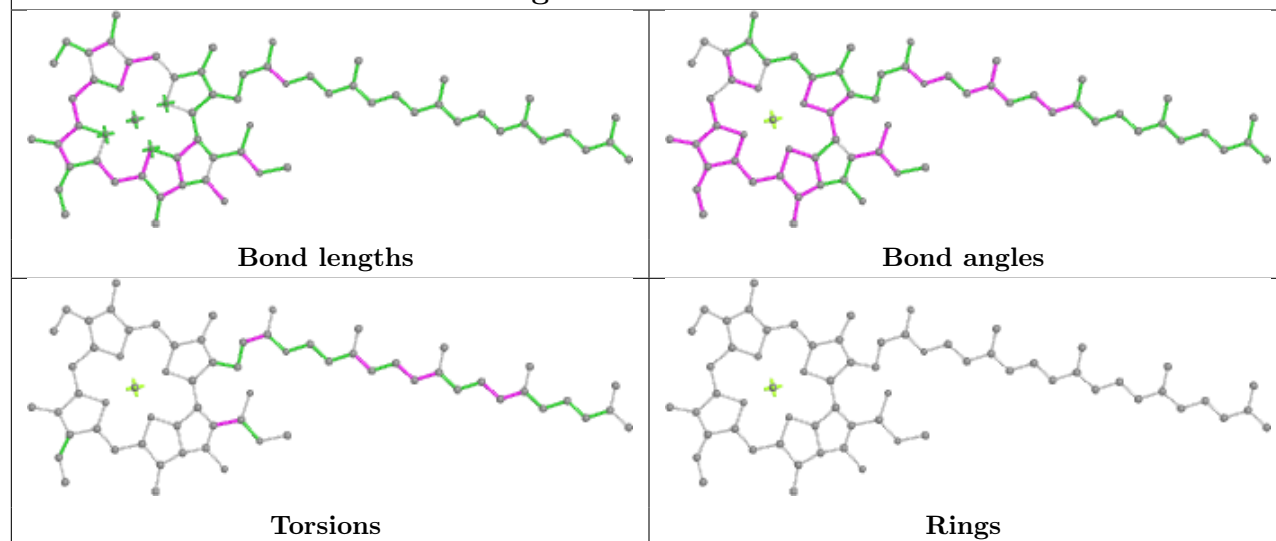
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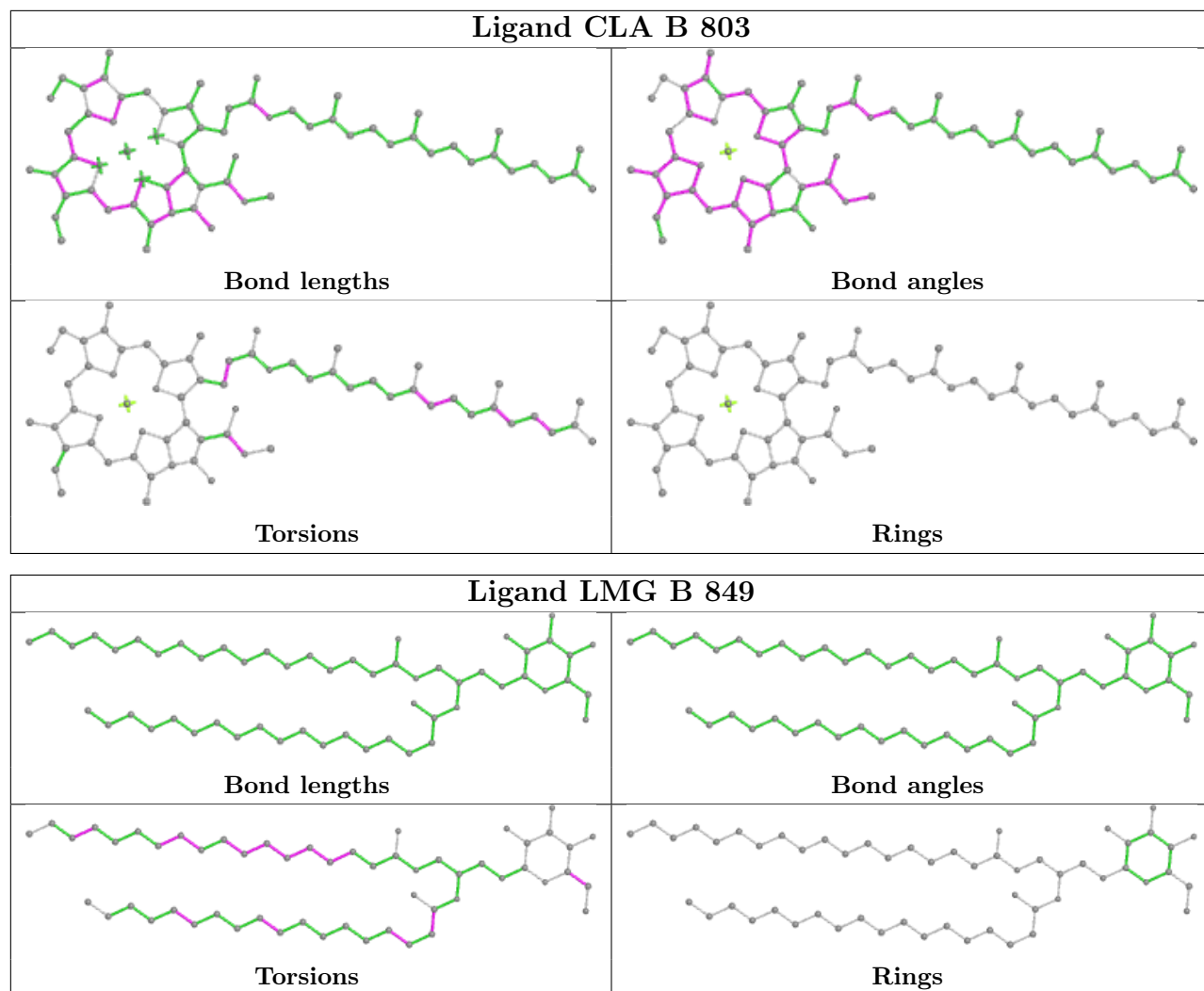


Ligand CLA B 804

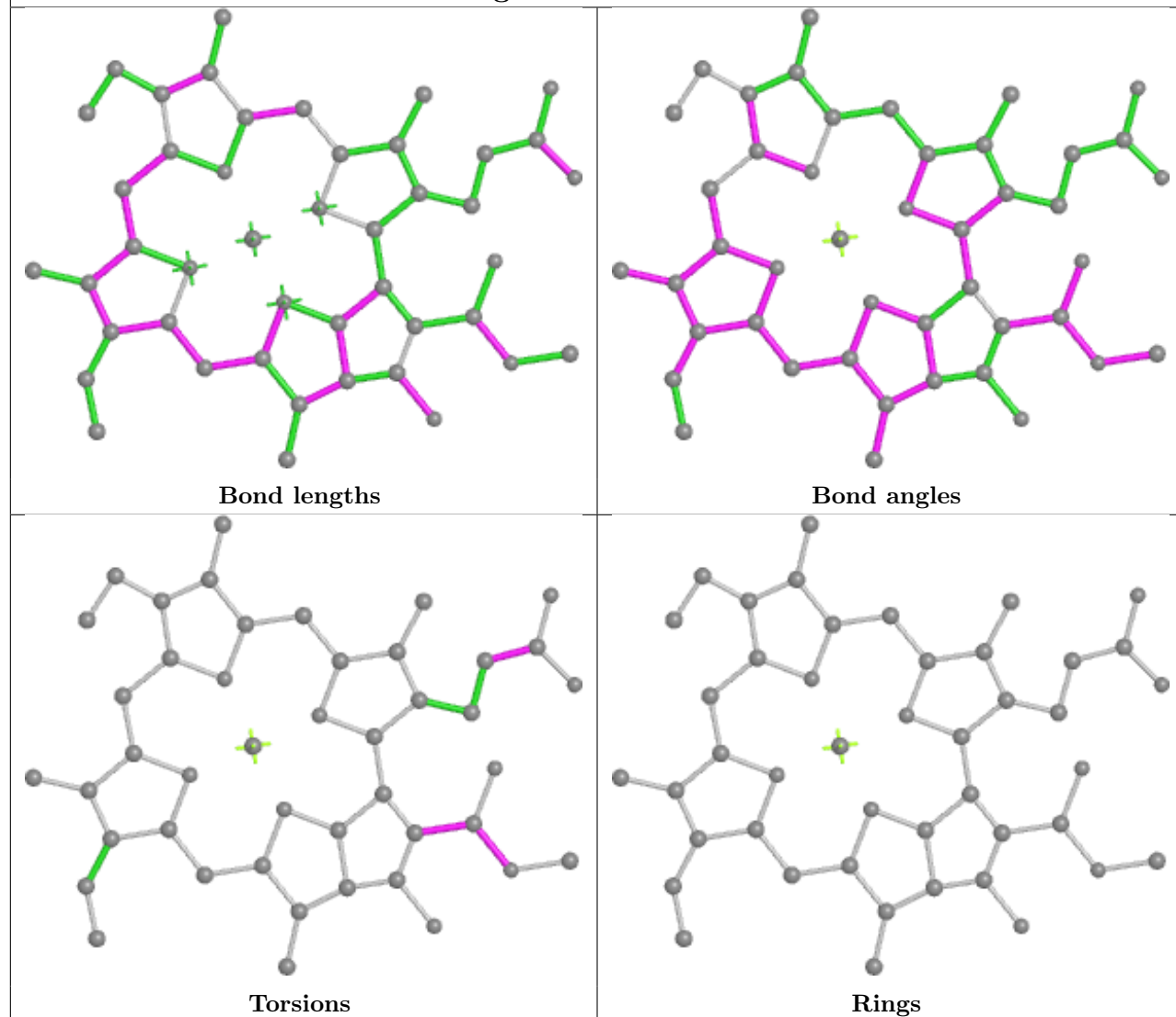


Ligand CLA A 839

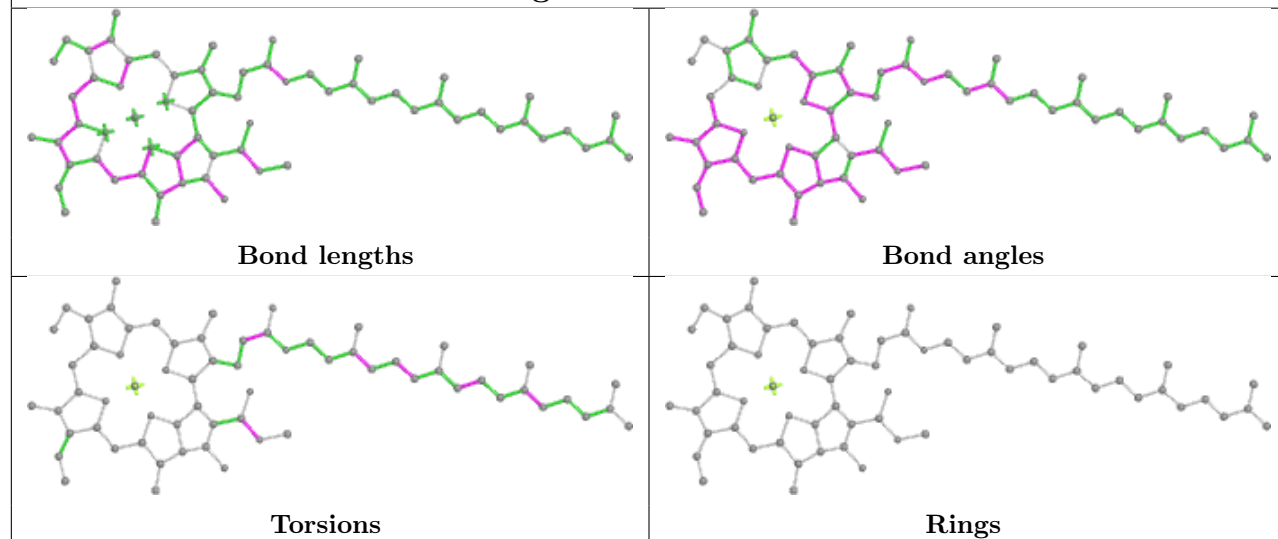




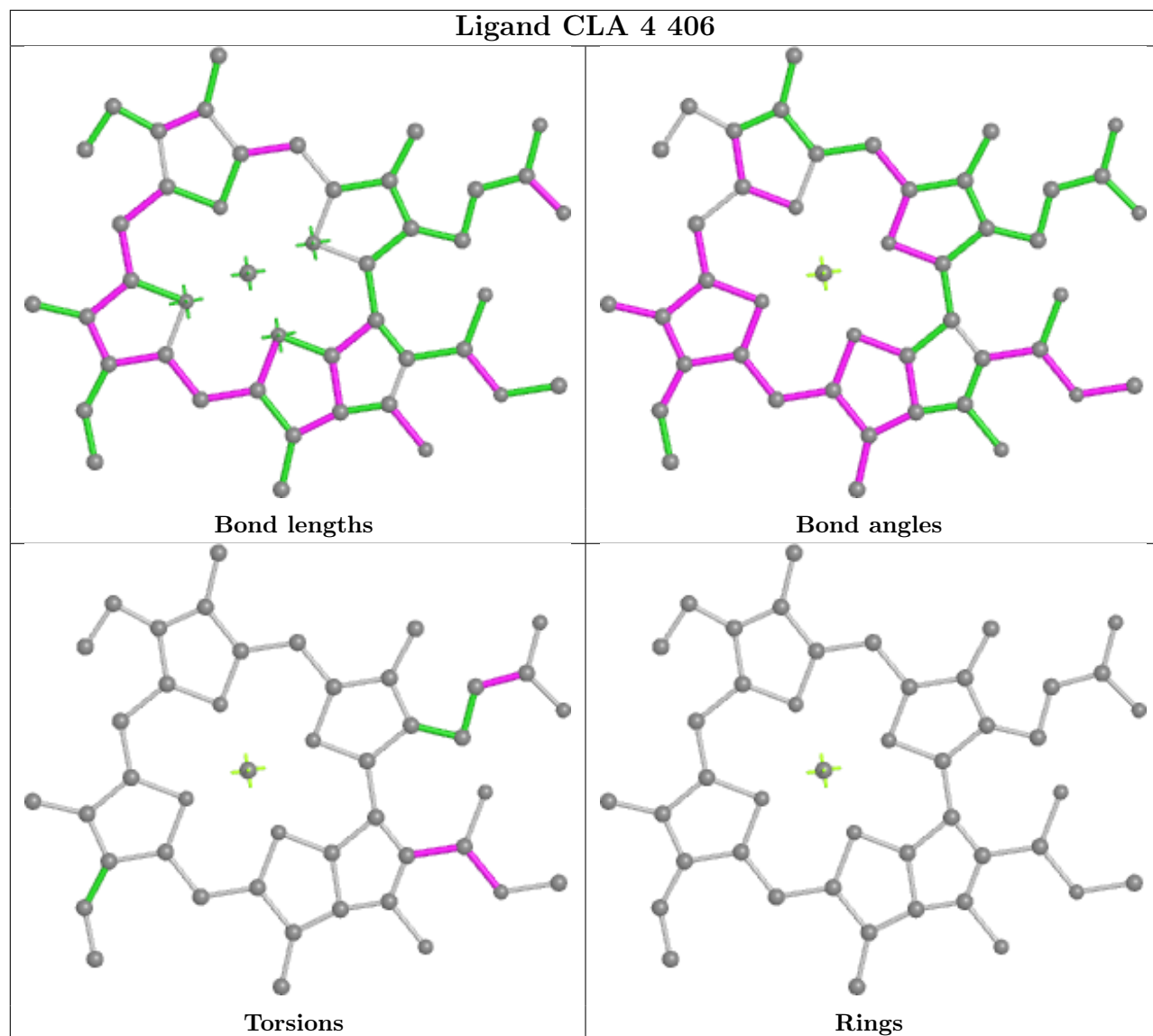
Ligand CLA 4 403



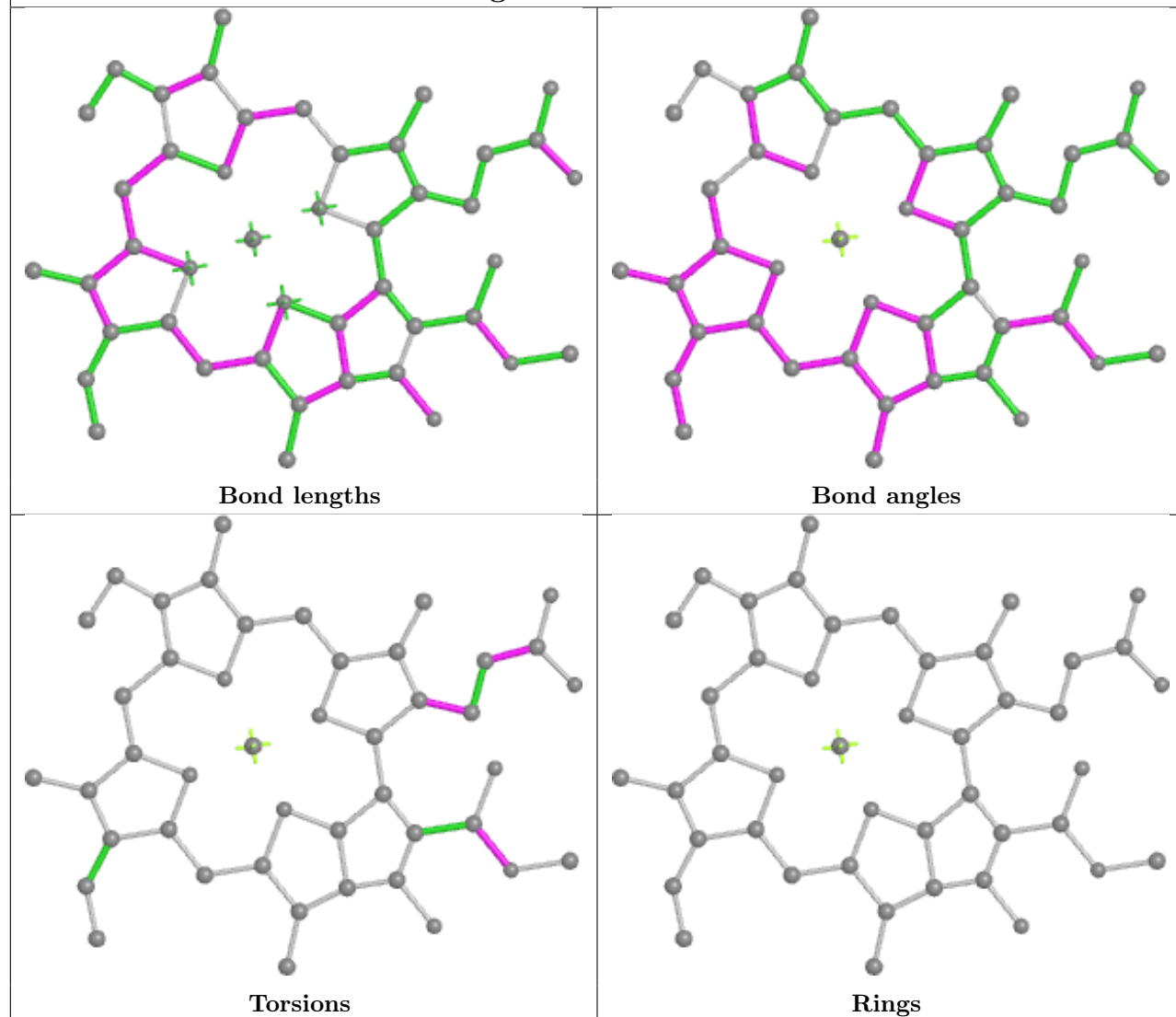
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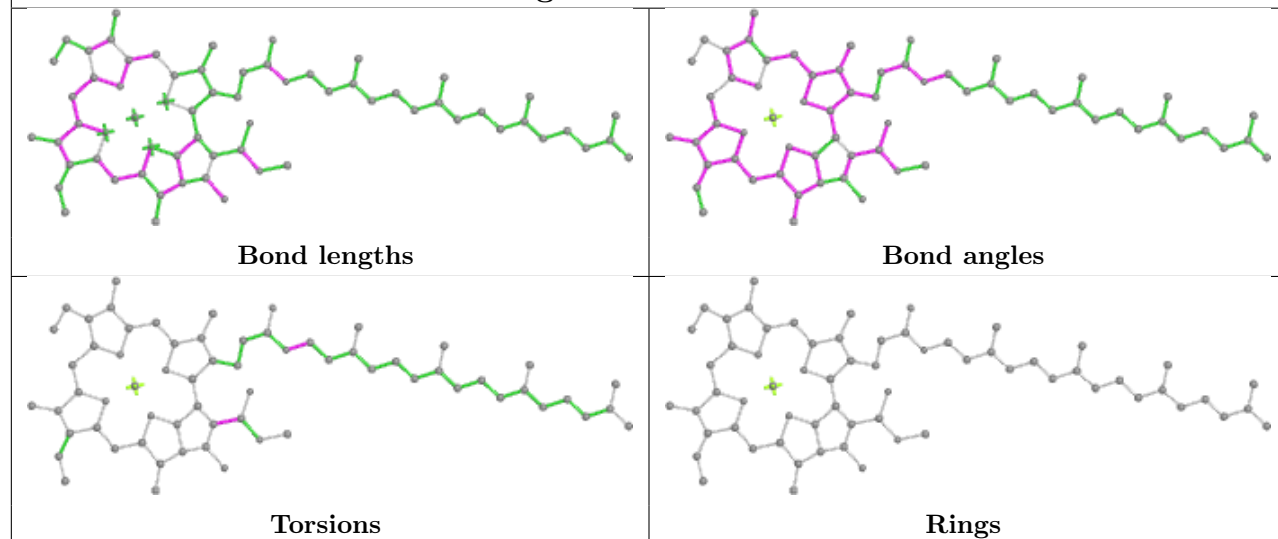
Ligand CLA 4 406



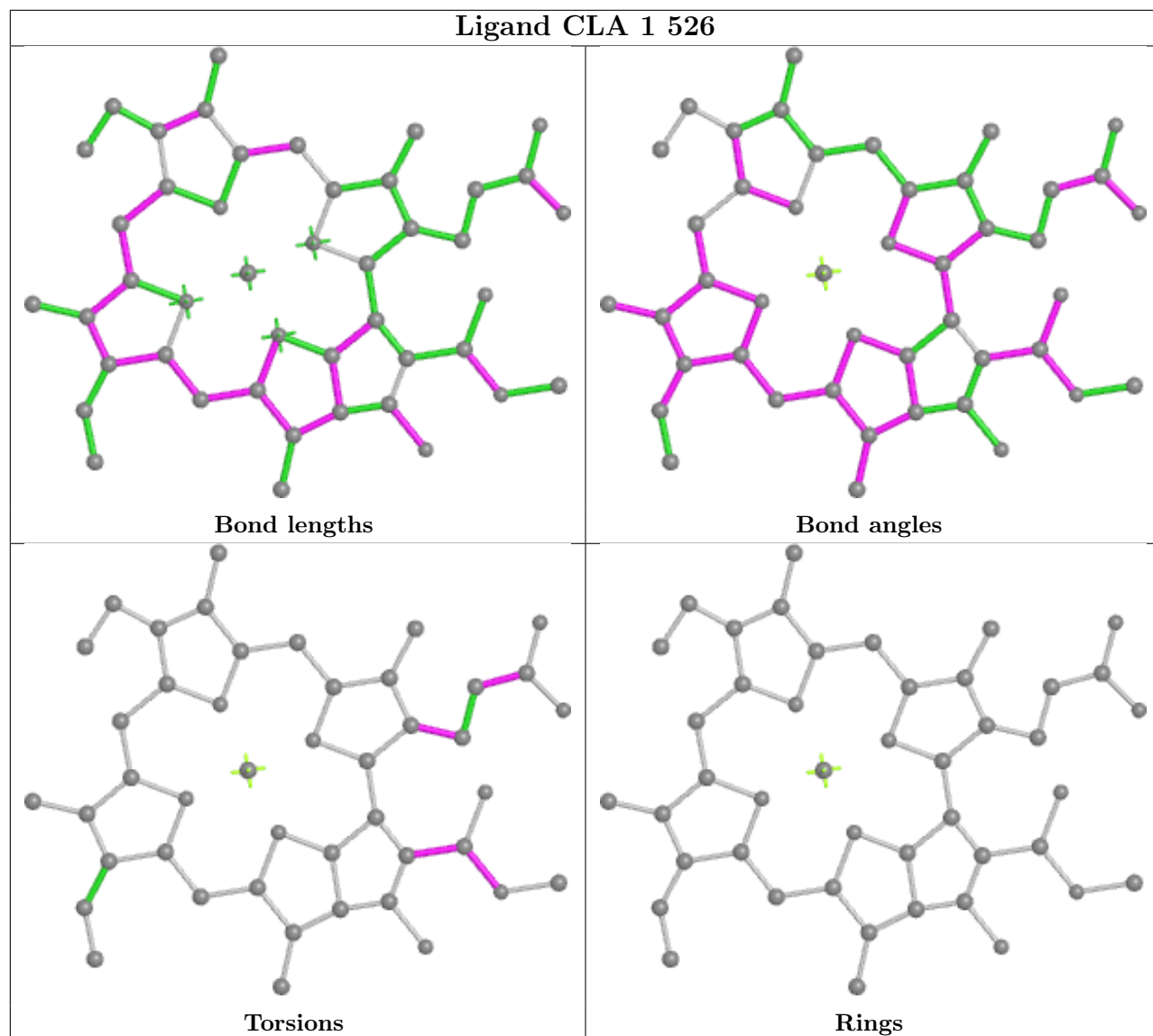
Ligand CLA B 835



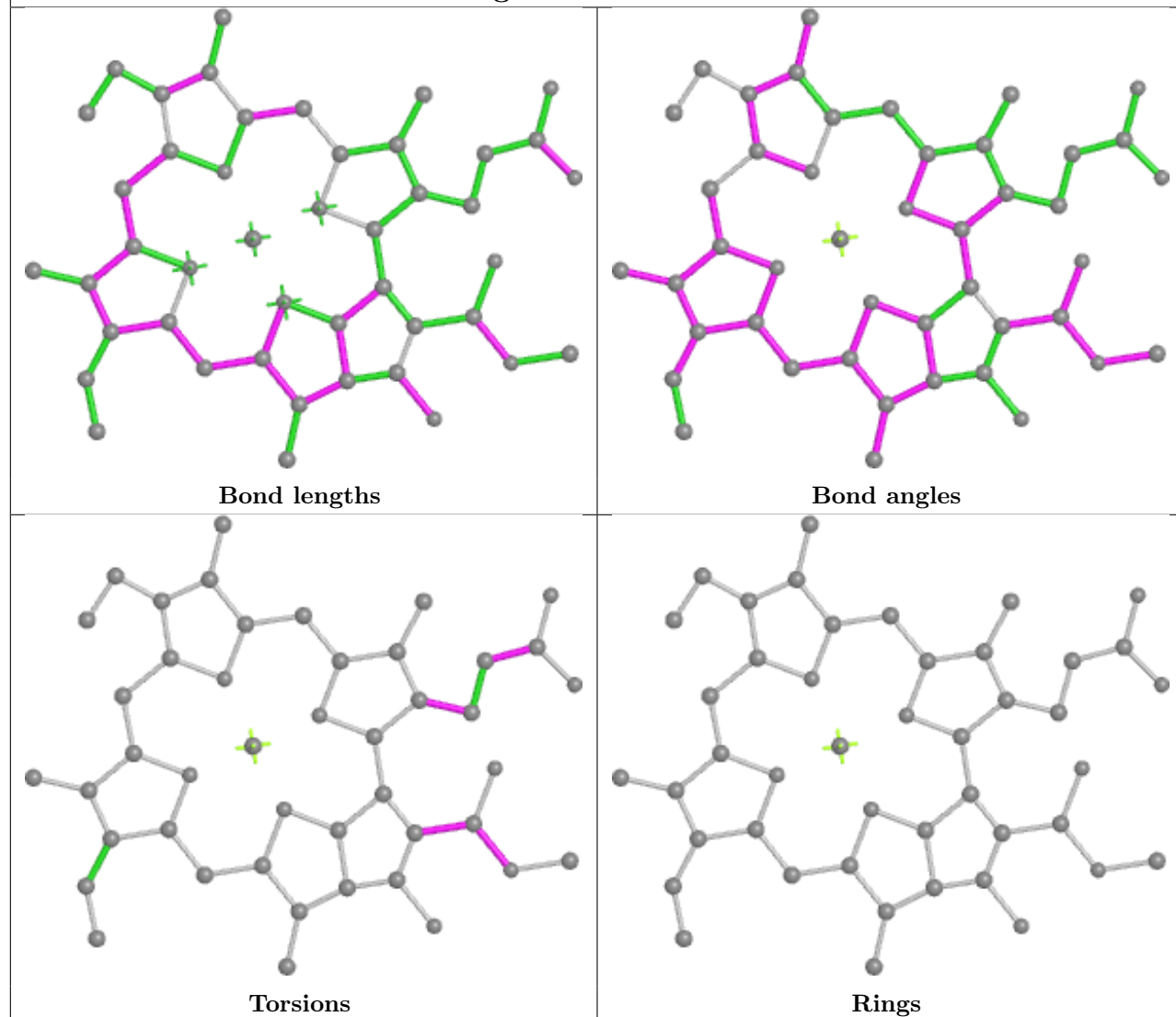
Ligand CL0 A 801



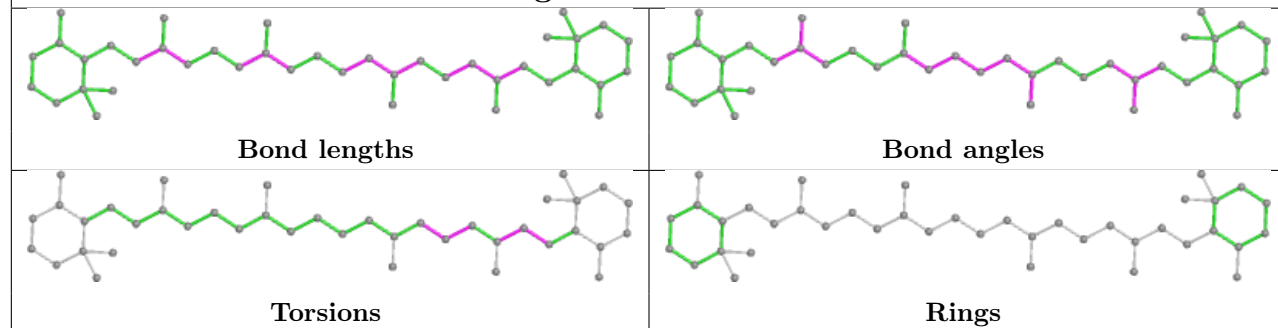
Ligand CLA 1 526



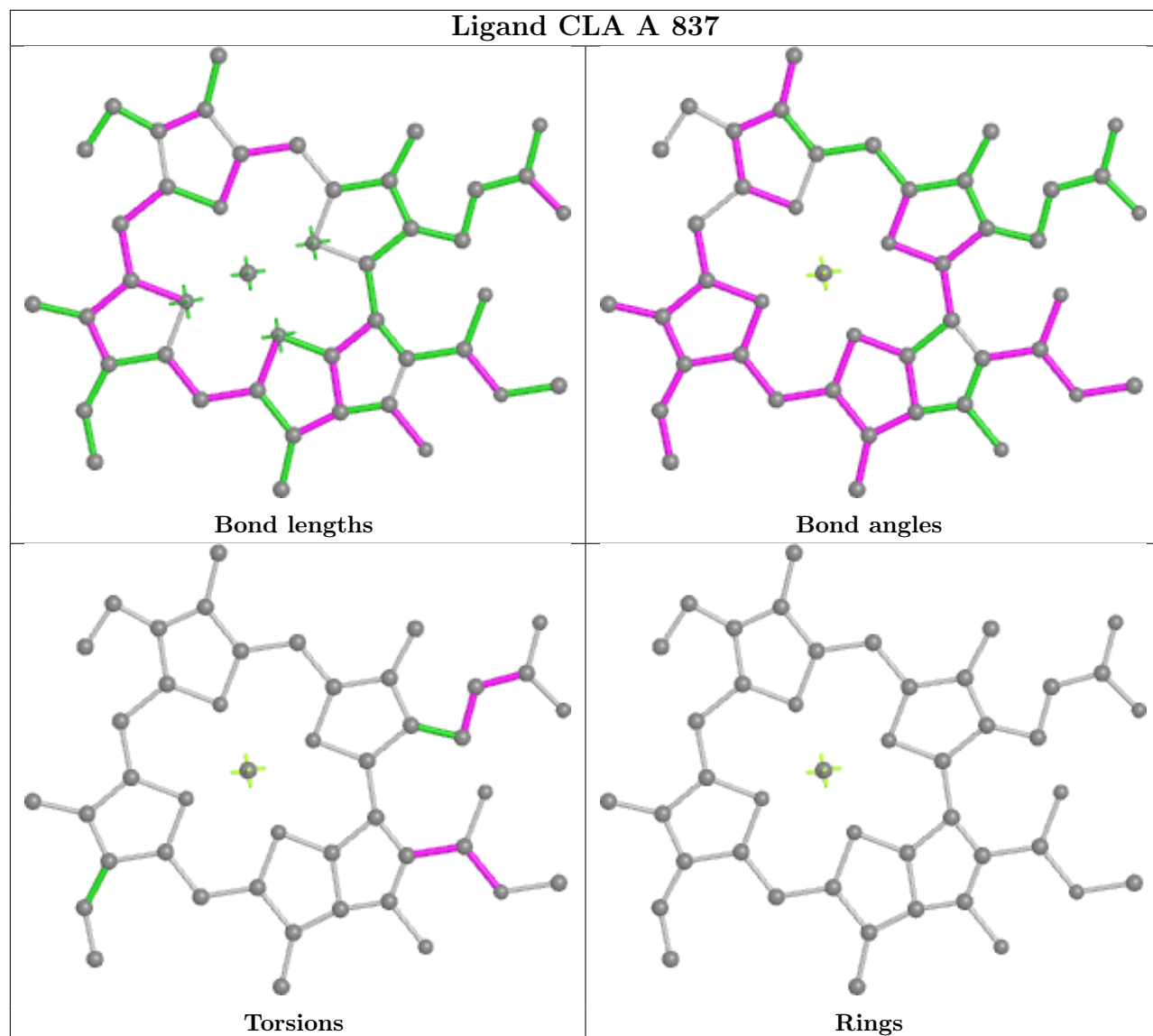
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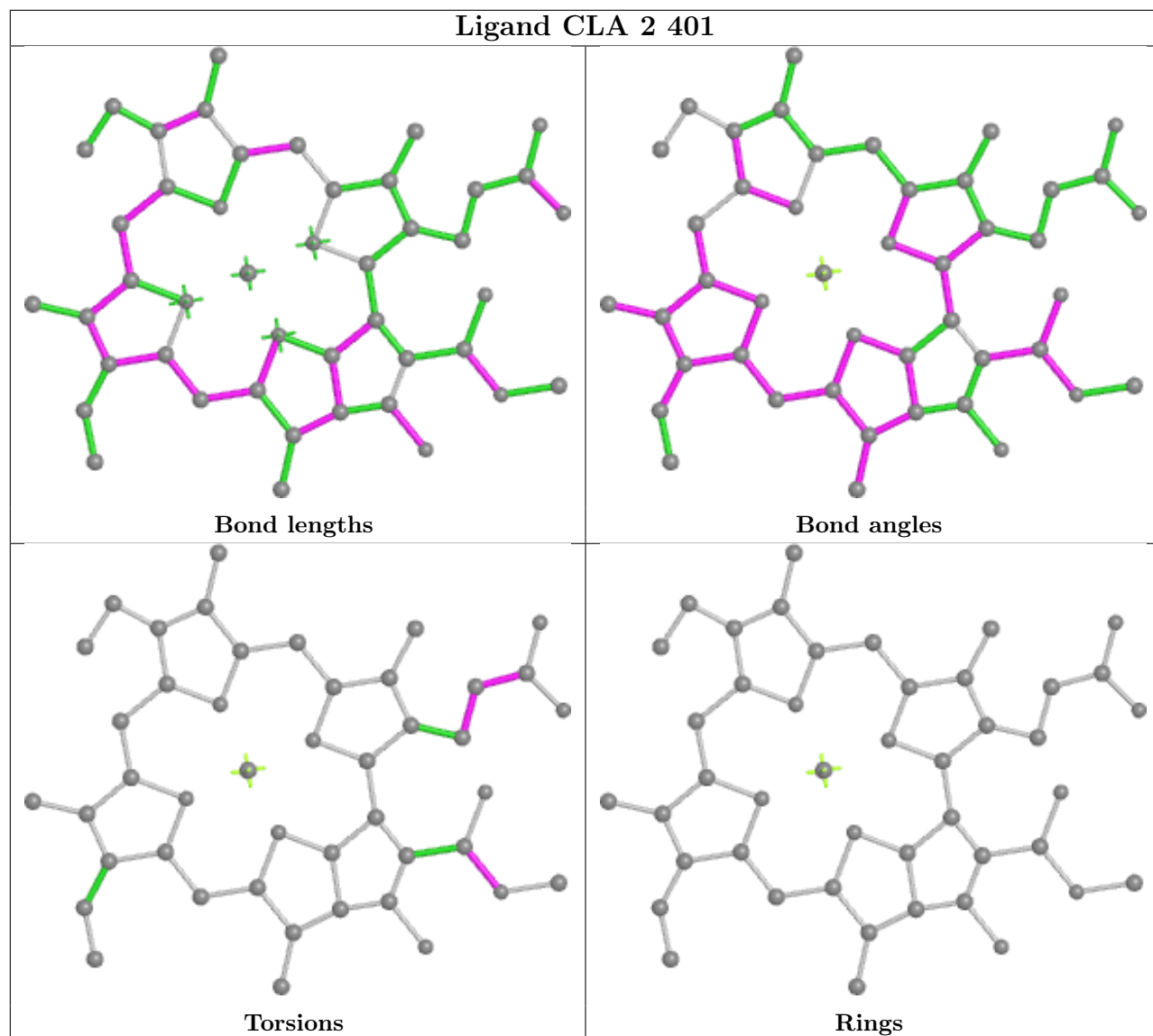
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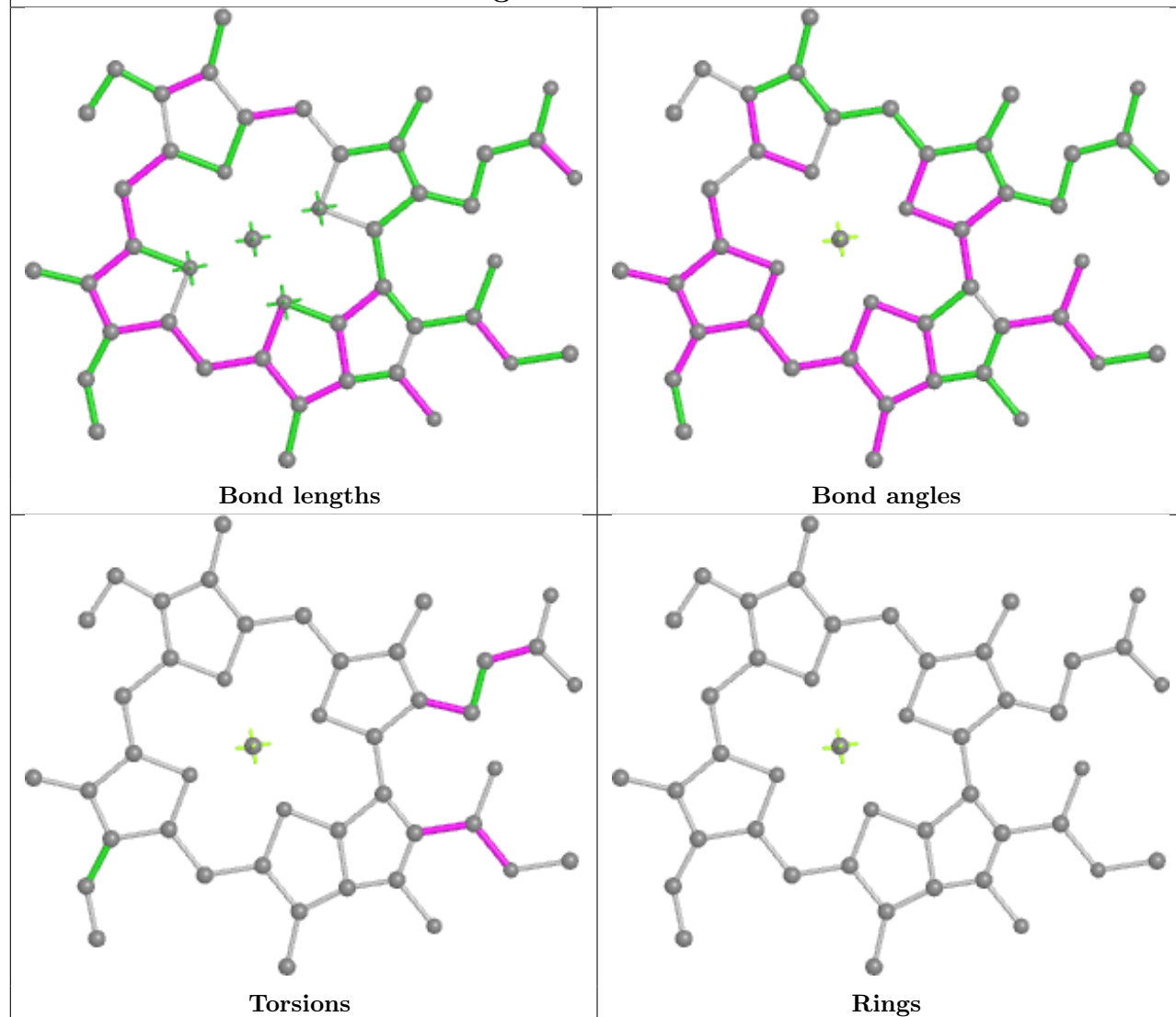
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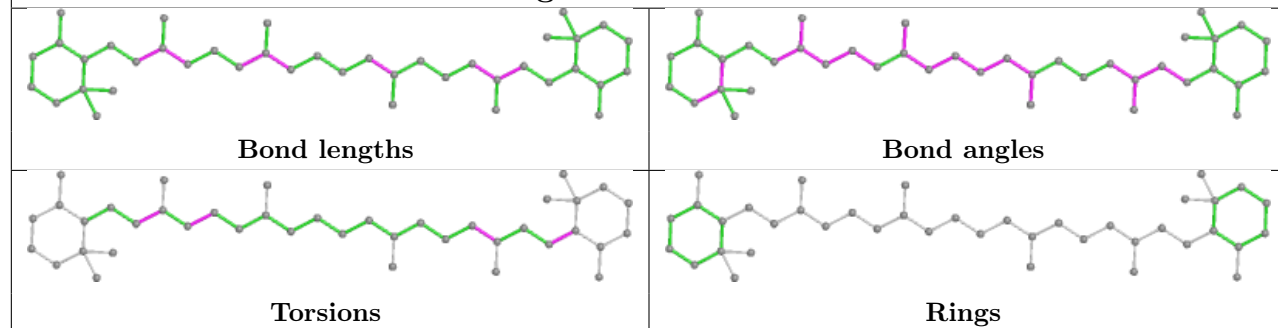
Ligand CLA 2 401

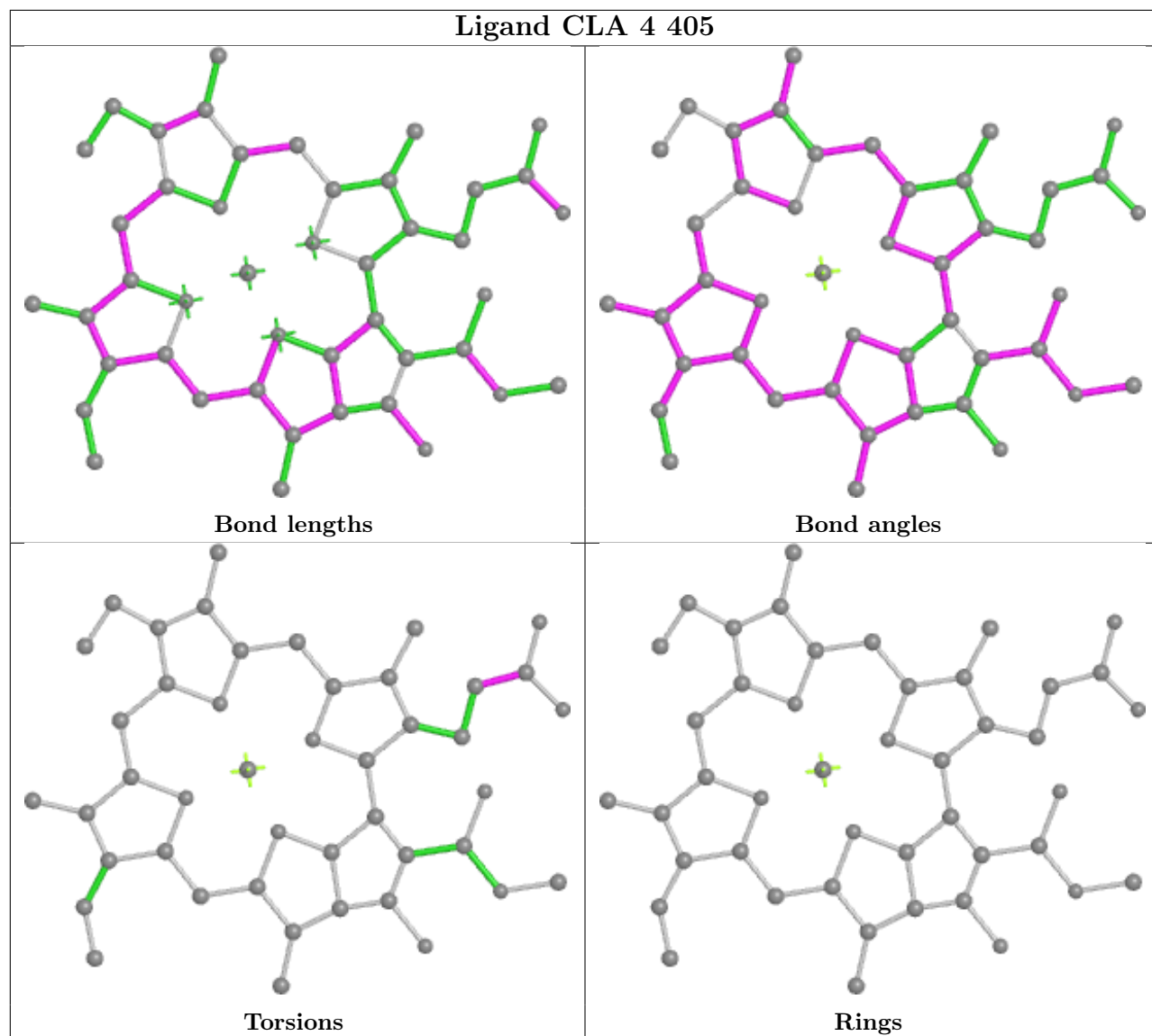
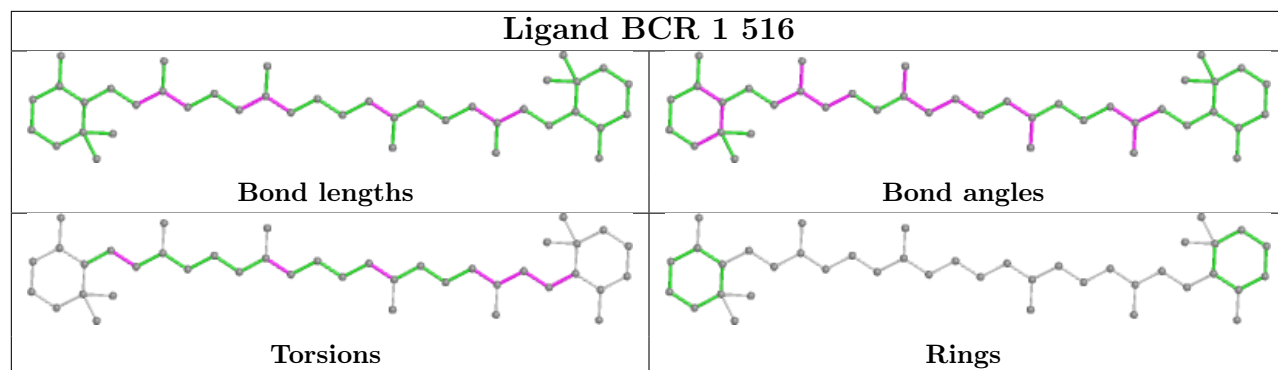


Ligand CLA 2 406

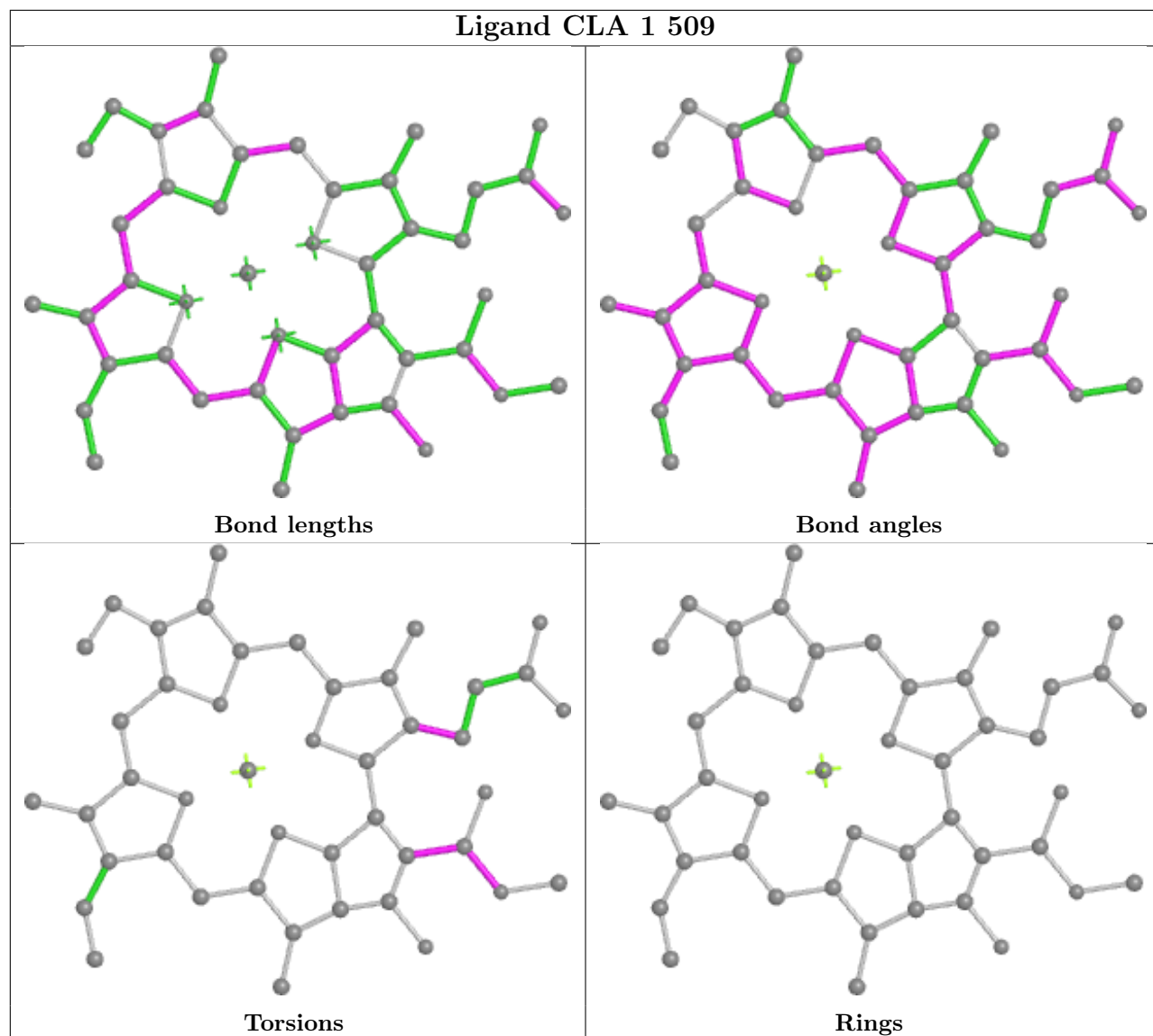


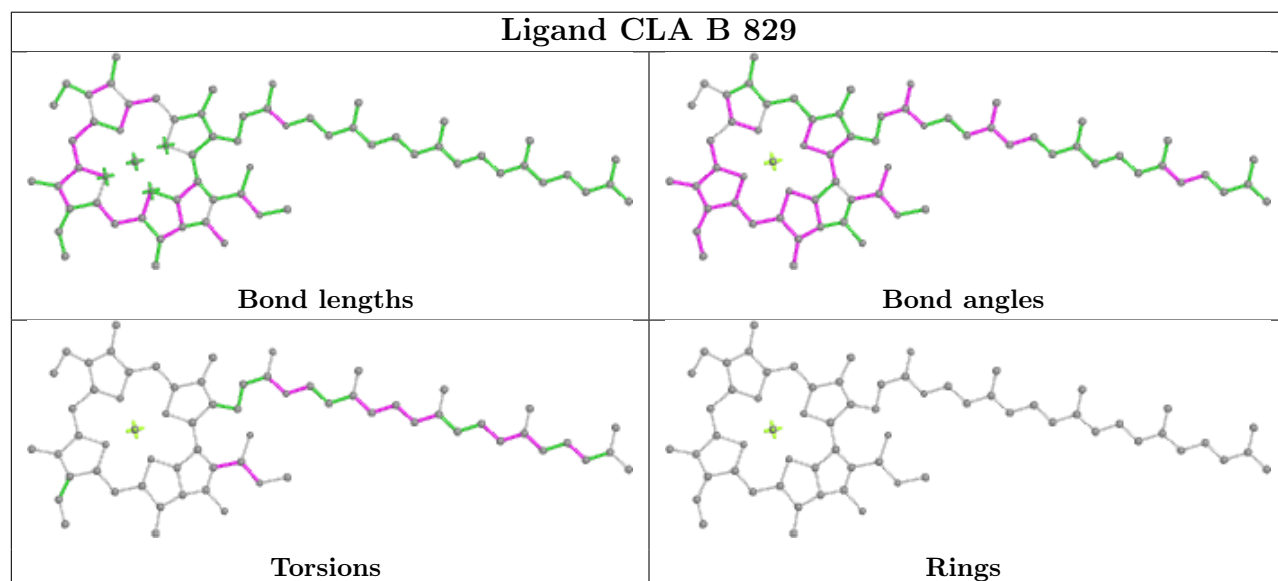
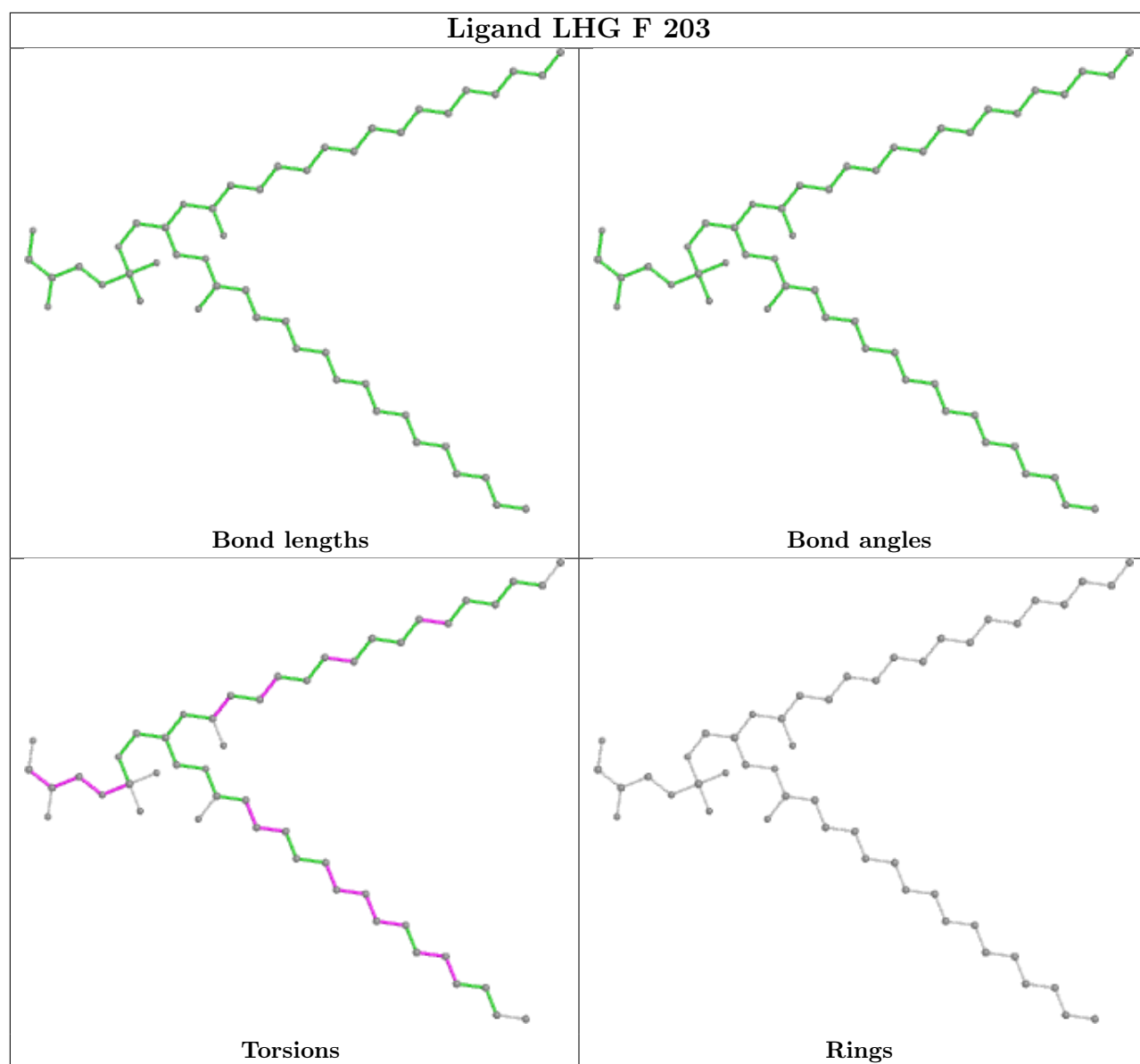
Ligand BCR I 102



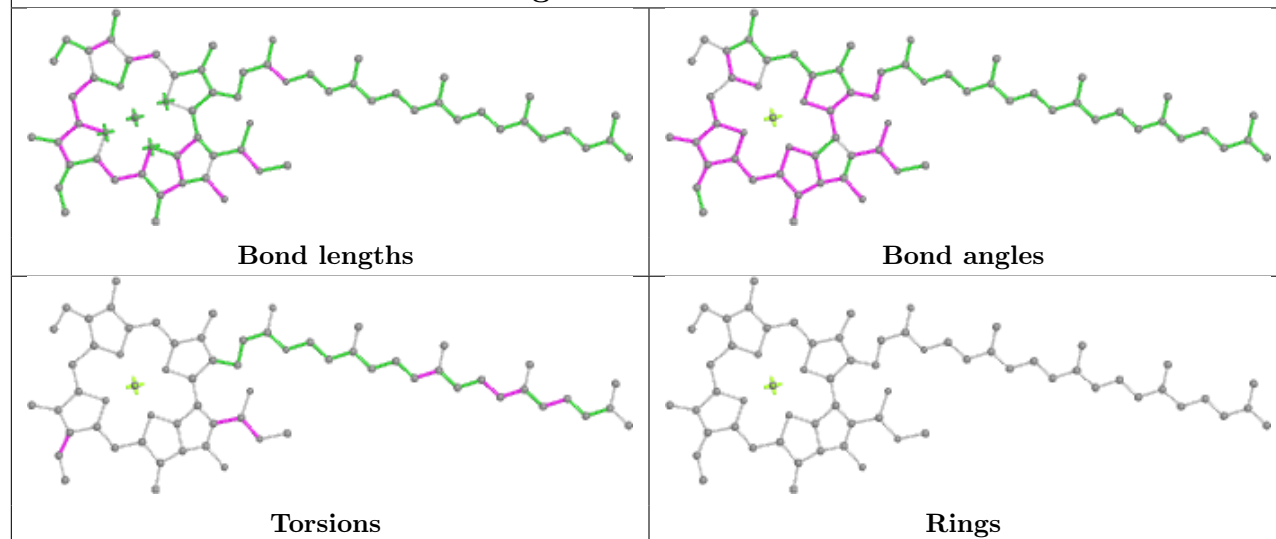


Ligand CLA 1 509

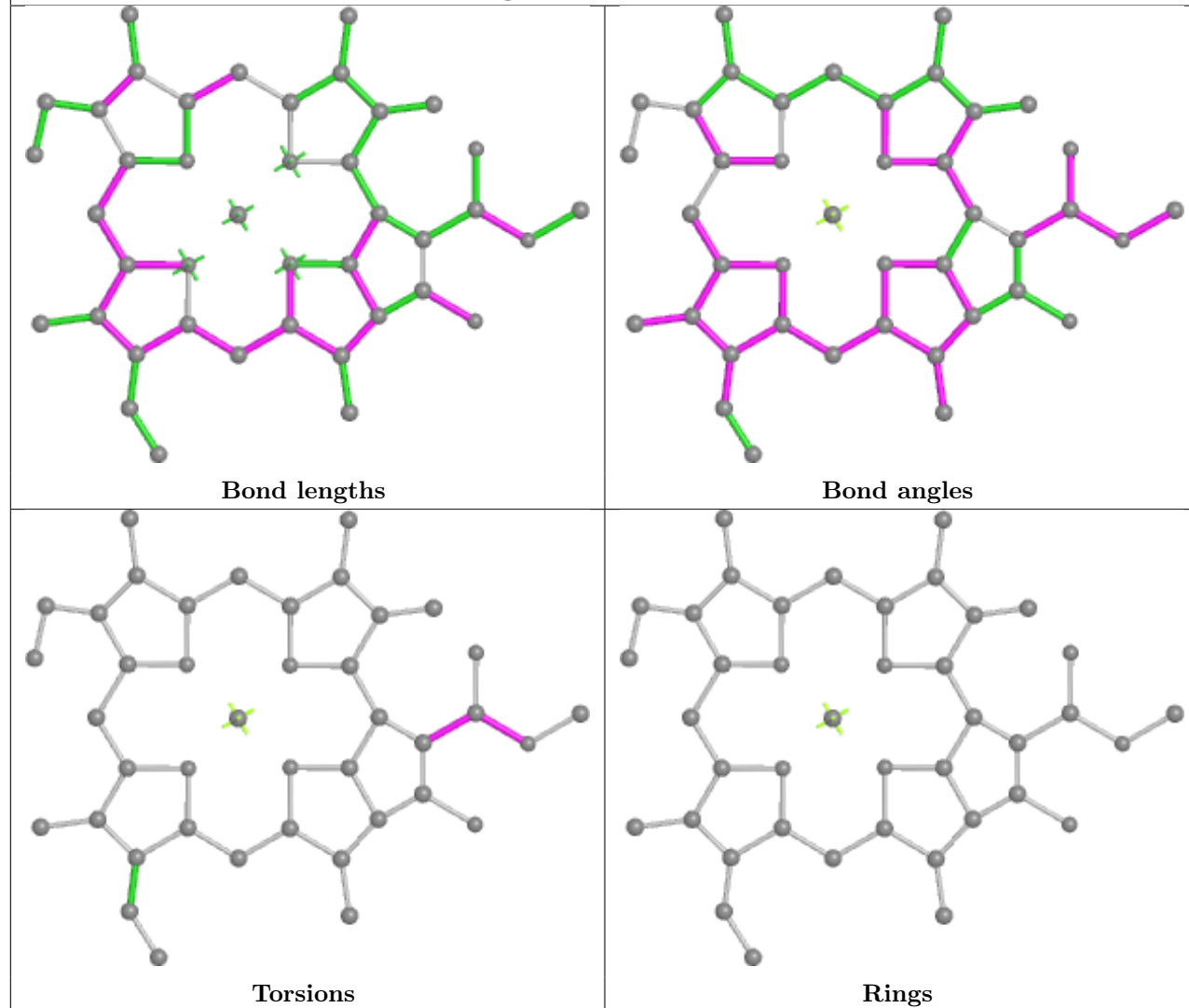


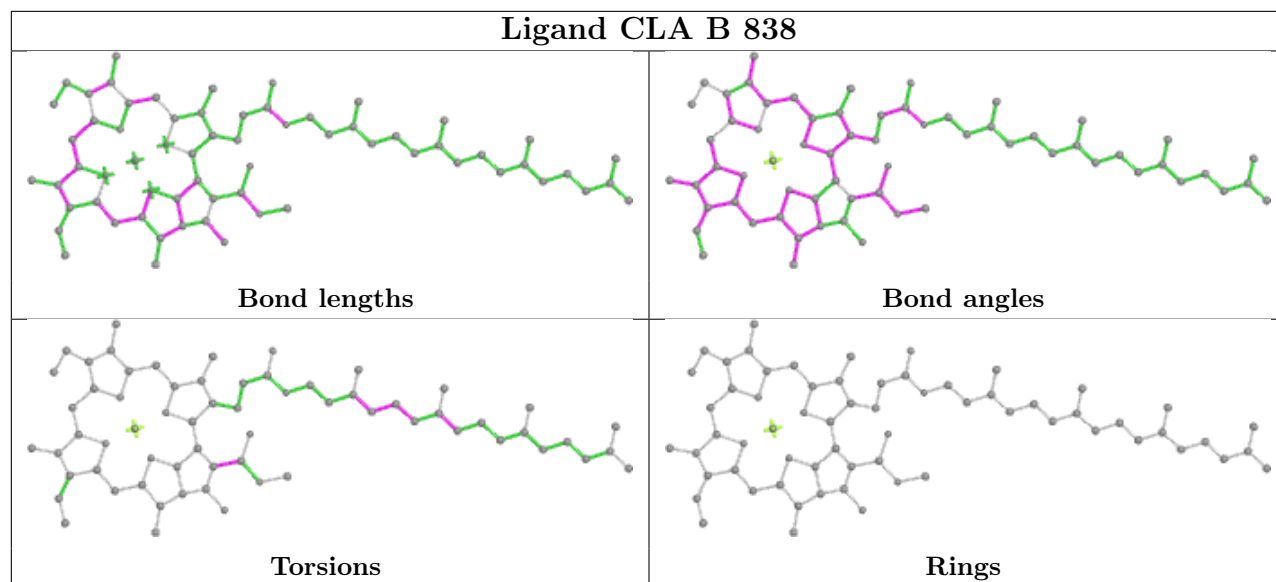
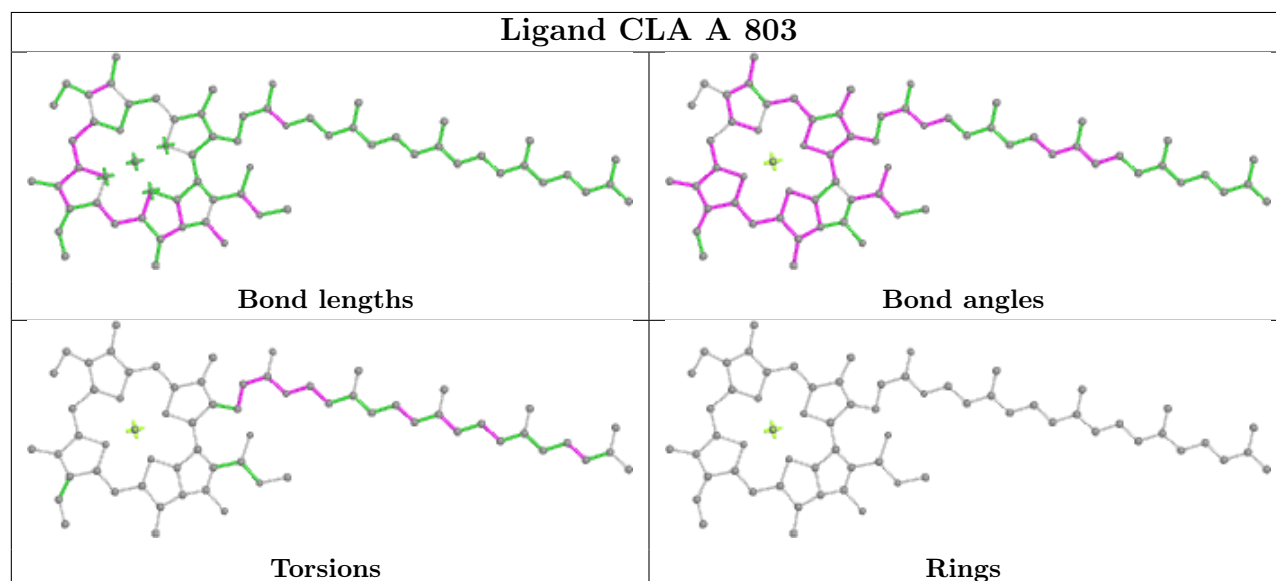


Ligand CLA B 826

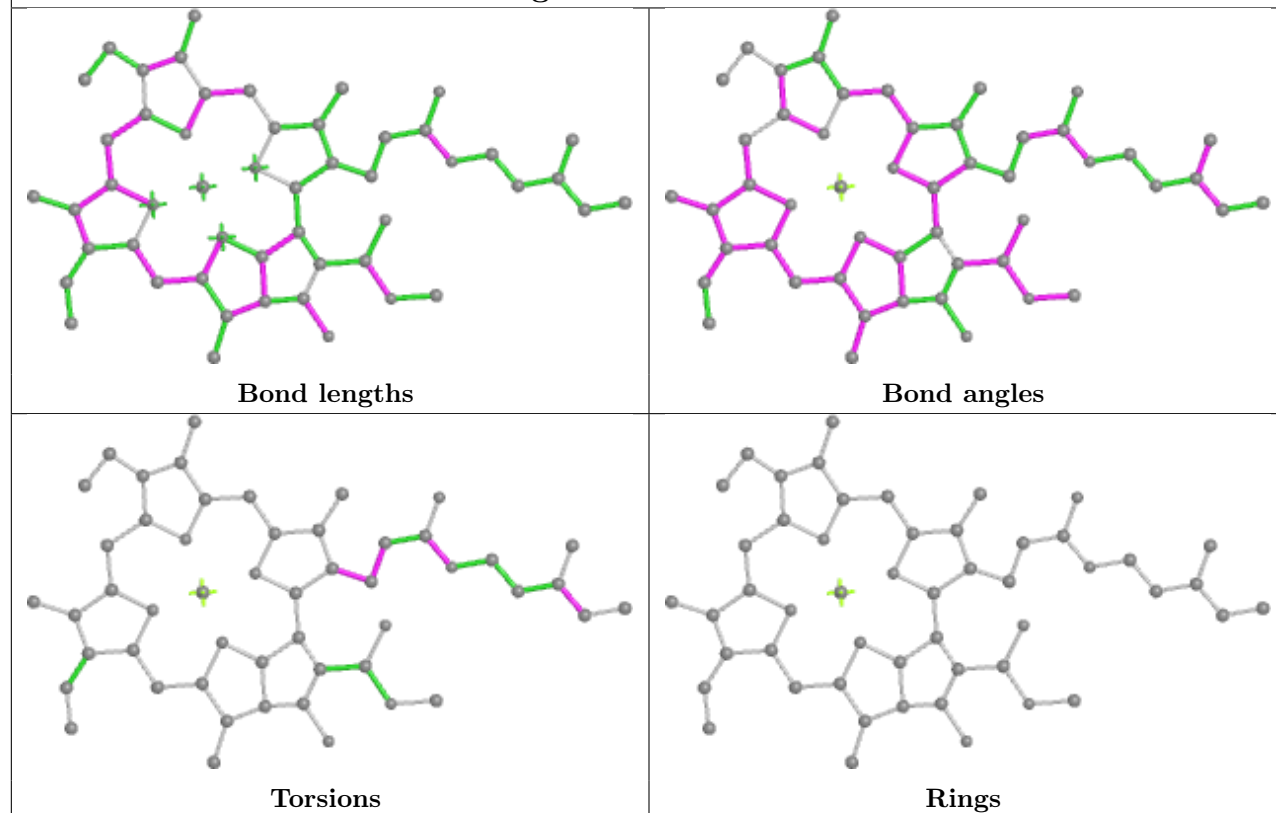


Ligand CLA 5 416

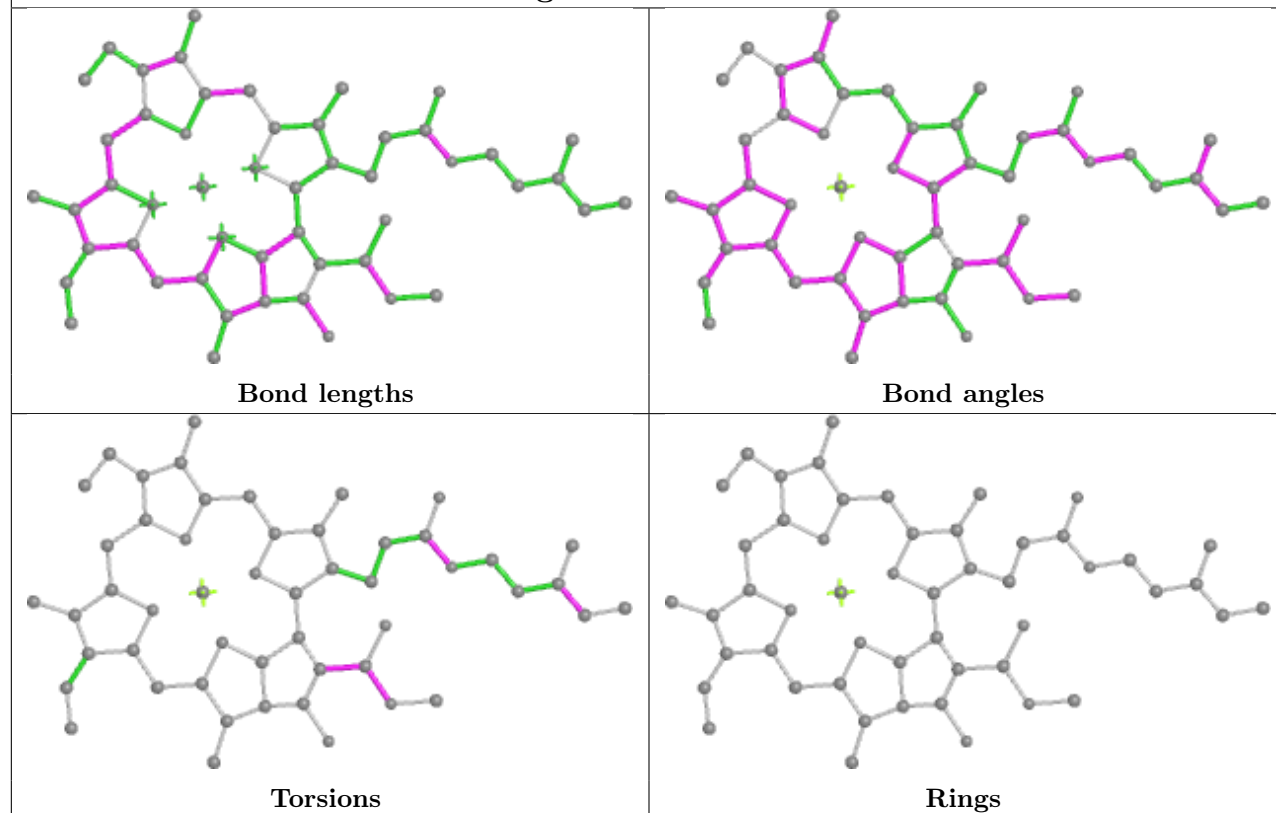


Ligand CLA B 838**Ligand CLA A 803**

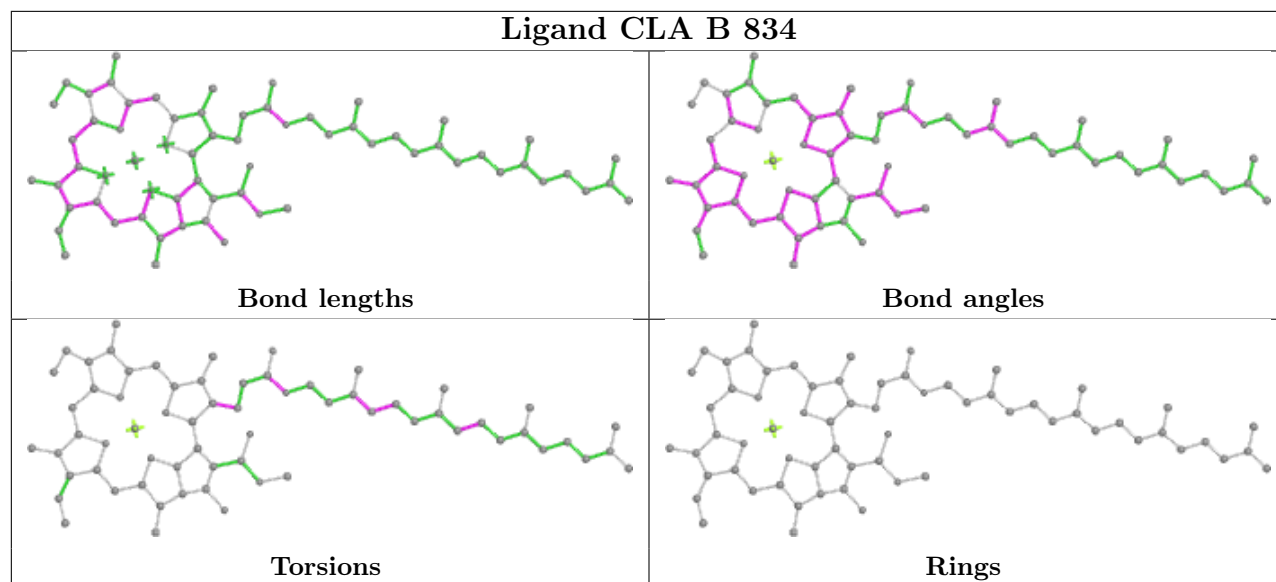
Ligand CLA A 838



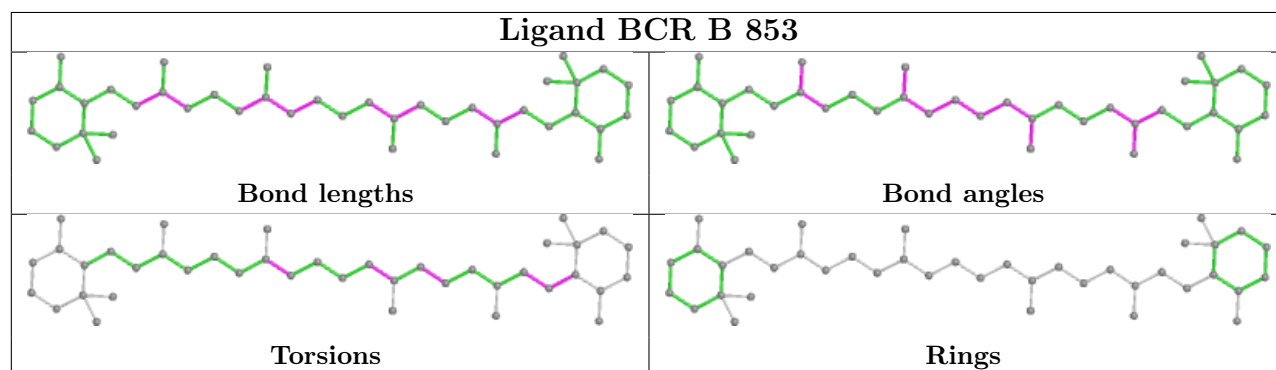
Ligand CLA 1 503



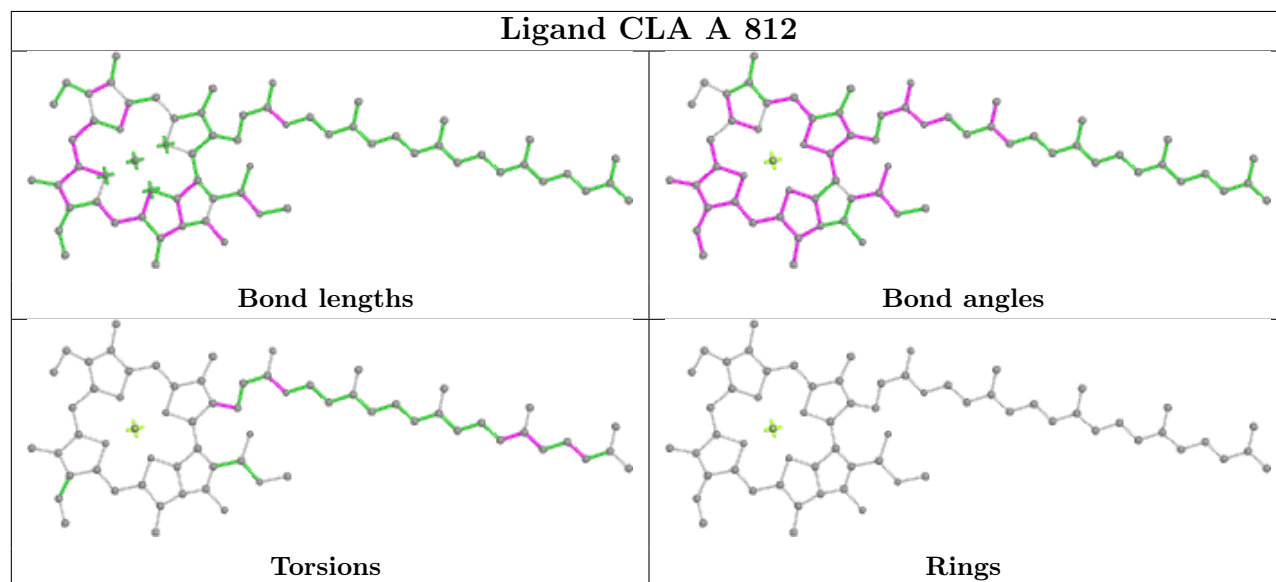
Ligand CLA B 834



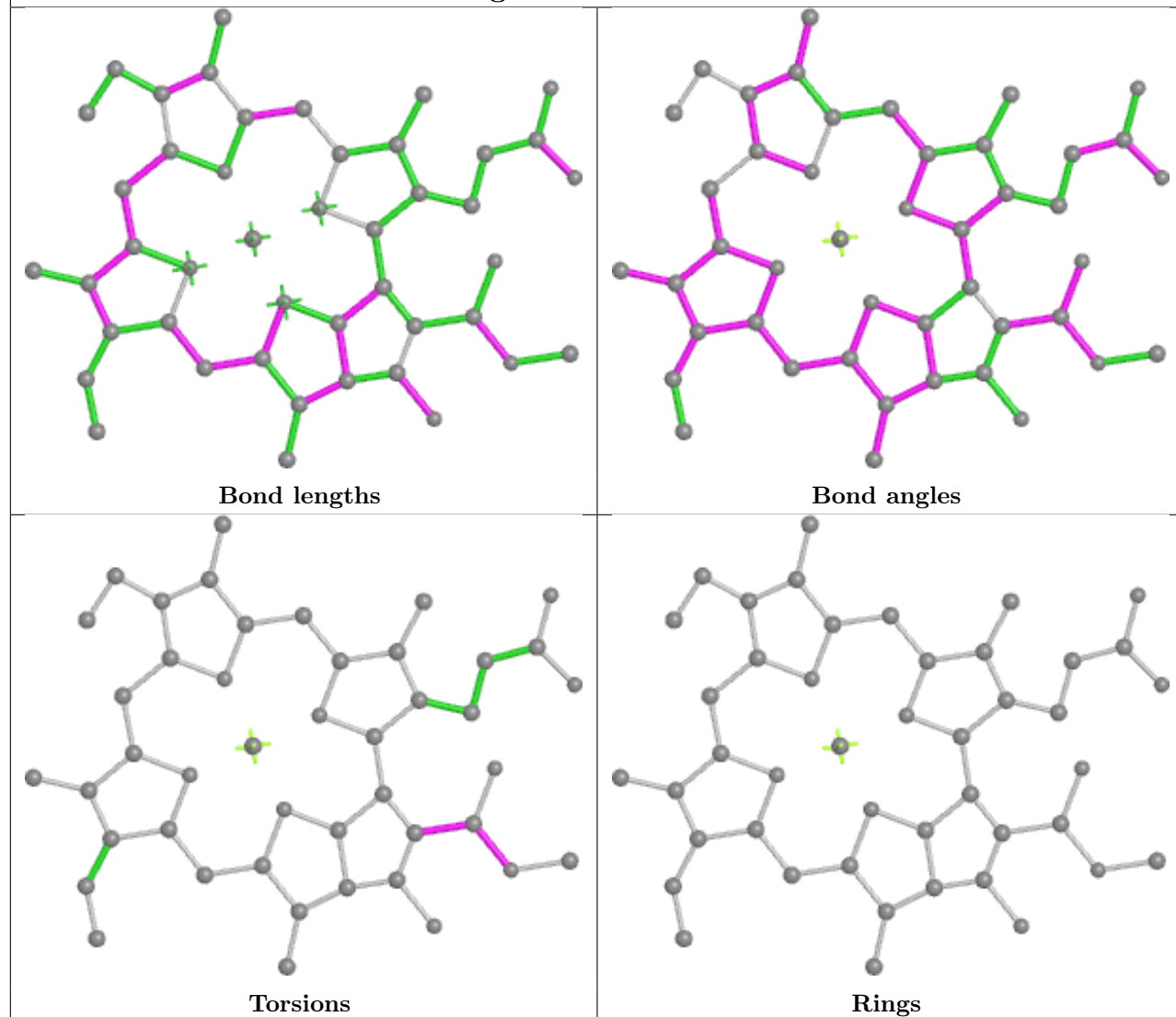
Ligand BCR B 853



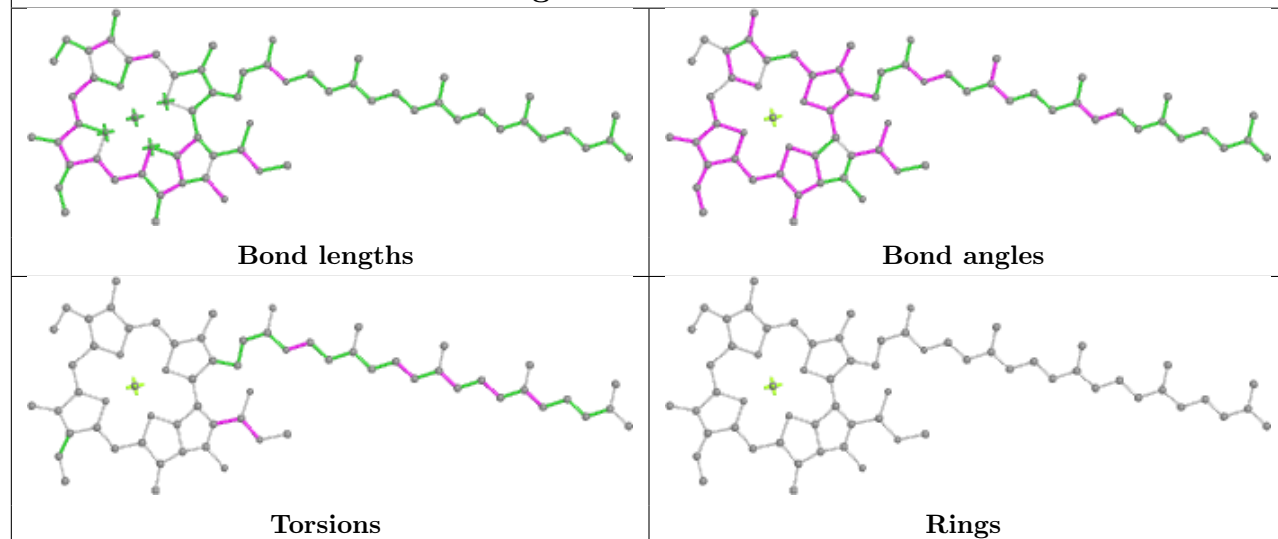
Ligand CLA A 812

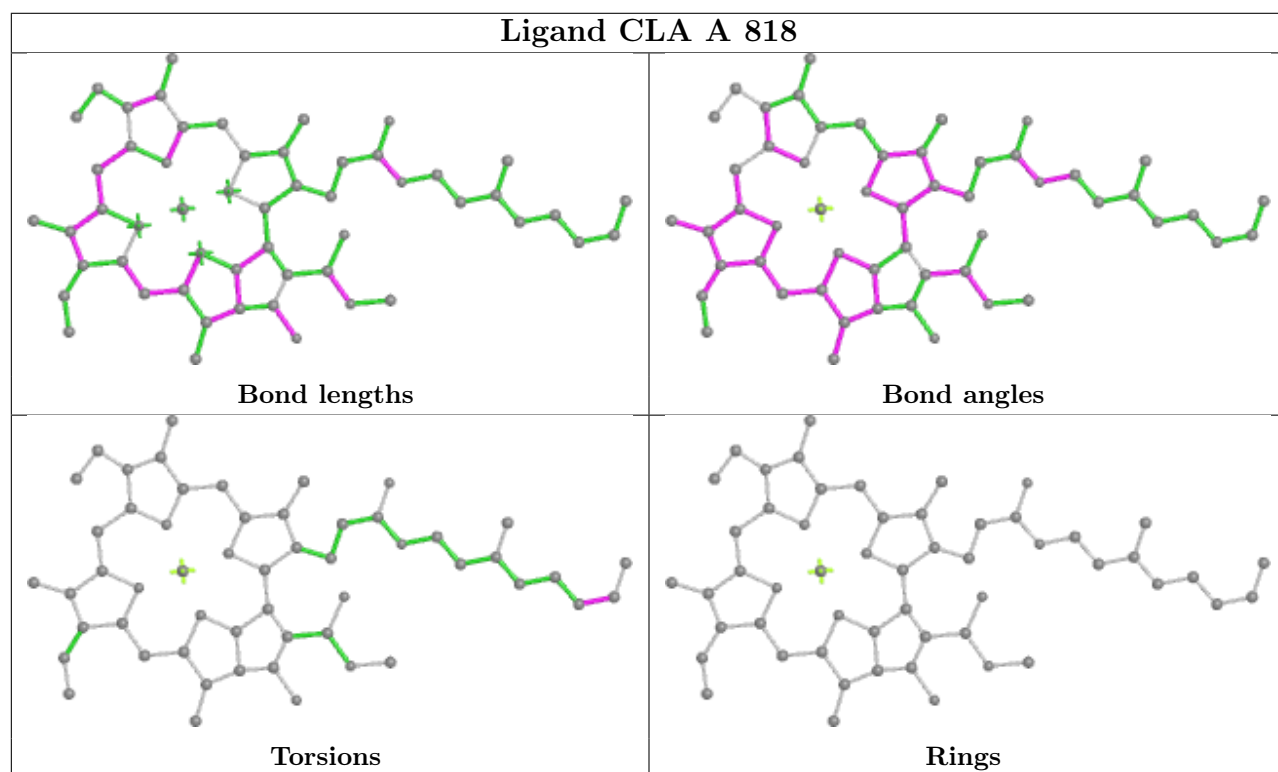
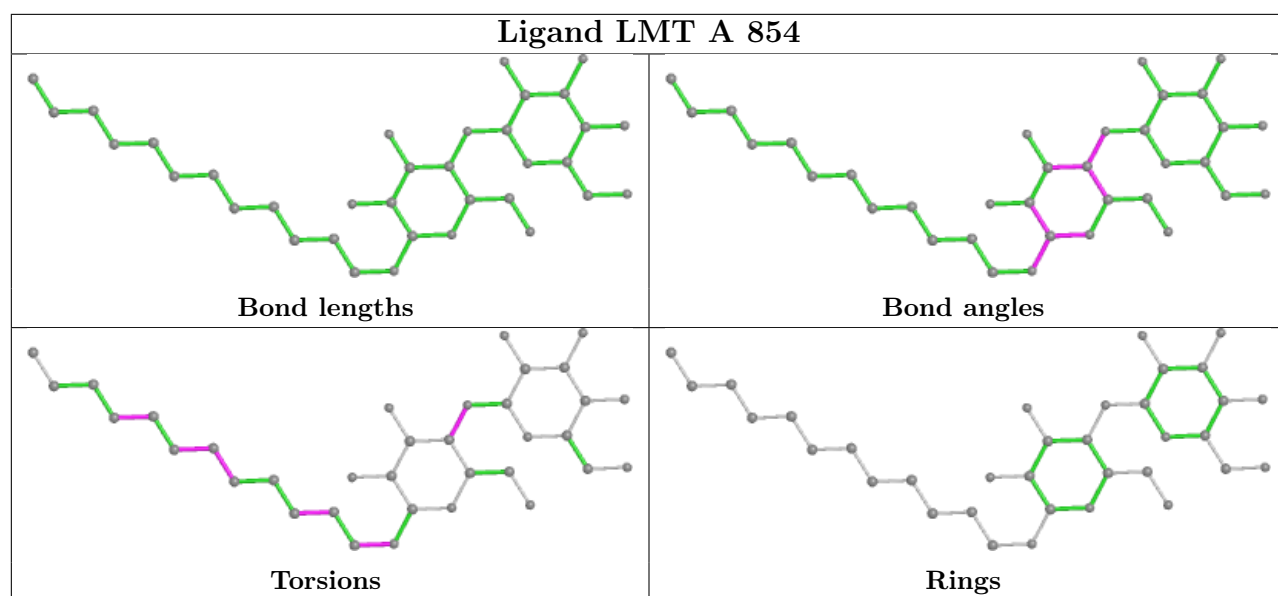


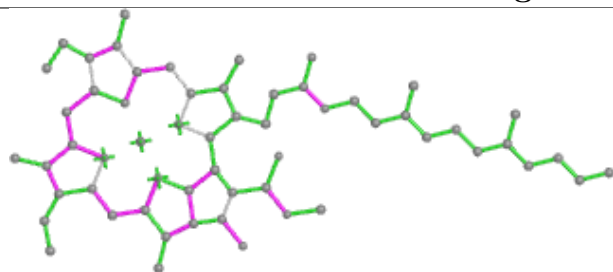
Ligand CLA B 821



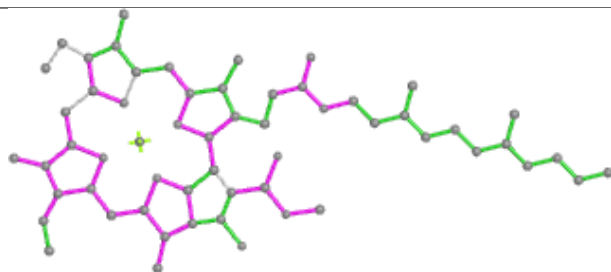
Ligand CLA B 801



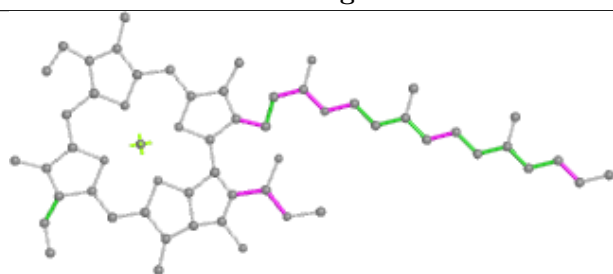


Ligand CLA B 833

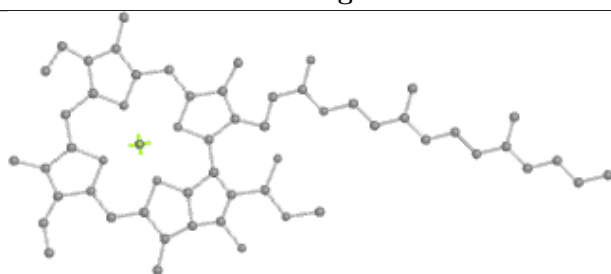
Bond lengths



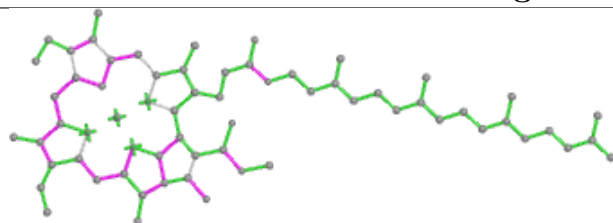
Bond angles



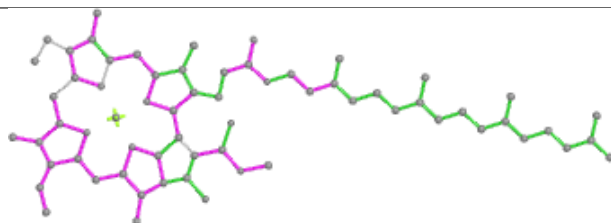
Torsions



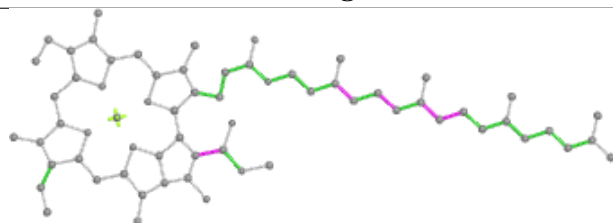
Rings

Ligand CLA A 841

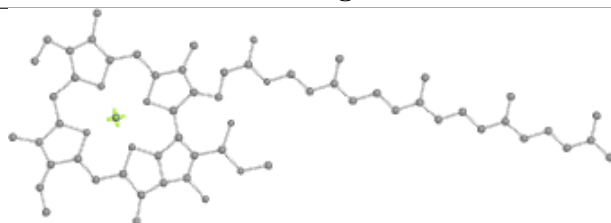
Bond lengths



Bond angles

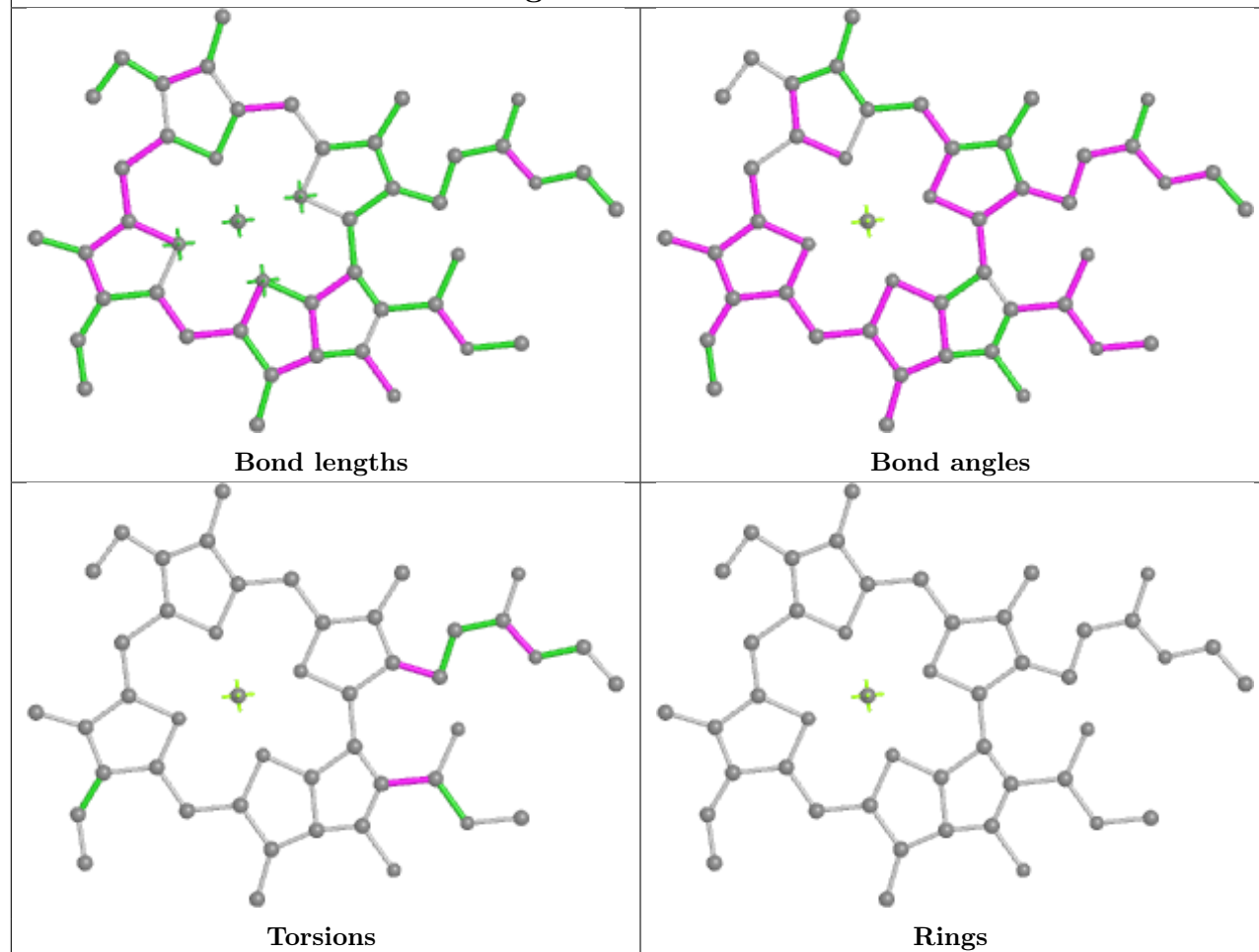


Torsions

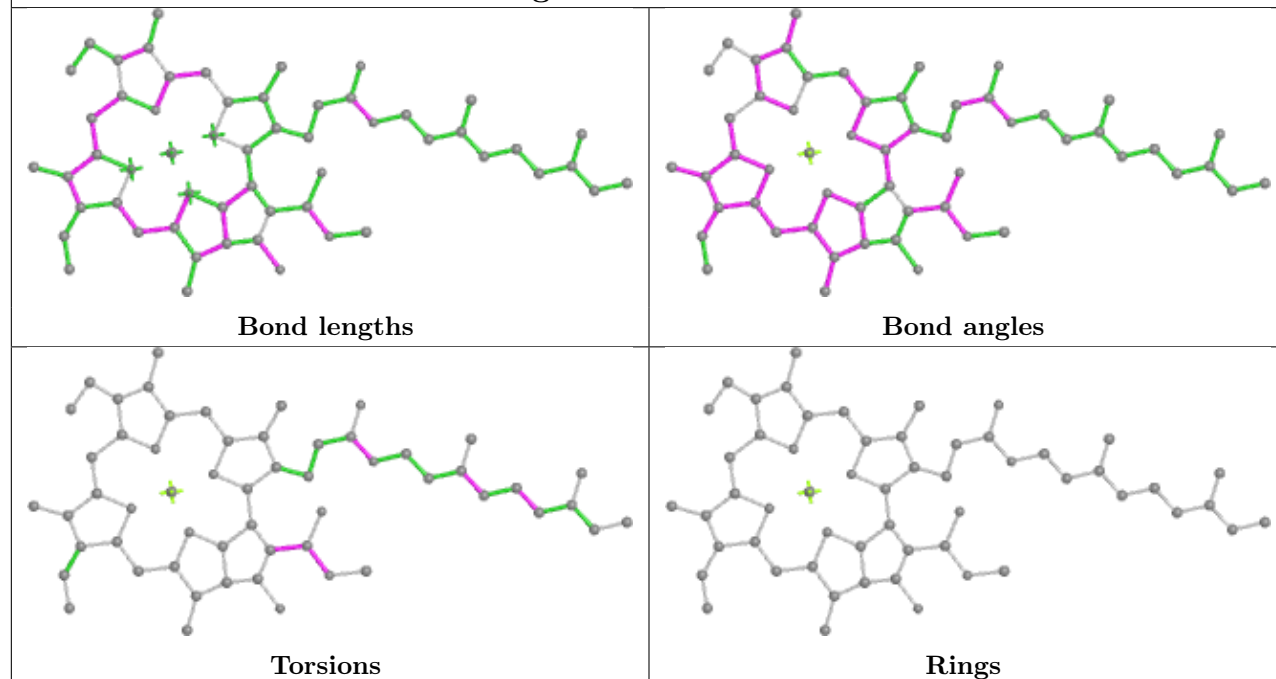


Rings

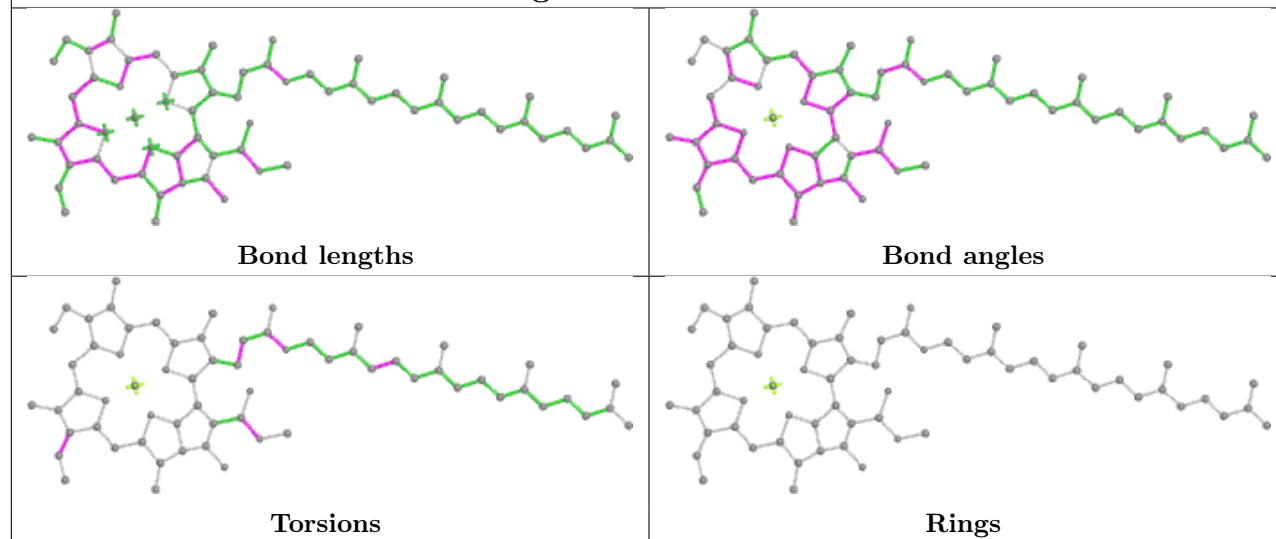
Ligand CLA B 820



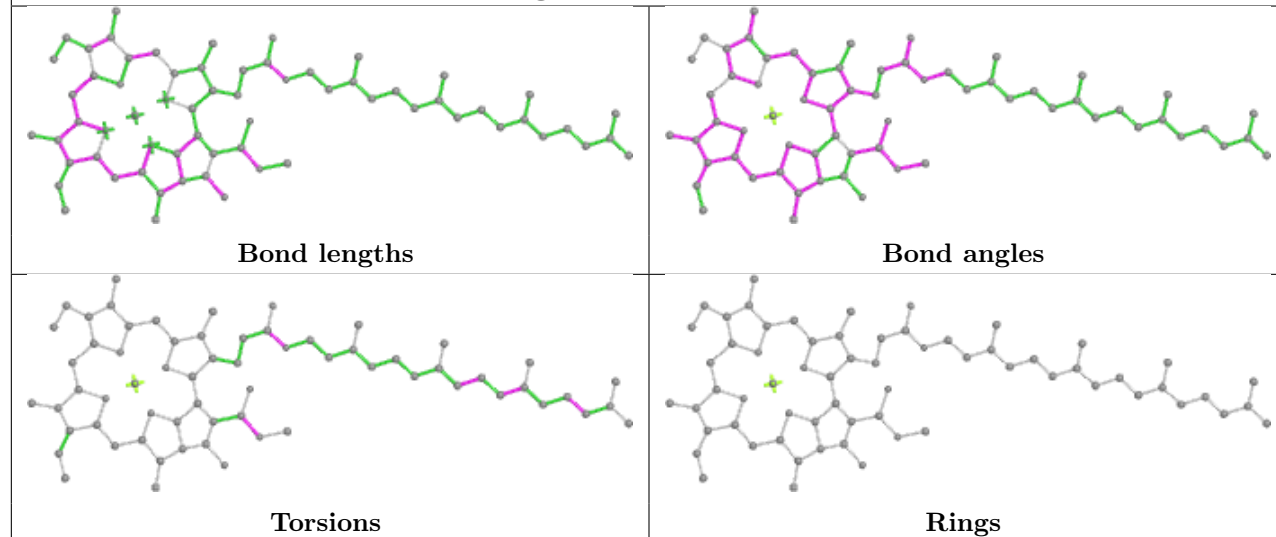
Ligand CLA B 814



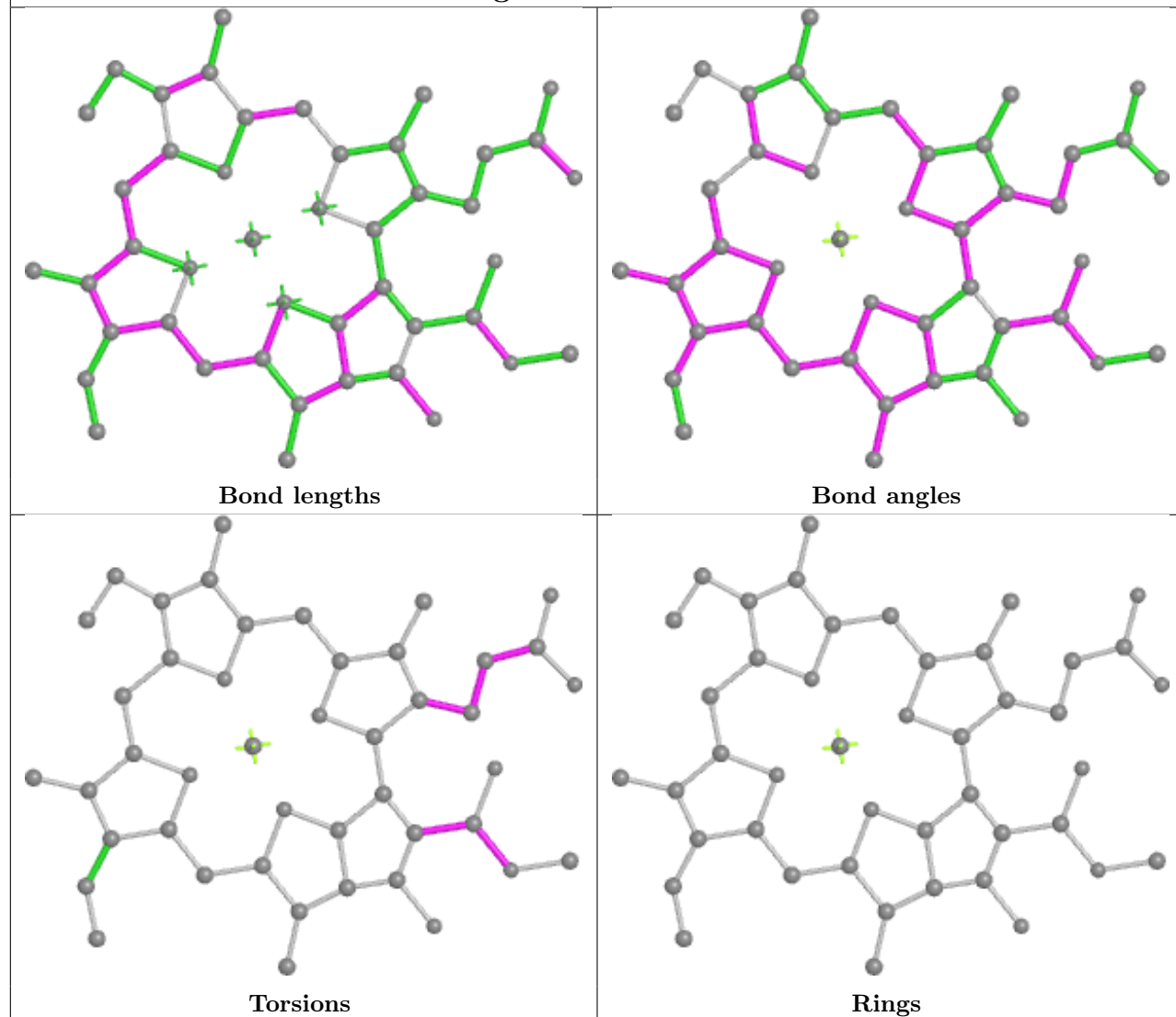
Ligand CLA B 841



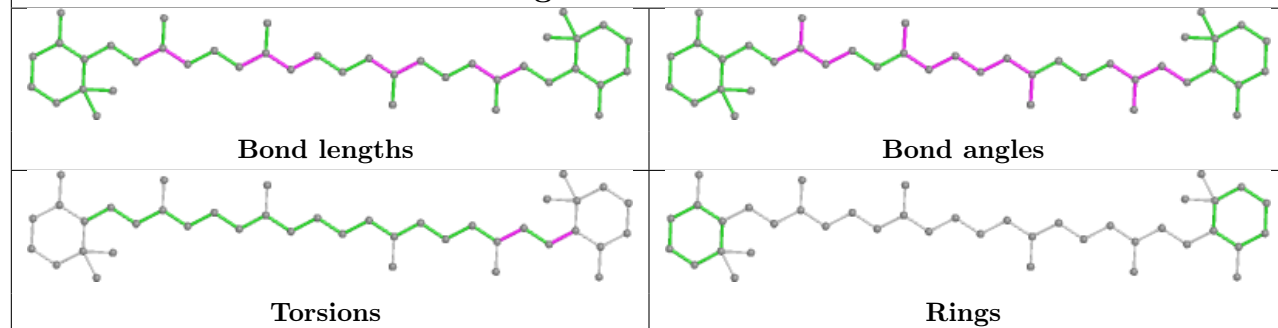
Ligand CLA B 831

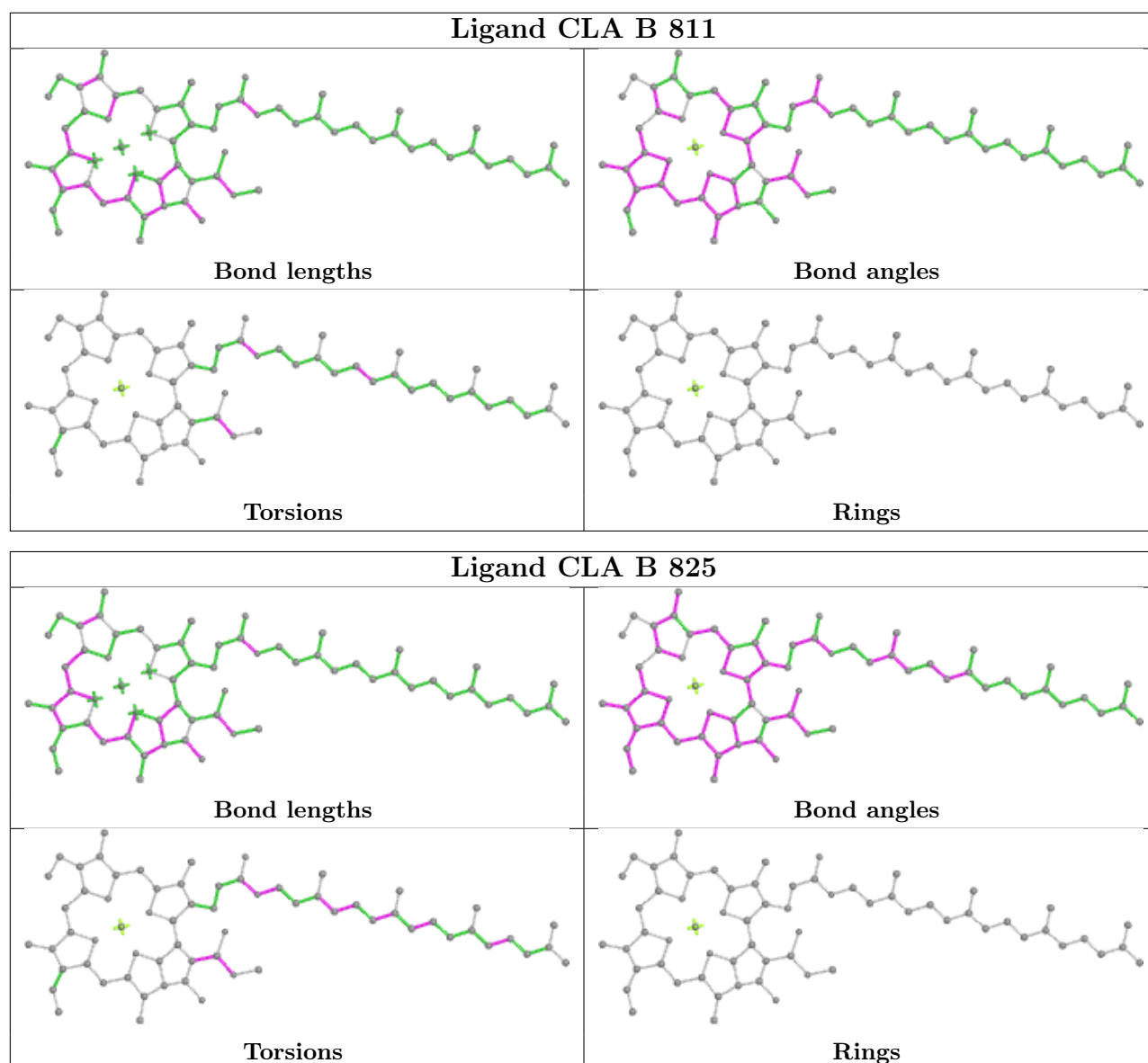


Ligand CLA 1 525



Ligand BCR 1 522





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

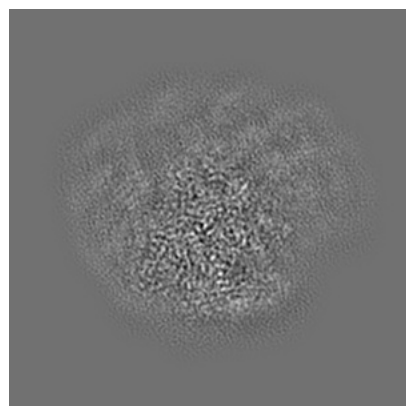
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33593. These allow visual inspection of the internal detail of the map and identification of artifacts.

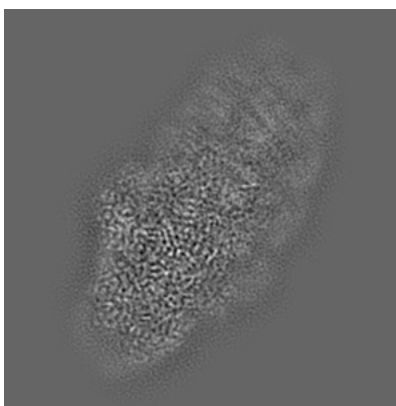
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

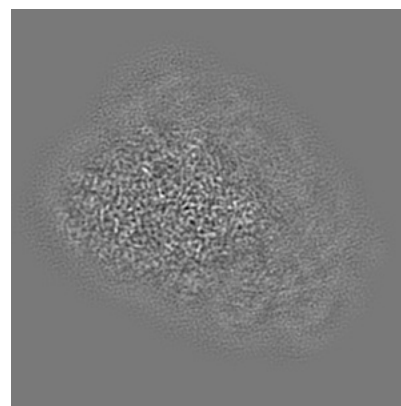
6.1.1 Primary map



X

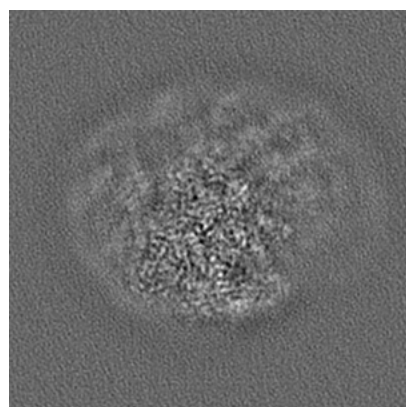


Y

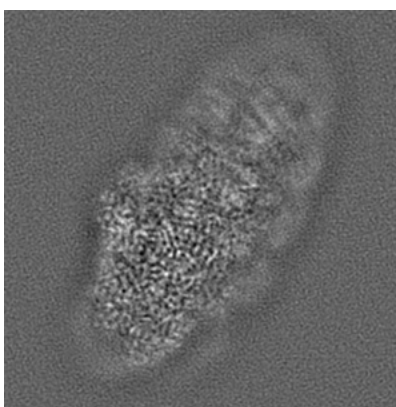


Z

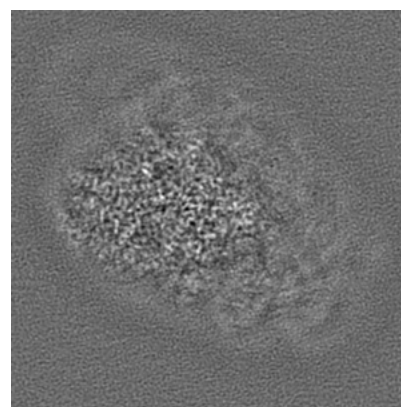
6.1.2 Raw map



X



Y

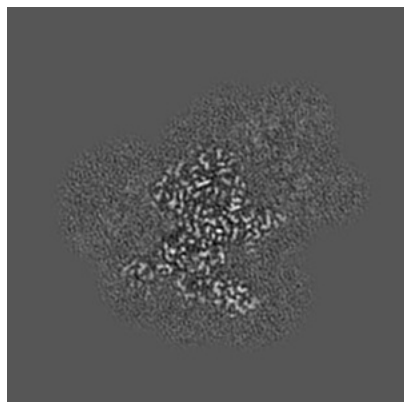


Z

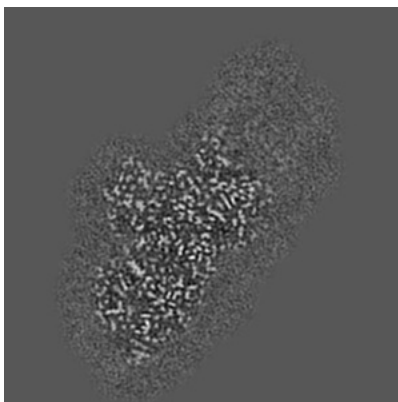
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

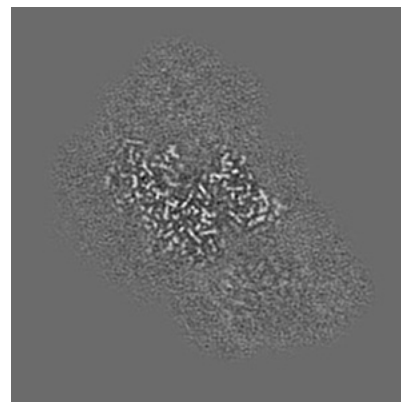
6.2.1 Primary map



X Index: 116

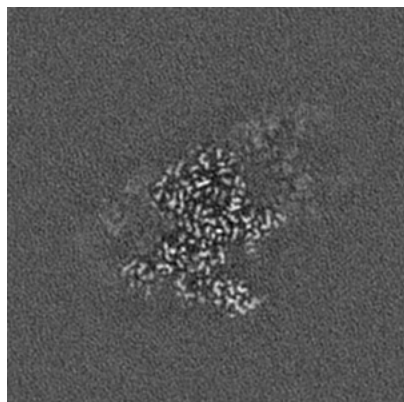


Y Index: 116

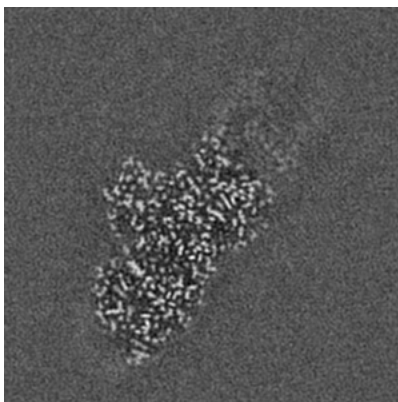


Z Index: 116

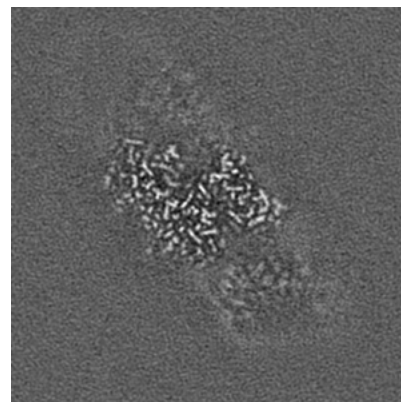
6.2.2 Raw map



X Index: 116



Y Index: 116

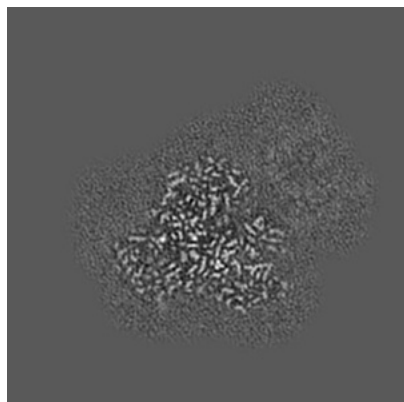


Z Index: 116

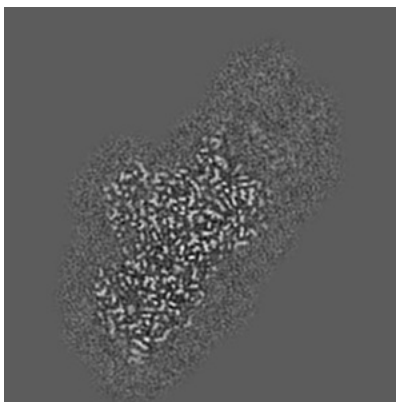
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

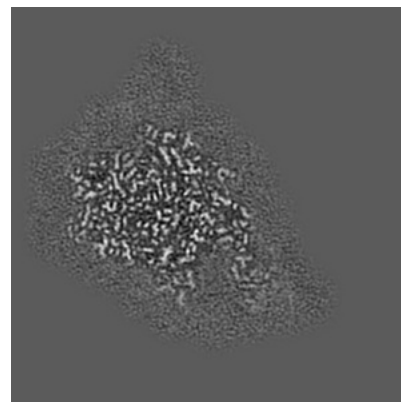
6.3.1 Primary map



X Index: 102

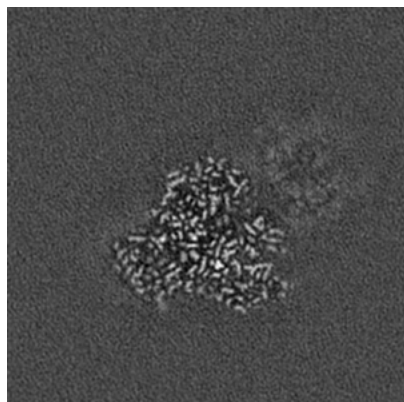


Y Index: 117

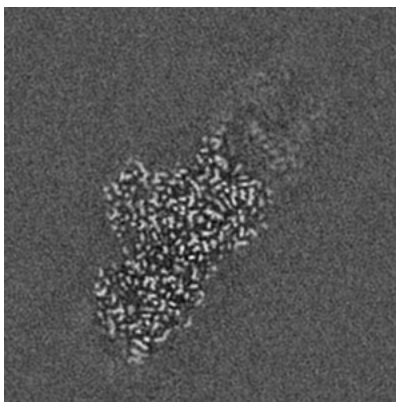


Z Index: 96

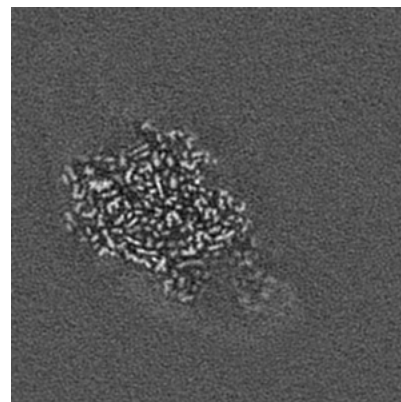
6.3.2 Raw map



X Index: 102



Y Index: 117

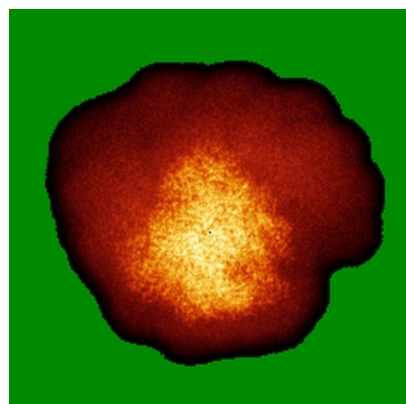


Z Index: 92

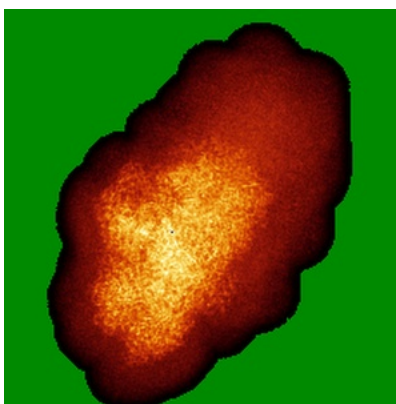
The images above show the largest variance slices of the map in three orthogonal directions.

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

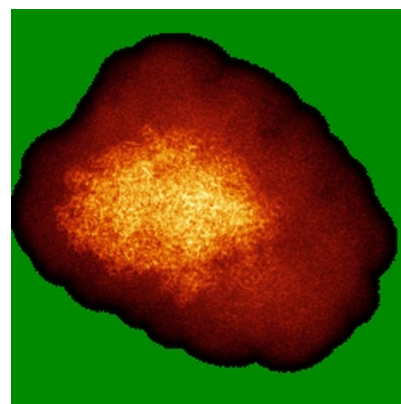
6.4.1 Primary map



X

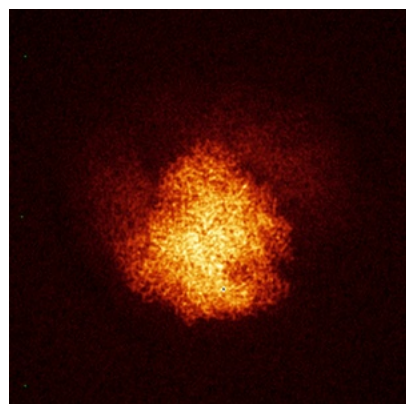


Y

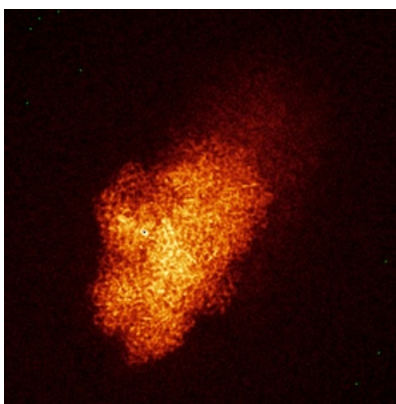


Z

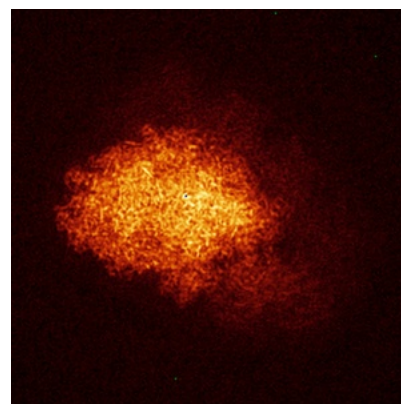
6.4.2 Raw map



X



Y

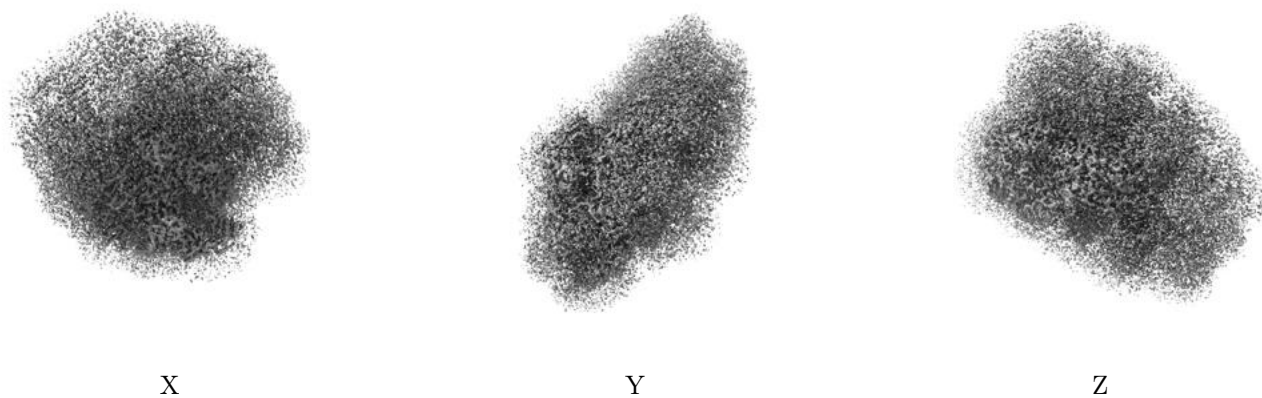


Z

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.

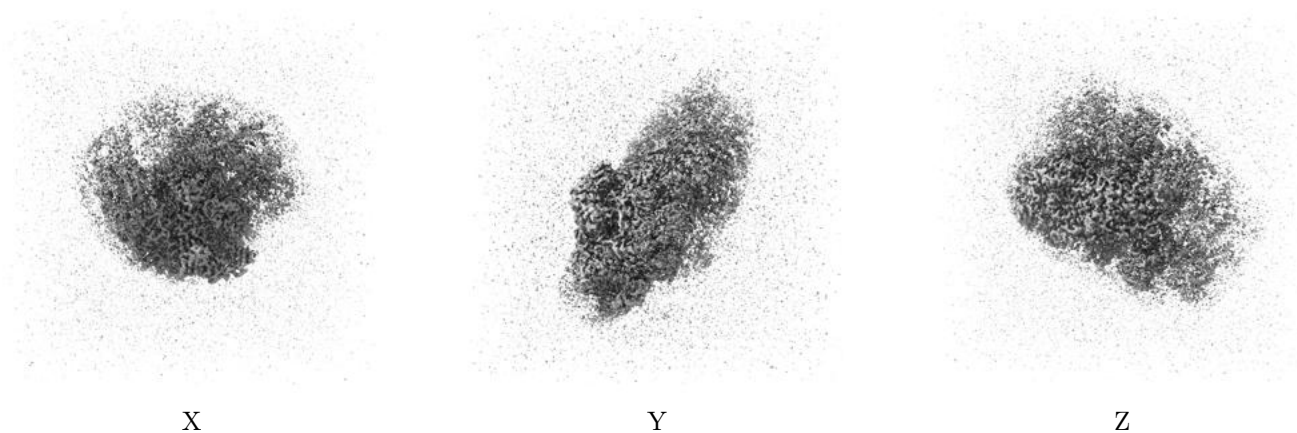
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

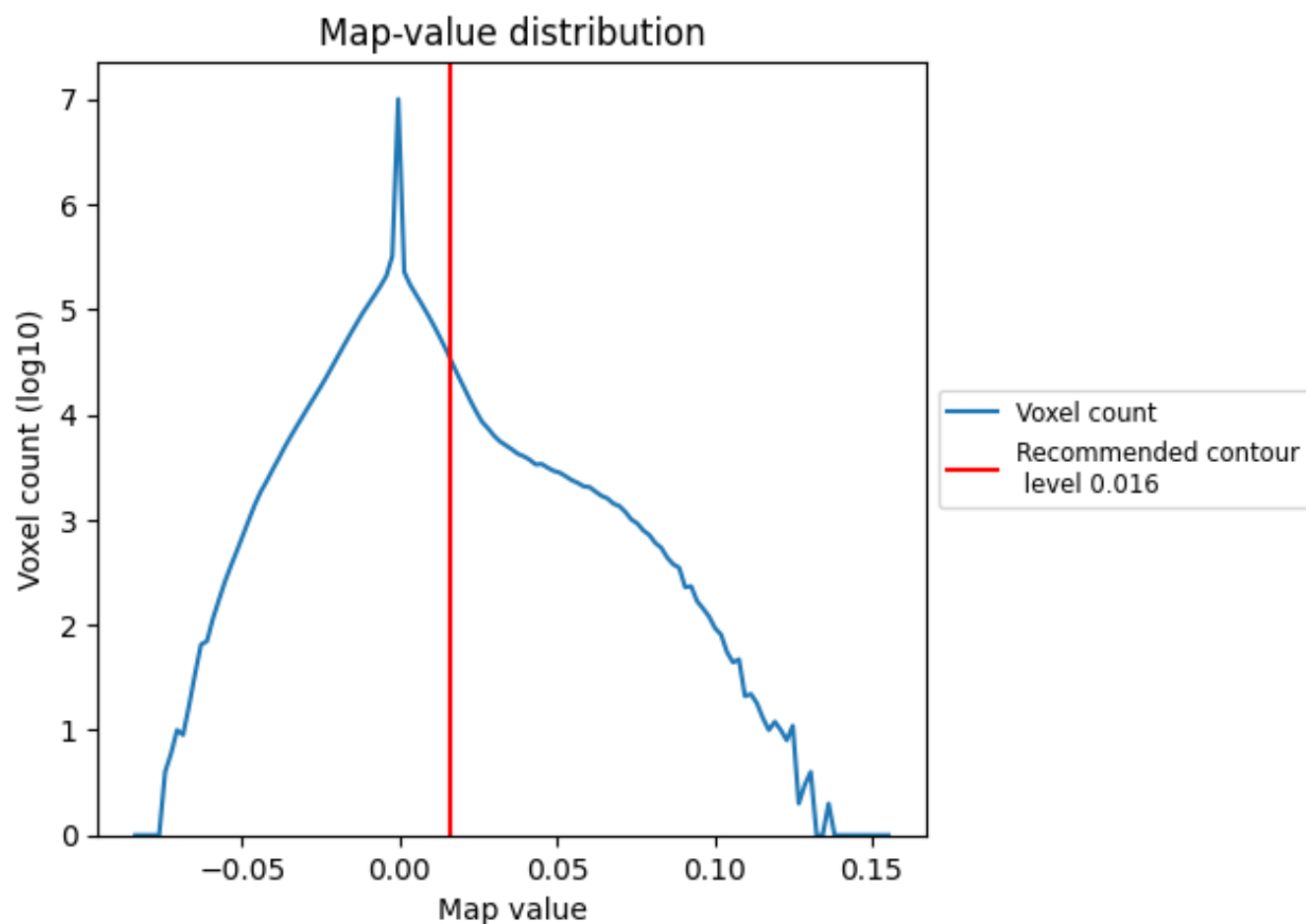
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

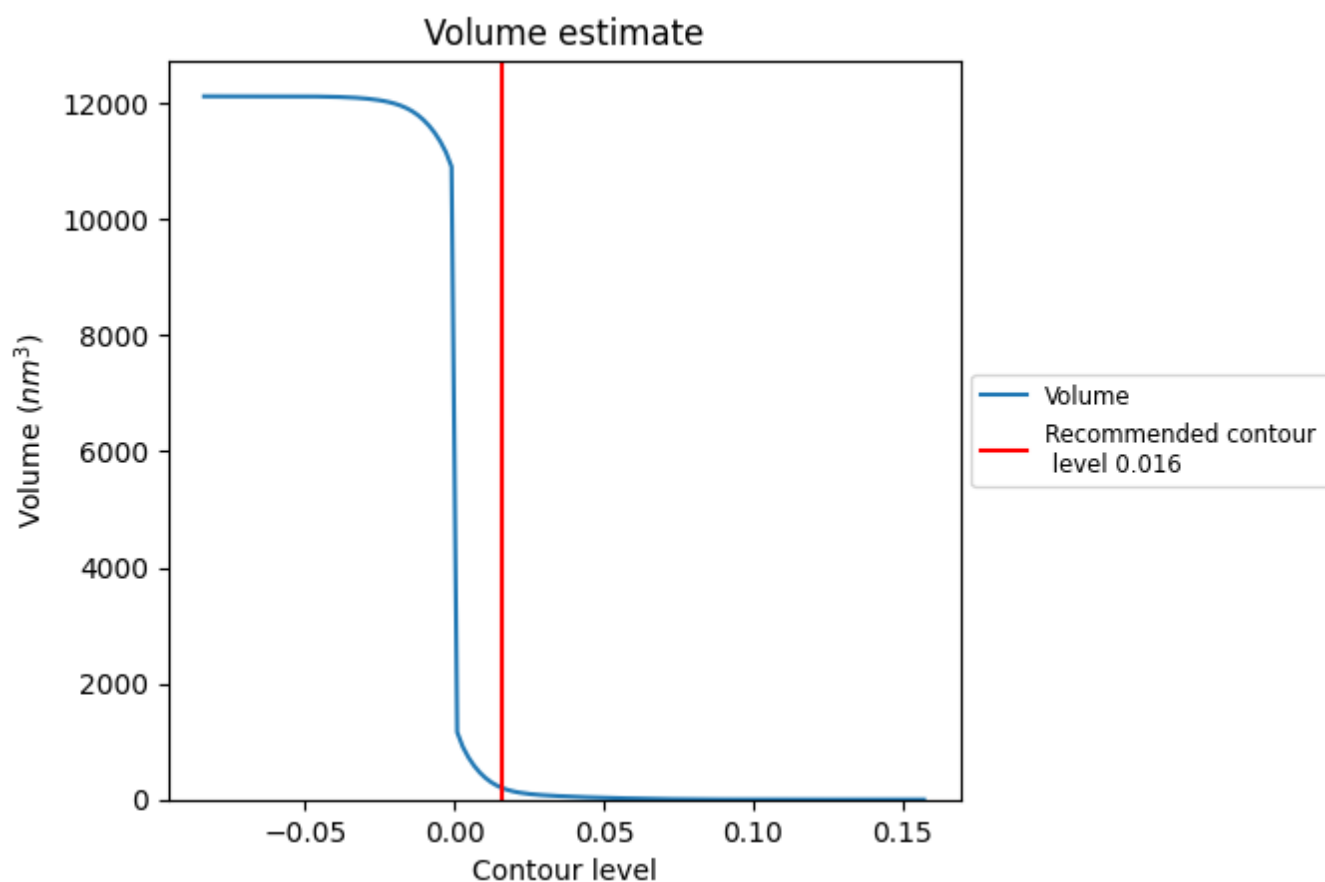
This section contains the results of statistical analysis of the map.

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.

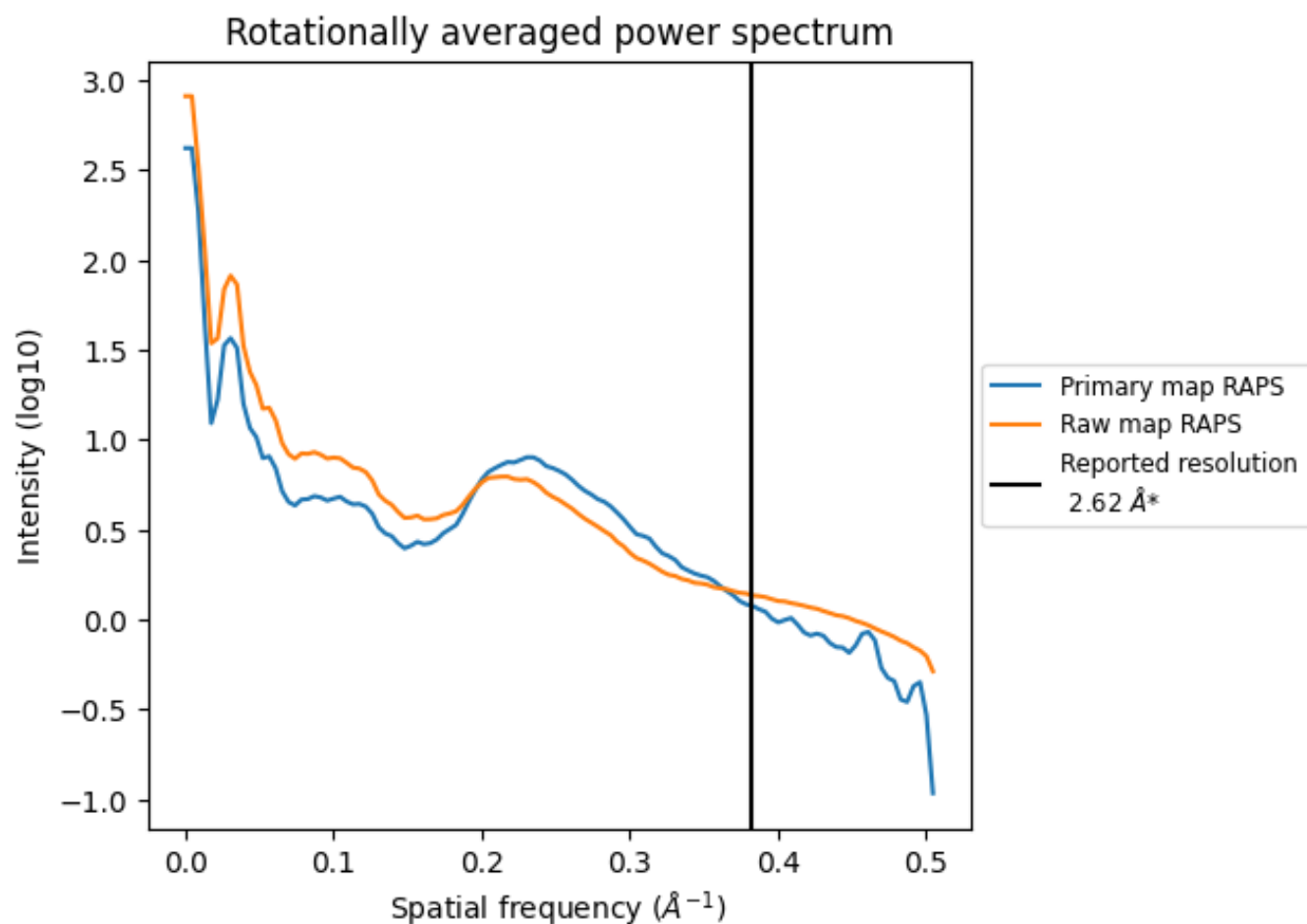
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 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 ⓘ

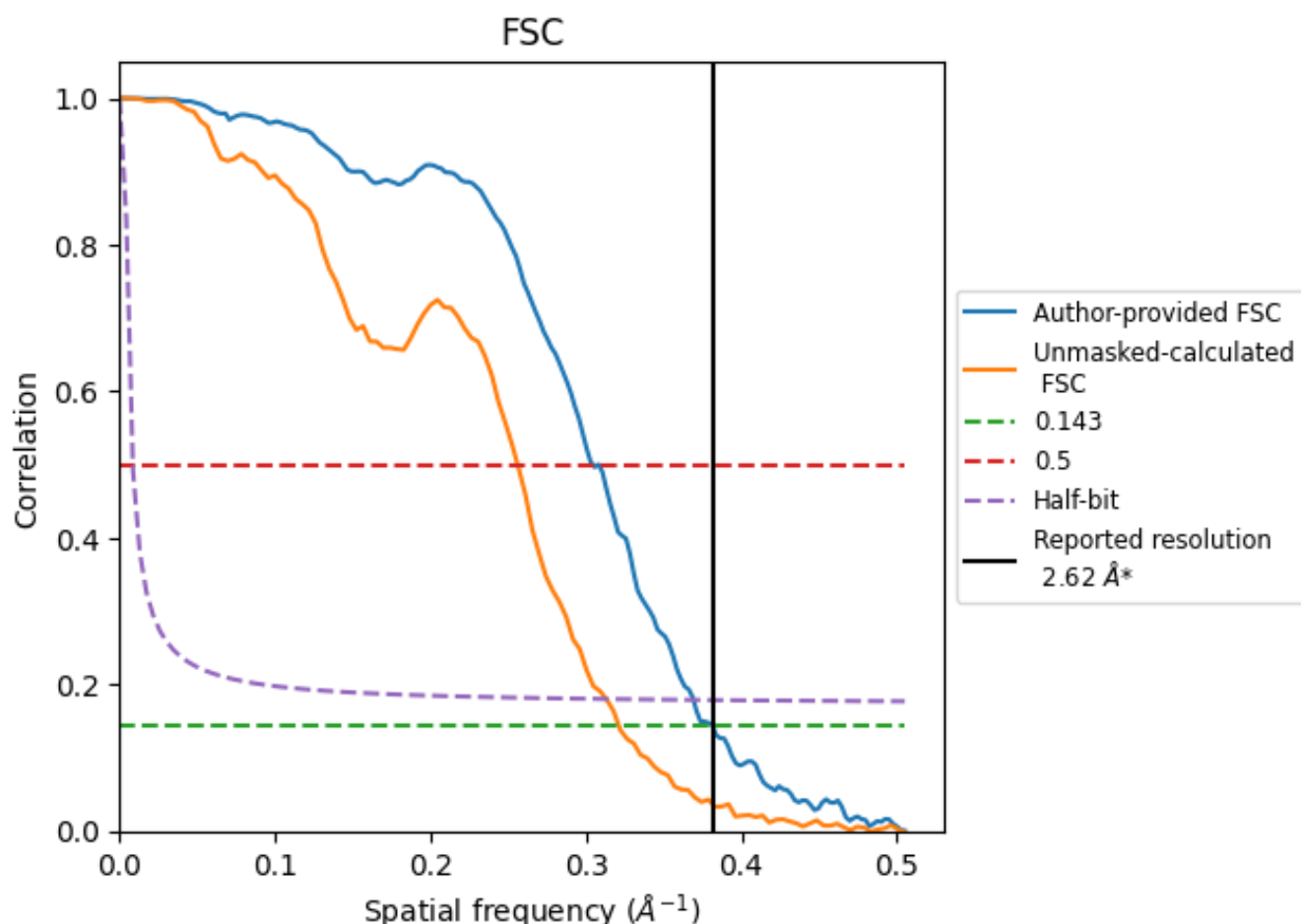


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

8.2 Resolution estimates [i](#)

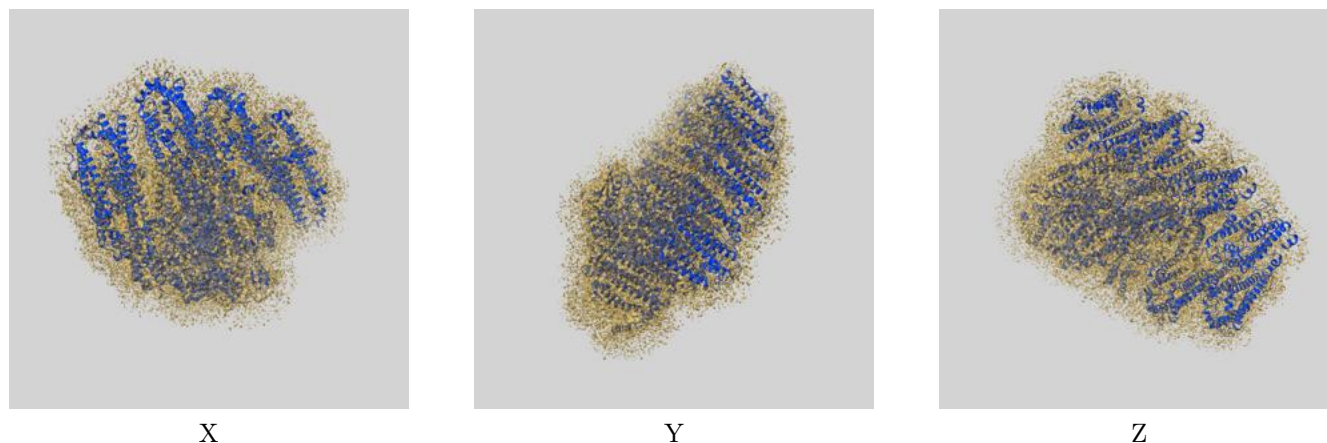
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	3.29	2.71
Unmasked-calculated*	3.11	3.91	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.62 by more than 10 %

9 Map-model fit [i](#)

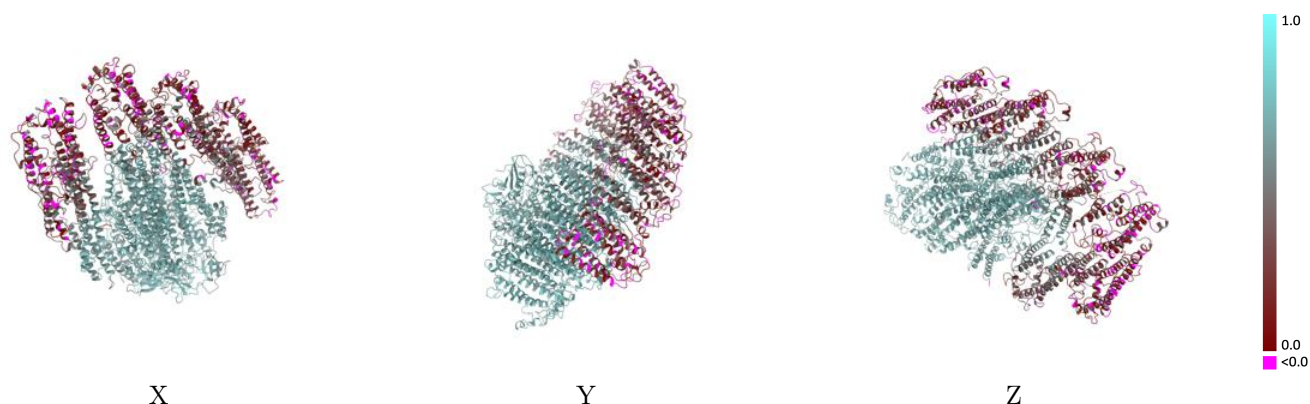
This section contains information regarding the fit between EMDB map EMD-33593 and PDB model 7Y3F. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



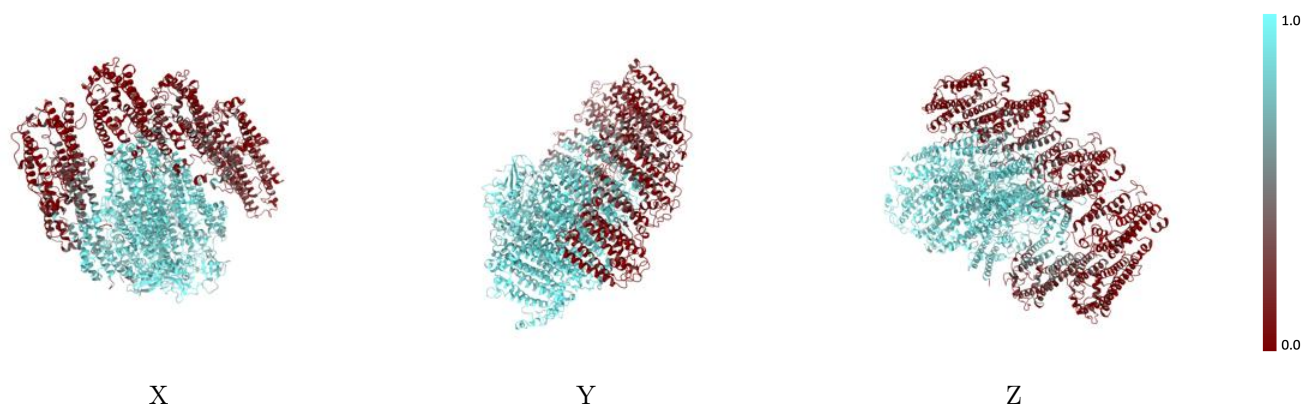
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



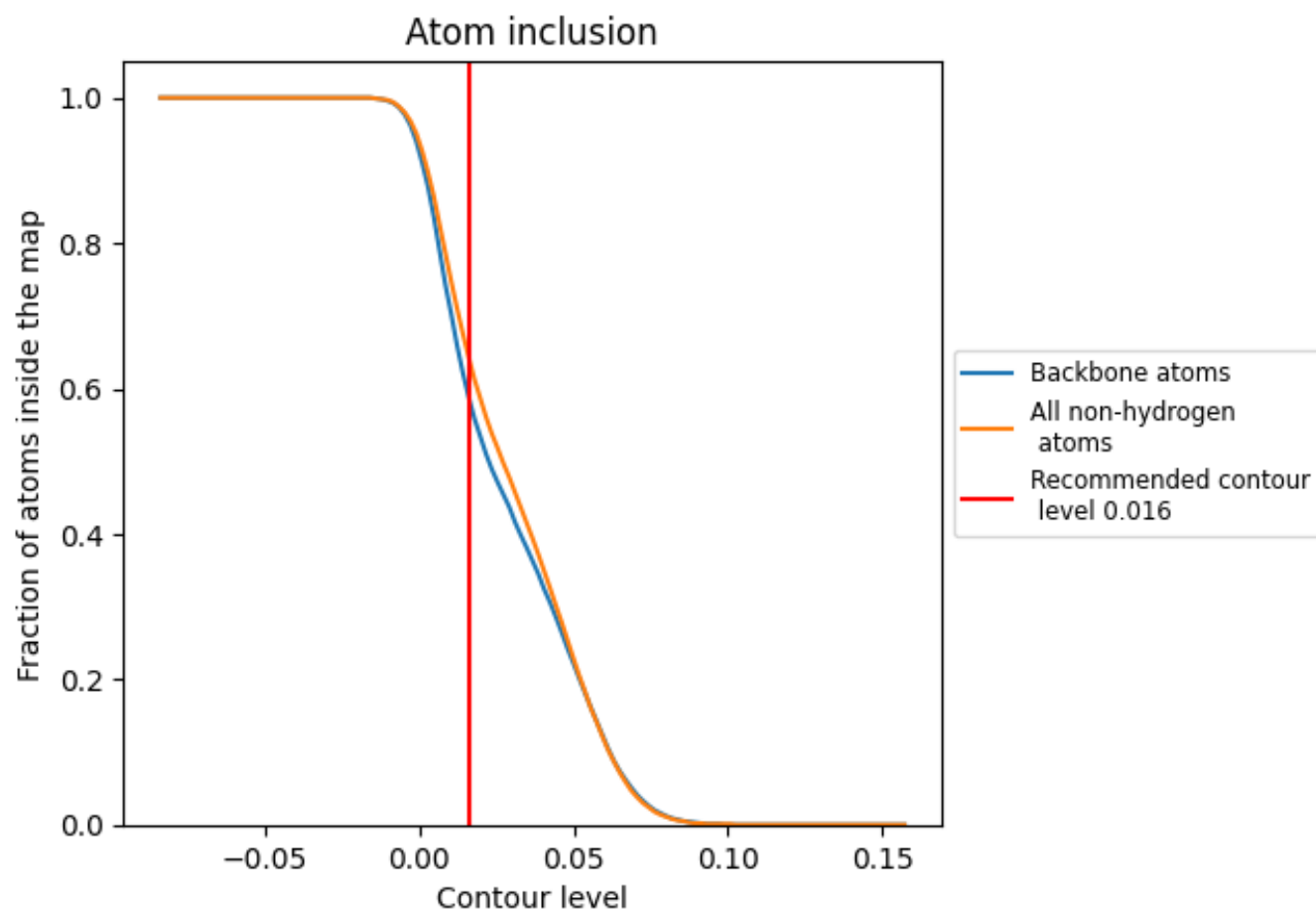
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 64% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6430	<div></div> 0.5260
1	<div></div> 0.5240	<div></div> 0.4830
2	<div></div> 0.1170	<div></div> 0.1960
3	<div></div> 0.0680	<div></div> 0.1850
4	<div></div> 0.1620	<div></div> 0.2490
5	<div></div> 0.2040	<div></div> 0.2940
6	<div></div> 0.0990	<div></div> 0.2000
A	<div></div> 0.9420	<div></div> 0.6910
B	<div></div> 0.9270	<div></div> 0.6830
C	<div></div> 0.9480	<div></div> 0.6910
D	<div></div> 0.8790	<div></div> 0.6540
E	<div></div> 0.8490	<div></div> 0.6230
F	<div></div> 0.8710	<div></div> 0.6580
I	<div></div> 0.8940	<div></div> 0.6640
J	<div></div> 0.9130	<div></div> 0.6690
K	<div></div> 0.8770	<div></div> 0.6230
M	<div></div> 0.8300	<div></div> 0.6290
X	<div></div> 0.8270	<div></div> 0.6290

1.0

0.0

<0.0