



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:28 PM UTC

PDB ID : 5ZGH / pdb_00005zgh
EMDB ID : EMD-6930
Title : Cryo-EM structure of the red algal PSI-LHCR
Authors : Pi, X.
Deposited on : 2018-03-09
Resolution : 3.82 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

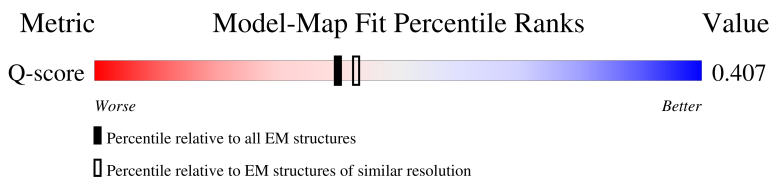
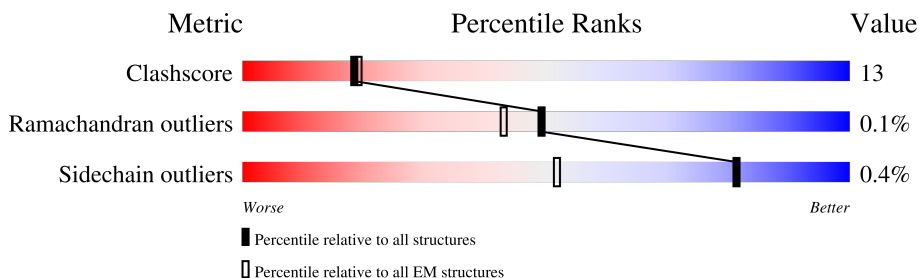
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.82 Å.

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



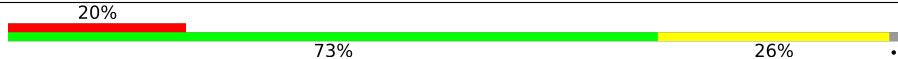
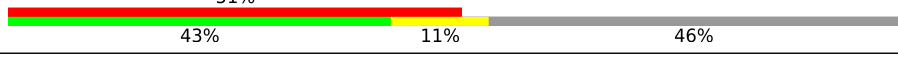
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11696 (3.13 - 4.13)

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	1	175	
2	2	199	
3	3	188	
4	A	748	

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Mol	Chain	Length	Quality of chain
5	B	732	
6	C	81	
7	D	139	
8	E	94	
9	F	185	
10	I	32	
11	J	38	
12	K	60	
13	L	140	
14	M	29	
15	O	155	

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
16	CLA	1	601	X	-	-	-
16	CLA	1	602	X	-	-	-
16	CLA	1	603	X	-	-	-
16	CLA	1	604	X	-	-	-
16	CLA	1	605	X	-	-	-
16	CLA	1	606	X	-	-	-
16	CLA	1	607	X	-	-	-
16	CLA	1	608	X	-	-	-
16	CLA	1	609	X	-	-	-
16	CLA	1	610	X	-	-	-
16	CLA	1	611	X	-	-	-
16	CLA	1	612	X	-	-	-
16	CLA	2	601	X	-	-	-
16	CLA	2	602	X	-	-	-
16	CLA	2	603	X	-	-	-
16	CLA	2	604	X	-	-	-
16	CLA	2	605	X	-	-	-
16	CLA	2	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	2	607	X	-	-	-
16	CLA	2	608	X	-	-	-
16	CLA	2	609	X	-	-	-
16	CLA	2	610	X	-	-	-
16	CLA	2	611	X	-	-	-
16	CLA	2	612	X	-	-	-
16	CLA	2	613	X	-	-	-
16	CLA	3	202	X	-	-	-
16	CLA	3	203	X	-	-	-
16	CLA	3	204	X	-	-	-
16	CLA	3	205	X	-	-	-
16	CLA	3	206	X	-	-	-
16	CLA	3	207	X	-	-	-
16	CLA	3	208	X	-	-	-
16	CLA	3	209	X	-	-	-
16	CLA	3	210	X	-	-	-
16	CLA	3	211	X	-	-	-
16	CLA	3	212	X	-	-	-
16	CLA	3	213	X	-	-	-
16	CLA	A	802	X	-	-	-
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	810	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	817	X	-	-	-
16	CLA	A	818	X	-	-	-
16	CLA	A	819	X	-	-	-
16	CLA	A	820	X	-	-	-
16	CLA	A	821	X	-	-	-
16	CLA	A	822	X	-	-	-
16	CLA	A	823	X	-	-	-
16	CLA	A	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	825	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	832	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	850	X	-	-	-
16	CLA	A	851	X	-	-	-
16	CLA	A	852	X	-	-	-
16	CLA	B	801	X	-	-	-
16	CLA	B	802	X	-	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	-	-	-
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	815	X	-	-	-
16	CLA	B	816	X	-	-	-
16	CLA	B	817	X	-	-	-
16	CLA	B	818	X	-	-	-
16	CLA	B	819	X	-	-	-
16	CLA	B	820	X	-	-	-
16	CLA	B	821	X	-	-	-
16	CLA	B	822	X	-	-	-
16	CLA	B	823	X	-	-	-
16	CLA	B	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	B	841	X	-	-	-
16	CLA	B	842	X	-	-	-
16	CLA	F	802	X	-	-	-
16	CLA	F	803	X	-	-	-
16	CLA	J	101	X	-	-	-
16	CLA	K	101	X	-	-	-
16	CLA	K	102	X	-	-	-
16	CLA	L	201	X	-	-	-
16	CLA	L	203	X	-	-	-
16	CLA	L	204	X	-	-	-
16	CLA	L	205	X	-	-	-
16	CLA	O	201	X	-	-	-
16	CLA	O	202	X	-	-	-
16	CLA	O	203	X	-	-	-
16	CLA	O	204	X	-	-	-
19	CL0	A	801	X	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 30757 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 Lhcr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	169	Total	C	N	O	S	0	0
			1351	887	227	229	8		

- Molecule 2 is a protein called Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	175	Total	C	N	O	S	0	0
			1371	892	233	239	7		

- Molecule 3 is a protein called Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	170	Total	C	N	O	S	0	0
			1303	845	219	232	7		

- Molecule 4 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	741	Total	C	N	O	S	0	0
			5798	3792	996	983	27		

- Molecule 5 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	731	Total	C	N	O	S	0	0
			5819	3827	982	991	19		

- Molecule 6 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	80	Total	C	N	O	S	0	0
			597	367	104	114	12		

- Molecule 7 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	119	Total	C	N	O	S	0	0
			950	600	167	179	4		

- Molecule 8 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	61	Total	C	N	O	0	0
			493	322	79	92		

- Molecule 9 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	154	Total	C	N	O	S	0	0
			1263	811	214	234	4		

- Molecule 10 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	31	Total	C	N	O	S	0	0
			230	158	32	39	1		

- Molecule 11 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	38	Total	C	N	O	S	0	0
			312	214	46	51	1		

- Molecule 12 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	59	Total	C	N	O	S	0	0
			428	279	70	74	5		

- Molecule 13 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	119	Total	C	N	O	S	0	0
			900	591	148	159	2		

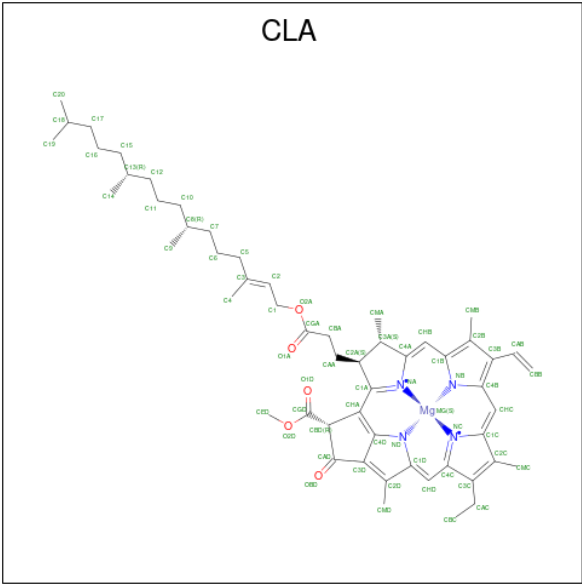
- Molecule 14 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	27	Total	C	N	O	S	0	0
			204	136	32	34	2		

- Molecule 15 is a protein called PsaO.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	83	Total	C	N	O	0	0
			641	439	97	105		

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			59	49	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
			42	34	1	4	3	
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
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
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	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			65	55	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
			42	34	1	4	3	
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
			50	40	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
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	3	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
16	3	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	

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Mol	Chain	Residues	Atoms					AltConf
16	3	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	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	3	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
			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
			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
			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
			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	
16	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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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
			62	52	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
			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
			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
			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
			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
			45	35	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 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 43	C 35	Mg 1	N 4	O 3	0
16	A	1	Total 61	C 51	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 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 55	C 45	Mg 1	N 4	O 5	0

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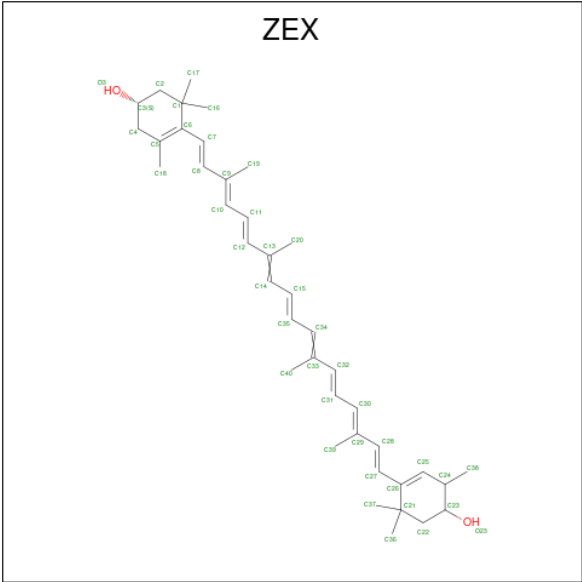
Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
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
			45	35	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	

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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
			60	50	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
			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	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	L	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 17 is (1R,2S)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: C₄₀H₅₆O₂).



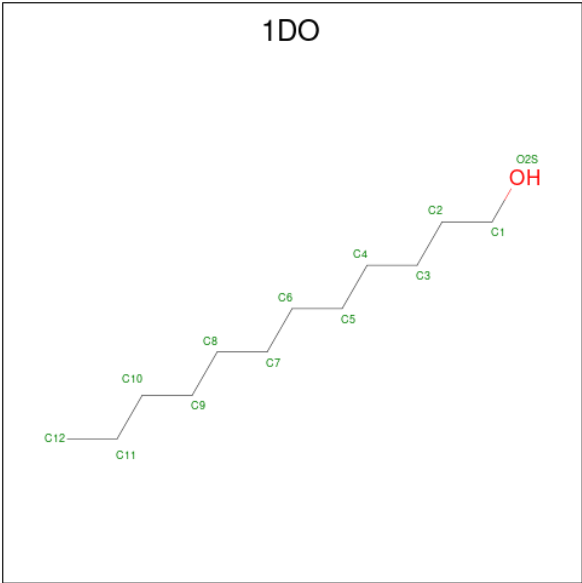
Mol	Chain	Residues	Atoms			AltConf
17	1	1	Total	C	O	0
			42	40	2	
17	1	1	Total	C	O	0
			42	40	2	
17	1	1	Total	C	O	0
			42	40	2	
17	1	1	Total	C	O	0
			42	40	2	
17	1	1	Total	C	O	0
			42	40	2	
17	2	1	Total	C	O	0
			42	40	2	
17	2	1	Total	C	O	0
			42	40	2	
17	2	1	Total	C	O	0
			42	40	2	
17	3	1	Total	C	O	0
			42	40	2	
17	3	1	Total	C	O	0
			42	40	2	
17	3	1	Total	C	O	0
			42	40	2	
17	3	1	Total	C	O	0
			42	40	2	

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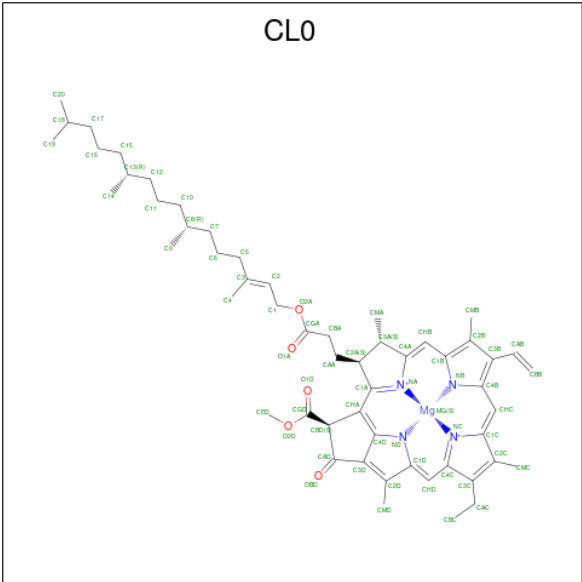
Mol	Chain	Residues	Atoms			AltConf
17	3	1	Total	C	O	0
			42	40	2	

- Molecule 18 is 1-DODECANOL (CCD ID: 1DO) (formula: C₁₂H₂₆O).



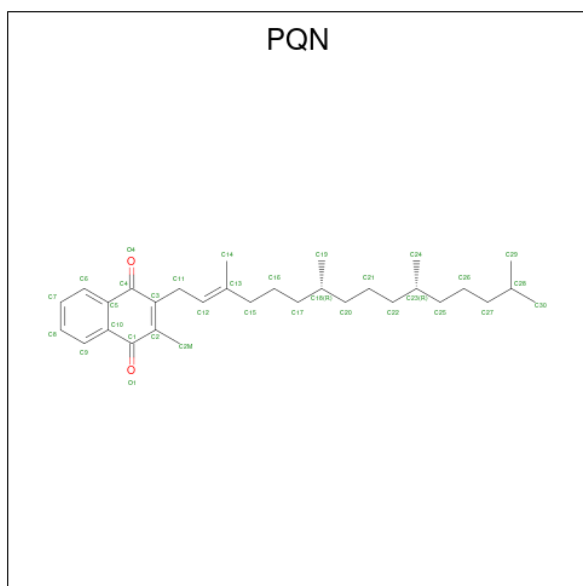
Mol	Chain	Residues	Atoms			AltConf
18	3	1	Total	C	O	0
			13	12	1	

- Molecule 19 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



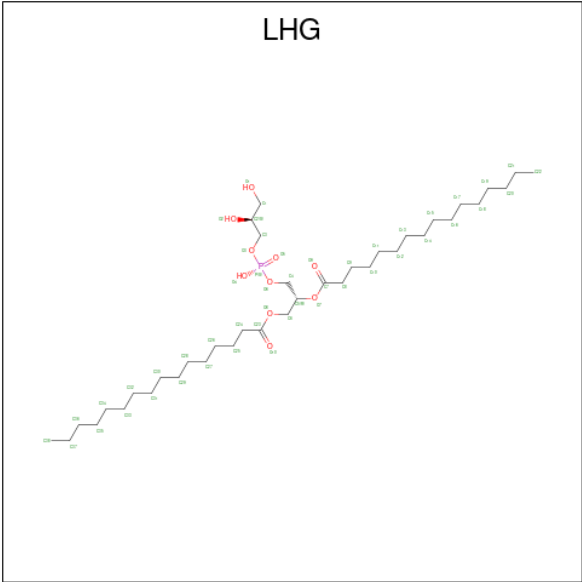
Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



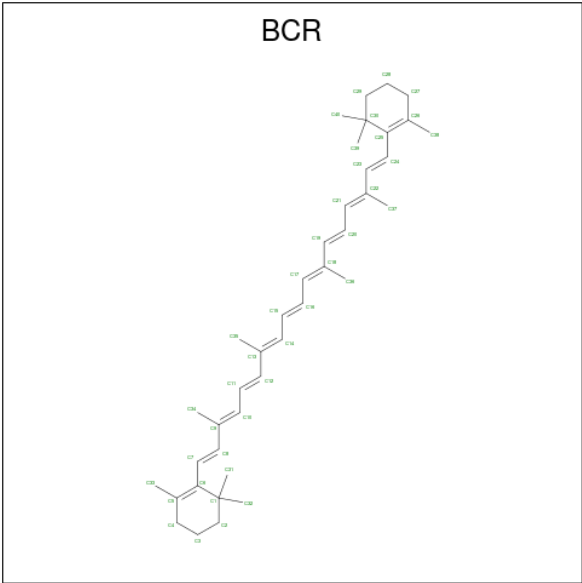
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	O	P	0
			49	38	10	1	
21	A	1	Total	C	O	P	0
			40	29	10	1	

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



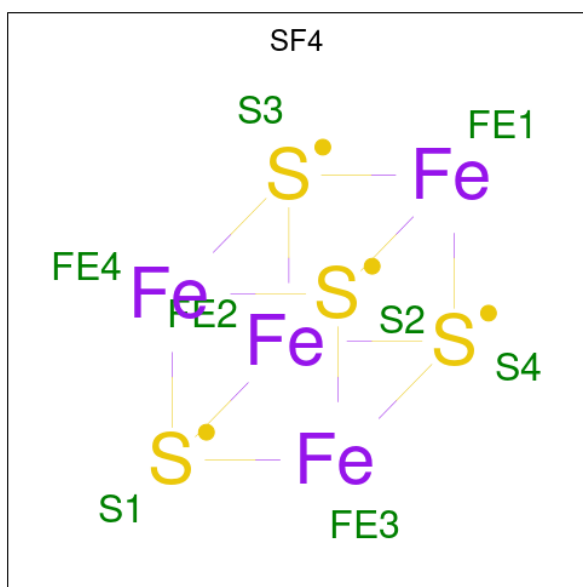
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	

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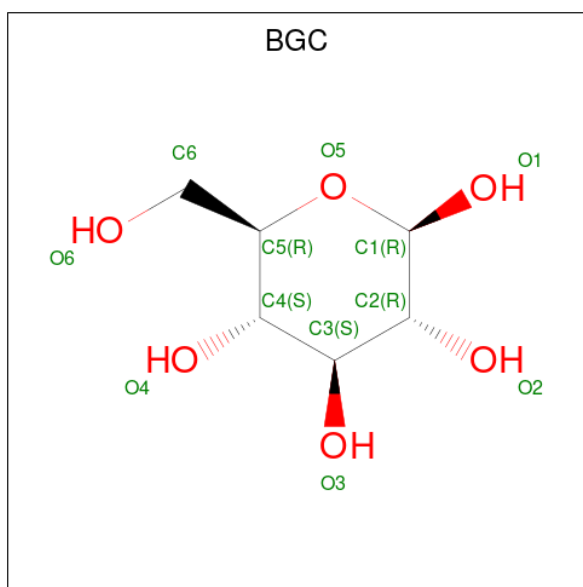
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	F	1	Total C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

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



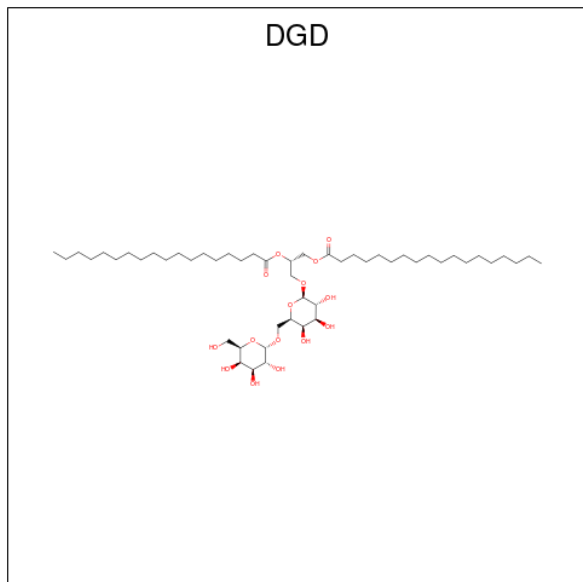
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 24 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



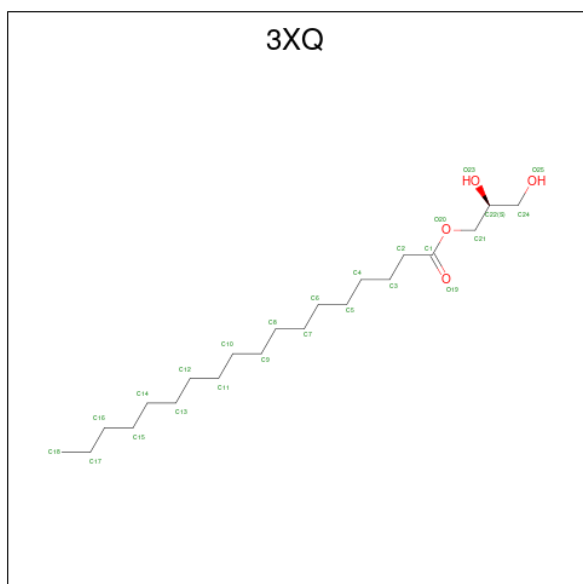
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			11	6	5	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 26 is (2S)-2,3-dihydroxypropyl octadecanoate (CCD ID: 3XQ) (formula: $C_{21}H_{42}O_4$).

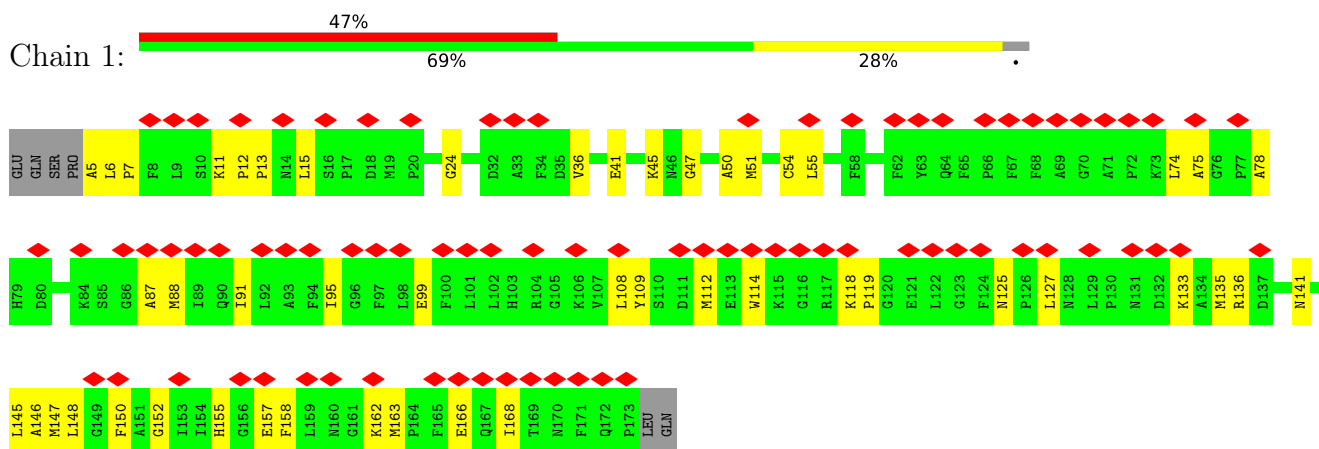


Mol	Chain	Residues	Atoms			AltConf
26	J	1	Total	C	O	0
			25	21	4	

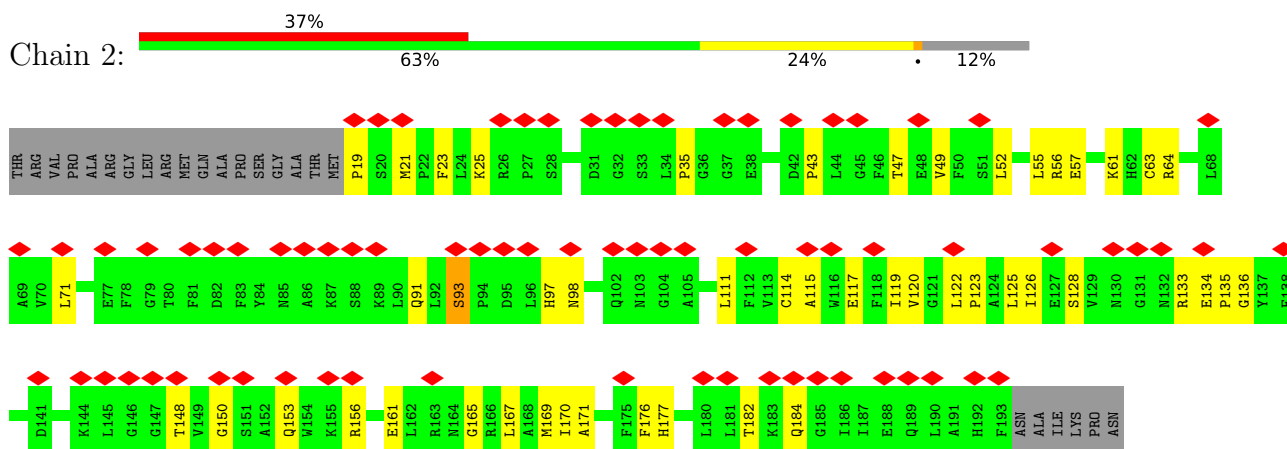
3 Residue-property plots

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.

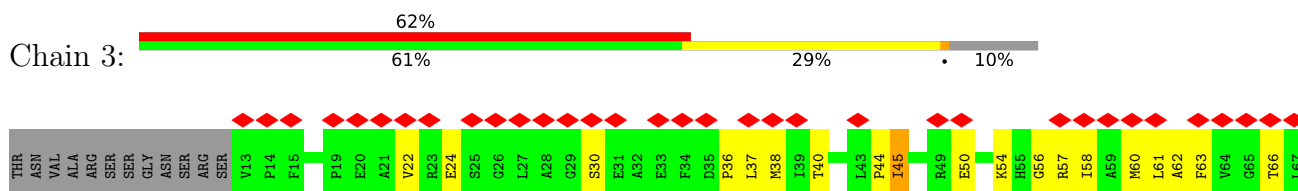
• Molecule 1: Lhcr1

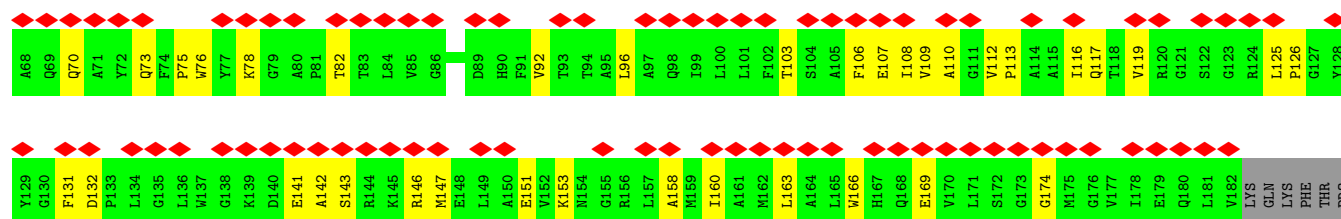


• Molecule 2: Lhcr2

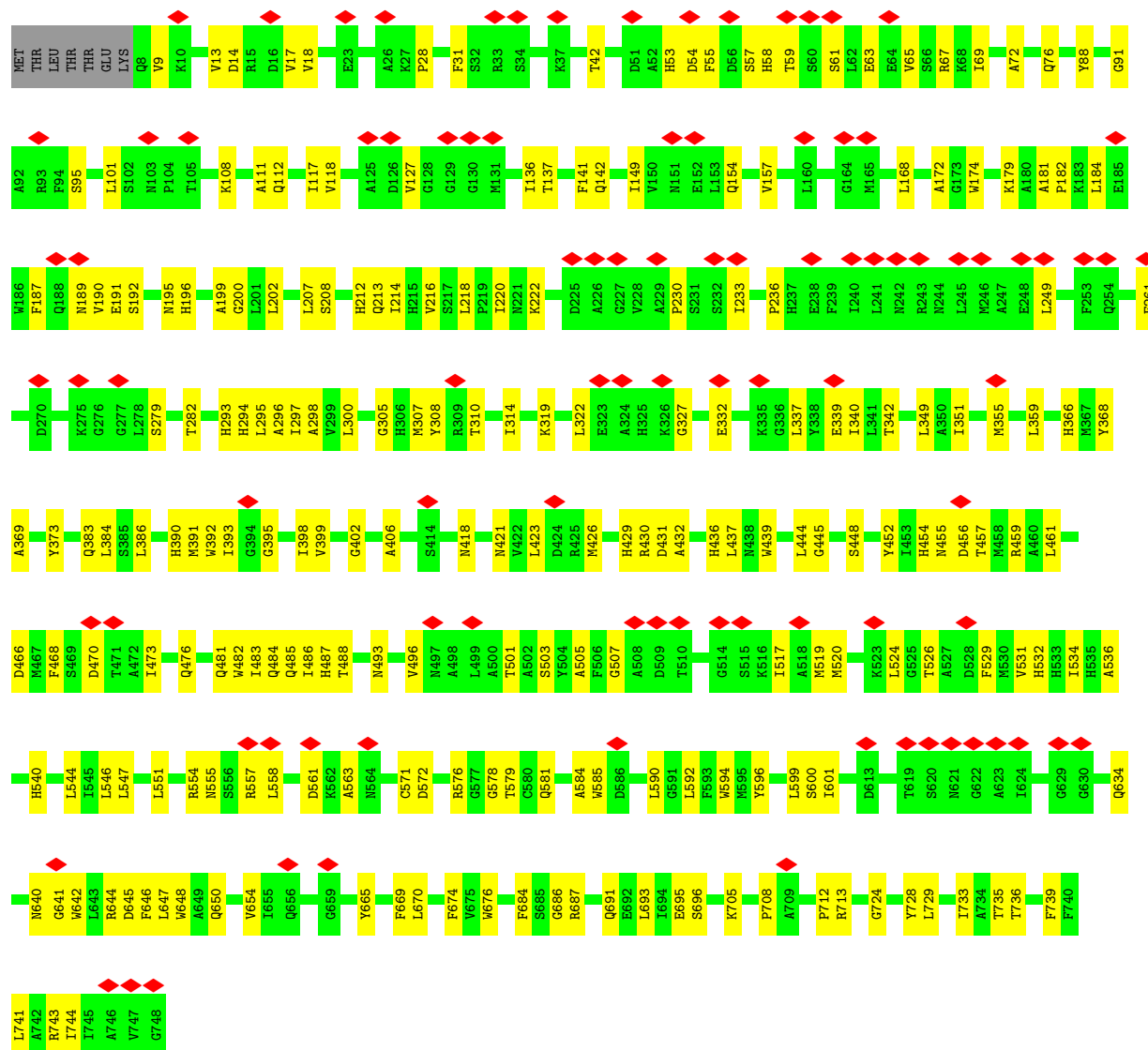


• Molecule 3: Lhcr3

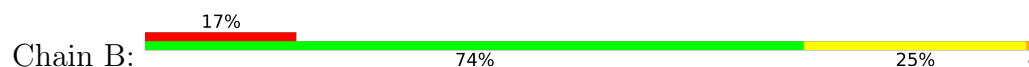


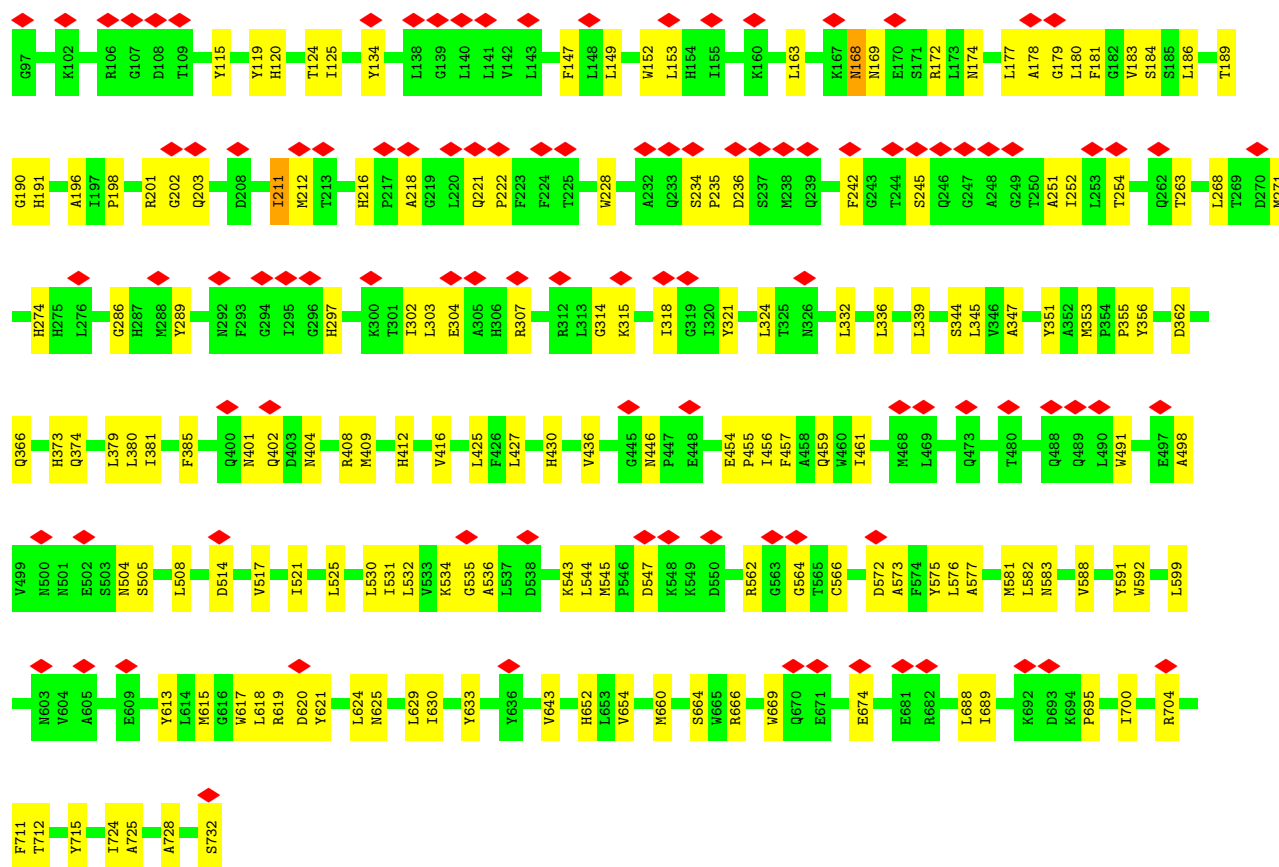


• Molecule 4: PsaA



• Molecule 5: PsaB

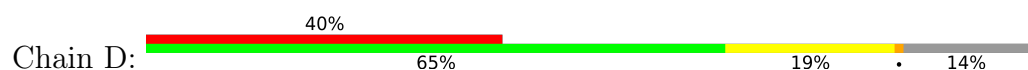




• Molecule 6: PsuC



• Molecule 7: PsuA



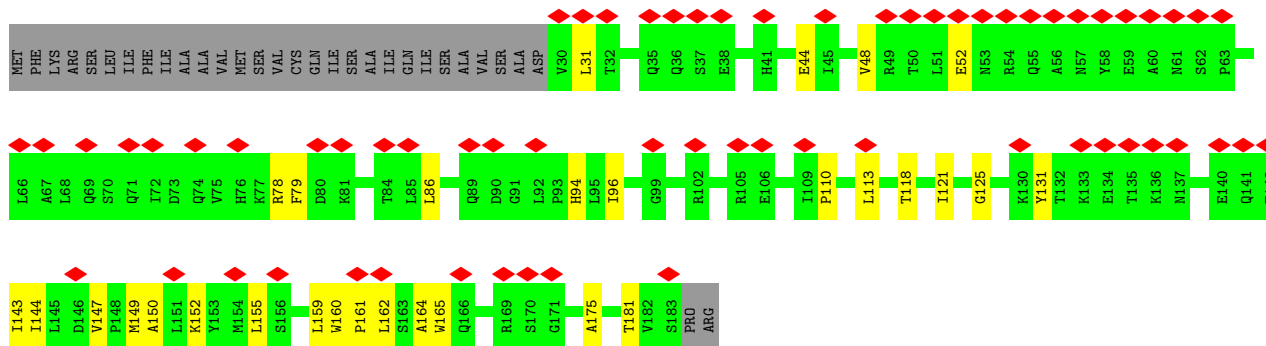
• Molecule 8: PsuB



PRO VAL LYS SER GLU VAL LYS ALA GLU LYS LYS ASN LYS LYS GLY GLY ALA

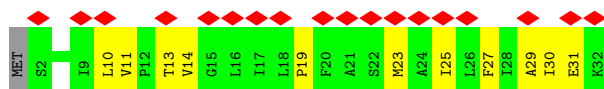
• Molecule 9: PsaF

Chain F: 



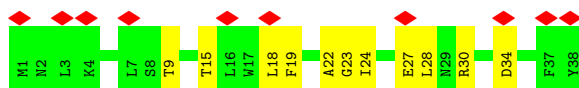
• Molecule 10: PsaI

Chain I: 



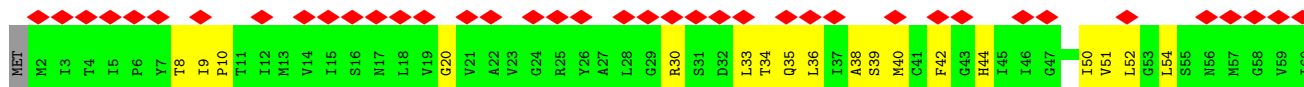
• Molecule 11: PsaJ

Chain J: 



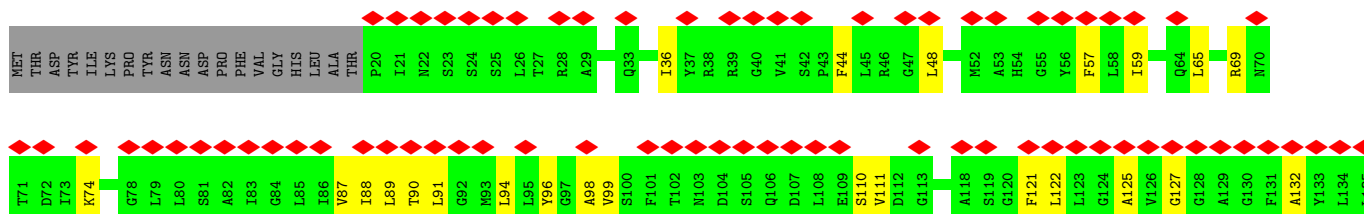
• Molecule 12: PsaK

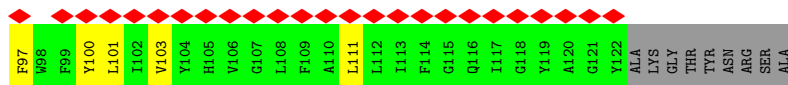
Chain K: 



• Molecule 13: PsaL

Chain L: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76079	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.17	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.584	Depositor
Minimum map value	-0.161	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.087	Depositor
Map size ($\text{\AA}$)	294.0, 294.0, 294.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, BCR, SF4, 1DO, LHG, ZEX, PQN, DGD, BGC, 3XQ, CLA

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	1	0.33	0/1395	0.73	0/1884
2	2	0.33	0/1407	0.72	1/1898 (0.1%)
3	3	0.31	0/1337	0.73	2/1817 (0.1%)
4	A	0.46	0/5985	0.62	1/8158 (0.0%)
5	B	0.42	0/6028	0.62	4/8236 (0.0%)
6	C	0.36	0/607	0.55	0/822
7	D	0.27	0/969	0.59	0/1307
8	E	0.30	0/502	0.54	0/680
9	F	0.30	0/1296	0.59	0/1760
10	I	0.32	0/235	0.82	1/321 (0.3%)
11	J	0.34	0/321	0.53	0/437
12	K	0.30	0/433	0.67	0/588
13	L	0.25	0/919	0.54	0/1247
14	M	0.17	0/205	0.49	0/277
15	O	0.29	0/664	0.69	0/913
All	All	0.39	0/22303	0.64	9/30345 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
5	B	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	14	VAL	N-CA-C	-6.05	106.91	112.96
4	A	571	CYS	CA-CB-SG	-5.37	102.06	114.40
5	B	168	ASN	CA-C-N	5.22	131.51	121.54
5	B	168	ASN	C-N-CA	5.22	131.51	121.54
3	3	131	PHE	CA-C-N	-5.05	117.67	122.37
3	3	131	PHE	C-N-CA	-5.05	117.67	122.37
2	2	93	SER	N-CA-C	5.02	120.90	109.81
5	B	402	GLN	CA-C-N	5.00	131.10	121.54
5	B	402	GLN	C-N-CA	5.00	131.10	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	135	PRO	Peptide
5	B	430	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1351	0	1322	36	0
2	2	1371	0	1362	34	0
3	3	1303	0	1305	43	0
4	A	5798	0	5727	188	0
5	B	5819	0	5648	167	0
6	C	597	0	584	19	0
7	D	950	0	944	24	0
8	E	493	0	509	8	0
9	F	1263	0	1236	24	0
10	I	230	0	253	12	0
11	J	312	0	327	13	0
12	K	428	0	464	14	0
13	L	900	0	931	20	0
14	M	204	0	226	4	0
15	O	641	0	650	9	0
16	1	565	0	443	12	0
16	2	600	0	466	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	3	565	0	440	16	0
16	A	2423	0	2452	111	0
16	B	2484	0	2521	155	0
16	F	86	0	62	4	0
16	J	42	0	31	1	0
16	K	87	0	64	2	0
16	L	228	0	215	3	0
16	O	188	0	144	2	0
17	1	210	0	280	17	0
17	2	168	0	224	11	0
17	3	252	0	336	25	0
18	3	13	0	25	0	0
19	A	65	0	71	55	0
20	A	33	0	46	2	0
20	B	33	0	46	4	0
21	A	89	0	127	3	0
22	A	240	0	336	14	0
22	B	240	0	336	19	0
22	F	80	0	112	3	0
22	I	40	0	56	1	0
22	J	80	0	112	6	0
22	K	40	0	56	4	0
22	L	120	0	168	11	0
23	A	8	0	0	0	0
23	C	16	0	0	1	0
24	A	11	0	9	0	0
25	B	66	0	96	4	0
26	J	25	0	0	0	0
All	All	30757	0	30762	808	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 13.

All (808) 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)
19:A:801:CL0:H66	16:B:802:CLA:CMB	1.58	1.33
4:A:642:TRP:CD1	19:A:801:CL0:H50	1.63	1.32
19:A:801:CL0:C19	16:B:802:CLA:CMB	2.13	1.26
5:B:4:LYS:HB2	5:B:13:ALA:HB1	1.25	1.11
19:A:801:CL0:C9	16:B:802:CLA:O1D	1.98	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:801:CL0:C19	16:B:802:CLA:HMB1	1.81	1.07
5:B:5:PHE:CD2	10:I:30:ILE:HG12	1.88	1.07
5:B:5:PHE:HD2	10:I:30:ILE:HG12	1.15	1.06
4:A:736:THR:HG22	19:A:801:CL0:OBD	1.59	1.02
5:B:5:PHE:HB3	5:B:6:PRO:HD3	1.43	1.01
5:B:4:LYS:HB2	5:B:13:ALA:CB	1.92	0.98
19:A:801:CL0:H66	16:B:802:CLA:HMB3	1.02	0.98
19:A:801:CL0:H47	16:B:802:CLA:O1D	1.63	0.97
4:A:642:TRP:CD1	19:A:801:CL0:C11	2.48	0.97
5:B:5:PHE:HB2	5:B:20:ARG:NH2	1.82	0.94
4:A:534:ILE:HG23	19:A:801:CL0:H69	1.51	0.92
3:3:113:PRO:O	3:3:117:GLN:HB2	1.71	0.90
5:B:4:LYS:CB	5:B:13:ALA:HB1	2.00	0.90
19:A:801:CL0:C19	16:B:802:CLA:HMB3	1.89	0.86
19:A:801:CL0:H65	16:B:802:CLA:CMB	2.05	0.86
19:A:801:CL0:H65	16:B:802:CLA:HMB1	1.59	0.83
4:A:642:TRP:HD1	19:A:801:CL0:H50	1.46	0.81
4:A:642:TRP:O	4:A:646:PHE:HB3	1.84	0.78
4:A:596:TYR:HE2	19:A:801:CL0:O2A	1.66	0.78
5:B:134:TYR:HH	14:M:2:ILE:N	1.84	0.75
10:I:23:MET:O	10:I:27:PHE:HB3	1.86	0.75
19:A:801:CL0:H46	16:B:802:CLA:O1D	1.87	0.74
16:2:608:CLA:HAB	17:2:614:ZEX:H12	1.70	0.74
11:J:23:GLY:HA3	16:J:101:CLA:HAB	1.69	0.74
4:A:601:ILE:HD13	19:A:801:CL0:H60	1.68	0.74
19:A:801:CL0:C19	16:B:802:CLA:C2B	2.65	0.73
22:A:849:BCR:H24C	12:K:42:PHE:HB2	1.70	0.73
9:F:48:VAL:O	9:F:52:GLU:HB2	1.88	0.72
11:J:24:ILE:O	11:J:28:LEU:HB2	1.90	0.71
1:1:47:GLY:O	1:1:51:MET:HB2	1.91	0.71
15:O:97:PHE:O	15:O:101:LEU:HB2	1.90	0.71
19:A:801:CL0:H65	16:B:802:CLA:C2B	2.21	0.71
3:3:106:PHE:O	3:3:110:ALA:HB3	1.90	0.70
5:B:228:TRP:HB3	16:B:818:CLA:H3A	1.72	0.70
16:B:808:CLA:H162	16:B:830:CLA:HBB2	1.72	0.70
5:B:5:PHE:CB	5:B:20:ARG:NH2	2.54	0.70
5:B:615:MET:O	5:B:619:ARG:HB3	1.92	0.69
5:B:521:ILE:HG21	16:B:837:CLA:HAB	1.74	0.68
5:B:545:MET:SD	6:C:66:ARG:NH2	2.66	0.68
7:D:30:MET:HA	7:D:83:ILE:HA	1.76	0.67
2:2:169:MET:HB3	17:2:615:ZEX:H403	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:807:CLA:H2	16:A:827:CLA:H52	1.74	0.67
5:B:491:TRP:HE1	16:B:835:CLA:HED1	1.60	0.67
19:A:801:CL0:O1A	16:B:802:CLA:HMD3	1.94	0.67
1:1:95:ILE:HD11	17:1:616:ZEX:H193	1.77	0.66
4:A:640:ASN:O	4:A:644:ARG:HB3	1.94	0.66
5:B:314:GLY:HA2	5:B:408:ARG:HH21	1.59	0.66
16:A:831:CLA:H142	22:B:849:BCR:H17C	1.77	0.66
16:A:825:CLA:HAB	22:A:846:BCR:HC7	1.77	0.65
5:B:545:MET:HG2	5:B:547:ASP:H	1.59	0.65
6:C:12:ILE:HG21	8:E:52:ASN:HD21	1.62	0.65
5:B:425:LEU:HB3	16:B:833:CLA:HED2	1.79	0.65
4:A:488:THR:HG22	4:A:507:GLY:HA2	1.79	0.65
4:A:349:LEU:HD11	16:A:829:CLA:HBB1	1.77	0.65
1:1:45:LYS:NZ	1:1:99:GLU:OE2	2.30	0.65
4:A:191:GLU:O	4:A:195:ASN:HB2	1.96	0.65
2:2:177:HIS:HE1	17:2:617:ZEX:H14	1.62	0.64
16:A:805:CLA:HBB	16:A:829:CLA:HAB	1.77	0.64
4:A:112:GLN:NE2	16:A:808:CLA:OBD	2.31	0.64
4:A:392:TRP:CD1	16:A:827:CLA:HAB	2.33	0.64
5:B:582:LEU:HD11	5:B:712:THR:HG22	1.80	0.64
5:B:5:PHE:H	5:B:20:ARG:HH21	1.45	0.63
16:A:831:CLA:HBB1	16:A:832:CLA:H2	1.79	0.63
16:B:832:CLA:HBB2	16:B:839:CLA:HHC	1.79	0.63
9:F:160:TRP:O	9:F:164:ALA:HB3	1.99	0.63
4:A:395:GLY:HA3	4:A:599:LEU:HD11	1.81	0.62
5:B:454:GLU:HG3	9:F:31:LEU:HD11	1.81	0.62
4:A:601:ILE:CD1	19:A:801:CL0:H70	2.29	0.62
4:A:735:THR:OG1	19:A:801:CL0:H28	1.99	0.62
1:1:133:LYS:HG3	1:1:135:MET:H	1.63	0.62
16:A:831:CLA:H201	25:B:850:DGD:HA91	1.81	0.62
5:B:530:LEU:O	5:B:534:LYS:HB2	1.99	0.62
17:1:615:ZEX:H34	16:2:605:CLA:HBC3	1.82	0.62
4:A:601:ILE:HD13	19:A:801:CL0:H70	1.81	0.62
4:A:191:GLU:HB3	4:A:308:TYR:HB3	1.81	0.62
3:3:142:ALA:O	3:3:146:ARG:HB2	2.00	0.61
3:3:103:THR:O	3:3:107:GLU:HB2	1.99	0.61
16:B:815:CLA:H42	22:B:845:BCR:H21C	1.83	0.61
5:B:178:ALA:HB2	5:B:286:GLY:HA3	1.83	0.61
5:B:221:GLN:HG2	5:B:222:PRO:HD3	1.81	0.61
4:A:398:ILE:HD12	22:A:846:BCR:H343	1.83	0.60
16:B:811:CLA:H93	16:B:831:CLA:H172	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:141:GLU:HG3	3:3:143:SER:H	1.64	0.60
16:A:806:CLA:HMC3	16:A:807:CLA:HBB	1.83	0.60
16:A:809:CLA:HBB1	16:A:812:CLA:H142	1.84	0.60
16:B:840:CLA:HAB	20:B:843:PQN:H151	1.84	0.60
12:K:35:GLN:O	12:K:39:SER:HB3	2.02	0.60
4:A:366:HIS:ND1	16:A:817:CLA:OBD	2.35	0.60
3:3:113:PRO:O	3:3:117:GLN:CB	2.49	0.60
4:A:641:GLY:O	4:A:645:ASP:HB3	2.02	0.60
4:A:384:LEU:HD22	4:A:744:ILE:HD12	1.84	0.60
22:B:848:BCR:H21C	22:B:848:BCR:H403	1.84	0.60
4:A:432:ALA:O	4:A:436:HIS:ND1	2.34	0.59
15:O:100:TYR:HA	15:O:103:VAL:HG12	1.84	0.59
2:2:47:THR:HG23	2:2:52:LEU:HB2	1.84	0.59
4:A:600:SER:OG	19:A:801:CL0:H29	2.01	0.59
16:B:840:CLA:H112	16:B:841:CLA:H121	1.83	0.59
4:A:355:MET:HG3	16:A:824:CLA:HBB	1.85	0.59
15:O:58:ALA:HB1	15:O:72:LEU:HB2	1.85	0.59
5:B:120:HIS:NE2	5:B:362:ASP:OD2	2.36	0.59
4:A:28:PRO:HG3	9:F:143:ILE:HG21	1.84	0.59
16:B:842:CLA:H2A	16:B:842:CLA:HED2	1.84	0.59
1:1:162:LYS:HG2	1:1:163:MET:HG2	1.84	0.59
16:B:841:CLA:HBB1	22:B:849:BCR:H363	1.85	0.59
19:A:801:CL0:H66	16:B:802:CLA:C2B	2.27	0.58
5:B:20:ARG:HH22	10:I:30:ILE:HG23	1.67	0.58
5:B:235:PRO:HB3	5:B:254:THR:HG21	1.84	0.58
7:D:123:ASN:OD1	7:D:139:ARG:NH1	2.35	0.58
3:3:58:ILE:O	3:3:62:ALA:HB3	2.04	0.58
4:A:319:LYS:NZ	4:A:339:GLU:OE2	2.37	0.58
4:A:483:ILE:O	4:A:487:HIS:ND1	2.31	0.58
16:B:815:CLA:H112	22:B:845:BCR:H381	1.85	0.58
16:B:830:CLA:H52	22:B:845:BCR:H23C	1.86	0.58
12:K:50:ILE:O	12:K:54:LEU:HB2	2.04	0.58
16:3:206:CLA:HAA2	17:3:217:ZEX:H25	1.84	0.57
5:B:347:ALA:HB2	5:B:373:HIS:HB2	1.85	0.57
7:D:82:LYS:NZ	7:D:83:ILE:O	2.33	0.57
2:2:57:GLU:OE2	2:2:61:LYS:NZ	2.36	0.57
2:2:64:ARG:NH1	2:2:161:GLU:OE2	2.37	0.57
16:A:830:CLA:HBB2	16:A:837:CLA:HHC	1.86	0.57
16:A:851:CLA:HBC1	16:B:827:CLA:H172	1.86	0.57
5:B:621:TYR:O	5:B:625:ASN:HB2	2.05	0.57
5:B:543:LYS:HG3	9:F:181:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:611:CLA:HAB	17:3:201:ZEX:H32	1.87	0.57
13:L:44:PHE:O	13:L:48:LEU:HB2	2.04	0.57
4:A:642:TRP:NE1	19:A:801:CL0:C11	2.67	0.57
4:A:676:TRP:CD2	19:A:801:CL0:H6	2.39	0.57
5:B:660:MET:O	5:B:664:SER:OG	2.22	0.57
3:3:22:VAL:HA	3:3:38:MET:HE1	1.87	0.57
4:A:596:TYR:OH	19:A:801:CL0:H7	2.04	0.57
5:B:436:VAL:HG12	16:B:834:CLA:HAC1	1.85	0.57
6:C:73:THR:H	6:C:76:SER:HG	1.52	0.57
9:F:31:LEU:HB3	9:F:86:LEU:HB3	1.85	0.57
6:C:64:SER:OG	23:C:102:SF4:S3	2.59	0.57
1:1:141:ASN:ND2	16:1:609:CLA:O1D	2.38	0.56
4:A:202:LEU:HD11	16:A:828:CLA:H191	1.87	0.56
16:A:808:CLA:H111	22:J:102:BCR:H332	1.87	0.56
16:1:603:CLA:HMC2	17:1:614:ZEX:H11	1.87	0.56
3:3:73:GLN:HG3	3:3:76:TRP:HE1	1.70	0.56
4:A:691:GLN:HE22	4:A:713:ARG:HA	1.70	0.56
16:A:808:CLA:H101	22:J:103:BCR:H372	1.87	0.56
16:A:834:CLA:H2A	16:A:834:CLA:HED3	1.86	0.56
5:B:85:LYS:HD3	5:B:732:SER:HB2	1.87	0.56
5:B:652:HIS:HB3	16:B:802:CLA:HBD	1.87	0.56
16:B:825:CLA:HBA1	22:B:847:BCR:H16C	1.87	0.56
2:2:21:MET:HB3	2:2:23:PHE:HD2	1.70	0.56
2:2:111:LEU:O	2:2:114:CYS:HB2	2.06	0.56
5:B:572:ASP:HA	5:B:575:TYR:HB3	1.88	0.56
16:O:203:CLA:H2A	16:O:203:CLA:HED2	1.86	0.56
16:2:602:CLA:H121	17:2:615:ZEX:H392	1.88	0.56
1:1:87:ALA:HB3	16:1:605:CLA:HBB1	1.88	0.56
5:B:37:MET:SD	5:B:45:LYS:NZ	2.77	0.56
5:B:412:HIS:HB3	16:B:832:CLA:HED1	1.88	0.56
8:E:2:ILE:N	8:E:60:GLU:OE2	2.39	0.56
10:I:25:ILE:O	10:I:29:ALA:HB2	2.06	0.56
5:B:304:GLU:HG3	5:B:318:ILE:HG12	1.88	0.56
17:3:201:ZEX:H403	16:3:206:CLA:HBB2	1.88	0.56
4:A:481:GLN:NE2	4:A:524:LEU:O	2.38	0.56
19:A:801:CL0:H46	19:A:801:CL0:H39	1.87	0.56
16:B:828:CLA:H191	16:B:842:CLA:H152	1.88	0.56
11:J:15:THR:O	11:J:19:PHE:CB	2.54	0.56
2:2:19:PRO:HG3	2:2:25:LYS:HA	1.87	0.55
4:A:213:GLN:NE2	16:A:818:CLA:O1D	2.38	0.55
19:A:801:CL0:H42	16:B:805:CLA:HBB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:618:LEU:HD12	16:B:804:CLA:HED2	1.89	0.55
2:2:93:SER:HB2	2:2:98:ASN:HB2	1.87	0.55
16:3:203:CLA:HAC2	17:3:216:ZEX:H381	1.88	0.55
4:A:572:ASP:OD2	4:A:576:ARG:NH2	2.39	0.55
5:B:172:ARG:HG3	16:B:815:CLA:HBC2	1.88	0.55
16:A:832:CLA:HAC2	16:B:811:CLA:HBB2	1.88	0.55
5:B:573:ALA:O	5:B:577:ALA:HB3	2.07	0.55
4:A:212:HIS:O	4:A:216:VAL:HB	2.07	0.55
11:J:27:GLU:OE1	11:J:30:ARG:NH2	2.39	0.55
3:3:54:LYS:NZ	3:3:107:GLU:OE2	2.34	0.55
3:3:61:LEU:HD23	16:3:205:CLA:HHC	1.87	0.55
22:A:847:BCR:H403	22:A:847:BCR:H371	1.89	0.55
5:B:4:LYS:CB	5:B:13:ALA:CB	2.73	0.55
7:D:30:MET:HE1	7:D:68:LEU:HD22	1.89	0.55
7:D:32:TRP:HH2	7:D:50:MET:HG3	1.71	0.55
1:1:74:LEU:HB3	1:1:78:ALA:HB2	1.89	0.54
6:C:18:VAL:HG22	6:C:26:LEU:HB3	1.88	0.54
4:A:72:ALA:HB1	16:A:804:CLA:HBB1	1.90	0.54
4:A:534:ILE:HG23	19:A:801:CL0:C20	2.31	0.54
4:A:578:GLY:O	5:B:666:ARG:NH2	2.31	0.54
16:B:834:CLA:H2A	16:B:834:CLA:HED2	1.88	0.54
11:J:15:THR:O	11:J:19:PHE:HB3	2.07	0.54
16:A:823:CLA:HAC1	22:A:845:BCR:H23C	1.89	0.54
4:A:459:ARG:NH2	4:A:634:GLN:O	2.37	0.54
16:A:834:CLA:HAC2	15:O:66:VAL:HG11	1.89	0.54
4:A:452:TYR:O	4:A:456:ASP:HB2	2.08	0.54
16:B:811:CLA:H203	22:L:206:BCR:HC7	1.89	0.54
8:E:8:VAL:HG22	8:E:60:GLU:HG3	1.89	0.54
5:B:5:PHE:N	5:B:20:ARG:HH21	2.06	0.54
13:L:121:PHE:O	13:L:125:ALA:HB2	2.08	0.54
4:A:650:GLN:OE1	4:A:743:ARG:NE	2.40	0.54
5:B:26:ALA:HA	16:B:831:CLA:H43	1.90	0.54
16:1:602:CLA:HMC1	17:1:614:ZEX:H32	1.89	0.54
4:A:647:LEU:HD11	19:A:801:CL0:H42	1.90	0.54
4:A:63:GLU:HG2	4:A:184:LEU:HB2	1.89	0.54
4:A:531:VAL:HG13	4:A:534:ILE:HD12	1.88	0.54
4:A:686:GLY:HA3	5:B:566:CYS:HB2	1.89	0.54
16:B:810:CLA:HAB	16:B:811:CLA:HAA2	1.89	0.54
4:A:431:ASP:OD2	4:A:557:ARG:NH2	2.40	0.53
5:B:401:ASN:OD1	5:B:404:ASN:ND2	2.38	0.53
17:3:215:ZEX:H192	17:3:218:ZEX:H393	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:55:PHE:HB3	4:A:65:VAL:HG13	1.91	0.53
4:A:192:SER:O	4:A:196:HIS:ND1	2.29	0.53
4:A:200:GLY:HA3	16:A:812:CLA:HBB1	1.91	0.53
16:A:802:CLA:H112	22:J:103:BCR:H19C	1.90	0.53
5:B:40:GLU:HG2	5:B:163:LEU:HB2	1.90	0.53
5:B:517:VAL:HG11	5:B:591:TYR:CG	2.43	0.53
3:3:147:MET:O	3:3:151:GLU:HB2	2.08	0.53
5:B:379:LEU:HD13	16:B:808:CLA:H122	1.91	0.53
1:1:50:ALA:HB2	17:1:614:ZEX:H202	1.90	0.53
4:A:88:TYR:HE2	22:A:843:BCR:HC42	1.74	0.53
5:B:66:PHE:HZ	14:M:7:VAL:HG13	1.72	0.53
5:B:613:TYR:OH	5:B:619:ARG:NH2	2.42	0.53
5:B:695:PRO:O	6:C:81:TYR:OH	2.27	0.53
20:B:843:PQN:H241	22:L:206:BCR:H11C	1.90	0.53
1:1:168:ILE:HG22	17:1:613:ZEX:H171	1.91	0.53
16:A:826:CLA:H143	16:A:833:CLA:H121	1.90	0.53
1:1:55:LEU:HB3	16:1:604:CLA:HMC2	1.91	0.53
16:A:826:CLA:H161	16:A:833:CLA:H142	1.91	0.53
5:B:71:GLN:NE2	16:B:809:CLA:O1D	2.41	0.53
5:B:216:HIS:ND1	5:B:218:ALA:O	2.42	0.53
5:B:615:MET:O	5:B:619:ARG:CB	2.55	0.53
5:B:700:ILE:HD12	5:B:704:ARG:HH12	1.73	0.52
3:3:132:ASP:OD1	17:3:214:ZEX:O3	2.26	0.52
20:B:843:PQN:H293	22:L:206:BCR:HC8	1.90	0.52
12:K:9:ILE:HD12	12:K:51:VAL:HG13	1.91	0.52
12:K:20:GLY:O	12:K:39:SER:OG	2.27	0.52
16:B:810:CLA:H121	16:B:829:CLA:H162	1.92	0.52
19:A:801:CL0:C4	16:B:802:CLA:ND	2.73	0.52
5:B:6:PRO:C	5:B:8:PHE:H	2.17	0.52
5:B:234:SER:H	5:B:251:ALA:HB2	1.73	0.52
4:A:536:ALA:O	4:A:540:HIS:ND1	2.28	0.52
10:I:25:ILE:O	10:I:29:ALA:CB	2.58	0.52
4:A:713:ARG:NH2	8:E:43:VAL:O	2.43	0.52
16:F:802:CLA:HHC	16:F:802:CLA:HBB1	1.92	0.52
5:B:149:LEU:O	5:B:153:LEU:HB2	2.10	0.52
5:B:307:ARG:HE	5:B:315:LYS:HA	1.75	0.52
16:A:818:CLA:HAB	16:A:818:CLA:H121	1.91	0.52
4:A:393:ILE:HD13	16:A:828:CLA:HHC	1.91	0.51
5:B:211:ILE:HD12	5:B:212:MET:HG2	1.92	0.51
6:C:8:TYR:HE2	7:D:120:ILE:HG13	1.74	0.51
16:1:606:CLA:HBB2	17:1:617:ZEX:H193	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:203:CLA:H2A	16:3:203:CLA:HED3	1.92	0.51
4:A:576:ARG:NH1	7:D:63:GLU:OE1	2.43	0.51
4:A:581:GLN:HE22	5:B:664:SER:HA	1.74	0.51
4:A:596:TYR:CE2	19:A:801:CL0:O2A	2.55	0.51
22:A:847:BCR:H21C	16:B:801:CLA:H93	1.91	0.51
5:B:374:GLN:HE21	5:B:588:VAL:HG11	1.76	0.51
2:2:117:GLU:O	2:2:122:LEU:N	2.44	0.51
4:A:17:VAL:HG21	4:A:181:ALA:HB3	1.91	0.51
4:A:187:PHE:HB3	16:A:824:CLA:H171	1.92	0.51
5:B:531:ILE:HG22	5:B:573:ALA:HA	1.92	0.51
16:B:824:CLA:HAB	16:B:842:CLA:HED1	1.92	0.51
7:D:21:CYS:SG	7:D:22:ALA:N	2.79	0.51
3:3:160:ILE:HA	17:3:218:ZEX:H403	1.93	0.51
4:A:199:ALA:HB2	4:A:305:GLY:HA3	1.91	0.51
16:3:204:CLA:HAC1	16:3:207:CLA:HAB	1.93	0.51
16:3:210:CLA:H2A	16:3:210:CLA:HED3	1.93	0.51
4:A:640:ASN:O	4:A:644:ARG:CB	2.58	0.51
4:A:708:PRO:HG2	4:A:712:PRO:HD3	1.93	0.51
5:B:436:VAL:HG22	16:B:804:CLA:H12	1.93	0.51
12:K:44:HIS:HD2	22:K:103:BCR:HC8	1.75	0.51
16:A:837:CLA:HMC2	16:L:201:CLA:HBC2	1.93	0.51
5:B:4:LYS:CG	5:B:13:ALA:HB1	2.40	0.51
2:2:115:ALA:HA	2:2:119:ILE:HD12	1.93	0.50
16:2:601:CLA:HAA2	17:3:201:ZEX:H221	1.93	0.50
4:A:332:GLU:HB3	4:A:421:ASN:HA	1.93	0.50
4:A:368:TYR:HA	4:A:383:GLN:HE21	1.76	0.50
16:A:816:CLA:C1D	16:A:817:CLA:HBB2	2.41	0.50
4:A:473:ILE:HG12	13:L:69:ARG:HH12	1.76	0.50
4:A:456:ASP:OD1	5:B:633:TYR:OH	2.20	0.50
2:2:148:THR:HB	2:2:153:GLN:HB3	1.94	0.50
16:B:807:CLA:H52	16:B:815:CLA:H61	1.94	0.50
4:A:585:TRP:HE1	16:A:829:CLA:HMD3	1.77	0.50
16:A:806:CLA:H142	16:A:806:CLA:H61	1.94	0.50
4:A:9:VAL:HG21	4:A:310:THR:HB	1.93	0.50
16:A:804:CLA:H202	16:A:812:CLA:H8	1.92	0.50
16:A:850:CLA:CGA	16:A:850:CLA:H3A	2.42	0.50
22:B:847:BCR:H24C	22:B:848:BCR:H402	1.93	0.50
13:L:89:LEU:HD22	22:L:206:BCR:H391	1.93	0.50
16:2:604:CLA:HED2	16:2:604:CLA:H2A	1.93	0.50
5:B:353:MET:HE3	16:B:828:CLA:HMC3	1.94	0.50
5:B:385:PHE:HZ	16:B:827:CLA:HAB	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:121:PHE:O	13:L:125:ALA:CB	2.60	0.50
2:2:148:THR:HG22	2:2:150:GLY:H	1.77	0.50
16:3:206:CLA:H2A	16:3:206:CLA:HED2	1.93	0.50
16:A:839:CLA:H41	16:B:840:CLA:H61	1.94	0.49
1:1:108:LEU:HD13	9:F:155:LEU:HB3	1.92	0.49
3:3:24:GLU:HB2	3:3:40:THR:HG21	1.93	0.49
2:2:91:GLN:HG2	2:2:176:PHE:HD1	1.77	0.49
4:A:576:ARG:O	5:B:666:ARG:NH2	2.44	0.49
3:3:57:ARG:NH1	3:3:151:GLU:OE2	2.45	0.49
4:A:373:TYR:OH	16:A:828:CLA:OBD	2.29	0.49
12:K:36:LEU:O	12:K:40:MET:HB2	2.12	0.49
5:B:216:HIS:HB2	5:B:252:ILE:HD11	1.94	0.49
5:B:532:LEU:HD23	5:B:573:ALA:HB1	1.94	0.49
6:C:7:ILE:HG12	6:C:65:ILE:HG12	1.94	0.49
6:C:17:CYS:SG	6:C:18:VAL:N	2.86	0.49
6:C:27:GLU:HG3	7:D:103:PRO:HB3	1.94	0.49
16:1:603:CLA:HAB	17:1:614:ZEX:H35	1.93	0.49
4:A:596:TYR:OH	19:A:801:CL0:O2D	2.30	0.49
4:A:644:ARG:O	4:A:648:TRP:HB3	2.13	0.49
5:B:5:PHE:HD2	10:I:30:ILE:CG1	2.05	0.49
6:C:3:HIS:HA	6:C:70:GLY:H	1.76	0.49
3:3:63:PHE:CE2	17:3:214:ZEX:H32	2.47	0.49
4:A:149:ILE:HG23	4:A:154:GLN:HB2	1.93	0.49
9:F:144:ILE:HG12	11:J:9:THR:HG22	1.93	0.49
3:3:78:LYS:HG3	16:3:205:CLA:HED2	1.95	0.49
4:A:470:ASP:OD1	4:A:476:GLN:NE2	2.46	0.49
4:A:687:ARG:NH1	4:A:691:GLN:OE1	2.46	0.49
5:B:168:ASN:HB3	16:B:815:CLA:HBC1	1.95	0.49
5:B:351:TYR:HA	5:B:366:GLN:HE21	1.78	0.49
2:2:153:GLN:HA	2:2:156:ARG:HG2	1.95	0.49
16:2:601:CLA:HMA1	17:2:617:ZEX:H221	1.94	0.49
4:A:457:THR:O	4:A:461:LEU:N	2.38	0.49
7:D:43:PRO:HD3	7:D:68:LEU:HD12	1.95	0.49
3:3:112:VAL:HG13	3:3:116:ILE:HD12	1.94	0.49
5:B:169:ASN:OD1	16:B:826:CLA:HHD	2.12	0.49
16:B:840:CLA:H152	16:B:841:CLA:H91	1.95	0.49
5:B:336:LEU:HD22	5:B:380:LEU:HD22	1.94	0.48
4:A:294:HIS:HA	4:A:297:ILE:HD12	1.95	0.48
4:A:496:VAL:N	16:A:834:CLA:O1D	2.46	0.48
4:A:505:ALA:HB2	4:A:519:MET:HE2	1.95	0.48
4:A:691:GLN:HB3	5:B:544:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:501:THR:OG1	4:A:503:SER:O	2.31	0.48
16:B:828:CLA:H71	22:B:848:BCR:H15C	1.94	0.48
4:A:359:LEU:HG	16:A:826:CLA:H41	1.95	0.48
16:B:829:CLA:H141	25:B:850:DGD:HAS1	1.96	0.48
3:3:112:VAL:O	3:3:116:ILE:HB	2.14	0.48
4:A:13:VAL:HA	4:A:182:PRO:HA	1.96	0.48
5:B:289:TYR:HA	5:B:297:HIS:H	1.78	0.48
4:A:484:GLN:NE2	4:A:505:ALA:O	2.46	0.48
16:A:826:CLA:HMA3	16:A:833:CLA:H62	1.96	0.48
5:B:351:TYR:O	5:B:505:SER:OG	2.25	0.48
7:D:33:SER:OG	7:D:54:ASP:OD1	2.31	0.48
16:B:828:CLA:H2	22:B:848:BCR:H351	1.96	0.48
4:A:437:LEU:HD11	4:A:547:LEU:HD12	1.94	0.48
4:A:642:TRP:NE1	19:A:801:CL0:H51	2.29	0.48
16:A:818:CLA:HAB	16:A:818:CLA:H8	1.96	0.48
5:B:29:HIS:HD2	16:B:807:CLA:HAB	1.79	0.48
4:A:337:LEU:HD23	4:A:340:ILE:HD12	1.94	0.47
16:A:831:CLA:H162	16:B:841:CLA:H2	1.94	0.47
5:B:324:LEU:HD22	16:B:826:CLA:HBC2	1.96	0.47
5:B:666:ARG:O	5:B:669:TRP:N	2.47	0.47
13:L:110:SER:OG	13:L:111:VAL:N	2.47	0.47
2:2:43:PRO:HD2	17:2:615:ZEX:H23	1.95	0.47
5:B:134:TYR:OH	14:M:2:ILE:N	2.45	0.47
16:B:804:CLA:H101	16:B:804:CLA:H41	1.96	0.47
16:B:821:CLA:H93	16:B:826:CLA:H152	1.97	0.47
15:O:82:ARG:NH2	15:O:94:ASP:OD1	2.47	0.47
2:2:117:GLU:HG2	16:2:607:CLA:NB	2.28	0.47
4:A:296:ALA:O	4:A:300:LEU:HB3	2.14	0.47
4:A:592:LEU:HD21	16:A:829:CLA:HBC1	1.96	0.47
19:A:801:CL0:C4	16:B:802:CLA:C4D	2.92	0.47
10:I:19:PRO:HG3	22:I:101:BCR:H14C	1.95	0.47
12:K:35:GLN:O	12:K:39:SER:CB	2.63	0.47
13:L:57:PHE:CE2	16:L:204:CLA:HBB1	2.50	0.47
2:2:57:GLU:HG2	2:2:125:LEU:HD13	1.97	0.47
16:A:827:CLA:H202	16:B:804:CLA:H152	1.95	0.47
3:3:75:PRO:HB3	17:3:217:ZEX:H393	1.96	0.47
3:3:106:PHE:O	3:3:110:ALA:CB	2.62	0.47
4:A:220:ILE:HD11	4:A:236:PRO:HG3	1.95	0.47
16:B:830:CLA:H3A	16:B:830:CLA:HBA2	1.58	0.47
16:A:802:CLA:H152	16:A:838:CLA:H203	1.95	0.47
16:B:803:CLA:H43	16:B:833:CLA:HED1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:161:PRO:O	9:F:165:TRP:HB2	2.14	0.47
12:K:34:THR:O	12:K:38:ALA:HB3	2.15	0.47
2:2:49:VAL:HG13	4:A:179:LYS:HD2	1.96	0.47
3:3:169:GLU:HB2	3:3:174:GLY:HA2	1.96	0.47
5:B:629:LEU:HD12	5:B:725:ALA:HB3	1.96	0.47
5:B:711:PHE:O	5:B:715:TYR:HB2	2.15	0.47
16:B:833:CLA:HBB1	22:F:801:BCR:H323	1.96	0.47
9:F:144:ILE:HA	11:J:9:THR:HA	1.95	0.47
9:F:161:PRO:O	9:F:165:TRP:CB	2.63	0.47
13:L:87:VAL:O	13:L:91:LEU:HB2	2.15	0.47
13:L:96:TYR:HB2	22:L:206:BCR:H361	1.95	0.47
19:A:801:CL0:H7	19:A:801:CL0:CGD	2.45	0.47
5:B:724:ILE:O	5:B:728:ALA:HB3	2.15	0.47
16:B:829:CLA:H142	16:B:831:CLA:H192	1.97	0.47
16:B:833:CLA:H201	16:B:838:CLA:H111	1.96	0.47
3:3:108:ILE:HG13	3:3:109:VAL:HG13	1.97	0.47
4:A:314:ILE:HG12	12:K:30:ARG:HH12	1.79	0.47
5:B:190:GLY:HA3	16:B:817:CLA:HAB	1.96	0.47
7:D:82:LYS:HD3	7:D:96:HIS:HB3	1.96	0.47
7:D:120:ILE:HG23	7:D:123:ASN:HD22	1.79	0.47
15:O:55:SER:HA	15:O:73:THR:HG21	1.95	0.47
15:O:91:PRO:HG2	15:O:93:LEU:HG	1.97	0.47
4:A:601:ILE:HG23	19:A:801:CL0:H55	1.96	0.47
16:B:802:CLA:H201	16:B:811:CLA:H3A	1.97	0.47
4:A:207:LEU:HD12	4:A:298:ALA:HB1	1.97	0.46
4:A:351:ILE:HG12	22:A:845:BCR:H371	1.95	0.46
16:A:822:CLA:H3A	16:A:822:CLA:HBA2	1.59	0.46
16:B:812:CLA:HHC	16:B:812:CLA:HBB1	1.97	0.46
7:D:82:LYS:HD2	7:D:83:ILE:HD12	1.96	0.46
22:J:102:BCR:H12C	22:J:103:BCR:H362	1.96	0.46
12:K:50:ILE:O	12:K:54:LEU:CB	2.63	0.46
1:1:148:LEU:HD13	17:1:615:ZEX:H12	1.97	0.46
4:A:214:ILE:HA	4:A:218:LEU:HD12	1.96	0.46
4:A:399:VAL:HG22	4:A:546:LEU:HD11	1.96	0.46
4:A:670:LEU:HD11	5:B:615:MET:HB2	1.97	0.46
6:C:27:GLU:OE2	6:C:44:ARG:NH2	2.48	0.46
2:2:93:SER:HA	2:2:97:HIS:HB3	1.96	0.46
4:A:261:PHE:HA	16:K:102:CLA:HBC3	1.98	0.46
4:A:351:ILE:HG12	22:A:845:BCR:H24C	1.97	0.46
4:A:418:ASN:HD21	4:A:423:LEU:HD13	1.80	0.46
4:A:529:PHE:HA	16:A:836:CLA:HED1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:825:CLA:HAB	22:A:846:BCR:C7	2.45	0.46
5:B:87:LEU:O	5:B:119:TYR:OH	2.31	0.46
4:A:327:GLY:HA3	21:A:842:LHG:HC32	1.97	0.46
4:A:402:GLY:HA3	4:A:546:LEU:HD22	1.97	0.46
5:B:4:LYS:HB2	5:B:13:ALA:HB2	1.91	0.46
16:B:818:CLA:CHD	16:B:819:CLA:HBB2	2.46	0.46
16:F:802:CLA:HBC2	11:J:18:LEU:HD21	1.97	0.46
19:A:801:CL0:H36	16:B:802:CLA:ND	2.31	0.46
5:B:115:TYR:H	16:B:810:CLA:HMD1	1.81	0.46
13:L:127:GLY:HA3	22:L:207:BCR:H312	1.96	0.46
4:A:322:LEU:HD13	4:A:337:LEU:HB2	1.96	0.46
16:A:851:CLA:OBD	16:B:832:CLA:H3A	2.16	0.46
16:B:836:CLA:HBA2	16:B:836:CLA:H3A	1.46	0.46
9:F:147:VAL:HA	9:F:150:ALA:HB3	1.97	0.46
4:A:17:VAL:HG12	4:A:18:VAL:HG23	1.97	0.46
4:A:293:HIS:CE1	4:A:297:ILE:HD11	2.51	0.46
4:A:386:LEU:O	4:A:390:HIS:ND1	2.39	0.46
4:A:391:MET:HG3	4:A:599:LEU:HD22	1.98	0.46
4:A:406:ALA:HB1	4:A:584:ALA:HB1	1.97	0.46
4:A:600:SER:HB3	19:A:801:CL0:CED	2.46	0.46
16:A:802:CLA:HBB2	16:A:810:CLA:H121	1.97	0.46
16:A:825:CLA:H3A	16:A:825:CLA:HBA2	1.63	0.46
5:B:303:LEU:HD12	5:B:321:TYR:HB2	1.97	0.46
16:B:829:CLA:CGA	16:B:829:CLA:H3A	2.44	0.46
2:2:134:GLU:O	2:2:136:GLY:N	2.47	0.46
16:3:212:CLA:HBA2	16:3:212:CLA:H3A	1.50	0.46
4:A:454:HIS:NE2	4:A:466:ASP:O	2.43	0.46
4:A:485:GLN:O	4:A:488:THR:OG1	2.27	0.46
5:B:177:LEU:HA	5:B:181:PHE:HD2	1.81	0.46
5:B:339:LEU:HD21	16:B:807:CLA:H51	1.97	0.46
19:A:801:CL0:H9	19:A:801:CL0:H72	1.30	0.46
16:B:809:CLA:HMB3	16:B:810:CLA:HHB	1.98	0.46
16:B:825:CLA:HAB	16:B:832:CLA:HMD1	1.98	0.46
4:A:76:GLN:HE21	16:A:804:CLA:HMB3	1.81	0.46
4:A:137:THR:HG21	4:A:741:LEU:HD22	1.98	0.46
4:A:174:TRP:HB2	16:A:810:CLA:HMC2	1.98	0.46
4:A:430:ARG:NH1	4:A:551:LEU:O	2.47	0.46
5:B:508:LEU:HD22	5:B:599:LEU:HD11	1.98	0.46
6:C:16:GLN:O	6:C:20:ALA:HB2	2.15	0.46
4:A:444:LEU:O	4:A:448:SER:OG	2.33	0.45
4:A:455:ASN:OD1	4:A:468:PHE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:19:ARG:NH1	6:C:77:MET:SD	2.73	0.45
5:B:620:ASP:HA	5:B:624:LEU:HD12	1.98	0.45
1:1:75:ALA:HB3	1:1:157:GLU:HG3	1.97	0.45
16:A:805:CLA:HBA2	16:A:805:CLA:HBD	1.97	0.45
5:B:4:LYS:CE	5:B:4:LYS:HA	2.42	0.45
5:B:498:ALA:O	5:B:504:ASN:ND2	2.48	0.45
16:B:825:CLA:H52	16:B:826:CLA:H151	1.97	0.45
6:C:16:GLN:O	6:C:20:ALA:CB	2.65	0.45
1:1:147:MET:HB3	17:1:614:ZEX:H403	1.97	0.45
3:3:158:ALA:HB2	17:3:214:ZEX:H403	1.97	0.45
4:A:9:VAL:HA	4:A:189:ASN:HD21	1.81	0.45
16:A:802:CLA:H122	16:A:802:CLA:H162	1.70	0.45
16:A:838:CLA:H202	11:J:18:LEU:HD22	1.98	0.45
5:B:531:ILE:HG12	16:B:801:CLA:HMD3	1.97	0.45
6:C:8:TYR:CE2	7:D:120:ILE:HG13	2.52	0.45
13:L:69:ARG:HA	13:L:74:LYS:HG2	1.98	0.45
2:2:182:THR:HG22	2:2:184:GLN:H	1.81	0.45
3:3:50:GLU:O	3:3:54:LYS:HB2	2.16	0.45
3:3:116:ILE:HA	3:3:119:VAL:HG12	1.99	0.45
16:A:826:CLA:H162	16:A:826:CLA:H121	1.70	0.45
5:B:124:THR:HG21	5:B:356:TYR:HA	1.98	0.45
5:B:454:GLU:HG2	9:F:94:HIS:HB3	1.98	0.45
5:B:455:PRO:HG3	5:B:514:ASP:HB3	1.99	0.45
1:1:15:LEU:HA	1:1:36:VAL:HG11	1.97	0.45
16:3:203:CLA:HAB	17:3:215:ZEX:H12	1.98	0.45
4:A:517:ILE:HG21	4:A:520:MET:HE3	1.99	0.45
16:B:811:CLA:H122	16:B:811:CLA:H8	1.80	0.45
2:2:167:LEU:O	2:2:171:ALA:CB	2.64	0.45
4:A:687:ARG:NH2	5:B:564:GLY:O	2.41	0.45
19:A:801:CL0:H46	19:A:801:CL0:C5	2.45	0.45
5:B:5:PHE:HB3	5:B:6:PRO:CD	2.28	0.45
5:B:592:TRP:HB2	16:B:837:CLA:HMC1	1.99	0.45
16:B:840:CLA:H18	16:B:841:CLA:H8	1.97	0.45
1:1:125:ASN:OD1	17:1:613:ZEX:O23	2.26	0.45
4:A:54:ASP:HB3	4:A:57:SER:HB3	1.98	0.45
4:A:594:TRP:HE1	16:A:850:CLA:CHD	2.30	0.45
16:B:812:CLA:H172	13:L:87:VAL:HG21	1.99	0.45
2:2:63:CYS:HB2	2:2:165:GLY:HA3	1.97	0.45
4:A:14:ASP:OD2	4:A:67:ARG:NH2	2.49	0.45
4:A:95:SER:HB2	4:A:141:PHE:HZ	1.82	0.45
16:A:833:CLA:H61	16:A:833:CLA:H41	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:73:THR:N	6:C:76:SER:OG	2.43	0.45
7:D:85:ARG:HB2	7:D:93:GLN:HB2	1.99	0.45
3:3:70:GLN:NE2	3:3:82:THR:O	2.49	0.45
4:A:111:ALA:HB2	4:A:136:ILE:HD11	1.99	0.45
5:B:201:ARG:HH12	5:B:236:ASP:HB2	1.82	0.45
16:B:835:CLA:H2	16:B:835:CLA:H61	1.76	0.45
1:1:127:LEU:HD12	17:1:613:ZEX:H382	1.99	0.45
3:3:37:LEU:HD12	17:3:215:ZEX:H21	1.99	0.45
4:A:208:SER:HB2	22:A:843:BCR:H14C	1.99	0.45
16:A:818:CLA:H142	16:A:818:CLA:HBB2	1.99	0.45
16:A:838:CLA:H11	16:B:801:CLA:H202	1.98	0.45
5:B:174:ASN:HD21	5:B:289:TYR:HB2	1.82	0.45
16:F:802:CLA:HBA1	16:F:802:CLA:H3A	1.67	0.45
16:O:204:CLA:HBA2	16:O:204:CLA:H3A	1.85	0.45
2:2:133:ARG:NH2	2:2:136:GLY:O	2.50	0.44
16:A:829:CLA:H121	21:A:841:LHG:H372	1.99	0.44
5:B:456:ILE:HD11	9:F:96:ILE:HA	1.99	0.44
16:B:808:CLA:H51	25:B:850:DGD:HB91	1.99	0.44
16:B:810:CLA:H171	16:B:829:CLA:H161	2.00	0.44
2:2:119:ILE:HG22	2:2:120:VAL:HG13	1.98	0.44
4:A:695:GLU:OE1	8:E:45:TYR:OH	2.29	0.44
20:A:840:PQN:H111	22:F:801:BCR:H281	1.99	0.44
16:B:803:CLA:H62	16:B:833:CLA:H42	1.99	0.44
4:A:724:GLY:O	4:A:728:TYR:HB2	2.17	0.44
16:A:850:CLA:HED2	16:A:850:CLA:HBD	1.89	0.44
5:B:5:PHE:CB	5:B:6:PRO:HD3	2.26	0.44
5:B:689:ILE:HD11	22:L:206:BCR:H382	1.99	0.44
16:B:803:CLA:H52	16:B:833:CLA:HAA2	1.99	0.44
7:D:28:TYR:O	7:D:59:LEU:N	2.48	0.44
3:3:153:LYS:NZ	17:3:216:ZEX:O23	2.45	0.44
4:A:426:MET:HA	4:A:429:HIS:CE1	2.52	0.44
4:A:601:ILE:HG23	19:A:801:CL0:C14	2.47	0.44
16:A:807:CLA:HMC2	16:A:827:CLA:H121	2.00	0.44
16:A:836:CLA:H62	16:A:836:CLA:H41	1.75	0.44
20:A:840:PQN:H191	20:A:840:PQN:H212	1.86	0.44
16:B:801:CLA:H41	16:B:801:CLA:H62	1.80	0.44
3:3:45:ILE:H	3:3:45:ILE:HG13	1.59	0.44
3:3:50:GLU:O	3:3:54:LYS:CB	2.65	0.44
3:3:125:LEU:HD12	3:3:126:PRO:HD2	1.98	0.44
17:3:218:ZEX:H15	17:3:218:ZEX:H201	1.81	0.44
4:A:222:LYS:HD3	4:A:249:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:557:ARG:HD2	5:B:674:GLU:HB3	2.00	0.44
4:A:676:TRP:CE3	19:A:801:CL0:H6	2.53	0.44
16:A:836:CLA:H141	16:A:836:CLA:H162	1.80	0.44
7:D:82:LYS:HE3	7:D:95:LEU:H	1.82	0.44
13:L:94:LEU:O	13:L:98:ALA:HB2	2.17	0.44
17:1:614:ZEX:H11	17:1:614:ZEX:H191	1.85	0.44
2:2:170:ILE:HG21	17:3:201:ZEX:H32	2.00	0.44
3:3:36:PRO:HD2	17:3:215:ZEX:H3	2.00	0.44
4:A:190:VAL:HG21	4:A:342:THR:HG22	2.00	0.44
4:A:200:GLY:HA2	16:A:819:CLA:HBC1	1.99	0.44
19:A:801:CL0:H44	19:A:801:CL0:H52	1.59	0.44
9:F:118:THR:HG22	9:F:121:ILE:HD12	2.00	0.44
2:2:55:LEU:HD22	16:2:602:CLA:H43	2.00	0.44
17:2:617:ZEX:H25	17:3:201:ZEX:H31	1.98	0.44
6:C:11:CYS:HB3	6:C:39:MET:HG3	2.00	0.44
2:2:35:PRO:HD2	2:2:56:ARG:HH12	1.82	0.44
4:A:437:LEU:HD13	4:A:544:LEU:HA	2.00	0.44
16:A:816:CLA:H62	16:A:816:CLA:H41	1.56	0.44
16:A:825:CLA:H51	16:A:835:CLA:H42	2.00	0.44
5:B:152:TRP:CE2	14:M:23:LYS:HE2	2.53	0.44
16:B:827:CLA:HBB1	16:B:839:CLA:HHB	2.00	0.44
12:K:8:THR:HG23	12:K:10:PRO:HD2	1.99	0.44
16:2:601:CLA:H2A	17:3:201:ZEX:H361	2.00	0.44
3:3:30:SER:OG	16:3:203:CLA:O1D	2.30	0.44
16:A:807:CLA:H3A	16:A:807:CLA:HBA2	1.43	0.44
5:B:544:LEU:O	5:B:562:ARG:NH1	2.51	0.44
5:B:688:LEU:HD21	13:L:36:ILE:HG21	1.99	0.44
4:A:108:LYS:HB2	4:A:127:VAL:HB	2.00	0.43
4:A:157:VAL:HG11	16:A:815:CLA:HAA2	2.00	0.43
19:A:801:CL0:H34	19:A:801:CL0:H30	2.00	0.43
7:D:73:ARG:HB2	7:D:78:ILE:HD11	2.00	0.43
22:K:103:BCR:H403	22:K:103:BCR:H371	2.00	0.43
4:A:91:GLY:O	4:A:95:SER:OG	2.29	0.43
4:A:601:ILE:HD12	19:A:801:CL0:H70	2.00	0.43
4:A:654:VAL:HG21	4:A:739:PHE:HA	2.00	0.43
5:B:344:SER:OG	16:B:827:CLA:O1D	2.31	0.43
5:B:643:VAL:HG22	16:B:811:CLA:HAC1	2.00	0.43
20:B:843:PQN:H112	20:B:843:PQN:H142	1.77	0.43
8:E:33:LEU:O	8:E:54:SER:OG	2.35	0.43
1:1:155:HIS:CD2	16:1:611:CLA:HAC2	2.53	0.43
2:2:176:PHE:CE1	17:2:617:ZEX:H7	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:802:CLA:HED3	16:A:852:CLA:H3A	2.00	0.43
5:B:535:GLY:HA3	5:B:573:ALA:HB2	1.99	0.43
19:A:801:CL0:C4	16:B:802:CLA:C1D	2.96	0.43
5:B:355:PRO:HG3	16:B:820:CLA:HBA1	2.01	0.43
16:B:805:CLA:H152	16:B:805:CLA:H112	1.53	0.43
16:B:828:CLA:H52	22:B:848:BCR:H15C	1.99	0.43
16:B:841:CLA:H202	13:L:88:ILE:HG23	2.01	0.43
22:B:846:BCR:H15C	22:B:846:BCR:H351	1.90	0.43
4:A:439:TRP:NE1	16:A:831:CLA:OBD	2.36	0.43
16:A:817:CLA:H3A	16:A:817:CLA:HBA2	1.46	0.43
5:B:446:ASN:HD21	9:F:78:ARG:HD2	1.84	0.43
16:B:803:CLA:H171	9:F:125:GLY:HA2	2.00	0.43
16:B:825:CLA:HBC3	22:B:847:BCR:H403	1.99	0.43
11:J:18:LEU:O	11:J:22:ALA:HB2	2.18	0.43
1:1:6:LEU:HA	1:1:7:PRO:HD3	1.89	0.43
4:A:295:LEU:HD23	4:A:295:LEU:HA	1.77	0.43
4:A:676:TRP:CG	19:A:801:CL0:H6	2.54	0.43
19:A:801:CL0:C9	19:A:801:CL0:H39	2.46	0.43
16:A:819:CLA:HBA2	16:A:819:CLA:H3A	1.50	0.43
7:D:72:LEU:HD13	7:D:78:ILE:HG21	2.00	0.43
1:1:5:ALA:HB3	1:1:24:GLY:HA3	1.99	0.43
16:A:820:CLA:H42	16:A:833:CLA:H122	2.01	0.43
5:B:4:LYS:HG2	5:B:13:ALA:HB1	2.01	0.43
5:B:180:LEU:O	5:B:184:SER:OG	2.27	0.43
5:B:724:ILE:O	5:B:728:ALA:CB	2.66	0.43
16:B:803:CLA:C1B	16:B:833:CLA:H41	2.48	0.43
16:B:841:CLA:H171	22:L:206:BCR:H351	2.01	0.43
13:L:90:THR:HG21	13:L:122:LEU:HB2	2.01	0.43
4:A:592:LEU:HA	4:A:592:LEU:HD23	1.82	0.43
16:A:804:CLA:H112	16:A:804:CLA:H71	1.82	0.43
5:B:427:LEU:HD11	16:B:838:CLA:HMB1	2.01	0.43
16:B:824:CLA:HBC1	16:B:825:CLA:H43	2.01	0.43
16:3:209:CLA:HBB2	17:3:214:ZEX:H14	2.01	0.43
16:A:834:CLA:H3A	16:A:834:CLA:HBA2	1.56	0.43
5:B:576:LEU:HB3	16:B:801:CLA:HMD1	2.00	0.43
16:B:807:CLA:H52	16:B:815:CLA:H2	2.01	0.43
6:C:7:ILE:HG23	6:C:65:ILE:HG12	2.00	0.43
1:1:108:LEU:HD12	16:1:607:CLA:CGA	2.48	0.43
4:A:31:PHE:HB2	4:A:58:HIS:CD2	2.53	0.43
16:B:811:CLA:H72	16:B:829:CLA:H191	2.01	0.43
8:E:57:GLU:H	8:E:57:GLU:HG2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:482:TRP:CZ2	4:A:486:ILE:HD11	2.54	0.42
16:A:850:CLA:H141	16:A:850:CLA:H161	1.83	0.42
22:K:103:BCR:H342	22:K:103:BCR:H331	2.01	0.42
22:L:206:BCR:H351	22:L:206:BCR:H15C	1.85	0.42
1:1:118:LYS:HD3	1:1:136:ARG:HH21	1.84	0.42
1:1:118:LYS:HD2	1:1:119:PRO:HD2	2.00	0.42
16:2:602:CLA:H102	16:2:602:CLA:H61	1.75	0.42
3:3:56:GLY:O	3:3:60:MET:HG2	2.20	0.42
3:3:166:TRP:CH2	17:3:218:ZEX:H7	2.55	0.42
16:3:208:CLA:HBA2	16:3:208:CLA:H3A	1.43	0.42
17:3:216:ZEX:H30	17:3:218:ZEX:H362	2.01	0.42
4:A:117:ILE:HG22	4:A:118:VAL:H	1.83	0.42
4:A:665:TYR:O	4:A:669:PHE:HB2	2.19	0.42
5:B:125:ILE:HG23	5:B:191:HIS:NE2	2.34	0.42
4:A:561:ASP:OD1	4:A:561:ASP:N	2.52	0.42
16:A:802:CLA:H192	22:J:102:BCR:H20C	2.02	0.42
5:B:583:ASN:HB2	16:B:804:CLA:HBC2	1.99	0.42
16:B:803:CLA:H51	22:F:801:BCR:H19C	2.01	0.42
16:B:820:CLA:H3A	16:B:820:CLA:HBA2	1.47	0.42
10:I:31:GLU:HG3	13:L:99:VAL:HG13	2.01	0.42
17:3:201:ZEX:H362	17:3:201:ZEX:H27	1.84	0.42
4:A:53:HIS:CD2	16:A:804:CLA:HBB2	2.54	0.42
4:A:168:LEU:O	4:A:172:ALA:HB2	2.18	0.42
4:A:674:PHE:HB2	16:B:804:CLA:HAA1	2.01	0.42
5:B:5:PHE:HB2	5:B:20:ARG:HH22	1.71	0.42
5:B:416:VAL:HG13	16:B:839:CLA:HBB2	2.01	0.42
5:B:660:MET:HE2	5:B:660:MET:HB3	1.83	0.42
7:D:102:LEU:HA	7:D:103:PRO:HD3	1.93	0.42
15:O:60:ILE:HG13	15:O:61:PRO:HD3	2.00	0.42
1:1:152:GLY:HA3	17:1:613:ZEX:H181	2.01	0.42
2:2:71:LEU:HD22	17:2:614:ZEX:H203	2.02	0.42
2:2:123:PRO:O	2:2:126:ILE:HB	2.19	0.42
4:A:554:ARG:HG3	4:A:563:ALA:HB2	2.01	0.42
16:A:827:CLA:H8	16:A:827:CLA:H51	1.85	0.42
16:A:833:CLA:H162	16:A:833:CLA:H141	1.81	0.42
5:B:532:LEU:HD23	5:B:532:LEU:HA	1.90	0.42
5:B:573:ALA:O	5:B:577:ALA:CB	2.66	0.42
13:L:59:ILE:HG13	13:L:132:ALA:HB3	2.01	0.42
16:3:206:CLA:HBA1	16:3:206:CLA:H3A	1.79	0.42
4:A:644:ARG:HB2	5:B:630:ILE:HG13	2.01	0.42
4:A:676:TRP:CG	19:A:801:CL0:CMA	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:705:LYS:HE2	9:F:175:ALA:HB2	2.01	0.42
19:A:801:CL0:CMB	16:B:804:CLA:HMD3	2.50	0.42
16:A:804:CLA:HBA1	16:A:804:CLA:H3A	1.66	0.42
16:A:805:CLA:H2	16:A:805:CLA:HMA2	2.02	0.42
5:B:43:TYR:HA	5:B:46:ILE:HG12	2.02	0.42
5:B:461:ILE:HD13	16:B:835:CLA:HAB	2.02	0.42
16:B:802:CLA:H3A	16:B:802:CLA:O1A	2.20	0.42
25:B:850:DGD:HA92	25:B:850:DGD:HAW2	1.78	0.42
7:D:72:LEU:HB3	7:D:78:ILE:HG12	2.02	0.42
11:J:30:ARG:HD3	22:J:103:BCR:H312	2.01	0.42
2:2:71:LEU:HB3	16:2:604:CLA:HMC2	2.02	0.42
4:A:101:LEU:HD23	4:A:230:PRO:HB3	2.01	0.42
4:A:729:LEU:O	4:A:733:ILE:HB	2.18	0.42
16:A:816:CLA:H143	16:A:816:CLA:H111	1.89	0.42
16:A:832:CLA:HMA2	13:L:65:LEU:HD23	2.01	0.42
16:A:852:CLA:HMD3	16:B:803:CLA:HBB1	2.02	0.42
5:B:198:PRO:HB2	5:B:203:GLN:HB2	2.01	0.42
9:F:44:GLU:HA	9:F:79:PHE:CE2	2.55	0.42
12:K:40:MET:O	12:K:44:HIS:HB2	2.20	0.42
16:B:812:CLA:H62	16:B:812:CLA:H102	1.83	0.42
1:1:109:TYR:CD2	9:F:152:LYS:HA	2.55	0.42
16:2:607:CLA:HBC3	17:2:616:ZEX:H381	2.02	0.42
4:A:483:ILE:HA	4:A:486:ILE:HD12	2.01	0.42
16:A:827:CLA:H93	16:A:827:CLA:H111	1.91	0.42
5:B:38:THR:OG1	5:B:41:ASN:OD1	2.33	0.42
5:B:65:LEU:HD11	22:B:846:BCR:H271	2.02	0.42
5:B:345:LEU:HD22	16:B:820:CLA:H62	2.02	0.42
5:B:525:LEU:HD12	16:B:839:CLA:HED3	2.01	0.42
9:F:110:PRO:HA	9:F:113:LEU:HB3	2.01	0.42
4:A:199:ALA:HB1	16:A:819:CLA:HBC3	2.02	0.42
16:A:818:CLA:HBA2	16:A:818:CLA:H3A	1.53	0.42
16:B:807:CLA:H12	22:B:845:BCR:H24C	2.02	0.42
3:3:163:LEU:HB2	17:3:218:ZEX:C15	2.50	0.41
4:A:590:LEU:HD23	4:A:590:LEU:HA	1.79	0.41
4:A:601:ILE:CG2	19:A:801:CL0:H55	2.50	0.41
16:A:826:CLA:H61	16:A:826:CLA:H2	1.60	0.41
5:B:5:PHE:CE2	10:I:30:ILE:HG12	2.49	0.41
5:B:29:HIS:CD2	16:B:807:CLA:HAB	2.55	0.41
16:B:809:CLA:HAA1	10:I:11:VAL:HG22	2.01	0.41
16:B:828:CLA:H92	16:B:828:CLA:H62	1.83	0.41
9:F:78:ARG:HG3	11:J:34:ASP:CG	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:159:LEU:HG	9:F:162:LEU:HG	2.01	0.41
16:K:102:CLA:HMC2	22:K:103:BCR:H332	2.02	0.41
4:A:168:LEU:HD22	16:A:809:CLA:HBC1	2.01	0.41
4:A:307:MET:HB3	16:A:821:CLA:HAC2	2.02	0.41
16:A:802:CLA:H8	11:J:15:THR:HG22	2.02	0.41
7:D:51:ASN:HB3	7:D:55:ASN:HB3	2.01	0.41
1:1:54:CYS:HB3	1:1:150:PHE:HB2	2.02	0.41
4:A:439:TRP:CE2	16:L:201:CLA:HAB	2.55	0.41
4:A:42:THR:HB	16:A:852:CLA:HBB1	2.02	0.41
4:A:230:PRO:HA	4:A:233:ILE:HD12	2.01	0.41
4:A:279:SER:OG	4:A:282:THR:OG1	2.31	0.41
4:A:693:LEU:O	4:A:696:SER:OG	2.29	0.41
16:A:810:CLA:H92	16:A:810:CLA:H62	1.85	0.41
5:B:202:GLY:HA3	5:B:245:SER:HB3	2.02	0.41
5:B:457:PHE:CZ	16:F:803:CLA:HAB	2.55	0.41
16:B:801:CLA:H92	16:B:801:CLA:H61	1.87	0.41
16:B:807:CLA:H143	16:B:807:CLA:H161	1.88	0.41
16:B:829:CLA:H2	16:B:829:CLA:H62	1.86	0.41
16:B:840:CLA:H122	22:L:202:BCR:H361	2.02	0.41
1:1:163:MET:HG3	1:1:166:GLU:HB2	2.01	0.41
3:3:58:ILE:O	3:3:62:ALA:CB	2.68	0.41
4:A:445:GLY:HA3	16:A:850:CLA:H11	2.02	0.41
4:A:558:LEU:HD21	4:A:579:THR:HG22	2.03	0.41
5:B:60:TRP:NE1	16:B:829:CLA:OBD	2.53	0.41
5:B:179:GLY:O	5:B:183:VAL:HB	2.21	0.41
1:1:145:LEU:HD13	16:1:609:CLA:HBC1	2.01	0.41
3:3:63:PHE:O	3:3:66:THR:OG1	2.30	0.41
16:3:203:CLA:HAB	17:3:215:ZEX:C12	2.50	0.41
4:A:59:THR:HG22	4:A:61:SER:H	1.86	0.41
4:A:359:LEU:HD22	16:A:818:CLA:H72	2.02	0.41
4:A:430:ARG:NH2	4:A:555:ASN:O	2.40	0.41
16:A:804:CLA:H172	16:A:812:CLA:H51	2.01	0.41
16:A:839:CLA:H121	16:B:840:CLA:H102	2.02	0.41
5:B:271:MET:HA	5:B:274:HIS:HB3	2.03	0.41
16:B:805:CLA:H111	16:B:805:CLA:H72	1.82	0.41
16:B:815:CLA:H192	16:B:815:CLA:H162	1.87	0.41
22:B:847:BCR:H15C	22:B:847:BCR:H351	1.89	0.41
10:I:10:LEU:HA	10:I:13:THR:HG22	2.02	0.41
16:1:612:CLA:H3A	16:1:612:CLA:HBA1	1.86	0.41
4:A:9:VAL:HG22	4:A:189:ASN:HD21	1.85	0.41
4:A:95:SER:HA	4:A:111:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:850:CLA:H121	22:B:849:BCR:H362	2.03	0.41
5:B:65:LEU:O	5:B:69:ALA:HB2	2.20	0.41
5:B:302:ILE:HD12	5:B:302:ILE:HA	1.89	0.41
5:B:532:LEU:O	5:B:536:ALA:CB	2.68	0.41
5:B:652:HIS:HE1	16:B:805:CLA:NA	2.18	0.41
16:B:842:CLA:H8	16:B:842:CLA:H52	1.88	0.41
8:E:53:PHE:HB3	8:E:57:GLU:HG3	2.02	0.41
13:L:89:LEU:HB3	22:L:206:BCR:H401	2.02	0.41
2:2:125:LEU:HA	2:2:128:SER:HB3	2.02	0.41
3:3:92:VAL:HG22	3:3:96:LEU:HD22	2.01	0.41
4:A:293:HIS:NE2	4:A:297:ILE:HD11	2.35	0.41
16:A:829:CLA:H192	22:A:847:BCR:H341	2.02	0.41
21:A:842:LHG:H102	21:A:842:LHG:H131	1.79	0.41
5:B:196:ALA:HB1	5:B:268:LEU:HD13	2.01	0.41
1:1:41:GLU:HG2	1:1:119:PRO:HB3	2.02	0.41
1:1:88:MET:HG2	16:1:606:CLA:HMD3	2.03	0.41
1:1:146:ALA:HB2	17:1:613:ZEX:H202	2.03	0.41
16:2:602:CLA:H62	17:2:615:ZEX:H362	2.03	0.41
4:A:644:ARG:HG3	5:B:630:ILE:HG23	2.02	0.41
4:A:684:PHE:HB2	16:B:801:CLA:HBC1	2.03	0.41
19:A:801:CL0:H36	16:B:802:CLA:C1D	2.50	0.41
16:A:836:CLA:HBA2	16:A:836:CLA:H3A	1.81	0.41
5:B:186:LEU:O	5:B:189:THR:OG1	2.32	0.41
5:B:242:PHE:HB2	5:B:263:THR:HG21	2.03	0.41
5:B:385:PHE:CZ	16:B:827:CLA:HAB	2.55	0.41
16:B:805:CLA:H62	16:B:805:CLA:H2	1.85	0.41
16:B:821:CLA:H2A	16:B:821:CLA:HED3	2.03	0.41
16:B:833:CLA:H62	16:B:833:CLA:H2	1.73	0.41
9:F:131:TYR:CZ	9:F:149:MET:HG2	2.56	0.41
4:A:369:ALA:O	4:A:503:SER:OG	2.38	0.41
5:B:50:HIS:HD2	16:B:807:CLA:HAA1	1.85	0.41
16:B:801:CLA:H3A	16:B:801:CLA:CGA	2.51	0.41
16:B:827:CLA:H42	16:B:835:CLA:HBB2	2.03	0.41
3:3:44:PRO:HG3	3:3:119:VAL:HG23	2.03	0.40
22:A:845:BCR:H15C	22:A:845:BCR:H351	1.89	0.40
5:B:147:PHE:HD1	5:B:147:PHE:HA	1.77	0.40
5:B:332:LEU:HB2	16:B:807:CLA:HMD2	2.03	0.40
16:B:802:CLA:H72	16:B:802:CLA:H111	1.87	0.40
16:B:832:CLA:HBC1	22:B:847:BCR:H21C	2.02	0.40
1:1:11:LYS:C	1:1:13:PRO:HD3	2.46	0.40
16:2:607:CLA:H3A	16:2:607:CLA:HBA1	1.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:493:ASN:HB3	15:O:67:LEU:HD12	2.03	0.40
5:B:409:MET:HA	5:B:412:HIS:CE1	2.56	0.40
5:B:654:VAL:HG22	16:B:841:CLA:HMB3	2.03	0.40
16:B:816:CLA:C1B	22:B:846:BCR:H19C	2.51	0.40
16:B:833:CLA:H161	16:B:833:CLA:H202	1.84	0.40
16:A:818:CLA:H111	16:A:818:CLA:H152	1.88	0.40
5:B:617:TRP:O	5:B:621:TYR:HB3	2.21	0.40
1:1:112:MET:HE1	1:1:114:TRP:HE3	1.86	0.40
4:A:142:GLN:HB3	4:A:373:TYR:HB3	2.03	0.40
4:A:532:HIS:CG	16:A:836:CLA:HED2	2.56	0.40
16:A:805:CLA:H151	16:A:828:CLA:HBB2	2.03	0.40
16:A:817:CLA:H151	16:A:817:CLA:H111	1.81	0.40
5:B:5:PHE:CB	5:B:6:PRO:CD	2.95	0.40
5:B:577:ALA:O	5:B:581:MET:HB2	2.21	0.40
16:B:835:CLA:HBA1	16:B:835:CLA:H3A	1.94	0.40
1:1:91:ILE:HD12	1:1:91:ILE:HA	2.00	0.40
1:1:158:PHE:HZ	17:1:617:ZEX:H8	1.86	0.40
17:1:613:ZEX:H15	17:1:613:ZEX:H201	1.85	0.40
3:3:37:LEU:HB3	12:K:33:LEU:HD13	2.02	0.40
16:A:820:CLA:HBC3	16:A:826:CLA:H171	2.04	0.40
22:A:843:BCR:H20C	22:A:843:BCR:H361	1.86	0.40
5:B:4:LYS:HB3	5:B:5:PHE:H	1.64	0.40
5:B:454:GLU:OE1	5:B:459:GLN:NE2	2.52	0.40
7:D:72:LEU:HB3	7:D:78:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	167/175 (95%)	129 (77%)	37 (22%)	1 (1%)	21 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	173/199 (87%)	134 (78%)	39 (22%)	0	100	100
3	3	168/188 (89%)	141 (84%)	27 (16%)	0	100	100
4	A	739/748 (99%)	686 (93%)	52 (7%)	1 (0%)	48	79
5	B	729/732 (100%)	663 (91%)	65 (9%)	1 (0%)	48	79
6	C	78/81 (96%)	67 (86%)	11 (14%)	0	100	100
7	D	117/139 (84%)	103 (88%)	14 (12%)	0	100	100
8	E	59/94 (63%)	53 (90%)	6 (10%)	0	100	100
9	F	152/185 (82%)	136 (90%)	16 (10%)	0	100	100
10	I	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
11	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	K	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
13	L	117/140 (84%)	107 (92%)	10 (8%)	0	100	100
14	M	25/29 (86%)	23 (92%)	2 (8%)	0	100	100
15	O	81/155 (52%)	67 (83%)	14 (17%)	0	100	100
All	All	2727/2995 (91%)	2421 (89%)	303 (11%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	12	PRO
5	B	7	LYS
4	A	526	THR

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	1	139/145 (96%)	139 (100%)	0	100	100
2	2	142/160 (89%)	142 (100%)	0	100	100
3	3	132/148 (89%)	131 (99%)	1 (1%)	73	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	598/605 (99%)	597 (100%)	1 (0%)	87	87
5	B	598/599 (100%)	593 (99%)	5 (1%)	73	75
6	C	66/67 (98%)	66 (100%)	0	100	100
7	D	101/118 (86%)	100 (99%)	1 (1%)	68	74
8	E	58/87 (67%)	58 (100%)	0	100	100
9	F	136/162 (84%)	136 (100%)	0	100	100
10	I	26/27 (96%)	26 (100%)	0	100	100
11	J	34/34 (100%)	34 (100%)	0	100	100
12	K	48/49 (98%)	47 (98%)	1 (2%)	47	64
13	L	94/113 (83%)	94 (100%)	0	100	100
14	M	22/23 (96%)	22 (100%)	0	100	100
15	O	64/121 (53%)	63 (98%)	1 (2%)	55	68
All	All	2258/2458 (92%)	2248 (100%)	10 (0%)	81	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	45	ILE
4	A	69	ILE
5	B	3	THR
5	B	4	LYS
5	B	7	LYS
5	B	211	ILE
5	B	381	ILE
7	D	78	ILE
12	K	52	LEU
15	O	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	64	GLN
1	1	79	HIS
1	1	167	GLN
2	2	85	ASN
2	2	99	GLN
2	2	184	GLN

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Mol	Chain	Res	Type
3	3	98	GLN
4	A	76	GLN
4	A	112	GLN
4	A	189	ASN
4	A	352	ASN
4	A	383	GLN
4	A	484	GLN
4	A	493	ASN
4	A	535	HIS
5	B	53	HIS
5	B	98	GLN
5	B	194	HIS
5	B	233	GLN
5	B	374	GLN
5	B	488	GLN
6	C	38	GLN
7	D	71	GLN
7	D	75	GLN
7	D	79	GLN
7	D	112	GLN
8	E	52	ASN
9	F	46	ASN
13	L	22	ASN
14	M	6	GLN

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 ⓘ

181 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
16	CLA	A	831	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	7 (8%)
16	CLA	2	612	-	49,53,73	1.36	9 (18%)	58,89,113	1.56	6 (10%)
22	BCR	L	206	-	41,41,41	1.13	3 (7%)	56,56,56	1.51	10 (17%)
16	CLA	A	827	-	69,73,73	1.20	9 (13%)	82,113,113	1.56	8 (9%)
16	CLA	B	831	-	69,73,73	1.24	8 (11%)	82,113,113	1.66	16 (19%)
16	CLA	1	607	-	49,53,73	1.36	10 (20%)	58,89,113	1.62	6 (10%)
22	BCR	A	843	-	41,41,41	1.15	4 (9%)	56,56,56	1.33	6 (10%)
16	CLA	A	829	-	69,73,73	1.35	10 (14%)	82,113,113	1.74	25 (30%)
16	CLA	B	830	-	69,73,73	1.24	9 (13%)	82,113,113	1.45	9 (10%)
16	CLA	1	610	-	49,53,73	1.38	10 (20%)	58,89,113	1.59	8 (13%)
16	CLA	3	206	-	49,53,73	1.46	8 (16%)	58,89,113	1.70	12 (20%)
16	CLA	A	819	-	49,53,73	1.37	9 (18%)	58,89,113	1.59	5 (8%)
16	CLA	B	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.45	10 (12%)
16	CLA	3	205	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	9 (15%)
26	3XQ	J	104	-	24,24,24	0.60	1 (4%)	25,25,25	1.14	1 (4%)
22	BCR	A	849	-	41,41,41	1.19	3 (7%)	56,56,56	1.36	7 (12%)
16	CLA	2	602	-	69,73,73	1.18	10 (14%)	82,113,113	1.42	7 (8%)
16	CLA	A	816	-	66,70,73	1.18	11 (16%)	78,109,113	1.44	8 (10%)
16	CLA	2	606	-	49,53,73	1.35	8 (16%)	58,89,113	1.54	7 (12%)
16	CLA	B	802	-	69,73,73	1.27	8 (11%)	82,113,113	1.58	18 (21%)
17	ZEX	2	615	-	43,43,43	3.74	18 (41%)	51,60,60	5.52	29 (56%)
22	BCR	I	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	7 (12%)
16	CLA	O	201	-	56,60,73	1.28	11 (19%)	65,97,113	1.49	10 (15%)
16	CLA	L	201	-	60,64,73	1.22	9 (15%)	71,102,113	1.40	7 (9%)
24	BGC	A	853	18	11,11,12	1.57	3 (27%)	15,15,17	0.94	0
16	CLA	B	803	-	69,73,73	1.14	9 (13%)	82,113,113	1.49	8 (9%)
16	CLA	1	602	-	63,67,73	1.19	9 (14%)	74,105,113	1.47	7 (9%)
22	BCR	J	102	-	41,41,41	1.24	4 (9%)	56,56,56	1.35	6 (10%)
16	CLA	B	833	-	69,73,73	1.19	10 (14%)	82,113,113	1.40	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	820	-	64,68,73	1.21	10 (15%)	76,107,113	1.52	10 (13%)
22	BCR	A	847	-	41,41,41	1.31	3 (7%)	56,56,56	1.30	7 (12%)
16	CLA	B	812	-	69,73,73	1.19	10 (14%)	82,113,113	1.40	8 (9%)
22	BCR	A	846	-	41,41,41	1.27	3 (7%)	56,56,56	1.34	6 (10%)
19	CL0	A	801	-	58,73,73	3.60	26 (44%)	60,113,113	3.54	25 (41%)
17	ZEX	1	617	-	43,43,43	3.80	18 (41%)	51,60,60	5.82	26 (50%)
16	CLA	A	836	-	69,73,73	1.17	8 (11%)	82,113,113	1.46	12 (14%)
16	CLA	B	839	-	51,55,73	1.31	8 (15%)	60,91,113	1.57	9 (15%)
16	CLA	3	212	-	50,54,73	1.34	8 (16%)	59,90,113	1.50	5 (8%)
17	ZEX	1	613	-	43,43,43	3.85	19 (44%)	51,60,60	5.52	30 (58%)
16	CLA	B	837	-	64,68,73	1.24	8 (12%)	76,107,113	1.57	11 (14%)
16	CLA	A	810	-	69,73,73	1.15	9 (13%)	82,113,113	1.45	7 (8%)
16	CLA	3	207	-	49,53,73	1.36	8 (16%)	58,89,113	1.60	6 (10%)
16	CLA	2	608	-	54,58,73	1.29	10 (18%)	64,95,113	1.59	10 (15%)
21	LHG	A	842	-	39,39,48	0.76	1 (2%)	42,45,54	1.33	6 (14%)
23	SF4	C	101	-	0,12,12	-	-	-	-	-
16	CLA	K	101	-	49,53,73	1.35	8 (16%)	58,89,113	1.60	7 (12%)
16	CLA	A	806	-	69,73,73	1.21	9 (13%)	82,113,113	1.58	17 (20%)
16	CLA	B	832	-	49,53,73	1.38	11 (22%)	58,89,113	1.56	6 (10%)
16	CLA	O	203	-	54,58,73	1.32	8 (14%)	64,95,113	1.44	8 (12%)
16	CLA	O	202	-	45,49,73	1.41	8 (17%)	54,84,113	1.62	7 (12%)
16	CLA	A	826	-	69,73,73	1.18	9 (13%)	82,113,113	1.44	7 (8%)
16	CLA	A	835	-	55,59,73	1.26	9 (16%)	64,96,113	1.64	11 (17%)
16	CLA	2	609	-	45,49,73	1.39	7 (15%)	54,84,113	1.65	7 (12%)
16	CLA	A	803	-	59,63,73	1.25	11 (18%)	70,101,113	1.60	10 (14%)
16	CLA	A	852	-	65,69,73	1.19	9 (13%)	77,108,113	1.45	10 (12%)
16	CLA	A	820	-	69,73,73	1.19	9 (13%)	82,113,113	1.48	9 (10%)
17	ZEX	3	201	-	43,43,43	4.04	20 (46%)	51,60,60	5.58	28 (54%)
16	CLA	A	807	4	69,73,73	1.14	9 (13%)	82,113,113	1.43	8 (9%)
16	CLA	2	605	-	49,53,73	1.35	8 (16%)	58,89,113	1.71	7 (12%)
20	PQN	B	843	-	34,34,34	2.81	10 (29%)	43,45,45	2.12	6 (13%)
16	CLA	2	613	-	49,53,73	1.37	8 (16%)	58,89,113	1.54	5 (8%)
16	CLA	B	808	-	69,73,73	1.20	7 (10%)	82,113,113	1.43	10 (12%)
17	ZEX	3	214	-	43,43,43	3.94	19 (44%)	51,60,60	5.57	30 (58%)
22	BCR	B	849	-	41,41,41	1.24	4 (9%)	56,56,56	1.52	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	823	-	59,63,73	1.24	9 (15%)	70,101,113	1.53	6 (8%)
17	ZEX	3	218	-	43,43,43	4.17	20 (46%)	51,60,60	4.87	28 (54%)
16	CLA	A	802	-	69,73,73	1.18	9 (13%)	82,113,113	1.51	10 (12%)
16	CLA	B	827	-	69,73,73	1.19	9 (13%)	82,113,113	1.44	9 (10%)
17	ZEX	3	216	-	43,43,43	3.97	19 (44%)	51,60,60	5.45	27 (52%)
22	BCR	J	103	-	41,41,41	1.29	3 (7%)	56,56,56	1.31	5 (8%)
22	BCR	B	848	-	41,41,41	1.20	4 (9%)	56,56,56	1.54	10 (17%)
16	CLA	1	606	-	49,53,73	1.38	9 (18%)	58,89,113	1.57	7 (12%)
16	CLA	A	832	-	69,73,73	1.16	8 (11%)	82,113,113	1.55	10 (12%)
16	CLA	B	813	-	58,62,73	1.35	9 (15%)	71,100,113	1.45	9 (12%)
22	BCR	B	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	7 (12%)
16	CLA	A	804	-	69,73,73	1.20	10 (14%)	82,113,113	1.55	11 (13%)
16	CLA	A	833	-	69,73,73	1.14	11 (15%)	82,113,113	1.45	9 (10%)
16	CLA	B	817	-	46,50,73	1.37	9 (19%)	53,85,113	1.55	5 (9%)
16	CLA	B	834	-	62,66,73	1.23	8 (12%)	73,104,113	1.49	7 (9%)
22	BCR	F	801	-	41,41,41	1.26	4 (9%)	56,56,56	1.48	8 (14%)
16	CLA	A	812	-	69,73,73	1.17	9 (13%)	82,113,113	1.42	9 (10%)
16	CLA	A	822	-	55,59,73	1.32	8 (14%)	64,96,113	1.47	5 (7%)
16	CLA	B	838	-	69,73,73	1.19	10 (14%)	82,113,113	1.43	8 (9%)
16	CLA	B	822	-	49,53,73	1.35	10 (20%)	58,89,113	1.58	5 (8%)
16	CLA	F	803	-	45,49,73	1.38	9 (20%)	54,84,113	1.60	5 (9%)
16	CLA	1	603	-	49,53,73	1.39	9 (18%)	58,89,113	1.52	6 (10%)
16	CLA	A	808	4	69,73,73	1.21	8 (11%)	82,113,113	1.57	13 (15%)
16	CLA	B	818	-	59,63,73	1.23	9 (15%)	70,101,113	1.45	9 (12%)
17	ZEX	1	616	-	43,43,43	3.92	18 (41%)	51,60,60	5.57	26 (50%)
16	CLA	A	824	-	69,73,73	1.21	9 (13%)	82,113,113	1.44	12 (14%)
16	CLA	3	204	-	49,53,73	1.36	9 (18%)	58,89,113	1.61	5 (8%)
17	ZEX	1	614	-	43,43,43	3.89	19 (44%)	51,60,60	5.97	27 (52%)
16	CLA	A	830	-	54,58,73	1.33	10 (18%)	64,95,113	1.46	8 (12%)
16	CLA	B	801	-	69,73,73	1.24	9 (13%)	82,113,113	1.80	16 (19%)
16	CLA	1	604	-	49,53,73	1.34	9 (18%)	58,89,113	1.63	8 (13%)
16	CLA	1	612	-	49,53,73	1.38	8 (16%)	58,89,113	1.53	7 (12%)
16	CLA	K	102	-	46,50,73	1.40	9 (19%)	53,85,113	1.55	4 (7%)
16	CLA	F	802	-	49,53,73	1.38	9 (18%)	58,89,113	1.60	11 (18%)
21	LHG	A	841	-	48,48,48	0.71	1 (2%)	51,54,54	1.31	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	L	203	-	61,65,73	1.21	8 (13%)	72,103,113	1.43	6 (8%)
16	CLA	L	205	-	54,58,73	1.30	9 (16%)	64,95,113	1.54	11 (17%)
16	CLA	A	850	-	69,73,73	1.24	8 (11%)	82,113,113	1.99	16 (19%)
16	CLA	B	825	-	59,63,73	1.25	10 (16%)	70,101,113	1.44	7 (10%)
16	CLA	J	101	-	46,50,73	1.36	9 (19%)	53,85,113	1.51	6 (11%)
18	1DO	3	219	24	12,12,12	0.29	0	11,11,11	0.83	0
16	CLA	B	816	-	49,53,73	1.37	10 (20%)	58,89,113	1.51	7 (12%)
17	ZEX	1	615	-	43,43,43	3.84	18 (41%)	51,60,60	5.53	29 (56%)
22	BCR	B	847	-	41,41,41	1.15	3 (7%)	56,56,56	1.34	7 (12%)
16	CLA	3	211	-	46,50,73	1.37	8 (17%)	53,85,113	1.52	6 (11%)
16	CLA	3	210	-	45,49,73	1.39	9 (20%)	54,84,113	1.63	6 (11%)
16	CLA	A	821	-	53,57,73	1.30	9 (16%)	61,93,113	1.59	7 (11%)
25	DGD	B	850	-	67,67,67	0.99	4 (5%)	81,81,81	1.49	13 (16%)
20	PQN	A	840	-	34,34,34	2.81	10 (29%)	43,45,45	2.08	6 (13%)
22	BCR	L	207	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	5 (8%)
16	CLA	B	824	-	47,51,73	1.38	9 (19%)	55,86,113	1.59	6 (10%)
16	CLA	1	611	-	49,53,73	1.35	9 (18%)	58,89,113	1.58	6 (10%)
16	CLA	B	806	-	49,53,73	1.35	10 (20%)	58,89,113	1.62	8 (13%)
16	CLA	1	601	-	52,56,73	1.32	8 (15%)	61,92,113	1.91	10 (16%)
16	CLA	A	834	-	49,53,73	1.37	11 (22%)	58,89,113	1.63	11 (18%)
16	CLA	A	813	-	49,53,73	1.36	9 (18%)	58,89,113	1.58	11 (18%)
16	CLA	B	809	-	69,73,73	1.13	9 (13%)	82,113,113	1.37	8 (9%)
22	BCR	A	845	-	41,41,41	1.26	4 (9%)	56,56,56	1.45	9 (16%)
17	ZEX	2	616	-	43,43,43	3.97	20 (46%)	51,60,60	5.62	27 (52%)
16	CLA	3	209	-	56,60,73	1.25	8 (14%)	65,97,113	1.52	8 (12%)
16	CLA	B	826	-	69,73,73	1.20	9 (13%)	82,113,113	1.40	7 (8%)
17	ZEX	3	215	-	43,43,43	3.94	19 (44%)	51,60,60	5.57	29 (56%)
16	CLA	B	840	-	69,73,73	1.15	11 (15%)	82,113,113	1.44	7 (8%)
16	CLA	A	838	-	69,73,73	1.14	8 (11%)	82,113,113	1.47	8 (9%)
16	CLA	B	810	-	69,73,73	1.16	9 (13%)	82,113,113	1.59	9 (10%)
16	CLA	B	811	-	69,73,73	1.18	9 (13%)	82,113,113	1.44	9 (10%)
16	CLA	B	807	-	69,73,73	1.15	9 (13%)	82,113,113	1.49	9 (10%)
16	CLA	A	828	-	69,73,73	1.27	9 (13%)	82,113,113	1.51	17 (20%)
16	CLA	A	818	-	69,73,73	1.23	7 (10%)	82,113,113	1.47	11 (13%)
16	CLA	B	828	-	69,73,73	1.18	11 (15%)	82,113,113	1.41	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	2	604	-	46,50,73	1.33	9 (19%)	53,85,113	1.58	6 (11%)
16	CLA	A	811	-	58,62,73	1.25	10 (17%)	68,99,113	1.42	6 (8%)
22	BCR	K	103	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	5 (8%)
16	CLA	B	835	-	69,73,73	1.14	9 (13%)	82,113,113	1.40	7 (8%)
16	CLA	2	603	-	49,53,73	1.39	9 (18%)	58,89,113	1.57	7 (12%)
16	CLA	3	203	-	67,71,73	1.17	10 (14%)	79,110,113	1.46	9 (11%)
22	BCR	B	844	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	8 (14%)
22	BCR	F	804	-	41,41,41	1.12	2 (4%)	56,56,56	1.42	10 (17%)
22	BCR	A	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.44	10 (17%)
16	CLA	A	825	-	59,63,73	1.25	10 (16%)	70,101,113	1.61	8 (11%)
16	CLA	B	804	-	69,73,73	1.24	10 (14%)	82,113,113	1.55	15 (18%)
17	ZEX	3	217	-	43,43,43	3.93	18 (41%)	51,60,60	5.26	27 (52%)
16	CLA	2	611	-	49,53,73	1.35	9 (18%)	58,89,113	1.72	8 (13%)
16	CLA	B	836	-	49,53,73	1.38	9 (18%)	58,89,113	1.55	5 (8%)
16	CLA	B	815	-	69,73,73	1.16	7 (10%)	82,113,113	1.43	8 (9%)
16	CLA	B	823	-	50,54,73	1.33	9 (18%)	59,90,113	1.50	6 (10%)
16	CLA	3	208	-	49,53,73	1.39	10 (20%)	58,89,113	1.50	6 (10%)
16	CLA	1	609	-	45,49,73	1.38	9 (20%)	54,84,113	1.66	6 (11%)
16	CLA	2	601	-	49,53,73	1.36	9 (18%)	58,89,113	1.68	6 (10%)
16	CLA	A	805	-	69,73,73	1.18	9 (13%)	82,113,113	1.54	10 (12%)
16	CLA	A	815	-	49,53,73	1.37	10 (20%)	58,89,113	1.69	8 (13%)
16	CLA	O	204	-	49,53,73	1.38	9 (18%)	58,89,113	1.45	5 (8%)
17	ZEX	2	617	-	43,43,43	3.78	18 (41%)	51,60,60	5.65	29 (56%)
16	CLA	L	204	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	6 (7%)
16	CLA	2	610	-	46,50,73	1.39	9 (19%)	53,85,113	1.59	5 (9%)
16	CLA	B	821	-	69,73,73	1.17	8 (11%)	82,113,113	1.39	7 (8%)
22	BCR	L	202	-	41,41,41	1.24	2 (4%)	56,56,56	1.35	6 (10%)
16	CLA	A	817	-	69,73,73	1.19	7 (10%)	82,113,113	1.41	12 (14%)
23	SF4	C	102	-	0,12,12	-	-	-	-	-
16	CLA	A	814	-	46,50,73	1.37	8 (17%)	53,85,113	1.73	6 (11%)
16	CLA	A	837	-	69,73,73	1.15	10 (14%)	82,113,113	1.38	10 (12%)
16	CLA	B	819	-	63,67,73	1.24	8 (12%)	74,105,113	1.50	11 (14%)
16	CLA	A	851	-	47,51,73	1.38	10 (21%)	55,86,113	1.59	8 (14%)
16	CLA	3	213	-	55,59,73	1.29	8 (14%)	64,96,113	1.50	6 (9%)
16	CLA	3	202	-	49,53,73	1.39	9 (18%)	58,89,113	1.55	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	1	608	-	64,68,73	1.19	10 (15%)	76,107,113	1.45	6 (7%)
16	CLA	2	607	-	49,53,73	1.35	10 (20%)	58,89,113	1.48	8 (13%)
16	CLA	A	809	-	59,63,73	1.24	8 (13%)	70,101,113	1.42	6 (8%)
16	CLA	1	605	-	45,50,73	1.42	7 (15%)	52,85,113	1.55	6 (11%)
16	CLA	B	814	-	59,63,73	1.23	11 (18%)	70,101,113	1.53	7 (10%)
22	BCR	B	846	-	41,41,41	1.11	3 (7%)	56,56,56	1.34	8 (14%)
16	CLA	A	839	-	69,73,73	1.17	9 (13%)	82,113,113	1.51	8 (9%)
17	ZEX	2	614	-	43,43,43	3.83	18 (41%)	51,60,60	5.57	31 (60%)
16	CLA	B	842	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
16	CLA	B	841	-	69,73,73	1.19	9 (13%)	82,113,113	1.44	9 (10%)
16	CLA	B	805	-	69,73,73	1.24	8 (11%)	82,113,113	1.85	15 (18%)
23	SF4	A	848	-	0,12,12	-	-	-	-	-

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
16	CLA	A	831	-	1/1/15/20	17/39/115/115	-
16	CLA	2	612	-	1/1/11/20	9/15/91/115	-
22	BCR	L	206	-	-	18/29/63/63	0/2/2/2
16	CLA	A	827	-	1/1/15/20	12/39/115/115	-
16	CLA	B	831	-	1/1/15/20	12/39/115/115	-
16	CLA	1	607	-	1/1/11/20	9/15/91/115	-
22	BCR	A	843	-	-	13/29/63/63	0/2/2/2
16	CLA	A	829	-	1/1/15/20	13/39/115/115	-
16	CLA	B	830	-	1/1/15/20	15/39/115/115	-
16	CLA	1	610	-	1/1/11/20	6/15/91/115	-
16	CLA	3	206	-	1/1/11/20	7/15/91/115	-
16	CLA	A	819	-	1/1/11/20	9/15/91/115	-
16	CLA	B	829	-	1/1/15/20	22/39/115/115	-
16	CLA	3	205	-	1/1/11/20	6/15/91/115	-
26	3XQ	J	104	-	-	14/24/24/24	-
22	BCR	A	849	-	-	15/29/63/63	0/2/2/2
16	CLA	2	602	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	816	-	1/1/14/20	11/36/112/115	-
16	CLA	2	606	-	1/1/11/20	7/15/91/115	-
16	CLA	B	802	-	1/1/15/20	13/39/115/115	-
17	ZEX	2	615	-	-	20/29/67/67	0/2/2/2
22	BCR	I	101	-	-	18/29/63/63	0/2/2/2
16	CLA	O	201	-	1/1/12/20	7/24/100/115	-
16	CLA	L	201	-	1/1/13/20	6/29/105/115	-
24	BGC	A	853	18	-	2/2/19/22	0/1/1/1
16	CLA	B	803	-	1/1/15/20	15/39/115/115	-
16	CLA	1	602	-	1/1/13/20	8/32/108/115	-
22	BCR	J	102	-	-	16/29/63/63	0/2/2/2
16	CLA	B	833	-	1/1/15/20	18/39/115/115	-
16	CLA	B	820	-	1/1/14/20	11/33/109/115	-
22	BCR	A	847	-	-	18/29/63/63	0/2/2/2
16	CLA	B	812	-	1/1/15/20	15/39/115/115	-
22	BCR	A	846	-	-	15/29/63/63	0/2/2/2
19	CL0	A	801	-	3/3/20/25	11/37/135/135	-
17	ZEX	1	617	-	-	17/29/67/67	0/2/2/2
16	CLA	A	836	-	1/1/15/20	16/39/115/115	-
16	CLA	B	839	-	1/1/11/20	2/18/94/115	-
16	CLA	3	212	-	1/1/11/20	8/17/93/115	-
17	ZEX	1	613	-	-	18/29/67/67	0/2/2/2
16	CLA	B	837	-	1/1/14/20	15/33/109/115	-
16	CLA	A	810	-	1/1/15/20	16/39/115/115	-
16	CLA	3	207	-	1/1/11/20	6/15/91/115	-
16	CLA	2	608	-	1/1/12/20	7/21/97/115	-
21	LHG	A	842	-	-	17/44/44/53	-
23	SF4	C	101	-	-	-	0/6/5/5
16	CLA	K	101	-	1/1/11/20	6/15/91/115	-
16	CLA	A	806	-	1/1/15/20	18/39/115/115	-
16	CLA	B	832	-	1/1/11/20	6/15/91/115	-
16	CLA	O	203	-	1/1/12/20	8/21/97/115	-
16	CLA	O	202	-	1/1/10/20	4/10/86/115	-
16	CLA	A	826	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	835	-	1/1/12/20	7/23/99/115	-
16	CLA	2	609	-	1/1/10/20	4/10/86/115	-
16	CLA	A	803	-	1/1/13/20	7/27/103/115	-
16	CLA	A	852	-	1/1/14/20	15/35/111/115	-
16	CLA	A	820	-	1/1/15/20	16/39/115/115	-
17	ZEX	3	201	-	-	18/29/67/67	0/2/2/2
16	CLA	A	807	4	1/1/15/20	15/39/115/115	-
16	CLA	2	605	-	1/1/11/20	7/15/91/115	-
20	PQN	B	843	-	-	7/23/43/43	0/2/2/2
16	CLA	2	613	-	1/1/11/20	4/15/91/115	-
16	CLA	B	808	-	1/1/15/20	18/39/115/115	-
17	ZEX	3	214	-	-	14/29/67/67	0/2/2/2
22	BCR	B	849	-	-	13/29/63/63	0/2/2/2
16	CLA	A	823	-	1/1/13/20	7/27/103/115	-
17	ZEX	3	218	-	-	17/29/67/67	0/2/2/2
16	CLA	A	802	-	1/1/15/20	20/39/115/115	-
16	CLA	B	827	-	1/1/15/20	10/39/115/115	-
17	ZEX	3	216	-	-	15/29/67/67	0/2/2/2
22	BCR	J	103	-	-	15/29/63/63	0/2/2/2
22	BCR	B	848	-	-	23/29/63/63	0/2/2/2
16	CLA	1	606	-	1/1/11/20	7/15/91/115	-
16	CLA	A	832	-	1/1/15/20	14/39/115/115	-
16	CLA	B	813	-	1/1/13/20	6/25/101/115	-
22	BCR	B	845	-	-	11/29/63/63	0/2/2/2
16	CLA	A	804	-	1/1/15/20	7/39/115/115	-
16	CLA	A	833	-	1/1/15/20	10/39/115/115	-
16	CLA	B	817	-	1/1/10/20	5/12/88/115	-
16	CLA	B	834	-	1/1/13/20	11/31/107/115	-
22	BCR	F	801	-	-	17/29/63/63	0/2/2/2
16	CLA	A	812	-	1/1/15/20	10/39/115/115	-
16	CLA	A	822	-	1/1/12/20	11/23/99/115	-
16	CLA	B	838	-	1/1/15/20	10/39/115/115	-
16	CLA	B	822	-	1/1/11/20	5/15/91/115	-
16	CLA	F	803	-	1/1/10/20	6/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	1	603	-	1/1/11/20	8/15/91/115	-
16	CLA	A	808	4	1/1/15/20	17/39/115/115	-
16	CLA	B	818	-	1/1/13/20	11/27/103/115	-
17	ZEX	1	616	-	-	17/29/67/67	0/2/2/2
16	CLA	A	824	-	1/1/15/20	16/39/115/115	-
16	CLA	3	204	-	1/1/11/20	10/15/91/115	-
17	ZEX	1	614	-	-	17/29/67/67	0/2/2/2
16	CLA	A	830	-	1/1/12/20	7/21/97/115	-
16	CLA	B	801	-	1/1/15/20	14/39/115/115	-
16	CLA	1	604	-	1/1/11/20	6/15/91/115	-
16	CLA	1	612	-	1/1/11/20	8/15/91/115	-
16	CLA	K	102	-	1/1/10/20	3/12/88/115	-
16	CLA	F	802	-	1/1/11/20	3/15/91/115	-
21	LHG	A	841	-	-	28/53/53/53	-
16	CLA	L	203	-	1/1/13/20	15/30/106/115	-
16	CLA	L	205	-	1/1/12/20	7/21/97/115	-
16	CLA	A	850	-	1/1/15/20	11/39/115/115	-
16	CLA	B	825	-	1/1/13/20	12/27/103/115	-
16	CLA	J	101	-	1/1/10/20	8/12/88/115	-
18	IDO	3	219	24	-	1/10/10/10	-
16	CLA	B	816	-	1/1/11/20	3/15/91/115	-
17	ZEX	1	615	-	-	18/29/67/67	0/2/2/2
22	BCR	B	847	-	-	16/29/63/63	0/2/2/2
16	CLA	3	211	-	1/1/10/20	2/12/88/115	-
16	CLA	3	210	-	1/1/10/20	4/10/86/115	-
16	CLA	A	821	-	1/1/11/20	8/20/96/115	-
25	DGD	B	850	-	-	30/55/95/95	0/2/2/2
20	PQN	A	840	-	-	8/23/43/43	0/2/2/2
22	BCR	L	207	-	-	16/29/63/63	0/2/2/2
16	CLA	B	824	-	1/1/10/20	4/13/89/115	-
16	CLA	1	611	-	1/1/11/20	8/15/91/115	-
16	CLA	B	806	-	1/1/11/20	5/15/91/115	-
16	CLA	1	601	-	1/1/11/20	6/19/95/115	-
16	CLA	A	834	-	1/1/11/20	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	813	-	1/1/11/20	8/15/91/115	-
16	CLA	B	809	-	1/1/15/20	15/39/115/115	-
22	BCR	A	845	-	-	18/29/63/63	0/2/2/2
17	ZEX	2	616	-	-	20/29/67/67	0/2/2/2
16	CLA	3	209	-	1/1/12/20	6/24/100/115	-
16	CLA	B	826	-	1/1/15/20	13/39/115/115	-
17	ZEX	3	215	-	-	16/29/67/67	0/2/2/2
16	CLA	B	840	-	1/1/15/20	15/39/115/115	-
16	CLA	A	838	-	1/1/15/20	12/39/115/115	-
16	CLA	B	810	-	1/1/15/20	13/39/115/115	-
16	CLA	B	811	-	1/1/15/20	15/39/115/115	-
16	CLA	B	807	-	1/1/15/20	16/39/115/115	-
16	CLA	A	828	-	1/1/15/20	18/39/115/115	-
16	CLA	A	818	-	1/1/15/20	15/39/115/115	-
16	CLA	B	828	-	1/1/15/20	12/39/115/115	-
16	CLA	2	604	-	1/1/10/20	5/12/88/115	-
16	CLA	A	811	-	1/1/12/20	8/26/102/115	-
22	BCR	K	103	-	-	18/29/63/63	0/2/2/2
16	CLA	B	835	-	1/1/15/20	16/39/115/115	-
16	CLA	2	603	-	1/1/11/20	6/15/91/115	-
16	CLA	3	203	-	1/1/14/20	19/37/113/115	-
22	BCR	B	844	-	-	13/29/63/63	0/2/2/2
22	BCR	F	804	-	-	19/29/63/63	0/2/2/2
22	BCR	A	844	-	-	17/29/63/63	0/2/2/2
16	CLA	A	825	-	1/1/13/20	5/27/103/115	-
16	CLA	B	804	-	1/1/15/20	15/39/115/115	-
17	ZEX	3	217	-	-	16/29/67/67	0/2/2/2
16	CLA	2	611	-	1/1/11/20	8/15/91/115	-
16	CLA	B	836	-	1/1/11/20	9/15/91/115	-
16	CLA	B	815	-	1/1/15/20	22/39/115/115	-
16	CLA	B	823	-	1/1/11/20	8/17/93/115	-
16	CLA	3	208	-	1/1/11/20	9/15/91/115	-
16	CLA	1	609	-	1/1/10/20	2/10/86/115	-
16	CLA	2	601	-	1/1/11/20	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	805	-	1/1/15/20	17/39/115/115	-
16	CLA	A	815	-	1/1/11/20	8/15/91/115	-
16	CLA	O	204	-	1/1/11/20	6/15/91/115	-
17	ZEX	2	617	-	-	16/29/67/67	0/2/2/2
16	CLA	L	204	-	1/1/15/20	17/39/115/115	-
16	CLA	2	610	-	1/1/10/20	6/12/88/115	-
16	CLA	B	821	-	1/1/15/20	13/39/115/115	-
22	BCR	L	202	-	-	20/29/63/63	0/2/2/2
16	CLA	A	817	-	1/1/15/20	13/39/115/115	-
23	SF4	C	102	-	-	-	0/6/5/5
16	CLA	A	814	-	1/1/10/20	3/12/88/115	-
16	CLA	A	837	-	1/1/15/20	9/39/115/115	-
16	CLA	B	819	-	1/1/13/20	14/32/108/115	-
16	CLA	A	851	-	1/1/10/20	4/13/89/115	-
16	CLA	3	213	-	1/1/12/20	9/23/99/115	-
16	CLA	3	202	-	1/1/11/20	7/15/91/115	-
16	CLA	1	608	-	1/1/14/20	11/33/109/115	-
16	CLA	2	607	-	1/1/11/20	8/15/91/115	-
16	CLA	A	809	-	1/1/13/20	8/27/103/115	-
16	CLA	1	605	-	1/1/10/20	6/11/87/115	-
16	CLA	B	814	-	1/1/13/20	6/27/103/115	-
22	BCR	B	846	-	-	20/29/63/63	0/2/2/2
16	CLA	A	839	-	1/1/15/20	21/39/115/115	-
17	ZEX	2	614	-	-	17/29/67/67	0/2/2/2
16	CLA	B	842	-	1/1/15/20	15/39/115/115	-
16	CLA	B	841	-	1/1/15/20	12/39/115/115	-
16	CLA	B	805	-	1/1/15/20	19/39/115/115	-
23	SF4	A	848	-	-	-	0/6/5/5

All (1595) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	801	CL0	C3A-C2A	-14.58	1.42	1.54
17	3	215	ZEX	C5-C6	12.77	1.55	1.34
17	3	216	ZEX	C25-C26	12.29	1.53	1.34
17	2	615	ZEX	C5-C6	12.23	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	217	ZEX	C5-C6	12.18	1.54	1.34
17	3	201	ZEX	C25-C26	12.18	1.52	1.34
17	3	216	ZEX	C5-C6	12.12	1.54	1.34
17	1	614	ZEX	C5-C6	12.11	1.54	1.34
17	3	218	ZEX	C5-C6	12.11	1.54	1.34
17	2	616	ZEX	C5-C6	12.07	1.54	1.34
17	1	616	ZEX	C5-C6	12.07	1.54	1.34
17	3	214	ZEX	C25-C26	12.05	1.52	1.34
17	2	617	ZEX	C5-C6	12.04	1.54	1.34
17	1	615	ZEX	C5-C6	11.99	1.54	1.34
17	3	218	ZEX	C25-C26	11.97	1.52	1.34
17	3	215	ZEX	C25-C26	11.97	1.52	1.34
17	2	616	ZEX	C25-C26	11.93	1.52	1.34
17	3	214	ZEX	C5-C6	11.91	1.54	1.34
17	2	614	ZEX	C5-C6	11.88	1.54	1.34
17	1	613	ZEX	C25-C26	11.88	1.52	1.34
17	1	613	ZEX	C5-C6	11.76	1.54	1.34
17	1	616	ZEX	C25-C26	11.73	1.52	1.34
17	1	614	ZEX	C25-C26	11.71	1.52	1.34
17	3	217	ZEX	C25-C26	11.68	1.52	1.34
17	3	201	ZEX	C5-C6	11.63	1.54	1.34
17	1	617	ZEX	C25-C26	11.58	1.51	1.34
17	1	617	ZEX	C5-C6	11.51	1.53	1.34
17	2	614	ZEX	C25-C26	11.48	1.51	1.34
17	1	615	ZEX	C25-C26	11.43	1.51	1.34
17	2	617	ZEX	C25-C26	11.35	1.51	1.34
17	2	615	ZEX	C25-C26	10.92	1.50	1.34
17	3	218	ZEX	C14-C13	9.05	1.56	1.35
20	A	840	PQN	C12-C13	8.64	1.52	1.33
17	1	616	ZEX	C14-C13	8.46	1.55	1.35
17	3	201	ZEX	C14-C13	8.44	1.55	1.35
20	B	843	PQN	C12-C13	8.41	1.52	1.33
17	3	217	ZEX	C14-C13	8.31	1.55	1.35
20	B	843	PQN	O4-C4	8.31	1.40	1.23
17	2	616	ZEX	C14-C13	8.26	1.54	1.35
19	A	801	CL0	MG-NB	-8.24	1.89	2.05
17	3	218	ZEX	C10-C9	8.23	1.54	1.35
17	1	615	ZEX	C14-C13	8.22	1.54	1.35
17	1	617	ZEX	C14-C13	8.21	1.54	1.35
17	3	216	ZEX	C14-C13	8.20	1.54	1.35
17	1	614	ZEX	C14-C13	8.17	1.54	1.35
19	A	801	CL0	CBD-CGD	-8.16	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	214	ZEX	C14-C13	8.15	1.54	1.35
17	3	201	ZEX	C10-C9	8.12	1.54	1.35
17	2	614	ZEX	C14-C13	8.12	1.54	1.35
17	1	613	ZEX	C14-C13	8.07	1.54	1.35
17	1	613	ZEX	C10-C9	7.96	1.54	1.35
20	A	840	PQN	O4-C4	7.96	1.39	1.23
17	3	215	ZEX	C14-C13	7.94	1.54	1.35
17	2	615	ZEX	C14-C13	7.82	1.53	1.35
17	2	617	ZEX	C14-C13	7.81	1.53	1.35
19	A	801	CL0	CMA-C3A	-7.78	1.40	1.53
20	A	840	PQN	O1-C1	7.76	1.39	1.23
17	3	218	ZEX	C34-C33	7.70	1.53	1.35
17	1	614	ZEX	C10-C9	7.62	1.53	1.35
17	2	616	ZEX	C10-C9	7.60	1.53	1.35
17	3	217	ZEX	C10-C9	7.59	1.53	1.35
17	1	616	ZEX	C10-C9	7.57	1.53	1.35
17	3	214	ZEX	C10-C9	7.57	1.53	1.35
17	1	615	ZEX	C10-C9	7.55	1.53	1.35
20	B	843	PQN	O1-C1	7.53	1.38	1.23
17	3	216	ZEX	C10-C9	7.53	1.53	1.35
17	2	614	ZEX	C10-C9	7.52	1.53	1.35
17	3	215	ZEX	C10-C9	7.49	1.53	1.35
17	3	218	ZEX	C30-C29	7.44	1.53	1.35
17	2	615	ZEX	C10-C9	7.29	1.52	1.35
17	3	217	ZEX	C30-C29	7.28	1.52	1.35
17	1	617	ZEX	C10-C9	7.25	1.52	1.35
17	2	616	ZEX	C30-C29	7.24	1.52	1.35
17	2	617	ZEX	C10-C9	7.18	1.52	1.35
17	1	615	ZEX	C30-C29	7.18	1.52	1.35
17	3	201	ZEX	C30-C29	7.15	1.52	1.35
17	3	214	ZEX	C30-C29	7.12	1.52	1.35
17	1	616	ZEX	C30-C29	7.08	1.52	1.35
17	3	216	ZEX	C30-C29	7.05	1.52	1.35
17	3	201	ZEX	C34-C33	7.04	1.52	1.35
17	1	614	ZEX	C30-C29	7.04	1.52	1.35
17	3	215	ZEX	C30-C29	7.00	1.52	1.35
17	2	614	ZEX	C30-C29	6.99	1.52	1.35
17	2	616	ZEX	C34-C33	6.99	1.52	1.35
17	3	217	ZEX	C34-C33	6.95	1.51	1.35
17	3	214	ZEX	C34-C33	6.95	1.51	1.35
17	3	216	ZEX	C34-C33	6.94	1.51	1.35
17	1	617	ZEX	C30-C29	6.93	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	613	ZEX	C30-C29	6.92	1.51	1.35
17	1	616	ZEX	C34-C33	6.91	1.51	1.35
17	2	617	ZEX	C30-C29	6.88	1.51	1.35
17	1	614	ZEX	C34-C33	6.85	1.51	1.35
17	1	617	ZEX	C34-C33	6.85	1.51	1.35
17	2	617	ZEX	C34-C33	6.78	1.51	1.35
17	3	215	ZEX	C34-C33	6.77	1.51	1.35
17	1	615	ZEX	C34-C33	6.76	1.51	1.35
17	2	615	ZEX	C34-C33	6.72	1.51	1.35
17	1	613	ZEX	C34-C33	6.71	1.51	1.35
17	2	614	ZEX	C34-C33	6.68	1.51	1.35
17	2	615	ZEX	C30-C29	6.62	1.51	1.35
19	A	801	CL0	MG-ND	-6.17	1.93	2.05
19	A	801	CL0	C3D-C4D	-5.73	1.32	1.41
19	A	801	CL0	C4A-C3A	-5.39	1.40	1.51
17	3	201	ZEX	C27-C26	5.38	1.53	1.46
19	A	801	CL0	CMD-C2D	-4.95	1.41	1.51
17	3	218	ZEX	C27-C26	4.93	1.52	1.46
16	A	829	CLA	CMB-C2B	-4.44	1.41	1.50
19	A	801	CL0	C1A-C2A	-4.43	1.42	1.51
17	3	218	ZEX	C28-C29	4.40	1.55	1.46
19	A	801	CL0	CHA-CBD	-4.38	1.46	1.51
17	3	201	ZEX	C7-C6	4.37	1.60	1.45
17	2	616	ZEX	C27-C26	4.28	1.51	1.46
17	3	218	ZEX	C7-C6	4.25	1.59	1.45
17	3	217	ZEX	C27-C26	4.20	1.51	1.46
17	2	615	ZEX	C7-C6	4.20	1.59	1.45
17	3	214	ZEX	C27-C26	4.14	1.51	1.46
17	1	614	ZEX	C7-C6	4.13	1.59	1.45
17	1	617	ZEX	C7-C6	4.13	1.59	1.45
17	1	615	ZEX	C7-C6	4.12	1.59	1.45
17	3	215	ZEX	C27-C26	4.11	1.51	1.46
17	1	616	ZEX	C7-C6	4.10	1.59	1.45
17	3	215	ZEX	C7-C6	4.09	1.59	1.45
19	A	801	CL0	CHB-C4A	-4.08	1.33	1.38
17	2	614	ZEX	C7-C6	4.07	1.59	1.45
17	3	218	ZEX	C35-C34	4.07	1.55	1.43
17	1	613	ZEX	C7-C6	4.06	1.59	1.45
22	A	846	BCR	C30-C25	-4.05	1.48	1.53
17	2	616	ZEX	C28-C29	4.05	1.54	1.46
17	3	216	ZEX	C7-C6	4.04	1.58	1.45
17	3	214	ZEX	C7-C6	4.01	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	847	BCR	C30-C25	-4.00	1.48	1.53
17	3	216	ZEX	C27-C26	4.00	1.51	1.46
17	2	616	ZEX	C7-C6	3.97	1.58	1.45
17	3	217	ZEX	C7-C6	3.95	1.58	1.45
16	A	850	CLA	CMC-C2C	-3.92	1.42	1.50
22	F	801	BCR	C30-C25	-3.91	1.48	1.53
17	3	201	ZEX	C35-C34	3.91	1.55	1.43
22	A	847	BCR	C1-C6	-3.90	1.48	1.53
22	L	202	BCR	C30-C25	-3.89	1.48	1.53
22	J	103	BCR	C30-C25	-3.87	1.48	1.53
17	2	616	ZEX	C35-C34	3.86	1.55	1.43
17	1	617	ZEX	C27-C26	3.85	1.51	1.46
19	A	801	CL0	C3D-C2D	-3.85	1.33	1.39
17	2	614	ZEX	C35-C34	3.85	1.55	1.43
22	J	103	BCR	C1-C6	-3.84	1.48	1.53
17	1	616	ZEX	C27-C26	3.82	1.51	1.46
17	3	216	ZEX	C35-C34	3.82	1.55	1.43
22	A	845	BCR	C30-C25	-3.81	1.48	1.53
17	3	214	ZEX	C28-C29	3.81	1.54	1.46
17	3	217	ZEX	C35-C34	3.79	1.54	1.43
22	J	102	BCR	C1-C6	-3.78	1.48	1.53
17	1	617	ZEX	C35-C34	3.76	1.54	1.43
17	1	616	ZEX	C35-C34	3.76	1.54	1.43
17	3	218	ZEX	C8-C9	3.72	1.53	1.46
17	2	617	ZEX	C7-C6	3.71	1.57	1.45
20	B	843	PQN	C2-C1	-3.71	1.39	1.47
17	3	215	ZEX	C35-C34	3.66	1.54	1.43
17	2	617	ZEX	C28-C29	3.65	1.53	1.46
17	3	218	ZEX	C31-C30	3.65	1.54	1.43
16	O	202	CLA	C1D-ND	3.65	1.42	1.37
17	2	617	ZEX	C35-C34	3.65	1.54	1.43
17	1	613	ZEX	C35-C34	3.65	1.54	1.43
17	1	617	ZEX	C28-C29	3.64	1.53	1.46
17	1	615	ZEX	C35-C34	3.64	1.54	1.43
22	A	849	BCR	C1-C6	-3.64	1.49	1.53
17	2	614	ZEX	C28-C29	3.64	1.53	1.46
17	2	616	ZEX	C31-C30	3.63	1.54	1.43
17	2	617	ZEX	C27-C26	3.62	1.51	1.46
17	3	214	ZEX	C35-C34	3.62	1.54	1.43
16	A	829	CLA	C1B-NB	-3.62	1.33	1.37
17	3	201	ZEX	C28-C29	3.62	1.53	1.46
17	3	217	ZEX	C28-C29	3.61	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	615	ZEX	C35-C34	3.57	1.54	1.43
17	3	218	ZEX	C11-C10	3.57	1.54	1.43
22	I	101	BCR	C30-C25	-3.57	1.49	1.53
17	3	201	ZEX	C11-C10	3.56	1.54	1.43
22	B	848	BCR	C30-C25	-3.56	1.49	1.53
17	1	615	ZEX	C27-C26	3.56	1.50	1.46
22	A	846	BCR	C1-C6	-3.55	1.49	1.53
17	1	614	ZEX	C35-C34	3.54	1.54	1.43
16	2	609	CLA	C1D-ND	3.54	1.42	1.37
16	O	203	CLA	C1D-ND	3.54	1.42	1.37
17	3	216	ZEX	C28-C29	3.53	1.53	1.46
22	L	202	BCR	C1-C6	-3.52	1.49	1.53
17	3	216	ZEX	C31-C30	3.52	1.54	1.43
22	B	849	BCR	C30-C25	-3.52	1.49	1.53
17	1	614	ZEX	C8-C9	3.52	1.53	1.46
17	1	615	ZEX	C28-C29	3.52	1.53	1.46
22	A	843	BCR	C1-C6	-3.52	1.49	1.53
20	B	843	PQN	C10-C1	-3.51	1.41	1.48
19	A	801	CL0	CMB-C2B	-3.51	1.44	1.51
17	1	614	ZEX	C31-C30	3.51	1.54	1.43
22	B	846	BCR	C30-C25	-3.50	1.49	1.53
17	3	201	ZEX	C8-C9	3.50	1.53	1.46
17	1	616	ZEX	C28-C29	3.50	1.53	1.46
17	3	218	ZEX	C15-C14	3.50	1.54	1.43
17	1	613	ZEX	C27-C26	3.50	1.50	1.46
16	A	829	CLA	MG-NB	-3.49	1.98	2.05
16	B	831	CLA	CMB-C2B	-3.49	1.43	1.50
17	2	614	ZEX	C27-C26	3.48	1.50	1.46
16	A	828	CLA	CMD-C2D	-3.48	1.43	1.50
17	3	214	ZEX	C31-C30	3.48	1.54	1.43
19	A	801	CL0	C1B-C2B	3.48	1.43	1.39
16	B	801	CLA	C1B-NB	-3.47	1.33	1.37
17	1	616	ZEX	C31-C30	3.47	1.53	1.43
20	A	840	PQN	C3-C4	-3.47	1.38	1.47
17	2	617	ZEX	C31-C30	3.46	1.53	1.43
17	3	217	ZEX	C31-C30	3.46	1.53	1.43
16	1	605	CLA	C1D-ND	3.46	1.42	1.37
17	3	201	ZEX	C31-C30	3.46	1.53	1.43
16	3	206	CLA	CMB-C2B	-3.45	1.43	1.50
20	A	840	PQN	C2-C1	-3.43	1.39	1.47
16	3	202	CLA	C1D-ND	3.41	1.42	1.37
17	3	215	ZEX	C31-C30	3.41	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	801	CLA	CMD-C2D	-3.39	1.43	1.50
17	1	614	ZEX	C27-C26	3.39	1.50	1.46
17	3	201	ZEX	C15-C14	3.38	1.53	1.43
17	1	615	ZEX	C31-C30	3.38	1.53	1.43
22	L	207	BCR	C1-C6	-3.37	1.49	1.53
16	B	813	CLA	CAB-C3B	-3.37	1.43	1.50
17	2	616	ZEX	C11-C10	3.36	1.53	1.43
16	2	613	CLA	C1D-ND	3.35	1.42	1.37
17	1	616	ZEX	C8-C9	3.33	1.53	1.46
17	1	616	ZEX	C11-C10	3.33	1.53	1.43
16	B	802	CLA	MG-NB	-3.33	1.99	2.05
16	3	210	CLA	C1D-ND	3.32	1.42	1.37
16	A	818	CLA	MG-NB	-3.32	1.99	2.05
16	A	829	CLA	MG-ND	-3.32	1.99	2.05
17	1	617	ZEX	C31-C30	3.32	1.53	1.43
19	A	801	CL0	CBB-CAB	3.31	1.50	1.29
16	B	841	CLA	CMB-C2B	-3.31	1.44	1.50
17	1	613	ZEX	C11-C10	3.31	1.53	1.43
16	A	818	CLA	CMB-C2B	-3.31	1.44	1.50
17	2	614	ZEX	C31-C30	3.31	1.53	1.43
16	2	610	CLA	C1D-ND	3.30	1.42	1.37
17	2	615	ZEX	C8-C9	3.30	1.53	1.46
16	A	822	CLA	C1D-ND	3.29	1.42	1.37
16	3	213	CLA	C1D-ND	3.29	1.42	1.37
17	1	613	ZEX	C28-C29	3.29	1.53	1.46
17	3	216	ZEX	C8-C9	3.28	1.53	1.46
22	A	845	BCR	C1-C6	-3.28	1.49	1.53
20	B	843	PQN	C3-C4	-3.27	1.39	1.47
16	A	818	CLA	C1B-NB	-3.26	1.33	1.37
22	F	804	BCR	C30-C25	-3.26	1.49	1.53
16	3	208	CLA	C1D-ND	3.26	1.42	1.37
16	B	830	CLA	CMB-C2B	-3.26	1.44	1.50
17	2	614	ZEX	C15-C14	3.26	1.53	1.43
16	3	212	CLA	C1D-ND	3.25	1.42	1.37
16	B	834	CLA	C1D-ND	3.25	1.42	1.37
16	K	102	CLA	C1D-ND	3.25	1.42	1.37
17	3	218	ZEX	C32-C33	3.24	1.52	1.46
16	L	203	CLA	C1D-ND	3.23	1.42	1.37
17	1	614	ZEX	C11-C10	3.23	1.53	1.43
17	3	216	ZEX	C11-C10	3.23	1.53	1.43
17	1	615	ZEX	C8-C9	3.23	1.52	1.46
17	3	215	ZEX	C28-C29	3.22	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	828	CLA	MG-NB	-3.22	1.99	2.05
16	B	835	CLA	C1D-ND	3.20	1.42	1.37
20	A	840	PQN	C10-C1	-3.20	1.41	1.48
16	2	605	CLA	C1D-ND	3.20	1.42	1.37
16	B	827	CLA	CMD-C2D	-3.19	1.44	1.50
17	3	217	ZEX	C11-C10	3.19	1.53	1.43
17	2	614	ZEX	C11-C10	3.19	1.53	1.43
16	1	601	CLA	C1D-ND	3.19	1.42	1.37
17	1	614	ZEX	C28-C29	3.19	1.52	1.46
16	O	204	CLA	C1D-ND	3.18	1.42	1.37
17	3	215	ZEX	C11-C10	3.18	1.53	1.43
17	2	615	ZEX	C28-C29	3.18	1.52	1.46
16	B	805	CLA	CMD-C2D	-3.18	1.44	1.50
17	1	613	ZEX	C31-C30	3.18	1.53	1.43
16	1	607	CLA	C1D-ND	3.18	1.42	1.37
22	B	847	BCR	C30-C25	-3.17	1.49	1.53
17	2	615	ZEX	C11-C10	3.16	1.53	1.43
17	1	616	ZEX	C15-C14	3.16	1.53	1.43
22	K	103	BCR	C30-C25	-3.16	1.49	1.53
16	A	808	CLA	MG-NB	-3.16	1.99	2.05
17	3	217	ZEX	C8-C9	3.16	1.52	1.46
17	1	613	ZEX	C8-C9	3.15	1.52	1.46
17	2	617	ZEX	C11-C10	3.14	1.52	1.43
16	1	612	CLA	C1D-ND	3.14	1.42	1.37
17	2	616	ZEX	C8-C9	3.14	1.52	1.46
16	1	610	CLA	C1D-ND	3.14	1.42	1.37
16	B	813	CLA	C1D-ND	3.14	1.42	1.37
17	3	214	ZEX	C15-C14	3.13	1.52	1.43
16	3	211	CLA	C1D-ND	3.13	1.42	1.37
16	1	606	CLA	C1D-ND	3.13	1.42	1.37
19	A	801	CL0	CBD-CAD	-3.13	1.42	1.53
22	K	103	BCR	C1-C6	-3.13	1.49	1.53
22	B	844	BCR	C1-C6	-3.13	1.49	1.53
17	1	615	ZEX	C11-C10	3.12	1.52	1.43
17	1	617	ZEX	C8-C9	3.12	1.52	1.46
17	3	218	ZEX	C12-C13	3.12	1.52	1.46
16	A	815	CLA	C1D-ND	3.12	1.42	1.37
17	3	216	ZEX	C15-C14	3.11	1.52	1.43
22	F	801	BCR	C1-C6	-3.11	1.49	1.53
17	3	214	ZEX	C11-C10	3.11	1.52	1.43
17	3	217	ZEX	C15-C14	3.11	1.52	1.43
16	2	612	CLA	C1D-ND	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	828	CLA	C1B-NB	-3.10	1.33	1.37
17	2	616	ZEX	C15-C14	3.10	1.52	1.43
16	B	830	CLA	CMD-C2D	-3.10	1.44	1.50
22	A	844	BCR	C1-C6	-3.10	1.49	1.53
16	A	823	CLA	C1D-ND	3.10	1.41	1.37
17	2	614	ZEX	C8-C9	3.10	1.52	1.46
16	3	207	CLA	C1D-ND	3.09	1.41	1.37
16	3	205	CLA	C1D-ND	3.09	1.41	1.37
22	B	847	BCR	C1-C6	-3.09	1.49	1.53
16	2	607	CLA	C1D-ND	3.09	1.41	1.37
17	1	614	ZEX	C15-C14	3.09	1.52	1.43
16	L	205	CLA	C1D-ND	3.09	1.41	1.37
17	1	617	ZEX	C15-C14	3.09	1.52	1.43
16	B	812	CLA	C1D-ND	3.08	1.41	1.37
16	1	609	CLA	C1D-ND	3.08	1.41	1.37
16	A	836	CLA	CMB-C2B	-3.07	1.44	1.50
17	3	216	ZEX	C1-C6	3.07	1.57	1.53
17	3	201	ZEX	C32-C33	3.07	1.52	1.46
16	A	832	CLA	C1D-ND	3.07	1.41	1.37
16	A	809	CLA	C1D-ND	3.06	1.41	1.37
16	A	805	CLA	C1D-ND	3.06	1.41	1.37
16	A	806	CLA	MG-NB	-3.05	1.99	2.05
16	F	803	CLA	C1D-ND	3.05	1.41	1.37
17	3	215	ZEX	C15-C14	3.05	1.52	1.43
17	1	617	ZEX	C11-C10	3.05	1.52	1.43
17	3	218	ZEX	C8-C7	3.05	1.42	1.33
16	B	836	CLA	C1D-ND	3.04	1.41	1.37
19	A	801	CL0	CAA-C2A	-3.04	1.47	1.54
16	B	821	CLA	CMB-C2B	-3.04	1.44	1.50
25	B	850	DGD	O2G-C2G	-3.03	1.39	1.46
16	B	823	CLA	C1D-ND	3.03	1.41	1.37
17	2	615	ZEX	C31-C30	3.02	1.52	1.43
17	3	214	ZEX	C8-C9	3.02	1.52	1.46
16	B	842	CLA	C1D-ND	3.02	1.41	1.37
16	2	603	CLA	MG-NB	-3.02	1.99	2.05
21	A	841	LHG	O7-C5	-3.02	1.39	1.46
17	1	615	ZEX	C15-C14	3.02	1.52	1.43
16	1	605	CLA	C4B-NB	3.01	1.41	1.37
16	A	834	CLA	C1D-ND	3.01	1.41	1.37
16	A	828	CLA	CMB-C2B	-3.01	1.44	1.50
17	3	214	ZEX	C32-C33	3.00	1.52	1.46
16	B	831	CLA	CMD-C2D	-3.00	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	101	CLA	C1D-ND	2.99	1.41	1.37
17	1	614	ZEX	C1-C6	2.99	1.57	1.53
16	2	606	CLA	C1D-ND	2.99	1.41	1.37
22	A	849	BCR	C30-C25	-2.99	1.50	1.53
16	B	819	CLA	CMB-C2B	-2.98	1.44	1.50
16	A	802	CLA	C1D-ND	2.98	1.41	1.37
16	B	815	CLA	C1D-ND	2.98	1.41	1.37
17	3	201	ZEX	C8-C7	2.98	1.42	1.33
16	O	204	CLA	C4B-NB	2.97	1.41	1.37
22	J	102	BCR	C30-C25	-2.97	1.50	1.53
17	1	613	ZEX	C15-C14	2.97	1.52	1.43
17	3	217	ZEX	C1-C6	2.97	1.57	1.53
16	B	829	CLA	MG-NB	-2.97	1.99	2.05
16	A	817	CLA	MG-ND	-2.96	1.99	2.05
16	2	608	CLA	C1D-ND	2.96	1.41	1.37
16	A	808	CLA	C1D-ND	2.96	1.41	1.37
16	A	810	CLA	C1D-ND	2.96	1.41	1.37
16	B	825	CLA	C1D-ND	2.96	1.41	1.37
22	B	848	BCR	C1-C6	-2.96	1.50	1.53
16	F	802	CLA	C1D-ND	2.96	1.41	1.37
16	3	203	CLA	C1D-ND	2.96	1.41	1.37
16	B	814	CLA	C1D-ND	2.96	1.41	1.37
16	B	833	CLA	C4B-NB	2.95	1.41	1.37
16	A	829	CLA	CMD-C2D	-2.95	1.44	1.50
22	L	207	BCR	C30-C25	-2.95	1.50	1.53
22	L	206	BCR	C1-C6	-2.95	1.50	1.53
16	B	830	CLA	MG-NB	-2.94	2.00	2.05
16	A	851	CLA	C1D-ND	2.94	1.41	1.37
17	2	615	ZEX	C27-C26	2.94	1.50	1.46
16	A	819	CLA	C1D-ND	2.93	1.41	1.37
16	3	206	CLA	C1D-ND	2.93	1.41	1.37
16	1	604	CLA	C1D-ND	2.93	1.41	1.37
22	B	845	BCR	C1-C6	-2.93	1.50	1.53
16	2	603	CLA	C1D-ND	2.92	1.41	1.37
16	B	817	CLA	C1D-ND	2.92	1.41	1.37
16	B	831	CLA	C1B-NB	-2.92	1.34	1.37
16	B	839	CLA	MG-NB	-2.92	2.00	2.05
16	1	608	CLA	C1D-ND	2.92	1.41	1.37
16	O	201	CLA	C1D-ND	2.92	1.41	1.37
16	B	840	CLA	CMC-C2C	-2.92	1.44	1.50
24	A	853	BGC	O2-C2	-2.92	1.37	1.43
16	O	203	CLA	C4B-NB	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	822	CLA	C1D-ND	2.91	1.41	1.37
17	3	215	ZEX	C8-C9	2.91	1.52	1.46
16	A	814	CLA	C1D-ND	2.91	1.41	1.37
16	B	810	CLA	CMD-C2D	-2.91	1.44	1.50
16	B	841	CLA	MG-NB	-2.91	2.00	2.05
22	A	843	BCR	C30-C25	-2.90	1.50	1.53
16	O	202	CLA	C4B-NB	2.90	1.41	1.37
16	B	827	CLA	MG-NB	-2.90	2.00	2.05
17	2	617	ZEX	C15-C14	2.90	1.52	1.43
16	3	209	CLA	C1D-ND	2.90	1.41	1.37
19	A	801	CL0	CAC-C3C	-2.90	1.46	1.51
16	B	806	CLA	C1D-ND	2.90	1.41	1.37
16	A	828	CLA	MG-ND	-2.89	2.00	2.05
20	B	843	PQN	C10-C5	-2.89	1.36	1.40
17	2	615	ZEX	C15-C14	2.89	1.52	1.43
17	2	616	ZEX	C32-C33	2.89	1.52	1.46
16	A	837	CLA	MG-NB	-2.88	2.00	2.05
16	1	601	CLA	CMC-C2C	-2.88	1.44	1.50
17	1	616	ZEX	C32-C33	2.88	1.52	1.46
16	3	206	CLA	MG-NB	-2.88	2.00	2.05
16	2	611	CLA	C1D-ND	2.88	1.41	1.37
16	A	813	CLA	C1D-ND	2.88	1.41	1.37
16	A	824	CLA	C1D-ND	2.88	1.41	1.37
22	B	849	BCR	C1-C6	-2.88	1.50	1.53
16	B	802	CLA	CMB-C2B	-2.88	1.44	1.50
16	A	830	CLA	MG-NB	-2.88	2.00	2.05
16	B	804	CLA	MG-NB	-2.87	2.00	2.05
16	A	817	CLA	C1D-ND	2.87	1.41	1.37
17	3	214	ZEX	C1-C6	2.87	1.57	1.53
16	B	818	CLA	C1D-ND	2.87	1.41	1.37
16	A	836	CLA	MG-NB	-2.87	2.00	2.05
16	3	210	CLA	C4B-NB	2.86	1.41	1.37
16	B	819	CLA	MG-NB	-2.86	2.00	2.05
16	A	827	CLA	CMC-C2C	-2.86	1.44	1.50
16	A	806	CLA	CMD-C2D	-2.86	1.44	1.50
16	B	837	CLA	MG-NB	-2.86	2.00	2.05
22	L	206	BCR	C30-C25	-2.86	1.50	1.53
16	3	204	CLA	C1D-ND	2.86	1.41	1.37
16	A	831	CLA	C1D-ND	2.86	1.41	1.37
16	B	824	CLA	MG-NB	-2.85	2.00	2.05
19	A	801	CL0	CHD-C4C	-2.85	1.33	1.39
16	B	821	CLA	MG-NB	-2.85	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	825	CLA	MG-NB	-2.85	2.00	2.05
16	A	826	CLA	CMC-C2C	-2.85	1.44	1.50
17	3	216	ZEX	C32-C33	2.85	1.52	1.46
16	A	835	CLA	MG-NB	-2.85	2.00	2.05
20	A	840	PQN	C3-C2	2.84	1.40	1.35
16	B	801	CLA	MG-ND	-2.84	2.00	2.05
20	A	840	PQN	C10-C5	-2.84	1.36	1.40
16	1	607	CLA	CMD-C2D	-2.84	1.45	1.50
20	B	843	PQN	C3-C2	2.83	1.40	1.35
16	2	601	CLA	C1B-C2B	2.83	1.49	1.43
17	3	217	ZEX	C32-C33	2.83	1.52	1.46
17	3	201	ZEX	C12-C13	2.83	1.52	1.46
16	A	834	CLA	C4B-NB	2.83	1.41	1.37
16	2	602	CLA	C1D-ND	2.83	1.41	1.37
17	1	617	ZEX	C8-C7	2.83	1.41	1.33
16	B	833	CLA	C3B-C4B	2.83	1.50	1.42
16	B	808	CLA	C1D-ND	2.82	1.41	1.37
17	1	614	ZEX	C32-C33	2.82	1.52	1.46
16	A	852	CLA	MG-NB	-2.82	2.00	2.05
16	B	805	CLA	CMC-C2C	-2.82	1.45	1.50
16	A	803	CLA	C1D-ND	2.82	1.41	1.37
16	3	206	CLA	C4B-NB	2.82	1.41	1.37
16	B	802	CLA	MG-ND	-2.81	2.00	2.05
16	A	821	CLA	MG-NB	-2.81	2.00	2.05
16	B	813	CLA	C4B-NB	2.81	1.41	1.37
16	B	813	CLA	C1B-C2B	2.81	1.49	1.43
16	B	811	CLA	MG-NB	-2.81	2.00	2.05
16	B	812	CLA	C4B-NB	2.81	1.41	1.37
16	B	826	CLA	MG-NB	-2.81	2.00	2.05
16	B	832	CLA	C1D-ND	2.81	1.41	1.37
17	2	616	ZEX	C1-C6	2.81	1.57	1.53
16	A	806	CLA	CMB-C2B	-2.81	1.45	1.50
16	B	831	CLA	MG-NB	-2.81	2.00	2.05
16	B	808	CLA	MG-NB	-2.80	2.00	2.05
16	3	208	CLA	C4B-NB	2.80	1.41	1.37
16	A	824	CLA	CMD-C2D	-2.80	1.45	1.50
16	A	812	CLA	C1D-ND	2.80	1.41	1.37
22	F	804	BCR	C1-C6	-2.80	1.50	1.53
16	A	820	CLA	C1D-ND	2.80	1.41	1.37
16	B	840	CLA	C1D-ND	2.79	1.41	1.37
16	B	801	CLA	MG-NB	-2.79	2.00	2.05
16	1	603	CLA	MG-NB	-2.79	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	830	CLA	C1D-ND	2.79	1.41	1.37
16	A	817	CLA	MG-NB	-2.79	2.00	2.05
16	B	805	CLA	C1B-C2B	2.79	1.49	1.43
16	B	838	CLA	C1D-ND	2.78	1.41	1.37
16	A	820	CLA	MG-NB	-2.78	2.00	2.05
16	A	836	CLA	C1D-ND	2.78	1.41	1.37
16	A	827	CLA	MG-NB	-2.78	2.00	2.05
17	2	617	ZEX	C32-C33	2.78	1.51	1.46
16	A	811	CLA	C1D-ND	2.78	1.41	1.37
16	A	804	CLA	CMC-C2C	-2.78	1.45	1.50
16	A	839	CLA	MG-NB	-2.78	2.00	2.05
16	2	610	CLA	C4B-NB	2.77	1.41	1.37
16	B	811	CLA	C1D-ND	2.77	1.41	1.37
16	2	604	CLA	C1D-ND	2.77	1.41	1.37
16	3	212	CLA	C4B-NB	2.76	1.41	1.37
16	A	802	CLA	MG-NB	-2.76	2.00	2.05
16	2	613	CLA	C4B-NB	2.76	1.41	1.37
16	L	204	CLA	MG-NB	-2.76	2.00	2.05
16	A	850	CLA	MG-ND	-2.76	2.00	2.05
16	A	822	CLA	C4B-NB	2.76	1.41	1.37
16	B	826	CLA	CMB-C2B	-2.76	1.45	1.50
16	B	830	CLA	C1B-NB	-2.76	1.34	1.37
16	L	201	CLA	MG-NB	-2.75	2.00	2.05
16	B	819	CLA	C1D-ND	2.75	1.41	1.37
16	A	832	CLA	MG-NB	-2.75	2.00	2.05
16	3	211	CLA	C4B-NB	2.75	1.41	1.37
16	A	802	CLA	CMC-C2C	-2.75	1.45	1.50
16	3	208	CLA	CMC-C2C	-2.75	1.45	1.50
25	B	850	DGD	O1G-C1G	-2.74	1.39	1.45
16	A	806	CLA	C1D-ND	2.74	1.41	1.37
17	1	614	ZEX	C8-C7	2.74	1.41	1.33
16	B	826	CLA	CMD-C2D	-2.74	1.45	1.50
17	1	613	ZEX	C8-C7	2.74	1.41	1.33
16	B	805	CLA	MG-ND	-2.74	2.00	2.05
16	1	610	CLA	C4B-NB	2.74	1.41	1.37
16	A	838	CLA	MG-NB	-2.74	2.00	2.05
16	A	820	CLA	CMC-C2C	-2.73	1.45	1.50
16	1	602	CLA	C1D-ND	2.73	1.41	1.37
16	A	852	CLA	C1D-ND	2.73	1.41	1.37
16	B	801	CLA	CMB-C2B	-2.73	1.45	1.50
17	3	214	ZEX	C24-C25	2.73	1.54	1.50
16	A	813	CLA	MG-NB	-2.73	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	617	ZEX	C1-C6	2.73	1.57	1.53
17	1	615	ZEX	C32-C33	2.73	1.51	1.46
16	B	816	CLA	C1D-ND	2.72	1.41	1.37
16	F	803	CLA	C4B-NB	2.72	1.41	1.37
16	1	602	CLA	MG-NB	-2.72	2.00	2.05
16	A	824	CLA	MG-NB	-2.72	2.00	2.05
16	2	602	CLA	C4B-NB	2.72	1.41	1.37
16	B	816	CLA	CMD-C2D	-2.72	1.45	1.50
16	B	837	CLA	CMC-C2C	-2.72	1.45	1.50
16	B	841	CLA	C1D-ND	2.72	1.41	1.37
16	B	839	CLA	C1D-ND	2.72	1.41	1.37
22	B	845	BCR	C30-C25	-2.72	1.50	1.53
16	O	201	CLA	C4B-NB	2.72	1.41	1.37
16	3	209	CLA	C4B-NB	2.71	1.41	1.37
16	A	833	CLA	C1D-ND	2.71	1.41	1.37
16	B	824	CLA	CMB-C2B	-2.71	1.45	1.50
16	A	807	CLA	MG-NB	-2.71	2.00	2.05
17	2	615	ZEX	C8-C7	2.71	1.41	1.33
17	2	616	ZEX	C24-C25	2.71	1.54	1.50
16	B	828	CLA	MG-NB	-2.71	2.00	2.05
16	A	811	CLA	MG-NB	-2.71	2.00	2.05
16	A	806	CLA	MG-ND	-2.71	2.00	2.05
16	B	823	CLA	C4B-NB	2.71	1.41	1.37
16	A	839	CLA	CMB-C2B	-2.71	1.45	1.50
17	1	616	ZEX	C8-C7	2.70	1.41	1.33
16	B	830	CLA	MG-ND	-2.70	2.00	2.05
17	2	614	ZEX	C32-C33	2.70	1.51	1.46
17	3	218	ZEX	C1-C6	2.70	1.57	1.53
16	A	804	CLA	CMB-C2B	-2.70	1.45	1.50
19	A	801	CL0	CHB-C1B	-2.70	1.35	1.39
16	B	808	CLA	MG-ND	-2.70	2.00	2.05
16	B	832	CLA	MG-NB	-2.70	2.00	2.05
16	1	611	CLA	C1D-ND	2.70	1.41	1.37
16	O	204	CLA	C1B-C2B	2.70	1.49	1.43
16	1	609	CLA	C1B-C2B	2.69	1.49	1.43
16	B	805	CLA	MG-NB	-2.69	2.00	2.05
16	A	820	CLA	CMB-C2B	-2.69	1.45	1.50
16	A	826	CLA	C1D-ND	2.69	1.41	1.37
16	B	828	CLA	C1D-ND	2.69	1.41	1.37
16	B	821	CLA	C1D-ND	2.69	1.41	1.37
16	B	831	CLA	MG-ND	-2.69	2.00	2.05
16	3	213	CLA	C4B-NB	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	802	CLA	C4B-NB	2.69	1.41	1.37
16	B	803	CLA	MG-NB	-2.68	2.00	2.05
17	1	616	ZEX	C12-C13	2.68	1.51	1.46
16	A	826	CLA	MG-NB	-2.68	2.00	2.05
16	B	820	CLA	C1B-NB	-2.68	1.34	1.37
16	B	838	CLA	MG-NB	-2.68	2.00	2.05
17	3	216	ZEX	C8-C7	2.68	1.41	1.33
16	B	836	CLA	C4B-NB	2.68	1.41	1.37
16	O	202	CLA	C1B-C2B	2.67	1.49	1.43
16	A	808	CLA	CMD-C2D	-2.67	1.45	1.50
16	B	829	CLA	CMC-C2C	-2.67	1.45	1.50
16	B	838	CLA	CMC-C2C	-2.67	1.45	1.50
16	A	837	CLA	C1D-ND	2.67	1.41	1.37
16	A	829	CLA	CMC-C2C	-2.67	1.45	1.50
16	B	820	CLA	C1D-ND	2.67	1.41	1.37
16	B	838	CLA	CMB-C2B	-2.67	1.45	1.50
16	B	820	CLA	MG-NB	-2.66	2.00	2.05
16	A	850	CLA	CMD-C2D	-2.66	1.45	1.50
16	A	806	CLA	C1B-NB	-2.66	1.34	1.37
16	A	818	CLA	MG-ND	-2.66	2.00	2.05
16	1	603	CLA	C1D-ND	2.66	1.41	1.37
16	B	816	CLA	MG-NB	-2.66	2.00	2.05
17	1	617	ZEX	C32-C33	2.66	1.51	1.46
16	A	804	CLA	CMD-C2D	-2.66	1.45	1.50
16	3	204	CLA	C4B-NB	2.66	1.41	1.37
16	O	203	CLA	C1B-C2B	2.65	1.49	1.43
16	A	816	CLA	MG-NB	-2.65	2.00	2.05
16	3	213	CLA	C1B-C2B	2.65	1.49	1.43
17	3	217	ZEX	C8-C7	2.65	1.41	1.33
16	K	102	CLA	MG-NB	-2.65	2.00	2.05
16	A	838	CLA	CMC-C2C	-2.65	1.45	1.50
16	B	841	CLA	CMD-C2D	-2.65	1.45	1.50
16	L	203	CLA	C4B-NB	2.65	1.41	1.37
16	2	610	CLA	C1B-C2B	2.65	1.49	1.43
22	B	844	BCR	C30-C25	-2.65	1.50	1.53
16	K	101	CLA	C1D-ND	2.65	1.41	1.37
16	3	205	CLA	CMC-C2C	-2.64	1.45	1.50
16	A	816	CLA	CMD-C2D	-2.64	1.45	1.50
16	B	840	CLA	MG-NB	-2.64	2.00	2.05
16	B	822	CLA	C4B-NB	2.64	1.41	1.37
16	A	808	CLA	CMB-C2B	-2.64	1.45	1.50
16	3	205	CLA	C4B-NB	2.64	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3	204	CLA	C1B-C2B	2.64	1.49	1.43
16	B	817	CLA	C1B-C2B	2.64	1.49	1.43
16	B	812	CLA	C3B-C4B	2.64	1.50	1.42
16	A	830	CLA	CMD-C2D	-2.64	1.45	1.50
20	B	843	PQN	C5-C4	-2.64	1.43	1.48
16	B	819	CLA	MG-ND	-2.63	2.00	2.05
16	2	606	CLA	MG-NB	-2.63	2.00	2.05
16	A	804	CLA	MG-NB	-2.63	2.00	2.05
16	A	810	CLA	CMD-C2D	-2.63	1.45	1.50
16	B	815	CLA	MG-NB	-2.63	2.00	2.05
16	A	819	CLA	CMD-C2D	-2.63	1.45	1.50
16	1	609	CLA	C4B-NB	2.63	1.41	1.37
16	L	205	CLA	MG-NB	-2.63	2.00	2.05
16	B	810	CLA	C1D-ND	2.63	1.41	1.37
16	3	202	CLA	C4B-NB	2.63	1.41	1.37
17	2	614	ZEX	C1-C6	2.63	1.57	1.53
16	2	601	CLA	C1D-ND	2.63	1.41	1.37
16	B	802	CLA	C1D-ND	2.62	1.41	1.37
16	A	804	CLA	C1D-ND	2.62	1.41	1.37
16	B	837	CLA	CMB-C2B	-2.62	1.45	1.50
16	1	603	CLA	CMD-C2D	-2.62	1.45	1.50
16	B	825	CLA	C4B-NB	2.62	1.41	1.37
17	1	613	ZEX	C32-C33	2.62	1.51	1.46
16	B	807	CLA	C1D-ND	2.62	1.41	1.37
16	A	831	CLA	MG-NB	-2.62	2.00	2.05
16	3	212	CLA	C1B-C2B	2.62	1.49	1.43
16	B	817	CLA	C4B-NB	2.62	1.41	1.37
16	A	810	CLA	MG-NB	-2.61	2.00	2.05
17	3	215	ZEX	C32-C33	2.61	1.51	1.46
16	A	850	CLA	MG-NB	-2.61	2.00	2.05
16	L	204	CLA	C1D-ND	2.61	1.41	1.37
16	3	207	CLA	MG-NB	-2.61	2.00	2.05
16	B	807	CLA	MG-NB	-2.61	2.00	2.05
16	B	834	CLA	CMC-C2C	-2.61	1.45	1.50
16	A	812	CLA	MG-NB	-2.61	2.00	2.05
16	A	827	CLA	CMD-C2D	-2.61	1.45	1.50
16	3	206	CLA	C1B-NB	-2.61	1.34	1.37
16	2	612	CLA	C4B-NB	2.61	1.41	1.37
16	1	612	CLA	C1B-C2B	2.60	1.49	1.43
16	L	201	CLA	C1D-ND	2.60	1.41	1.37
19	A	801	CL0	C5-C3	-2.60	1.45	1.51
16	B	802	CLA	C1B-NB	-2.60	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	829	CLA	MG-ND	-2.60	2.00	2.05
16	A	822	CLA	C1B-C2B	2.60	1.49	1.43
16	A	814	CLA	CMC-C2C	-2.60	1.45	1.50
16	B	804	CLA	C1B-NB	-2.60	1.34	1.37
16	1	612	CLA	C4B-NB	2.60	1.41	1.37
17	2	614	ZEX	C8-C7	2.60	1.40	1.33
16	B	836	CLA	CMB-C2B	-2.60	1.45	1.50
16	B	837	CLA	MG-ND	-2.60	2.00	2.05
17	2	617	ZEX	C8-C9	2.60	1.51	1.46
16	3	202	CLA	C1B-C2B	2.60	1.49	1.43
16	2	602	CLA	MG-NB	-2.60	2.00	2.05
16	B	814	CLA	C4B-NB	2.59	1.41	1.37
16	3	203	CLA	CMC-C2C	-2.59	1.45	1.50
16	1	605	CLA	C1B-C2B	2.59	1.49	1.43
17	2	616	ZEX	C8-C7	2.59	1.40	1.33
19	A	801	CL0	CHC-C4B	-2.59	1.35	1.39
16	1	606	CLA	MG-NB	-2.59	2.00	2.05
16	B	837	CLA	C1D-ND	2.58	1.41	1.37
16	B	818	CLA	MG-NB	-2.58	2.00	2.05
16	1	608	CLA	C4B-NB	2.58	1.41	1.37
16	2	604	CLA	MG-NB	-2.58	2.00	2.05
16	A	851	CLA	CMB-C2B	-2.58	1.45	1.50
16	3	205	CLA	C3B-C4B	2.58	1.50	1.42
16	K	101	CLA	MG-NB	-2.58	2.00	2.05
16	B	811	CLA	CMB-C2B	-2.57	1.45	1.50
16	B	820	CLA	CMD-C2D	-2.57	1.45	1.50
16	3	210	CLA	C1B-C2B	2.57	1.49	1.43
16	B	809	CLA	MG-NB	-2.57	2.00	2.05
16	2	611	CLA	MG-NB	-2.57	2.00	2.05
16	A	826	CLA	MG-ND	-2.57	2.00	2.05
17	3	214	ZEX	C8-C7	2.57	1.40	1.33
16	B	842	CLA	C1B-C2B	2.57	1.49	1.43
16	B	804	CLA	CMC-C2C	-2.57	1.45	1.50
17	3	217	ZEX	C12-C13	2.57	1.51	1.46
17	3	215	ZEX	C12-C13	2.57	1.51	1.46
17	1	615	ZEX	C8-C7	2.57	1.40	1.33
16	A	814	CLA	MG-NB	-2.57	2.00	2.05
16	B	842	CLA	C4B-NB	2.56	1.41	1.37
16	2	601	CLA	C4B-NB	2.56	1.41	1.37
16	F	802	CLA	C3B-C4B	2.56	1.50	1.42
16	2	613	CLA	C1B-C2B	2.56	1.49	1.43
16	A	816	CLA	CMC-C2C	-2.56	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	606	CLA	C1B-C2B	2.56	1.49	1.43
16	A	836	CLA	C1B-NB	-2.56	1.34	1.37
16	A	815	CLA	C4B-NB	2.56	1.41	1.37
16	K	101	CLA	CMD-C2D	-2.56	1.45	1.50
16	2	608	CLA	MG-NB	-2.56	2.00	2.05
16	B	825	CLA	MG-NB	-2.55	2.00	2.05
16	B	802	CLA	CAB-C3B	-2.55	1.40	1.47
16	B	832	CLA	CMD-C2D	-2.55	1.45	1.50
16	B	831	CLA	C1D-ND	2.55	1.41	1.37
16	A	808	CLA	MG-ND	-2.55	2.00	2.05
16	K	101	CLA	C4B-NB	2.55	1.41	1.37
16	B	817	CLA	CMC-C2C	-2.55	1.45	1.50
16	1	611	CLA	C1B-C2B	2.55	1.49	1.43
22	A	844	BCR	C30-C25	-2.55	1.50	1.53
16	B	842	CLA	MG-NB	-2.55	2.00	2.05
16	A	823	CLA	CMC-C2C	-2.55	1.45	1.50
16	A	850	CLA	C1B-NB	-2.55	1.34	1.37
16	A	813	CLA	CMD-C2D	-2.55	1.45	1.50
16	A	839	CLA	C1D-ND	2.55	1.41	1.37
16	B	803	CLA	C1D-ND	2.55	1.41	1.37
16	A	819	CLA	C4B-NB	2.54	1.41	1.37
16	A	805	CLA	MG-NB	-2.54	2.00	2.05
16	A	817	CLA	CMD-C2D	-2.54	1.45	1.50
16	1	611	CLA	C4B-NB	2.54	1.41	1.37
16	A	835	CLA	C1D-ND	2.54	1.41	1.37
16	K	102	CLA	C4B-NB	2.54	1.41	1.37
19	A	801	CL0	C3B-C2B	2.54	1.43	1.40
16	B	804	CLA	CHC-C1C	2.54	1.43	1.38
16	1	603	CLA	CMB-C2B	-2.54	1.45	1.50
16	A	807	CLA	CMB-C2B	-2.54	1.45	1.50
16	B	828	CLA	C4B-NB	2.54	1.41	1.37
16	A	807	CLA	CMD-C2D	-2.53	1.45	1.50
16	2	609	CLA	C4B-NB	2.53	1.41	1.37
17	1	614	ZEX	C24-C25	2.53	1.54	1.50
16	B	820	CLA	CMB-C2B	-2.53	1.45	1.50
16	B	824	CLA	CMD-C2D	-2.53	1.45	1.50
16	3	206	CLA	MG-ND	-2.53	2.00	2.05
16	J	101	CLA	MG-NB	-2.53	2.00	2.05
16	B	806	CLA	MG-NB	-2.53	2.00	2.05
16	3	203	CLA	MG-NB	-2.53	2.00	2.05
16	2	606	CLA	C4B-NB	2.53	1.41	1.37
16	2	609	CLA	C1B-C2B	2.53	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	603	CLA	CMB-C2B	-2.52	1.45	1.50
16	B	835	CLA	MG-NB	-2.52	2.00	2.05
16	B	833	CLA	C1D-ND	2.52	1.41	1.37
16	1	607	CLA	MG-NB	-2.52	2.00	2.05
17	2	616	ZEX	C12-C13	2.52	1.51	1.46
16	O	201	CLA	MG-NB	-2.52	2.00	2.05
16	1	604	CLA	C1B-C2B	2.52	1.49	1.43
16	B	807	CLA	C1B-NB	-2.52	1.34	1.37
16	A	805	CLA	CMC-C2C	-2.52	1.45	1.50
16	F	802	CLA	MG-NB	-2.52	2.00	2.05
16	O	204	CLA	CMD-C2D	-2.52	1.45	1.50
16	A	833	CLA	CMB-C2B	-2.52	1.45	1.50
17	3	216	ZEX	C24-C25	2.52	1.54	1.50
16	B	831	CLA	CMC-C2C	-2.52	1.45	1.50
16	A	815	CLA	MG-NB	-2.51	2.00	2.05
16	A	832	CLA	CMB-C2B	-2.51	1.45	1.50
16	F	802	CLA	CMD-C2D	-2.51	1.45	1.50
16	A	826	CLA	CMD-C2D	-2.51	1.45	1.50
17	3	214	ZEX	C12-C13	2.51	1.51	1.46
16	A	819	CLA	MG-NB	-2.51	2.00	2.05
16	B	829	CLA	C1D-ND	2.51	1.41	1.37
16	A	803	CLA	MG-NB	-2.51	2.00	2.05
16	3	204	CLA	MG-NB	-2.51	2.00	2.05
16	A	809	CLA	C1B-C2B	2.51	1.49	1.43
16	B	806	CLA	C4B-NB	2.50	1.41	1.37
16	B	805	CLA	CMB-C2B	-2.50	1.45	1.50
17	1	616	ZEX	C1-C6	2.50	1.57	1.53
16	A	823	CLA	MG-NB	-2.50	2.00	2.05
16	F	803	CLA	C1B-C2B	2.50	1.49	1.43
16	A	802	CLA	CMD-C2D	-2.50	1.45	1.50
16	3	204	CLA	CMD-C2D	-2.50	1.45	1.50
17	1	615	ZEX	C12-C13	2.50	1.51	1.46
16	3	206	CLA	CMD-C2D	-2.50	1.45	1.50
16	2	605	CLA	C1B-C2B	2.50	1.49	1.43
16	K	102	CLA	C1B-C2B	2.50	1.49	1.43
16	B	830	CLA	C4B-NB	2.50	1.41	1.37
16	A	811	CLA	CMD-C2D	-2.50	1.45	1.50
16	A	816	CLA	C4B-NB	2.49	1.41	1.37
16	A	827	CLA	C1D-ND	2.49	1.41	1.37
16	1	606	CLA	CMD-C2D	-2.49	1.45	1.50
16	B	812	CLA	C1B-NB	-2.49	1.34	1.37
16	A	837	CLA	CMB-C2B	-2.49	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	810	CLA	CMB-C2B	-2.49	1.45	1.50
16	B	823	CLA	C1B-C2B	2.49	1.49	1.43
16	2	603	CLA	CMC-C2C	-2.49	1.45	1.50
16	B	801	CLA	CAC-C3C	-2.49	1.44	1.51
16	A	834	CLA	CMB-C2B	-2.49	1.45	1.50
16	3	207	CLA	C1B-C2B	2.49	1.49	1.43
16	A	818	CLA	CMD-C2D	-2.48	1.45	1.50
16	A	851	CLA	C4B-NB	2.48	1.41	1.37
17	1	613	ZEX	C12-C13	2.48	1.51	1.46
16	A	815	CLA	CMD-C2D	-2.48	1.45	1.50
16	B	818	CLA	C4B-NB	2.48	1.41	1.37
16	B	802	CLA	CMD-C2D	-2.48	1.45	1.50
24	A	853	BGC	O3-C3	-2.48	1.36	1.43
16	1	604	CLA	MG-ND	-2.48	2.00	2.05
16	A	832	CLA	C1B-C2B	2.48	1.48	1.43
16	F	802	CLA	CMB-C2B	-2.48	1.45	1.50
25	B	850	DGD	C4D-C5D	2.48	1.58	1.53
16	A	815	CLA	C1B-C2B	2.48	1.48	1.43
16	A	831	CLA	MG-ND	-2.48	2.00	2.05
16	3	207	CLA	C4B-NB	2.48	1.41	1.37
16	B	810	CLA	MG-NB	-2.48	2.00	2.05
16	2	606	CLA	C1B-C2B	2.48	1.48	1.43
16	1	606	CLA	C4B-NB	2.48	1.41	1.37
16	B	824	CLA	C4B-NB	2.48	1.41	1.37
16	B	824	CLA	C1D-ND	2.48	1.41	1.37
16	A	814	CLA	C1B-C2B	2.48	1.48	1.43
16	A	852	CLA	CMB-C2B	-2.48	1.45	1.50
16	A	839	CLA	CMD-C2D	-2.47	1.45	1.50
16	A	812	CLA	CMB-C2B	-2.47	1.45	1.50
16	B	838	CLA	C4B-NB	2.47	1.41	1.37
16	2	603	CLA	CMD-C2D	-2.47	1.45	1.50
16	B	801	CLA	CMC-C2C	-2.47	1.45	1.50
17	3	216	ZEX	C12-C13	2.47	1.51	1.46
16	B	809	CLA	C1D-ND	2.47	1.41	1.37
16	A	809	CLA	C4B-NB	2.47	1.41	1.37
16	B	833	CLA	MG-NB	-2.47	2.00	2.05
16	3	203	CLA	C4B-NB	2.46	1.41	1.37
16	A	804	CLA	MG-ND	-2.46	2.00	2.05
16	A	838	CLA	CMB-C2B	-2.46	1.45	1.50
16	B	828	CLA	CMC-C2C	-2.46	1.45	1.50
16	B	841	CLA	C4B-NB	2.46	1.41	1.37
16	B	830	CLA	C1D-ND	2.46	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	203	CLA	C1B-C2B	2.46	1.48	1.43
16	A	817	CLA	C1B-NB	-2.46	1.34	1.37
16	A	824	CLA	C1B-NB	-2.46	1.34	1.37
16	A	831	CLA	CMB-C2B	-2.46	1.45	1.50
16	L	205	CLA	C4B-NB	2.46	1.41	1.37
16	A	812	CLA	CMD-C2D	-2.46	1.45	1.50
16	B	808	CLA	CMB-C2B	-2.46	1.45	1.50
16	B	822	CLA	MG-NB	-2.46	2.00	2.05
16	B	808	CLA	CMC-C2C	-2.46	1.45	1.50
16	A	818	CLA	C1D-ND	2.46	1.41	1.37
16	B	826	CLA	C4B-NB	2.45	1.41	1.37
16	A	833	CLA	MG-NB	-2.45	2.00	2.05
16	A	822	CLA	MG-NB	-2.45	2.00	2.05
16	A	803	CLA	CMD-C2D	-2.45	1.45	1.50
16	B	836	CLA	MG-NB	-2.45	2.00	2.05
16	A	851	CLA	CMC-C2C	-2.45	1.45	1.50
16	3	209	CLA	C1B-C2B	2.45	1.48	1.43
16	A	809	CLA	CMB-C2B	-2.45	1.45	1.50
16	B	834	CLA	C1B-C2B	2.45	1.48	1.43
16	1	603	CLA	C4B-NB	2.45	1.41	1.37
16	A	834	CLA	MG-NB	-2.45	2.00	2.05
16	A	807	CLA	C1D-ND	2.45	1.41	1.37
16	1	611	CLA	MG-NB	-2.44	2.00	2.05
16	B	826	CLA	MG-ND	-2.44	2.00	2.05
16	B	826	CLA	C1B-NB	-2.44	1.34	1.37
16	B	819	CLA	C1B-NB	-2.44	1.34	1.37
16	B	833	CLA	CMD-C2D	-2.44	1.45	1.50
16	B	809	CLA	C1B-C2B	2.44	1.48	1.43
16	A	808	CLA	C1B-NB	-2.44	1.34	1.37
16	J	101	CLA	C4B-NB	2.44	1.41	1.37
16	1	601	CLA	C4B-NB	2.44	1.41	1.37
16	B	839	CLA	CMD-C2D	-2.44	1.45	1.50
16	3	208	CLA	C1B-C2B	2.44	1.48	1.43
17	2	615	ZEX	C1-C6	2.44	1.56	1.53
16	B	827	CLA	MG-ND	-2.44	2.01	2.05
16	2	602	CLA	C1B-C2B	2.44	1.48	1.43
16	B	813	CLA	C4B-C3B	2.44	1.48	1.43
16	B	810	CLA	CMC-C2C	-2.43	1.45	1.50
16	A	838	CLA	CMD-C2D	-2.43	1.45	1.50
17	1	614	ZEX	C12-C13	2.43	1.51	1.46
16	B	804	CLA	CMD-C2D	-2.43	1.45	1.50
16	B	834	CLA	CMD-C2D	-2.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	601	CLA	C1B-C2B	2.43	1.48	1.43
16	B	810	CLA	C1B-C2B	2.43	1.48	1.43
16	1	611	CLA	CMD-C2D	-2.43	1.45	1.50
16	B	826	CLA	C1D-ND	2.43	1.41	1.37
17	2	617	ZEX	C8-C7	2.43	1.40	1.33
19	A	801	CL0	OBD-CAD	-2.43	1.19	1.22
16	A	835	CLA	CMD-C2D	-2.43	1.45	1.50
16	3	208	CLA	MG-NB	-2.43	2.01	2.05
16	B	814	CLA	MG-NB	-2.43	2.01	2.05
16	A	824	CLA	C4B-NB	2.43	1.41	1.37
16	A	821	CLA	C4B-NB	2.43	1.41	1.37
16	A	813	CLA	MG-ND	-2.42	2.01	2.05
16	A	821	CLA	C1B-C2B	2.42	1.48	1.43
16	B	833	CLA	CMB-C2B	-2.42	1.45	1.50
16	1	603	CLA	MG-ND	-2.42	2.01	2.05
16	L	203	CLA	MG-NB	-2.42	2.01	2.05
16	A	836	CLA	CMC-C2C	-2.42	1.45	1.50
16	A	809	CLA	MG-NB	-2.42	2.01	2.05
16	A	851	CLA	MG-NB	-2.42	2.01	2.05
16	A	838	CLA	C1D-ND	2.42	1.41	1.37
16	B	841	CLA	C1B-NB	-2.42	1.34	1.37
16	1	609	CLA	MG-NB	-2.42	2.01	2.05
16	A	816	CLA	C1D-ND	2.42	1.41	1.37
16	K	101	CLA	C1B-C2B	2.41	1.48	1.43
16	B	829	CLA	CMD-C2D	-2.41	1.45	1.50
16	A	820	CLA	C4B-NB	2.41	1.41	1.37
16	1	608	CLA	MG-NB	-2.41	2.01	2.05
16	B	817	CLA	MG-NB	-2.41	2.01	2.05
16	A	833	CLA	C4B-NB	2.41	1.41	1.37
16	B	837	CLA	CMD-C2D	-2.41	1.45	1.50
16	3	211	CLA	C1B-C2B	2.41	1.48	1.43
16	A	827	CLA	MG-ND	-2.41	2.01	2.05
16	B	808	CLA	C1B-C2B	2.41	1.48	1.43
16	A	812	CLA	CMC-C2C	-2.41	1.45	1.50
17	3	215	ZEX	C8-C7	2.41	1.40	1.33
16	F	802	CLA	C1B-NB	-2.41	1.34	1.37
16	2	607	CLA	CMD-C2D	-2.41	1.45	1.50
16	2	611	CLA	C4B-NB	2.41	1.41	1.37
16	L	201	CLA	CMB-C2B	-2.40	1.45	1.50
16	B	807	CLA	CMD-C2D	-2.40	1.45	1.50
16	A	830	CLA	MG-ND	-2.40	2.01	2.05
17	2	615	ZEX	C12-C13	2.40	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	828	CLA	CMC-C2C	-2.40	1.45	1.50
16	B	823	CLA	MG-NB	-2.40	2.01	2.05
16	O	204	CLA	MG-NB	-2.40	2.01	2.05
16	2	605	CLA	C4B-NB	2.40	1.41	1.37
16	1	603	CLA	C1B-C2B	2.40	1.48	1.43
16	2	609	CLA	MG-NB	-2.40	2.01	2.05
16	B	834	CLA	MG-NB	-2.40	2.01	2.05
16	B	803	CLA	CMD-C2D	-2.40	1.45	1.50
16	1	610	CLA	MG-NB	-2.40	2.01	2.05
16	B	828	CLA	CMD-C2D	-2.40	1.45	1.50
16	A	827	CLA	CMB-C2B	-2.40	1.45	1.50
16	B	811	CLA	CMD-C2D	-2.40	1.45	1.50
16	3	205	CLA	MG-NB	-2.40	2.01	2.05
16	2	611	CLA	C1B-C2B	2.40	1.48	1.43
21	A	842	LHG	O7-C5	-2.40	1.41	1.46
16	O	203	CLA	C3B-C4B	2.40	1.49	1.42
16	B	821	CLA	C4B-NB	2.39	1.41	1.37
19	A	801	CL0	C1A-CHA	2.39	1.42	1.40
16	1	612	CLA	MG-NB	-2.39	2.01	2.05
16	2	602	CLA	CMB-C2B	-2.39	1.45	1.50
16	B	807	CLA	CMB-C2B	-2.39	1.45	1.50
16	B	822	CLA	C1B-C2B	2.39	1.48	1.43
17	2	615	ZEX	C32-C33	2.39	1.51	1.46
16	B	805	CLA	C4B-NB	2.39	1.41	1.37
16	1	607	CLA	C1B-C2B	2.39	1.48	1.43
16	O	201	CLA	CMD-C2D	-2.39	1.45	1.50
16	B	812	CLA	C1B-C2B	2.39	1.48	1.43
16	B	816	CLA	MG-ND	-2.38	2.01	2.05
16	A	834	CLA	C3B-C4B	2.38	1.49	1.42
16	O	202	CLA	C3B-C4B	2.38	1.49	1.42
19	A	801	CL0	C3B-C4B	-2.38	1.39	1.41
16	B	828	CLA	MG-ND	-2.38	2.01	2.05
16	A	839	CLA	CMC-C2C	-2.38	1.45	1.50
16	A	806	CLA	C4B-NB	2.38	1.41	1.37
16	1	604	CLA	MG-NB	-2.38	2.01	2.05
16	B	840	CLA	CMD-C2D	-2.38	1.45	1.50
16	L	204	CLA	CMD-C2D	-2.38	1.45	1.50
16	A	852	CLA	C1B-NB	-2.38	1.34	1.37
16	A	808	CLA	CMC-C2C	-2.38	1.45	1.50
16	B	835	CLA	C1B-C2B	2.37	1.48	1.43
16	3	211	CLA	MG-NB	-2.37	2.01	2.05
16	2	612	CLA	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	606	CLA	CMD-C2D	-2.37	1.45	1.50
16	B	825	CLA	CMD-C2D	-2.37	1.45	1.50
16	A	831	CLA	CMD-C2D	-2.37	1.45	1.50
16	B	821	CLA	CMC-C2C	-2.37	1.45	1.50
16	3	209	CLA	MG-NB	-2.37	2.01	2.05
16	B	803	CLA	CMC-C2C	-2.37	1.45	1.50
16	3	205	CLA	CHC-C1C	2.37	1.43	1.38
16	B	807	CLA	MG-ND	-2.37	2.01	2.05
16	A	810	CLA	CMC-C2C	-2.37	1.45	1.50
16	B	833	CLA	CMC-C2C	-2.37	1.45	1.50
16	B	825	CLA	C1B-C2B	2.37	1.48	1.43
16	A	813	CLA	C1B-NB	-2.37	1.34	1.37
16	1	602	CLA	C1B-C2B	2.37	1.48	1.43
16	B	839	CLA	CMB-C2B	-2.37	1.45	1.50
16	1	608	CLA	C3B-C4B	2.37	1.49	1.42
16	3	207	CLA	CMB-C2B	-2.37	1.45	1.50
16	A	821	CLA	CMD-C2D	-2.37	1.45	1.50
16	A	803	CLA	CMC-C2C	-2.37	1.45	1.50
16	A	821	CLA	MG-ND	-2.36	2.01	2.05
16	A	821	CLA	C1B-NB	-2.36	1.34	1.37
16	B	820	CLA	CMC-C2C	-2.36	1.45	1.50
16	A	829	CLA	CHC-C4B	-2.36	1.34	1.39
16	B	811	CLA	C1B-NB	-2.36	1.34	1.37
16	1	602	CLA	CMC-C2C	-2.36	1.45	1.50
16	A	821	CLA	C1D-ND	2.36	1.41	1.37
16	2	611	CLA	CMC-C2C	-2.36	1.45	1.50
16	A	817	CLA	CMB-C2B	-2.36	1.45	1.50
16	A	830	CLA	CMC-C2C	-2.36	1.45	1.50
16	2	612	CLA	MG-NB	-2.36	2.01	2.05
16	2	612	CLA	CMC-C2C	-2.36	1.45	1.50
16	A	802	CLA	CMB-C2B	-2.36	1.45	1.50
16	3	203	CLA	C3B-C4B	2.36	1.49	1.42
16	L	205	CLA	CMB-C2B	-2.36	1.45	1.50
16	A	814	CLA	C4B-NB	2.36	1.41	1.37
16	A	832	CLA	CMC-C2C	-2.35	1.45	1.50
16	2	602	CLA	CMC-C2C	-2.35	1.45	1.50
16	2	607	CLA	MG-NB	-2.35	2.01	2.05
16	1	610	CLA	CMC-C2C	-2.35	1.45	1.50
16	B	827	CLA	CMB-C2B	-2.35	1.45	1.50
16	A	830	CLA	C4B-NB	2.35	1.41	1.37
16	B	816	CLA	C4B-NB	2.35	1.41	1.37
16	2	603	CLA	C1B-C2B	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	818	CLA	CMC-C2C	-2.35	1.45	1.50
20	A	840	PQN	C11-C12	2.35	1.54	1.50
16	A	837	CLA	CMD-C2D	-2.35	1.46	1.50
16	A	806	CLA	CMC-C2C	-2.35	1.46	1.50
16	L	204	CLA	C4B-NB	2.35	1.40	1.37
16	1	612	CLA	CMD-C2D	-2.35	1.46	1.50
16	B	811	CLA	MG-ND	-2.35	2.01	2.05
16	B	812	CLA	CMD-C2D	-2.35	1.46	1.50
16	A	837	CLA	C1B-NB	-2.35	1.34	1.37
16	2	605	CLA	MG-NB	-2.35	2.01	2.05
16	3	203	CLA	CHC-C1C	2.35	1.43	1.38
16	L	203	CLA	CMB-C2B	-2.35	1.46	1.50
16	1	607	CLA	C4B-NB	2.34	1.40	1.37
16	A	814	CLA	CMD-C2D	-2.34	1.46	1.50
16	3	213	CLA	MG-NB	-2.34	2.01	2.05
16	B	838	CLA	CMD-C2D	-2.34	1.46	1.50
17	3	215	ZEX	C24-C25	2.34	1.54	1.50
16	B	818	CLA	C1B-C2B	2.34	1.48	1.43
17	3	201	ZEX	C24-C25	2.34	1.54	1.50
16	B	804	CLA	C3B-C4B	2.34	1.49	1.42
16	O	203	CLA	CHC-C1C	2.34	1.43	1.38
16	2	604	CLA	CMD-C2D	-2.34	1.46	1.50
16	3	210	CLA	MG-NB	-2.34	2.01	2.05
16	A	852	CLA	CMD-C2D	-2.34	1.46	1.50
16	A	807	CLA	C1B-NB	-2.34	1.34	1.37
16	A	825	CLA	MG-ND	-2.34	2.01	2.05
16	B	813	CLA	MG-NB	-2.34	2.01	2.05
16	A	837	CLA	MG-ND	-2.34	2.01	2.05
16	B	803	CLA	MG-ND	-2.34	2.01	2.05
16	B	837	CLA	C1B-C2B	2.33	1.48	1.43
16	A	822	CLA	CMD-C2D	-2.33	1.46	1.50
16	1	608	CLA	C1B-C2B	2.33	1.48	1.43
16	A	828	CLA	CHC-C1C	2.33	1.43	1.38
16	B	829	CLA	CMB-C2B	-2.33	1.46	1.50
16	L	201	CLA	CMC-C2C	-2.33	1.46	1.50
16	A	819	CLA	C1B-C2B	2.33	1.48	1.43
16	2	608	CLA	CMC-C2C	-2.33	1.46	1.50
16	B	824	CLA	MG-ND	-2.33	2.01	2.05
16	A	820	CLA	C3B-C4B	2.33	1.49	1.42
16	A	804	CLA	C1B-NB	-2.33	1.34	1.37
16	K	102	CLA	CMC-C2C	-2.33	1.46	1.50
16	L	201	CLA	MG-ND	-2.33	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	607	CLA	C4B-NB	2.33	1.40	1.37
16	B	808	CLA	CMD-C2D	-2.33	1.46	1.50
16	B	827	CLA	C3B-C4B	2.33	1.49	1.42
16	A	830	CLA	C1B-C2B	2.33	1.48	1.43
16	A	821	CLA	CMB-C2B	-2.32	1.46	1.50
16	2	603	CLA	MG-ND	-2.32	2.01	2.05
16	B	806	CLA	CMD-C2D	-2.32	1.46	1.50
16	B	806	CLA	CMC-C2C	-2.32	1.46	1.50
16	B	836	CLA	C1B-C2B	2.32	1.48	1.43
16	B	809	CLA	C4B-NB	2.32	1.40	1.37
16	B	809	CLA	CMB-C2B	-2.32	1.46	1.50
16	J	101	CLA	C1B-C2B	2.32	1.48	1.43
16	1	606	CLA	MG-ND	-2.32	2.01	2.05
16	A	811	CLA	MG-ND	-2.32	2.01	2.05
16	2	613	CLA	MG-NB	-2.32	2.01	2.05
16	A	823	CLA	CMD-C2D	-2.31	1.46	1.50
16	A	826	CLA	C1B-C2B	2.31	1.48	1.43
22	B	846	BCR	C1-C6	-2.31	1.50	1.53
16	2	603	CLA	C4B-NB	2.31	1.40	1.37
16	A	832	CLA	MG-ND	-2.31	2.01	2.05
16	A	851	CLA	MG-ND	-2.31	2.01	2.05
16	A	839	CLA	C1B-NB	-2.31	1.34	1.37
16	A	828	CLA	C4B-NB	2.31	1.40	1.37
16	A	825	CLA	C1D-ND	2.31	1.40	1.37
16	B	839	CLA	MG-ND	-2.31	2.01	2.05
16	B	824	CLA	C1B-C2B	2.31	1.48	1.43
16	B	803	CLA	CMB-C2B	-2.31	1.46	1.50
16	B	821	CLA	MG-ND	-2.31	2.01	2.05
16	B	819	CLA	C4B-NB	2.31	1.40	1.37
16	1	602	CLA	CMD-C2D	-2.31	1.46	1.50
16	1	604	CLA	CMD-C2D	-2.31	1.46	1.50
16	B	832	CLA	CMC-C2C	-2.31	1.46	1.50
16	B	832	CLA	CMB-C2B	-2.30	1.46	1.50
16	3	212	CLA	MG-NB	-2.30	2.01	2.05
16	A	824	CLA	CMB-C2B	-2.30	1.46	1.50
16	L	204	CLA	C1B-C2B	2.30	1.48	1.43
16	A	805	CLA	CMD-C2D	-2.30	1.46	1.50
16	F	803	CLA	MG-NB	-2.30	2.01	2.05
16	A	811	CLA	C1B-C2B	2.30	1.48	1.43
16	B	812	CLA	MG-NB	-2.30	2.01	2.05
16	B	814	CLA	C1B-C2B	2.30	1.48	1.43
16	2	610	CLA	C3B-C4B	2.30	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	811	CLA	CMB-C2B	-2.30	1.46	1.50
16	B	815	CLA	CMB-C2B	-2.30	1.46	1.50
16	2	610	CLA	CMC-C2C	-2.30	1.46	1.50
16	A	852	CLA	CMC-C2C	-2.30	1.46	1.50
16	B	812	CLA	CMC-C2C	-2.30	1.46	1.50
16	A	805	CLA	MG-ND	-2.30	2.01	2.05
16	1	604	CLA	CMC-C2C	-2.30	1.46	1.50
16	B	822	CLA	CMD-C2D	-2.30	1.46	1.50
16	B	840	CLA	CMB-C2B	-2.30	1.46	1.50
16	B	841	CLA	CMC-C2C	-2.29	1.46	1.50
16	B	809	CLA	CMD-C2D	-2.29	1.46	1.50
16	B	804	CLA	C1D-ND	2.29	1.40	1.37
16	A	802	CLA	MG-ND	-2.29	2.01	2.05
16	B	815	CLA	CMD-C2D	-2.29	1.46	1.50
16	F	803	CLA	C3B-C4B	2.29	1.49	1.42
16	1	608	CLA	CMC-C2C	-2.29	1.46	1.50
16	L	201	CLA	CMD-C2D	-2.29	1.46	1.50
16	K	101	CLA	MG-ND	-2.29	2.01	2.05
16	2	604	CLA	CMB-C2B	-2.29	1.46	1.50
16	B	813	CLA	CMC-C2C	-2.29	1.46	1.50
16	O	201	CLA	CHC-C1C	2.29	1.43	1.38
16	B	827	CLA	C1B-NB	-2.29	1.34	1.37
16	2	613	CLA	CMC-C2C	-2.29	1.46	1.50
16	1	611	CLA	CMC-C2C	-2.29	1.46	1.50
16	2	604	CLA	C1B-C2B	2.28	1.48	1.43
22	J	102	BCR	C38-C26	-2.28	1.47	1.50
16	A	832	CLA	CMD-C2D	-2.28	1.46	1.50
16	B	830	CLA	C3B-C4B	2.28	1.49	1.42
16	A	824	CLA	MG-ND	-2.28	2.01	2.05
16	A	810	CLA	C4B-NB	2.28	1.40	1.37
16	A	814	CLA	C1B-NB	-2.28	1.34	1.37
16	2	601	CLA	MG-NB	-2.28	2.01	2.05
16	B	815	CLA	C1B-C2B	2.28	1.48	1.43
17	3	218	ZEX	C27-C28	2.28	1.39	1.33
16	A	807	CLA	C1B-C2B	2.28	1.48	1.43
16	A	839	CLA	C1B-C2B	2.28	1.48	1.43
17	2	617	ZEX	C12-C13	2.28	1.50	1.46
16	2	608	CLA	C4B-NB	2.28	1.40	1.37
16	A	815	CLA	CMB-C2B	-2.27	1.46	1.50
16	A	824	CLA	CMC-C2C	-2.27	1.46	1.50
16	A	830	CLA	CMB-C2B	-2.27	1.46	1.50
16	A	813	CLA	CMB-C2B	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	805	CLA	C1B-NB	-2.27	1.34	1.37
16	1	610	CLA	CMD-C2D	-2.27	1.46	1.50
17	1	615	ZEX	C1-C6	2.27	1.56	1.53
16	2	608	CLA	CHC-C1C	2.27	1.43	1.38
16	1	604	CLA	C1B-NB	-2.27	1.34	1.37
16	A	831	CLA	CMC-C2C	-2.27	1.46	1.50
17	3	215	ZEX	C1-C6	2.27	1.56	1.53
16	A	850	CLA	CMB-C2B	-2.27	1.46	1.50
16	2	612	CLA	CMD-C2D	-2.27	1.46	1.50
16	3	205	CLA	CMB-C2B	-2.27	1.46	1.50
16	B	829	CLA	C1B-C2B	2.27	1.48	1.43
16	1	601	CLA	CMB-C2B	-2.27	1.46	1.50
16	A	839	CLA	MG-ND	-2.27	2.01	2.05
16	A	835	CLA	C1B-NB	-2.27	1.34	1.37
16	B	802	CLA	CMC-C2C	-2.27	1.46	1.50
16	B	840	CLA	C4B-NB	2.27	1.40	1.37
16	O	201	CLA	C3B-C4B	2.27	1.49	1.42
16	B	810	CLA	C4B-NB	2.27	1.40	1.37
16	B	833	CLA	C1B-NB	-2.27	1.34	1.37
16	A	835	CLA	MG-ND	-2.27	2.01	2.05
16	A	825	CLA	CMB-C2B	-2.26	1.46	1.50
16	L	201	CLA	C4B-NB	2.26	1.40	1.37
16	3	213	CLA	CMC-C2C	-2.26	1.46	1.50
16	A	807	CLA	MG-ND	-2.26	2.01	2.05
16	B	842	CLA	CMD-C2D	-2.26	1.46	1.50
22	A	847	BCR	C33-C5	-2.26	1.47	1.50
16	A	851	CLA	CMD-C2D	-2.26	1.46	1.50
16	B	816	CLA	CMC-C2C	-2.26	1.46	1.50
16	1	602	CLA	C1B-NB	-2.26	1.34	1.37
16	A	833	CLA	CMD-C2D	-2.26	1.46	1.50
16	B	831	CLA	C4B-NB	2.26	1.40	1.37
16	A	819	CLA	CMB-C2B	-2.26	1.46	1.50
16	A	822	CLA	CMB-C2B	-2.26	1.46	1.50
16	A	852	CLA	MG-ND	-2.26	2.01	2.05
16	O	202	CLA	MG-NB	-2.26	2.01	2.05
16	B	815	CLA	CMC-C2C	-2.26	1.46	1.50
16	3	208	CLA	C3B-C4B	2.26	1.49	1.42
16	A	826	CLA	CMB-C2B	-2.25	1.46	1.50
16	B	816	CLA	C1B-C2B	2.25	1.48	1.43
16	3	204	CLA	CMC-C2C	-2.25	1.46	1.50
16	B	813	CLA	CMB-C2B	-2.25	1.46	1.50
17	2	614	ZEX	C12-C13	2.25	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	809	CLA	MG-ND	-2.25	2.01	2.05
16	2	605	CLA	CMD-C2D	-2.25	1.46	1.50
16	B	836	CLA	CMD-C2D	-2.25	1.46	1.50
16	A	823	CLA	CMB-C2B	-2.25	1.46	1.50
16	B	835	CLA	CMB-C2B	-2.25	1.46	1.50
16	B	841	CLA	MG-ND	-2.25	2.01	2.05
16	K	102	CLA	CMD-C2D	-2.25	1.46	1.50
16	A	839	CLA	C4B-NB	2.25	1.40	1.37
16	B	842	CLA	C3B-C4B	2.25	1.49	1.42
16	B	810	CLA	CMB-C2B	-2.24	1.46	1.50
16	B	819	CLA	CMD-C2D	-2.24	1.46	1.50
16	A	804	CLA	C4B-NB	2.24	1.40	1.37
16	A	811	CLA	C4B-NB	2.24	1.40	1.37
16	A	812	CLA	C1B-NB	-2.24	1.34	1.37
16	A	819	CLA	C1B-NB	-2.24	1.34	1.37
16	O	201	CLA	CMB-C2B	-2.24	1.46	1.50
16	2	612	CLA	C3B-C4B	2.24	1.49	1.42
16	B	825	CLA	CMB-C2B	-2.24	1.46	1.50
16	2	602	CLA	MG-ND	-2.24	2.01	2.05
16	L	205	CLA	CMD-C2D	-2.24	1.46	1.50
20	B	843	PQN	C11-C12	2.24	1.54	1.50
16	3	208	CLA	CMB-C2B	-2.24	1.46	1.50
16	A	816	CLA	CMB-C2B	-2.24	1.46	1.50
16	B	825	CLA	CHC-C1C	2.24	1.43	1.38
16	A	816	CLA	C1B-C2B	2.24	1.48	1.43
16	1	610	CLA	C1B-C2B	2.24	1.48	1.43
16	B	806	CLA	CHC-C1C	2.23	1.43	1.38
16	A	833	CLA	CMC-C2C	-2.23	1.46	1.50
16	1	605	CLA	MG-NB	-2.23	2.01	2.05
16	A	809	CLA	CMD-C2D	-2.23	1.46	1.50
16	B	804	CLA	CMB-C2B	-2.23	1.46	1.50
16	3	210	CLA	C3B-C4B	2.23	1.49	1.42
16	B	804	CLA	MG-ND	-2.23	2.01	2.05
16	B	835	CLA	CMD-C2D	-2.23	1.46	1.50
16	J	101	CLA	CMB-C2B	-2.23	1.46	1.50
16	L	204	CLA	CMB-C2B	-2.23	1.46	1.50
16	3	209	CLA	CMD-C2D	-2.23	1.46	1.50
16	A	820	CLA	CMD-C2D	-2.23	1.46	1.50
16	A	821	CLA	CMC-C2C	-2.23	1.46	1.50
16	1	609	CLA	CMD-C2D	-2.23	1.46	1.50
16	1	610	CLA	CMB-C2B	-2.23	1.46	1.50
16	A	811	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	832	CLA	MG-ND	-2.23	2.01	2.05
16	A	825	CLA	CHC-C1C	2.23	1.42	1.38
16	2	608	CLA	C3B-C4B	2.23	1.49	1.42
16	A	805	CLA	CMB-C2B	-2.23	1.46	1.50
16	B	820	CLA	MG-ND	-2.23	2.01	2.05
16	B	828	CLA	C3B-C4B	2.22	1.49	1.42
16	A	816	CLA	CHC-C1C	2.22	1.42	1.38
16	A	802	CLA	C4B-NB	2.22	1.40	1.37
16	3	202	CLA	C3B-C4B	2.22	1.49	1.42
16	A	813	CLA	CMC-C2C	-2.22	1.46	1.50
16	F	803	CLA	CMB-C2B	-2.22	1.46	1.50
16	2	607	CLA	MG-ND	-2.22	2.01	2.05
16	2	607	CLA	C1B-C2B	2.22	1.48	1.43
16	3	202	CLA	MG-NB	-2.22	2.01	2.05
16	3	202	CLA	CMD-C2D	-2.22	1.46	1.50
16	B	818	CLA	CMD-C2D	-2.22	1.46	1.50
16	3	210	CLA	CMD-C2D	-2.22	1.46	1.50
16	1	604	CLA	C3B-C4B	2.22	1.49	1.42
16	B	822	CLA	MG-ND	-2.22	2.01	2.05
16	2	611	CLA	CMD-C2D	-2.22	1.46	1.50
16	1	611	CLA	MG-ND	-2.22	2.01	2.05
16	2	607	CLA	CMB-C2B	-2.22	1.46	1.50
16	2	604	CLA	MG-ND	-2.22	2.01	2.05
16	2	609	CLA	C3B-C4B	2.22	1.49	1.42
16	F	802	CLA	MG-ND	-2.22	2.01	2.05
16	3	207	CLA	CMD-C2D	-2.22	1.46	1.50
16	A	851	CLA	C1B-NB	-2.22	1.34	1.37
17	1	617	ZEX	C1-C6	2.22	1.56	1.53
16	A	812	CLA	MG-ND	-2.22	2.01	2.05
16	2	601	CLA	CMC-C2C	-2.22	1.46	1.50
16	3	209	CLA	C3B-C4B	2.21	1.49	1.42
16	2	612	CLA	CMB-C2B	-2.21	1.46	1.50
16	B	839	CLA	CMC-C2C	-2.21	1.46	1.50
16	A	803	CLA	C3B-C4B	2.21	1.49	1.42
16	B	814	CLA	CMD-C2D	-2.21	1.46	1.50
16	2	609	CLA	CMD-C2D	-2.21	1.46	1.50
16	B	806	CLA	C3B-C4B	2.21	1.49	1.42
16	B	828	CLA	CMB-C2B	-2.21	1.46	1.50
16	B	832	CLA	C3B-C4B	2.21	1.49	1.42
16	J	101	CLA	CMC-C2C	-2.21	1.46	1.50
16	B	820	CLA	CAC-C3C	-2.21	1.45	1.51
16	3	208	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	824	CLA	C1B-NB	-2.21	1.35	1.37
16	O	204	CLA	C3B-C4B	2.21	1.49	1.42
16	B	823	CLA	C3B-C4B	2.21	1.49	1.42
16	A	819	CLA	MG-ND	-2.20	2.01	2.05
16	B	807	CLA	CMC-C2C	-2.20	1.46	1.50
16	B	814	CLA	C1B-NB	-2.20	1.35	1.37
16	A	852	CLA	C1B-C2B	2.20	1.48	1.43
16	B	812	CLA	CMB-C2B	-2.20	1.46	1.50
16	B	826	CLA	C1B-C2B	2.20	1.48	1.43
16	3	212	CLA	C3B-C4B	2.20	1.49	1.42
16	A	803	CLA	CMB-C2B	-2.20	1.46	1.50
17	3	218	ZEX	C24-C25	2.20	1.53	1.50
16	A	808	CLA	C4B-NB	2.20	1.40	1.37
16	A	831	CLA	C4B-NB	2.20	1.40	1.37
16	B	827	CLA	C1D-ND	2.20	1.40	1.37
16	A	816	CLA	C3B-C4B	2.20	1.49	1.42
16	B	825	CLA	C3B-C4B	2.20	1.49	1.42
16	A	838	CLA	MG-ND	-2.20	2.01	2.05
16	B	811	CLA	CMC-C2C	-2.20	1.46	1.50
16	A	836	CLA	CMD-C2D	-2.20	1.46	1.50
16	B	823	CLA	CMD-C2D	-2.20	1.46	1.50
16	A	837	CLA	CMC-C2C	-2.20	1.46	1.50
16	B	811	CLA	C1B-C2B	2.19	1.48	1.43
16	2	608	CLA	CMD-C2D	-2.19	1.46	1.50
16	1	604	CLA	C4B-NB	2.19	1.40	1.37
16	2	610	CLA	MG-NB	-2.19	2.01	2.05
16	B	837	CLA	C1B-NB	-2.19	1.35	1.37
16	F	803	CLA	CMD-C2D	-2.19	1.46	1.50
16	A	816	CLA	MG-ND	-2.19	2.01	2.05
16	2	607	CLA	C3B-C4B	2.19	1.49	1.42
16	L	204	CLA	CMC-C2C	-2.19	1.46	1.50
16	A	820	CLA	MG-ND	-2.19	2.01	2.05
16	A	812	CLA	C1B-C2B	2.19	1.48	1.43
16	B	814	CLA	CMC-C2C	-2.19	1.46	1.50
16	B	825	CLA	CMC-C2C	-2.19	1.46	1.50
16	3	205	CLA	C1B-C2B	2.19	1.48	1.43
16	1	606	CLA	CMC-C2C	-2.19	1.46	1.50
16	B	810	CLA	MG-ND	-2.19	2.01	2.05
16	B	822	CLA	CMB-C2B	-2.19	1.46	1.50
16	A	803	CLA	CHC-C1C	2.19	1.42	1.38
16	B	820	CLA	C1B-C2B	2.19	1.48	1.43
16	1	608	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	834	CLA	C4B-NB	2.18	1.40	1.37
16	2	602	CLA	CMD-C2D	-2.18	1.46	1.50
16	A	851	CLA	C3B-C4B	2.18	1.49	1.42
16	B	832	CLA	C1B-NB	-2.18	1.35	1.37
16	A	836	CLA	MG-ND	-2.18	2.01	2.05
16	A	825	CLA	C3B-C4B	2.18	1.49	1.42
16	K	101	CLA	CMB-C2B	-2.18	1.46	1.50
16	B	839	CLA	C1B-C2B	2.18	1.48	1.43
16	1	610	CLA	C3B-C4B	2.18	1.49	1.42
16	B	832	CLA	C4B-NB	2.18	1.40	1.37
16	A	825	CLA	C1B-NB	-2.18	1.35	1.37
16	B	822	CLA	CMC-C2C	-2.18	1.46	1.50
16	A	834	CLA	CMD-C2D	-2.18	1.46	1.50
16	B	828	CLA	C1B-C2B	2.18	1.48	1.43
16	B	805	CLA	CMA-C3A	-2.18	1.48	1.53
16	B	803	CLA	C4B-NB	2.18	1.40	1.37
17	1	613	ZEX	C24-C25	2.18	1.53	1.50
16	B	829	CLA	CAB-C3B	-2.18	1.41	1.47
16	1	611	CLA	CMB-C2B	-2.18	1.46	1.50
16	A	834	CLA	CMC-C2C	-2.18	1.46	1.50
16	A	831	CLA	C1B-C2B	2.18	1.48	1.43
16	A	833	CLA	C1B-C2B	2.17	1.48	1.43
16	B	827	CLA	CMC-C2C	-2.17	1.46	1.50
16	B	838	CLA	C3B-C4B	2.17	1.49	1.42
16	B	806	CLA	C1B-C2B	2.17	1.48	1.43
16	3	211	CLA	C3B-C4B	2.17	1.49	1.42
16	B	817	CLA	CMD-C2D	-2.17	1.46	1.50
16	B	818	CLA	C3B-C4B	2.17	1.49	1.42
16	A	829	CLA	C1D-ND	2.17	1.40	1.37
25	B	850	DGD	O5D-C6D	-2.17	1.40	1.43
16	A	823	CLA	C1B-C2B	2.17	1.48	1.43
16	A	825	CLA	CMD-C2D	-2.17	1.46	1.50
16	L	204	CLA	MG-ND	-2.17	2.01	2.05
16	1	605	CLA	C3B-C4B	2.17	1.49	1.42
16	A	805	CLA	C4B-NB	2.17	1.40	1.37
16	A	829	CLA	CAC-C3C	-2.17	1.45	1.51
16	B	838	CLA	CHC-C1C	2.17	1.42	1.38
16	B	811	CLA	C4B-NB	2.17	1.40	1.37
16	J	101	CLA	CMD-C2D	-2.17	1.46	1.50
16	A	828	CLA	C3B-C4B	2.17	1.49	1.42
16	1	602	CLA	MG-ND	-2.16	2.01	2.05
16	3	209	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	836	CLA	C4B-NB	2.16	1.40	1.37
16	3	205	CLA	CMD-C2D	-2.16	1.46	1.50
16	B	809	CLA	CMC-C2C	-2.16	1.46	1.50
16	F	802	CLA	CMC-C2C	-2.16	1.46	1.50
16	L	205	CLA	MG-ND	-2.16	2.01	2.05
16	2	604	CLA	CMC-C2C	-2.16	1.46	1.50
16	B	814	CLA	MG-ND	-2.16	2.01	2.05
16	A	807	CLA	CMC-C2C	-2.16	1.46	1.50
16	A	827	CLA	C1B-NB	-2.16	1.35	1.37
16	B	817	CLA	MG-ND	-2.16	2.01	2.05
22	I	101	BCR	C1-C6	-2.16	1.51	1.53
16	B	816	CLA	C1B-NB	-2.16	1.35	1.37
16	B	815	CLA	MG-ND	-2.16	2.01	2.05
16	B	821	CLA	CMD-C2D	-2.16	1.46	1.50
22	A	845	BCR	C38-C26	-2.16	1.47	1.50
22	J	103	BCR	C33-C5	-2.16	1.47	1.50
16	2	610	CLA	CMD-C2D	-2.16	1.46	1.50
16	A	805	CLA	C1B-C2B	2.16	1.48	1.43
16	A	825	CLA	CMC-C2C	-2.16	1.46	1.50
16	1	607	CLA	CMB-C2B	-2.15	1.46	1.50
16	3	204	CLA	CMB-C2B	-2.15	1.46	1.50
16	1	608	CLA	CHC-C1C	2.15	1.42	1.38
22	J	102	BCR	C27-C26	-2.15	1.47	1.51
16	2	613	CLA	CMD-C2D	-2.15	1.46	1.50
16	B	809	CLA	C3B-C4B	2.15	1.49	1.42
16	K	102	CLA	MG-ND	-2.15	2.01	2.05
16	A	811	CLA	C1B-NB	-2.15	1.35	1.37
16	2	608	CLA	C1B-C2B	2.15	1.48	1.43
16	B	816	CLA	CMB-C2B	-2.15	1.46	1.50
16	B	814	CLA	CMB-C2B	-2.15	1.46	1.50
16	A	813	CLA	C3B-C4B	2.15	1.49	1.42
16	B	835	CLA	CMC-C2C	-2.15	1.46	1.50
16	2	613	CLA	C3B-C4B	2.15	1.49	1.42
16	2	606	CLA	CMC-C2C	-2.15	1.46	1.50
16	B	812	CLA	MG-ND	-2.15	2.01	2.05
16	1	605	CLA	CMB-C2B	-2.15	1.46	1.50
16	A	817	CLA	CMC-C2C	-2.15	1.46	1.50
16	A	822	CLA	C3B-C4B	2.15	1.49	1.42
16	B	801	CLA	C3B-C4B	2.15	1.49	1.42
16	3	211	CLA	CMB-C2B	-2.15	1.46	1.50
16	L	205	CLA	C1B-C2B	2.15	1.48	1.43
16	B	832	CLA	C1B-C2B	2.14	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	851	CLA	C1B-C2B	2.14	1.48	1.43
16	A	850	CLA	CHC-C4B	-2.14	1.34	1.39
16	B	818	CLA	CMC-C2C	-2.14	1.46	1.50
16	A	802	CLA	C1B-NB	-2.14	1.35	1.37
16	O	202	CLA	CHC-C1C	2.14	1.42	1.38
16	1	603	CLA	CMC-C2C	-2.14	1.46	1.50
16	L	203	CLA	C3B-C4B	2.14	1.49	1.42
16	B	828	CLA	C1B-NB	-2.14	1.35	1.37
16	A	819	CLA	CMC-C2C	-2.14	1.46	1.50
16	A	826	CLA	C4B-NB	2.14	1.40	1.37
16	A	833	CLA	C3B-C4B	2.14	1.49	1.42
16	2	612	CLA	MG-ND	-2.14	2.01	2.05
16	A	826	CLA	C3B-C4B	2.14	1.49	1.42
16	A	822	CLA	CMC-C2C	-2.14	1.46	1.50
16	O	202	CLA	CMD-C2D	-2.13	1.46	1.50
16	3	212	CLA	CMD-C2D	-2.13	1.46	1.50
16	B	832	CLA	CHC-C1C	2.13	1.42	1.38
22	F	801	BCR	C4-C5	-2.13	1.47	1.51
16	B	842	CLA	CMB-C2B	-2.13	1.46	1.50
16	B	842	CLA	MG-ND	-2.13	2.01	2.05
16	1	609	CLA	C3B-C4B	2.13	1.49	1.42
16	B	823	CLA	CMB-C2B	-2.13	1.46	1.50
16	B	826	CLA	CMC-C2C	-2.13	1.46	1.50
16	1	612	CLA	CMB-C2B	-2.13	1.46	1.50
16	2	606	CLA	CMB-C2B	-2.13	1.46	1.50
16	B	833	CLA	CHC-C1C	2.13	1.42	1.38
16	1	601	CLA	MG-NB	-2.13	2.01	2.05
16	B	824	CLA	CMC-C2C	-2.13	1.46	1.50
16	2	605	CLA	CMB-C2B	-2.13	1.46	1.50
16	3	212	CLA	CMC-C2C	-2.13	1.46	1.50
16	L	204	CLA	C1B-NB	-2.13	1.35	1.37
16	1	606	CLA	CMB-C2B	-2.13	1.46	1.50
16	A	833	CLA	MG-ND	-2.13	2.01	2.05
16	2	602	CLA	C1B-NB	-2.13	1.35	1.37
16	B	839	CLA	C1B-NB	-2.13	1.35	1.37
16	1	608	CLA	CMB-C2B	-2.13	1.46	1.50
16	2	613	CLA	CMB-C2B	-2.13	1.46	1.50
16	O	201	CLA	C1B-C2B	2.12	1.48	1.43
16	K	101	CLA	CMC-C2C	-2.12	1.46	1.50
16	A	831	CLA	C1B-NB	-2.12	1.35	1.37
16	O	203	CLA	MG-NB	-2.12	2.01	2.05
16	2	603	CLA	C1B-NB	-2.12	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	830	CLA	C1B-NB	-2.12	1.35	1.37
16	3	208	CLA	CHC-C1C	2.12	1.42	1.38
16	B	828	CLA	CHC-C1C	2.12	1.42	1.38
16	1	602	CLA	CMB-C2B	-2.12	1.46	1.50
16	A	834	CLA	C1B-C2B	2.12	1.48	1.43
16	B	836	CLA	CMC-C2C	-2.12	1.46	1.50
16	3	213	CLA	CMB-C2B	-2.12	1.46	1.50
16	A	838	CLA	C4B-NB	2.12	1.40	1.37
16	2	605	CLA	CMC-C2C	-2.12	1.46	1.50
16	A	835	CLA	CMC-C2C	-2.12	1.46	1.50
16	1	611	CLA	C3B-C4B	2.12	1.48	1.42
16	B	835	CLA	MG-ND	-2.12	2.01	2.05
16	J	101	CLA	MG-ND	-2.12	2.01	2.05
16	O	201	CLA	C1B-NB	-2.12	1.35	1.37
16	B	803	CLA	C1B-NB	-2.12	1.35	1.37
16	B	814	CLA	C3B-C4B	2.12	1.48	1.42
20	A	840	PQN	C5-C4	-2.12	1.44	1.48
16	B	817	CLA	CMB-C2B	-2.12	1.46	1.50
16	1	602	CLA	C4B-NB	2.11	1.40	1.37
16	A	815	CLA	C3B-C4B	2.11	1.48	1.42
26	J	104	3XQ	O20-C21	-2.11	1.40	1.45
16	2	604	CLA	C4B-NB	2.11	1.40	1.37
16	A	829	CLA	C4B-NB	2.11	1.40	1.37
17	1	617	ZEX	C12-C13	2.11	1.50	1.46
16	B	818	CLA	CHC-C1C	2.11	1.42	1.38
16	B	819	CLA	CMC-C2C	-2.11	1.46	1.50
16	B	838	CLA	C1B-NB	-2.11	1.35	1.37
16	A	824	CLA	C1B-C2B	2.11	1.48	1.43
16	2	601	CLA	CMB-C2B	-2.11	1.46	1.50
16	B	806	CLA	MG-ND	-2.11	2.01	2.05
16	L	201	CLA	C3B-C4B	2.10	1.48	1.42
16	A	825	CLA	C4B-NB	2.10	1.40	1.37
16	2	601	CLA	MG-ND	-2.10	2.01	2.05
16	F	803	CLA	CHC-C1C	2.10	1.42	1.38
16	1	606	CLA	C3B-C4B	2.10	1.48	1.42
16	2	606	CLA	MG-ND	-2.10	2.01	2.05
16	O	201	CLA	CMC-C2C	-2.10	1.46	1.50
16	1	612	CLA	C3B-C4B	2.10	1.48	1.42
16	B	803	CLA	C1B-C2B	2.10	1.48	1.43
16	A	802	CLA	C1B-C2B	2.10	1.48	1.43
16	2	610	CLA	CMB-C2B	-2.10	1.46	1.50
16	B	820	CLA	C4B-NB	2.10	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	830	CLA	CMC-C2C	-2.10	1.46	1.50
16	B	836	CLA	C3B-C4B	2.10	1.48	1.42
16	2	607	CLA	CMC-C2C	-2.10	1.46	1.50
16	2	601	CLA	CMD-C2D	-2.10	1.46	1.50
16	2	611	CLA	CMB-C2B	-2.09	1.46	1.50
16	1	609	CLA	MG-ND	-2.09	2.01	2.05
16	3	204	CLA	MG-ND	-2.09	2.01	2.05
17	1	613	ZEX	C1-C6	2.09	1.56	1.53
16	B	840	CLA	C1B-NB	-2.09	1.35	1.37
16	3	202	CLA	CMB-C2B	-2.09	1.46	1.50
16	K	102	CLA	CMB-C2B	-2.09	1.46	1.50
16	3	208	CLA	MG-ND	-2.09	2.01	2.05
16	B	816	CLA	C3B-C4B	2.09	1.48	1.42
16	A	827	CLA	CAB-C3B	-2.09	1.41	1.47
16	A	803	CLA	C1B-NB	-2.09	1.35	1.37
16	A	835	CLA	C1B-C2B	2.09	1.48	1.43
16	A	815	CLA	C1B-NB	-2.09	1.35	1.37
16	B	807	CLA	C4B-NB	2.09	1.40	1.37
16	B	835	CLA	C4B-NB	2.09	1.40	1.37
16	B	836	CLA	MG-ND	-2.09	2.01	2.05
16	3	211	CLA	CMD-C2D	-2.09	1.46	1.50
16	B	834	CLA	CMB-C2B	-2.09	1.46	1.50
16	A	809	CLA	C3B-C4B	2.09	1.48	1.42
16	B	807	CLA	C1B-C2B	2.09	1.48	1.43
16	A	803	CLA	C4B-NB	2.09	1.40	1.37
16	B	817	CLA	C3B-C4B	2.09	1.48	1.42
16	A	815	CLA	MG-ND	-2.09	2.01	2.05
16	O	203	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	849	BCR	C36-C18	-2.09	1.46	1.50
16	A	834	CLA	CHC-C1C	2.09	1.42	1.38
16	B	838	CLA	MG-ND	-2.09	2.01	2.05
16	B	840	CLA	MG-ND	-2.09	2.01	2.05
22	A	845	BCR	C27-C26	-2.09	1.47	1.51
16	2	608	CLA	CMB-C2B	-2.08	1.46	1.50
16	3	210	CLA	CMB-C2B	-2.08	1.46	1.50
16	J	101	CLA	C3B-C4B	2.08	1.48	1.42
16	B	801	CLA	C4B-NB	2.08	1.40	1.37
16	B	834	CLA	MG-ND	-2.08	2.01	2.05
16	1	601	CLA	C3B-C4B	2.08	1.48	1.42
16	L	205	CLA	C1B-NB	-2.08	1.35	1.37
17	3	201	ZEX	C1-C6	2.08	1.56	1.53
16	B	818	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	827	CLA	CHC-C1C	2.08	1.42	1.38
17	2	616	ZEX	C27-C28	2.08	1.39	1.33
16	3	203	CLA	CMB-C2B	-2.07	1.46	1.50
16	A	834	CLA	C1B-NB	-2.07	1.35	1.37
16	A	837	CLA	C1B-C2B	2.07	1.48	1.43
16	A	810	CLA	MG-ND	-2.07	2.01	2.05
16	A	803	CLA	MG-ND	-2.07	2.01	2.05
16	A	823	CLA	C4B-NB	2.07	1.40	1.37
16	2	602	CLA	CHC-C1C	2.07	1.42	1.38
16	1	607	CLA	C3B-C4B	2.07	1.48	1.42
16	B	804	CLA	CAB-C3B	-2.07	1.41	1.47
16	A	850	CLA	C1D-ND	2.07	1.40	1.37
16	3	203	CLA	CMD-C2D	-2.07	1.46	1.50
16	B	806	CLA	CMB-C2B	-2.07	1.46	1.50
16	B	810	CLA	C1B-NB	-2.07	1.35	1.37
16	A	814	CLA	MG-ND	-2.07	2.01	2.05
16	1	607	CLA	MG-ND	-2.06	2.01	2.05
16	A	835	CLA	CMB-C2B	-2.06	1.46	1.50
16	2	609	CLA	CMB-C2B	-2.06	1.46	1.50
16	1	610	CLA	MG-ND	-2.06	2.01	2.05
22	B	848	BCR	C33-C5	-2.06	1.47	1.50
16	B	840	CLA	CHC-C1C	2.06	1.42	1.38
17	3	201	ZEX	C27-C28	2.06	1.39	1.33
22	B	847	BCR	C38-C26	-2.06	1.47	1.50
16	B	840	CLA	C3B-C4B	2.06	1.48	1.42
16	B	823	CLA	CMC-C2C	-2.06	1.46	1.50
22	L	206	BCR	C38-C26	-2.06	1.47	1.50
16	A	810	CLA	C1B-C2B	2.06	1.48	1.43
16	B	814	CLA	CHC-C1C	2.06	1.42	1.38
16	A	804	CLA	C1B-C2B	2.06	1.48	1.43
16	A	823	CLA	MG-ND	-2.06	2.01	2.05
16	A	809	CLA	CMC-C2C	-2.06	1.46	1.50
16	B	825	CLA	MG-ND	-2.06	2.01	2.05
16	3	210	CLA	CHC-C1C	2.06	1.42	1.38
16	1	607	CLA	CMC-C2C	-2.06	1.46	1.50
16	A	823	CLA	C1B-NB	-2.06	1.35	1.37
16	A	834	CLA	MG-ND	-2.06	2.01	2.05
16	A	835	CLA	C4B-NB	2.05	1.40	1.37
16	F	803	CLA	CMC-C2C	-2.05	1.46	1.50
22	A	843	BCR	C38-C26	-2.05	1.47	1.50
16	2	601	CLA	C3B-C4B	2.05	1.48	1.42
16	2	608	CLA	MG-ND	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	O	203	CLA	CMC-C2C	-2.05	1.46	1.50
22	F	801	BCR	C33-C5	-2.05	1.47	1.50
16	3	213	CLA	C3B-C4B	2.05	1.48	1.42
16	1	601	CLA	CMD-C2D	-2.05	1.46	1.50
16	2	611	CLA	CHC-C1C	2.05	1.42	1.38
16	3	204	CLA	C3B-C4B	2.05	1.48	1.42
16	B	835	CLA	C3B-C4B	2.05	1.48	1.42
16	A	816	CLA	C1B-NB	-2.05	1.35	1.37
16	L	203	CLA	CMD-C2D	-2.05	1.46	1.50
16	K	102	CLA	C3B-C4B	2.05	1.48	1.42
16	3	207	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	846	BCR	C38-C26	-2.05	1.47	1.50
16	O	204	CLA	CHC-C1C	2.04	1.42	1.38
16	B	813	CLA	CMD-C2D	-2.04	1.46	1.50
16	2	610	CLA	MG-ND	-2.04	2.01	2.05
16	B	833	CLA	MG-ND	-2.04	2.01	2.05
22	A	846	BCR	C38-C26	-2.04	1.47	1.50
16	A	813	CLA	C4B-NB	2.04	1.40	1.37
16	A	815	CLA	CMC-C2C	-2.04	1.46	1.50
16	A	852	CLA	C4B-NB	2.04	1.40	1.37
16	B	840	CLA	C1B-C2B	2.04	1.47	1.43
16	3	210	CLA	CMC-C2C	-2.04	1.46	1.50
16	B	822	CLA	C3B-C4B	2.04	1.48	1.42
16	3	211	CLA	CMC-C2C	-2.03	1.46	1.50
16	3	206	CLA	C3B-C4B	2.03	1.48	1.42
16	1	605	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	849	BCR	C38-C26	-2.03	1.47	1.50
16	A	830	CLA	CHC-C1C	2.03	1.42	1.38
16	A	837	CLA	C3B-C4B	2.03	1.48	1.42
16	1	603	CLA	C1B-NB	-2.03	1.35	1.37
16	L	203	CLA	MG-ND	-2.03	2.01	2.05
16	O	202	CLA	CMB-C2B	-2.03	1.46	1.50
16	3	202	CLA	MG-ND	-2.03	2.01	2.05
16	B	821	CLA	C1B-C2B	2.03	1.47	1.43
16	A	820	CLA	C1B-NB	-2.03	1.35	1.37
24	A	853	BGC	C2-C3	2.03	1.55	1.52
16	A	832	CLA	CHC-C4B	-2.03	1.34	1.39
16	B	823	CLA	MG-ND	-2.03	2.01	2.05
16	A	812	CLA	C3B-C4B	2.03	1.48	1.42
16	A	811	CLA	C3B-C4B	2.03	1.48	1.42
16	3	212	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	848	BCR	C38-C26	-2.02	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	842	CLA	CHC-C1C	2.02	1.42	1.38
16	1	610	CLA	CHC-C1C	2.02	1.42	1.38
16	B	829	CLA	C1B-NB	-2.02	1.35	1.37
16	2	611	CLA	C3B-C4B	2.02	1.48	1.42
16	A	806	CLA	C3B-C4B	2.02	1.48	1.42
16	3	203	CLA	MG-ND	-2.02	2.01	2.05
16	L	205	CLA	CMC-C2C	-2.02	1.46	1.50
16	1	612	CLA	CMC-C2C	-2.02	1.46	1.50
22	A	849	BCR	C33-C5	-2.02	1.47	1.50
16	B	822	CLA	CHC-C1C	2.02	1.42	1.38
16	A	827	CLA	CHC-C1C	2.02	1.42	1.38
16	2	607	CLA	CHC-C1C	2.02	1.42	1.38
16	3	207	CLA	MG-ND	-2.01	2.01	2.05
16	A	837	CLA	C4B-NB	2.01	1.40	1.37
16	2	604	CLA	C3B-C4B	2.01	1.48	1.42
16	3	203	CLA	C1B-C2B	2.01	1.47	1.43
16	1	609	CLA	CMC-C2C	-2.01	1.46	1.50
16	A	833	CLA	CHC-C1C	2.01	1.42	1.38
16	1	608	CLA	MG-ND	-2.01	2.01	2.05
16	L	201	CLA	CHC-C1C	2.01	1.42	1.38
22	A	843	BCR	C33-C5	-2.01	1.47	1.50
16	A	803	CLA	C1B-C2B	2.01	1.47	1.43
16	1	609	CLA	CMB-C2B	-2.01	1.46	1.50
16	O	204	CLA	CMC-C2C	-2.01	1.46	1.50
16	O	204	CLA	MG-ND	-2.01	2.01	2.05
16	B	841	CLA	C1B-C2B	2.01	1.47	1.43
16	3	202	CLA	CHC-C1C	2.01	1.42	1.38
16	A	810	CLA	C1B-NB	-2.01	1.35	1.37
16	A	804	CLA	CAC-C3C	-2.00	1.46	1.51
16	A	838	CLA	C1B-C2B	2.00	1.47	1.43
16	3	209	CLA	CMB-C2B	-2.00	1.46	1.50
16	O	201	CLA	MG-ND	-2.00	2.01	2.05
16	2	605	CLA	C3B-C4B	2.00	1.48	1.42
16	1	607	CLA	CHC-C1C	2.00	1.42	1.38
16	3	213	CLA	CMD-C2D	-2.00	1.46	1.50
16	A	807	CLA	C4B-NB	2.00	1.40	1.37
16	A	833	CLA	C1B-NB	-2.00	1.35	1.37

All (1763) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	616	ZEX	C21-C26-C25	-18.85	108.27	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	214	ZEX	C21-C26-C25	-16.89	109.78	122.84
17	1	617	ZEX	C21-C26-C25	-16.87	109.80	122.84
17	1	614	ZEX	C31-C30-C29	-16.82	103.68	127.28
17	1	615	ZEX	C21-C26-C25	-16.61	110.00	122.84
17	2	617	ZEX	C21-C26-C25	-16.59	110.01	122.84
17	1	616	ZEX	C21-C26-C25	-16.58	110.03	122.84
17	1	614	ZEX	C21-C26-C25	-16.11	110.39	122.84
17	3	218	ZEX	C21-C26-C25	-15.94	110.51	122.84
17	3	201	ZEX	C21-C26-C25	-15.40	110.93	122.84
17	3	217	ZEX	C21-C26-C25	-15.19	111.10	122.84
17	3	216	ZEX	C21-C26-C25	-14.97	111.27	122.84
17	3	215	ZEX	C21-C26-C25	-14.89	111.33	122.84
17	2	614	ZEX	C21-C26-C25	-14.57	111.58	122.84
19	A	801	CL0	C1B-CHB-C4A	14.51	130.65	121.32
17	2	615	ZEX	C21-C26-C25	-14.45	111.67	122.84
17	1	617	ZEX	C31-C30-C29	-13.99	107.66	127.28
17	1	615	ZEX	C18-C5-C6	-13.42	109.84	124.48
17	3	201	ZEX	C31-C30-C29	-13.40	108.48	127.28
17	1	613	ZEX	C21-C26-C25	-13.27	112.58	122.84
17	1	613	ZEX	C31-C30-C29	-13.23	108.72	127.28
17	1	613	ZEX	C18-C5-C6	-12.96	110.35	124.48
17	3	216	ZEX	C18-C5-C6	-12.93	110.38	124.48
17	1	617	ZEX	C11-C10-C9	-12.90	109.19	127.28
17	2	615	ZEX	C31-C30-C29	-12.85	109.26	127.28
17	2	614	ZEX	C18-C5-C6	-12.77	110.55	124.48
17	3	215	ZEX	C11-C10-C9	-12.71	109.45	127.28
17	1	617	ZEX	C18-C5-C6	-12.57	110.77	124.48
17	3	201	ZEX	C18-C5-C6	-12.51	110.83	124.48
17	2	617	ZEX	C18-C5-C6	-12.50	110.85	124.48
17	2	616	ZEX	C18-C5-C6	-12.43	110.92	124.48
17	1	614	ZEX	C18-C5-C6	-12.22	111.15	124.48
17	3	214	ZEX	C18-C5-C6	-12.08	111.31	124.48
17	1	615	ZEX	C11-C10-C9	-12.05	110.38	127.28
17	1	616	ZEX	C18-C5-C6	-11.95	111.45	124.48
17	2	617	ZEX	C35-C34-C33	-11.91	110.57	127.28
17	3	217	ZEX	C18-C5-C6	-11.90	111.50	124.48
17	3	215	ZEX	C18-C5-C6	-11.90	111.50	124.48
17	1	614	ZEX	C39-C29-C28	-11.71	100.19	118.09
17	1	616	ZEX	C11-C10-C9	-11.58	111.04	127.28
17	2	616	ZEX	C11-C10-C9	-11.47	111.20	127.28
17	2	614	ZEX	C31-C30-C29	-11.37	111.33	127.28
17	2	614	ZEX	C11-C10-C9	-11.36	111.35	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	214	ZEX	C11-C10-C9	-11.35	111.37	127.28
17	1	614	ZEX	C35-C34-C33	-11.25	111.50	127.28
17	1	614	ZEX	C11-C10-C9	-11.23	111.53	127.28
17	1	614	ZEX	C28-C27-C26	-11.22	108.89	126.94
17	3	217	ZEX	C11-C10-C9	-11.12	111.69	127.28
17	1	615	ZEX	C15-C14-C13	-11.09	111.73	127.28
17	1	616	ZEX	C35-C34-C33	-11.08	111.74	127.28
17	2	615	ZEX	C18-C5-C6	-11.05	112.43	124.48
17	3	218	ZEX	C18-C5-C6	-11.04	112.43	124.48
17	2	616	ZEX	C31-C30-C29	-10.93	111.95	127.28
17	3	214	ZEX	C35-C34-C33	-10.88	112.02	127.28
17	3	201	ZEX	C35-C34-C33	-10.83	112.09	127.28
17	2	615	ZEX	C15-C14-C13	-10.80	112.13	127.28
17	1	616	ZEX	C31-C30-C29	-10.65	112.34	127.28
17	3	214	ZEX	C31-C30-C29	-10.64	112.36	127.28
17	3	216	ZEX	C31-C30-C29	-10.61	112.39	127.28
17	3	216	ZEX	C35-C34-C33	-10.60	112.41	127.28
17	3	215	ZEX	C20-C13-C14	-10.55	105.72	122.82
17	1	617	ZEX	C15-C14-C13	-10.50	112.55	127.28
17	3	217	ZEX	C15-C14-C13	-10.48	112.58	127.28
17	3	215	ZEX	C15-C14-C13	-10.40	112.70	127.28
17	1	616	ZEX	C15-C14-C13	-10.39	112.71	127.28
17	2	615	ZEX	C11-C10-C9	-10.39	112.71	127.28
17	2	617	ZEX	C15-C14-C13	-10.15	113.04	127.28
17	2	616	ZEX	C35-C34-C33	-10.07	113.16	127.28
16	1	601	CLA	C4A-NA-C1A	10.06	111.27	106.68
17	1	615	ZEX	C31-C30-C29	-10.04	113.19	127.28
17	3	216	ZEX	C15-C14-C13	-9.89	113.40	127.28
17	3	201	ZEX	C15-C14-C13	-9.89	113.41	127.28
17	3	217	ZEX	C35-C34-C33	-9.85	113.46	127.28
17	3	215	ZEX	C35-C34-C33	-9.82	113.51	127.28
17	1	613	ZEX	C15-C14-C13	-9.79	113.55	127.28
17	3	214	ZEX	C15-C14-C13	-9.69	113.69	127.28
19	A	801	CL0	O2D-CGD-CBD	9.69	121.59	110.95
17	3	215	ZEX	C31-C30-C29	-9.68	113.70	127.28
19	A	801	CL0	CBC-CAC-C3C	-9.65	99.06	112.87
16	B	805	CLA	C4A-NA-C1A	9.58	111.05	106.68
17	3	201	ZEX	C39-C29-C30	-9.52	107.39	122.82
17	2	617	ZEX	C31-C30-C29	-9.50	113.95	127.28
17	2	616	ZEX	C15-C14-C13	-9.46	114.01	127.28
17	3	218	ZEX	C15-C14-C13	-9.42	114.07	127.28
17	1	617	ZEX	C35-C34-C33	-9.31	114.22	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	615	ZEX	C35-C34-C33	-9.26	114.29	127.28
17	3	218	ZEX	C31-C30-C29	-9.26	114.30	127.28
17	1	613	ZEX	C11-C10-C9	-9.21	114.37	127.28
17	1	614	ZEX	C39-C29-C30	-9.12	108.04	122.82
17	2	617	ZEX	C11-C10-C9	-9.01	114.64	127.28
17	2	614	ZEX	C15-C14-C13	-8.99	114.67	127.28
17	1	613	ZEX	C35-C34-C33	-8.98	114.68	127.28
17	3	201	ZEX	C1-C6-C5	-8.89	110.50	122.64
17	3	218	ZEX	C39-C29-C30	-8.88	108.42	122.82
17	2	614	ZEX	C40-C33-C34	-8.87	108.44	122.82
17	2	617	ZEX	C39-C29-C30	-8.85	108.48	122.82
17	3	214	ZEX	C20-C13-C14	-8.85	108.48	122.82
17	3	214	ZEX	C39-C29-C30	-8.81	108.54	122.82
17	2	614	ZEX	C19-C9-C10	-8.74	108.66	122.82
20	B	843	PQN	C11-C12-C13	-8.72	111.80	126.83
17	1	616	ZEX	C39-C29-C30	-8.72	108.69	122.82
17	2	614	ZEX	C35-C34-C33	-8.68	115.11	127.28
17	2	614	ZEX	C20-C13-C14	-8.61	108.86	122.82
20	A	840	PQN	C11-C12-C13	-8.61	112.00	126.83
16	B	810	CLA	C4A-NA-C1A	8.59	110.60	106.68
16	A	850	CLA	C4A-NA-C1A	8.58	110.59	106.68
17	1	616	ZEX	C19-C9-C10	-8.58	108.92	122.82
17	2	617	ZEX	C40-C33-C34	-8.56	108.94	122.82
17	1	617	ZEX	C1-C6-C5	-8.56	110.94	122.64
16	A	814	CLA	C4A-NA-C1A	8.55	110.58	106.68
17	1	617	ZEX	C39-C29-C30	-8.53	108.99	122.82
17	2	614	ZEX	C39-C29-C30	-8.52	109.01	122.82
17	2	615	ZEX	C19-C9-C10	-8.52	109.01	122.82
17	1	613	ZEX	C19-C9-C8	-8.51	105.08	118.09
17	2	615	ZEX	C39-C29-C30	-8.44	109.14	122.82
17	3	217	ZEX	C40-C33-C34	-8.44	109.15	122.82
16	2	605	CLA	C4A-NA-C1A	8.41	110.52	106.68
17	2	615	ZEX	C20-C13-C14	-8.41	109.19	122.82
16	A	832	CLA	C4A-NA-C1A	8.37	110.50	106.68
17	1	617	ZEX	C19-C9-C10	-8.37	109.25	122.82
16	A	839	CLA	C4A-NA-C1A	8.34	110.48	106.68
17	3	216	ZEX	C11-C10-C9	-8.33	115.60	127.28
17	3	201	ZEX	C40-C33-C34	-8.31	109.35	122.82
17	3	216	ZEX	C20-C13-C14	-8.25	109.44	122.82
17	3	216	ZEX	C19-C9-C10	-8.25	109.44	122.82
17	1	613	ZEX	C1-C6-C5	-8.25	111.36	122.64
17	3	201	ZEX	C11-C10-C9	-8.23	115.74	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	201	ZEX	C20-C13-C14	-8.23	109.49	122.82
17	3	216	ZEX	C40-C33-C34	-8.19	109.54	122.82
17	2	616	ZEX	C19-C9-C10	-8.19	109.55	122.82
17	1	613	ZEX	C39-C29-C30	-8.17	109.57	122.82
17	1	616	ZEX	C40-C33-C34	-8.11	109.68	122.82
17	2	615	ZEX	C28-C29-C30	-8.09	106.28	119.01
17	3	216	ZEX	C8-C9-C10	-8.08	106.30	119.01
17	2	617	ZEX	C19-C9-C10	-8.05	109.77	122.82
17	3	215	ZEX	C19-C9-C10	-8.05	109.77	122.82
17	3	216	ZEX	C39-C29-C30	-8.04	109.79	122.82
16	A	850	CLA	CAC-C3C-C4C	8.03	135.24	124.79
17	3	215	ZEX	C40-C33-C34	-8.02	109.83	122.82
17	1	615	ZEX	C20-C13-C14	-8.00	109.85	122.82
16	A	821	CLA	C4A-NA-C1A	8.00	110.33	106.68
17	2	617	ZEX	C20-C13-C14	-8.00	109.86	122.82
16	2	601	CLA	C4A-NA-C1A	7.98	110.32	106.68
17	3	215	ZEX	C39-C29-C28	-7.97	105.91	118.09
17	2	617	ZEX	C19-C9-C8	-7.95	105.94	118.09
17	3	214	ZEX	C19-C9-C10	-7.94	109.96	122.82
17	1	615	ZEX	C39-C29-C28	-7.94	105.97	118.09
16	A	827	CLA	C4A-NA-C1A	7.89	110.28	106.68
17	3	217	ZEX	C20-C13-C14	-7.88	110.05	122.82
17	3	217	ZEX	C19-C9-C10	-7.86	110.08	122.82
16	B	814	CLA	C4A-NA-C1A	7.84	110.25	106.68
17	2	616	ZEX	C20-C13-C14	-7.81	110.16	122.82
17	1	614	ZEX	C40-C33-C34	-7.80	110.17	122.82
17	2	614	ZEX	C40-C33-C32	-7.77	106.22	118.09
17	2	616	ZEX	C40-C33-C34	-7.77	110.23	122.82
17	1	616	ZEX	C20-C13-C14	-7.76	110.24	122.82
17	3	217	ZEX	C31-C30-C29	-7.75	116.42	127.28
17	1	613	ZEX	C40-C33-C34	-7.72	110.31	122.82
16	A	823	CLA	C4A-NA-C1A	7.72	110.20	106.68
16	3	204	CLA	C4A-NA-C1A	7.70	110.19	106.68
16	2	610	CLA	C4A-NA-C1A	7.69	110.19	106.68
16	B	820	CLA	C4A-NA-C1A	7.68	110.18	106.68
16	B	841	CLA	C4A-NA-C1A	7.67	110.18	106.68
16	B	822	CLA	C4A-NA-C1A	7.67	110.18	106.68
17	1	614	ZEX	C15-C14-C13	-7.66	116.54	127.28
17	1	613	ZEX	C20-C13-C14	-7.63	110.45	122.82
17	1	615	ZEX	C19-C9-C10	-7.61	110.49	122.82
17	3	216	ZEX	C39-C29-C28	-7.60	106.48	118.09
16	A	838	CLA	C4A-NA-C1A	7.60	110.14	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	836	CLA	C4A-NA-C1A	7.60	110.14	106.68
16	B	837	CLA	C4A-NA-C1A	7.59	110.14	106.68
16	A	815	CLA	C4A-NA-C1A	7.58	110.14	106.68
17	3	218	ZEX	C40-C33-C32	-7.57	106.53	118.09
16	3	213	CLA	C4A-NA-C1A	7.56	110.13	106.68
16	A	807	CLA	C4A-NA-C1A	7.56	110.13	106.68
16	B	840	CLA	C4A-NA-C1A	7.55	110.12	106.68
17	2	617	ZEX	C8-C9-C10	-7.54	107.14	119.01
16	1	604	CLA	C4A-NA-C1A	7.52	110.11	106.68
17	1	617	ZEX	C40-C33-C34	-7.51	110.64	122.82
17	1	615	ZEX	C39-C29-C30	-7.51	110.65	122.82
17	3	214	ZEX	C40-C33-C34	-7.48	110.70	122.82
16	L	203	CLA	C4A-NA-C1A	7.46	110.08	106.68
16	2	602	CLA	C4A-NA-C1A	7.46	110.08	106.68
17	1	614	ZEX	C19-C9-C10	-7.46	110.73	122.82
16	1	608	CLA	C4A-NA-C1A	7.45	110.08	106.68
16	B	817	CLA	C4A-NA-C1A	7.44	110.07	106.68
17	1	615	ZEX	C32-C33-C34	-7.43	107.32	119.01
16	B	803	CLA	C4A-NA-C1A	7.43	110.07	106.68
16	3	207	CLA	C4A-NA-C1A	7.42	110.06	106.68
17	3	218	ZEX	C11-C10-C9	-7.42	116.88	127.28
17	3	201	ZEX	C19-C9-C8	-7.41	106.76	118.09
16	2	604	CLA	C4A-NA-C1A	7.38	110.04	106.68
17	2	616	ZEX	C39-C29-C30	-7.37	110.88	122.82
16	3	212	CLA	C4A-NA-C1A	7.33	110.03	106.68
16	A	822	CLA	C4A-NA-C1A	7.33	110.02	106.68
16	B	824	CLA	C4A-NA-C1A	7.33	110.02	106.68
17	1	614	ZEX	C12-C13-C14	-7.33	107.48	119.01
17	3	201	ZEX	C39-C29-C28	-7.32	106.91	118.09
17	1	617	ZEX	C20-C13-C14	-7.31	110.97	122.82
16	A	833	CLA	C4A-NA-C1A	7.31	110.01	106.68
16	A	819	CLA	C4A-NA-C1A	7.29	110.00	106.68
16	K	102	CLA	C4A-NA-C1A	7.27	110.00	106.68
16	B	809	CLA	C4A-NA-C1A	7.27	110.00	106.68
16	A	802	CLA	C4A-NA-C1A	7.26	109.99	106.68
16	A	808	CLA	C4A-NA-C1A	7.23	109.98	106.68
16	2	613	CLA	C4A-NA-C1A	7.21	109.97	106.68
16	A	826	CLA	C4A-NA-C1A	7.21	109.97	106.68
17	3	215	ZEX	C39-C29-C30	-7.20	111.15	122.82
16	1	602	CLA	C4A-NA-C1A	7.18	109.95	106.68
16	1	605	CLA	C4A-NA-C1A	7.18	109.95	106.68
16	1	611	CLA	C4A-NA-C1A	7.18	109.95	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	803	CLA	C4A-NA-C1A	7.17	109.95	106.68
16	B	806	CLA	C4A-NA-C1A	7.17	109.95	106.68
16	A	834	CLA	C4A-NA-C1A	7.16	109.95	106.68
16	A	804	CLA	C4A-NA-C1A	7.15	109.94	106.68
16	B	835	CLA	C4A-NA-C1A	7.15	109.94	106.68
16	L	204	CLA	C4A-NA-C1A	7.15	109.94	106.68
16	B	834	CLA	C4A-NA-C1A	7.14	109.94	106.68
16	B	813	CLA	C4A-NA-C1A	7.12	109.93	106.68
17	3	218	ZEX	C35-C34-C33	-7.10	117.31	127.28
16	B	833	CLA	C4A-NA-C1A	7.08	109.91	106.68
16	2	606	CLA	C4A-NA-C1A	7.08	109.91	106.68
16	B	831	CLA	C4A-NA-C1A	7.07	109.90	106.68
16	1	612	CLA	C4A-NA-C1A	7.06	109.90	106.68
16	B	807	CLA	C4A-NA-C1A	7.06	109.90	106.68
16	B	823	CLA	C4A-NA-C1A	7.05	109.90	106.68
17	3	215	ZEX	C32-C33-C34	-7.04	107.94	119.01
16	2	612	CLA	C4A-NA-C1A	7.03	109.89	106.68
16	3	209	CLA	C4A-NA-C1A	7.03	109.88	106.68
17	1	617	ZEX	C28-C27-C26	-7.02	115.64	126.94
16	A	809	CLA	C4A-NA-C1A	7.00	109.87	106.68
17	3	218	ZEX	C20-C13-C14	-7.00	111.48	122.82
16	1	609	CLA	C4A-NA-C1A	6.99	109.87	106.68
16	A	810	CLA	C4A-NA-C1A	6.99	109.87	106.68
17	3	218	ZEX	C40-C33-C34	-6.98	111.50	122.82
17	1	614	ZEX	C20-C13-C14	-6.97	111.52	122.82
16	B	821	CLA	C4A-NA-C1A	6.96	109.86	106.68
17	1	615	ZEX	C35-C34-C33	-6.96	117.51	127.28
19	A	801	CL0	CBA-CAA-C2A	-6.96	93.27	113.78
17	1	613	ZEX	C28-C29-C30	-6.96	108.07	119.01
16	B	826	CLA	C4A-NA-C1A	6.95	109.85	106.68
16	3	211	CLA	C4A-NA-C1A	6.94	109.85	106.68
16	A	824	CLA	C4A-NA-C1A	6.92	109.84	106.68
16	B	829	CLA	C4A-NA-C1A	6.92	109.84	106.68
16	B	801	CLA	C4A-NA-C1A	6.92	109.83	106.68
16	A	836	CLA	C4A-NA-C1A	6.91	109.83	106.68
16	B	819	CLA	C4A-NA-C1A	6.90	109.83	106.68
16	2	603	CLA	C4A-NA-C1A	6.90	109.83	106.68
16	A	812	CLA	C4A-NA-C1A	6.90	109.83	106.68
17	3	215	ZEX	C19-C9-C8	-6.89	107.56	118.09
17	3	201	ZEX	C20-C13-C12	-6.88	107.58	118.09
17	2	615	ZEX	C12-C13-C14	-6.86	108.22	119.01
16	2	609	CLA	C4A-NA-C1A	6.86	109.81	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	617	ZEX	C28-C29-C30	-6.86	108.22	119.01
17	2	615	ZEX	C32-C33-C34	-6.85	108.23	119.01
16	1	610	CLA	C4A-NA-C1A	6.83	109.79	106.68
16	2	608	CLA	C4A-NA-C1A	6.80	109.78	106.68
17	1	613	ZEX	C40-C33-C32	-6.80	107.69	118.09
16	O	202	CLA	C4A-NA-C1A	6.80	109.78	106.68
16	A	851	CLA	C4A-NA-C1A	6.79	109.78	106.68
17	3	218	ZEX	C19-C9-C10	-6.79	111.82	122.82
17	2	617	ZEX	C12-C13-C14	-6.78	108.34	119.01
17	2	614	ZEX	C20-C13-C12	-6.77	107.74	118.09
16	3	208	CLA	C4A-NA-C1A	6.77	109.77	106.68
16	A	816	CLA	C4A-NA-C1A	6.77	109.77	106.68
16	B	842	CLA	C4A-NA-C1A	6.75	109.76	106.68
16	B	812	CLA	C4A-NA-C1A	6.74	109.75	106.68
17	1	617	ZEX	C40-C33-C32	-6.74	107.79	118.09
16	3	210	CLA	C4A-NA-C1A	6.74	109.75	106.68
16	A	820	CLA	C4A-NA-C1A	6.74	109.75	106.68
16	K	101	CLA	C4A-NA-C1A	6.74	109.75	106.68
17	3	216	ZEX	C12-C13-C14	-6.72	108.43	119.01
16	A	831	CLA	C4A-NA-C1A	6.72	109.75	106.68
17	3	214	ZEX	C20-C13-C12	-6.72	107.82	118.09
17	1	617	ZEX	C20-C13-C12	-6.72	107.83	118.09
17	3	217	ZEX	C32-C33-C34	-6.71	108.45	119.01
16	A	837	CLA	C4A-NA-C1A	6.70	109.74	106.68
16	3	205	CLA	C4A-NA-C1A	6.70	109.73	106.68
16	L	205	CLA	C4A-NA-C1A	6.70	109.73	106.68
16	A	852	CLA	C4A-NA-C1A	6.69	109.73	106.68
16	B	828	CLA	C4A-NA-C1A	6.69	109.73	106.68
17	2	615	ZEX	C28-C27-C26	-6.68	116.18	126.94
17	2	614	ZEX	C28-C29-C30	-6.68	108.50	119.01
16	B	808	CLA	C4A-NA-C1A	6.68	109.72	106.68
17	3	217	ZEX	C28-C29-C30	-6.67	108.51	119.01
16	3	202	CLA	C4A-NA-C1A	6.65	109.71	106.68
17	3	215	ZEX	C20-C13-C12	-6.64	107.94	118.09
17	3	218	ZEX	C19-C9-C8	-6.64	107.95	118.09
17	3	201	ZEX	C7-C8-C9	-6.63	116.42	126.23
16	B	818	CLA	C4A-NA-C1A	6.62	109.70	106.68
16	A	806	CLA	C4A-NA-C1A	6.61	109.69	106.68
17	2	616	ZEX	C28-C27-C26	-6.60	116.32	126.94
17	3	201	ZEX	C19-C9-C10	-6.60	112.13	122.82
16	1	607	CLA	C4A-NA-C1A	6.59	109.69	106.68
17	1	615	ZEX	C40-C33-C34	-6.59	112.14	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	614	ZEX	C32-C33-C34	-6.57	108.68	119.01
16	1	606	CLA	C4A-NA-C1A	6.57	109.67	106.68
16	A	835	CLA	C4A-NA-C1A	6.55	109.67	106.68
16	J	101	CLA	C4A-NA-C1A	6.54	109.66	106.68
16	A	805	CLA	C4A-NA-C1A	6.53	109.66	106.68
17	3	214	ZEX	C8-C9-C10	-6.53	108.74	119.01
16	F	803	CLA	C4A-NA-C1A	6.53	109.66	106.68
16	O	203	CLA	C4A-NA-C1A	6.52	109.65	106.68
16	B	839	CLA	C4A-NA-C1A	6.48	109.64	106.68
17	3	214	ZEX	C39-C29-C28	-6.47	108.20	118.09
16	A	818	CLA	C4A-NA-C1A	6.44	109.62	106.68
16	1	603	CLA	C4A-NA-C1A	6.44	109.62	106.68
17	1	613	ZEX	C32-C33-C34	-6.39	108.95	119.01
17	2	617	ZEX	C40-C33-C32	-6.39	108.33	118.09
16	B	838	CLA	C4A-NA-C1A	6.38	109.59	106.68
17	1	616	ZEX	C28-C29-C30	-6.37	108.99	119.01
17	3	217	ZEX	C39-C29-C30	-6.37	112.50	122.82
17	1	617	ZEX	C39-C29-C28	-6.37	108.36	118.09
17	2	615	ZEX	C40-C33-C34	-6.35	112.52	122.82
17	2	616	ZEX	C40-C33-C32	-6.35	108.39	118.09
16	B	811	CLA	C4A-NA-C1A	6.35	109.57	106.68
16	F	802	CLA	C4A-NA-C1A	6.33	109.57	106.68
17	1	615	ZEX	C28-C27-C26	-6.32	116.76	126.94
17	1	616	ZEX	C39-C29-C28	-6.30	108.46	118.09
16	B	832	CLA	C4A-NA-C1A	6.28	109.55	106.68
17	1	613	ZEX	C27-C28-C29	-6.28	116.95	126.23
17	3	218	ZEX	C20-C13-C12	-6.25	108.53	118.09
16	2	611	CLA	C4A-NA-C1A	6.21	109.51	106.68
17	2	616	ZEX	C12-C13-C14	-6.20	109.25	119.01
16	A	817	CLA	C4A-NA-C1A	6.20	109.51	106.68
17	1	613	ZEX	C20-C13-C12	-6.20	108.62	118.09
16	B	825	CLA	C4A-NA-C1A	6.20	109.51	106.68
16	L	201	CLA	C4A-NA-C1A	6.18	109.50	106.68
16	B	830	CLA	C4A-NA-C1A	6.17	109.49	106.68
16	A	825	CLA	C4A-NA-C1A	6.15	109.49	106.68
17	2	614	ZEX	C8-C9-C10	-6.14	109.36	119.01
16	3	203	CLA	C4A-NA-C1A	6.12	109.47	106.68
17	2	614	ZEX	C27-C28-C29	-6.00	117.36	126.23
16	A	830	CLA	C4A-NA-C1A	5.99	109.41	106.68
17	3	217	ZEX	C12-C13-C14	-5.98	109.60	119.01
17	1	616	ZEX	C20-C13-C12	-5.97	108.96	118.09
17	2	616	ZEX	C39-C29-C28	-5.97	108.97	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	616	ZEX	C32-C33-C34	-5.96	109.63	119.01
16	A	811	CLA	C4A-NA-C1A	5.96	109.40	106.68
17	3	217	ZEX	C39-C29-C28	-5.96	108.99	118.09
16	B	815	CLA	C4A-NA-C1A	5.95	109.39	106.68
17	2	616	ZEX	C19-C9-C8	-5.90	109.08	118.09
16	A	829	CLA	C4A-NA-C1A	5.89	109.37	106.68
17	1	617	ZEX	C32-C33-C34	-5.88	109.76	119.01
17	1	615	ZEX	C12-C13-C14	-5.86	109.79	119.01
20	B	843	PQN	C14-C13-C12	-5.86	108.58	123.63
17	3	217	ZEX	C1-C6-C5	-5.85	114.65	122.64
17	3	217	ZEX	C8-C9-C10	-5.83	109.84	119.01
16	O	201	CLA	C4A-NA-C1A	5.81	109.33	106.68
17	3	215	ZEX	C28-C29-C30	-5.80	109.88	119.01
16	2	607	CLA	C4A-NA-C1A	5.80	109.32	106.68
19	A	801	CL0	C4D-CHA-CBD	5.77	114.78	108.97
16	O	204	CLA	C4A-NA-C1A	5.75	109.30	106.68
17	3	216	ZEX	C28-C27-C26	-5.74	117.70	126.94
16	B	827	CLA	C4A-NA-C1A	5.73	109.29	106.68
17	3	216	ZEX	C32-C33-C34	-5.71	110.02	119.01
16	B	816	CLA	C4A-NA-C1A	5.70	109.28	106.68
17	1	613	ZEX	C12-C13-C14	-5.70	110.05	119.01
17	3	214	ZEX	C32-C33-C34	-5.68	110.07	119.01
17	1	615	ZEX	C19-C9-C8	-5.66	109.45	118.09
17	1	613	ZEX	C19-C9-C10	-5.65	113.67	122.82
17	1	614	ZEX	C20-C13-C12	-5.63	109.49	118.09
17	3	201	ZEX	C40-C33-C32	-5.63	109.49	118.09
17	1	616	ZEX	C27-C28-C29	-5.62	117.92	126.23
17	3	215	ZEX	C40-C33-C32	-5.58	109.56	118.09
17	1	616	ZEX	C1-C6-C5	-5.57	115.03	122.64
17	2	616	ZEX	C8-C9-C10	-5.56	110.26	119.01
17	1	613	ZEX	C39-C29-C28	-5.56	109.59	118.09
17	1	614	ZEX	C1-C6-C5	-5.56	115.04	122.64
17	1	615	ZEX	C28-C29-C30	-5.56	110.27	119.01
17	2	614	ZEX	C12-C13-C14	-5.52	110.32	119.01
17	2	614	ZEX	C1-C6-C5	-5.52	115.10	122.64
20	B	843	PQN	C15-C13-C12	-5.52	108.78	121.17
20	A	840	PQN	C15-C13-C12	-5.50	108.82	121.17
17	3	214	ZEX	C19-C9-C8	-5.49	109.71	118.09
16	B	801	CLA	CMB-C2B-C1B	-5.48	117.07	125.42
17	1	616	ZEX	C40-C33-C32	-5.47	109.73	118.09
17	2	617	ZEX	C32-C33-C34	-5.46	110.42	119.01
17	2	615	ZEX	C8-C9-C10	-5.46	110.42	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	615	ZEX	C19-C9-C8	-5.43	109.79	118.09
19	A	801	CL0	C6-C5-C3	-5.43	100.23	113.47
17	2	614	ZEX	C19-C9-C8	-5.42	109.81	118.09
17	2	616	ZEX	C32-C33-C34	-5.41	110.50	119.01
17	2	614	ZEX	C32-C33-C34	-5.40	110.51	119.01
20	A	840	PQN	C14-C13-C12	-5.39	109.78	123.63
17	2	616	ZEX	C1-C6-C5	-5.38	115.28	122.64
17	3	216	ZEX	C20-C13-C12	-5.38	109.87	118.09
17	3	216	ZEX	C40-C33-C32	-5.36	109.90	118.09
16	A	825	CLA	CAA-C2A-C3A	-5.34	98.58	113.00
16	3	206	CLA	C4A-NA-C1A	5.32	109.11	106.68
17	3	217	ZEX	C20-C13-C12	-5.31	109.97	118.09
17	2	616	ZEX	C20-C13-C12	-5.29	110.01	118.09
19	A	801	CL0	O1D-CGD-CBD	-5.28	116.71	124.72
16	B	831	CLA	CMB-C2B-C1B	-5.27	117.39	125.42
16	A	813	CLA	C4A-NA-C1A	5.27	109.08	106.68
17	1	615	ZEX	C20-C13-C12	-5.27	110.04	118.09
17	3	216	ZEX	C1-C6-C5	-5.25	115.46	122.64
17	3	217	ZEX	C19-C9-C8	-5.24	110.08	118.09
17	1	617	ZEX	C12-C13-C14	-5.23	110.78	119.01
17	2	617	ZEX	C1-C6-C5	-5.22	115.50	122.64
17	2	615	ZEX	C39-C29-C28	-5.20	110.14	118.09
17	3	216	ZEX	C28-C29-C30	-5.19	110.84	119.01
17	1	614	ZEX	C19-C9-C8	-5.17	110.18	118.09
17	3	214	ZEX	C12-C13-C14	-5.16	110.89	119.01
17	1	617	ZEX	C8-C9-C10	-5.14	110.92	119.01
17	2	617	ZEX	C39-C29-C28	-5.14	110.24	118.09
16	A	805	CLA	CAA-C2A-C3A	-5.12	99.15	113.00
17	1	616	ZEX	C19-C9-C8	-5.12	110.26	118.09
17	3	218	ZEX	C39-C29-C28	-5.10	110.29	118.09
16	2	611	CLA	CAC-C3C-C4C	5.07	131.39	124.79
17	1	615	ZEX	C40-C33-C32	-5.02	110.41	118.09
17	3	215	ZEX	C28-C27-C26	-5.02	118.86	126.94
16	A	829	CLA	CMB-C2B-C1B	-4.99	117.83	125.42
17	3	214	ZEX	C28-C27-C26	-4.98	118.93	126.94
17	2	617	ZEX	C20-C13-C12	-4.95	110.52	118.09
17	3	217	ZEX	C40-C33-C32	-4.95	110.53	118.09
17	1	615	ZEX	C8-C9-C10	-4.92	111.27	119.01
17	3	214	ZEX	C7-C6-C5	-4.91	110.24	121.56
17	2	616	ZEX	C7-C8-C9	-4.90	118.99	126.23
17	1	616	ZEX	C12-C13-C14	-4.90	111.31	119.01
17	1	615	ZEX	C1-C6-C5	-4.89	115.95	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	216	ZEX	C7-C6-C5	-4.89	110.29	121.56
17	2	617	ZEX	C7-C6-C5	-4.86	110.36	121.56
16	B	827	CLA	CAA-C2A-C3A	-4.84	99.91	113.00
16	B	802	CLA	C3B-C4B-NB	-4.84	106.21	110.53
17	2	614	ZEX	C39-C29-C28	-4.81	110.74	118.09
17	2	615	ZEX	C40-C33-C32	-4.80	110.76	118.09
17	2	614	ZEX	C7-C8-C9	-4.79	119.15	126.23
17	2	615	ZEX	C20-C13-C12	-4.78	110.79	118.09
17	2	615	ZEX	C1-C6-C5	-4.77	116.12	122.64
16	A	828	CLA	C3B-C4B-NB	-4.76	106.28	110.53
17	3	214	ZEX	C7-C8-C9	-4.73	119.24	126.23
17	2	614	ZEX	C7-C6-C5	-4.72	110.69	121.56
16	A	850	CLA	CHB-C4A-NA	4.72	131.21	124.40
17	3	214	ZEX	C28-C29-C30	-4.71	111.60	119.01
17	2	615	ZEX	C27-C28-C29	-4.69	119.29	126.23
17	1	615	ZEX	C7-C6-C5	-4.69	110.75	121.56
17	1	617	ZEX	C19-C9-C8	-4.65	110.99	118.09
17	3	214	ZEX	C40-C33-C32	-4.64	110.99	118.09
17	3	214	ZEX	C1-C6-C5	-4.64	116.30	122.64
16	3	210	CLA	CAA-C2A-C3A	-4.60	105.67	116.23
16	B	805	CLA	CMA-C3A-C4A	-4.60	99.41	111.77
17	3	215	ZEX	C1-C6-C5	-4.59	116.36	122.64
16	2	609	CLA	CAA-C2A-C3A	-4.59	105.70	116.23
17	1	613	ZEX	C8-C9-C10	-4.56	111.84	119.01
17	1	616	ZEX	C8-C9-C10	-4.53	111.89	119.01
17	3	201	ZEX	C32-C33-C34	-4.52	111.90	119.01
16	1	609	CLA	CAA-C2A-C3A	-4.51	105.89	116.23
17	3	216	ZEX	C19-C9-C8	-4.51	111.20	118.09
17	3	215	ZEX	C27-C28-C29	-4.50	119.58	126.23
16	A	828	CLA	C4A-NA-C1A	4.48	108.72	106.68
21	A	841	LHG	O4-P-O5	4.48	133.29	112.44
17	2	615	ZEX	C7-C6-C5	-4.47	111.26	121.56
21	A	842	LHG	O4-P-O5	4.42	132.99	112.44
22	K	103	BCR	C2-C1-C6	4.39	116.82	110.44
16	B	801	CLA	CHB-C4A-NA	4.39	130.74	124.40
17	3	215	ZEX	C8-C9-C10	-4.38	112.11	119.01
17	3	201	ZEX	C28-C27-C26	-4.38	119.89	126.94
16	B	804	CLA	C4A-NA-C1A	4.37	108.67	106.68
17	3	215	ZEX	C8-C7-C6	-4.37	115.33	127.00
17	2	616	ZEX	C7-C6-C5	-4.37	111.50	121.56
17	1	616	ZEX	C7-C6-C5	-4.35	111.54	121.56
17	3	218	ZEX	C28-C29-C30	-4.35	112.17	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	804	CLA	C3B-C4B-NB	-4.34	106.66	110.53
19	A	801	CL0	C11-C10-C8	-4.31	101.63	115.97
16	F	803	CLA	CAA-C2A-C3A	-4.30	106.37	116.23
17	1	614	ZEX	C40-C33-C32	-4.26	111.58	118.09
17	3	215	ZEX	C18-C5-C4	-4.24	106.63	114.42
17	2	617	ZEX	C28-C27-C26	-4.24	120.12	126.94
16	O	202	CLA	CAA-C2A-C3A	-4.22	106.55	116.23
22	L	206	BCR	C24-C23-C22	-4.21	120.00	126.23
16	A	815	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
16	B	805	CLA	CHB-C4A-NA	4.19	130.44	124.40
17	2	617	ZEX	C8-C7-C6	-4.16	115.89	127.00
17	1	613	ZEX	C8-C7-C6	-4.16	115.89	127.00
16	B	827	CLA	C3B-C4B-NB	-4.16	106.82	110.53
16	A	850	CLA	CAC-C3C-C2C	-4.15	119.94	127.56
19	A	801	CL0	CGD-CBD-CAD	-4.14	97.45	110.85
22	B	849	BCR	C24-C23-C22	-4.12	120.14	126.23
16	A	827	CLA	C3B-C4B-NB	-4.12	106.86	110.53
17	2	615	ZEX	C18-C5-C4	-4.11	106.86	114.42
17	2	617	ZEX	C27-C28-C29	-4.11	120.16	126.23
16	B	801	CLA	CMB-C2B-C3B	4.10	136.19	126.55
16	3	206	CLA	CMB-C2B-C1B	-4.09	119.19	125.42
17	3	218	ZEX	C8-C9-C10	-4.09	112.58	119.01
16	A	825	CLA	C3B-C4B-NB	-4.08	106.89	110.53
17	1	616	ZEX	C28-C27-C26	-4.05	120.42	126.94
17	3	218	ZEX	C1-C6-C5	-4.05	117.10	122.64
17	1	617	ZEX	C28-C29-C30	-4.03	112.66	119.01
17	3	215	ZEX	C12-C13-C14	-4.03	112.67	119.01
16	B	807	CLA	CMA-C3A-C4A	-4.03	100.95	111.77
16	A	806	CLA	C3B-C4B-NB	-4.01	106.95	110.53
16	1	601	CLA	CHB-C4A-NA	3.97	130.13	124.40
17	3	201	ZEX	C28-C29-C30	-3.96	112.78	119.01
17	2	616	ZEX	C28-C29-C30	-3.95	112.80	119.01
16	A	808	CLA	C3B-C4B-NB	-3.93	107.02	110.53
16	A	832	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
16	3	203	CLA	C3B-C4B-NB	-3.93	107.03	110.53
22	F	801	BCR	C3-C4-C5	-3.92	107.06	114.06
16	A	803	CLA	CHB-C4A-NA	3.92	130.06	124.40
17	3	216	ZEX	C27-C28-C29	-3.92	120.44	126.23
22	L	206	BCR	C2-C1-C6	3.90	116.11	110.44
16	B	812	CLA	CAA-C2A-C3A	-3.90	102.46	113.00
16	B	804	CLA	CMA-C3A-C4A	-3.89	101.31	111.77
16	B	838	CLA	C3B-C4B-NB	-3.88	107.06	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	218	ZEX	C7-C6-C5	-3.87	112.65	121.56
25	B	850	DGD	O5D-C6D-C5D	-3.85	100.75	109.42
16	B	828	CLA	C3B-C4B-NB	-3.84	107.11	110.53
16	B	833	CLA	C3B-C4B-NB	-3.83	107.11	110.53
17	1	617	ZEX	C4-C5-C6	-3.83	112.89	120.76
16	A	806	CLA	CMB-C2B-C1B	-3.83	119.59	125.42
19	A	801	CL0	CMB-C2B-C3B	3.82	132.32	124.68
16	B	815	CLA	CAA-C2A-C3A	-3.82	102.69	113.00
22	F	801	BCR	C2-C1-C6	3.81	115.97	110.44
17	3	217	ZEX	C7-C6-C5	-3.78	112.84	121.56
16	B	803	CLA	CHB-C4A-NA	3.78	129.86	124.40
17	1	613	ZEX	C18-C5-C4	-3.76	107.50	114.42
16	A	816	CLA	C3B-C4B-NB	-3.76	107.17	110.53
16	A	852	CLA	CAA-C2A-C3A	-3.76	102.84	113.00
16	A	829	CLA	C1D-ND-C4D	3.76	108.95	106.31
22	B	848	BCR	C2-C1-C6	3.76	115.90	110.44
17	3	201	ZEX	C4-C5-C6	-3.75	113.06	120.76
17	3	217	ZEX	C8-C7-C6	-3.74	117.01	127.00
16	B	805	CLA	C3B-C4B-NB	-3.72	107.21	110.53
16	A	835	CLA	CMB-C2B-C1B	-3.71	119.77	125.42
16	B	805	CLA	CMA-C3A-C2A	-3.71	99.66	113.98
17	1	617	ZEX	C18-C5-C4	-3.70	107.62	114.42
16	A	810	CLA	CAA-C2A-C3A	-3.69	103.02	113.00
19	A	801	CL0	C1C-CHC-C4B	3.68	129.23	116.07
16	A	830	CLA	C3B-C4B-NB	-3.66	107.26	110.53
16	A	813	CLA	CMB-C2B-C1B	-3.66	119.85	125.42
17	1	616	ZEX	C8-C7-C6	-3.65	117.24	127.00
16	B	832	CLA	C3B-C4B-NB	-3.65	107.27	110.53
16	B	801	CLA	CBC-CAC-C3C	-3.64	102.54	112.42
16	2	605	CLA	CHB-C4A-NA	3.64	129.66	124.40
22	B	848	BCR	C24-C23-C22	-3.64	120.85	126.23
17	1	617	ZEX	C8-C7-C6	-3.64	117.28	127.00
17	1	613	ZEX	C28-C27-C26	-3.63	121.09	126.94
16	B	829	CLA	C3B-C4B-NB	-3.61	107.31	110.53
17	1	615	ZEX	C7-C8-C9	-3.61	120.90	126.23
16	B	835	CLA	CHB-C4A-NA	3.61	129.60	124.40
17	1	614	ZEX	C18-C5-C4	-3.60	107.80	114.42
19	A	801	CL0	C4D-ND-C1D	-3.60	102.49	105.22
16	B	810	CLA	CHB-C4A-NA	3.60	129.59	124.40
16	B	814	CLA	CMB-C2B-C1B	-3.59	119.95	125.42
16	B	807	CLA	CHB-C4A-NA	3.58	129.57	124.40
16	1	607	CLA	CAA-CBA-CGA	3.58	122.03	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	201	ZEX	C8-C9-C10	-3.58	113.38	119.01
16	B	825	CLA	C3B-C4B-NB	-3.57	107.34	110.53
17	1	617	ZEX	C7-C6-C5	-3.57	113.33	121.56
16	3	203	CLA	CAA-C2A-C3A	-3.57	103.36	113.00
17	3	201	ZEX	C27-C28-C29	-3.55	120.98	126.23
16	3	205	CLA	C3B-C4B-NB	-3.55	107.36	110.53
17	1	613	ZEX	C31-C32-C33	-3.54	116.66	126.36
16	B	839	CLA	C3B-C4B-NB	-3.54	107.37	110.53
16	A	827	CLA	CHB-C4A-NA	3.53	129.50	124.40
16	F	802	CLA	C3B-C4B-NB	-3.53	107.38	110.53
16	B	805	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
19	A	801	CL0	CMA-C3A-C4A	-3.52	107.02	114.61
16	A	833	CLA	CAA-C2A-C3A	-3.51	103.52	113.00
17	3	218	ZEX	C27-C28-C29	-3.50	121.05	126.23
16	A	811	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
16	A	839	CLA	CHB-C4A-NA	3.49	129.44	124.40
16	A	832	CLA	CHB-C4A-NA	3.49	129.44	124.40
22	I	101	BCR	C31-C1-C6	3.48	115.70	110.24
16	B	840	CLA	C3B-C4B-NB	-3.48	107.42	110.53
17	1	615	ZEX	C18-C5-C4	-3.47	108.03	114.42
16	A	812	CLA	CHB-C4A-NA	3.47	129.41	124.40
16	K	101	CLA	C3B-C4B-NB	-3.46	107.44	110.53
16	A	850	CLA	CAA-C2A-C3A	-3.46	103.64	113.00
16	B	821	CLA	C3B-C4B-NB	-3.46	107.44	110.53
16	B	830	CLA	C3B-C4B-NB	-3.46	107.44	110.53
22	A	849	BCR	C15-C14-C13	-3.46	122.43	127.28
16	A	802	CLA	CHB-C4A-NA	3.45	129.38	124.40
16	A	804	CLA	CAA-C2A-C3A	-3.44	103.71	113.00
16	A	823	CLA	CAA-C2A-C3A	-3.43	103.74	113.00
16	B	802	CLA	C4A-NA-C1A	3.43	108.24	106.68
16	A	835	CLA	CMB-C2B-C3B	3.42	134.59	126.55
17	3	201	ZEX	C11-C12-C13	-3.42	116.99	126.36
17	2	615	ZEX	C31-C32-C33	-3.41	117.01	126.36
16	A	838	CLA	C3B-C4B-NB	-3.41	107.49	110.53
16	B	806	CLA	C3B-C4B-NB	-3.41	107.49	110.53
22	A	845	BCR	C28-C27-C26	-3.40	107.99	114.06
17	3	217	ZEX	C27-C28-C29	-3.39	121.22	126.23
16	1	608	CLA	CAA-C2A-C3A	-3.38	103.86	113.00
16	F	802	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
16	A	837	CLA	CMB-C2B-C1B	-3.38	120.27	125.42
16	B	805	CLA	C1-C2-C3	-3.38	120.67	126.20
16	A	806	CLA	CAA-C2A-C3A	-3.37	103.90	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	604	CLA	CMB-C2B-C1B	-3.37	120.29	125.42
22	A	846	BCR	C11-C10-C9	-3.36	122.56	127.28
16	B	836	CLA	CHB-C4A-NA	3.36	129.26	124.40
17	3	216	ZEX	C8-C7-C6	-3.36	118.01	127.00
16	A	850	CLA	CHC-C1C-NC	3.36	129.37	124.31
22	B	848	BCR	C15-C14-C13	-3.36	122.57	127.28
22	A	845	BCR	C24-C23-C22	-3.35	121.28	126.23
16	B	833	CLA	CHB-C4A-NA	3.34	129.22	124.40
16	A	817	CLA	CHB-C4A-NA	3.34	129.22	124.40
16	A	820	CLA	C3B-C4B-NB	-3.34	107.55	110.53
17	2	617	ZEX	C7-C8-C9	-3.33	121.31	126.23
16	A	817	CLA	C3B-C4B-NB	-3.33	107.56	110.53
16	2	611	CLA	C3B-C4B-NB	-3.32	107.57	110.53
16	1	607	CLA	CAA-C2A-C3A	-3.32	104.03	113.00
16	O	201	CLA	C3B-C4B-NB	-3.32	107.57	110.53
16	A	820	CLA	CHB-C4A-NA	3.31	129.18	124.40
16	2	608	CLA	C3B-C4B-NB	-3.31	107.58	110.53
16	B	805	CLA	C2A-C3A-C4A	3.31	107.21	101.87
16	B	804	CLA	CHB-C4A-NA	3.31	129.17	124.40
16	A	823	CLA	CHB-C4A-NA	3.30	129.17	124.40
22	B	847	BCR	C15-C16-C17	-3.30	116.76	123.52
16	B	832	CLA	CHB-C4A-NA	3.30	129.16	124.40
16	A	829	CLA	CHB-C1B-NB	3.30	129.00	124.05
16	A	808	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
17	3	217	ZEX	C28-C27-C26	-3.30	121.63	126.94
16	A	835	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
16	B	819	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
16	A	828	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
16	L	201	CLA	C3B-C4B-NB	-3.29	107.59	110.53
16	B	819	CLA	CHB-C4A-NA	3.29	129.14	124.40
16	A	838	CLA	O2D-CGD-O1D	-3.28	117.45	123.85
16	3	205	CLA	CAA-C2A-C3A	-3.28	104.15	113.00
16	2	604	CLA	CHB-C4A-NA	3.28	129.13	124.40
17	3	214	ZEX	C18-C5-C4	-3.27	108.40	114.42
19	A	801	CL0	CAA-C2A-C3A	3.27	121.85	113.00
25	B	850	DGD	O3G-C3G-C2G	-3.27	102.86	110.82
16	A	832	CLA	O2D-CGD-CBD	3.27	116.95	111.23
22	F	801	BCR	C24-C23-C22	-3.27	121.40	126.23
16	2	607	CLA	C3B-C4B-NB	-3.27	107.61	110.53
16	A	835	CLA	C3B-C4B-NB	-3.26	107.62	110.53
16	A	833	CLA	CHB-C4A-NA	3.26	129.11	124.40
16	2	608	CLA	CAA-C2A-C3A	-3.26	104.20	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	602	CLA	C3B-C4B-NB	-3.26	107.62	110.53
20	A	840	PQN	C14-C13-C15	-3.26	109.58	115.23
16	2	601	CLA	CHB-C4A-NA	3.25	129.09	124.40
16	B	803	CLA	C3B-C4B-NB	-3.25	107.63	110.53
16	B	828	CLA	CHB-C4A-NA	3.25	129.09	124.40
17	2	614	ZEX	C28-C27-C26	-3.25	121.72	126.94
22	J	103	BCR	C24-C23-C22	-3.24	121.44	126.23
16	A	815	CLA	O2D-CGD-CBD	3.24	116.89	111.23
17	1	614	ZEX	C8-C9-C10	-3.24	113.91	119.01
16	B	831	CLA	CMB-C2B-C3B	3.24	134.16	126.55
16	B	810	CLA	CAA-C2A-C3A	-3.24	104.25	113.00
16	A	806	CLA	CHB-C1B-NB	3.24	128.90	124.05
22	A	849	BCR	C15-C16-C17	-3.23	116.91	123.52
16	A	826	CLA	CHB-C4A-NA	3.23	129.06	124.40
22	A	844	BCR	C11-C10-C9	-3.23	122.75	127.28
16	A	814	CLA	CMB-C2B-C1B	-3.23	120.51	125.42
16	2	612	CLA	CHB-C4A-NA	3.22	129.05	124.40
16	A	815	CLA	CHB-C4A-NA	3.22	129.05	124.40
16	A	828	CLA	CMB-C2B-C1B	-3.22	120.52	125.42
16	B	816	CLA	C3B-C4B-NB	-3.22	107.66	110.53
16	2	601	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
16	1	608	CLA	CHB-C4A-NA	3.22	129.04	124.40
17	3	215	ZEX	C7-C6-C5	-3.21	114.15	121.56
16	3	208	CLA	C3B-C4B-NB	-3.21	107.67	110.53
16	A	813	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
16	B	804	CLA	OBD-CAD-C3D	3.21	135.91	128.42
16	B	805	CLA	O2D-CGD-CBD	3.21	116.83	111.23
16	A	803	CLA	C3B-C4B-NB	-3.20	107.67	110.53
16	L	204	CLA	C3B-C4B-NB	-3.20	107.67	110.53
16	1	603	CLA	C3B-C4B-NB	-3.20	107.67	110.53
16	A	834	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
16	B	809	CLA	CHB-C4A-NA	3.19	129.00	124.40
17	2	614	ZEX	C18-C5-C4	-3.19	108.56	114.42
16	A	818	CLA	CMB-C2B-C1B	-3.18	120.57	125.42
16	A	828	CLA	CHB-C1B-NB	3.18	128.83	124.05
16	B	819	CLA	C3B-C4B-NB	-3.18	107.69	110.53
16	J	101	CLA	C3B-C4B-NB	-3.18	107.69	110.53
16	B	821	CLA	CAA-C2A-C3A	-3.18	104.41	113.00
16	B	831	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
16	B	826	CLA	CHB-C4A-NA	3.18	128.99	124.40
16	B	818	CLA	C3B-C4B-NB	-3.17	107.70	110.53
16	F	803	CLA	C3B-C4B-NB	-3.17	107.70	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	601	CLA	CMC-C2C-C1C	-3.16	120.10	125.03
17	2	616	ZEX	C18-C5-C4	-3.16	108.62	114.42
22	J	102	BCR	C28-C27-C26	-3.15	108.43	114.06
16	A	805	CLA	CHB-C4A-NA	3.15	128.95	124.40
17	3	214	ZEX	C27-C28-C29	-3.15	121.57	126.23
25	B	850	DGD	O6D-C1D-O3G	-3.15	102.60	110.04
16	B	815	CLA	C3B-C4B-NB	-3.15	107.72	110.53
16	B	831	CLA	CHB-C4A-NA	3.15	128.94	124.40
16	B	810	CLA	O2A-CGA-O1A	-3.15	115.76	123.63
16	2	610	CLA	CHB-C4A-NA	3.14	128.94	124.40
16	A	834	CLA	CHB-C4A-NA	3.14	128.94	124.40
16	L	203	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
17	1	615	ZEX	C15-C35-C34	-3.14	117.09	123.52
16	2	603	CLA	C3B-C4B-NB	-3.14	107.73	110.53
17	2	615	ZEX	C37-C21-C26	-3.14	105.33	110.25
16	3	206	CLA	C3B-C4B-NB	-3.14	107.73	110.53
16	B	808	CLA	C3B-C4B-NB	-3.14	107.73	110.53
19	A	801	CL0	CMA-C3A-C2A	-3.14	102.02	114.13
16	3	202	CLA	CHB-C4A-NA	3.14	128.93	124.40
16	B	820	CLA	CHB-C4A-NA	3.14	128.93	124.40
17	1	616	ZEX	C18-C5-C4	-3.13	108.66	114.42
16	A	806	CLA	CHB-C4A-NA	3.13	128.91	124.40
20	B	843	PQN	C11-C3-C2	-3.13	119.53	124.89
16	B	834	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
16	B	834	CLA	CHB-C4A-NA	3.12	128.91	124.40
16	B	837	CLA	C3B-C4B-NB	-3.12	107.74	110.53
16	B	841	CLA	C3B-C4B-NB	-3.12	107.75	110.53
16	B	837	CLA	CHB-C4A-NA	3.12	128.90	124.40
16	2	608	CLA	CHB-C4A-NA	3.12	128.90	124.40
16	3	213	CLA	CHB-C4A-NA	3.11	128.89	124.40
16	A	813	CLA	CMB-C2B-C3B	3.11	133.86	126.55
17	1	614	ZEX	C31-C32-C33	-3.11	117.84	126.36
22	I	101	BCR	C15-C16-C17	-3.10	117.17	123.52
16	A	804	CLA	C3B-C4B-NB	-3.10	107.76	110.53
16	3	205	CLA	CHB-C4A-NA	3.10	128.87	124.40
16	A	819	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
16	B	808	CLA	CHB-C4A-NA	3.09	128.87	124.40
16	2	612	CLA	C3B-C4B-NB	-3.09	107.77	110.53
16	A	804	CLA	CHB-C4A-NA	3.09	128.86	124.40
16	J	101	CLA	CHB-C4A-NA	3.09	128.86	124.40
16	1	608	CLA	C3B-C4B-NB	-3.09	107.77	110.53
16	B	837	CLA	C1-C2-C3	-3.08	121.15	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	202	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
16	A	833	CLA	C3B-C4B-NB	-3.08	107.78	110.53
17	2	617	ZEX	C18-C5-C4	-3.08	108.76	114.42
16	3	206	CLA	CHB-C1B-NB	3.08	128.67	124.05
16	A	851	CLA	CHB-C4A-NA	3.08	128.84	124.40
22	B	846	BCR	C2-C1-C6	3.07	114.91	110.44
16	B	802	CLA	CHB-C1B-NB	3.07	128.66	124.05
16	A	804	CLA	CAA-CBA-CGA	-3.07	104.48	113.21
16	A	831	CLA	CHB-C4A-NA	3.07	128.83	124.40
16	A	819	CLA	C3B-C4B-NB	-3.07	107.79	110.53
16	B	822	CLA	CHB-C4A-NA	3.07	128.83	124.40
16	A	835	CLA	CHB-C4A-NA	3.07	128.82	124.40
16	A	829	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
16	A	824	CLA	C3B-C4B-NB	-3.06	107.80	110.53
16	B	806	CLA	CHB-C4A-NA	3.06	128.81	124.40
16	L	203	CLA	CHB-C4A-NA	3.06	128.81	124.40
16	B	811	CLA	CAA-C2A-C3A	-3.05	104.75	113.00
16	A	806	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
16	A	807	CLA	CHB-C4A-NA	3.05	128.80	124.40
16	A	807	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
16	B	818	CLA	CHB-C4A-NA	3.05	128.80	124.40
22	L	206	BCR	C11-C10-C9	-3.05	123.01	127.28
16	B	814	CLA	CHB-C4A-NA	3.04	128.79	124.40
16	A	819	CLA	CHB-C4A-NA	3.04	128.79	124.40
16	A	838	CLA	CHB-C4A-NA	3.04	128.79	124.40
16	A	839	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
16	B	810	CLA	C3B-C4B-NB	-3.04	107.82	110.53
17	2	614	ZEX	C31-C32-C33	-3.04	118.04	126.36
16	2	613	CLA	CHB-C4A-NA	3.03	128.78	124.40
16	1	610	CLA	C3B-C4B-NB	-3.03	107.82	110.53
16	B	842	CLA	C3B-C4B-NB	-3.03	107.82	110.53
25	B	850	DGD	C1E-O6E-C5E	3.03	119.64	113.72
19	A	801	CL0	C1-C2-C3	-3.03	121.23	126.20
16	B	809	CLA	C3B-C4B-NB	-3.03	107.83	110.53
16	A	822	CLA	CHB-C4A-NA	3.03	128.77	124.40
22	B	846	BCR	C27-C26-C25	3.03	126.79	122.70
17	1	613	ZEX	C4-C5-C6	-3.03	114.54	120.76
16	3	203	CLA	CHB-C4A-NA	3.02	128.76	124.40
16	3	202	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
16	B	829	CLA	CHB-C4A-NA	3.02	128.76	124.40
16	3	207	CLA	C3B-C4B-NB	-3.02	107.83	110.53
17	1	617	ZEX	C11-C12-C13	-3.02	118.09	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	807	CLA	C3B-C4B-NB	-3.02	107.84	110.53
16	B	834	CLA	C3B-C4B-NB	-3.01	107.84	110.53
16	B	831	CLA	CAA-C2A-C3A	-3.01	104.87	113.00
16	3	212	CLA	CHB-C4A-NA	3.01	128.74	124.40
16	B	824	CLA	C3B-C4B-NB	-3.00	107.85	110.53
16	O	204	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
16	B	825	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
16	A	825	CLA	CAA-C2A-C1A	-3.00	102.15	111.97
22	B	847	BCR	C30-C25-C26	-3.00	118.54	122.64
16	B	802	CLA	CHB-C4A-NA	2.99	128.72	124.40
16	A	827	CLA	C1-C2-C3	-2.99	121.29	126.20
16	B	827	CLA	CAA-C2A-C1A	-2.99	102.17	111.97
16	1	602	CLA	CAA-C2A-C3A	-2.99	104.92	113.00
22	L	202	BCR	C15-C16-C17	-2.99	117.41	123.52
16	O	202	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	A	810	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	B	840	CLA	CHB-C4A-NA	2.98	128.70	124.40
16	B	840	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
16	L	203	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	2	611	CLA	CAC-C3C-C2C	-2.98	122.09	127.56
16	B	810	CLA	C1-C2-C3	-2.97	121.32	126.20
16	1	606	CLA	C3B-C4B-NB	-2.97	107.88	110.53
17	1	613	ZEX	C11-C12-C13	-2.97	118.21	126.36
22	J	103	BCR	C15-C14-C13	-2.97	123.11	127.28
16	1	607	CLA	O2D-CGD-CBD	2.97	116.42	111.23
22	A	843	BCR	C27-C26-C25	2.97	126.71	122.70
16	3	209	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
16	B	823	CLA	C3B-C4B-NB	-2.97	107.88	110.53
16	1	612	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
17	1	614	ZEX	C8-C7-C6	-2.97	119.08	127.00
16	O	201	CLA	CMB-C2B-C1B	-2.96	120.91	125.42
16	B	801	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
16	B	823	CLA	CHB-C4A-NA	2.96	128.67	124.40
22	L	206	BCR	C27-C26-C25	2.96	126.70	122.70
16	1	611	CLA	CHB-C4A-NA	2.96	128.67	124.40
16	A	803	CLA	CMA-C3A-C4A	-2.96	103.82	111.77
16	L	205	CLA	C3B-C4B-NB	-2.96	107.89	110.53
17	3	218	ZEX	C31-C32-C33	-2.96	118.26	126.36
16	A	814	CLA	CHB-C4A-NA	2.96	128.67	124.40
16	3	209	CLA	CHB-C4A-NA	2.96	128.66	124.40
17	1	613	ZEX	C17-C1-C6	-2.95	105.61	110.24
16	A	834	CLA	C3B-C4B-NB	-2.95	107.89	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	803	CLA	CHB-C4A-NA	2.95	128.66	124.40
16	A	810	CLA	CHB-C4A-NA	2.95	128.66	124.40
16	B	817	CLA	CHB-C4A-NA	2.95	128.66	124.40
16	2	610	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
16	2	613	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
16	L	204	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
16	A	809	CLA	CHB-C4A-NA	2.95	128.65	124.40
16	3	211	CLA	C3B-C4B-NB	-2.95	107.90	110.53
16	B	820	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
16	B	821	CLA	CHB-C4A-NA	2.94	128.65	124.40
16	B	824	CLA	CHB-C4A-NA	2.94	128.65	124.40
16	2	602	CLA	CHB-C4A-NA	2.94	128.65	124.40
16	2	611	CLA	CBC-CAC-C3C	2.94	120.40	112.42
16	B	834	CLA	CAA-C2A-C3A	-2.94	105.05	113.00
16	A	825	CLA	CHB-C4A-NA	2.94	128.64	124.40
22	B	848	BCR	C15-C16-C17	-2.94	117.51	123.52
16	2	608	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
16	1	612	CLA	CHB-C4A-NA	2.94	128.64	124.40
16	A	804	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
16	B	828	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
16	K	102	CLA	C3B-C4B-NB	-2.94	107.91	110.53
22	L	206	BCR	C15-C16-C17	-2.94	117.51	123.52
16	L	201	CLA	CAA-C2A-C3A	-2.93	105.08	113.00
16	1	610	CLA	CHB-C4A-NA	2.93	128.63	124.40
16	B	836	CLA	C3B-C4B-NB	-2.93	107.92	110.53
16	A	816	CLA	CHB-C4A-NA	2.93	128.62	124.40
16	L	205	CLA	CHB-C4A-NA	2.93	128.62	124.40
16	F	803	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
16	B	822	CLA	C3B-C4B-NB	-2.93	107.92	110.53
17	3	214	ZEX	C11-C12-C13	-2.93	118.34	126.36
22	A	844	BCR	C15-C14-C13	-2.93	123.17	127.28
16	A	850	CLA	C1C-C2C-C3C	2.93	110.06	106.98
16	3	203	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
16	2	603	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
16	A	837	CLA	C3B-C4B-NB	-2.92	107.92	110.53
22	B	844	BCR	C15-C16-C17	-2.92	117.55	123.52
17	2	617	ZEX	C35-C15-C14	-2.92	117.55	123.52
16	A	802	CLA	C3B-C4B-NB	-2.92	107.93	110.53
22	F	801	BCR	C16-C15-C14	-2.91	117.56	123.52
17	1	617	ZEX	C31-C32-C33	-2.91	118.38	126.36
17	3	201	ZEX	C31-C32-C33	-2.91	118.38	126.36
16	A	813	CLA	CHB-C4A-NA	2.91	128.60	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	849	BCR	C2-C1-C6	2.91	114.66	110.44
17	3	218	ZEX	C12-C13-C14	-2.91	114.43	119.01
16	2	608	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
16	2	613	CLA	C3B-C4B-NB	-2.91	107.93	110.53
16	A	826	CLA	C3B-C4B-NB	-2.91	107.93	110.53
16	A	831	CLA	C3B-C4B-NB	-2.91	107.94	110.53
16	B	807	CLA	O2A-CGA-O1A	-2.91	116.36	123.63
16	A	802	CLA	CAA-C2A-C3A	-2.91	105.14	113.00
22	B	847	BCR	C27-C26-C25	2.90	126.63	122.70
17	1	613	ZEX	C15-C35-C34	-2.90	117.58	123.52
16	2	602	CLA	CAA-C2A-C3A	-2.90	105.16	113.00
16	B	830	CLA	CMB-C2B-C1B	-2.90	121.00	125.42
16	3	207	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
16	A	821	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
17	1	614	ZEX	C11-C12-C13	-2.89	118.43	126.36
22	B	847	BCR	C15-C14-C13	-2.89	123.22	127.28
16	B	826	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	B	850	DGD	CDB-CCB-CBB	-2.89	99.75	114.37
16	1	609	CLA	CHB-C4A-NA	2.89	128.57	124.40
16	3	210	CLA	CHB-C4A-NA	2.89	128.57	124.40
21	A	842	LHG	O8-C23-C24	2.89	120.64	111.83
16	3	213	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	B	849	BCR	C15-C16-C17	-2.89	117.61	123.52
22	A	844	BCR	C2-C1-C6	2.88	114.63	110.44
16	A	805	CLA	C3B-C4B-NB	-2.88	107.96	110.53
16	B	802	CLA	C1D-ND-C4D	2.88	108.33	106.31
16	B	840	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
16	B	807	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	F	801	BCR	C11-C10-C9	-2.88	123.24	127.28
16	2	606	CLA	CHB-C4A-NA	2.88	128.56	124.40
17	2	615	ZEX	C8-C7-C6	-2.88	119.31	127.00
16	1	602	CLA	CMB-C2B-C1B	-2.88	121.04	125.42
16	A	813	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	B	844	BCR	C27-C26-C25	2.88	126.59	122.70
16	K	101	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
16	O	203	CLA	C3B-C4B-NB	-2.87	107.97	110.53
16	3	210	CLA	C3B-C4B-NB	-2.87	107.97	110.53
16	1	611	CLA	CAC-C3C-C4C	2.87	128.52	124.79
16	3	211	CLA	CHB-C4A-NA	2.87	128.53	124.40
16	2	607	CLA	CHB-C4A-NA	2.86	128.53	124.40
16	O	203	CLA	CHB-C4A-NA	2.86	128.53	124.40
16	1	601	CLA	O2D-CGD-O1D	-2.86	118.28	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	607	CLA	CHB-C4A-NA	2.86	128.53	124.40
16	A	832	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
16	O	204	CLA	C3B-C4B-NB	-2.86	107.98	110.53
16	K	102	CLA	CHB-C4A-NA	2.86	128.52	124.40
16	B	835	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
16	B	835	CLA	C3B-C4B-NB	-2.85	107.98	110.53
16	2	609	CLA	CHB-C4A-NA	2.85	128.52	124.40
16	1	602	CLA	C3B-C4B-NB	-2.85	107.98	110.53
16	3	207	CLA	CHB-C4A-NA	2.85	128.51	124.40
16	3	204	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
16	1	606	CLA	CHB-C4A-NA	2.85	128.51	124.40
16	B	816	CLA	CAA-C2A-C3A	-2.85	105.31	113.00
16	1	604	CLA	CHB-C4A-NA	2.85	128.51	124.40
22	A	843	BCR	C11-C10-C9	-2.85	123.29	127.28
16	A	803	CLA	CMB-C2B-C1B	-2.84	121.09	125.42
16	3	204	CLA	CAA-C2A-C3A	-2.84	105.32	113.00
17	3	217	ZEX	C7-C8-C9	-2.84	122.03	126.23
16	2	606	CLA	C3B-C4B-NB	-2.84	107.99	110.53
16	A	836	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
16	L	204	CLA	CAA-C2A-C3A	-2.84	105.32	113.00
16	A	815	CLA	C3B-C4B-NB	-2.84	108.00	110.53
17	1	615	ZEX	C31-C32-C33	-2.84	118.59	126.36
16	A	822	CLA	C3B-C4B-NB	-2.84	108.00	110.53
16	3	206	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
16	A	820	CLA	CAA-C2A-C3A	-2.83	105.34	113.00
16	O	202	CLA	CHB-C4A-NA	2.83	128.49	124.40
16	3	209	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
16	B	812	CLA	CHB-C4A-NA	2.82	128.47	124.40
16	1	604	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
16	B	839	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
16	B	814	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	F	804	BCR	C15-C16-C17	-2.82	117.75	123.52
16	1	602	CLA	CHB-C4A-NA	2.82	128.47	124.40
16	1	607	CLA	C3B-C4B-NB	-2.82	108.01	110.53
16	1	610	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
16	1	611	CLA	C3B-C4B-NB	-2.82	108.02	110.53
16	B	811	CLA	CHB-C4A-NA	2.82	128.47	124.40
16	B	814	CLA	CMB-C2B-C3B	2.82	133.17	126.55
17	3	217	ZEX	C4-C5-C6	-2.81	114.97	120.76
16	B	841	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
16	A	828	CLA	C1-C2-C3	-2.81	121.59	126.20
16	B	811	CLA	O2D-CGD-O1D	-2.81	118.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	804	CLA	O1D-CGD-CBD	2.81	130.06	124.52
16	A	836	CLA	C3B-C4B-NB	-2.81	108.02	110.53
16	B	815	CLA	C1-C2-C3	-2.81	121.60	126.20
16	1	601	CLA	CHC-C1C-NC	2.81	128.54	124.31
16	B	842	CLA	CHB-C4A-NA	2.81	128.45	124.40
22	A	846	BCR	C27-C26-C25	2.80	126.49	122.70
19	A	801	CL0	C1A-CHA-C4D	-2.80	114.31	118.98
16	2	601	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	A	812	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	A	803	CLA	CMB-C2B-C3B	2.80	133.14	126.55
17	2	615	ZEX	C15-C35-C34	-2.80	117.79	123.52
22	F	804	BCR	C31-C1-C6	2.80	114.63	110.24
16	2	604	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	1	608	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
16	A	826	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
17	3	218	ZEX	C32-C33-C34	-2.80	114.61	119.01
16	A	824	CLA	CHB-C4A-NA	2.79	128.43	124.40
22	B	849	BCR	C11-C10-C9	-2.79	123.36	127.28
22	B	849	BCR	C15-C14-C13	-2.79	123.36	127.28
16	A	830	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
16	B	813	CLA	CHB-C4A-NA	2.79	128.43	124.40
22	B	848	BCR	C11-C10-C9	-2.79	123.37	127.28
22	F	804	BCR	C24-C23-C22	-2.79	122.11	126.23
22	J	102	BCR	C15-C16-C17	-2.79	117.82	123.52
16	A	808	CLA	CAA-C2A-C3A	-2.78	105.47	113.00
16	B	806	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
16	1	602	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
22	L	207	BCR	C27-C26-C25	2.78	126.46	122.70
16	2	604	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
16	F	802	CLA	CHB-C4A-NA	2.78	128.41	124.40
16	A	802	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
16	B	815	CLA	CHB-C4A-NA	2.77	128.40	124.40
16	L	204	CLA	CHB-C4A-NA	2.77	128.40	124.40
16	L	201	CLA	CHB-C4A-NA	2.77	128.40	124.40
16	B	838	CLA	CHB-C4A-NA	2.77	128.40	124.40
16	1	604	CLA	CMB-C2B-C3B	2.77	133.06	126.55
16	3	204	CLA	CHB-C4A-NA	2.77	128.39	124.40
16	2	611	CLA	CHB-C4A-NA	2.77	128.39	124.40
17	1	614	ZEX	C35-C15-C14	-2.77	117.86	123.52
16	2	611	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
16	A	809	CLA	CAA-C2A-C3A	-2.76	105.53	113.00
22	A	844	BCR	C15-C16-C17	-2.76	117.87	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	207	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
16	A	836	CLA	CMB-C2B-C1B	-2.76	121.21	125.42
16	O	203	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
16	L	201	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
16	B	803	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
16	2	605	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
16	3	210	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
16	A	823	CLA	C3B-C4B-NB	-2.76	108.07	110.53
16	A	850	CLA	CHD-C4C-C3C	2.75	128.79	124.77
22	I	101	BCR	C15-C14-C13	-2.75	123.42	127.28
16	2	605	CLA	C3B-C4B-NB	-2.75	108.07	110.53
16	2	603	CLA	CHB-C4A-NA	2.75	128.37	124.40
16	1	605	CLA	C3B-C4B-NB	-2.75	108.07	110.53
22	A	846	BCR	C15-C16-C17	-2.75	117.90	123.52
22	B	848	BCR	C3-C4-C5	-2.75	109.16	114.06
16	B	823	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
16	A	821	CLA	CHB-C4A-NA	2.74	128.36	124.40
16	2	606	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
16	A	834	CLA	CMB-C2B-C1B	-2.74	121.24	125.42
16	1	603	CLA	CAA-C2A-C3A	-2.74	105.59	113.00
17	1	614	ZEX	C38-C24-C25	-2.74	106.09	110.76
16	B	841	CLA	CAA-C2A-C3A	-2.74	105.59	113.00
16	A	852	CLA	CHB-C4A-NA	2.74	128.35	124.40
16	B	808	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
16	B	838	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	3	217	ZEX	C18-C5-C4	-2.74	109.39	114.42
16	3	205	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	3	218	ZEX	C7-C8-C9	-2.74	122.19	126.23
16	B	818	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	3	201	ZEX	C38-C24-C25	-2.74	106.10	110.76
16	2	602	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
22	B	848	BCR	C37-C22-C21	-2.73	118.39	122.82
16	A	818	CLA	C3B-C4B-NB	-2.73	108.09	110.53
16	A	818	CLA	CHB-C4A-NA	2.73	128.34	124.40
17	3	215	ZEX	C37-C21-C26	-2.73	105.97	110.25
16	2	610	CLA	C3B-C4B-NB	-2.73	108.09	110.53
16	A	838	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
16	3	208	CLA	CHB-C4A-NA	2.73	128.33	124.40
16	B	816	CLA	CHB-C4A-NA	2.72	128.33	124.40
16	B	804	CLA	C4D-C3D-CAD	-2.72	105.15	108.11
16	A	833	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
16	B	801	CLA	CMA-C3A-C4A	-2.72	104.46	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	612	CLA	C3B-C4B-NB	-2.72	108.11	110.53
16	A	833	CLA	CMA-C3A-C2A	-2.72	103.48	113.98
16	3	206	CLA	CHB-C4A-NA	2.71	128.32	124.40
16	A	818	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
16	B	816	CLA	CMB-C2B-C1B	-2.71	121.29	125.42
16	B	839	CLA	CHB-C4A-NA	2.71	128.31	124.40
16	A	837	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
17	3	218	ZEX	C4-C5-C6	-2.71	115.20	120.76
16	2	609	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
16	3	206	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
16	A	850	CLA	CMB-C2B-C3B	2.70	132.91	126.55
22	L	202	BCR	C27-C26-C25	2.70	126.36	122.70
22	A	843	BCR	C15-C16-C17	-2.70	117.98	123.52
16	A	851	CLA	CMB-C2B-C1B	-2.70	121.30	125.42
16	A	838	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
16	A	837	CLA	CMB-C2B-C3B	2.70	132.91	126.55
16	A	826	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
16	B	829	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
16	1	606	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
17	2	614	ZEX	C11-C12-C13	-2.70	118.96	126.36
16	B	826	CLA	C1-C2-C3	-2.70	121.77	126.20
16	1	605	CLA	CHB-C4A-NA	2.70	128.30	124.40
25	B	850	DGD	C3G-C2G-C1G	-2.70	105.49	111.78
17	1	615	ZEX	C11-C12-C13	-2.70	118.96	126.36
16	3	203	CLA	CMB-C2B-C3B	2.70	132.90	126.55
16	A	838	CLA	C1-C2-C3	-2.69	121.78	126.20
22	K	103	BCR	C15-C16-C17	-2.69	118.01	123.52
17	3	216	ZEX	C18-C5-C4	-2.69	109.47	114.42
16	B	841	CLA	CHB-C4A-NA	2.69	128.28	124.40
16	B	806	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
16	A	818	CLA	CHB-C1B-NB	2.69	128.09	124.05
16	1	601	CLA	C3A-C2A-C1A	2.69	105.37	101.34
16	B	825	CLA	CHB-C4A-NA	2.69	128.28	124.40
16	A	814	CLA	CMB-C2B-C3B	2.69	132.87	126.55
16	2	611	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
16	3	213	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
16	B	801	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
22	K	103	BCR	C15-C14-C13	-2.69	123.51	127.28
16	A	823	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
16	K	101	CLA	CHB-C4A-NA	2.68	128.27	124.40
16	B	820	CLA	CAA-CBA-CGA	-2.68	105.59	113.21
16	2	603	CLA	CAA-C2A-C3A	-2.68	105.76	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	810	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
22	F	804	BCR	C27-C26-C25	2.68	126.33	122.70
16	1	603	CLA	CHB-C4A-NA	2.68	128.27	124.40
16	2	612	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
16	1	609	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
16	3	212	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
22	A	843	BCR	C15-C14-C13	-2.68	123.53	127.28
16	A	811	CLA	CHB-C4A-NA	2.67	128.26	124.40
16	B	842	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
22	L	207	BCR	C15-C14-C13	-2.67	123.53	127.28
22	A	847	BCR	C33-C5-C6	-2.67	121.57	124.48
16	3	209	CLA	C3B-C4B-NB	-2.67	108.14	110.53
16	A	806	CLA	CMB-C2B-C3B	2.67	132.83	126.55
17	1	614	ZEX	C7-C8-C9	-2.67	122.29	126.23
16	B	812	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
16	B	807	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
16	B	817	CLA	C3B-C4B-NB	-2.66	108.15	110.53
16	B	829	CLA	CHC-C4B-NB	2.66	128.04	124.05
16	B	803	CLA	C1-C2-C3	-2.66	121.84	126.20
16	B	832	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
16	B	806	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
16	A	807	CLA	O2D-CGD-CBD	2.66	115.88	111.23
16	A	829	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
16	2	608	CLA	CMB-C2B-C3B	2.66	132.80	126.55
17	3	201	ZEX	C12-C13-C14	-2.66	114.83	119.01
16	A	821	CLA	C3B-C4B-NB	-2.66	108.16	110.53
16	B	815	CLA	CBC-CAC-C3C	2.66	119.63	112.42
16	O	201	CLA	CHB-C4A-NA	2.66	128.24	124.40
16	A	805	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
16	B	813	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
19	A	801	CL0	C16-C17-C18	-2.66	104.08	115.94
16	B	805	CLA	CAA-C2A-C3A	-2.65	105.83	113.00
16	B	801	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	A	801	CL0	C11-C12-C13	-2.65	107.15	115.97
16	A	816	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
16	B	824	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
16	B	832	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
16	B	802	CLA	CHA-C1A-NA	-2.65	120.39	126.39
16	1	603	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
16	A	811	CLA	C3B-C4B-NB	-2.65	108.17	110.53
16	A	825	CLA	C3A-C2A-C1A	2.65	105.30	101.34
22	L	206	BCR	C15-C14-C13	-2.65	123.57	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	801	BCR	C27-C26-C25	2.64	126.28	122.70
22	J	103	BCR	C15-C16-C17	-2.64	118.12	123.52
16	A	805	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
16	A	850	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
16	2	608	CLA	C1-C2-C3	-2.64	122.49	126.76
16	B	816	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
16	A	817	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
16	O	204	CLA	CHB-C4A-NA	2.63	128.20	124.40
25	B	850	DGD	CAB-C9B-C8B	-2.63	101.06	114.37
22	L	206	BCR	C3-C4-C5	-2.63	109.36	114.06
16	A	807	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
16	1	605	CLA	O2D-CGD-O1D	-2.63	118.12	124.08
16	O	201	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
16	B	811	CLA	C3B-C4B-NB	-2.62	108.19	110.53
16	A	827	CLA	CAA-C2A-C3A	-2.62	105.91	113.00
16	2	601	CLA	O1D-CGD-CBD	2.62	129.69	124.52
16	1	611	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
16	3	205	CLA	O2D-CGD-CBD	2.62	115.82	111.23
16	A	825	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
22	A	845	BCR	C29-C30-C25	2.62	114.25	110.44
16	A	824	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
16	B	809	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
16	B	808	CLA	CAA-C2A-C3A	-2.62	105.93	113.00
22	J	103	BCR	C27-C26-C25	2.62	126.24	122.70
17	2	616	ZEX	C35-C15-C14	-2.61	118.17	123.52
17	2	614	ZEX	C21-C26-C27	-2.61	108.56	115.65
16	B	802	CLA	CAA-CBA-CGA	-2.61	105.80	113.21
16	O	201	CLA	CAA-C2A-C3A	-2.61	105.95	113.00
22	B	848	BCR	C27-C26-C25	2.61	126.23	122.70
16	B	801	CLA	CGD-CBD-CAD	2.61	119.29	110.85
17	3	215	ZEX	C11-C12-C13	-2.61	119.22	126.36
16	B	827	CLA	O1D-CGD-CBD	2.61	129.66	124.52
22	F	804	BCR	C15-C14-C13	-2.61	123.62	127.28
16	B	831	CLA	CHB-C1B-NB	2.60	127.96	124.05
16	L	205	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
16	B	830	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
16	A	806	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
16	B	834	CLA	O2D-CGD-CBD	2.60	115.77	111.23
16	A	808	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
16	A	836	CLA	CHB-C4A-NA	2.60	128.15	124.40
20	A	840	PQN	C2M-C2-C3	-2.60	120.18	124.45
16	B	802	CLA	O2A-CGA-O1A	-2.60	117.14	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	830	CLA	CHB-C1B-NB	2.60	127.94	124.05
16	B	822	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
16	A	831	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
16	1	602	CLA	CMB-C2B-C3B	2.59	132.63	126.55
17	2	614	ZEX	C37-C21-C26	-2.58	106.20	110.25
16	A	802	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
16	A	829	CLA	C2D-C1D-ND	-2.58	107.57	110.13
16	A	817	CLA	C2A-C1A-CHA	2.58	128.34	123.87
16	3	212	CLA	C3B-C4B-NB	-2.58	108.23	110.53
16	A	821	CLA	O2D-CGD-CBD	2.58	115.73	111.23
16	3	211	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
16	A	820	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
16	A	837	CLA	CHB-C4A-NA	2.58	128.12	124.40
22	J	102	BCR	C20-C21-C22	-2.58	123.67	127.28
16	B	833	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
16	1	604	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
16	A	814	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
17	3	218	ZEX	C8-C7-C6	-2.57	120.12	127.00
22	A	849	BCR	C7-C8-C9	-2.57	122.43	126.23
16	2	612	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
16	B	839	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
17	2	615	ZEX	C7-C8-C9	-2.56	122.44	126.23
16	B	839	CLA	CAA-C2A-C3A	-2.56	106.08	113.00
16	L	205	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
16	A	803	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
22	A	845	BCR	C16-C17-C18	-2.56	123.69	127.28
16	B	802	CLA	CMA-C3A-C4A	-2.56	104.90	111.77
22	B	847	BCR	C40-C30-C25	2.55	114.25	110.24
16	B	837	CLA	CAC-C3C-C4C	2.55	128.11	124.79
22	A	845	BCR	C16-C15-C14	-2.55	118.30	123.52
16	A	816	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
21	A	841	LHG	O8-C23-C24	2.55	119.60	111.83
17	3	218	ZEX	C18-C5-C4	-2.55	109.74	114.42
21	A	841	LHG	C11-C10-C9	-2.55	101.50	114.37
16	B	833	CLA	CAA-C2A-C3A	-2.54	106.12	113.00
19	A	801	CL0	OBD-CAD-CBD	-2.54	122.09	125.82
16	1	612	CLA	C2A-C1A-CHA	2.54	128.28	123.87
16	B	839	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
16	B	837	CLA	CBA-CAA-C2A	-2.54	106.24	113.79
16	A	850	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
22	A	845	BCR	C7-C8-C9	-2.54	122.48	126.23
16	B	837	CLA	O2D-CGD-O1D	-2.53	118.92	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	844	BCR	C30-C25-C26	-2.53	119.17	122.64
16	A	851	CLA	C3B-C4B-NB	-2.53	108.27	110.53
16	A	829	CLA	O2D-CGD-CBD	2.53	115.65	111.23
16	A	829	CLA	CHC-C1C-NC	2.53	128.12	124.31
16	B	812	CLA	C3B-C4B-NB	-2.53	108.28	110.53
16	A	809	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
16	B	839	CLA	O2D-CGD-CBD	2.52	115.64	111.23
16	A	836	CLA	O2D-CGD-CBD	2.52	115.64	111.23
22	A	847	BCR	C7-C8-C9	-2.52	122.50	126.23
16	B	806	CLA	CMB-C2B-C3B	2.52	132.48	126.55
17	3	214	ZEX	C8-C7-C6	-2.52	120.27	127.00
16	B	825	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
22	K	103	BCR	C27-C26-C25	2.51	126.10	122.70
16	A	830	CLA	CHB-C4A-NA	2.51	128.03	124.40
16	B	831	CLA	C2D-C1D-ND	-2.51	107.64	110.13
16	A	835	CLA	C2A-C1A-CHA	2.51	128.23	123.87
16	1	610	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
16	A	832	CLA	C3B-C4B-NB	-2.51	108.29	110.53
16	A	812	CLA	CAA-C2A-C3A	-2.50	106.23	113.00
17	1	613	ZEX	C7-C6-C5	-2.50	115.79	121.56
16	3	209	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
16	3	209	CLA	CMB-C2B-C3B	2.50	132.43	126.55
16	B	805	CLA	C16-C15-C13	-2.50	107.65	115.97
22	A	844	BCR	C16-C15-C14	-2.50	118.41	123.52
16	2	606	CLA	CAA-C2A-C3A	-2.49	106.26	113.00
16	A	828	CLA	CMD-C2D-C1D	-2.49	120.34	124.73
22	B	848	BCR	C20-C21-C22	-2.49	123.79	127.28
16	F	802	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
17	2	617	ZEX	C4-C5-C6	-2.49	115.65	120.76
16	A	809	CLA	C3B-C4B-NB	-2.48	108.31	110.53
16	B	838	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
17	2	617	ZEX	C31-C32-C33	-2.48	119.56	126.36
16	A	851	CLA	CAA-C2A-C3A	-2.48	106.30	113.00
16	A	852	CLA	C3B-C4B-NB	-2.48	108.32	110.53
22	A	849	BCR	C27-C26-C25	2.48	126.06	122.70
16	A	839	CLA	C3B-C4B-NB	-2.48	108.32	110.53
16	1	601	CLA	CAA-C2A-C3A	-2.48	106.31	113.00
16	A	827	CLA	O2D-CGD-CBD	2.48	115.56	111.23
16	A	828	CLA	CMA-C3A-C2A	-2.48	104.41	113.98
16	B	802	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
16	B	830	CLA	CAA-C2A-C3A	-2.47	106.31	113.00
16	3	203	CLA	O2D-CGD-O1D	-2.47	119.03	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	852	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
16	A	804	CLA	C1-C2-C3	-2.47	122.15	126.20
16	A	829	CLA	C1-C2-C3	-2.47	122.15	126.20
16	B	830	CLA	CHB-C4A-NA	2.47	127.96	124.40
16	B	822	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
17	2	615	ZEX	C3-C4-C5	2.46	118.31	112.18
16	3	206	CLA	C1D-ND-C4D	2.46	108.04	106.31
22	B	846	BCR	C15-C16-C17	-2.46	118.48	123.52
16	B	813	CLA	CAB-C3B-C2B	2.46	130.08	123.53
16	A	827	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
22	B	849	BCR	C31-C1-C6	2.46	114.11	110.24
16	A	850	CLA	C2A-C1A-CHA	2.46	128.14	123.87
16	B	837	CLA	C2A-C1A-CHA	2.46	128.14	123.87
16	A	804	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
16	A	850	CLA	C3B-C4B-NB	-2.46	108.34	110.53
22	A	847	BCR	C16-C15-C14	-2.45	118.50	123.52
16	1	609	CLA	C3B-C4B-NB	-2.45	108.34	110.53
22	A	843	BCR	C33-C5-C6	-2.45	121.81	124.48
22	B	844	BCR	C7-C8-C9	-2.45	122.61	126.23
16	B	828	CLA	O2D-CGD-CBD	2.45	115.52	111.23
16	B	818	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
16	B	839	CLA	CMB-C2B-C3B	2.45	132.31	126.55
16	2	609	CLA	C3B-C4B-NB	-2.45	108.35	110.53
16	J	101	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
16	2	607	CLA	CAA-C2A-C3A	-2.44	106.39	113.00
16	B	829	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
16	O	201	CLA	CMB-C2B-C3B	2.44	132.29	126.55
22	L	202	BCR	C24-C23-C22	-2.44	122.63	126.23
16	3	206	CLA	CMB-C2B-C3B	2.44	132.28	126.55
19	A	801	CL0	C4C-C3C-C2C	-2.44	103.75	113.37
21	A	841	LHG	C20-C19-C18	-2.43	102.06	114.37
16	A	825	CLA	CBC-CAC-C3C	2.43	119.02	112.42
16	1	605	CLA	CAA-C2A-C3A	-2.43	106.43	113.00
17	1	615	ZEX	C17-C1-C6	-2.43	106.43	110.24
16	B	804	CLA	CHA-C1A-NA	-2.43	120.89	126.39
16	K	102	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
16	A	816	CLA	CAC-C3C-C4C	2.43	127.95	124.79
16	F	802	CLA	O2D-CGD-CBD	2.43	115.48	111.23
16	A	824	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
16	3	206	CLA	C2A-C1A-CHA	2.43	128.08	123.87
22	L	202	BCR	C10-C11-C12	-2.43	116.17	123.20
19	A	801	CL0	C4C-CHD-C1D	2.43	124.75	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	831	CLA	CHC-C1C-NC	2.43	127.97	124.31
16	A	829	CLA	C2A-C1A-CHA	2.43	128.08	123.87
16	B	802	CLA	CAA-C2A-C1A	2.42	119.92	111.97
16	3	202	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
22	J	102	BCR	C29-C30-C25	2.42	113.96	110.44
16	B	828	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
16	B	818	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
22	I	101	BCR	C27-C26-C25	2.42	125.97	122.70
16	B	827	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	A	849	BCR	C24-C23-C22	-2.41	122.67	126.23
16	A	808	CLA	CHB-C4A-NA	2.41	127.88	124.40
16	A	829	CLA	CMD-C2D-C1D	-2.41	120.49	124.73
16	A	829	CLA	CHB-C4A-NA	2.41	127.87	124.40
22	A	847	BCR	C27-C26-C25	2.41	125.96	122.70
16	A	813	CLA	CAA-C2A-C3A	-2.41	106.50	113.00
16	B	842	CLA	CAA-C2A-C3A	-2.41	106.50	113.00
16	A	829	CLA	CMB-C2B-C3B	2.41	132.21	126.55
16	A	839	CLA	C1-O2A-CGA	2.40	122.46	116.65
16	F	802	CLA	CHB-C1B-NB	2.40	127.65	124.05
16	A	829	CLA	CMC-C2C-C1C	-2.40	121.29	125.03
16	B	801	CLA	C3C-C4C-NC	-2.40	107.36	110.43
16	3	204	CLA	C3B-C4B-NB	-2.40	108.39	110.53
16	A	805	CLA	C1-C2-C3	-2.40	122.27	126.20
16	B	825	CLA	C1-C2-C3	-2.39	122.28	126.20
17	1	615	ZEX	C27-C28-C29	-2.39	122.69	126.23
16	B	810	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
16	A	808	CLA	CMA-C3A-C4A	2.39	118.20	111.77
16	B	816	CLA	CMB-C2B-C3B	2.39	132.17	126.55
16	A	804	CLA	CAC-C3C-C4C	2.39	127.90	124.79
16	B	829	CLA	C2A-C1A-CHA	2.39	128.01	123.87
22	L	207	BCR	C7-C8-C9	-2.39	122.71	126.23
25	B	850	DGD	CFB-CEB-CDB	-2.38	102.32	114.37
22	B	845	BCR	C28-C27-C26	-2.38	109.81	114.06
16	A	836	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
21	A	841	LHG	C18-C17-C16	-2.38	102.32	114.37
16	A	839	CLA	C1-C2-C3	-2.38	122.30	126.20
16	A	828	CLA	CAA-CBA-CGA	-2.38	106.45	113.21
16	B	821	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
22	B	846	BCR	C24-C23-C22	-2.38	122.72	126.23
16	B	824	CLA	CAA-C2A-C3A	-2.38	106.58	113.00
16	A	836	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
21	A	842	LHG	C11-C10-C9	-2.38	102.36	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	604	CLA	C3B-C4B-NB	-2.37	108.41	110.53
16	A	807	CLA	CAA-C2A-C1A	-2.37	104.20	111.97
16	B	827	CLA	C3A-C2A-C1A	2.37	104.89	101.34
16	3	202	CLA	C3B-C4B-NB	-2.37	108.41	110.53
16	A	829	CLA	C3B-C2B-C1B	2.37	109.97	107.17
16	K	101	CLA	CGD-CBD-CAD	2.37	118.52	110.85
16	B	809	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
16	A	837	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
16	B	830	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
16	F	802	CLA	C2A-C1A-CHA	2.37	127.98	123.87
16	A	818	CLA	C2A-C1A-CHA	2.37	127.97	123.87
21	A	842	LHG	C20-C19-C18	-2.36	102.41	114.37
22	B	846	BCR	C31-C1-C6	2.36	113.95	110.24
16	A	806	CLA	C1D-ND-C4D	2.36	107.97	106.31
16	A	811	CLA	O2D-CGD-CBD	2.36	115.36	111.23
16	A	820	CLA	CAC-C3C-C4C	2.36	127.86	124.79
22	B	848	BCR	C30-C25-C26	-2.36	119.41	122.64
17	3	218	ZEX	C11-C12-C13	-2.36	119.89	126.36
16	B	803	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
22	B	846	BCR	C15-C14-C13	-2.35	123.98	127.28
16	B	804	CLA	CHB-C1B-NB	2.35	127.57	124.05
16	B	801	CLA	CAA-CBA-CGA	-2.35	106.54	113.21
16	A	829	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
16	B	807	CLA	C2A-C1A-CHA	2.35	127.94	123.87
16	1	609	CLA	CMA-C3A-C2A	-2.34	110.85	116.23
22	B	844	BCR	C15-C14-C13	-2.34	123.99	127.28
16	A	836	CLA	C2A-C1A-CHA	2.34	127.93	123.87
16	B	801	CLA	C2D-C1D-ND	-2.34	107.81	110.13
16	B	804	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
16	A	817	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
16	O	203	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
16	A	851	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
22	K	103	BCR	C3-C4-C5	-2.34	109.89	114.06
16	A	852	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
16	A	828	CLA	CHB-C4A-NA	2.34	127.77	124.40
16	B	831	CLA	C1D-ND-C4D	2.34	107.95	106.31
16	B	823	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
16	A	852	CLA	CAA-CBA-CGA	-2.33	106.58	113.21
16	B	802	CLA	C2D-C1D-ND	-2.33	107.82	110.13
16	L	205	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
16	B	836	CLA	C2A-C1A-CHA	2.33	127.91	123.87
16	B	820	CLA	CMB-C2B-C3B	2.33	132.03	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	808	CLA	CHC-C4B-NB	2.33	127.54	124.05
16	A	850	CLA	CBC-CAC-C3C	2.33	118.73	112.42
17	1	615	ZEX	C8-C7-C6	-2.33	120.78	127.00
16	B	802	CLA	C4D-CHA-C1A	2.33	124.02	121.24
16	B	803	CLA	CAA-C2A-C3A	-2.32	106.72	113.00
16	A	836	CLA	CHB-C1B-NB	2.32	127.53	124.05
16	B	809	CLA	CAC-C3C-C4C	2.32	127.81	124.79
16	B	814	CLA	C3B-C4B-NB	-2.32	108.46	110.53
22	L	207	BCR	C24-C23-C22	-2.32	122.80	126.23
16	B	802	CLA	C4D-C3D-CAD	-2.32	105.59	108.11
16	B	836	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
22	B	845	BCR	C15-C14-C13	-2.32	124.03	127.28
16	A	820	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
16	B	811	CLA	CAC-C3C-C4C	2.32	127.80	124.79
22	A	847	BCR	C23-C22-C21	-2.31	115.37	119.01
16	2	609	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
16	L	205	CLA	C2A-C1A-CHA	2.31	127.87	123.87
25	B	850	DGD	C8B-C7B-C6B	-2.31	102.71	114.37
16	A	828	CLA	CMB-C2B-C3B	2.31	131.98	126.55
16	B	802	CLA	C2A-C1A-CHA	2.31	127.87	123.87
16	B	835	CLA	CAA-C2A-C3A	-2.30	106.77	113.00
16	A	822	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
16	2	602	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
16	2	608	CLA	O1D-CGD-CBD	2.30	129.06	124.52
26	J	104	3XQ	O25-C24-C22	-2.30	100.02	110.38
16	B	818	CLA	CMB-C2B-C3B	2.30	131.96	126.55
16	A	806	CLA	C2A-C1A-CHA	2.30	127.86	123.87
16	A	831	CLA	C2A-C1A-CHA	2.30	127.85	123.87
22	B	849	BCR	C3-C4-C5	-2.30	109.96	114.06
16	2	603	CLA	O2D-CGD-CBD	2.30	115.24	111.23
17	1	614	ZEX	C7-C6-C5	-2.29	116.27	121.56
16	B	829	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
16	A	824	CLA	C7-C6-C5	-2.29	107.15	113.26
16	A	839	CLA	CAA-C2A-C3A	-2.29	106.81	113.00
22	F	804	BCR	C2-C1-C6	2.29	113.76	110.44
17	3	214	ZEX	C35-C15-C14	-2.29	118.84	123.52
22	A	845	BCR	C15-C14-C13	-2.29	124.07	127.28
22	A	846	BCR	C33-C5-C6	-2.29	121.99	124.48
16	B	802	CLA	CHB-C1B-C2B	-2.29	120.79	127.43
16	B	819	CLA	C2A-C1A-CHA	2.29	127.83	123.87
16	B	805	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
17	3	217	ZEX	C11-C12-C13	-2.28	120.11	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	808	CLA	CMA-C3A-C2A	-2.28	105.16	113.98
22	L	202	BCR	C7-C8-C9	-2.28	122.86	126.23
16	A	808	CLA	CHB-C1B-NB	2.28	127.47	124.05
16	A	821	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
16	B	820	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
16	A	802	CLA	CMB-C2B-C3B	2.28	131.91	126.55
22	A	846	BCR	C15-C14-C13	-2.28	124.08	127.28
16	A	808	CLA	C1-C2-C3	-2.28	122.47	126.20
16	1	610	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
16	2	608	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
16	A	830	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
16	B	831	CLA	CMC-C2C-C1C	-2.27	121.48	125.03
19	A	801	CL0	C1-O2A-CGA	2.27	122.15	116.65
22	I	101	BCR	C11-C10-C9	-2.27	124.09	127.28
16	A	851	CLA	C2A-C1A-CHA	2.27	127.81	123.87
16	A	832	CLA	CMC-C2C-C1C	-2.27	121.49	125.03
16	L	201	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
16	A	829	CLA	CMC-C2C-C3C	2.27	132.28	126.15
16	A	824	CLA	CAA-CBA-CGA	-2.27	106.78	113.21
16	J	101	CLA	C2A-C1A-CHA	2.26	127.80	123.87
16	A	803	CLA	CAA-C2A-C3A	-2.26	106.88	113.00
16	A	835	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
16	B	833	CLA	CHB-C1B-NB	2.26	127.44	124.05
16	3	210	CLA	CMA-C3A-C2A	-2.26	111.05	116.23
22	F	801	BCR	C16-C17-C18	-2.26	124.11	127.28
16	A	817	CLA	CHA-C1A-NA	-2.26	121.28	126.39
22	A	849	BCR	C35-C13-C14	-2.26	119.16	122.82
16	A	831	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
16	A	817	CLA	CMB-C2B-C3B	2.25	131.85	126.55
16	A	808	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
22	A	847	BCR	C20-C21-C22	-2.25	124.12	127.28
17	3	215	ZEX	C3-C4-C5	2.25	117.78	112.18
21	A	841	LHG	C27-C26-C25	-2.25	103.00	114.37
16	A	812	CLA	C2A-C1A-CHA	2.25	127.77	123.87
16	A	829	CLA	C3B-C4B-NB	-2.25	108.52	110.53
16	B	830	CLA	CMA-C3A-C2A	-2.25	105.29	113.98
16	B	805	CLA	CHC-C4B-NB	2.25	127.42	124.05
16	A	807	CLA	C3A-C2A-C1A	2.25	104.70	101.34
22	A	844	BCR	C1-C6-C5	-2.25	119.57	122.64
16	A	802	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
16	A	805	CLA	CMB-C2B-C3B	2.24	131.83	126.55
25	B	850	DGD	O6E-C5E-C4E	2.24	113.74	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	212	CLA	C2A-C1A-CHA	2.24	127.76	123.87
16	3	213	CLA	C2A-C1A-CHA	2.24	127.76	123.87
17	3	216	ZEX	C31-C32-C33	-2.24	120.21	126.36
16	2	613	CLA	C2A-C1A-CHA	2.24	127.76	123.87
16	1	601	CLA	C3B-C4B-NB	-2.24	108.53	110.53
22	B	846	BCR	C11-C10-C9	-2.24	124.14	127.28
17	3	216	ZEX	C4-C5-C6	-2.24	116.16	120.76
22	I	101	BCR	C1-C6-C5	-2.24	119.58	122.64
16	A	834	CLA	CAA-C2A-C3A	-2.24	106.96	113.00
16	B	826	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
22	L	207	BCR	C15-C16-C17	-2.23	118.95	123.52
16	A	802	CLA	O1D-CGD-CBD	2.23	128.92	124.52
17	3	214	ZEX	C17-C1-C6	-2.23	106.75	110.24
16	1	610	CLA	C2A-C1A-CHA	2.23	127.74	123.87
16	2	605	CLA	C2A-C1A-CHA	2.23	127.74	123.87
16	B	811	CLA	O1D-CGD-CBD	2.23	128.91	124.52
16	O	202	CLA	C2A-C1A-CHA	2.23	127.72	123.86
17	2	616	ZEX	C4-C5-C6	-2.23	116.18	120.76
17	2	616	ZEX	C8-C7-C6	-2.23	121.05	127.00
20	B	843	PQN	C14-C13-C15	-2.22	111.37	115.23
16	B	805	CLA	CMD-C2D-C1D	-2.22	120.81	124.73
16	3	206	CLA	C2D-C1D-ND	-2.22	107.92	110.13
17	3	218	ZEX	C17-C1-C6	-2.22	106.76	110.24
19	A	801	CL0	O2A-C1-C2	2.22	116.66	108.11
16	B	815	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
16	B	813	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
16	B	819	CLA	CHB-C1B-NB	2.22	127.38	124.05
20	A	840	PQN	C11-C3-C2	-2.22	121.08	124.89
16	B	813	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
22	F	801	BCR	C7-C8-C9	-2.22	122.96	126.23
16	1	601	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
16	B	827	CLA	CMB-C2B-C3B	2.21	131.76	126.55
16	1	612	CLA	CHA-C1A-NA	-2.21	121.38	126.39
16	A	831	CLA	CAA-C2A-C3A	-2.21	107.02	113.00
16	1	608	CLA	C2A-C1A-CHA	2.21	127.71	123.87
16	B	820	CLA	C1-C2-C3	-2.21	122.58	126.20
22	B	844	BCR	C40-C30-C25	2.21	113.71	110.24
22	L	206	BCR	C39-C30-C25	2.21	113.71	110.24
16	F	802	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
16	A	827	CLA	CMA-C3A-C2A	-2.21	105.44	113.98
16	B	828	CLA	C2A-C1A-CHA	2.21	127.70	123.87
16	3	208	CLA	O2D-CGD-O1D	-2.21	119.55	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	803	CLA	O1D-CGD-CBD	2.21	128.87	124.52
16	B	814	CLA	C2A-C1A-CHA	2.21	127.70	123.87
16	B	813	CLA	CMA-C3A-C2A	-2.20	105.46	113.98
16	A	824	CLA	O1D-CGD-CBD	2.20	128.86	124.52
16	B	835	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	A	806	CLA	O2D-CGD-CBD	2.20	115.08	111.23
22	A	849	BCR	C20-C21-C22	-2.20	124.19	127.28
16	A	810	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
16	2	607	CLA	CHA-C1A-NA	-2.20	121.42	126.39
21	A	842	LHG	C27-C26-C25	-2.20	103.26	114.37
16	A	824	CLA	C2A-C1A-CHA	2.19	127.68	123.87
16	L	204	CLA	O2D-CGD-CBD	2.19	115.07	111.23
16	A	833	CLA	CMA-C3A-C4A	-2.19	105.87	111.77
16	B	804	CLA	CAA-C2A-C3A	-2.19	107.07	113.00
16	A	830	CLA	O2D-CGD-CBD	2.19	115.06	111.23
16	B	817	CLA	C2A-C1A-CHA	2.19	127.67	123.87
16	A	805	CLA	CBA-CAA-C2A	2.19	120.32	113.79
16	B	819	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
17	1	616	ZEX	C4-C5-C6	-2.19	116.26	120.76
16	A	832	CLA	CMC-C2C-C3C	2.19	132.07	126.15
16	1	606	CLA	C2A-C1A-CHA	2.19	127.67	123.87
16	B	811	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
22	F	804	BCR	C11-C10-C9	-2.19	124.21	127.28
16	B	840	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	B	815	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
22	B	844	BCR	C11-C10-C9	-2.19	124.21	127.28
16	B	807	CLA	CHA-C1A-NA	-2.19	121.44	126.39
16	A	835	CLA	CHA-C1A-NA	-2.18	121.44	126.39
16	3	205	CLA	C3A-C2A-C1A	2.18	104.61	101.34
16	B	819	CLA	CAA-C2A-C3A	-2.18	107.10	113.00
16	A	820	CLA	CHB-C1B-NB	2.18	127.32	124.05
16	L	203	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
16	B	804	CLA	CMD-C2D-C1D	-2.18	120.89	124.73
16	2	612	CLA	C2A-C1A-CHA	2.18	127.65	123.87
16	O	203	CLA	C2A-C1A-CHA	2.18	127.64	123.87
17	3	201	ZEX	C18-C5-C4	-2.18	110.42	114.42
22	F	804	BCR	C16-C15-C14	-2.18	119.07	123.52
16	A	806	CLA	CHA-C4D-ND	2.17	137.03	132.55
16	1	605	CLA	C2A-C1A-CHA	2.17	127.64	123.87
16	A	812	CLA	CHA-C1A-NA	-2.17	121.47	126.39
16	A	834	CLA	CHB-C1B-NB	2.17	127.31	124.05
16	2	605	CLA	CAA-C2A-C3A	-2.17	107.13	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	808	CLA	CHA-C4D-ND	2.17	137.02	132.55
16	A	815	CLA	C2A-C1A-CHA	2.17	127.63	123.87
16	2	607	CLA	O2A-CGA-O1A	-2.17	117.76	123.33
22	A	844	BCR	C29-C30-C25	2.17	113.59	110.44
22	A	843	BCR	C7-C8-C9	-2.17	123.03	126.23
16	B	810	CLA	CBA-CAA-C2A	2.17	120.24	113.79
16	2	601	CLA	CAC-C3C-C4C	2.17	127.61	124.79
22	J	102	BCR	C10-C11-C12	-2.17	116.93	123.20
16	L	201	CLA	CHB-C1B-NB	2.16	127.30	124.05
16	3	202	CLA	C2A-C1A-CHA	2.16	127.62	123.87
16	3	207	CLA	CHC-C4B-NB	2.16	127.29	124.05
16	A	812	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	B	837	CLA	CHA-C1A-NA	-2.16	121.50	126.39
16	A	835	CLA	CHC-C4B-NB	2.16	127.29	124.05
16	B	841	CLA	CHB-C1B-NB	2.16	127.29	124.05
16	B	801	CLA	O1D-CGD-CBD	2.16	128.78	124.52
16	3	203	CLA	CHB-C1B-NB	2.16	127.29	124.05
16	B	831	CLA	C6-C7-C8	-2.16	108.79	115.97
22	B	849	BCR	C28-C27-C26	-2.16	110.21	114.06
16	A	816	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
16	B	825	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
17	3	214	ZEX	C3-C4-C5	2.15	117.54	112.18
16	A	822	CLA	C1-C2-C3	-2.15	122.67	126.20
16	A	820	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
16	A	852	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
22	B	847	BCR	C7-C8-C9	-2.15	123.06	126.23
16	B	804	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
16	B	820	CLA	CMA-C3A-C4A	-2.15	106.00	111.77
16	A	813	CLA	O2A-CGA-O1A	-2.15	117.81	123.33
16	A	829	CLA	C4B-C3B-C2B	-2.14	104.64	107.30
16	A	828	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
16	O	201	CLA	CAC-C3C-C4C	2.14	127.58	124.79
17	2	614	ZEX	C8-C7-C6	-2.14	121.28	127.00
16	F	802	CLA	O2A-CGA-O1A	-2.14	117.82	123.33
22	L	202	BCR	C15-C14-C13	-2.14	124.28	127.28
17	1	613	ZEX	C21-C26-C27	-2.14	109.85	115.65
16	B	804	CLA	CMD-C2D-C3D	2.14	132.59	127.69
16	A	818	CLA	C1D-ND-C4D	2.14	107.81	106.31
22	B	844	BCR	C38-C26-C27	-2.14	109.04	113.60
16	A	806	CLA	C2D-C1D-ND	-2.14	108.01	110.13
16	O	201	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
16	L	205	CLA	O2A-CGA-O1A	-2.13	118.29	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	808	CLA	C2A-C1A-CHA	2.13	127.57	123.87
16	L	203	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
16	B	820	CLA	C3B-C4B-NB	-2.13	108.63	110.53
16	A	850	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
16	A	832	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	B	808	CLA	CHA-C1A-NA	-2.13	121.57	126.39
16	A	830	CLA	C1-C2-C3	-2.13	123.32	126.76
16	2	602	CLA	C1-C2-C3	-2.13	122.71	126.20
16	A	817	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	B	817	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
16	B	812	CLA	O2D-CGD-CBD	2.13	114.95	111.23
16	3	206	CLA	CHA-C1A-NA	-2.13	121.57	126.39
16	A	828	CLA	C2D-C1D-ND	-2.13	108.02	110.13
22	B	845	BCR	C7-C8-C9	-2.12	123.09	126.23
16	2	605	CLA	O2A-CGA-O1A	-2.12	117.87	123.33
16	B	820	CLA	C2A-C1A-CHA	2.12	127.55	123.87
16	B	821	CLA	CHB-C1B-NB	2.12	127.23	124.05
16	2	603	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
16	L	205	CLA	CMB-C2B-C3B	2.12	131.54	126.55
16	B	838	CLA	CHB-C1B-NB	2.12	127.23	124.05
16	B	829	CLA	O2D-CGD-CBD	2.12	114.94	111.23
16	A	809	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	A	844	BCR	C24-C23-C22	-2.12	123.10	126.23
16	A	832	CLA	C3A-C2A-C1A	2.12	104.51	101.34
16	B	801	CLA	CMA-C3A-C2A	-2.12	105.80	113.98
22	A	844	BCR	C27-C26-C25	2.11	125.56	122.70
16	B	809	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
17	3	215	ZEX	C15-C35-C34	-2.11	119.19	123.52
22	B	845	BCR	C27-C26-C25	2.11	125.56	122.70
16	A	818	CLA	CHC-C1C-NC	2.11	127.49	124.31
16	A	851	CLA	CMB-C2B-C3B	2.11	131.51	126.55
25	B	850	DGD	C5B-C4B-C3B	-2.11	103.71	114.37
16	2	609	CLA	CMB-C2B-C3B	2.11	131.51	126.55
16	B	810	CLA	O2A-CGA-CBA	2.11	118.26	111.83
17	2	616	ZEX	C17-C1-C6	-2.11	106.94	110.24
16	A	837	CLA	C2A-C1A-CHA	2.11	127.52	123.87
16	L	205	CLA	CHB-C1B-NB	2.11	127.21	124.05
22	J	103	BCR	C33-C5-C6	-2.11	122.19	124.48
16	1	601	CLA	CMC-C2C-C3C	2.11	131.84	126.15
16	A	836	CLA	C3A-C2A-C1A	2.10	104.49	101.34
16	J	101	CLA	CHA-C1A-NA	-2.10	121.63	126.39
16	B	833	CLA	O1D-CGD-CBD	2.10	128.66	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	206	BCR	C30-C25-C26	-2.10	119.76	122.64
16	K	101	CLA	CAA-C2A-C3A	-2.10	107.32	113.00
17	3	215	ZEX	C31-C32-C33	-2.10	120.60	126.36
16	B	837	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	A	817	CLA	C1D-ND-C4D	2.10	107.78	106.31
16	A	804	CLA	CMB-C2B-C3B	2.10	131.48	126.55
16	A	815	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
16	2	607	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
16	B	831	CLA	C3B-C4B-NB	-2.10	108.66	110.53
21	A	842	LHG	C18-C17-C16	-2.10	103.78	114.37
17	2	617	ZEX	C11-C12-C13	-2.09	120.63	126.36
22	B	845	BCR	C15-C16-C17	-2.09	119.24	123.52
16	A	806	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
16	A	821	CLA	CMD-C2D-C3D	2.09	132.48	127.69
16	B	802	CLA	C1-C2-C3	-2.09	122.78	126.20
16	3	213	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	A	805	CLA	CHA-C1A-NA	-2.09	121.67	126.39
16	A	830	CLA	CHA-C1A-NA	-2.09	121.67	126.39
16	3	203	CLA	CAC-C3C-C4C	2.09	127.50	124.79
16	B	829	CLA	CHA-C1A-NA	-2.09	121.67	126.39
16	3	208	CLA	C2A-C1A-CHA	2.09	127.49	123.87
16	B	804	CLA	C1-C2-C3	-2.08	122.78	126.20
16	B	808	CLA	CHC-C4B-NB	2.08	127.17	124.05
16	B	812	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	B	837	CLA	CBC-CAC-C3C	2.08	118.06	112.42
17	2	614	ZEX	C35-C15-C14	-2.08	119.26	123.52
16	B	802	CLA	OBD-CAD-C3D	2.08	133.28	128.42
25	B	850	DGD	CBB-CAB-C9B	-2.08	103.85	114.37
16	L	205	CLA	CHA-C1A-NA	-2.08	121.68	126.39
22	A	845	BCR	C10-C11-C12	-2.08	117.18	123.20
22	A	847	BCR	C37-C22-C21	-2.08	119.45	122.82
25	B	850	DGD	C7A-C6A-C5A	-2.08	103.86	114.37
16	A	824	CLA	C1-C2-C3	-2.08	122.79	126.20
16	B	818	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	O	202	CLA	CHA-C1A-NA	-2.08	121.69	126.39
16	A	817	CLA	CAA-C2A-C3A	-2.08	107.39	113.00
16	A	811	CLA	CHA-C1A-NA	-2.08	121.69	126.39
16	A	823	CLA	C2A-C1A-CHA	2.07	127.47	123.87
16	A	817	CLA	CHB-C1B-NB	2.07	127.16	124.05
16	O	203	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
16	A	834	CLA	O2A-CGA-O1A	-2.07	118.00	123.33
16	A	829	CLA	CHA-C4D-ND	2.07	136.82	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	846	BCR	C3-C4-C5	-2.07	110.36	114.06
16	1	603	CLA	O1D-CGD-CBD	2.07	128.60	124.52
17	3	214	ZEX	C4-C5-C6	-2.07	116.50	120.76
16	A	813	CLA	CHA-C1A-NA	-2.07	121.70	126.39
16	A	850	CLA	CMC-C2C-C1C	-2.07	121.80	125.03
16	A	829	CLA	C3A-C2A-C1A	2.07	104.44	101.34
16	A	803	CLA	C2A-C1A-CHA	2.07	127.46	123.87
22	F	804	BCR	C20-C21-C22	-2.07	124.38	127.28
16	A	806	CLA	CAC-C3C-C4C	2.07	127.48	124.79
16	O	204	CLA	CHA-C1A-NA	-2.07	121.71	126.39
16	A	813	CLA	C2D-C1D-ND	-2.07	108.08	110.13
16	3	211	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
16	F	802	CLA	CHA-C1A-NA	-2.07	121.71	126.39
16	A	819	CLA	C2A-C1A-CHA	2.07	127.45	123.87
16	B	811	CLA	CHA-C1A-NA	-2.07	121.71	126.39
16	A	824	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
16	1	604	CLA	C2A-C1A-CHA	2.06	127.45	123.87
16	A	835	CLA	O2D-CGD-CBD	2.06	114.84	111.23
16	B	804	CLA	C2A-C1A-CHA	2.06	127.45	123.87
16	B	801	CLA	C2A-C3A-C4A	2.06	105.20	101.87
16	A	829	CLA	CHA-C1A-NA	-2.06	121.72	126.39
16	A	834	CLA	CMB-C2B-C3B	2.06	131.40	126.55
16	B	819	CLA	C1D-ND-C4D	2.06	107.76	106.31
16	A	829	CLA	CHC-C1C-C2C	-2.06	121.09	126.95
22	A	845	BCR	C21-C20-C19	-2.06	117.23	123.20
16	B	821	CLA	C2A-C1A-CHA	2.06	127.44	123.87
22	A	846	BCR	C7-C8-C9	-2.06	123.19	126.23
17	1	616	ZEX	C31-C32-C33	-2.06	120.73	126.36
16	B	841	CLA	CHC-C4B-NB	2.06	127.13	124.05
20	B	843	PQN	C2M-C2-C3	-2.06	121.07	124.45
22	I	101	BCR	C2-C1-C6	2.05	113.42	110.44
17	3	216	ZEX	C7-C8-C9	-2.05	123.20	126.23
22	F	804	BCR	C1-C6-C5	-2.05	119.83	122.64
16	A	818	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	B	841	CLA	C2A-C1A-CHA	2.05	127.43	123.87
16	A	806	CLA	C3A-C2A-C1A	2.05	104.41	101.34
16	B	840	CLA	C3A-C2A-C1A	2.05	104.41	101.34
16	2	610	CLA	C2A-C1A-CHA	2.05	127.43	123.87
16	A	802	CLA	C1-C2-C3	-2.05	122.84	126.20
22	A	844	BCR	C28-C27-C26	-2.05	110.40	114.06
17	2	614	ZEX	C17-C1-C6	-2.05	107.03	110.24
22	J	102	BCR	C33-C5-C6	-2.05	122.25	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	834	CLA	O2D-CGD-CBD	2.05	114.81	111.23
16	B	813	CLA	CMB-C2B-C3B	2.05	128.98	123.53
16	B	831	CLA	C2A-C1A-CHA	2.05	127.42	123.87
16	A	813	CLA	O2D-CGD-CBD	2.05	114.81	111.23
16	1	606	CLA	CHA-C1A-NA	-2.05	121.75	126.39
16	B	808	CLA	C2A-C1A-CHA	2.05	127.42	123.87
16	B	827	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
22	B	849	BCR	C29-C30-C25	2.05	113.41	110.44
16	B	808	CLA	CMA-C3A-C4A	-2.05	106.28	111.77
16	2	606	CLA	O2A-CGA-O1A	-2.04	118.07	123.33
22	B	849	BCR	C27-C26-C25	2.04	125.47	122.70
16	A	833	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
16	3	205	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
16	3	205	CLA	CHB-C1B-NB	2.04	127.11	124.05
19	A	801	CL0	C4-C3-C5	2.04	118.77	115.23
16	B	819	CLA	O2D-CGD-CBD	2.04	114.80	111.23
16	A	810	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
16	B	838	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	1	606	CLA	CAC-C3C-C4C	2.04	127.45	124.79
16	1	612	CLA	O2A-CGA-O1A	-2.04	118.08	123.33
16	1	610	CLA	C3A-C2A-C1A	2.04	104.40	101.34
22	L	206	BCR	C7-C8-C9	-2.04	123.22	126.23
16	1	611	CLA	C2A-C1A-CHA	2.04	127.41	123.87
16	A	839	CLA	O2D-CGD-CBD	2.04	114.79	111.23
16	A	826	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	3	209	CLA	C1-C2-C3	-2.04	122.86	126.20
16	2	606	CLA	C2A-C1A-CHA	2.04	127.40	123.87
16	3	208	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
16	B	813	CLA	C3B-C4B-NB	-2.04	108.22	110.33
16	A	834	CLA	C2A-C1A-CHA	2.04	127.40	123.87
16	B	806	CLA	O1D-CGD-CBD	2.03	128.53	124.52
16	A	836	CLA	C1-C2-C3	-2.03	122.87	126.20
16	B	818	CLA	C2A-C1A-CHA	2.03	127.39	123.87
16	A	828	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	A	828	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
22	B	845	BCR	C33-C5-C6	-2.03	122.27	124.48
16	A	816	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
16	B	819	CLA	CHA-C4D-ND	2.03	136.74	132.55
16	B	805	CLA	CMD-C2D-C3D	2.03	132.34	127.69
22	B	847	BCR	C38-C26-C27	-2.03	109.27	113.60
16	B	831	CLA	CMC-C2C-C3C	2.03	131.63	126.15
22	B	845	BCR	C11-C10-C9	-2.03	124.44	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	826	CLA	C2A-C1A-CHA	2.03	127.38	123.87
16	B	807	CLA	C11-C12-C13	-2.03	109.23	115.97
16	2	607	CLA	C2A-C1A-CHA	2.02	127.38	123.87
16	B	835	CLA	CMA-C3A-C4A	-2.02	106.34	111.77
16	A	818	CLA	CMB-C2B-C3B	2.02	131.31	126.55
16	B	841	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	A	824	CLA	C11-C10-C8	-2.02	109.25	115.97
16	A	829	CLA	CMD-C2D-C3D	2.02	132.32	127.69
16	A	852	CLA	O2D-CGD-CBD	2.02	114.76	111.23
16	3	211	CLA	C2A-C1A-CHA	2.02	127.37	123.87
16	A	814	CLA	C3B-C4B-NB	-2.02	108.73	110.53
16	2	604	CLA	C2A-C1A-CHA	2.02	127.37	123.87
16	A	826	CLA	C2A-C1A-CHA	2.02	127.37	123.87
16	A	803	CLA	C1-C2-C3	-2.02	122.89	126.20
16	A	837	CLA	C1-C2-C3	-2.02	122.89	126.20
16	B	832	CLA	CAC-C3C-C4C	2.02	127.42	124.79
16	O	201	CLA	CHB-C1B-NB	2.02	127.07	124.05
16	B	824	CLA	C2A-C1A-CHA	2.01	127.36	123.87
16	B	838	CLA	OBD-CAD-C3D	2.01	133.12	128.42
16	2	604	CLA	O1D-CGD-CBD	2.01	128.48	124.52
16	A	812	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
16	B	812	CLA	C2A-C1A-CHA	2.01	127.35	123.87
16	A	837	CLA	C3A-C2A-C1A	2.01	104.35	101.34
16	O	203	CLA	CHA-C1A-NA	-2.01	121.84	126.39
16	K	101	CLA	C2A-C1A-CHA	2.01	127.35	123.87
16	A	828	CLA	CHA-C1A-NA	-2.01	121.84	126.39
16	B	826	CLA	O1D-CGD-CBD	2.01	128.48	124.52
16	B	809	CLA	O2D-CGD-CBD	2.01	114.74	111.23
16	B	823	CLA	C2A-C1A-CHA	2.01	127.35	123.87
16	B	831	CLA	C3A-C2A-C1A	2.01	104.34	101.34
16	A	812	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
16	B	833	CLA	C2A-C1A-CHA	2.01	127.35	123.87
16	A	828	CLA	O2D-CGD-CBD	2.00	114.73	111.23
16	B	834	CLA	CHC-C1C-NC	2.00	127.33	124.31
16	A	852	CLA	CMB-C2B-C3B	2.00	131.26	126.55
16	B	842	CLA	C2A-C1A-CHA	2.00	127.34	123.87
17	3	201	ZEX	C7-C6-C5	-2.00	116.94	121.56
16	A	833	CLA	CHD-C1D-ND	-2.00	121.99	124.80
16	A	815	CLA	O2A-CGA-O1A	-2.00	118.19	123.33
16	A	838	CLA	O2D-CGD-CBD	2.00	114.73	111.23

All (136) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	1	601	CLA	ND
16	1	602	CLA	ND
16	1	603	CLA	ND
16	1	604	CLA	ND
16	1	605	CLA	ND
16	1	606	CLA	ND
16	1	607	CLA	ND
16	1	608	CLA	ND
16	1	609	CLA	ND
16	1	610	CLA	ND
16	1	611	CLA	ND
16	1	612	CLA	ND
16	2	601	CLA	ND
16	2	602	CLA	ND
16	2	603	CLA	ND
16	2	604	CLA	ND
16	2	605	CLA	ND
16	2	606	CLA	ND
16	2	607	CLA	ND
16	2	608	CLA	ND
16	2	609	CLA	ND
16	2	610	CLA	ND
16	2	611	CLA	ND
16	2	612	CLA	ND
16	2	613	CLA	ND
16	3	202	CLA	ND
16	3	203	CLA	ND
16	3	204	CLA	ND
16	3	205	CLA	ND
16	3	206	CLA	ND
16	3	207	CLA	ND
16	3	208	CLA	ND
16	3	209	CLA	ND
16	3	210	CLA	ND
16	3	211	CLA	ND
16	3	212	CLA	ND
16	3	213	CLA	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

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Mol	Chain	Res	Type	Atom
16	A	808	CLA	ND
16	A	809	CLA	ND
16	A	810	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	817	CLA	ND
16	A	818	CLA	ND
16	A	819	CLA	ND
16	A	820	CLA	ND
16	A	821	CLA	ND
16	A	822	CLA	ND
16	A	823	CLA	ND
16	A	824	CLA	ND
16	A	825	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	832	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	850	CLA	ND
16	A	851	CLA	ND
16	A	852	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
16	B	806	CLA	ND
16	B	807	CLA	ND

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Mol	Chain	Res	Type	Atom
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	815	CLA	ND
16	B	816	CLA	ND
16	B	817	CLA	ND
16	B	818	CLA	ND
16	B	819	CLA	ND
16	B	820	CLA	ND
16	B	821	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	B	841	CLA	ND
16	B	842	CLA	ND
16	F	802	CLA	ND
16	F	803	CLA	ND
16	J	101	CLA	ND
16	K	101	CLA	ND
16	K	102	CLA	ND
16	L	201	CLA	ND
16	L	203	CLA	ND

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Mol	Chain	Res	Type	Atom
16	L	204	CLA	ND
16	L	205	CLA	ND
16	O	201	CLA	ND
16	O	202	CLA	ND
16	O	203	CLA	ND
16	O	204	CLA	ND
19	A	801	CL0	NA
19	A	801	CL0	ND
19	A	801	CL0	NC

All (2070) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	601	CLA	C2B-C3B-CAB-CBB
16	1	601	CLA	C4B-C3B-CAB-CBB
16	1	601	CLA	CBD-CGD-O2D-CED
16	1	602	CLA	CBD-CGD-O2D-CED
16	1	603	CLA	C4B-C3B-CAB-CBB
16	1	603	CLA	CBD-CGD-O2D-CED
16	1	604	CLA	C1A-C2A-CAA-CBA
16	1	604	CLA	CBD-CGD-O2D-CED
16	1	605	CLA	C2B-C3B-CAB-CBB
16	1	605	CLA	C4B-C3B-CAB-CBB
16	1	606	CLA	CBD-CGD-O2D-CED
16	1	607	CLA	C2B-C3B-CAB-CBB
16	1	607	CLA	C4B-C3B-CAB-CBB
16	1	607	CLA	CHA-CBD-CGD-O1D
16	1	607	CLA	CHA-CBD-CGD-O2D
16	1	608	CLA	CBD-CGD-O2D-CED
16	1	610	CLA	C4B-C3B-CAB-CBB
16	1	611	CLA	C1A-C2A-CAA-CBA
16	1	611	CLA	C3A-C2A-CAA-CBA
16	1	612	CLA	C2B-C3B-CAB-CBB
16	1	612	CLA	C4B-C3B-CAB-CBB
16	1	612	CLA	CHA-CBD-CGD-O2D
16	2	601	CLA	C2B-C3B-CAB-CBB
16	2	601	CLA	C4B-C3B-CAB-CBB
16	2	602	CLA	CAD-CBD-CGD-O2D
16	2	603	CLA	CHA-CBD-CGD-O1D
16	2	603	CLA	CHA-CBD-CGD-O2D
16	2	604	CLA	C1A-C2A-CAA-CBA
16	2	605	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	2	605	CLA	C4B-C3B-CAB-CBB
16	2	606	CLA	C1A-C2A-CAA-CBA
16	2	606	CLA	C3A-C2A-CAA-CBA
16	2	606	CLA	C2B-C3B-CAB-CBB
16	2	606	CLA	C4B-C3B-CAB-CBB
16	2	607	CLA	C1A-C2A-CAA-CBA
16	2	607	CLA	C3A-C2A-CAA-CBA
16	2	607	CLA	C2B-C3B-CAB-CBB
16	2	607	CLA	C4B-C3B-CAB-CBB
16	2	607	CLA	CBD-CGD-O2D-CED
16	2	609	CLA	CHA-CBD-CGD-O1D
16	2	609	CLA	CHA-CBD-CGD-O2D
16	2	610	CLA	C3A-C2A-CAA-CBA
16	2	610	CLA	CBD-CGD-O2D-CED
16	2	611	CLA	C2B-C3B-CAB-CBB
16	2	611	CLA	C4B-C3B-CAB-CBB
16	2	611	CLA	CBD-CGD-O2D-CED
16	2	612	CLA	C2B-C3B-CAB-CBB
16	2	612	CLA	C4B-C3B-CAB-CBB
16	2	612	CLA	CHA-CBD-CGD-O1D
16	2	612	CLA	CHA-CBD-CGD-O2D
16	2	613	CLA	C4B-C3B-CAB-CBB
16	3	202	CLA	C4B-C3B-CAB-CBB
16	3	202	CLA	CBD-CGD-O2D-CED
16	3	204	CLA	CAD-CBD-CGD-O1D
16	3	204	CLA	CAD-CBD-CGD-O2D
16	3	206	CLA	CHA-CBD-CGD-O1D
16	3	206	CLA	CHA-CBD-CGD-O2D
16	3	207	CLA	CBD-CGD-O2D-CED
16	3	207	CLA	O1D-CGD-O2D-CED
16	3	208	CLA	C1A-C2A-CAA-CBA
16	3	208	CLA	C3A-C2A-CAA-CBA
16	3	208	CLA	C4B-C3B-CAB-CBB
16	3	209	CLA	CBD-CGD-O2D-CED
16	3	210	CLA	C2B-C3B-CAB-CBB
16	3	210	CLA	C4B-C3B-CAB-CBB
16	3	211	CLA	C2B-C3B-CAB-CBB
16	3	211	CLA	C4B-C3B-CAB-CBB
16	3	212	CLA	C1A-C2A-CAA-CBA
16	3	212	CLA	C3A-C2A-CAA-CBA
16	3	212	CLA	CBA-CGA-O2A-C1
16	3	212	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	3	212	CLA	C2B-C3B-CAB-CBB
16	3	212	CLA	C4B-C3B-CAB-CBB
16	3	212	CLA	CBD-CGD-O2D-CED
16	3	212	CLA	O1D-CGD-O2D-CED
16	3	213	CLA	CHA-CBD-CGD-O1D
16	3	213	CLA	CHA-CBD-CGD-O2D
16	A	802	CLA	CAD-CBD-CGD-O1D
16	A	802	CLA	CAD-CBD-CGD-O2D
16	A	803	CLA	CHA-CBD-CGD-O1D
16	A	803	CLA	CHA-CBD-CGD-O2D
16	A	805	CLA	C1A-C2A-CAA-CBA
16	A	806	CLA	CAD-CBD-CGD-O1D
16	A	806	CLA	CAD-CBD-CGD-O2D
16	A	806	CLA	CBD-CGD-O2D-CED
16	A	807	CLA	C3A-C2A-CAA-CBA
16	A	807	CLA	CHA-CBD-CGD-O1D
16	A	807	CLA	CHA-CBD-CGD-O2D
16	A	808	CLA	CAD-CBD-CGD-O1D
16	A	808	CLA	CAD-CBD-CGD-O2D
16	A	809	CLA	CBD-CGD-O2D-CED
16	A	809	CLA	O1D-CGD-O2D-CED
16	A	811	CLA	C1A-C2A-CAA-CBA
16	A	811	CLA	C3A-C2A-CAA-CBA
16	A	812	CLA	CBD-CGD-O2D-CED
16	A	813	CLA	CHA-CBD-CGD-O1D
16	A	813	CLA	CHA-CBD-CGD-O2D
16	A	814	CLA	CBD-CGD-O2D-CED
16	A	815	CLA	C2B-C3B-CAB-CBB
16	A	815	CLA	C4B-C3B-CAB-CBB
16	A	817	CLA	C3A-C2A-CAA-CBA
16	A	818	CLA	C1A-C2A-CAA-CBA
16	A	818	CLA	C3A-C2A-CAA-CBA
16	A	819	CLA	C1A-C2A-CAA-CBA
16	A	819	CLA	C2B-C3B-CAB-CBB
16	A	819	CLA	C4B-C3B-CAB-CBB
16	A	819	CLA	CAD-CBD-CGD-O1D
16	A	819	CLA	CAD-CBD-CGD-O2D
16	A	821	CLA	C2B-C3B-CAB-CBB
16	A	821	CLA	C4B-C3B-CAB-CBB
16	A	821	CLA	CHA-CBD-CGD-O1D
16	A	821	CLA	CHA-CBD-CGD-O2D
16	A	822	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	A	822	CLA	CBD-CGD-O2D-CED
16	A	824	CLA	C1A-C2A-CAA-CBA
16	A	824	CLA	C3A-C2A-CAA-CBA
16	A	824	CLA	CHA-CBD-CGD-O2D
16	A	824	CLA	CBD-CGD-O2D-CED
16	A	825	CLA	C4B-C3B-CAB-CBB
16	A	827	CLA	C1A-C2A-CAA-CBA
16	A	827	CLA	C4B-C3B-CAB-CBB
16	A	828	CLA	C1A-C2A-CAA-CBA
16	A	829	CLA	CHA-CBD-CGD-O1D
16	A	829	CLA	CHA-CBD-CGD-O2D
16	A	830	CLA	C2B-C3B-CAB-CBB
16	A	830	CLA	C4B-C3B-CAB-CBB
16	A	831	CLA	C1A-C2A-CAA-CBA
16	A	831	CLA	C3A-C2A-CAA-CBA
16	A	832	CLA	C2B-C3B-CAB-CBB
16	A	832	CLA	C4B-C3B-CAB-CBB
16	A	832	CLA	CHA-CBD-CGD-O1D
16	A	832	CLA	CHA-CBD-CGD-O2D
16	A	834	CLA	C1A-C2A-CAA-CBA
16	A	835	CLA	CAD-CBD-CGD-O1D
16	A	835	CLA	CAD-CBD-CGD-O2D
16	A	838	CLA	C4B-C3B-CAB-CBB
16	A	839	CLA	C2-C1-O2A-CGA
16	A	850	CLA	CBD-CGD-O2D-CED
16	A	852	CLA	CBD-CGD-O2D-CED
16	A	852	CLA	C6-C7-C8-C9
16	B	802	CLA	C2B-C3B-CAB-CBB
16	B	802	CLA	C4B-C3B-CAB-CBB
16	B	803	CLA	C2B-C3B-CAB-CBB
16	B	803	CLA	C4B-C3B-CAB-CBB
16	B	804	CLA	C4B-C3B-CAB-CBB
16	B	804	CLA	CBD-CGD-O2D-CED
16	B	805	CLA	C4B-C3B-CAB-CBB
16	B	805	CLA	CBD-CGD-O2D-CED
16	B	807	CLA	C1A-C2A-CAA-CBA
16	B	807	CLA	C3A-C2A-CAA-CBA
16	B	807	CLA	CHA-CBD-CGD-O1D
16	B	807	CLA	CHA-CBD-CGD-O2D
16	B	808	CLA	C2B-C3B-CAB-CBB
16	B	808	CLA	C4B-C3B-CAB-CBB
16	B	808	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	B	809	CLA	C2B-C3B-CAB-CBB
16	B	809	CLA	C4B-C3B-CAB-CBB
16	B	810	CLA	C2B-C3B-CAB-CBB
16	B	810	CLA	C4B-C3B-CAB-CBB
16	B	810	CLA	CHA-CBD-CGD-O2D
16	B	811	CLA	CBD-CGD-O2D-CED
16	B	811	CLA	O1D-CGD-O2D-CED
16	B	813	CLA	O1A-CGA-O2A-C1
16	B	814	CLA	C1A-C2A-CAA-CBA
16	B	814	CLA	C3A-C2A-CAA-CBA
16	B	814	CLA	CBD-CGD-O2D-CED
16	B	814	CLA	O1D-CGD-O2D-CED
16	B	816	CLA	CBD-CGD-O2D-CED
16	B	817	CLA	CBD-CGD-O2D-CED
16	B	819	CLA	C1A-C2A-CAA-CBA
16	B	819	CLA	C11-C10-C8-C9
16	B	820	CLA	C1A-C2A-CAA-CBA
16	B	820	CLA	C3A-C2A-CAA-CBA
16	B	821	CLA	C4B-C3B-CAB-CBB
16	B	822	CLA	C2B-C3B-CAB-CBB
16	B	822	CLA	C4B-C3B-CAB-CBB
16	B	823	CLA	C4B-C3B-CAB-CBB
16	B	823	CLA	CBD-CGD-O2D-CED
16	B	824	CLA	C2B-C3B-CAB-CBB
16	B	824	CLA	C4B-C3B-CAB-CBB
16	B	824	CLA	CBD-CGD-O2D-CED
16	B	825	CLA	CBD-CGD-O2D-CED
16	B	826	CLA	C4B-C3B-CAB-CBB
16	B	826	CLA	CHA-CBD-CGD-O1D
16	B	826	CLA	CHA-CBD-CGD-O2D
16	B	828	CLA	CAD-CBD-CGD-O1D
16	B	828	CLA	CAD-CBD-CGD-O2D
16	B	829	CLA	C11-C10-C8-C9
16	B	830	CLA	C1A-C2A-CAA-CBA
16	B	830	CLA	C3A-C2A-CAA-CBA
16	B	831	CLA	CBD-CGD-O2D-CED
16	B	832	CLA	C2B-C3B-CAB-CBB
16	B	832	CLA	C4B-C3B-CAB-CBB
16	B	832	CLA	CHA-CBD-CGD-O1D
16	B	832	CLA	CHA-CBD-CGD-O2D
16	B	834	CLA	C2B-C3B-CAB-CBB
16	B	834	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	B	834	CLA	CHA-CBD-CGD-O1D
16	B	834	CLA	CHA-CBD-CGD-O2D
16	B	835	CLA	CBD-CGD-O2D-CED
16	B	836	CLA	C1A-C2A-CAA-CBA
16	B	836	CLA	C3A-C2A-CAA-CBA
16	B	836	CLA	C2B-C3B-CAB-CBB
16	B	836	CLA	C4B-C3B-CAB-CBB
16	B	836	CLA	CBD-CGD-O2D-CED
16	B	836	CLA	O1D-CGD-O2D-CED
16	B	837	CLA	C2B-C3B-CAB-CBB
16	B	837	CLA	C4B-C3B-CAB-CBB
16	B	837	CLA	CAD-CBD-CGD-O1D
16	B	837	CLA	CAD-CBD-CGD-O2D
16	B	838	CLA	C2B-C3B-CAB-CBB
16	B	838	CLA	C4B-C3B-CAB-CBB
16	B	841	CLA	C2B-C3B-CAB-CBB
16	B	841	CLA	C4B-C3B-CAB-CBB
16	B	841	CLA	CAD-CBD-CGD-O1D
16	B	841	CLA	CAD-CBD-CGD-O2D
16	B	841	CLA	CBD-CGD-O2D-CED
16	B	842	CLA	C4B-C3B-CAB-CBB
16	J	101	CLA	C1A-C2A-CAA-CBA
16	J	101	CLA	C3A-C2A-CAA-CBA
16	J	101	CLA	C2B-C3B-CAB-CBB
16	J	101	CLA	C4B-C3B-CAB-CBB
16	J	101	CLA	CAD-CBD-CGD-O2D
16	J	101	CLA	CBD-CGD-O2D-CED
16	K	101	CLA	C2B-C3B-CAB-CBB
16	K	101	CLA	C4B-C3B-CAB-CBB
16	K	102	CLA	C2B-C3B-CAB-CBB
16	K	102	CLA	C4B-C3B-CAB-CBB
16	L	203	CLA	C2B-C3B-CAB-CBB
16	L	203	CLA	C4B-C3B-CAB-CBB
16	L	203	CLA	CAD-CBD-CGD-O1D
16	L	203	CLA	CAD-CBD-CGD-O2D
16	L	203	CLA	CBD-CGD-O2D-CED
16	L	205	CLA	CBD-CGD-O2D-CED
16	O	201	CLA	CBD-CGD-O2D-CED
16	O	202	CLA	C4B-C3B-CAB-CBB
17	1	613	ZEX	C5-C6-C7-C8
17	1	613	ZEX	C25-C26-C27-C28
17	1	613	ZEX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
17	1	613	ZEX	C20-C13-C14-C15
17	1	613	ZEX	C40-C33-C34-C35
17	1	613	ZEX	C39-C29-C30-C31
17	1	614	ZEX	C5-C6-C7-C8
17	1	614	ZEX	C25-C26-C27-C28
17	1	614	ZEX	C11-C10-C9-C19
17	1	614	ZEX	C12-C13-C14-C15
17	1	614	ZEX	C33-C34-C35-C15
17	1	614	ZEX	C40-C33-C34-C35
17	1	614	ZEX	C31-C32-C33-C40
17	1	614	ZEX	C29-C30-C31-C32
17	1	614	ZEX	C39-C29-C30-C31
17	1	614	ZEX	C27-C28-C29-C39
17	1	615	ZEX	C21-C26-C27-C28
17	1	615	ZEX	C25-C26-C27-C28
17	1	615	ZEX	C11-C10-C9-C19
17	1	615	ZEX	C20-C13-C14-C15
17	1	615	ZEX	C29-C30-C31-C32
17	1	615	ZEX	C39-C29-C30-C31
17	1	616	ZEX	C7-C8-C9-C19
17	1	616	ZEX	C11-C10-C9-C19
17	1	616	ZEX	C11-C12-C13-C20
17	1	616	ZEX	C20-C13-C14-C15
17	1	616	ZEX	C40-C33-C34-C35
17	1	616	ZEX	C32-C33-C34-C35
17	1	616	ZEX	C31-C32-C33-C34
17	1	616	ZEX	C31-C32-C33-C40
17	1	616	ZEX	C39-C29-C30-C31
17	1	617	ZEX	C5-C6-C7-C8
17	1	617	ZEX	C25-C26-C27-C28
17	1	617	ZEX	C7-C8-C9-C10
17	1	617	ZEX	C11-C10-C9-C19
17	1	617	ZEX	C9-C10-C11-C12
17	1	617	ZEX	C11-C12-C13-C20
17	1	617	ZEX	C11-C12-C13-C14
17	1	617	ZEX	C20-C13-C14-C15
17	1	617	ZEX	C40-C33-C34-C35
17	1	617	ZEX	C39-C29-C30-C31
17	1	617	ZEX	C27-C28-C29-C39
17	2	614	ZEX	C25-C26-C27-C28
17	2	614	ZEX	C11-C10-C9-C19
17	2	614	ZEX	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
17	2	614	ZEX	C33-C34-C35-C15
17	2	614	ZEX	C40-C33-C34-C35
17	2	614	ZEX	C29-C30-C31-C32
17	2	614	ZEX	C39-C29-C30-C31
17	2	614	ZEX	C27-C28-C29-C30
17	2	614	ZEX	C27-C28-C29-C39
17	2	615	ZEX	C25-C26-C27-C28
17	2	615	ZEX	C11-C10-C9-C19
17	2	615	ZEX	C11-C12-C13-C14
17	2	615	ZEX	C20-C13-C14-C15
17	2	615	ZEX	C40-C33-C34-C35
17	2	615	ZEX	C39-C29-C30-C31
17	2	615	ZEX	C27-C28-C29-C30
17	2	615	ZEX	C27-C28-C29-C39
17	2	616	ZEX	C25-C26-C27-C28
17	2	616	ZEX	C11-C10-C9-C19
17	2	616	ZEX	C11-C12-C13-C20
17	2	616	ZEX	C11-C12-C13-C14
17	2	616	ZEX	C20-C13-C14-C15
17	2	616	ZEX	C40-C33-C34-C35
17	2	616	ZEX	C39-C29-C30-C31
17	2	616	ZEX	C27-C28-C29-C30
17	2	616	ZEX	C27-C28-C29-C39
17	2	617	ZEX	C25-C26-C27-C28
17	2	617	ZEX	C7-C8-C9-C19
17	2	617	ZEX	C11-C10-C9-C19
17	2	617	ZEX	C11-C12-C13-C20
17	2	617	ZEX	C20-C13-C14-C15
17	2	617	ZEX	C40-C33-C34-C35
17	2	617	ZEX	C39-C29-C30-C31
17	2	617	ZEX	C27-C28-C29-C30
17	3	201	ZEX	C11-C10-C9-C8
17	3	201	ZEX	C20-C13-C14-C15
17	3	201	ZEX	C13-C14-C15-C35
17	3	201	ZEX	C40-C33-C34-C35
17	3	201	ZEX	C31-C32-C33-C40
17	3	201	ZEX	C29-C30-C31-C32
17	3	201	ZEX	C39-C29-C30-C31
17	3	201	ZEX	C27-C28-C29-C30
17	3	201	ZEX	C27-C28-C29-C39
17	3	214	ZEX	C25-C26-C27-C28
17	3	214	ZEX	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
17	3	214	ZEX	C11-C12-C13-C20
17	3	214	ZEX	C20-C13-C14-C15
17	3	214	ZEX	C40-C33-C34-C35
17	3	214	ZEX	C31-C32-C33-C34
17	3	214	ZEX	C39-C29-C30-C31
17	3	214	ZEX	C27-C28-C29-C39
17	3	215	ZEX	C5-C6-C7-C8
17	3	215	ZEX	C25-C26-C27-C28
17	3	215	ZEX	C11-C10-C9-C19
17	3	215	ZEX	C11-C12-C13-C20
17	3	215	ZEX	C20-C13-C14-C15
17	3	215	ZEX	C40-C33-C34-C35
17	3	215	ZEX	C31-C32-C33-C40
17	3	215	ZEX	C29-C30-C31-C32
17	3	215	ZEX	C39-C29-C30-C31
17	3	215	ZEX	C27-C28-C29-C39
17	3	216	ZEX	C25-C26-C27-C28
17	3	216	ZEX	C11-C10-C9-C19
17	3	216	ZEX	C20-C13-C14-C15
17	3	216	ZEX	C33-C34-C35-C15
17	3	216	ZEX	C40-C33-C34-C35
17	3	216	ZEX	C39-C29-C30-C31
17	3	216	ZEX	C28-C29-C30-C31
17	3	217	ZEX	C25-C26-C27-C28
17	3	217	ZEX	C7-C8-C9-C10
17	3	217	ZEX	C11-C10-C9-C19
17	3	217	ZEX	C11-C12-C13-C20
17	3	217	ZEX	C20-C13-C14-C15
17	3	217	ZEX	C13-C14-C15-C35
17	3	217	ZEX	C40-C33-C34-C35
17	3	217	ZEX	C32-C33-C34-C35
17	3	217	ZEX	C31-C32-C33-C34
17	3	217	ZEX	C28-C29-C30-C31
17	3	217	ZEX	C27-C28-C29-C39
17	3	218	ZEX	C5-C6-C7-C8
17	3	218	ZEX	C7-C8-C9-C19
17	3	218	ZEX	C7-C8-C9-C10
17	3	218	ZEX	C11-C10-C9-C8
17	3	218	ZEX	C11-C12-C13-C20
17	3	218	ZEX	C20-C13-C14-C15
17	3	218	ZEX	C32-C33-C34-C35
17	3	218	ZEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
17	3	218	ZEX	C28-C29-C30-C31
17	3	218	ZEX	C27-C28-C29-C30
21	A	841	LHG	C1-C2-C3-O3
21	A	841	LHG	C3-O3-P-O6
21	A	841	LHG	C4-O6-P-O5
21	A	842	LHG	O1-C1-C2-O2
21	A	842	LHG	O1-C1-C2-C3
22	A	843	BCR	C6-C7-C8-C9
22	A	843	BCR	C7-C8-C9-C34
22	A	843	BCR	C14-C15-C16-C17
22	A	843	BCR	C22-C23-C24-C25
22	A	844	BCR	C6-C7-C8-C9
22	A	844	BCR	C7-C8-C9-C34
22	A	844	BCR	C12-C13-C14-C15
22	A	844	BCR	C35-C13-C14-C15
22	A	844	BCR	C14-C15-C16-C17
22	A	844	BCR	C20-C21-C22-C23
22	A	844	BCR	C20-C21-C22-C37
22	A	844	BCR	C21-C22-C23-C24
22	A	844	BCR	C22-C23-C24-C25
22	A	845	BCR	C6-C7-C8-C9
22	A	845	BCR	C7-C8-C9-C34
22	A	845	BCR	C20-C21-C22-C37
22	A	845	BCR	C21-C22-C23-C24
22	A	845	BCR	C22-C23-C24-C25
22	A	846	BCR	C18-C19-C20-C21
22	A	846	BCR	C20-C21-C22-C23
22	A	846	BCR	C22-C23-C24-C25
22	A	847	BCR	C6-C7-C8-C9
22	A	847	BCR	C7-C8-C9-C10
22	A	847	BCR	C12-C13-C14-C15
22	A	847	BCR	C18-C19-C20-C21
22	A	847	BCR	C20-C21-C22-C23
22	A	847	BCR	C20-C21-C22-C37
22	A	847	BCR	C22-C23-C24-C25
22	A	849	BCR	C7-C8-C9-C34
22	A	849	BCR	C22-C23-C24-C25
22	B	844	BCR	C6-C7-C8-C9
22	B	844	BCR	C7-C8-C9-C10
22	B	844	BCR	C20-C21-C22-C37
22	B	844	BCR	C22-C23-C24-C25
22	B	845	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
22	B	846	BCR	C6-C7-C8-C9
22	B	846	BCR	C7-C8-C9-C10
22	B	846	BCR	C7-C8-C9-C34
22	B	846	BCR	C10-C11-C12-C13
22	B	846	BCR	C16-C17-C18-C19
22	B	846	BCR	C16-C17-C18-C36
22	B	846	BCR	C18-C19-C20-C21
22	B	846	BCR	C21-C22-C23-C24
22	B	847	BCR	C6-C7-C8-C9
22	B	847	BCR	C7-C8-C9-C34
22	B	847	BCR	C11-C12-C13-C35
22	B	847	BCR	C21-C22-C23-C24
22	B	847	BCR	C22-C23-C24-C25
22	B	848	BCR	C6-C7-C8-C9
22	B	848	BCR	C7-C8-C9-C34
22	B	848	BCR	C10-C11-C12-C13
22	B	848	BCR	C11-C12-C13-C35
22	B	848	BCR	C16-C17-C18-C19
22	B	848	BCR	C16-C17-C18-C36
22	B	848	BCR	C36-C18-C19-C20
22	B	848	BCR	C18-C19-C20-C21
22	B	848	BCR	C22-C23-C24-C25
22	B	848	BCR	C23-C24-C25-C26
22	B	848	BCR	C23-C24-C25-C30
22	B	849	BCR	C10-C11-C12-C13
22	B	849	BCR	C14-C15-C16-C17
22	B	849	BCR	C37-C22-C23-C24
22	F	801	BCR	C20-C21-C22-C37
22	F	801	BCR	C21-C22-C23-C24
22	F	801	BCR	C22-C23-C24-C25
22	F	804	BCR	C6-C7-C8-C9
22	F	804	BCR	C11-C12-C13-C14
22	F	804	BCR	C35-C13-C14-C15
22	F	804	BCR	C13-C14-C15-C16
22	F	804	BCR	C14-C15-C16-C17
22	F	804	BCR	C18-C19-C20-C21
22	F	804	BCR	C21-C22-C23-C24
22	F	804	BCR	C22-C23-C24-C25
22	I	101	BCR	C6-C7-C8-C9
22	I	101	BCR	C20-C21-C22-C37
22	I	101	BCR	C22-C23-C24-C25
22	J	102	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	J	102	BCR	C7-C8-C9-C34
22	J	102	BCR	C16-C17-C18-C36
22	J	102	BCR	C18-C19-C20-C21
22	J	102	BCR	C22-C23-C24-C25
22	J	103	BCR	C6-C7-C8-C9
22	J	103	BCR	C14-C15-C16-C17
22	J	103	BCR	C16-C17-C18-C19
22	J	103	BCR	C16-C17-C18-C36
22	J	103	BCR	C21-C22-C23-C24
22	J	103	BCR	C22-C23-C24-C25
22	K	103	BCR	C6-C7-C8-C9
22	K	103	BCR	C16-C17-C18-C19
22	K	103	BCR	C16-C17-C18-C36
22	K	103	BCR	C20-C21-C22-C37
22	K	103	BCR	C22-C23-C24-C25
22	L	202	BCR	C6-C7-C8-C9
22	L	202	BCR	C11-C10-C9-C8
22	L	202	BCR	C14-C15-C16-C17
22	L	202	BCR	C15-C16-C17-C18
22	L	202	BCR	C16-C17-C18-C36
22	L	202	BCR	C17-C18-C19-C20
22	L	202	BCR	C18-C19-C20-C21
22	L	202	BCR	C37-C22-C23-C24
22	L	202	BCR	C22-C23-C24-C25
22	L	206	BCR	C7-C8-C9-C10
22	L	206	BCR	C11-C12-C13-C14
22	L	206	BCR	C17-C18-C19-C20
22	L	206	BCR	C19-C20-C21-C22
22	L	206	BCR	C37-C22-C23-C24
22	L	206	BCR	C22-C23-C24-C25
22	L	206	BCR	C23-C24-C25-C26
22	L	206	BCR	C23-C24-C25-C30
22	L	207	BCR	C11-C10-C9-C8
22	L	207	BCR	C10-C11-C12-C13
22	L	207	BCR	C22-C23-C24-C25
25	B	850	DGD	C2B-C1B-O2G-C2G
25	B	850	DGD	O1B-C1B-O2G-C2G
26	J	104	3XQ	O20-C21-C22-O23
16	1	606	CLA	O1D-CGD-O2D-CED
16	2	605	CLA	O1D-CGD-O2D-CED
16	2	606	CLA	O1D-CGD-O2D-CED
16	2	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	2	611	CLA	O1D-CGD-O2D-CED
16	3	213	CLA	O1D-CGD-O2D-CED
16	A	814	CLA	O1D-CGD-O2D-CED
16	A	850	CLA	O1D-CGD-O2D-CED
16	A	852	CLA	O1D-CGD-O2D-CED
16	B	802	CLA	O1D-CGD-O2D-CED
16	B	807	CLA	O1D-CGD-O2D-CED
16	B	808	CLA	O1D-CGD-O2D-CED
16	B	822	CLA	O1D-CGD-O2D-CED
16	B	824	CLA	O1D-CGD-O2D-CED
16	B	831	CLA	O1D-CGD-O2D-CED
16	B	835	CLA	O1D-CGD-O2D-CED
16	F	803	CLA	O1D-CGD-O2D-CED
16	L	205	CLA	O1D-CGD-O2D-CED
16	A	850	CLA	C2C-C3C-CAC-CBC
16	1	608	CLA	O1D-CGD-O2D-CED
16	2	610	CLA	O1D-CGD-O2D-CED
16	3	204	CLA	O1D-CGD-O2D-CED
16	3	209	CLA	O1D-CGD-O2D-CED
16	A	822	CLA	O1D-CGD-O2D-CED
16	B	805	CLA	O1D-CGD-O2D-CED
16	O	204	CLA	O1D-CGD-O2D-CED
16	1	610	CLA	CBD-CGD-O2D-CED
16	1	611	CLA	CBD-CGD-O2D-CED
16	1	612	CLA	CBD-CGD-O2D-CED
16	2	601	CLA	CBD-CGD-O2D-CED
16	2	604	CLA	CBD-CGD-O2D-CED
16	2	605	CLA	CBD-CGD-O2D-CED
16	2	606	CLA	CBD-CGD-O2D-CED
16	2	608	CLA	CBD-CGD-O2D-CED
16	3	203	CLA	CBD-CGD-O2D-CED
16	3	204	CLA	CBD-CGD-O2D-CED
16	3	206	CLA	CBD-CGD-O2D-CED
16	3	208	CLA	CBD-CGD-O2D-CED
16	3	210	CLA	CBD-CGD-O2D-CED
16	3	213	CLA	CBD-CGD-O2D-CED
16	A	802	CLA	CBD-CGD-O2D-CED
16	A	804	CLA	CBD-CGD-O2D-CED
16	A	808	CLA	CBD-CGD-O2D-CED
16	A	815	CLA	CBD-CGD-O2D-CED
16	A	817	CLA	CBD-CGD-O2D-CED
16	A	819	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	A	820	CLA	CBD-CGD-O2D-CED
16	A	827	CLA	CBD-CGD-O2D-CED
16	A	828	CLA	CBD-CGD-O2D-CED
16	A	831	CLA	CBD-CGD-O2D-CED
16	A	832	CLA	CBD-CGD-O2D-CED
16	A	834	CLA	CBD-CGD-O2D-CED
16	B	802	CLA	CBD-CGD-O2D-CED
16	B	807	CLA	CBD-CGD-O2D-CED
16	B	818	CLA	CBD-CGD-O2D-CED
16	B	822	CLA	CBD-CGD-O2D-CED
16	B	830	CLA	CBD-CGD-O2D-CED
16	B	834	CLA	CBD-CGD-O2D-CED
16	B	838	CLA	CBD-CGD-O2D-CED
16	F	803	CLA	CBD-CGD-O2D-CED
16	L	201	CLA	CBD-CGD-O2D-CED
16	O	202	CLA	CBD-CGD-O2D-CED
16	O	203	CLA	CBD-CGD-O2D-CED
16	O	204	CLA	CBD-CGD-O2D-CED
16	A	838	CLA	O1A-CGA-O2A-C1
16	B	820	CLA	O1A-CGA-O2A-C1
16	3	202	CLA	O1D-CGD-O2D-CED
16	1	610	CLA	O1D-CGD-O2D-CED
16	1	611	CLA	O1D-CGD-O2D-CED
16	A	828	CLA	O1D-CGD-O2D-CED
16	B	830	CLA	O1D-CGD-O2D-CED
16	B	838	CLA	O1D-CGD-O2D-CED
16	O	202	CLA	O1D-CGD-O2D-CED
16	A	838	CLA	CBA-CGA-O2A-C1
16	B	820	CLA	CBA-CGA-O2A-C1
21	A	841	LHG	C24-C23-O8-C6
16	A	803	CLA	O1A-CGA-O2A-C1
16	A	808	CLA	O1A-CGA-O2A-C1
16	A	816	CLA	O1A-CGA-O2A-C1
16	A	835	CLA	O1A-CGA-O2A-C1
16	L	203	CLA	O1A-CGA-O2A-C1
26	J	104	3XQ	O19-C1-O20-C21
16	A	850	CLA	C4C-C3C-CAC-CBC
16	1	601	CLA	O1D-CGD-O2D-CED
16	1	603	CLA	O1D-CGD-O2D-CED
16	A	808	CLA	O1D-CGD-O2D-CED
16	A	820	CLA	O1D-CGD-O2D-CED
16	A	824	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	B	823	CLA	O1D-CGD-O2D-CED
16	J	101	CLA	O1D-CGD-O2D-CED
16	1	604	CLA	O1D-CGD-O2D-CED
16	A	806	CLA	O1D-CGD-O2D-CED
16	A	812	CLA	O1D-CGD-O2D-CED
16	B	804	CLA	O1D-CGD-O2D-CED
16	B	817	CLA	O1D-CGD-O2D-CED
16	B	825	CLA	O1D-CGD-O2D-CED
16	B	841	CLA	O1D-CGD-O2D-CED
16	L	203	CLA	O1D-CGD-O2D-CED
16	O	201	CLA	O1D-CGD-O2D-CED
16	1	602	CLA	O1D-CGD-O2D-CED
16	A	802	CLA	C3-C5-C6-C7
16	A	806	CLA	C3-C5-C6-C7
16	A	808	CLA	C3-C5-C6-C7
16	A	816	CLA	C3-C5-C6-C7
16	A	823	CLA	C3-C5-C6-C7
16	A	832	CLA	C3-C5-C6-C7
16	B	810	CLA	C3-C5-C6-C7
16	B	826	CLA	C3-C5-C6-C7
16	B	830	CLA	C3-C5-C6-C7
16	B	831	CLA	C3-C5-C6-C7
16	B	837	CLA	C3-C5-C6-C7
16	L	203	CLA	C3-C5-C6-C7
16	A	803	CLA	CBA-CGA-O2A-C1
16	A	816	CLA	CBA-CGA-O2A-C1
16	A	821	CLA	CBA-CGA-O2A-C1
16	A	839	CLA	CBA-CGA-O2A-C1
16	B	812	CLA	CBA-CGA-O2A-C1
16	B	813	CLA	CBA-CGA-O2A-C1
16	B	819	CLA	CBA-CGA-O2A-C1
16	L	203	CLA	CBA-CGA-O2A-C1
26	J	104	3XQ	C2-C1-O20-C21
16	1	607	CLA	CBD-CGD-O2D-CED
16	2	609	CLA	CBD-CGD-O2D-CED
16	A	807	CLA	CBD-CGD-O2D-CED
16	A	813	CLA	CBD-CGD-O2D-CED
16	B	812	CLA	CBD-CGD-O2D-CED
16	B	842	CLA	CBD-CGD-O2D-CED
16	B	816	CLA	O1D-CGD-O2D-CED
16	O	203	CLA	O1D-CGD-O2D-CED
16	B	818	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	A	836	CLA	C4-C3-C5-C6
16	B	820	CLA	C4-C3-C5-C6
16	B	825	CLA	C4-C3-C5-C6
16	B	842	CLA	C4-C3-C5-C6
16	B	820	CLA	C2-C3-C5-C6
16	B	825	CLA	C2-C3-C5-C6
16	B	823	CLA	CBA-CGA-O2A-C1
16	B	827	CLA	CBD-CGD-O2D-CED
16	B	837	CLA	CBD-CGD-O2D-CED
16	A	815	CLA	O1D-CGD-O2D-CED
16	A	827	CLA	O1D-CGD-O2D-CED
16	3	209	CLA	C3-C5-C6-C7
16	B	826	CLA	C2A-CAA-CBA-CGA
16	B	833	CLA	C2A-CAA-CBA-CGA
16	A	839	CLA	O1A-CGA-O2A-C1
16	A	826	CLA	C3-C5-C6-C7
16	B	819	CLA	C3-C5-C6-C7
16	B	820	CLA	C3-C5-C6-C7
16	B	828	CLA	C3-C5-C6-C7
16	B	834	CLA	C3-C5-C6-C7
16	A	807	CLA	CBA-CGA-O2A-C1
16	A	808	CLA	CBA-CGA-O2A-C1
16	A	810	CLA	CBA-CGA-O2A-C1
16	A	818	CLA	CBA-CGA-O2A-C1
16	A	829	CLA	CBA-CGA-O2A-C1
16	A	835	CLA	CBA-CGA-O2A-C1
16	B	818	CLA	CBA-CGA-O2A-C1
20	A	840	PQN	C11-C12-C13-C14
20	B	843	PQN	C11-C12-C13-C14
17	1	615	ZEX	C13-C14-C15-C35
17	1	616	ZEX	C9-C10-C11-C12
17	1	616	ZEX	C33-C34-C35-C15
17	2	615	ZEX	C13-C14-C15-C35
17	2	616	ZEX	C33-C34-C35-C15
17	2	617	ZEX	C9-C10-C11-C12
17	3	201	ZEX	C9-C10-C11-C12
17	3	216	ZEX	C29-C30-C31-C32
17	3	218	ZEX	C29-C30-C31-C32
22	A	843	BCR	C13-C14-C15-C16
22	A	846	BCR	C19-C20-C21-C22
22	B	844	BCR	C15-C16-C17-C18
22	B	846	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	J	102	BCR	C15-C16-C17-C18
16	A	810	CLA	O1A-CGA-O2A-C1
16	A	818	CLA	O1A-CGA-O2A-C1
16	B	818	CLA	O1A-CGA-O2A-C1
16	B	819	CLA	O1A-CGA-O2A-C1
21	A	841	LHG	O10-C23-O8-C6
16	A	804	CLA	O1D-CGD-O2D-CED
16	A	817	CLA	O1D-CGD-O2D-CED
16	3	208	CLA	O1D-CGD-O2D-CED
16	A	832	CLA	O1D-CGD-O2D-CED
16	A	837	CLA	C3-C5-C6-C7
16	A	805	CLA	CBD-CGD-O2D-CED
16	F	802	CLA	CBD-CGD-O2D-CED
21	A	841	LHG	O2-C2-C3-O3
16	1	612	CLA	O1D-CGD-O2D-CED
16	2	608	CLA	O1D-CGD-O2D-CED
16	A	831	CLA	O1D-CGD-O2D-CED
16	B	834	CLA	O1D-CGD-O2D-CED
16	A	827	CLA	CBA-CGA-O2A-C1
16	B	805	CLA	CBA-CGA-O2A-C1
16	B	825	CLA	CBA-CGA-O2A-C1
16	B	840	CLA	CBA-CGA-O2A-C1
25	B	850	DGD	O6E-C5E-C6E-O5E
16	A	821	CLA	O1A-CGA-O2A-C1
16	B	812	CLA	O1A-CGA-O2A-C1
16	2	601	CLA	O1D-CGD-O2D-CED
16	A	834	CLA	O1D-CGD-O2D-CED
16	B	815	CLA	CBD-CGD-O2D-CED
16	B	821	CLA	CBD-CGD-O2D-CED
16	B	805	CLA	O1A-CGA-O2A-C1
16	B	825	CLA	O1A-CGA-O2A-C1
16	2	604	CLA	O1D-CGD-O2D-CED
16	3	203	CLA	O1D-CGD-O2D-CED
16	A	802	CLA	O1D-CGD-O2D-CED
16	A	803	CLA	C3-C5-C6-C7
16	A	839	CLA	C3-C5-C6-C7
21	A	841	LHG	C23-C24-C25-C26
16	3	206	CLA	O1D-CGD-O2D-CED
16	L	201	CLA	O1D-CGD-O2D-CED
16	A	808	CLA	C4-C3-C5-C6
16	A	816	CLA	C4-C3-C5-C6
16	A	816	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	A	836	CLA	C2-C3-C5-C6
16	A	807	CLA	O1A-CGA-O2A-C1
16	A	829	CLA	O1A-CGA-O2A-C1
16	3	210	CLA	O1D-CGD-O2D-CED
16	A	823	CLA	CBD-CGD-O2D-CED
16	B	813	CLA	CBD-CGD-O2D-CED
16	2	612	CLA	C2A-CAA-CBA-CGA
16	A	819	CLA	O1D-CGD-O2D-CED
16	A	827	CLA	O1A-CGA-O2A-C1
16	B	840	CLA	O1A-CGA-O2A-C1
16	A	820	CLA	CBA-CGA-O2A-C1
16	O	201	CLA	CBA-CGA-O2A-C1
16	A	818	CLA	CBD-CGD-O2D-CED
16	B	833	CLA	CBD-CGD-O2D-CED
16	K	101	CLA	CBD-CGD-O2D-CED
25	B	850	DGD	C4E-C5E-C6E-O5E
16	B	823	CLA	O1A-CGA-O2A-C1
17	2	615	ZEX	C9-C10-C11-C12
17	2	615	ZEX	C29-C30-C31-C32
22	B	848	BCR	C19-C20-C21-C22
22	K	103	BCR	C13-C14-C15-C16
22	L	207	BCR	C13-C14-C15-C16
16	A	820	CLA	O1A-CGA-O2A-C1
16	A	831	CLA	CBA-CGA-O2A-C1
16	A	836	CLA	CBA-CGA-O2A-C1
16	B	804	CLA	CBA-CGA-O2A-C1
16	B	811	CLA	CBA-CGA-O2A-C1
16	A	835	CLA	CBD-CGD-O2D-CED
16	A	837	CLA	CBD-CGD-O2D-CED
16	B	806	CLA	CBD-CGD-O2D-CED
16	B	840	CLA	CBD-CGD-O2D-CED
16	A	813	CLA	O1D-CGD-O2D-CED
16	B	842	CLA	C2-C3-C5-C6
16	A	802	CLA	C6-C7-C8-C9
16	B	804	CLA	C14-C13-C15-C16
16	B	810	CLA	C14-C13-C15-C16
19	A	801	CL0	C14-C13-C15-C16
21	A	842	LHG	O2-C2-C3-O3
17	1	613	ZEX	C31-C32-C33-C40
17	1	613	ZEX	C27-C28-C29-C39
17	1	615	ZEX	C11-C12-C13-C20
17	1	616	ZEX	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
17	1	617	ZEX	C7-C8-C9-C19
17	1	617	ZEX	C31-C32-C33-C40
17	2	614	ZEX	C7-C8-C9-C19
17	2	614	ZEX	C31-C32-C33-C40
17	2	615	ZEX	C11-C12-C13-C20
17	2	615	ZEX	C31-C32-C33-C40
17	2	616	ZEX	C7-C8-C9-C19
17	3	201	ZEX	C7-C8-C9-C19
17	3	201	ZEX	C11-C12-C13-C20
17	3	214	ZEX	C7-C8-C9-C19
17	3	215	ZEX	C7-C8-C9-C19
17	3	216	ZEX	C31-C32-C33-C40
17	3	216	ZEX	C27-C28-C29-C39
17	3	217	ZEX	C7-C8-C9-C19
22	A	846	BCR	C37-C22-C23-C24
22	A	847	BCR	C37-C22-C23-C24
22	B	844	BCR	C7-C8-C9-C34
22	B	844	BCR	C36-C18-C19-C20
22	B	845	BCR	C7-C8-C9-C34
22	B	845	BCR	C37-C22-C23-C24
22	B	846	BCR	C37-C22-C23-C24
22	B	847	BCR	C37-C22-C23-C24
22	B	849	BCR	C7-C8-C9-C34
22	F	801	BCR	C11-C12-C13-C35
22	F	801	BCR	C37-C22-C23-C24
22	F	804	BCR	C7-C8-C9-C34
22	F	804	BCR	C37-C22-C23-C24
22	I	101	BCR	C11-C12-C13-C35
22	J	102	BCR	C36-C18-C19-C20
22	J	102	BCR	C37-C22-C23-C24
22	K	103	BCR	C7-C8-C9-C34
22	L	202	BCR	C36-C18-C19-C20
22	L	206	BCR	C7-C8-C9-C34
22	L	206	BCR	C36-C18-C19-C20
22	L	207	BCR	C11-C12-C13-C35
17	1	614	ZEX	C11-C12-C13-C14
17	1	614	ZEX	C31-C32-C33-C34
17	1	615	ZEX	C7-C8-C9-C10
17	1	615	ZEX	C31-C32-C33-C34
17	2	615	ZEX	C7-C8-C9-C10
17	3	215	ZEX	C7-C8-C9-C10
17	3	217	ZEX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
22	A	846	BCR	C21-C22-C23-C24
22	B	845	BCR	C21-C22-C23-C24
22	B	847	BCR	C7-C8-C9-C10
22	B	848	BCR	C21-C22-C23-C24
22	B	849	BCR	C7-C8-C9-C10
22	I	101	BCR	C7-C8-C9-C10
22	I	101	BCR	C11-C12-C13-C14
22	L	206	BCR	C21-C22-C23-C24
16	B	812	CLA	C2A-CAA-CBA-CGA
16	O	201	CLA	C3-C5-C6-C7
16	A	831	CLA	O1A-CGA-O2A-C1
16	A	836	CLA	O1A-CGA-O2A-C1
24	A	853	BGC	O5-C5-C6-O6
16	B	830	CLA	CBA-CGA-O2A-C1
16	A	802	CLA	C5-C6-C7-C8
16	B	812	CLA	O1D-CGD-O2D-CED
16	B	842	CLA	O1D-CGD-O2D-CED
16	B	810	CLA	CBD-CGD-O2D-CED
22	B	848	BCR	C14-C15-C16-C17
16	A	809	CLA	C5-C6-C7-C8
16	A	827	CLA	C10-C11-C12-C13
16	1	607	CLA	O1D-CGD-O2D-CED
16	B	811	CLA	O1A-CGA-O2A-C1
16	L	204	CLA	CBD-CGD-O2D-CED
16	B	805	CLA	C11-C12-C13-C15
17	1	613	ZEX	C9-C10-C11-C12
17	1	614	ZEX	C13-C14-C15-C35
17	2	614	ZEX	C9-C10-C11-C12
17	2	616	ZEX	C29-C30-C31-C32
17	3	217	ZEX	C29-C30-C31-C32
22	A	846	BCR	C9-C10-C11-C12
22	B	846	BCR	C15-C16-C17-C18
22	B	847	BCR	C9-C10-C11-C12
22	B	848	BCR	C9-C10-C11-C12
22	F	801	BCR	C9-C10-C11-C12
22	F	804	BCR	C19-C20-C21-C22
22	J	102	BCR	C19-C20-C21-C22
22	J	103	BCR	C19-C20-C21-C22
22	L	202	BCR	C9-C10-C11-C12
21	A	841	LHG	O9-C7-O7-C5
16	2	609	CLA	O1D-CGD-O2D-CED
16	B	833	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	A	820	CLA	C13-C15-C16-C17
16	A	829	CLA	C10-C11-C12-C13
16	B	811	CLA	C13-C15-C16-C17
16	B	814	CLA	C5-C6-C7-C8
16	B	819	CLA	C5-C6-C7-C8
16	B	835	CLA	C10-C11-C12-C13
16	2	601	CLA	C2A-CAA-CBA-CGA
16	2	605	CLA	C2A-CAA-CBA-CGA
16	2	606	CLA	C2A-CAA-CBA-CGA
16	2	613	CLA	C2A-CAA-CBA-CGA
16	A	827	CLA	C2A-CAA-CBA-CGA
16	A	828	CLA	C2A-CAA-CBA-CGA
16	A	830	CLA	C2A-CAA-CBA-CGA
16	A	839	CLA	C2A-CAA-CBA-CGA
16	B	804	CLA	C2A-CAA-CBA-CGA
16	B	818	CLA	C2A-CAA-CBA-CGA
22	A	845	BCR	C10-C11-C12-C13
22	L	207	BCR	C18-C19-C20-C21
16	A	828	CLA	C8-C10-C11-C12
16	B	803	CLA	C5-C6-C7-C8
16	B	811	CLA	C15-C16-C17-C18
16	L	204	CLA	C15-C16-C17-C18
16	F	802	CLA	O1D-CGD-O2D-CED
16	B	804	CLA	O1A-CGA-O2A-C1
16	A	807	CLA	O1D-CGD-O2D-CED
16	1	608	CLA	C10-C11-C12-C13
16	A	812	CLA	C8-C10-C11-C12
16	A	818	CLA	C13-C15-C16-C17
16	A	824	CLA	C13-C15-C16-C17
16	A	826	CLA	C15-C16-C17-C18
16	A	839	CLA	C5-C6-C7-C8
16	A	852	CLA	C8-C10-C11-C12
16	A	852	CLA	C10-C11-C12-C13
16	B	802	CLA	C5-C6-C7-C8
16	B	815	CLA	C15-C16-C17-C18
16	B	826	CLA	C15-C16-C17-C18
16	B	828	CLA	C15-C16-C17-C18
16	B	837	CLA	C10-C11-C12-C13
20	B	843	PQN	C18-C20-C21-C22
16	2	611	CLA	C2C-C3C-CAC-CBC
16	B	833	CLA	CBA-CGA-O2A-C1
19	A	801	CL0	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	O	201	CLA	O1A-CGA-O2A-C1
16	A	851	CLA	C2A-CAA-CBA-CGA
16	A	824	CLA	C15-C16-C17-C18
16	A	839	CLA	C15-C16-C17-C18
16	B	805	CLA	C15-C16-C17-C18
16	B	815	CLA	C10-C11-C12-C13
16	B	831	CLA	C8-C10-C11-C12
16	B	840	CLA	C13-C15-C16-C17
16	A	805	CLA	O1D-CGD-O2D-CED
16	A	810	CLA	C10-C11-C12-C13
16	A	812	CLA	C15-C16-C17-C18
16	B	804	CLA	C10-C11-C12-C13
16	B	828	CLA	C5-C6-C7-C8
16	B	831	CLA	C15-C16-C17-C18
20	B	843	PQN	C25-C26-C27-C28
16	B	827	CLA	O1D-CGD-O2D-CED
16	A	817	CLA	C10-C11-C12-C13
16	A	820	CLA	C8-C10-C11-C12
16	A	829	CLA	C13-C15-C16-C17
16	A	831	CLA	C15-C16-C17-C18
16	B	805	CLA	C13-C15-C16-C17
16	B	821	CLA	C5-C6-C7-C8
16	A	826	CLA	CBA-CGA-O2A-C1
21	A	841	LHG	C8-C7-O7-C5
16	B	830	CLA	O1A-CGA-O2A-C1
16	B	837	CLA	O1D-CGD-O2D-CED
16	B	821	CLA	O1D-CGD-O2D-CED
17	1	617	ZEX	C33-C34-C35-C15
22	I	101	BCR	C9-C10-C11-C12
22	L	207	BCR	C9-C10-C11-C12
16	A	837	CLA	C15-C16-C17-C18
20	B	843	PQN	C20-C21-C22-C23
16	3	203	CLA	C2A-CAA-CBA-CGA
16	B	802	CLA	C2A-CAA-CBA-CGA
16	3	203	CLA	CBA-CGA-O2A-C1
22	L	206	BCR	C14-C15-C16-C17
16	A	838	CLA	C5-C6-C7-C8
16	A	838	CLA	C15-C16-C17-C18
16	B	837	CLA	C5-C6-C7-C8
16	B	840	CLA	C8-C10-C11-C12
16	B	803	CLA	C3-C5-C6-C7
16	A	828	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	B	818	CLA	C5-C6-C7-C8
16	B	819	CLA	C8-C10-C11-C12
16	B	829	CLA	C8-C10-C11-C12
16	L	203	CLA	C5-C6-C7-C8
16	A	812	CLA	C5-C6-C7-C8
16	A	850	CLA	C10-C11-C12-C13
16	B	803	CLA	C8-C10-C11-C12
16	B	804	CLA	C13-C15-C16-C17
16	B	827	CLA	C13-C15-C16-C17
16	B	831	CLA	C10-C11-C12-C13
16	L	201	CLA	CBA-CGA-O2A-C1
16	A	808	CLA	C2-C3-C5-C6
16	B	805	CLA	C10-C11-C12-C13
20	A	840	PQN	C25-C26-C27-C28
26	J	104	3XQ	O20-C21-C22-C24
16	B	834	CLA	C5-C6-C7-C8
16	B	838	CLA	C13-C15-C16-C17
17	1	614	ZEX	C20-C13-C14-C15
17	1	615	ZEX	C40-C33-C34-C35
17	3	218	ZEX	C40-C33-C34-C35
22	A	843	BCR	C16-C17-C18-C36
22	A	845	BCR	C11-C10-C9-C34
22	A	845	BCR	C16-C17-C18-C36
22	A	846	BCR	C20-C21-C22-C37
22	A	847	BCR	C11-C10-C9-C34
22	A	847	BCR	C35-C13-C14-C15
22	B	845	BCR	C11-C10-C9-C34
22	B	848	BCR	C11-C10-C9-C34
22	B	849	BCR	C11-C10-C9-C34
22	F	804	BCR	C20-C21-C22-C37
22	L	207	BCR	C11-C10-C9-C34
22	L	207	BCR	C16-C17-C18-C36
16	A	823	CLA	O1D-CGD-O2D-CED
16	A	810	CLA	C13-C15-C16-C17
16	B	820	CLA	C10-C11-C12-C13
17	2	614	ZEX	C11-C12-C13-C20
17	2	616	ZEX	C31-C32-C33-C40
17	2	617	ZEX	C31-C32-C33-C40
17	3	216	ZEX	C11-C12-C13-C20
17	3	218	ZEX	C31-C32-C33-C40
22	A	845	BCR	C11-C12-C13-C35
22	A	846	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
22	A	849	BCR	C37-C22-C23-C24
22	B	844	BCR	C37-C22-C23-C24
22	F	801	BCR	C7-C8-C9-C34
22	I	101	BCR	C7-C8-C9-C34
16	1	605	CLA	C2A-CAA-CBA-CGA
17	1	613	ZEX	C7-C8-C9-C10
17	1	613	ZEX	C11-C12-C13-C14
17	1	613	ZEX	C27-C28-C29-C30
17	1	614	ZEX	C7-C8-C9-C10
17	1	614	ZEX	C27-C28-C29-C30
17	1	615	ZEX	C27-C28-C29-C30
17	1	616	ZEX	C7-C8-C9-C10
17	1	616	ZEX	C11-C12-C13-C14
17	1	617	ZEX	C27-C28-C29-C30
17	3	214	ZEX	C27-C28-C29-C30
17	3	216	ZEX	C7-C8-C9-C10
22	A	849	BCR	C7-C8-C9-C10
22	A	849	BCR	C21-C22-C23-C24
22	B	848	BCR	C7-C8-C9-C10
22	F	801	BCR	C7-C8-C9-C10
22	F	801	BCR	C11-C12-C13-C14
22	L	207	BCR	C11-C12-C13-C14
16	B	833	CLA	O1A-CGA-O2A-C1
16	B	815	CLA	O1D-CGD-O2D-CED
16	1	608	CLA	C2A-CAA-CBA-CGA
16	3	202	CLA	C2A-CAA-CBA-CGA
16	A	811	CLA	C2A-CAA-CBA-CGA
16	A	817	CLA	C2A-CAA-CBA-CGA
16	B	806	CLA	C2A-CAA-CBA-CGA
16	B	813	CLA	C2A-CAA-CBA-CGA
16	B	829	CLA	C2A-CAA-CBA-CGA
16	B	840	CLA	C2A-CAA-CBA-CGA
16	B	820	CLA	C5-C6-C7-C8
16	1	608	CLA	C11-C12-C13-C14
16	A	806	CLA	C16-C17-C18-C19
16	A	828	CLA	C16-C17-C18-C20
16	B	807	CLA	C16-C17-C18-C19
16	B	801	CLA	C15-C16-C17-C18
17	1	613	ZEX	C28-C29-C30-C31
17	1	615	ZEX	C32-C33-C34-C35
17	1	617	ZEX	C32-C33-C34-C35
17	2	615	ZEX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
17	2	616	ZEX	C32-C33-C34-C35
17	2	617	ZEX	C11-C10-C9-C8
17	2	617	ZEX	C28-C29-C30-C31
17	3	214	ZEX	C11-C10-C9-C8
17	3	215	ZEX	C28-C29-C30-C31
17	3	218	ZEX	C12-C13-C14-C15
22	A	843	BCR	C11-C10-C9-C8
22	A	844	BCR	C11-C10-C9-C8
22	A	844	BCR	C16-C17-C18-C19
22	A	849	BCR	C12-C13-C14-C15
22	B	846	BCR	C11-C10-C9-C8
22	B	847	BCR	C20-C21-C22-C23
22	B	848	BCR	C20-C21-C22-C23
22	F	801	BCR	C11-C10-C9-C8
22	F	801	BCR	C20-C21-C22-C23
22	I	101	BCR	C11-C10-C9-C8
22	I	101	BCR	C20-C21-C22-C23
22	J	102	BCR	C12-C13-C14-C15
22	J	102	BCR	C16-C17-C18-C19
22	K	103	BCR	C11-C10-C9-C8
22	K	103	BCR	C12-C13-C14-C15
22	K	103	BCR	C20-C21-C22-C23
22	L	207	BCR	C16-C17-C18-C19
20	A	840	PQN	C18-C20-C21-C22
16	B	802	CLA	CBA-CGA-O2A-C1
16	A	833	CLA	C5-C6-C7-C8
16	B	835	CLA	C3-C5-C6-C7
16	1	608	CLA	C11-C12-C13-C15
16	A	802	CLA	C16-C17-C18-C20
16	A	806	CLA	C16-C17-C18-C20
16	A	828	CLA	C16-C17-C18-C19
16	A	826	CLA	O1A-CGA-O2A-C1
19	A	801	CL0	O1A-CGA-O2A-C1
21	A	841	LHG	C29-C30-C31-C32
25	B	850	DGD	C5A-C6A-C7A-C8A
16	B	832	CLA	CBD-CGD-O2D-CED
22	B	847	BCR	C14-C15-C16-C17
22	I	101	BCR	C14-C15-C16-C17
22	K	103	BCR	C14-C15-C16-C17
16	A	818	CLA	O1D-CGD-O2D-CED
16	B	813	CLA	O1D-CGD-O2D-CED
16	A	809	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	A	841	LHG	C17-C18-C19-C20
25	B	850	DGD	C3A-C4A-C5A-C6A
16	1	606	CLA	C4B-C3B-CAB-CBB
16	2	610	CLA	C4B-C3B-CAB-CBB
16	3	204	CLA	C4B-C3B-CAB-CBB
16	3	206	CLA	C4B-C3B-CAB-CBB
16	3	207	CLA	C4B-C3B-CAB-CBB
16	3	213	CLA	C4B-C3B-CAB-CBB
16	A	808	CLA	C4B-C3B-CAB-CBB
16	A	809	CLA	C4B-C3B-CAB-CBB
16	A	812	CLA	C4B-C3B-CAB-CBB
16	A	817	CLA	C4B-C3B-CAB-CBB
16	A	823	CLA	C4B-C3B-CAB-CBB
16	A	831	CLA	C4B-C3B-CAB-CBB
16	A	834	CLA	C4B-C3B-CAB-CBB
16	A	839	CLA	C4B-C3B-CAB-CBB
16	A	852	CLA	C4B-C3B-CAB-CBB
16	B	807	CLA	C4B-C3B-CAB-CBB
16	B	811	CLA	C4B-C3B-CAB-CBB
16	B	815	CLA	C4B-C3B-CAB-CBB
16	B	819	CLA	C4B-C3B-CAB-CBB
16	B	825	CLA	C4B-C3B-CAB-CBB
16	B	829	CLA	C4B-C3B-CAB-CBB
16	B	840	CLA	C4B-C3B-CAB-CBB
16	F	803	CLA	C4B-C3B-CAB-CBB
16	L	201	CLA	C4B-C3B-CAB-CBB
16	B	807	CLA	C16-C17-C18-C20
16	A	820	CLA	C2A-CAA-CBA-CGA
16	A	825	CLA	C5-C6-C7-C8
16	B	801	CLA	C5-C6-C7-C8
16	B	804	CLA	C12-C13-C15-C16
26	J	104	3XQ	C14-C15-C16-C17
16	A	825	CLA	CBA-CGA-O2A-C1
16	A	832	CLA	CBA-CGA-O2A-C1
16	B	801	CLA	C3-C5-C6-C7
16	1	605	CLA	C3A-C2A-CAA-CBA
16	3	213	CLA	C3A-C2A-CAA-CBA
16	A	802	CLA	C3A-C2A-CAA-CBA
16	A	827	CLA	C3A-C2A-CAA-CBA
16	A	834	CLA	C3A-C2A-CAA-CBA
16	A	852	CLA	C3A-C2A-CAA-CBA
16	B	812	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	B	815	CLA	C3A-C2A-CAA-CBA
16	B	819	CLA	C3A-C2A-CAA-CBA
25	B	850	DGD	C2A-C3A-C4A-C5A
26	J	104	3XQ	C12-C13-C14-C15
16	B	803	CLA	C10-C11-C12-C13
16	B	842	CLA	C15-C16-C17-C18
17	3	201	ZEX	C33-C34-C35-C15
22	A	845	BCR	C9-C10-C11-C12
22	B	846	BCR	C9-C10-C11-C12
22	I	101	BCR	C13-C14-C15-C16
16	A	802	CLA	C16-C17-C18-C19
25	B	850	DGD	CBB-CCB-CDB-CEB
16	A	830	CLA	CBA-CGA-O2A-C1
16	A	852	CLA	CBA-CGA-O2A-C1
25	B	850	DGD	CCA-CDA-CEA-CFA
16	A	810	CLA	C8-C10-C11-C12
16	B	835	CLA	C5-C6-C7-C8
17	2	614	ZEX	C21-C26-C27-C28
17	2	615	ZEX	C21-C26-C27-C28
17	3	201	ZEX	C21-C26-C27-C28
16	B	833	CLA	O1D-CGD-O2D-CED
21	A	841	LHG	C14-C15-C16-C17
16	B	825	CLA	C6-C7-C8-C9
26	J	104	3XQ	C1-C2-C3-C4
16	3	203	CLA	O1A-CGA-O2A-C1
16	L	201	CLA	O1A-CGA-O2A-C1
16	1	603	CLA	C2B-C3B-CAB-CBB
16	1	606	CLA	C2B-C3B-CAB-CBB
16	1	610	CLA	C2B-C3B-CAB-CBB
16	2	610	CLA	C2B-C3B-CAB-CBB
16	2	613	CLA	C2B-C3B-CAB-CBB
16	3	202	CLA	C2B-C3B-CAB-CBB
16	3	204	CLA	C2B-C3B-CAB-CBB
16	3	208	CLA	C2B-C3B-CAB-CBB
16	3	213	CLA	C2B-C3B-CAB-CBB
16	A	806	CLA	C2B-C3B-CAB-CBB
16	A	809	CLA	C2B-C3B-CAB-CBB
16	A	822	CLA	C2B-C3B-CAB-CBB
16	A	825	CLA	C2B-C3B-CAB-CBB
16	A	827	CLA	C2B-C3B-CAB-CBB
16	A	834	CLA	C2B-C3B-CAB-CBB
16	A	838	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	A	852	CLA	C2B-C3B-CAB-CBB
16	B	804	CLA	C2B-C3B-CAB-CBB
16	B	805	CLA	C2B-C3B-CAB-CBB
16	B	807	CLA	C2B-C3B-CAB-CBB
16	B	821	CLA	C2B-C3B-CAB-CBB
16	B	823	CLA	C2B-C3B-CAB-CBB
16	B	826	CLA	C2B-C3B-CAB-CBB
16	B	842	CLA	C2B-C3B-CAB-CBB
16	O	202	CLA	C2B-C3B-CAB-CBB
17	1	615	ZEX	C5-C6-C7-C8
17	3	201	ZEX	C1-C6-C7-C8
17	3	217	ZEX	C5-C6-C7-C8
22	A	843	BCR	C1-C6-C7-C8
22	A	843	BCR	C5-C6-C7-C8
22	A	843	BCR	C23-C24-C25-C26
22	A	843	BCR	C23-C24-C25-C30
22	A	845	BCR	C23-C24-C25-C26
22	A	845	BCR	C23-C24-C25-C30
22	A	846	BCR	C1-C6-C7-C8
22	A	846	BCR	C5-C6-C7-C8
22	A	846	BCR	C23-C24-C25-C26
22	A	846	BCR	C23-C24-C25-C30
22	B	844	BCR	C1-C6-C7-C8
22	J	102	BCR	C23-C24-C25-C30
22	L	202	BCR	C23-C24-C25-C30
22	L	207	BCR	C1-C6-C7-C8
16	L	204	CLA	CBA-CGA-O2A-C1
16	A	823	CLA	C2A-CAA-CBA-CGA
16	B	815	CLA	C2A-CAA-CBA-CGA
21	A	842	LHG	C13-C14-C15-C16
16	A	809	CLA	O1A-CGA-O2A-C1
16	B	802	CLA	O1A-CGA-O2A-C1
22	A	844	BCR	C10-C11-C12-C13
22	A	845	BCR	C18-C19-C20-C21
22	A	849	BCR	C10-C11-C12-C13
22	B	844	BCR	C18-C19-C20-C21
22	B	847	BCR	C18-C19-C20-C21
22	B	849	BCR	C18-C19-C20-C21
22	F	804	BCR	C10-C11-C12-C13
16	B	821	CLA	C8-C10-C11-C12
16	B	825	CLA	C5-C6-C7-C8
25	B	850	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
16	2	608	CLA	CBA-CGA-O2A-C1
16	A	828	CLA	C5-C6-C7-C8
16	B	812	CLA	C13-C15-C16-C17
16	A	825	CLA	O1A-CGA-O2A-C1
16	A	832	CLA	O1A-CGA-O2A-C1
16	B	829	CLA	CBA-CGA-O2A-C1
22	A	846	BCR	C15-C16-C17-C18
22	B	849	BCR	C19-C20-C21-C22
22	J	103	BCR	C13-C14-C15-C16
16	A	817	CLA	C16-C17-C18-C19
16	A	808	CLA	C8-C10-C11-C12
16	B	829	CLA	C15-C16-C17-C18
17	1	615	ZEX	C7-C8-C9-C19
17	2	617	ZEX	C27-C28-C29-C39
22	A	845	BCR	C7-C8-C9-C10
22	A	846	BCR	C7-C8-C9-C10
22	A	847	BCR	C17-C18-C19-C20
22	B	848	BCR	C11-C12-C13-C14
22	I	101	BCR	C21-C22-C23-C24
22	J	102	BCR	C21-C22-C23-C24
25	B	850	DGD	C4A-C5A-C6A-C7A
25	B	850	DGD	CDA-CEA-CFA-CGA
16	A	817	CLA	C16-C17-C18-C20
16	A	831	CLA	C16-C17-C18-C20
16	B	825	CLA	C6-C7-C8-C10
16	A	852	CLA	C4-C3-C5-C6
18	3	219	IDO	C1-C2-C3-C4
16	A	808	CLA	C15-C16-C17-C18
16	B	809	CLA	C13-C15-C16-C17
21	A	841	LHG	C11-C10-C9-C8
16	A	830	CLA	O1A-CGA-O2A-C1
16	A	852	CLA	O1A-CGA-O2A-C1
16	A	804	CLA	C3-C5-C6-C7
16	A	818	CLA	C15-C16-C17-C18
16	B	838	CLA	C5-C6-C7-C8
16	A	837	CLA	O1D-CGD-O2D-CED
16	B	825	CLA	C3-C5-C6-C7
25	B	850	DGD	O2G-C2G-C3G-O3G
16	A	831	CLA	C16-C17-C18-C19
16	A	824	CLA	C8-C10-C11-C12
16	B	829	CLA	C5-C6-C7-C8
26	J	104	3XQ	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
17	3	218	ZEX	C25-C26-C27-C28
16	A	824	CLA	C4-C3-C5-C6
16	3	203	CLA	C13-C15-C16-C17
25	B	850	DGD	C2B-C3B-C4B-C5B
16	3	213	CLA	C2A-CAA-CBA-CGA
16	A	816	CLA	C2A-CAA-CBA-CGA
16	A	838	CLA	C2A-CAA-CBA-CGA
16	A	839	CLA	CBD-CGD-O2D-CED
16	A	817	CLA	CBA-CGA-O2A-C1
16	B	803	CLA	C13-C15-C16-C17
19	A	801	CL0	C5-C6-C7-C8
16	B	806	CLA	O1D-CGD-O2D-CED
21	A	841	LHG	C9-C10-C11-C12
20	B	843	PQN	C15-C16-C17-C18
16	2	608	CLA	O1A-CGA-O2A-C1
16	L	204	CLA	O1A-CGA-O2A-C1
16	A	852	CLA	C3-C5-C6-C7
16	1	605	CLA	C1A-C2A-CAA-CBA
16	1	607	CLA	C1A-C2A-CAA-CBA
16	1	608	CLA	C1A-C2A-CAA-CBA
16	2	602	CLA	C1A-C2A-CAA-CBA
16	3	203	CLA	C1A-C2A-CAA-CBA
16	3	205	CLA	C1A-C2A-CAA-CBA
16	3	209	CLA	C1A-C2A-CAA-CBA
16	3	213	CLA	C1A-C2A-CAA-CBA
16	A	802	CLA	C1A-C2A-CAA-CBA
16	A	806	CLA	C1A-C2A-CAA-CBA
16	A	807	CLA	C1A-C2A-CAA-CBA
16	A	810	CLA	C1A-C2A-CAA-CBA
16	A	813	CLA	C1A-C2A-CAA-CBA
16	A	817	CLA	C1A-C2A-CAA-CBA
16	A	822	CLA	C1A-C2A-CAA-CBA
16	A	823	CLA	C1A-C2A-CAA-CBA
16	A	830	CLA	C1A-C2A-CAA-CBA
16	A	833	CLA	C1A-C2A-CAA-CBA
16	A	852	CLA	C1A-C2A-CAA-CBA
16	B	812	CLA	C1A-C2A-CAA-CBA
16	B	815	CLA	C1A-C2A-CAA-CBA
16	B	821	CLA	C1A-C2A-CAA-CBA
16	B	834	CLA	C1A-C2A-CAA-CBA
20	A	840	PQN	C23-C25-C26-C27
16	A	839	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	3	203	CLA	C12-C13-C15-C16
16	A	807	CLA	C11-C12-C13-C15
16	A	818	CLA	C12-C13-C15-C16
16	A	833	CLA	C11-C12-C13-C15
16	B	819	CLA	C11-C10-C8-C7
16	B	826	CLA	C11-C12-C13-C15
16	B	828	CLA	C11-C12-C13-C15
16	B	835	CLA	C11-C10-C8-C7
16	B	840	CLA	C6-C7-C8-C10
16	B	841	CLA	C11-C10-C8-C7
16	L	203	CLA	C11-C10-C8-C7
19	A	801	CL0	C11-C10-C8-C7
21	A	841	LHG	C24-C25-C26-C27
16	A	802	CLA	C10-C11-C12-C13
20	A	840	PQN	C20-C21-C22-C23
16	B	830	CLA	C8-C10-C11-C12
21	A	841	LHG	C7-C8-C9-C10
16	B	818	CLA	C4-C3-C5-C6
16	B	829	CLA	C4-C3-C5-C6
16	B	830	CLA	C4-C3-C5-C6
16	A	824	CLA	C2-C3-C5-C6
16	A	852	CLA	C2-C3-C5-C6
16	B	829	CLA	C2-C3-C5-C6
16	B	830	CLA	C2-C3-C5-C6
16	1	602	CLA	C2A-CAA-CBA-CGA
16	2	602	CLA	C2A-CAA-CBA-CGA
16	2	608	CLA	C2A-CAA-CBA-CGA
16	A	807	CLA	C2A-CAA-CBA-CGA
16	1	602	CLA	C11-C10-C8-C9
16	A	818	CLA	C6-C7-C8-C9
16	A	833	CLA	C11-C10-C8-C9
16	B	820	CLA	C11-C10-C8-C9
16	B	821	CLA	C14-C13-C15-C16
16	B	833	CLA	C14-C13-C15-C16
16	B	835	CLA	C11-C10-C8-C9
16	L	203	CLA	C11-C10-C8-C9
16	A	822	CLA	CBA-CGA-O2A-C1
16	B	828	CLA	CBA-CGA-O2A-C1
16	A	802	CLA	C8-C10-C11-C12
16	B	810	CLA	O1D-CGD-O2D-CED
25	B	850	DGD	C1G-C2G-C3G-O3G
21	A	842	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
16	K	101	CLA	O1D-CGD-O2D-CED
16	B	840	CLA	O1D-CGD-O2D-CED
17	1	613	ZEX	C11-C10-C9-C19
19	A	801	CL0	CHA-CBD-CGD-O1D
19	A	801	CL0	CHA-CBD-CGD-O2D
22	L	202	BCR	C11-C10-C9-C34
16	B	812	CLA	C3-C5-C6-C7
16	B	805	CLA	C2-C3-C5-C6
16	L	203	CLA	C2-C3-C5-C6
16	A	838	CLA	C13-C15-C16-C17
16	B	821	CLA	C10-C11-C12-C13
17	1	613	ZEX	C7-C8-C9-C19
17	1	613	ZEX	C11-C12-C13-C20
17	1	614	ZEX	C11-C12-C13-C20
17	1	615	ZEX	C31-C32-C33-C40
17	1	615	ZEX	C27-C28-C29-C39
19	A	801	CL0	C16-C17-C18-C19
17	2	617	ZEX	C31-C32-C33-C34
17	3	214	ZEX	C7-C8-C9-C10
22	A	843	BCR	C7-C8-C9-C10
22	B	847	BCR	C11-C12-C13-C14
22	B	849	BCR	C21-C22-C23-C24
22	L	202	BCR	C21-C22-C23-C24
16	A	817	CLA	O1A-CGA-O2A-C1
16	B	836	CLA	C2A-CAA-CBA-CGA
16	A	805	CLA	CBA-CGA-O2A-C1
25	B	850	DGD	C4B-C5B-C6B-C7B
22	L	206	BCR	C10-C11-C12-C13
21	A	841	LHG	C18-C19-C20-C21
26	J	104	3XQ	C6-C7-C8-C9
22	B	848	BCR	C13-C14-C15-C16
22	K	103	BCR	C19-C20-C21-C22
16	2	612	CLA	CBD-CGD-O2D-CED
17	1	613	ZEX	C12-C13-C14-C15
17	3	201	ZEX	C12-C13-C14-C15
16	B	837	CLA	CBA-CGA-O2A-C1
16	A	827	CLA	C4-C3-C5-C6
16	B	805	CLA	C4-C3-C5-C6
16	A	827	CLA	C2-C3-C5-C6
16	B	815	CLA	C2-C3-C5-C6
16	B	818	CLA	C2-C3-C5-C6
16	B	835	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	B	818	CLA	C6-C7-C8-C9
25	B	850	DGD	C6A-C7A-C8A-C9A
25	B	850	DGD	C5B-C6B-C7B-C8B
25	B	850	DGD	O1G-C1G-C2G-O2G
16	A	805	CLA	CAA-CBA-CGA-O2A
16	A	822	CLA	O1A-CGA-O2A-C1
16	B	829	CLA	O1A-CGA-O2A-C1
21	A	841	LHG	C15-C16-C17-C18
16	B	812	CLA	C10-C11-C12-C13
16	B	835	CLA	C15-C16-C17-C18
17	2	617	ZEX	C29-C30-C31-C32
16	B	818	CLA	C6-C7-C8-C10
21	A	842	LHG	C12-C13-C14-C15
16	B	801	CLA	C4-C3-C5-C6
16	B	803	CLA	C4-C3-C5-C6
16	B	815	CLA	C4-C3-C5-C6
16	L	203	CLA	C4-C3-C5-C6
20	B	843	PQN	C14-C13-C15-C16
16	B	815	CLA	CBA-CGA-O2A-C1
16	B	805	CLA	C5-C6-C7-C8
25	B	850	DGD	CEB-CFB-CGB-CHB
16	3	203	CLA	C6-C7-C8-C9
16	3	203	CLA	C14-C13-C15-C16
16	A	805	CLA	C11-C10-C8-C9
16	A	807	CLA	C11-C12-C13-C14
16	A	808	CLA	C11-C10-C8-C9
16	A	810	CLA	C11-C10-C8-C9
16	A	818	CLA	C14-C13-C15-C16
16	A	820	CLA	C11-C12-C13-C14
16	A	824	CLA	C11-C10-C8-C9
16	A	832	CLA	C6-C7-C8-C9
16	A	833	CLA	C11-C12-C13-C14
16	A	839	CLA	C11-C12-C13-C14
16	B	805	CLA	C11-C12-C13-C14
16	B	808	CLA	C6-C7-C8-C9
16	B	809	CLA	C6-C7-C8-C9
16	B	811	CLA	C6-C7-C8-C9
16	B	826	CLA	C11-C12-C13-C14
16	B	828	CLA	C11-C12-C13-C14
16	B	835	CLA	C6-C7-C8-C9
16	B	840	CLA	C6-C7-C8-C9
16	B	841	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	801	CL0	C11-C10-C8-C9
16	B	831	CLA	C13-C15-C16-C17
16	B	828	CLA	O1A-CGA-O2A-C1
16	1	608	CLA	C4B-C3B-CAB-CBB
16	1	609	CLA	C4B-C3B-CAB-CBB
16	1	611	CLA	C4B-C3B-CAB-CBB
16	2	603	CLA	C4B-C3B-CAB-CBB
16	2	604	CLA	C4B-C3B-CAB-CBB
16	3	205	CLA	C4B-C3B-CAB-CBB
16	A	804	CLA	C4B-C3B-CAB-CBB
16	A	806	CLA	C4B-C3B-CAB-CBB
16	A	807	CLA	C4B-C3B-CAB-CBB
16	A	810	CLA	C4B-C3B-CAB-CBB
16	A	811	CLA	C4B-C3B-CAB-CBB
16	A	816	CLA	C4B-C3B-CAB-CBB
16	A	818	CLA	C4B-C3B-CAB-CBB
16	A	820	CLA	C4B-C3B-CAB-CBB
16	A	824	CLA	C4B-C3B-CAB-CBB
16	A	826	CLA	C4B-C3B-CAB-CBB
16	A	828	CLA	C4B-C3B-CAB-CBB
16	A	829	CLA	C4B-C3B-CAB-CBB
16	A	833	CLA	C4B-C3B-CAB-CBB
16	A	836	CLA	C4B-C3B-CAB-CBB
16	A	850	CLA	C4B-C3B-CAB-CBB
16	B	817	CLA	C4B-C3B-CAB-CBB
16	B	827	CLA	C4B-C3B-CAB-CBB
16	B	828	CLA	C4B-C3B-CAB-CBB
16	B	835	CLA	C4B-C3B-CAB-CBB
16	L	204	CLA	C4B-C3B-CAB-CBB
16	L	205	CLA	C4B-C3B-CAB-CBB
16	O	203	CLA	C4B-C3B-CAB-CBB
16	O	204	CLA	C4B-C3B-CAB-CBB
16	B	823	CLA	CAA-CBA-CGA-O2A
16	B	807	CLA	C15-C16-C17-C18
16	B	808	CLA	C8-C10-C11-C12
16	B	809	CLA	C5-C6-C7-C8
16	B	832	CLA	O1D-CGD-O2D-CED
16	1	602	CLA	C11-C10-C8-C7
16	3	203	CLA	C6-C7-C8-C10
16	A	805	CLA	C11-C10-C8-C7
16	A	808	CLA	C11-C10-C8-C7
16	A	818	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
16	A	820	CLA	C11-C12-C13-C15
16	A	832	CLA	C6-C7-C8-C10
16	A	839	CLA	C11-C12-C13-C15
16	A	852	CLA	C6-C7-C8-C10
16	B	805	CLA	C12-C13-C15-C16
16	B	808	CLA	C6-C7-C8-C10
16	B	809	CLA	C6-C7-C8-C10
16	B	810	CLA	C12-C13-C15-C16
16	B	811	CLA	C6-C7-C8-C10
16	B	811	CLA	C11-C12-C13-C15
16	B	820	CLA	C11-C10-C8-C7
16	B	821	CLA	C12-C13-C15-C16
16	B	829	CLA	C11-C10-C8-C7
16	B	833	CLA	C12-C13-C15-C16
16	B	835	CLA	C6-C7-C8-C10
16	A	813	CLA	C3A-C2A-CAA-CBA
16	A	819	CLA	C3A-C2A-CAA-CBA
16	A	822	CLA	C3A-C2A-CAA-CBA
16	A	828	CLA	C3A-C2A-CAA-CBA
16	A	839	CLA	C3A-C2A-CAA-CBA
16	B	829	CLA	C3A-C2A-CAA-CBA
16	B	835	CLA	C4-C3-C5-C6
16	A	831	CLA	C5-C6-C7-C8
16	B	801	CLA	C8-C10-C11-C12
21	A	841	LHG	C11-C12-C13-C14
16	A	835	CLA	O1D-CGD-O2D-CED
16	A	826	CLA	C5-C6-C7-C8
22	B	847	BCR	C19-C20-C21-C22
22	L	206	BCR	C11-C12-C13-C35
16	L	204	CLA	O1D-CGD-O2D-CED
17	1	616	ZEX	C25-C26-C27-C28
17	3	201	ZEX	C25-C26-C27-C28
16	A	838	CLA	C8-C10-C11-C12
25	B	850	DGD	O1G-C1G-C2G-C3G
16	3	203	CLA	C15-C16-C17-C18
16	B	842	CLA	C16-C17-C18-C20
17	1	616	ZEX	C21-C26-C27-C28
17	1	617	ZEX	C21-C26-C27-C28
20	A	840	PQN	C14-C13-C15-C16
16	A	805	CLA	O1A-CGA-O2A-C1
16	F	803	CLA	C2B-C3B-CAB-CBB
17	1	615	ZEX	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	845	BCR	C1-C6-C7-C8
22	A	847	BCR	C1-C6-C7-C8
22	A	849	BCR	C1-C6-C7-C8
22	B	845	BCR	C1-C6-C7-C8
22	B	846	BCR	C23-C24-C25-C30
22	B	847	BCR	C1-C6-C7-C8
22	B	848	BCR	C1-C6-C7-C8
22	F	801	BCR	C1-C6-C7-C8
22	F	801	BCR	C23-C24-C25-C30
22	F	804	BCR	C23-C24-C25-C30
22	J	102	BCR	C1-C6-C7-C8
22	J	103	BCR	C1-C6-C7-C8
22	L	202	BCR	C1-C6-C7-C8
22	L	206	BCR	C1-C6-C7-C8
22	L	207	BCR	C23-C24-C25-C30
16	B	804	CLA	C3-C5-C6-C7
16	A	831	CLA	C8-C10-C11-C12
26	J	104	3XQ	C11-C12-C13-C14
16	A	828	CLA	C15-C16-C17-C18
16	B	803	CLA	C2-C3-C5-C6
21	A	841	LHG	C10-C11-C12-C13
16	A	806	CLA	CBA-CGA-O2A-C1
16	A	828	CLA	CBA-CGA-O2A-C1
16	B	805	CLA	C14-C13-C15-C16
16	B	808	CLA	C14-C13-C15-C16
16	B	829	CLA	C14-C13-C15-C16
16	L	204	CLA	C14-C13-C15-C16
16	B	827	CLA	C10-C11-C12-C13
22	A	849	BCR	C6-C7-C8-C9
22	F	801	BCR	C6-C7-C8-C9
22	F	801	BCR	C14-C15-C16-C17
16	A	810	CLA	C5-C6-C7-C8
16	2	610	CLA	C1A-C2A-CAA-CBA
16	A	814	CLA	C1A-C2A-CAA-CBA
16	B	817	CLA	C1A-C2A-CAA-CBA
16	K	102	CLA	C1A-C2A-CAA-CBA
16	2	602	CLA	C15-C16-C17-C18
22	K	103	BCR	C15-C16-C17-C18
16	A	806	CLA	C15-C16-C17-C18
22	A	844	BCR	C16-C17-C18-C36
22	A	849	BCR	C11-C10-C9-C34
22	A	849	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
22	B	844	BCR	C16-C17-C18-C36
22	F	804	BCR	C16-C17-C18-C36
22	I	101	BCR	C35-C13-C14-C15
22	J	103	BCR	C11-C10-C9-C34
22	J	103	BCR	C20-C21-C22-C37
22	L	206	BCR	C20-C21-C22-C37
16	A	820	CLA	C3-C5-C6-C7
16	B	842	CLA	CAA-CBA-CGA-O2A
17	2	615	ZEX	C7-C8-C9-C19
22	B	848	BCR	C37-C22-C23-C24
16	A	810	CLA	C11-C10-C8-C7
16	A	824	CLA	C11-C10-C8-C7
16	A	829	CLA	C11-C12-C13-C15
16	B	801	CLA	C11-C10-C8-C7
16	B	805	CLA	C6-C7-C8-C10
16	B	808	CLA	C12-C13-C15-C16
16	B	812	CLA	C11-C10-C8-C7
16	B	815	CLA	C11-C10-C8-C7
16	B	829	CLA	C12-C13-C15-C16
16	B	840	CLA	C11-C10-C8-C7
16	L	204	CLA	C12-C13-C15-C16
21	A	842	LHG	C7-C8-C9-C10
17	1	616	ZEX	C27-C28-C29-C30
17	2	614	ZEX	C7-C8-C9-C10
17	2	616	ZEX	C31-C32-C33-C34
17	3	216	ZEX	C27-C28-C29-C30
22	A	845	BCR	C17-C18-C19-C20
21	A	842	LHG	C16-C17-C18-C19
16	A	819	CLA	C2A-CAA-CBA-CGA
16	B	842	CLA	C16-C17-C18-C19
16	A	828	CLA	O1A-CGA-O2A-C1
16	B	837	CLA	O1A-CGA-O2A-C1
16	B	810	CLA	C8-C10-C11-C12
16	B	801	CLA	C16-C17-C18-C19
16	B	821	CLA	C15-C16-C17-C18
17	2	616	ZEX	C12-C13-C14-C15
17	2	616	ZEX	C28-C29-C30-C31
22	L	202	BCR	C16-C17-C18-C19
21	A	841	LHG	O6-C4-C5-O7
16	A	805	CLA	C8-C10-C11-C12
16	B	815	CLA	O1A-CGA-O2A-C1
16	A	824	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	B	801	CLA	C11-C10-C8-C9
16	B	805	CLA	C6-C7-C8-C9
16	B	812	CLA	C14-C13-C15-C16
16	A	806	CLA	O1A-CGA-O2A-C1
16	A	820	CLA	C5-C6-C7-C8
16	L	204	CLA	C3-C5-C6-C7
16	A	818	CLA	C8-C10-C11-C12
16	2	611	CLA	C4C-C3C-CAC-CBC
16	A	836	CLA	C15-C16-C17-C18
16	L	205	CLA	CBA-CGA-O2A-C1
16	1	608	CLA	C5-C6-C7-C8
16	B	833	CLA	C3-C5-C6-C7
16	A	839	CLA	C16-C17-C18-C19
16	A	839	CLA	C16-C17-C18-C20
16	A	838	CLA	C3-C5-C6-C7
16	B	811	CLA	C5-C6-C7-C8
16	1	602	CLA	C1A-C2A-CAA-CBA
16	A	851	CLA	C1A-C2A-CAA-CBA
16	B	829	CLA	C1A-C2A-CAA-CBA
16	B	809	CLA	C4-C3-C5-C6
16	A	836	CLA	C13-C15-C16-C17
21	A	841	LHG	O6-C4-C5-C6
16	A	839	CLA	O1D-CGD-O2D-CED
16	A	835	CLA	C2-C3-C5-C6
16	A	810	CLA	C11-C12-C13-C15
16	B	802	CLA	C12-C13-C15-C16
16	B	807	CLA	C6-C7-C8-C10
16	B	809	CLA	C11-C12-C13-C15
16	B	827	CLA	C12-C13-C15-C16
16	B	830	CLA	C11-C10-C8-C7
16	B	831	CLA	C12-C13-C15-C16
16	B	841	CLA	C12-C13-C15-C16
16	B	815	CLA	C16-C17-C18-C19
16	A	803	CLA	CBD-CGD-O2D-CED
26	J	104	3XQ	C9-C10-C11-C12
16	A	820	CLA	C10-C11-C12-C13
16	3	203	CLA	C3-C5-C6-C7
16	A	810	CLA	C14-C13-C15-C16
16	B	812	CLA	C11-C10-C8-C9
16	B	840	CLA	C11-C10-C8-C9
16	L	205	CLA	O1A-CGA-O2A-C1
16	L	204	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	2	617	ZEX	C13-C14-C15-C35
22	A	843	BCR	C9-C10-C11-C12
16	2	612	CLA	O1D-CGD-O2D-CED
16	A	821	CLA	C1-C2-C3-C4
20	A	840	PQN	C26-C27-C28-C30
16	A	807	CLA	C13-C15-C16-C17
16	B	840	CLA	C5-C6-C7-C8
16	B	811	CLA	C3-C5-C6-C7
16	1	603	CLA	CAD-CBD-CGD-O2D
16	A	805	CLA	CAD-CBD-CGD-O2D
16	A	836	CLA	CAD-CBD-CGD-O2D
16	B	804	CLA	CAD-CBD-CGD-O2D
16	B	815	CLA	CAD-CBD-CGD-O2D
16	O	201	CLA	CAD-CBD-CGD-O2D
16	A	806	CLA	C5-C6-C7-C8
16	B	830	CLA	C10-C11-C12-C13
16	B	829	CLA	C13-C15-C16-C17
16	1	603	CLA	CAD-CBD-CGD-O1D
16	1	605	CLA	CHA-CBD-CGD-O2D
16	1	612	CLA	CHA-CBD-CGD-O1D
16	2	602	CLA	CAD-CBD-CGD-O1D
16	2	613	CLA	CHA-CBD-CGD-O1D
16	A	805	CLA	CAD-CBD-CGD-O1D
16	A	811	CLA	CHA-CBD-CGD-O1D
16	A	815	CLA	CAD-CBD-CGD-O1D
16	A	824	CLA	CHA-CBD-CGD-O1D
16	A	830	CLA	CHA-CBD-CGD-O2D
16	A	836	CLA	CAD-CBD-CGD-O1D
16	B	804	CLA	CAD-CBD-CGD-O1D
16	B	810	CLA	CHA-CBD-CGD-O1D
16	B	815	CLA	CAD-CBD-CGD-O1D
16	B	819	CLA	CAD-CBD-CGD-O1D
16	B	842	CLA	CHA-CBD-CGD-O1D
16	B	842	CLA	CHA-CBD-CGD-O2D
16	F	803	CLA	CHA-CBD-CGD-O1D
16	F	803	CLA	CHA-CBD-CGD-O2D
16	J	101	CLA	CAD-CBD-CGD-O1D
16	O	201	CLA	CAD-CBD-CGD-O1D
16	O	203	CLA	CHA-CBD-CGD-O1D
16	O	203	CLA	CHA-CBD-CGD-O2D
17	2	616	ZEX	C13-C14-C15-C35
17	3	214	ZEX	C33-C34-C35-C15

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Mol	Chain	Res	Type	Atoms
17	3	218	ZEX	C9-C10-C11-C12
17	3	218	ZEX	C33-C34-C35-C15
21	A	841	LHG	C3-O3-P-O5
21	A	842	LHG	C3-O3-P-O5
21	A	842	LHG	C4-O6-P-O5
22	A	844	BCR	C13-C14-C15-C16
22	B	849	BCR	C35-C13-C14-C15
16	A	833	CLA	C4-C3-C5-C6
16	2	604	CLA	C2B-C3B-CAB-CBB
16	3	206	CLA	C2B-C3B-CAB-CBB
16	3	207	CLA	C2B-C3B-CAB-CBB
16	A	807	CLA	C2B-C3B-CAB-CBB
16	A	808	CLA	C2B-C3B-CAB-CBB
16	A	812	CLA	C2B-C3B-CAB-CBB
16	A	817	CLA	C2B-C3B-CAB-CBB
16	A	823	CLA	C2B-C3B-CAB-CBB
16	A	828	CLA	C2B-C3B-CAB-CBB
16	A	831	CLA	C2B-C3B-CAB-CBB
16	A	839	CLA	C2B-C3B-CAB-CBB
16	B	811	CLA	C2B-C3B-CAB-CBB
16	B	815	CLA	C2B-C3B-CAB-CBB
16	B	819	CLA	C2B-C3B-CAB-CBB
16	B	825	CLA	C2B-C3B-CAB-CBB
16	B	829	CLA	C2B-C3B-CAB-CBB
16	B	835	CLA	C2B-C3B-CAB-CBB
16	B	840	CLA	C2B-C3B-CAB-CBB
16	L	201	CLA	C2B-C3B-CAB-CBB
16	O	203	CLA	C2B-C3B-CAB-CBB
22	J	102	BCR	C23-C24-C25-C26
22	J	103	BCR	C5-C6-C7-C8
16	A	831	CLA	C13-C15-C16-C17
16	A	816	CLA	C13-C15-C16-C17
22	A	844	BCR	C11-C12-C13-C14
16	A	832	CLA	C13-C15-C16-C17
16	A	816	CLA	C5-C6-C7-C8
16	A	821	CLA	O2A-C1-C2-C3
17	2	616	ZEX	C10-C11-C12-C13
16	A	850	CLA	C15-C16-C17-C18
16	B	801	CLA	C2-C3-C5-C6
17	2	615	ZEX	C33-C34-C35-C15
16	A	802	CLA	C11-C12-C13-C14
16	A	816	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
16	A	829	CLA	C11-C12-C13-C14
16	A	836	CLA	C6-C7-C8-C9
16	B	809	CLA	C11-C12-C13-C14
16	B	815	CLA	C11-C10-C8-C9
16	B	828	CLA	C6-C7-C8-C9
16	A	802	CLA	C11-C12-C13-C15
16	A	836	CLA	C6-C7-C8-C10
16	B	812	CLA	C12-C13-C15-C16
17	2	614	ZEX	C11-C10-C9-C8
22	F	804	BCR	C12-C13-C14-C15
22	L	206	BCR	C11-C10-C9-C8
21	A	842	LHG	C25-C26-C27-C28
20	A	840	PQN	C26-C27-C28-C29
21	A	841	LHG	C12-C13-C14-C15
16	A	837	CLA	C16-C17-C18-C19
16	B	835	CLA	C16-C17-C18-C19
16	B	829	CLA	O1D-CGD-O2D-CED
16	B	839	CLA	CBA-CGA-O2A-C1
22	L	202	BCR	C13-C14-C15-C16
16	B	801	CLA	C16-C17-C18-C20
16	B	829	CLA	CAA-CBA-CGA-O2A
16	B	833	CLA	C13-C15-C16-C17
16	2	602	CLA	C3-C5-C6-C7
16	B	805	CLA	CAA-CBA-CGA-O2A
16	B	809	CLA	C2C-C3C-CAC-CBC
25	B	850	DGD	C5D-C6D-O5D-C1E
16	3	209	CLA	C2A-CAA-CBA-CGA
16	A	812	CLA	C2A-CAA-CBA-CGA
16	B	809	CLA	C2A-CAA-CBA-CGA
17	1	613	ZEX	C29-C30-C31-C32
22	L	207	BCR	C15-C16-C17-C18
24	A	853	BGC	C4-C5-C6-O6
16	B	838	CLA	C15-C16-C17-C18
16	A	805	CLA	CAA-CBA-CGA-O1A
16	A	828	CLA	C11-C12-C13-C14
16	B	807	CLA	C6-C7-C8-C9
16	B	811	CLA	C11-C12-C13-C14
21	A	842	LHG	C2-C3-O3-P
16	2	602	CLA	C4B-C3B-CAB-CBB
16	A	851	CLA	C4B-C3B-CAB-CBB
25	B	850	DGD	CAB-CBB-CCB-CDB
26	J	104	3XQ	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
16	A	833	CLA	C13-C15-C16-C17
16	B	839	CLA	O1A-CGA-O2A-C1
16	B	809	CLA	C2-C3-C5-C6
16	A	806	CLA	C11-C12-C13-C15
16	B	837	CLA	C6-C7-C8-C10
16	3	203	CLA	C5-C6-C7-C8
16	A	837	CLA	C16-C17-C18-C20
16	A	802	CLA	O1A-CGA-O2A-C1
16	1	601	CLA	C3A-C2A-CAA-CBA
16	A	805	CLA	C3A-C2A-CAA-CBA
16	L	204	CLA	C4-C3-C5-C6
16	O	204	CLA	C3A-C2A-CAA-CBA
16	1	601	CLA	O2A-C1-C2-C3
16	2	601	CLA	C2C-C3C-CAC-CBC
22	B	846	BCR	C11-C10-C9-C34
22	B	847	BCR	C20-C21-C22-C37
16	A	838	CLA	C2-C1-O2A-CGA
17	3	214	ZEX	C9-C10-C11-C12
22	B	844	BCR	C19-C20-C21-C22
16	B	842	CLA	C10-C11-C12-C13
22	J	103	BCR	C7-C8-C9-C34
16	A	834	CLA	CAA-CBA-CGA-O1A
16	B	802	CLA	C15-C16-C17-C18
16	B	803	CLA	C2A-CAA-CBA-CGA
16	2	601	CLA	CAA-CBA-CGA-O1A
16	3	203	CLA	C10-C11-C12-C13
16	B	808	CLA	O1A-CGA-O2A-C1
16	A	806	CLA	C11-C12-C13-C14
16	B	831	CLA	C14-C13-C15-C16
16	B	837	CLA	C6-C7-C8-C9
16	A	850	CLA	C13-C15-C16-C17
16	1	604	CLA	CAA-CBA-CGA-O1A
16	1	606	CLA	CAA-CBA-CGA-O1A
17	3	216	ZEX	C21-C26-C27-C28
16	1	604	CLA	CAA-CBA-CGA-O2A
16	2	601	CLA	CAA-CBA-CGA-O2A
16	B	806	CLA	CAA-CBA-CGA-O1A
16	B	806	CLA	CAA-CBA-CGA-O2A
16	A	831	CLA	C2A-CAA-CBA-CGA
16	B	823	CLA	CAA-CBA-CGA-O1A
16	3	204	CLA	C1A-C2A-CAA-CBA
16	A	839	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	B	813	CLA	C1A-C2A-CAA-CBA
16	B	818	CLA	C1A-C2A-CAA-CBA
16	B	837	CLA	C1A-C2A-CAA-CBA
16	O	204	CLA	C1A-C2A-CAA-CBA
22	A	845	BCR	C20-C21-C22-C23
22	A	847	BCR	C11-C10-C9-C8
22	A	847	BCR	C16-C17-C18-C19
22	B	845	BCR	C11-C10-C9-C8
22	B	845	BCR	C20-C21-C22-C23
16	1	608	CLA	C2B-C3B-CAB-CBB
16	1	611	CLA	C2B-C3B-CAB-CBB
16	2	602	CLA	C2B-C3B-CAB-CBB
16	2	603	CLA	C2B-C3B-CAB-CBB
16	3	205	CLA	C2B-C3B-CAB-CBB
16	A	810	CLA	C2B-C3B-CAB-CBB
16	A	816	CLA	C2B-C3B-CAB-CBB
16	A	818	CLA	C2B-C3B-CAB-CBB
16	A	820	CLA	C2B-C3B-CAB-CBB
16	A	824	CLA	C2B-C3B-CAB-CBB
16	A	829	CLA	C2B-C3B-CAB-CBB
16	A	833	CLA	C2B-C3B-CAB-CBB
16	A	836	CLA	C2B-C3B-CAB-CBB
16	A	850	CLA	C2B-C3B-CAB-CBB
16	A	851	CLA	C2B-C3B-CAB-CBB
16	L	204	CLA	C2B-C3B-CAB-CBB
16	O	204	CLA	C2B-C3B-CAB-CBB
17	2	615	ZEX	C5-C6-C7-C8
22	A	844	BCR	C23-C24-C25-C30
22	A	845	BCR	C5-C6-C7-C8
22	A	847	BCR	C5-C6-C7-C8
22	A	849	BCR	C5-C6-C7-C8
22	B	844	BCR	C5-C6-C7-C8
22	B	845	BCR	C5-C6-C7-C8
22	B	846	BCR	C1-C6-C7-C8
22	B	846	BCR	C5-C6-C7-C8
22	B	846	BCR	C23-C24-C25-C26
22	B	847	BCR	C5-C6-C7-C8
22	B	848	BCR	C5-C6-C7-C8
22	B	849	BCR	C1-C6-C7-C8
22	F	801	BCR	C5-C6-C7-C8
22	F	801	BCR	C23-C24-C25-C26
22	F	804	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	I	101	BCR	C1-C6-C7-C8
22	I	101	BCR	C5-C6-C7-C8
22	J	102	BCR	C5-C6-C7-C8
22	J	103	BCR	C23-C24-C25-C30
22	K	103	BCR	C23-C24-C25-C30
22	L	202	BCR	C5-C6-C7-C8
22	L	202	BCR	C23-C24-C25-C26
22	L	206	BCR	C5-C6-C7-C8
22	L	207	BCR	C5-C6-C7-C8
22	L	207	BCR	C23-C24-C25-C26
16	1	606	CLA	CAA-CBA-CGA-O2A
16	3	202	CLA	CAA-CBA-CGA-O2A
16	3	208	CLA	CAA-CBA-CGA-O1A
16	A	834	CLA	CAA-CBA-CGA-O2A
16	B	808	CLA	CBA-CGA-O2A-C1
16	A	805	CLA	C13-C15-C16-C17
16	2	607	CLA	CAA-CBA-CGA-O2A
16	2	602	CLA	C4-C3-C5-C6
16	A	802	CLA	C4-C3-C5-C6
16	A	810	CLA	C4-C3-C5-C6
16	B	810	CLA	C4-C3-C5-C6
16	L	204	CLA	C2-C3-C5-C6
16	1	603	CLA	CAA-CBA-CGA-O2A
16	A	828	CLA	C11-C12-C13-C15
16	B	833	CLA	C11-C10-C8-C7
26	J	104	3XQ	C10-C11-C12-C13
16	A	850	CLA	C16-C17-C18-C20
19	A	801	CL0	C16-C17-C18-C20
16	2	607	CLA	CAA-CBA-CGA-O1A
25	B	850	DGD	C8A-C9A-CAA-CBA
16	L	204	CLA	C8-C10-C11-C12
16	3	207	CLA	CAA-CBA-CGA-O2A
16	B	808	CLA	C4-C3-C5-C6
16	B	841	CLA	C4-C3-C5-C6
16	B	810	CLA	C2-C3-C5-C6
16	B	821	CLA	C16-C17-C18-C19
16	A	806	CLA	CAA-CBA-CGA-O2A
16	A	837	CLA	C2A-CAA-CBA-CGA
16	3	208	CLA	CAA-CBA-CGA-O2A
16	K	101	CLA	CAA-CBA-CGA-O2A
16	B	819	CLA	C6-C7-C8-C9
16	L	204	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
16	B	807	CLA	C5-C6-C7-C8
16	A	836	CLA	C16-C17-C18-C20
16	3	202	CLA	CAA-CBA-CGA-O1A
16	A	820	CLA	C4-C3-C5-C6
16	B	826	CLA	C4-C3-C5-C6
16	B	827	CLA	C4-C3-C5-C6
19	A	801	CL0	C4-C3-C5-C6
16	1	603	CLA	CAA-CBA-CGA-O1A
16	3	207	CLA	CAA-CBA-CGA-O1A
16	B	826	CLA	C2-C3-C5-C6
16	B	840	CLA	C15-C16-C17-C18
16	A	803	CLA	O1D-CGD-O2D-CED
16	3	208	CLA	C2A-CAA-CBA-CGA
16	A	850	CLA	C2A-CAA-CBA-CGA
16	F	802	CLA	C2A-CAA-CBA-CGA
16	B	835	CLA	C16-C17-C18-C20
16	3	203	CLA	C4-C3-C5-C6
16	A	838	CLA	C4-C3-C5-C6
16	A	802	CLA	CBA-CGA-O2A-C1
21	A	842	LHG	C1-C2-C3-O3
17	3	217	ZEX	C39-C29-C30-C31
22	A	847	BCR	C16-C17-C18-C36
22	A	849	BCR	C16-C17-C18-C36
22	B	846	BCR	C20-C21-C22-C37
22	K	103	BCR	C11-C10-C9-C34
22	L	202	BCR	C20-C21-C22-C37
16	B	808	CLA	C15-C16-C17-C18
16	A	815	CLA	CAA-CBA-CGA-O2A
21	A	842	LHG	O6-C4-C5-C6
16	A	829	CLA	C5-C6-C7-C8
16	1	610	CLA	CAA-CBA-CGA-O2A
16	3	204	CLA	CAA-CBA-CGA-O2A
16	3	203	CLA	C2-C3-C5-C6
16	A	820	CLA	C2-C3-C5-C6
16	B	826	CLA	C5-C6-C7-C8
16	B	827	CLA	C11-C12-C13-C15
16	B	821	CLA	C16-C17-C18-C20
16	A	815	CLA	CAA-CBA-CGA-O1A
16	K	101	CLA	CAA-CBA-CGA-O1A
17	3	215	ZEX	C27-C28-C29-C30
16	B	815	CLA	C14-C13-C15-C16
16	B	830	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	B	833	CLA	C6-C7-C8-C9
16	1	611	CLA	CAA-CBA-CGA-O2A
16	2	603	CLA	CAA-CBA-CGA-O2A
16	A	806	CLA	C2A-CAA-CBA-CGA
16	A	809	CLA	C2-C1-O2A-CGA
16	B	803	CLA	C2-C1-O2A-CGA
16	B	841	CLA	C2-C1-O2A-CGA
16	L	204	CLA	C2-C1-O2A-CGA
16	A	839	CLA	C8-C10-C11-C12
16	3	204	CLA	C3A-C2A-CAA-CBA
16	B	803	CLA	C3A-C2A-CAA-CBA
16	B	803	CLA	C15-C16-C17-C18
16	B	811	CLA	C10-C11-C12-C13
16	B	831	CLA	CBA-CGA-O2A-C1
21	A	841	LHG	C35-C36-C37-C38
16	3	205	CLA	CAA-CBA-CGA-O2A
16	B	808	CLA	C10-C11-C12-C13
16	A	836	CLA	C16-C17-C18-C19
16	B	836	CLA	CAA-CBA-CGA-O2A
16	A	807	CLA	C8-C10-C11-C12
16	A	832	CLA	C2A-CAA-CBA-CGA
16	1	612	CLA	CAA-CBA-CGA-O2A
16	3	205	CLA	CAA-CBA-CGA-O1A
22	B	846	BCR	C20-C21-C22-C23
16	2	603	CLA	CAA-CBA-CGA-O1A
21	A	842	LHG	O6-C4-C5-O7
16	B	829	CLA	CBD-CGD-O2D-CED
25	B	850	DGD	CDB-CEB-CFB-CGB
16	A	805	CLA	C5-C6-C7-C8
16	B	833	CLA	CAA-CBA-CGA-O2A
16	1	612	CLA	CAA-CBA-CGA-O1A
17	2	614	ZEX	C13-C14-C15-C35
22	A	849	BCR	C13-C14-C15-C16
16	B	815	CLA	C4C-C3C-CAC-CBC
17	3	215	ZEX	C21-C26-C27-C28
26	J	104	3XQ	C13-C14-C15-C16
16	1	610	CLA	CAA-CBA-CGA-O1A
16	A	813	CLA	CAA-CBA-CGA-O2A
16	A	836	CLA	C3-C5-C6-C7
22	A	849	BCR	C14-C15-C16-C17
16	A	810	CLA	C11-C12-C13-C14
16	B	802	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
16	B	827	CLA	C14-C13-C15-C16
25	B	850	DGD	C3B-C4B-C5B-C6B
16	1	611	CLA	CAA-CBA-CGA-O1A
16	A	833	CLA	C2-C3-C5-C6
16	B	808	CLA	C2-C3-C5-C6
16	3	204	CLA	CAA-CBA-CGA-O1A
16	1	606	CLA	C2A-CAA-CBA-CGA
16	A	831	CLA	C11-C10-C8-C7
16	B	815	CLA	C12-C13-C15-C16
16	B	833	CLA	C6-C7-C8-C10
16	L	204	CLA	C11-C12-C13-C15
20	B	843	PQN	C21-C22-C23-C25
16	2	611	CLA	CAA-CBA-CGA-O2A
16	1	609	CLA	C2B-C3B-CAB-CBB
16	A	804	CLA	C2B-C3B-CAB-CBB
16	A	811	CLA	C2B-C3B-CAB-CBB
16	A	826	CLA	C2B-C3B-CAB-CBB
16	B	801	CLA	C2B-C3B-CAB-CBB
16	B	817	CLA	C2B-C3B-CAB-CBB
16	B	827	CLA	C2B-C3B-CAB-CBB
16	B	828	CLA	C2B-C3B-CAB-CBB
16	L	205	CLA	C2B-C3B-CAB-CBB
17	2	616	ZEX	C5-C6-C7-C8
17	3	216	ZEX	C5-C6-C7-C8
22	A	844	BCR	C23-C24-C25-C26
22	A	847	BCR	C23-C24-C25-C26
22	A	847	BCR	C23-C24-C25-C30
22	B	845	BCR	C23-C24-C25-C26
22	B	845	BCR	C23-C24-C25-C30
22	B	849	BCR	C23-C24-C25-C26
22	B	849	BCR	C23-C24-C25-C30
22	F	804	BCR	C1-C6-C7-C8
22	F	804	BCR	C5-C6-C7-C8
22	I	101	BCR	C23-C24-C25-C26
22	I	101	BCR	C23-C24-C25-C30
22	J	103	BCR	C23-C24-C25-C26
22	K	103	BCR	C1-C6-C7-C8
22	K	103	BCR	C5-C6-C7-C8
22	K	103	BCR	C23-C24-C25-C26
16	A	812	CLA	C2-C1-O2A-CGA
16	B	801	CLA	C2-C1-O2A-CGA
16	B	838	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
16	B	836	CLA	CAA-CBA-CGA-O1A
16	B	842	CLA	CAA-CBA-CGA-O1A
16	A	804	CLA	C4-C3-C5-C6
16	B	802	CLA	C2-C3-C5-C6
16	B	833	CLA	C2-C3-C5-C6
16	B	831	CLA	O1A-CGA-O2A-C1
16	B	809	CLA	C15-C16-C17-C18
16	O	203	CLA	CAA-CBA-CGA-O2A
16	A	805	CLA	C10-C11-C12-C13
16	1	602	CLA	C11-C12-C13-C14
16	A	808	CLA	C10-C11-C12-C13
21	A	841	LHG	O8-C23-C24-C25
16	B	802	CLA	C4-C3-C5-C6
16	A	811	CLA	CAA-CBA-CGA-O2A
16	B	803	CLA	CAA-CBA-CGA-O2A
16	B	808	CLA	CAA-CBA-CGA-O2A
16	A	804	CLA	C2-C3-C5-C6
16	A	810	CLA	C2-C3-C5-C6
16	A	813	CLA	CAA-CBA-CGA-O1A
16	A	839	CLA	C10-C11-C12-C13
16	L	203	CLA	C2A-CAA-CBA-CGA
16	2	602	CLA	C11-C12-C13-C14
16	A	828	CLA	C14-C13-C15-C16
16	3	203	CLA	CAA-CBA-CGA-O2A
16	A	808	CLA	C1A-C2A-CAA-CBA
16	A	826	CLA	C1A-C2A-CAA-CBA
16	A	829	CLA	C1A-C2A-CAA-CBA
16	B	816	CLA	C1A-C2A-CAA-CBA
16	1	607	CLA	CAA-CBA-CGA-O1A
16	2	605	CLA	CAA-CBA-CGA-O1A
16	A	805	CLA	C4-C3-C5-C6
16	B	833	CLA	C4-C3-C5-C6
16	2	602	CLA	CAA-CBA-CGA-O2A
16	2	608	CLA	CAA-CBA-CGA-O2A
16	A	822	CLA	CAA-CBA-CGA-O2A
17	2	615	ZEX	C31-C32-C33-C34
17	3	215	ZEX	C31-C32-C33-C34
16	A	836	CLA	C8-C10-C11-C12
16	B	834	CLA	C10-C11-C12-C13
16	A	837	CLA	CAA-CBA-CGA-O2A
16	B	807	CLA	CAA-CBA-CGA-O2A
16	B	809	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	B	838	CLA	CAA-CBA-CGA-O2A
16	B	826	CLA	O1D-CGD-O2D-CED
16	B	808	CLA	C16-C17-C18-C19
16	B	830	CLA	CAA-CBA-CGA-O2A
16	A	822	CLA	C2-C3-C5-C6
16	A	802	CLA	C2-C1-O2A-CGA
16	A	839	CLA	C12-C13-C15-C16
16	B	819	CLA	C6-C7-C8-C10
16	B	829	CLA	C11-C12-C13-C15
16	B	831	CLA	C6-C7-C8-C10
16	A	802	CLA	C2-C3-C5-C6
16	2	612	CLA	CAA-CBA-CGA-O2A
16	3	205	CLA	C2A-CAA-CBA-CGA
16	1	607	CLA	CAA-CBA-CGA-O2A
16	2	611	CLA	CAA-CBA-CGA-O1A
16	1	604	CLA	C3A-C2A-CAA-CBA
16	B	837	CLA	C3A-C2A-CAA-CBA
16	B	804	CLA	C15-C16-C17-C18
21	A	842	LHG	C18-C19-C20-C21
16	3	203	CLA	CAA-CBA-CGA-O1A
16	A	811	CLA	CAA-CBA-CGA-O1A
16	1	602	CLA	CBA-CGA-O2A-C1
21	A	842	LHG	C26-C27-C28-C29
25	B	850	DGD	CBA-CCA-CDA-CEA
16	B	808	CLA	CAA-CBA-CGA-O1A
16	B	829	CLA	C11-C12-C13-C14
16	B	833	CLA	C11-C10-C8-C9
16	B	841	CLA	C14-C13-C15-C16
16	2	602	CLA	CAA-CBA-CGA-O1A
16	A	832	CLA	C5-C6-C7-C8
16	B	834	CLA	C4-C3-C5-C6
16	B	833	CLA	CAA-CBA-CGA-O1A
16	B	842	CLA	C13-C15-C16-C17
17	3	201	ZEX	C7-C8-C9-C10
16	B	801	CLA	C10-C11-C12-C13
16	B	830	CLA	CAA-CBA-CGA-O1A
16	B	838	CLA	CAA-CBA-CGA-O1A
25	B	850	DGD	CFB-CGB-CHB-CIB
16	O	203	CLA	CAA-CBA-CGA-O1A
16	B	812	CLA	C4-C3-C5-C6
16	1	608	CLA	CAA-CBA-CGA-O2A
16	3	209	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	A	831	CLA	CAA-CBA-CGA-O2A
16	2	605	CLA	CAA-CBA-CGA-O2A
16	3	206	CLA	CAA-CBA-CGA-O1A
16	A	812	CLA	CAD-CBD-CGD-O2D
16	A	815	CLA	CAD-CBD-CGD-O2D
25	B	850	DGD	O2G-C1B-C2B-C3B
16	2	612	CLA	CAA-CBA-CGA-O1A
16	B	803	CLA	CAA-CBA-CGA-O1A
25	B	850	DGD	C7A-C8A-C9A-CAA
16	2	608	CLA	CAA-CBA-CGA-O1A
16	A	822	CLA	CAA-CBA-CGA-O1A
16	B	807	CLA	CAA-CBA-CGA-O1A
21	A	841	LHG	O10-C23-C24-C25
16	A	829	CLA	C8-C10-C11-C12
16	B	810	CLA	C15-C16-C17-C18
16	B	815	CLA	C2C-C3C-CAC-CBC
16	A	817	CLA	CAA-CBA-CGA-O2A
16	A	826	CLA	CAA-CBA-CGA-O2A
16	B	814	CLA	CAA-CBA-CGA-O2A
16	L	205	CLA	CAA-CBA-CGA-O2A
16	B	801	CLA	C13-C15-C16-C17
16	B	822	CLA	CAA-CBA-CGA-O2A
16	A	837	CLA	CAA-CBA-CGA-O1A
21	A	841	LHG	C32-C33-C34-C35
16	B	809	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

147 monomers are involved in 413 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	831	CLA	5	0
22	L	206	BCR	9	0
16	A	827	CLA	6	0
16	B	831	CLA	3	0
16	1	607	CLA	1	0
22	A	843	BCR	3	0
16	A	829	CLA	6	0
16	B	830	CLA	3	0
16	3	206	CLA	4	0
16	A	819	CLA	3	0
16	B	829	CLA	8	0
16	3	205	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	849	BCR	1	0
16	2	602	CLA	4	0
16	A	816	CLA	3	0
16	B	802	CLA	23	0
17	2	615	ZEX	4	0
22	I	101	BCR	1	0
16	L	201	CLA	2	0
16	B	803	CLA	7	0
16	1	602	CLA	1	0
22	J	102	BCR	3	0
16	B	833	CLA	9	0
16	B	820	CLA	3	0
22	A	847	BCR	3	0
16	B	812	CLA	3	0
22	A	846	BCR	3	0
19	A	801	CL0	55	0
17	1	617	ZEX	2	0
16	A	836	CLA	5	0
16	B	839	CLA	4	0
16	3	212	CLA	1	0
17	1	613	ZEX	6	0
16	B	837	CLA	2	0
16	A	810	CLA	3	0
16	3	207	CLA	1	0
16	2	608	CLA	1	0
21	A	842	LHG	2	0
16	A	806	CLA	2	0
16	B	832	CLA	5	0
16	O	203	CLA	1	0
16	A	826	CLA	7	0
16	A	835	CLA	1	0
16	A	852	CLA	3	0
16	A	820	CLA	2	0
17	3	201	ZEX	7	0
16	A	807	CLA	4	0
16	2	605	CLA	1	0
20	B	843	PQN	4	0
16	B	808	CLA	3	0
17	3	214	ZEX	4	0
22	B	849	BCR	3	0
16	A	823	CLA	1	0
17	3	218	ZEX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	802	CLA	7	0
16	B	827	CLA	6	0
17	3	216	ZEX	3	0
22	J	103	BCR	4	0
22	B	848	BCR	5	0
16	1	606	CLA	2	0
16	A	832	CLA	3	0
22	B	845	BCR	4	0
16	A	804	CLA	7	0
16	A	833	CLA	6	0
16	B	817	CLA	1	0
16	B	834	CLA	2	0
22	F	801	BCR	3	0
16	A	812	CLA	4	0
16	A	822	CLA	1	0
16	B	838	CLA	2	0
16	F	803	CLA	1	0
16	1	603	CLA	2	0
16	A	808	CLA	3	0
16	B	818	CLA	2	0
17	1	616	ZEX	1	0
16	A	824	CLA	2	0
16	3	204	CLA	1	0
17	1	614	ZEX	6	0
16	A	830	CLA	1	0
16	B	801	CLA	8	0
16	1	604	CLA	1	0
16	1	612	CLA	1	0
16	K	102	CLA	2	0
16	F	802	CLA	3	0
21	A	841	LHG	1	0
16	A	850	CLA	6	0
16	B	825	CLA	5	0
16	J	101	CLA	1	0
16	B	816	CLA	1	0
17	1	615	ZEX	2	0
22	B	847	BCR	5	0
16	3	210	CLA	1	0
16	A	821	CLA	1	0
25	B	850	DGD	4	0
20	A	840	PQN	2	0
22	L	207	BCR	1	0

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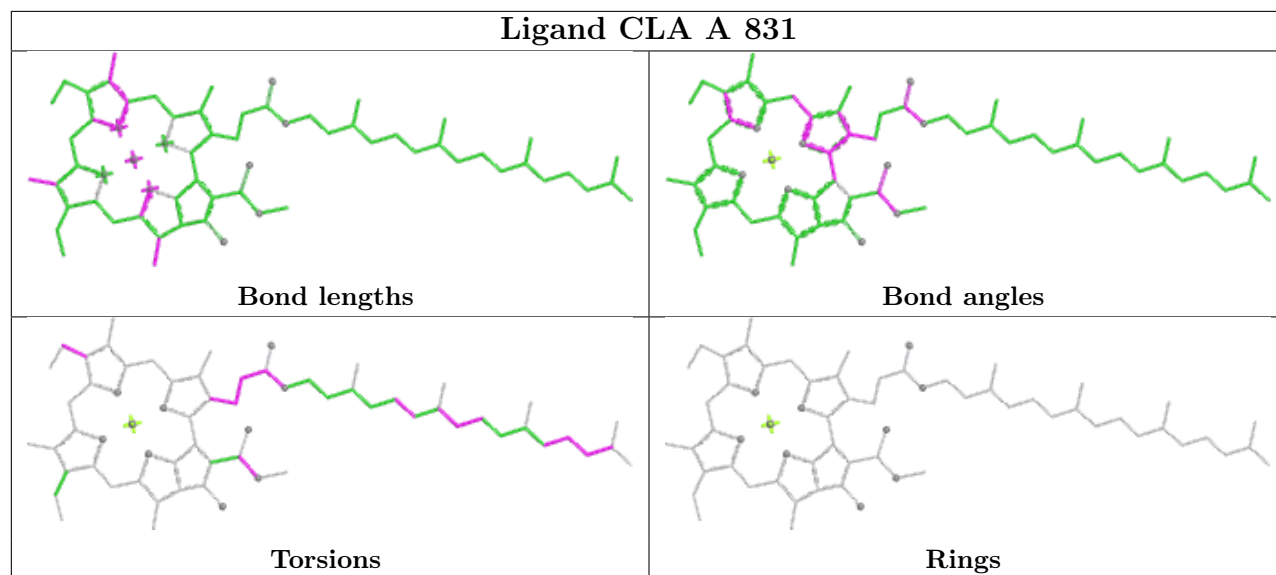
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	824	CLA	2	0
16	1	611	CLA	1	0
16	A	834	CLA	4	0
16	B	809	CLA	3	0
22	A	845	BCR	4	0
17	2	616	ZEX	1	0
16	3	209	CLA	1	0
16	B	826	CLA	4	0
17	3	215	ZEX	5	0
16	B	840	CLA	7	0
16	A	838	CLA	3	0
16	B	810	CLA	5	0
16	B	811	CLA	8	0
16	B	807	CLA	9	0
16	A	828	CLA	4	0
16	A	818	CLA	7	0
16	B	828	CLA	6	0
16	2	604	CLA	2	0
22	K	103	BCR	4	0
16	B	835	CLA	5	0
16	3	203	CLA	5	0
16	A	825	CLA	4	0
16	B	804	CLA	7	0
17	3	217	ZEX	2	0
16	2	611	CLA	1	0
16	B	836	CLA	1	0
16	B	815	CLA	7	0
16	3	208	CLA	1	0
16	1	609	CLA	2	0
16	2	601	CLA	3	0
16	A	805	CLA	4	0
16	A	815	CLA	1	0
16	O	204	CLA	1	0
17	2	617	ZEX	4	0
16	L	204	CLA	1	0
16	B	821	CLA	2	0
22	L	202	BCR	1	0
16	A	817	CLA	4	0
23	C	102	SF4	1	0
16	A	837	CLA	2	0
16	B	819	CLA	1	0
16	A	851	CLA	2	0

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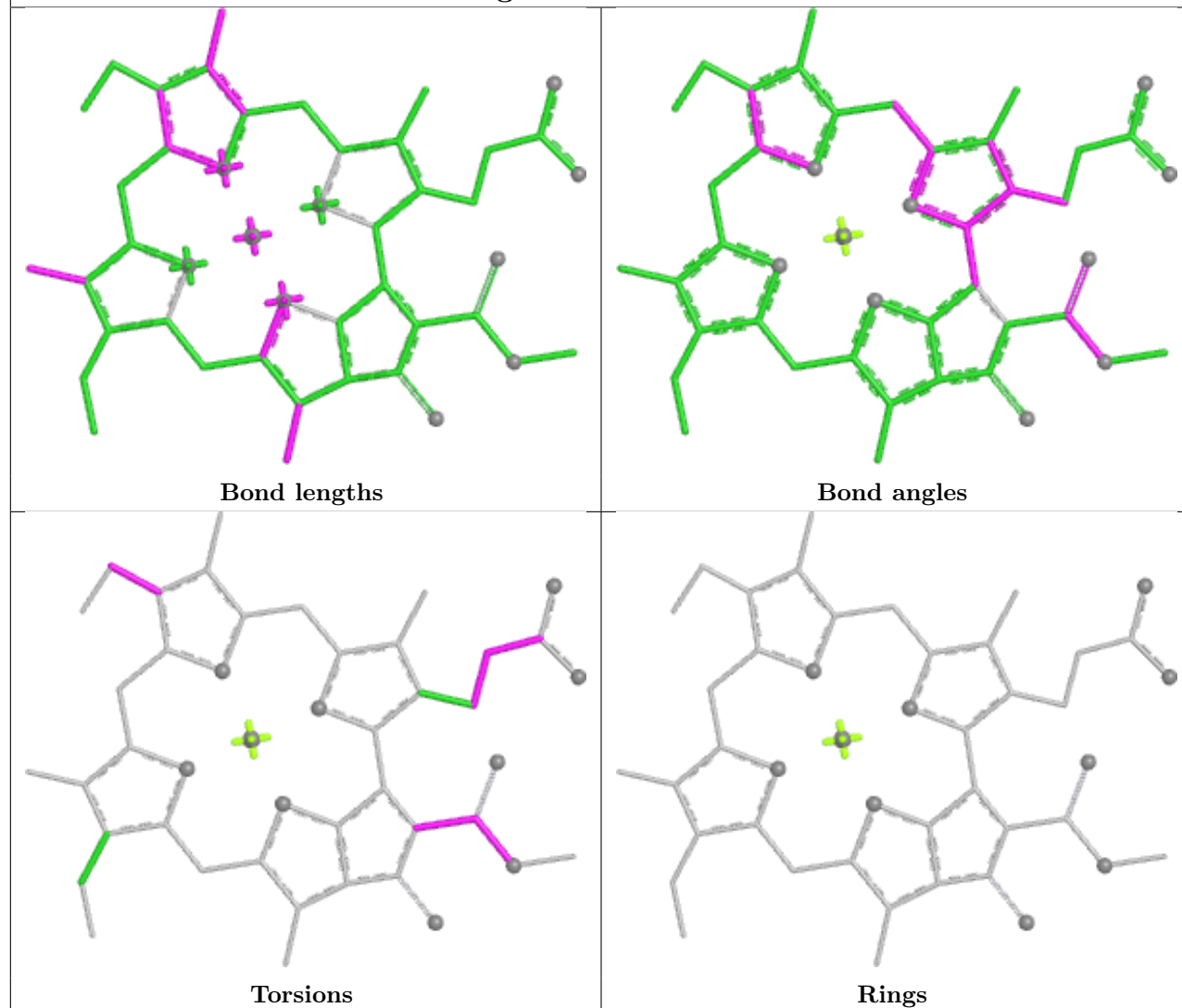
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	2	607	CLA	3	0
16	A	809	CLA	2	0
16	1	605	CLA	1	0
22	B	846	BCR	3	0
16	A	839	CLA	2	0
17	2	614	ZEX	2	0
16	B	842	CLA	4	0
16	B	841	CLA	8	0
16	B	805	CLA	5	0

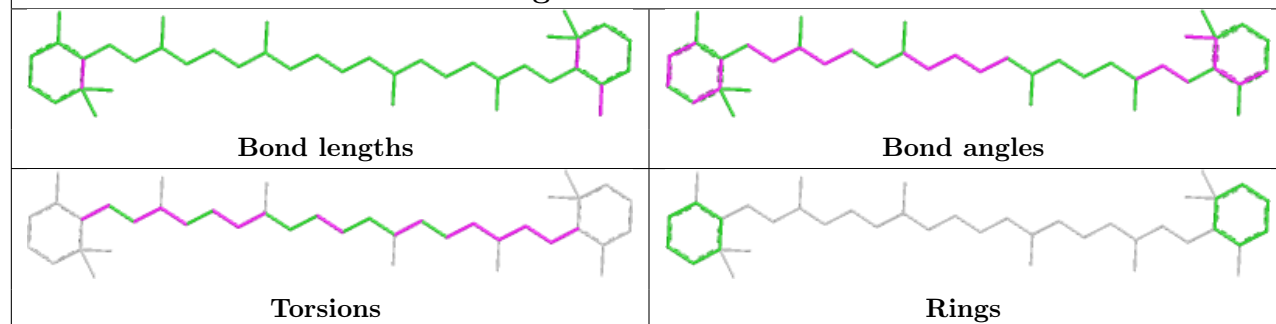
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

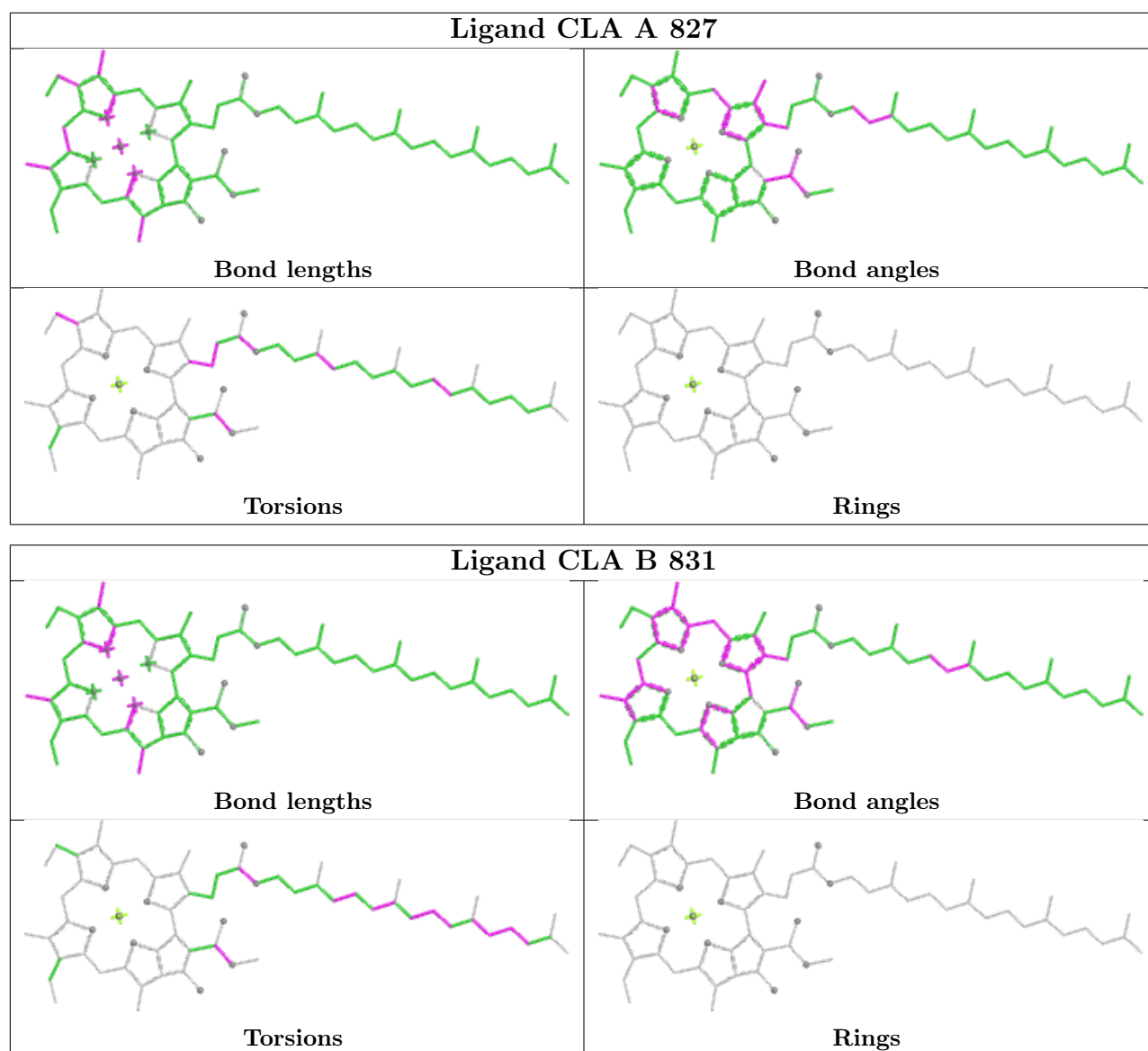


Ligand CLA 2 612

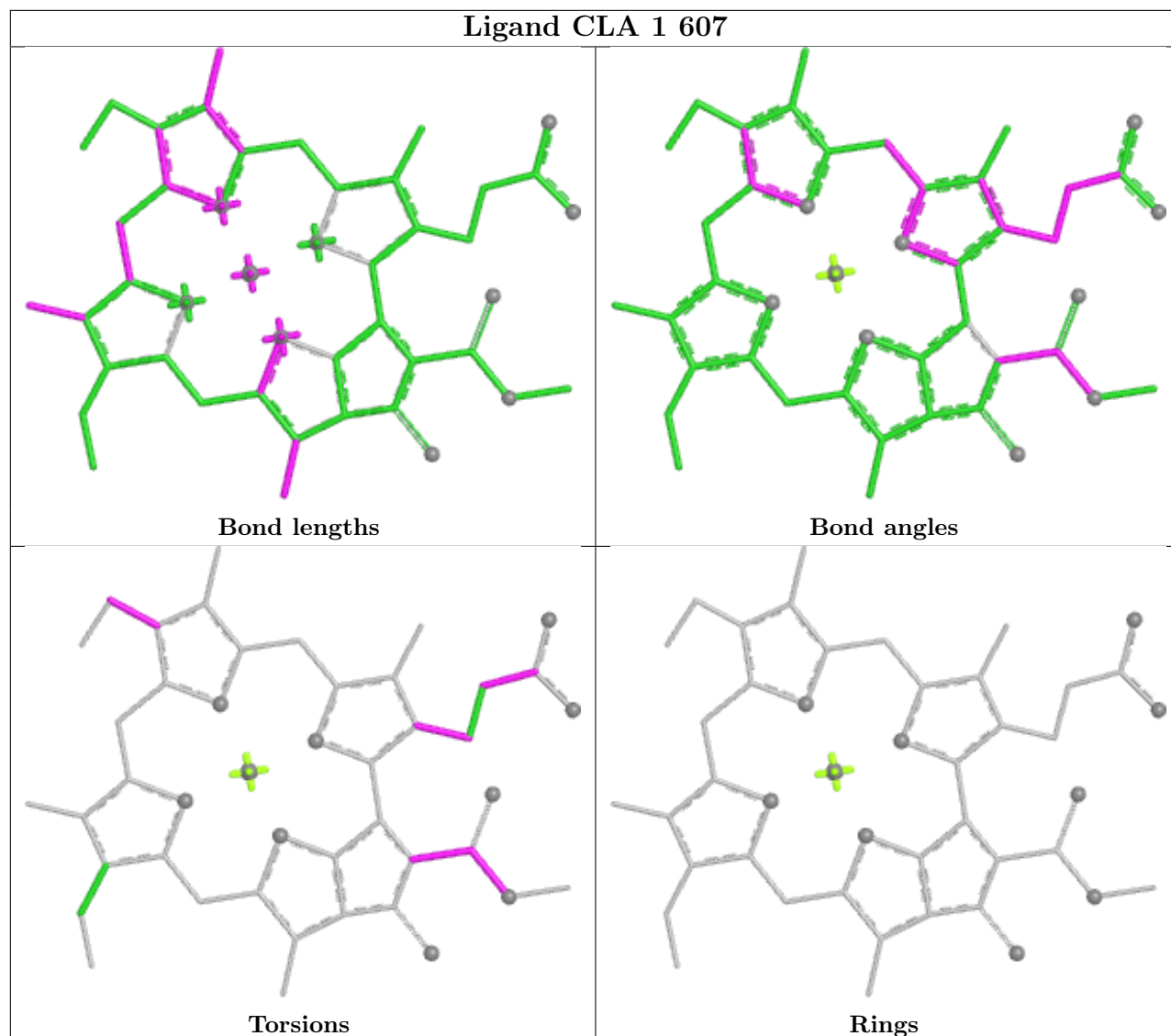


Ligand BCR L 206

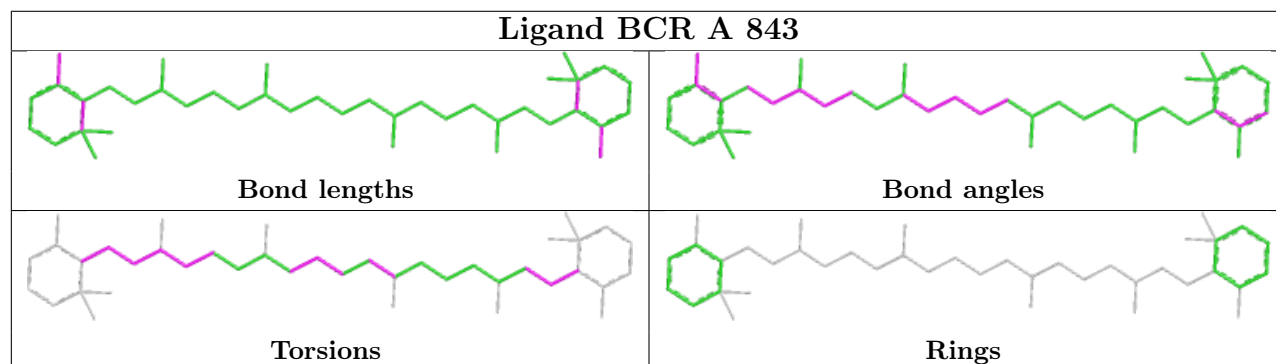


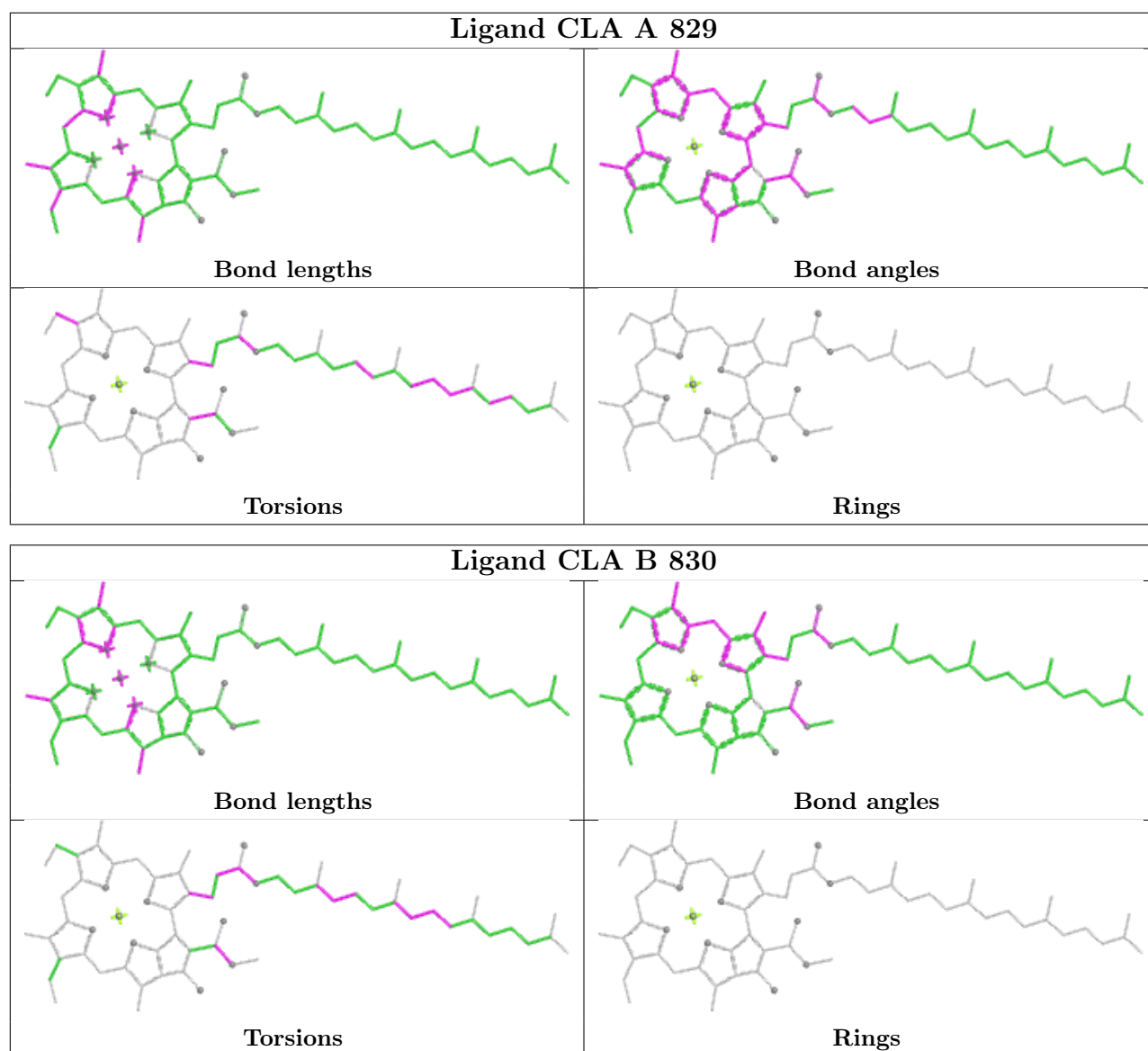


Ligand CLA 1 607

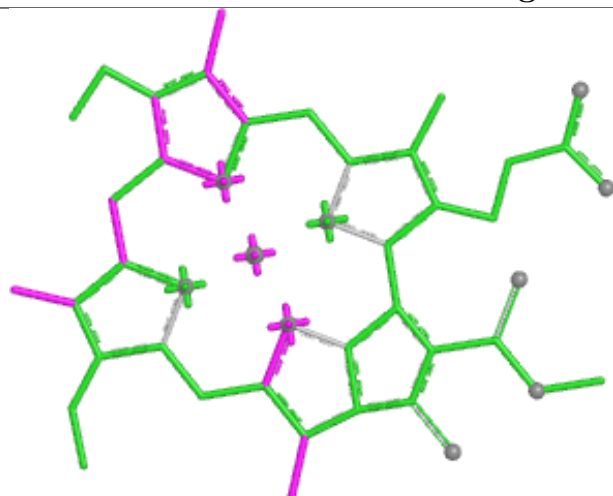


Ligand BCR A 843

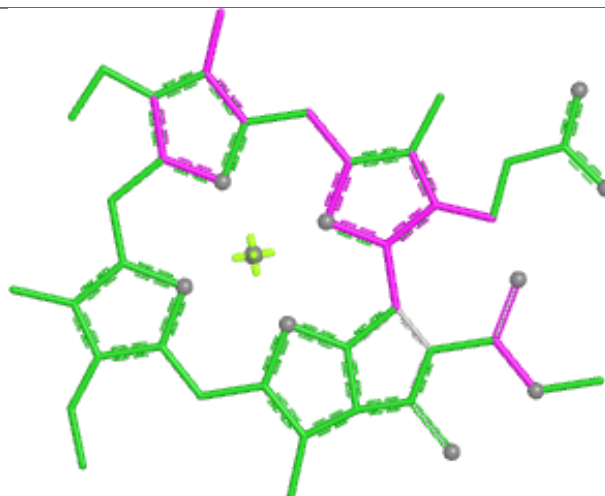




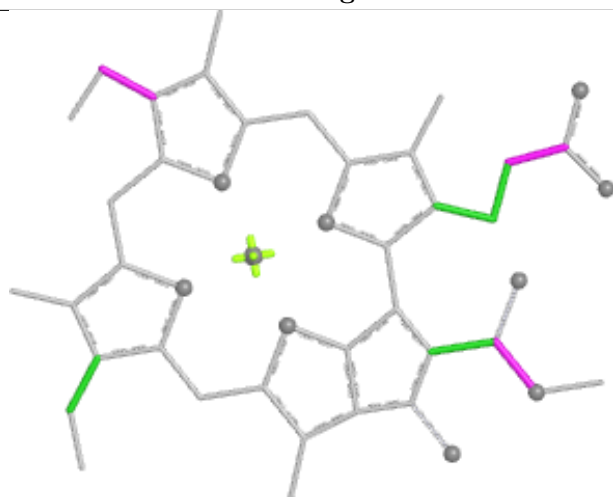
Ligand CLA 1 610



Bond lengths



Bond angles

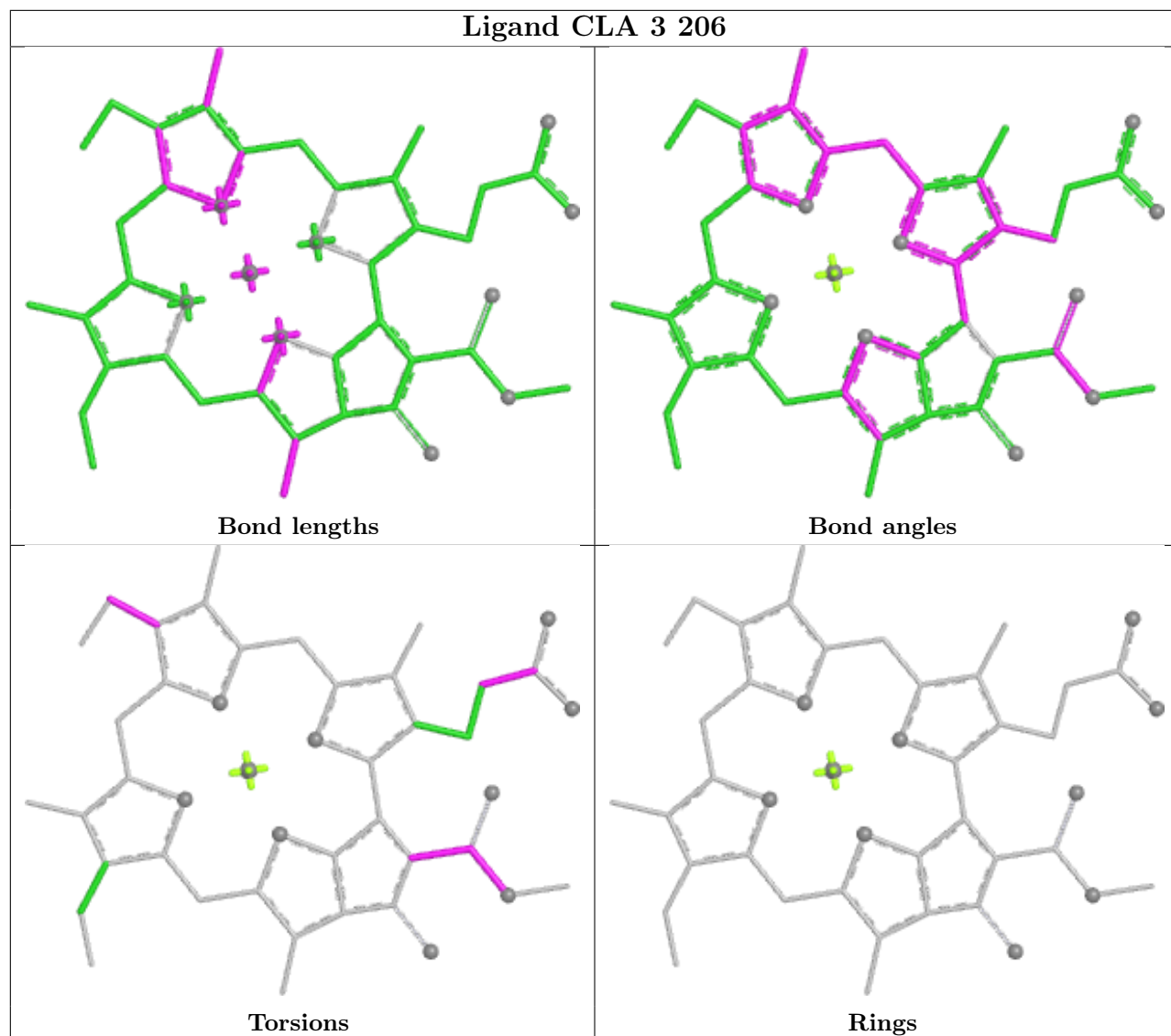


Torsions

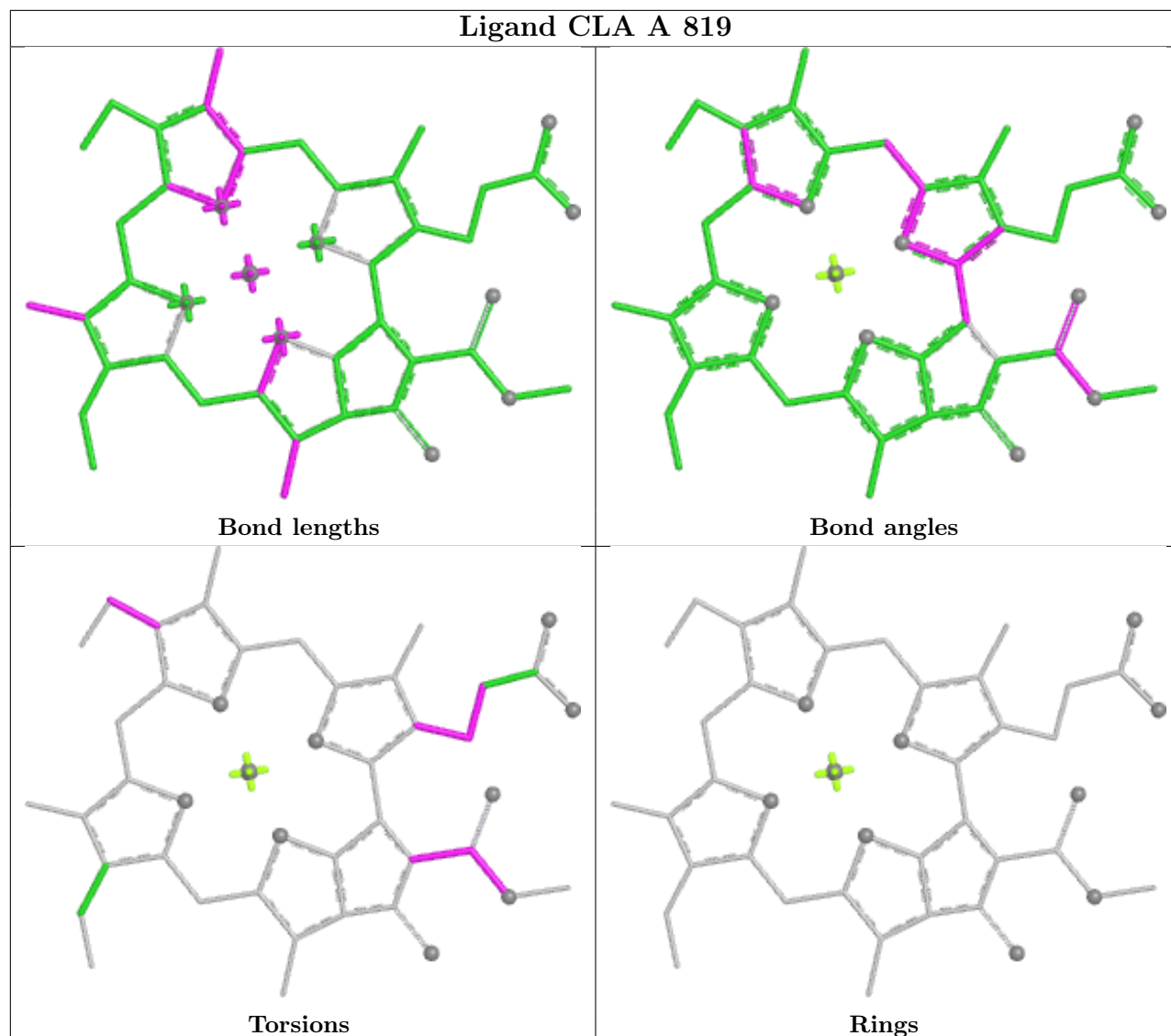


Rings

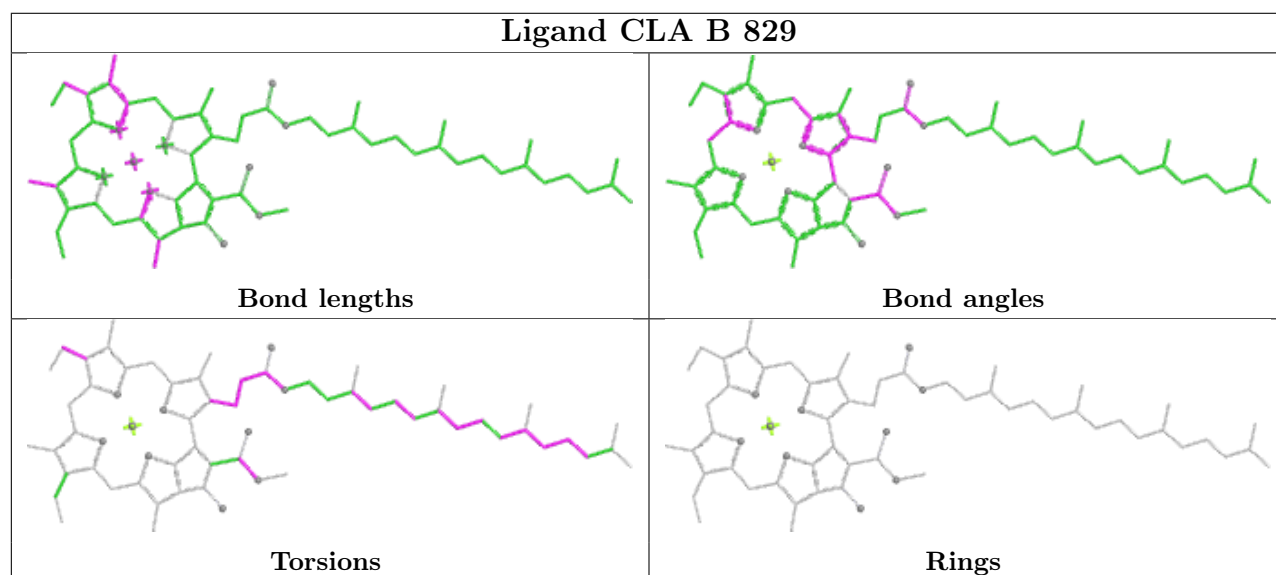
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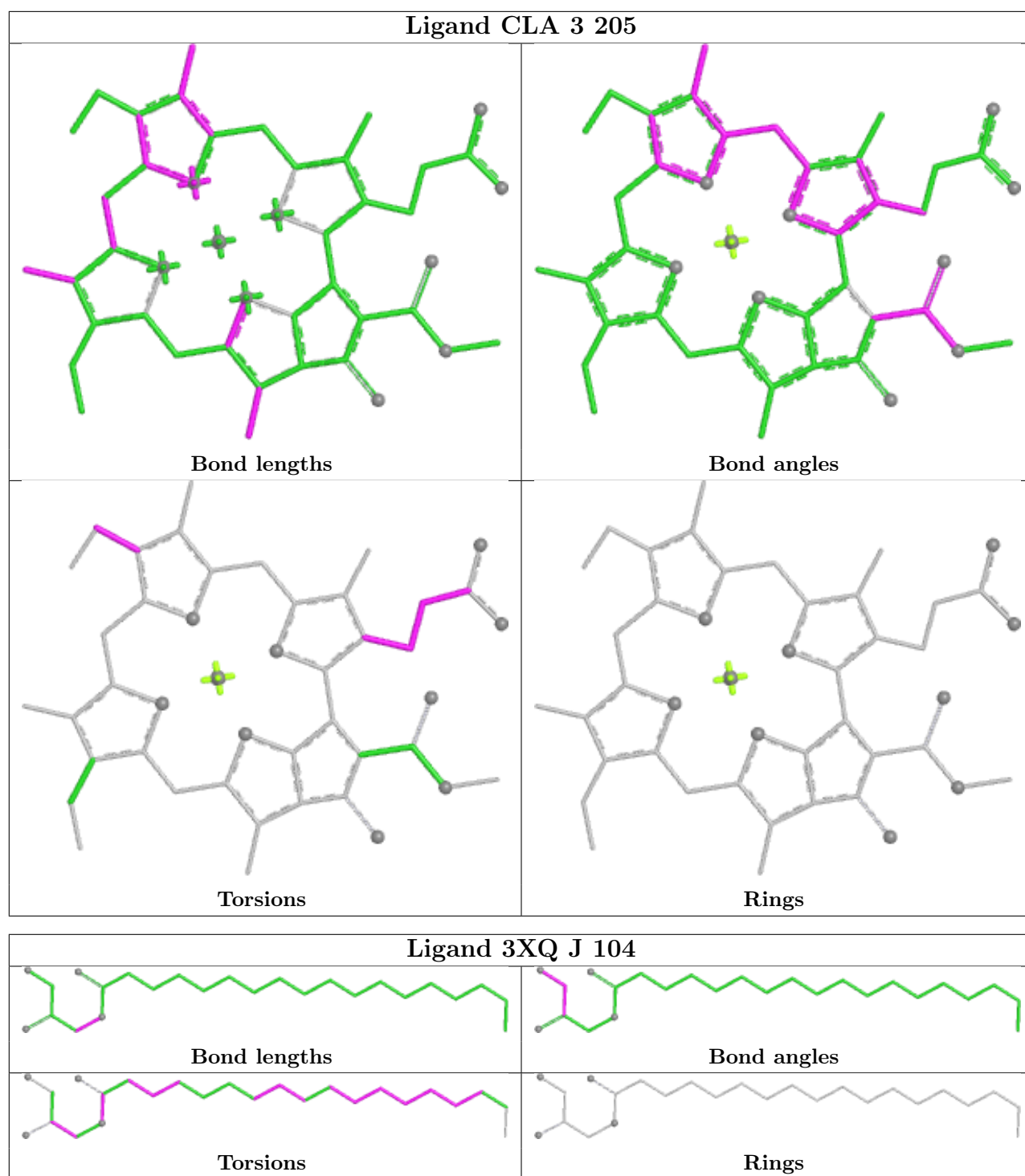


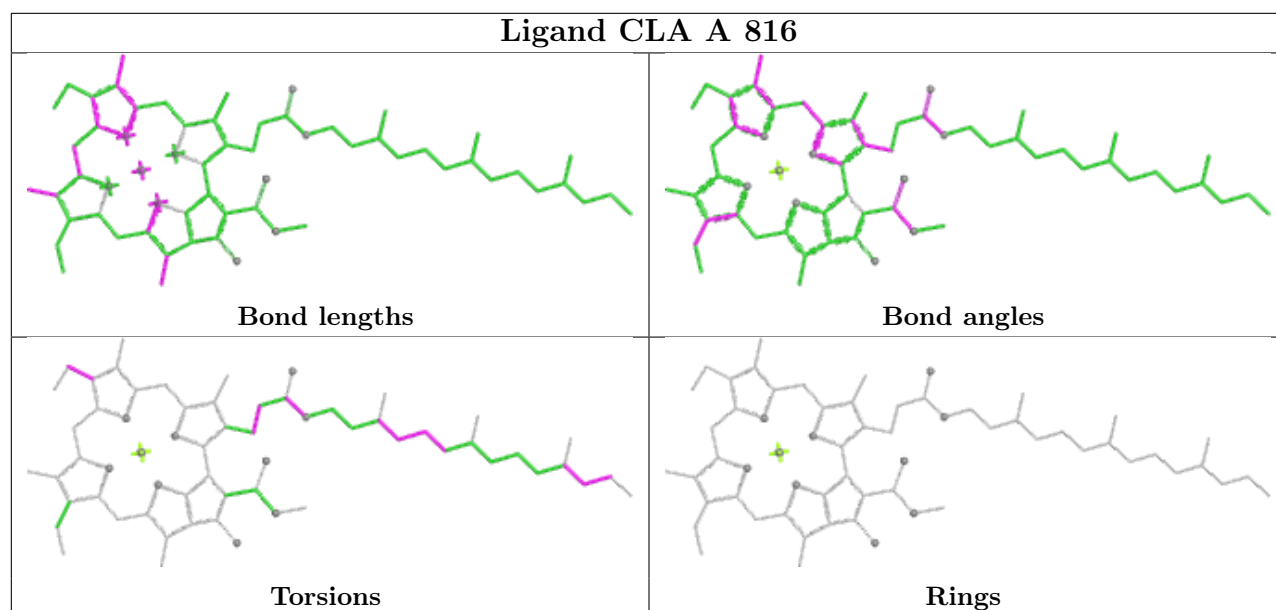
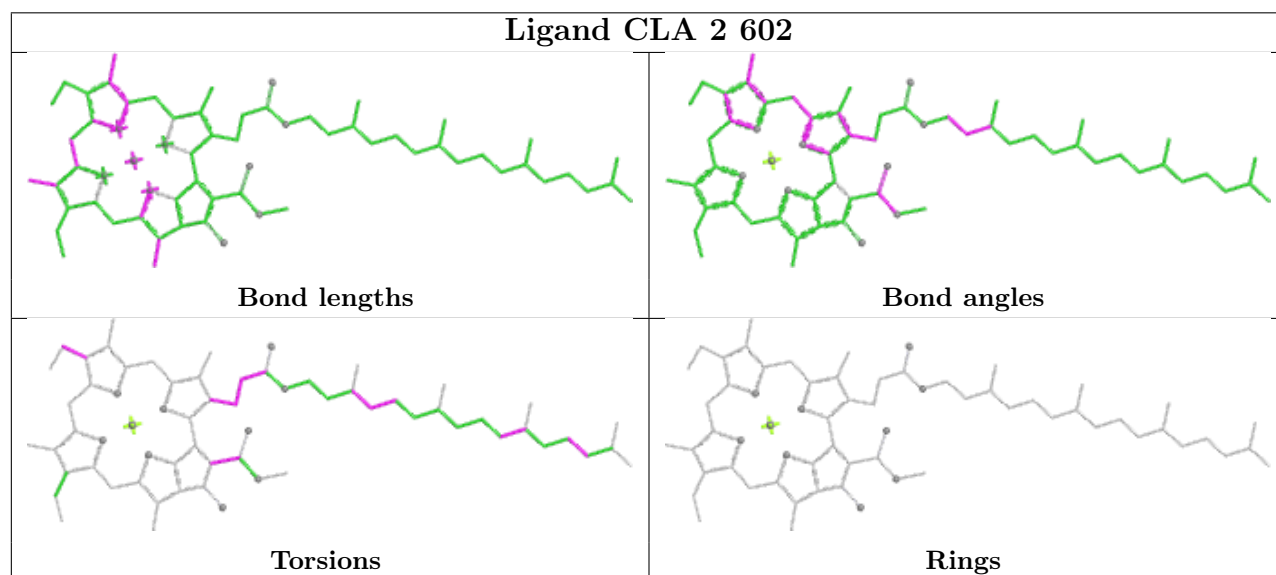
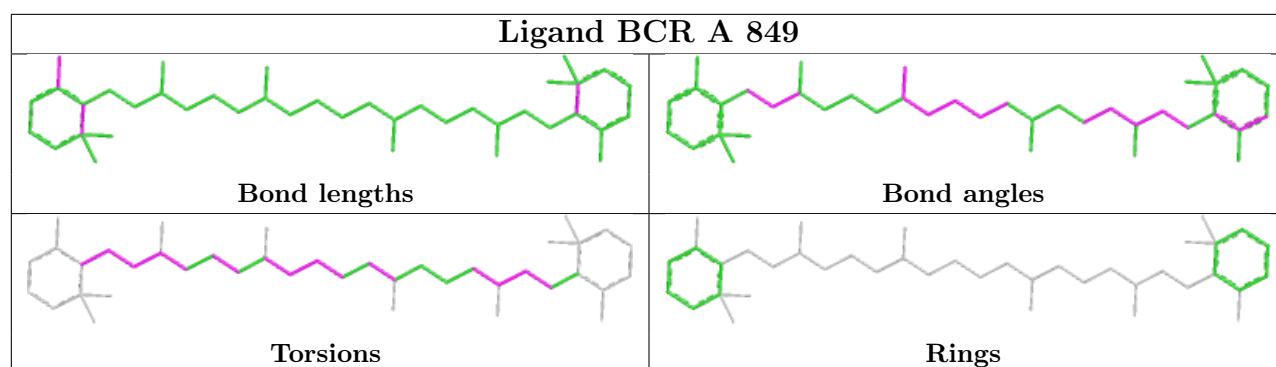
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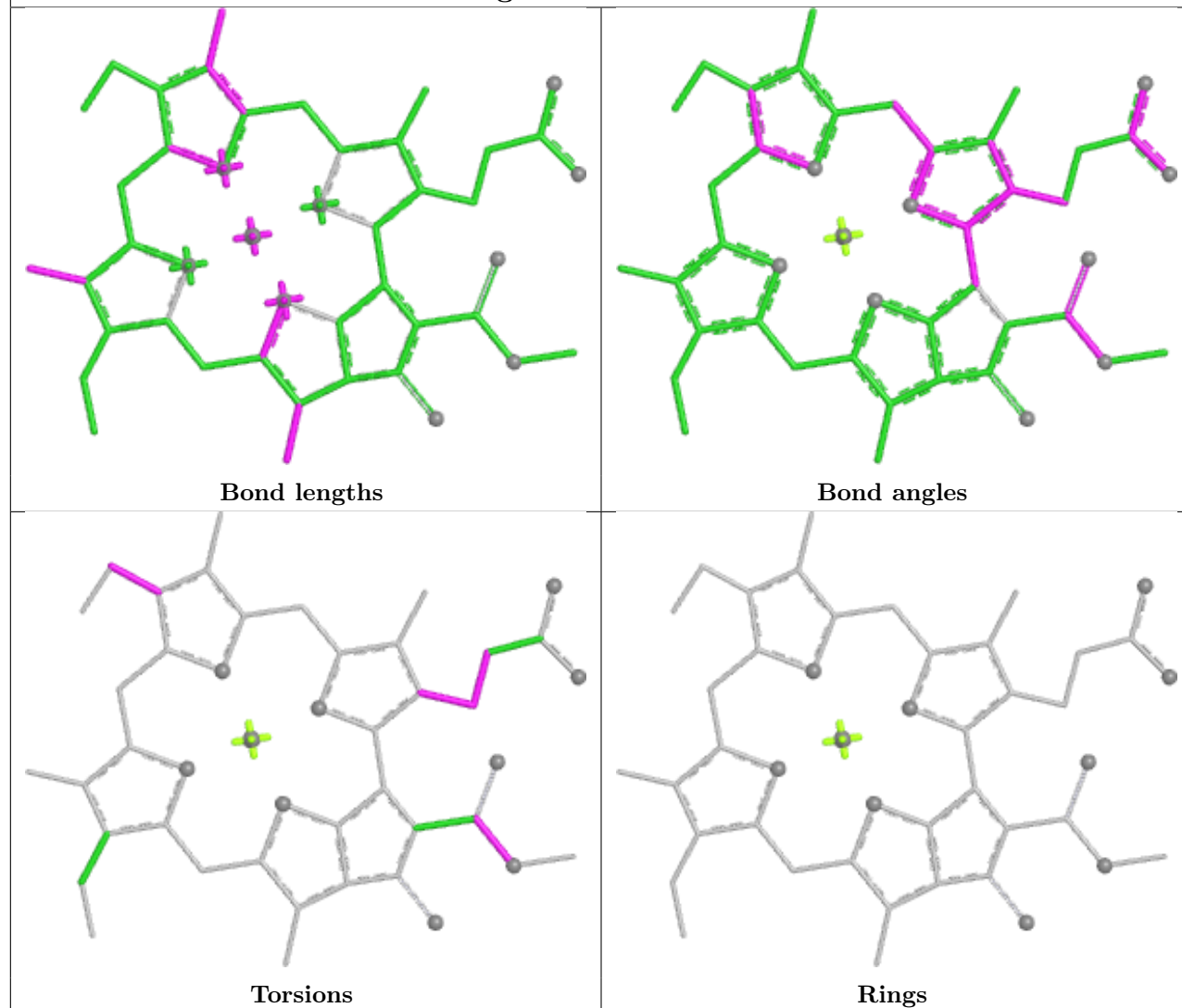
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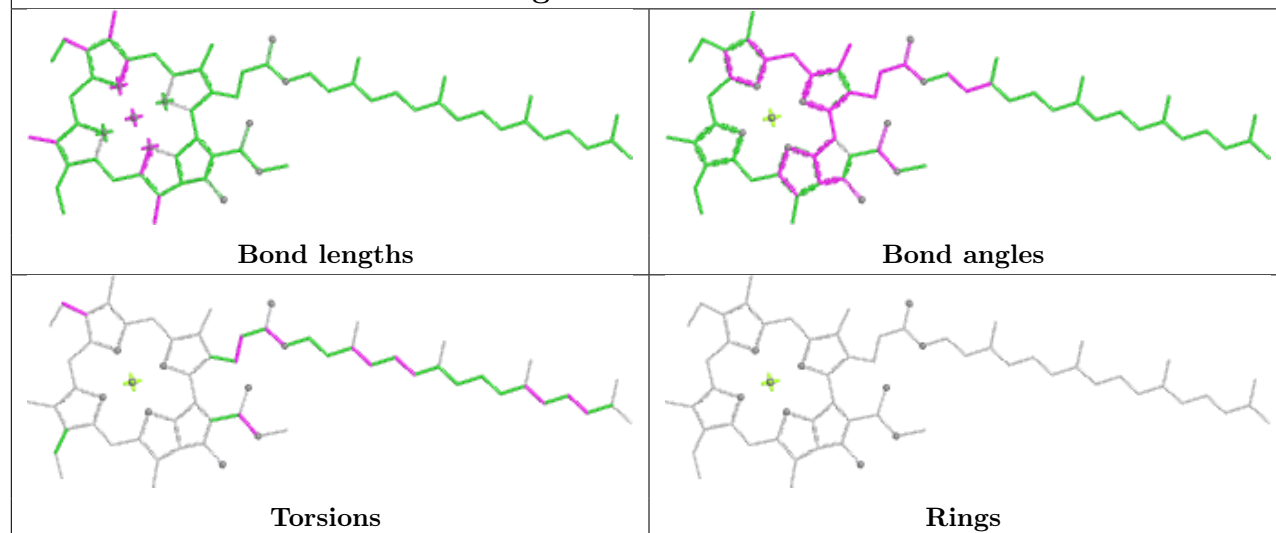


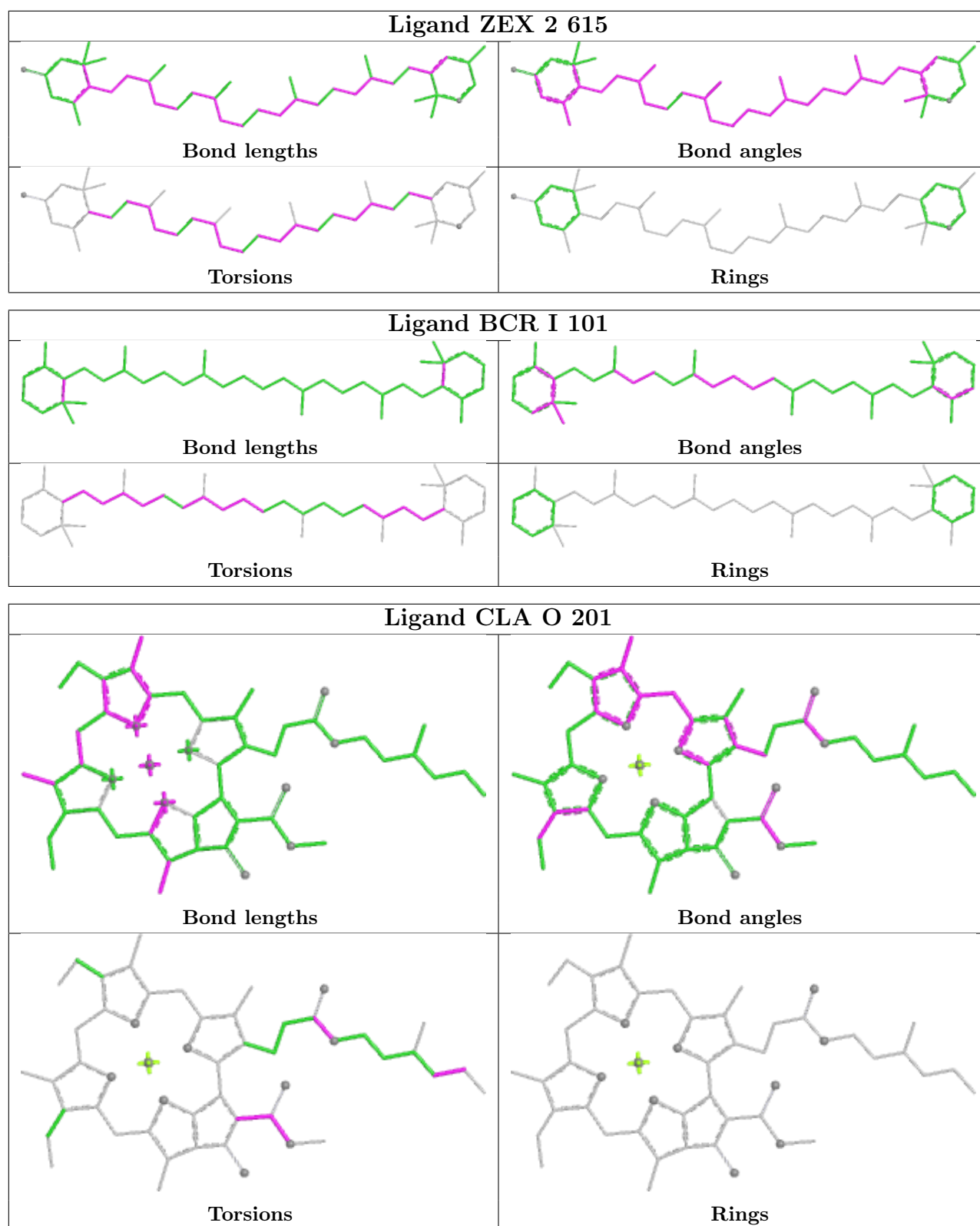


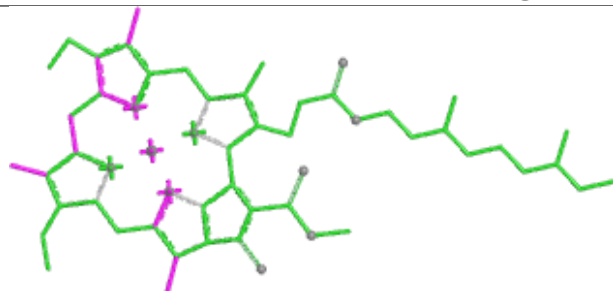
Ligand CLA 2 606



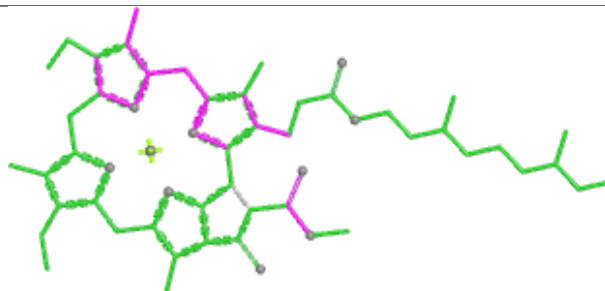
Ligand CLA B 802



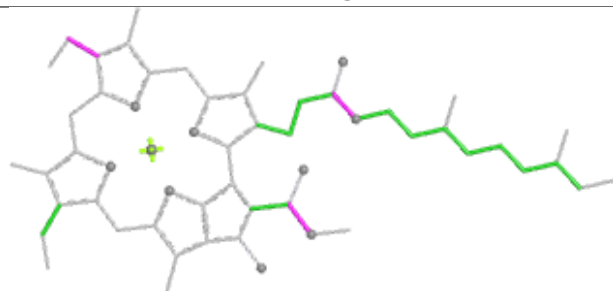


Ligand CLA L 201

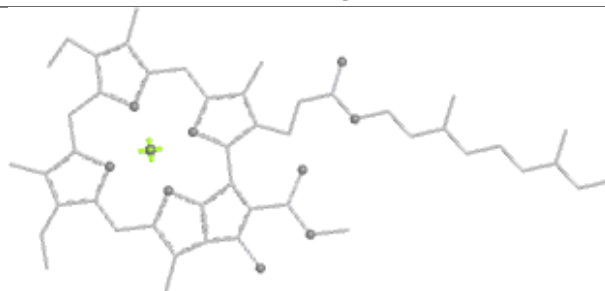
Bond lengths



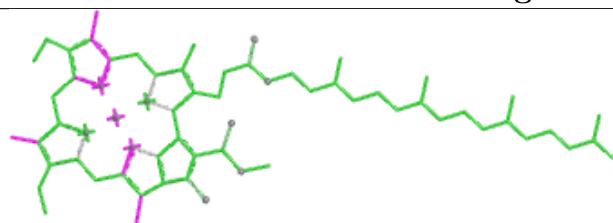
Bond angles



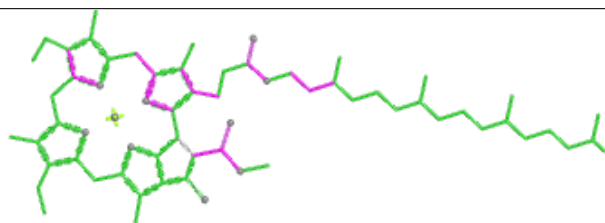
Torsions



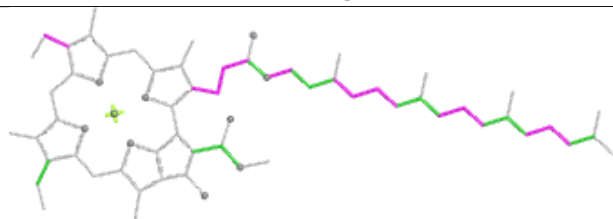
Rings

Ligand CLA B 803

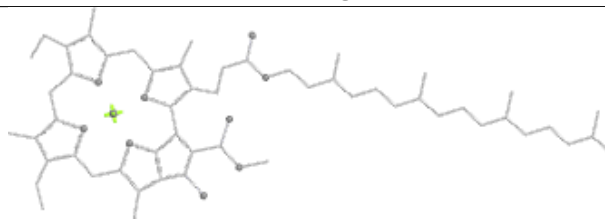
Bond lengths



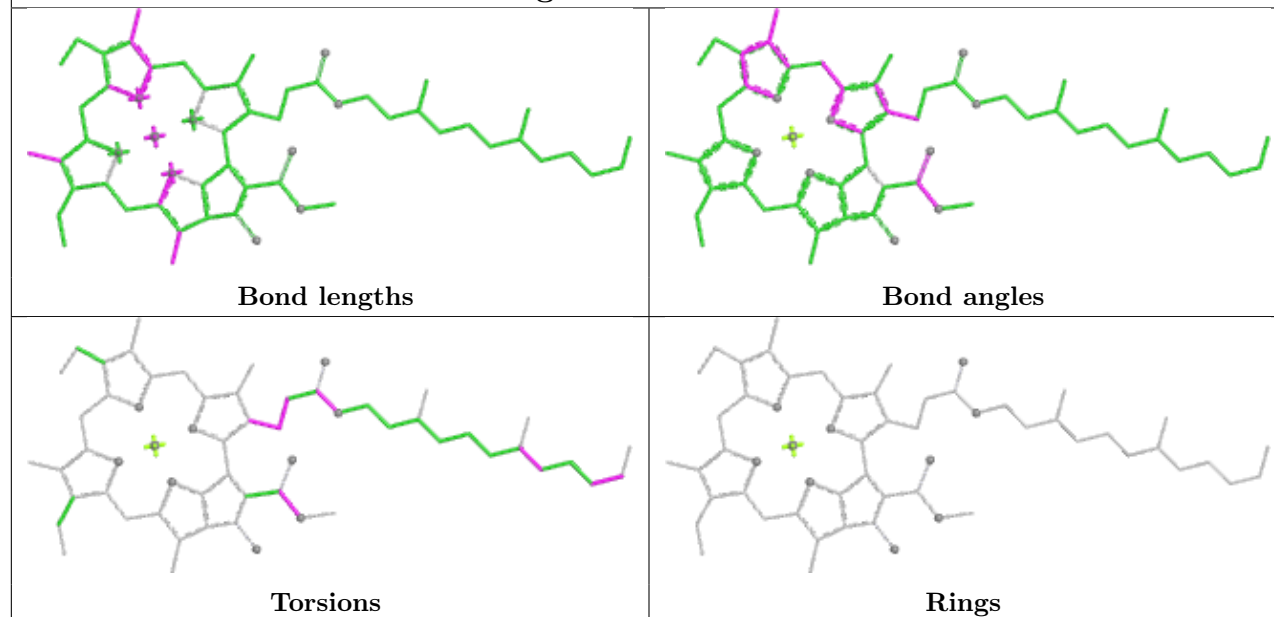
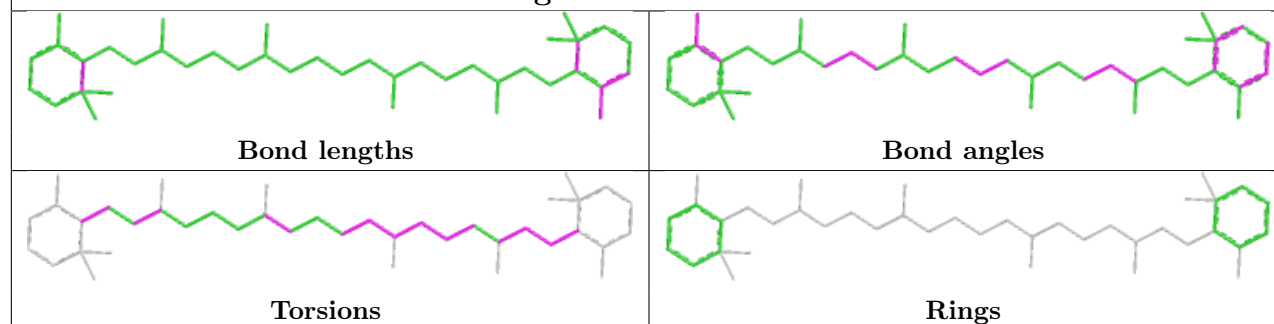
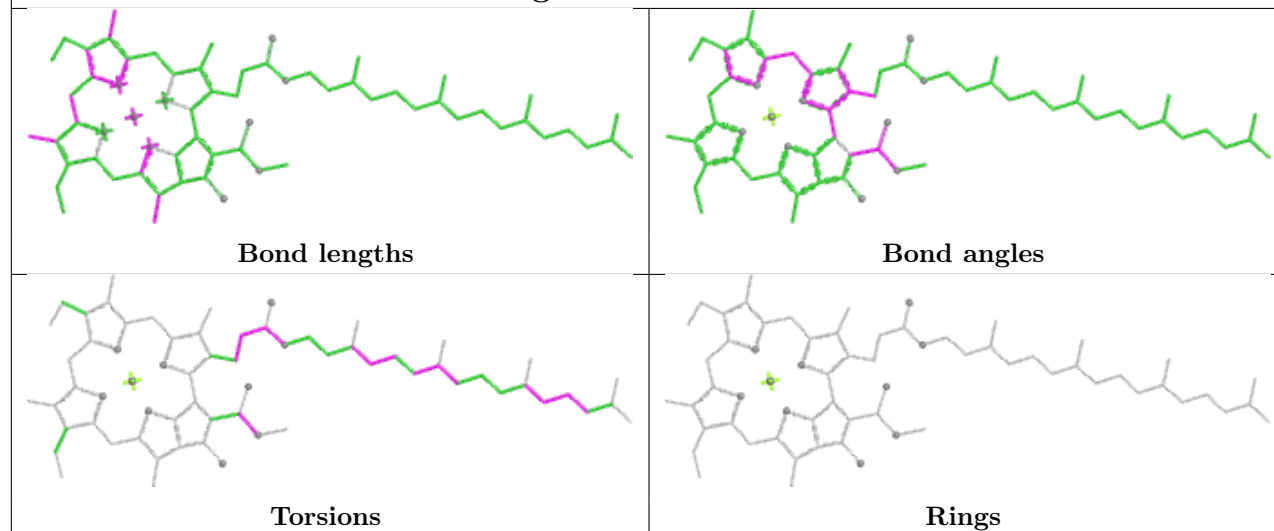
Bond angles

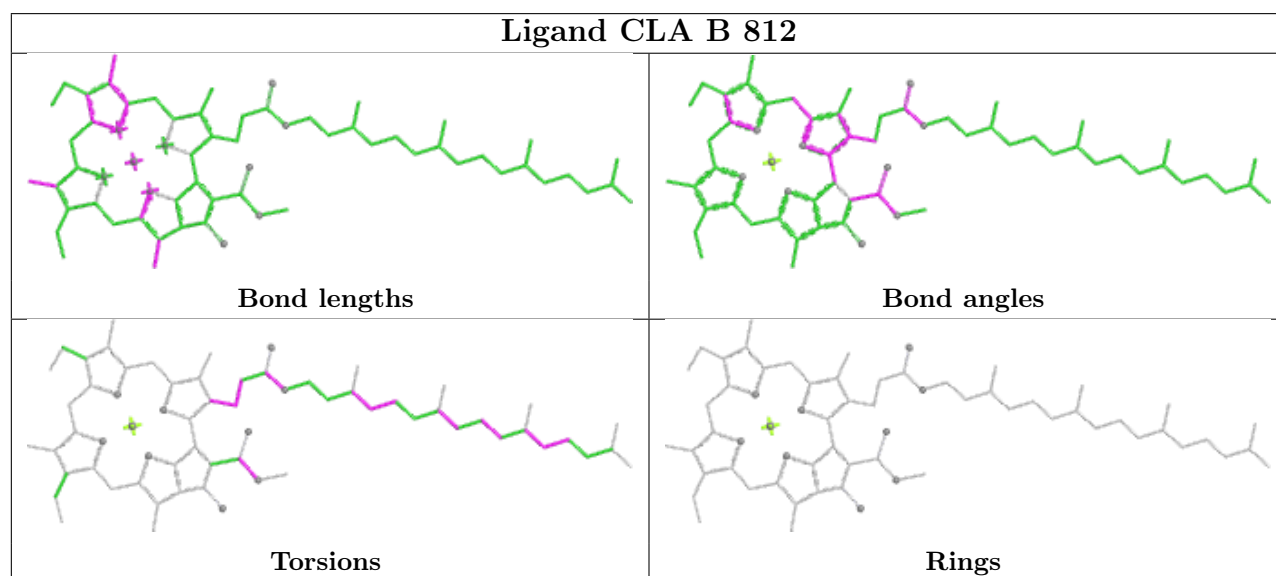
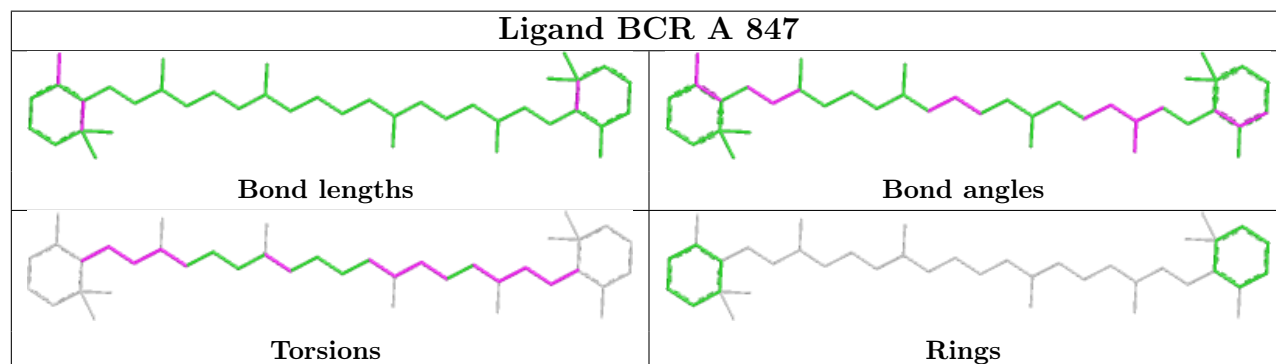
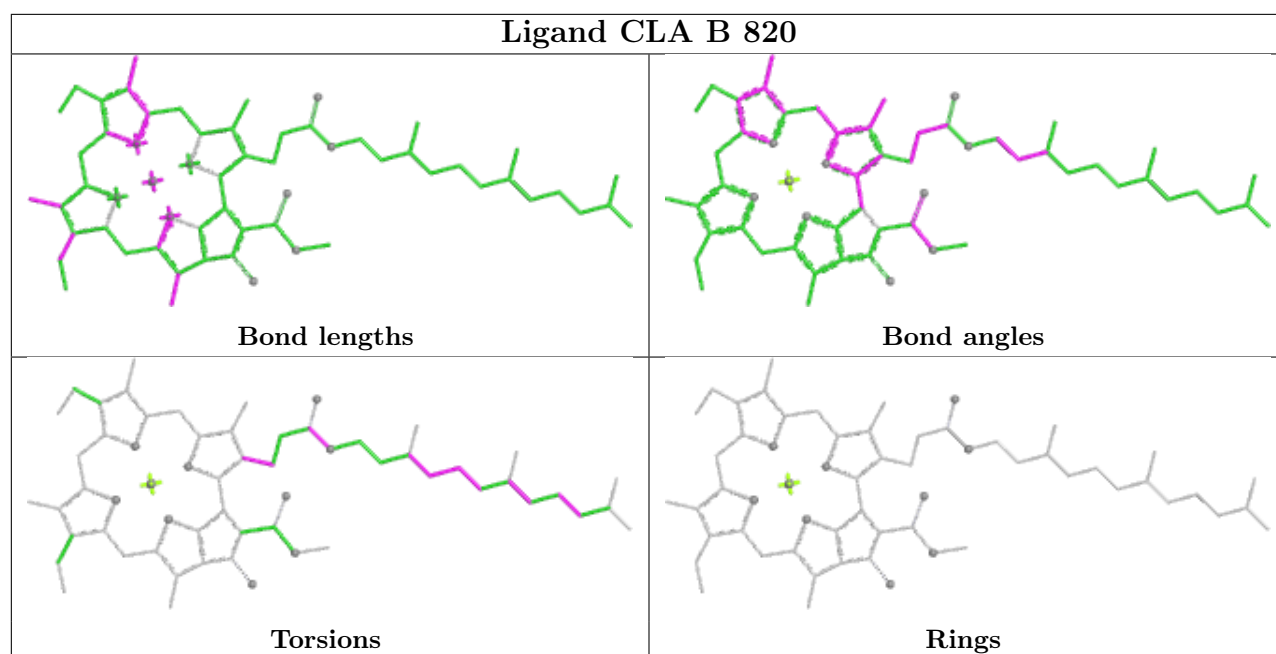


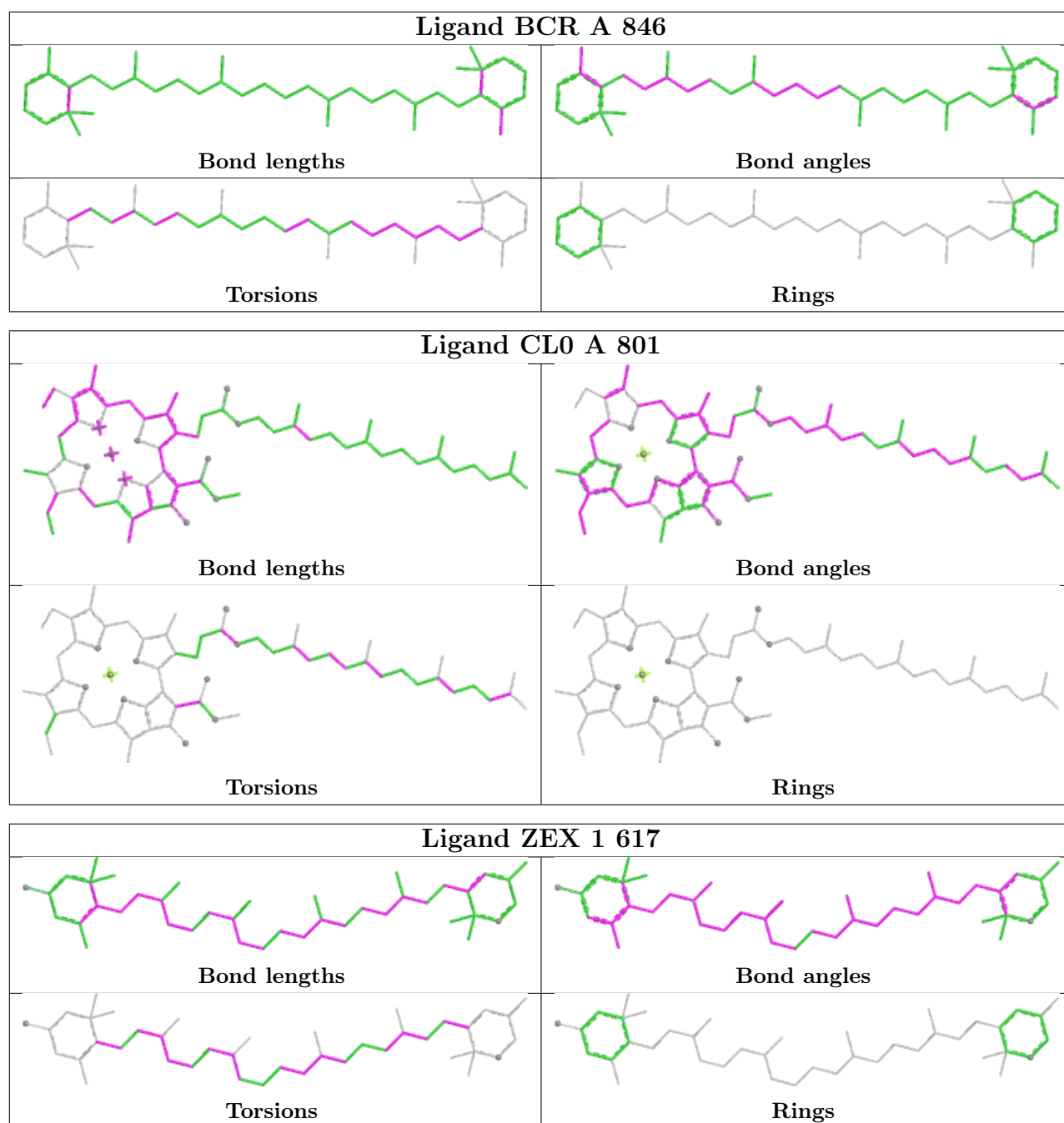
Torsions



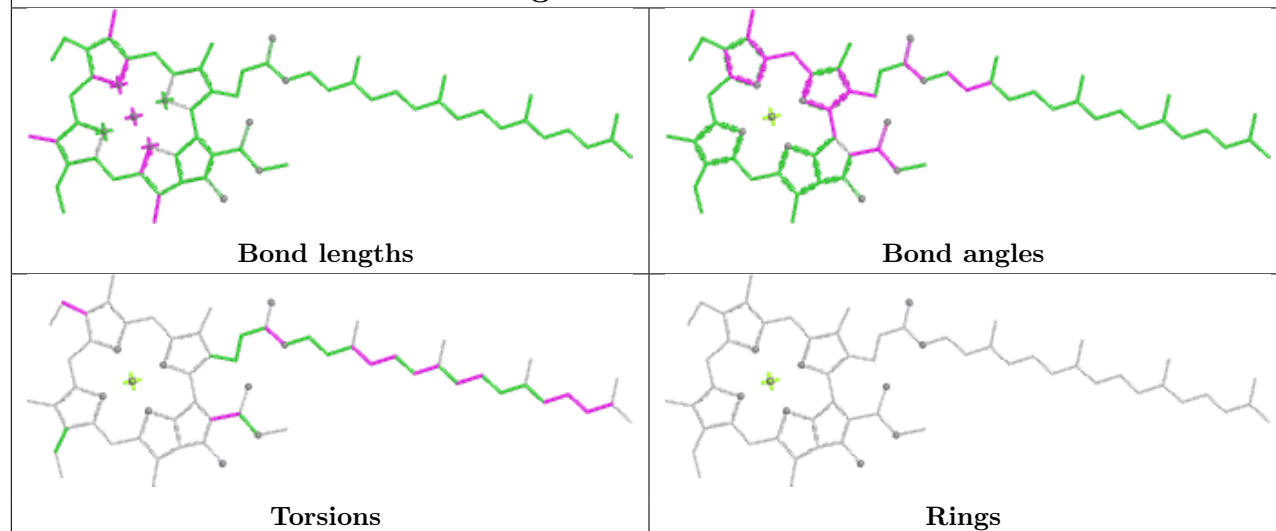
Rings

Ligand CLA 1 602**Ligand BCR J 102****Ligand CLA B 833**

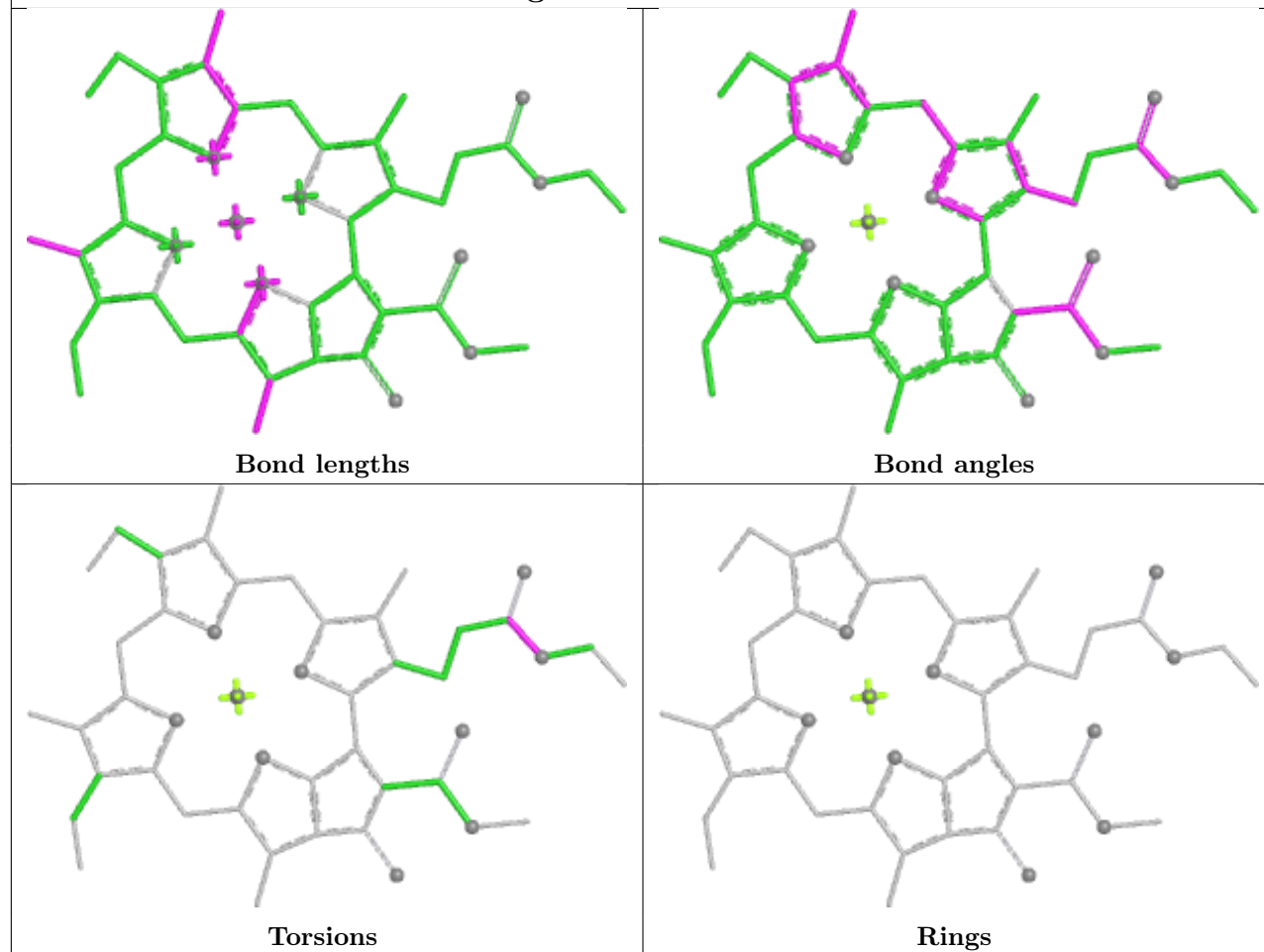




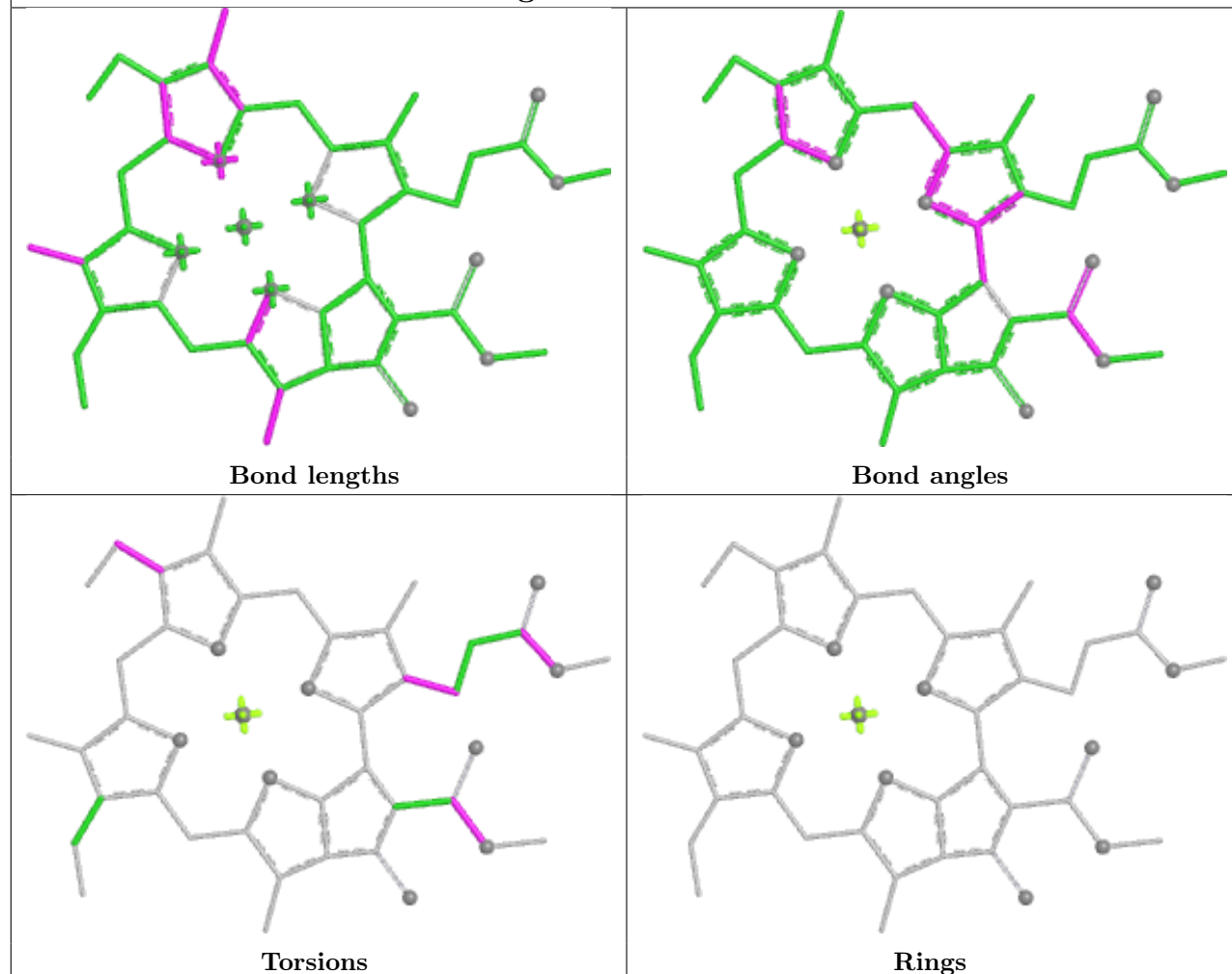
Ligand CLA A 836



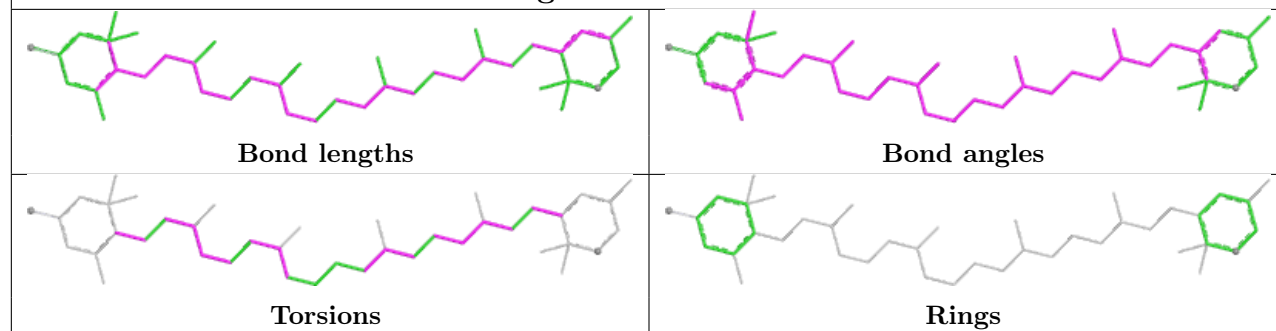
Ligand CLA B 839

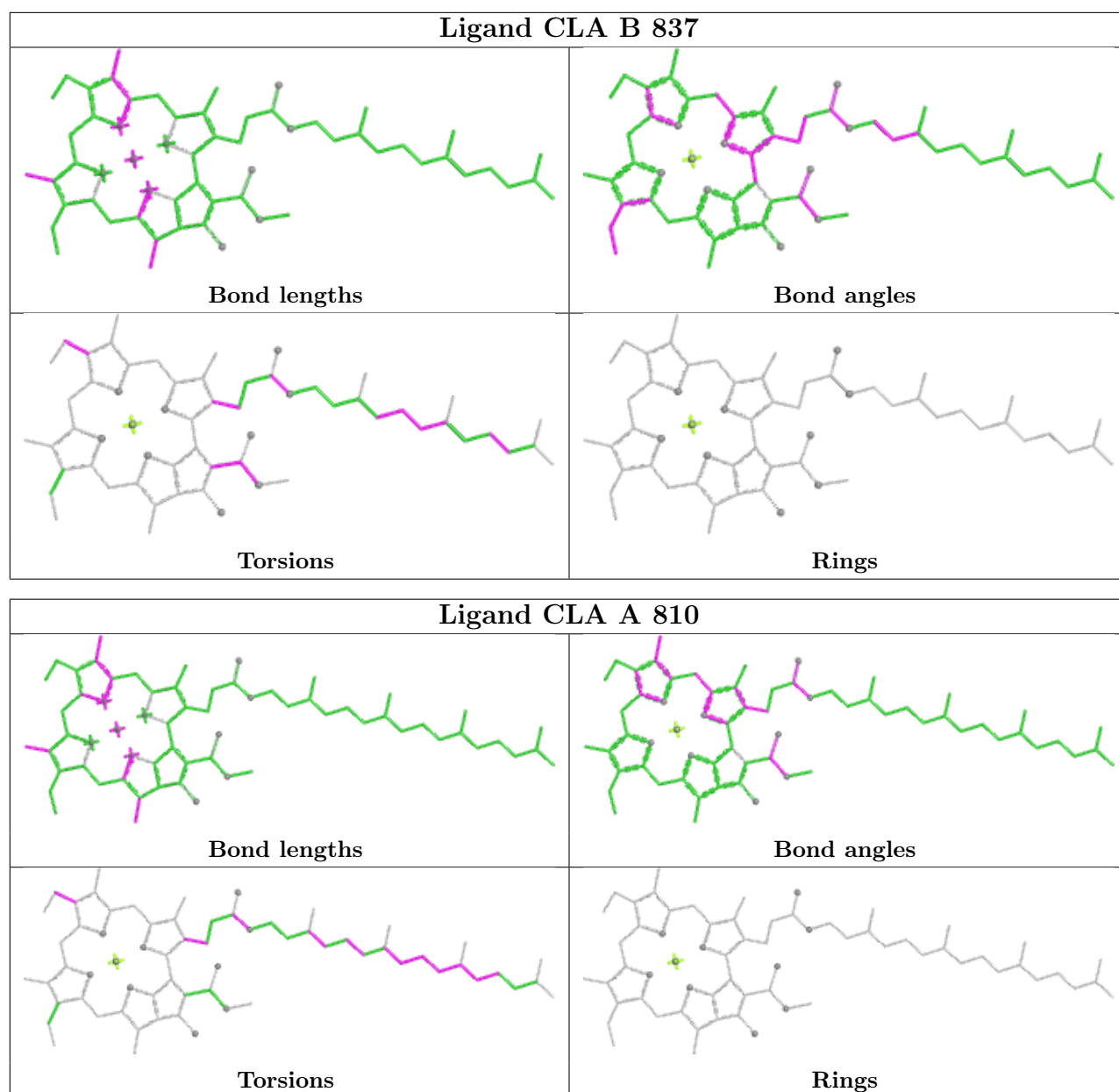


Ligand CLA 3 212

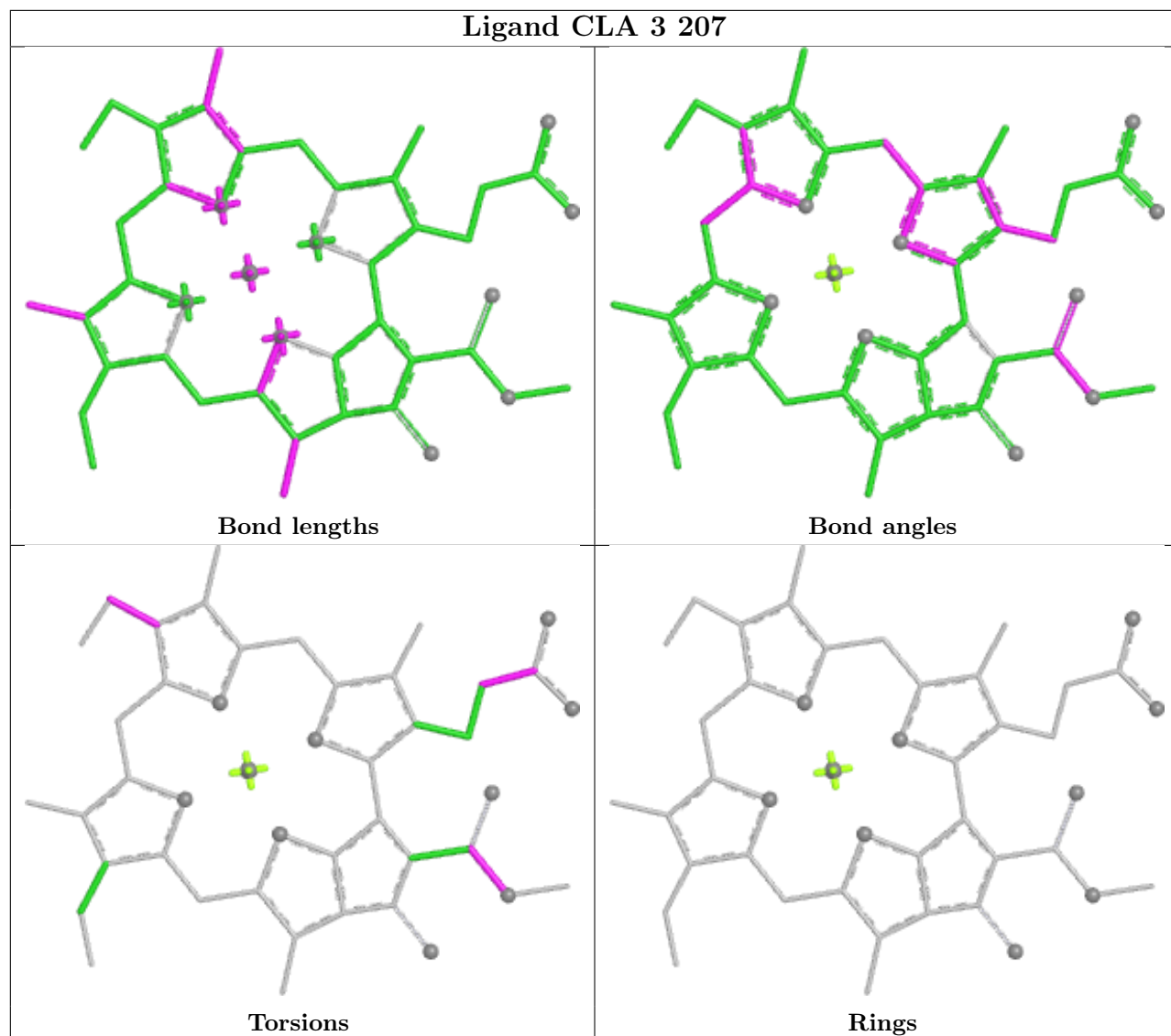


Ligand ZEX 1 613

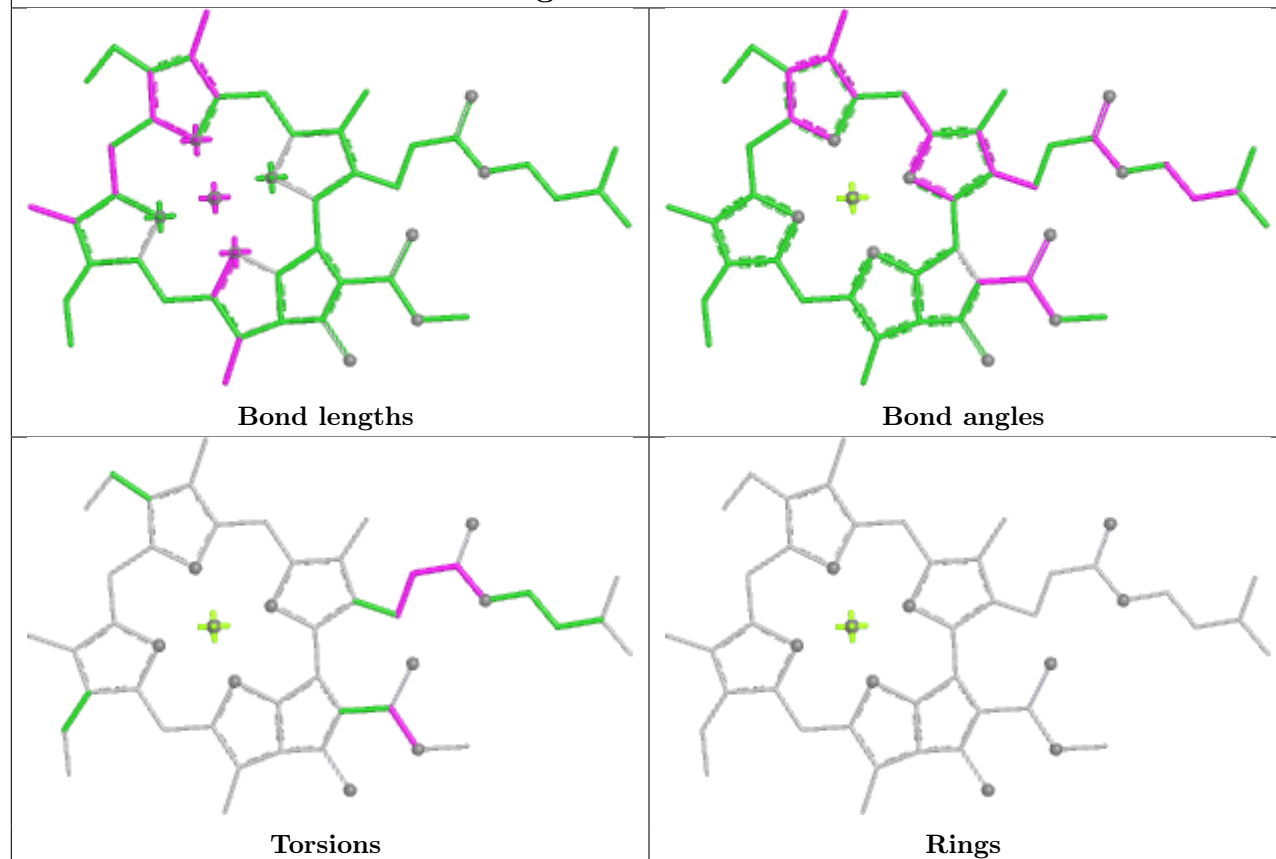




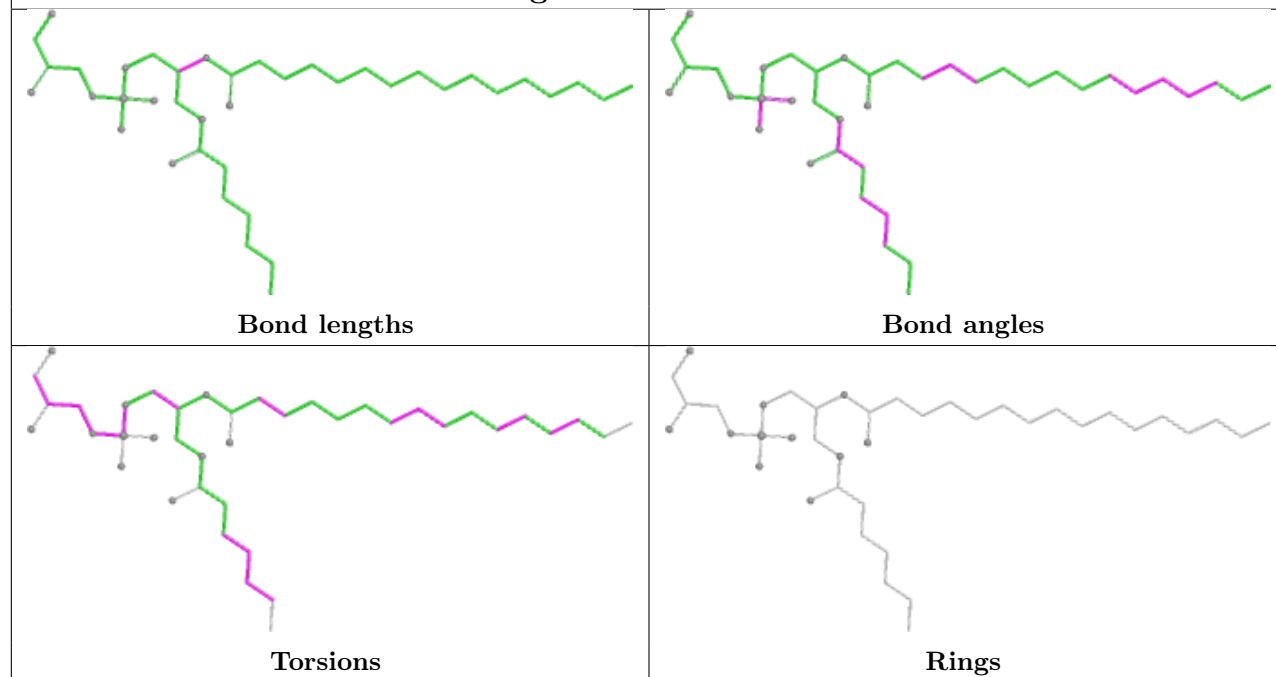
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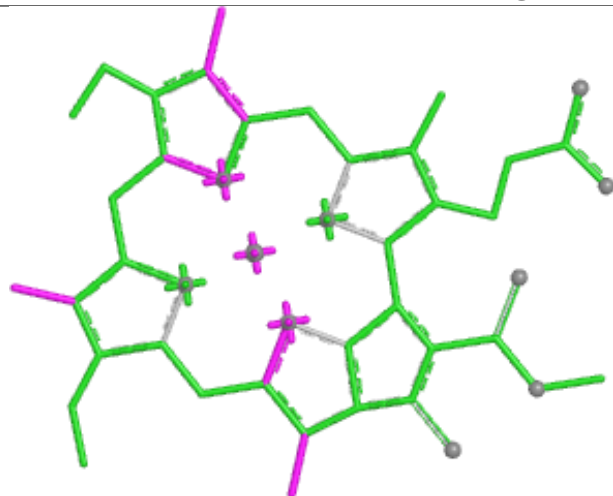
Ligand CLA 2 608



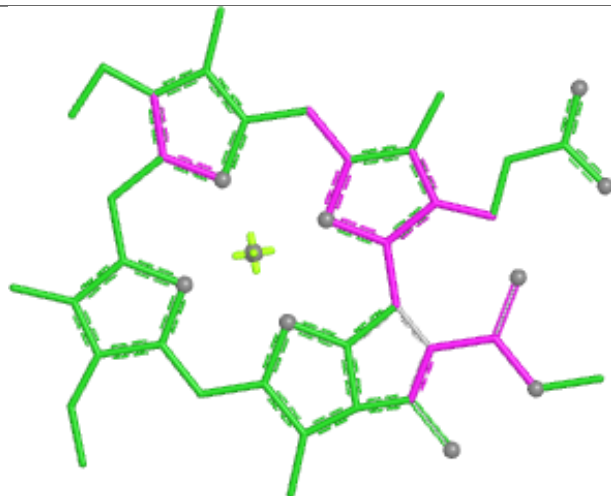
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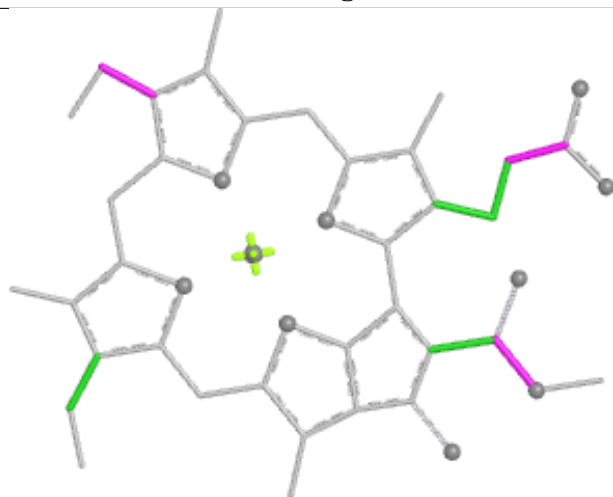
Ligand CLA K 101



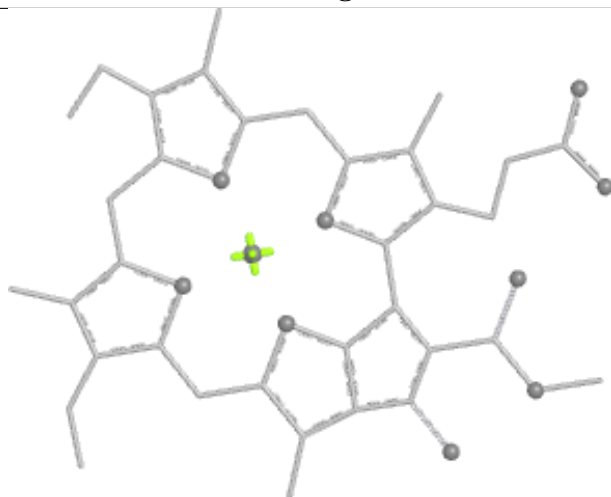
Bond lengths



Bond angles

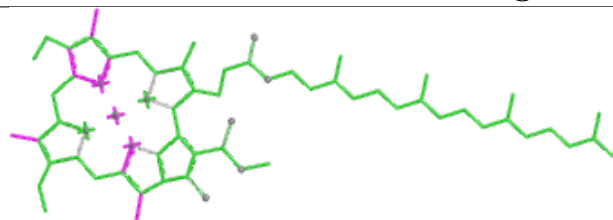


Torsions

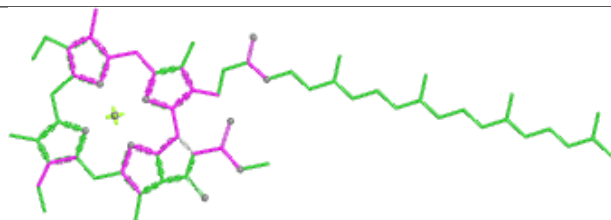


Rings

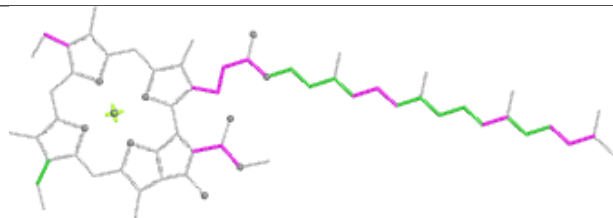
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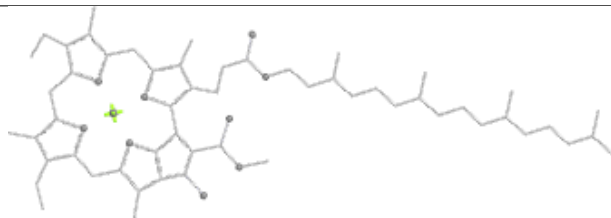
Bond lengths



Bond angles

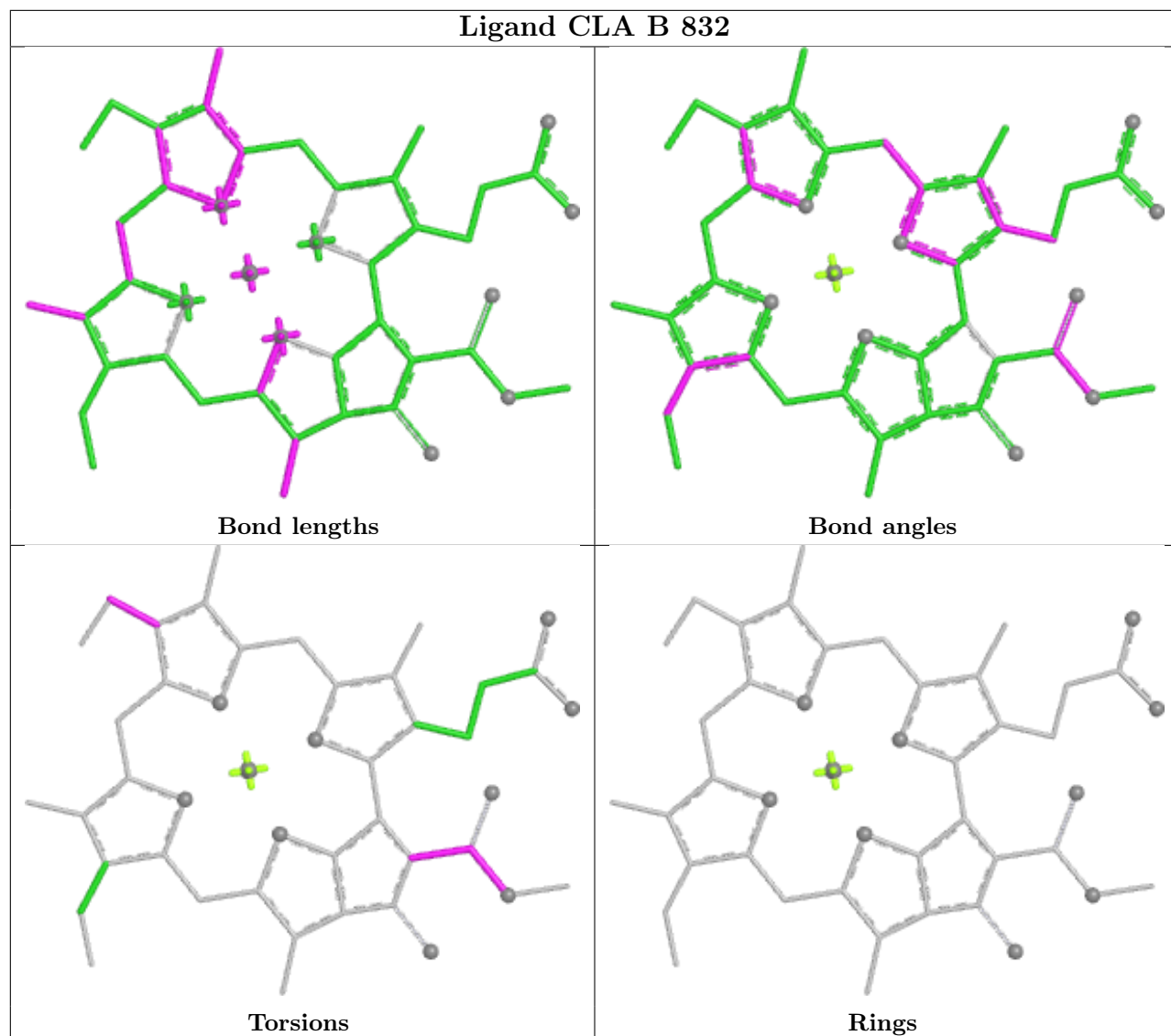


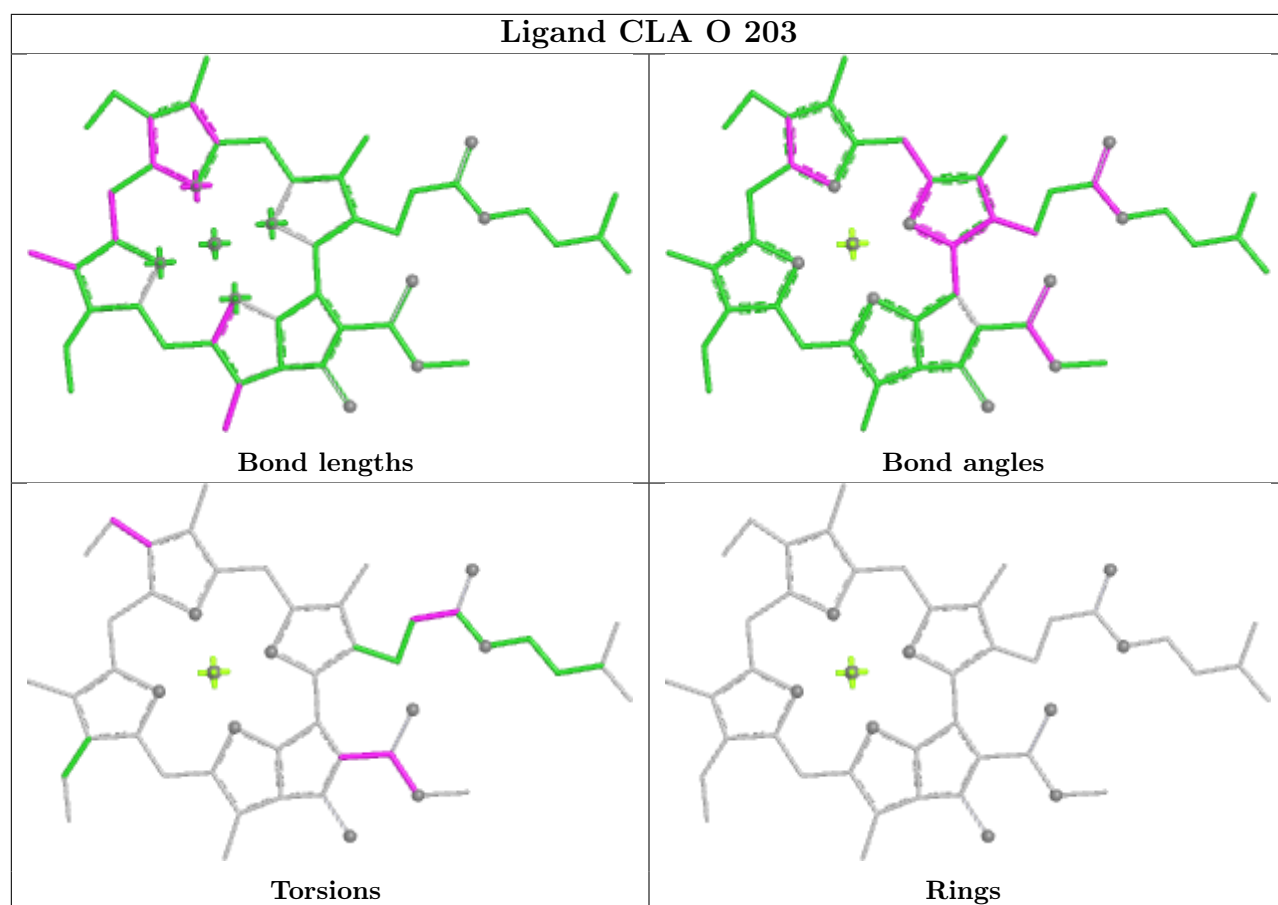
Torsions



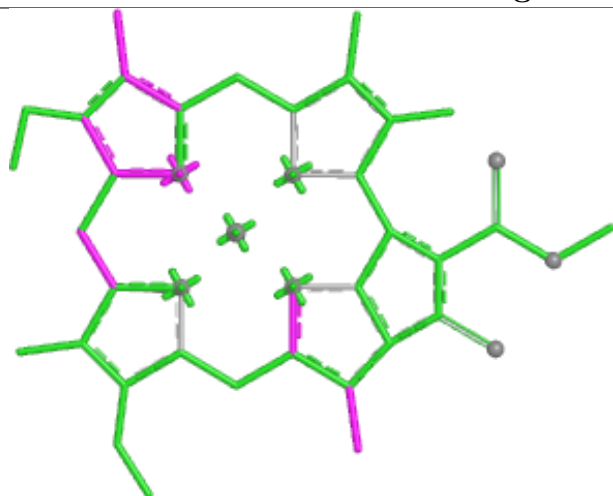
Rings

Ligand CLA B 832

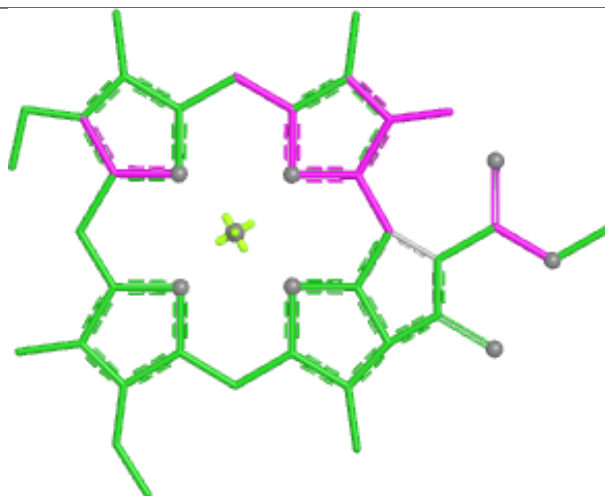




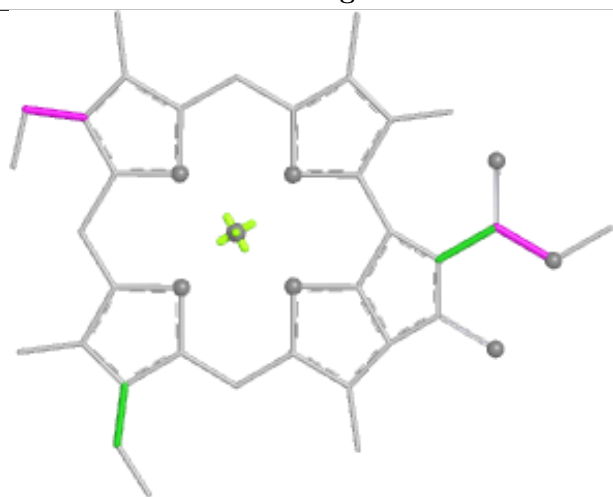
Ligand CLA O 202



Bond lengths



Bond angles

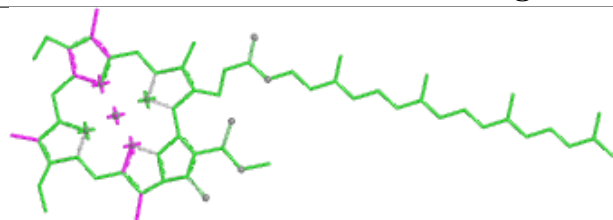


Torsions

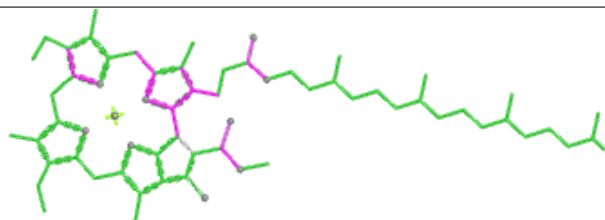


Rings

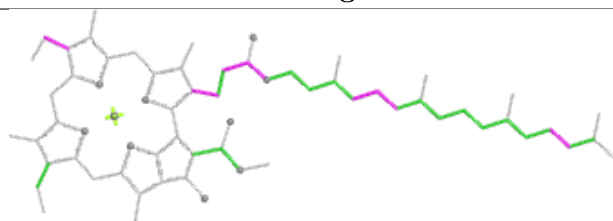
Ligand CLA A 826



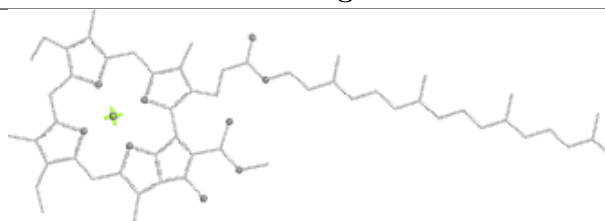
Bond lengths



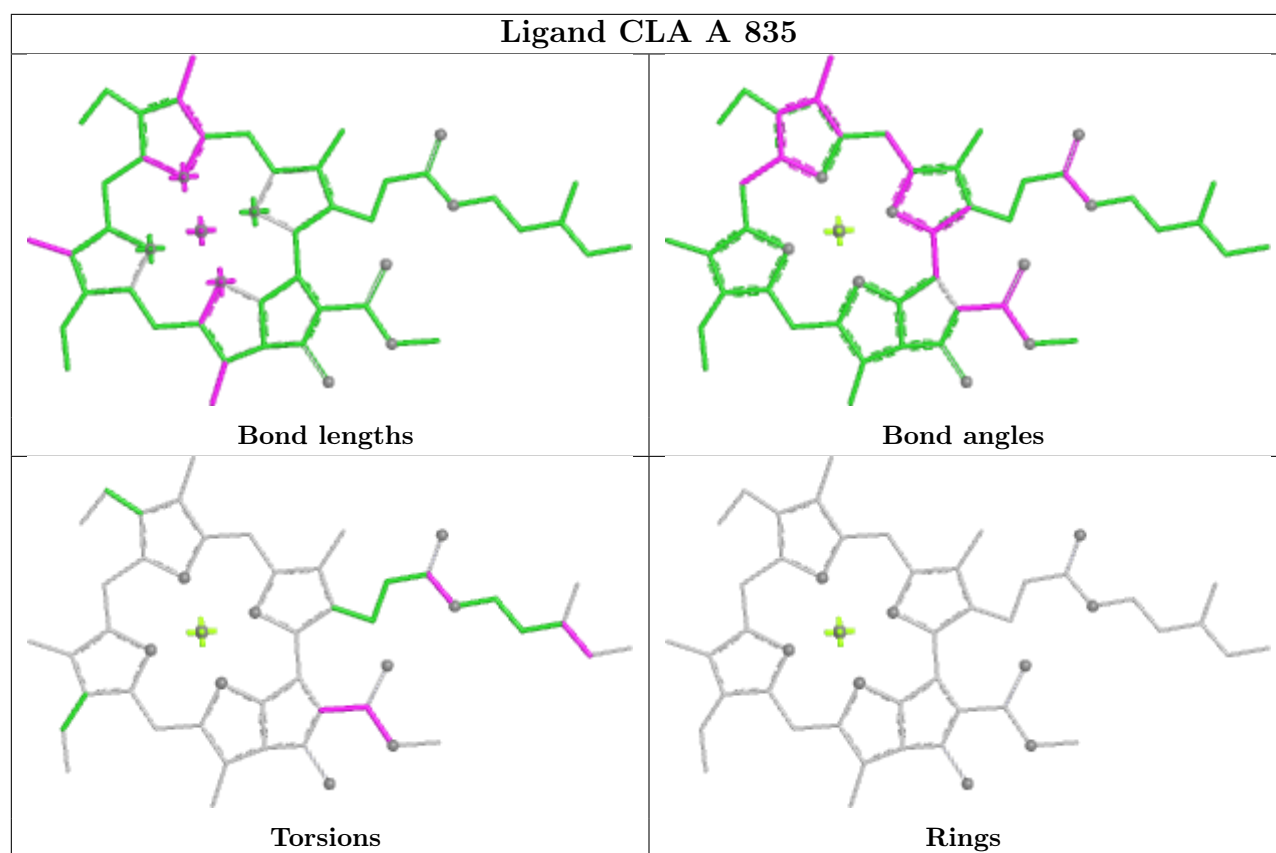
Bond angles



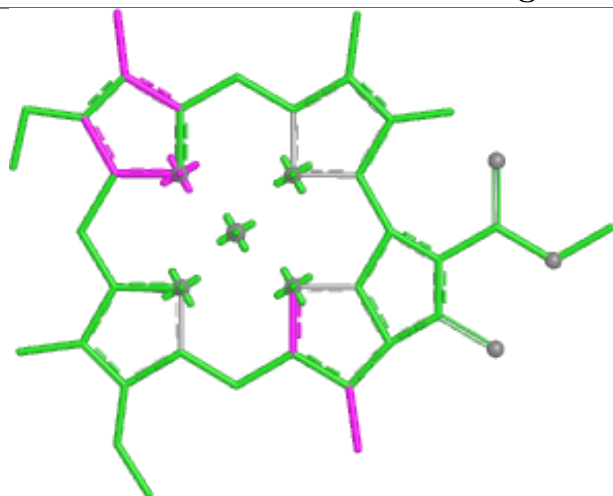
Torsions



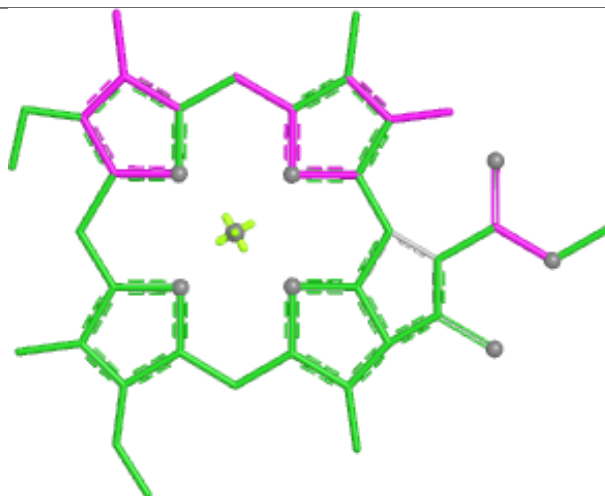
Rings



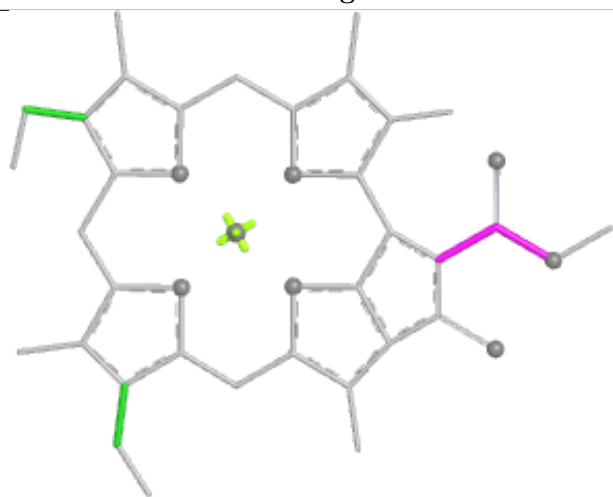
Ligand CLA 2 609



Bond lengths



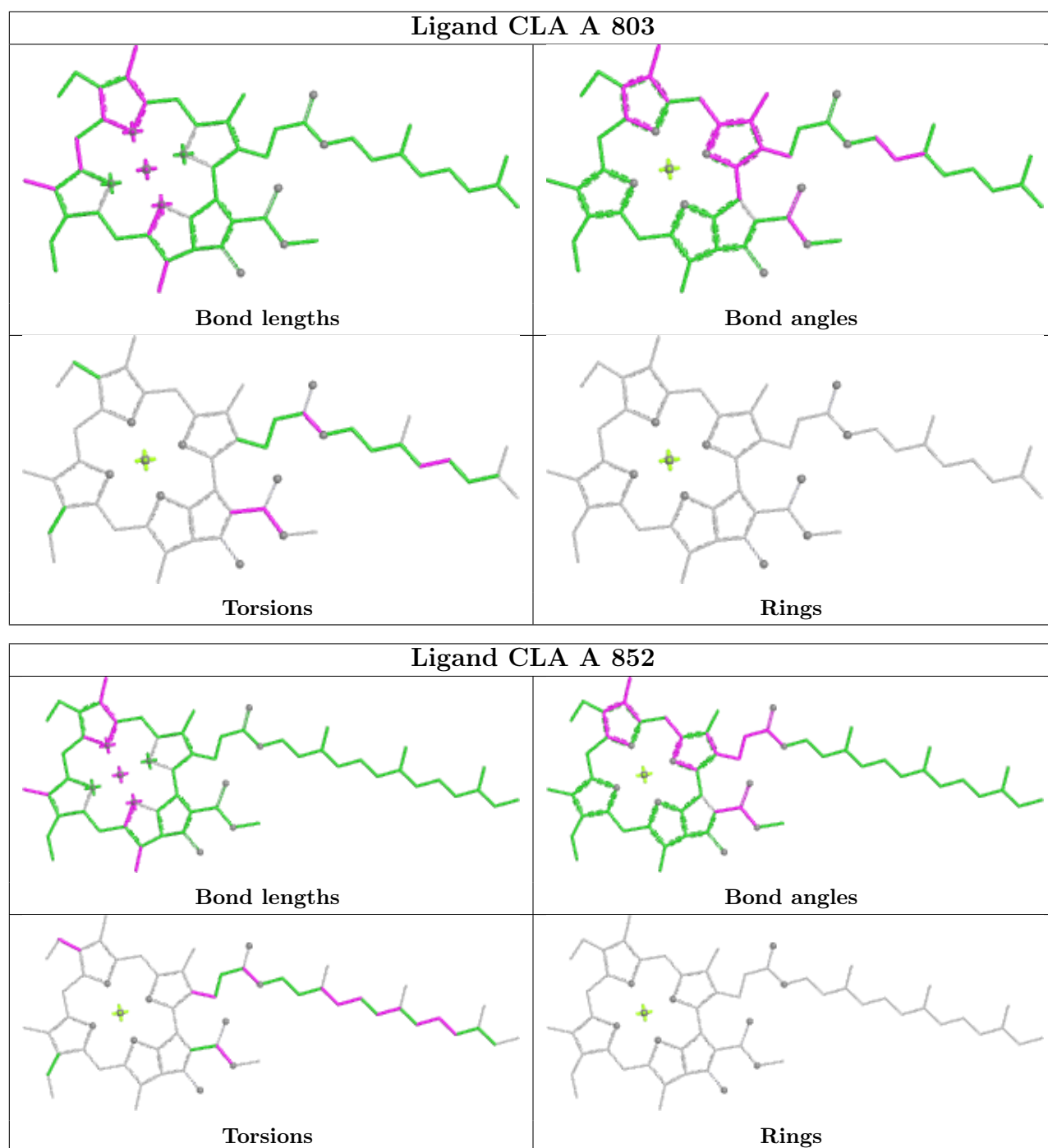
Bond angles

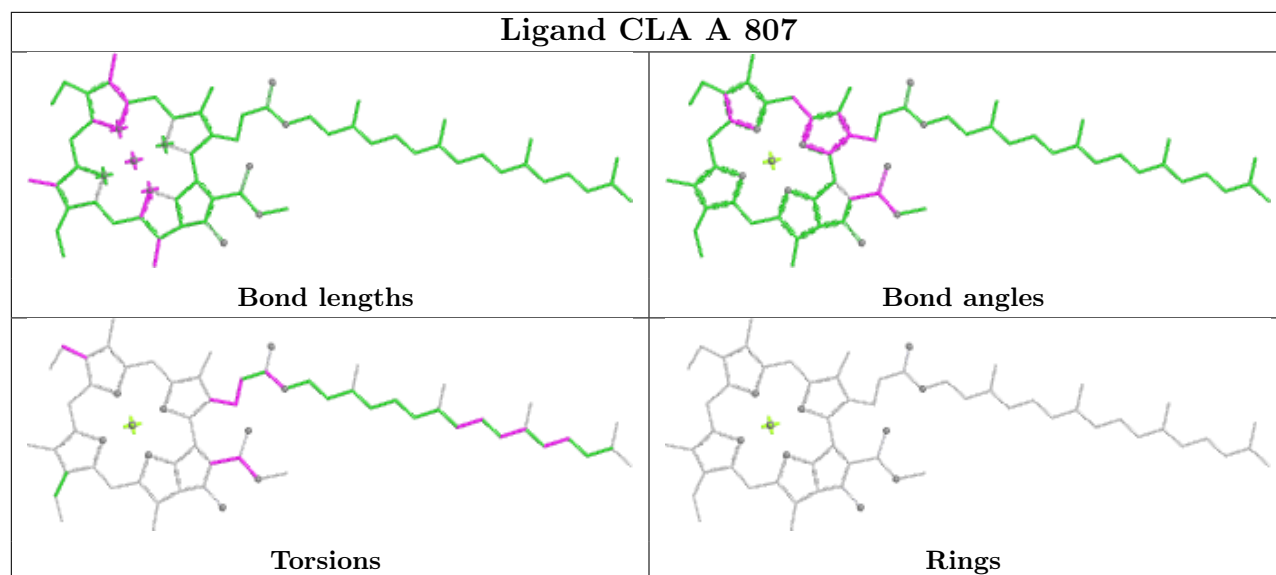
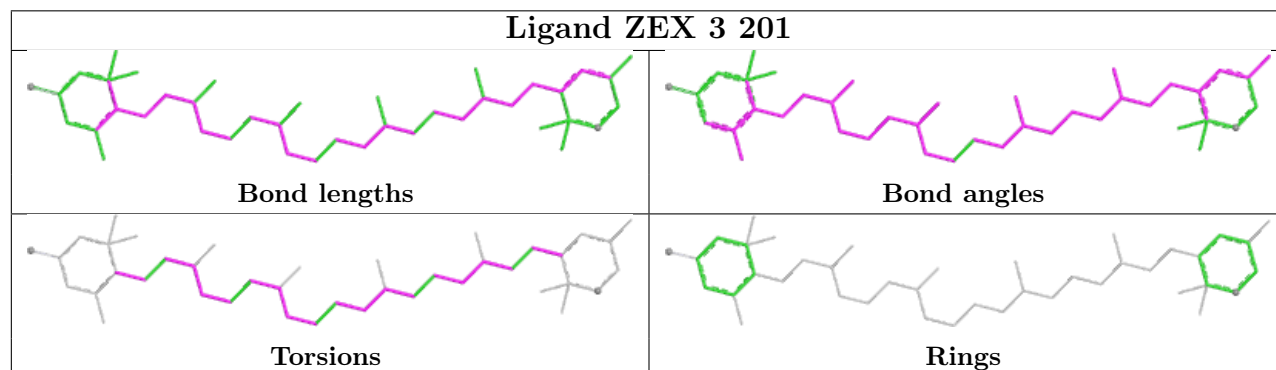
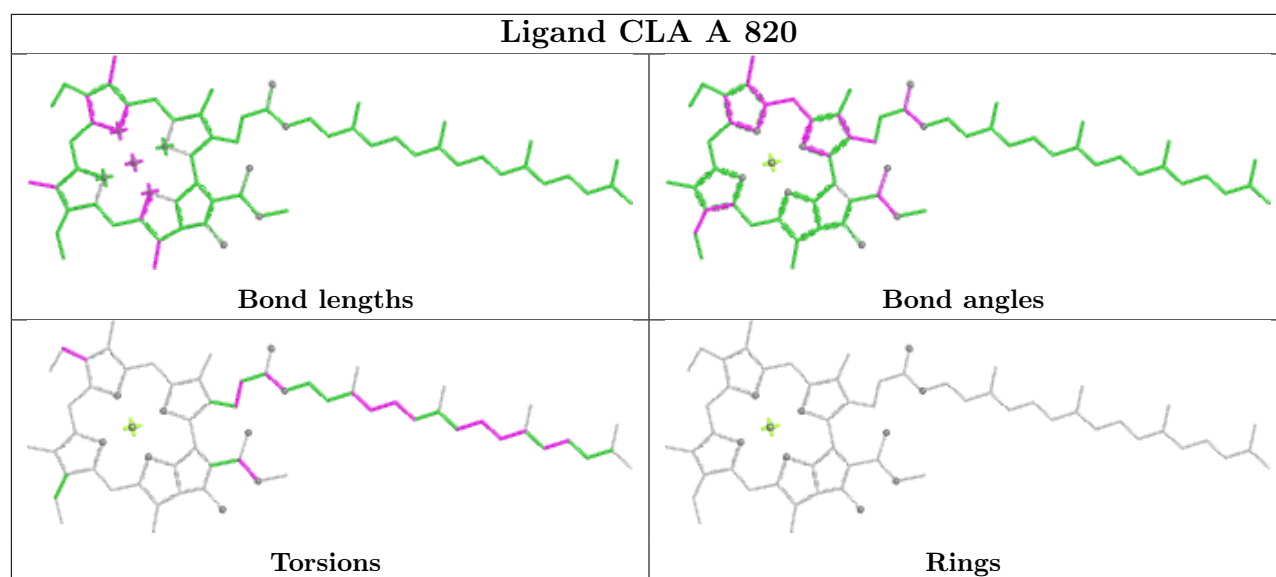


Torsions

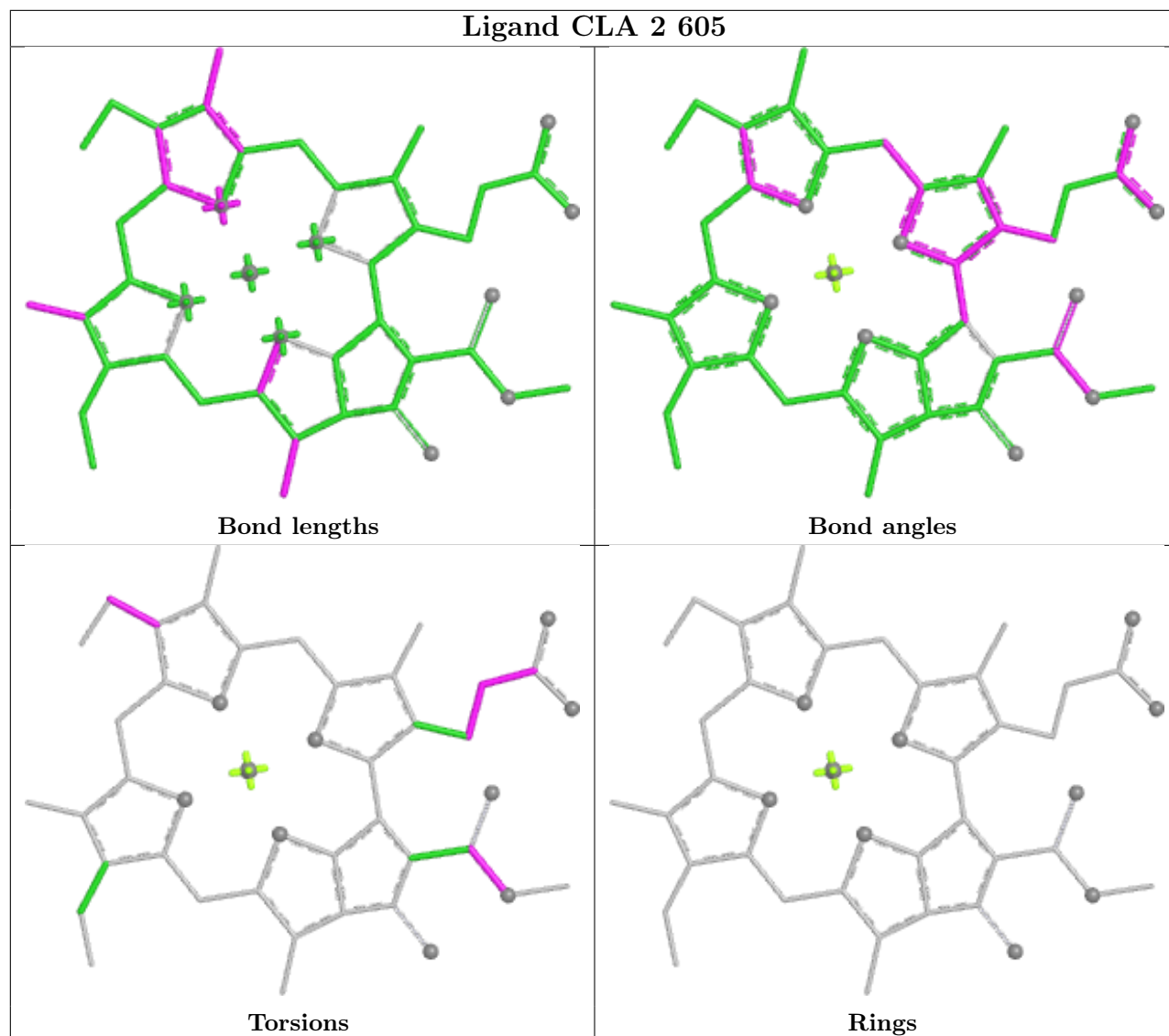


Rings

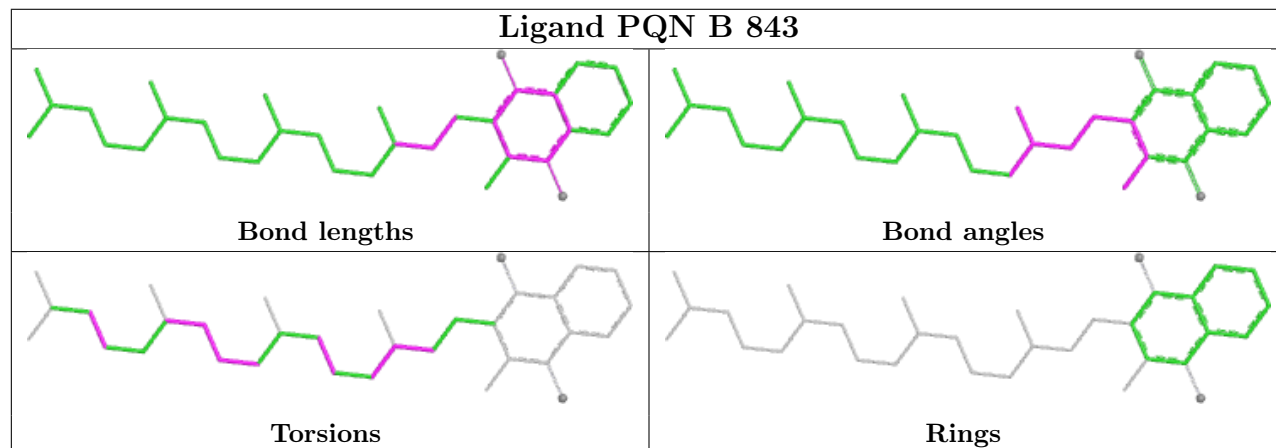




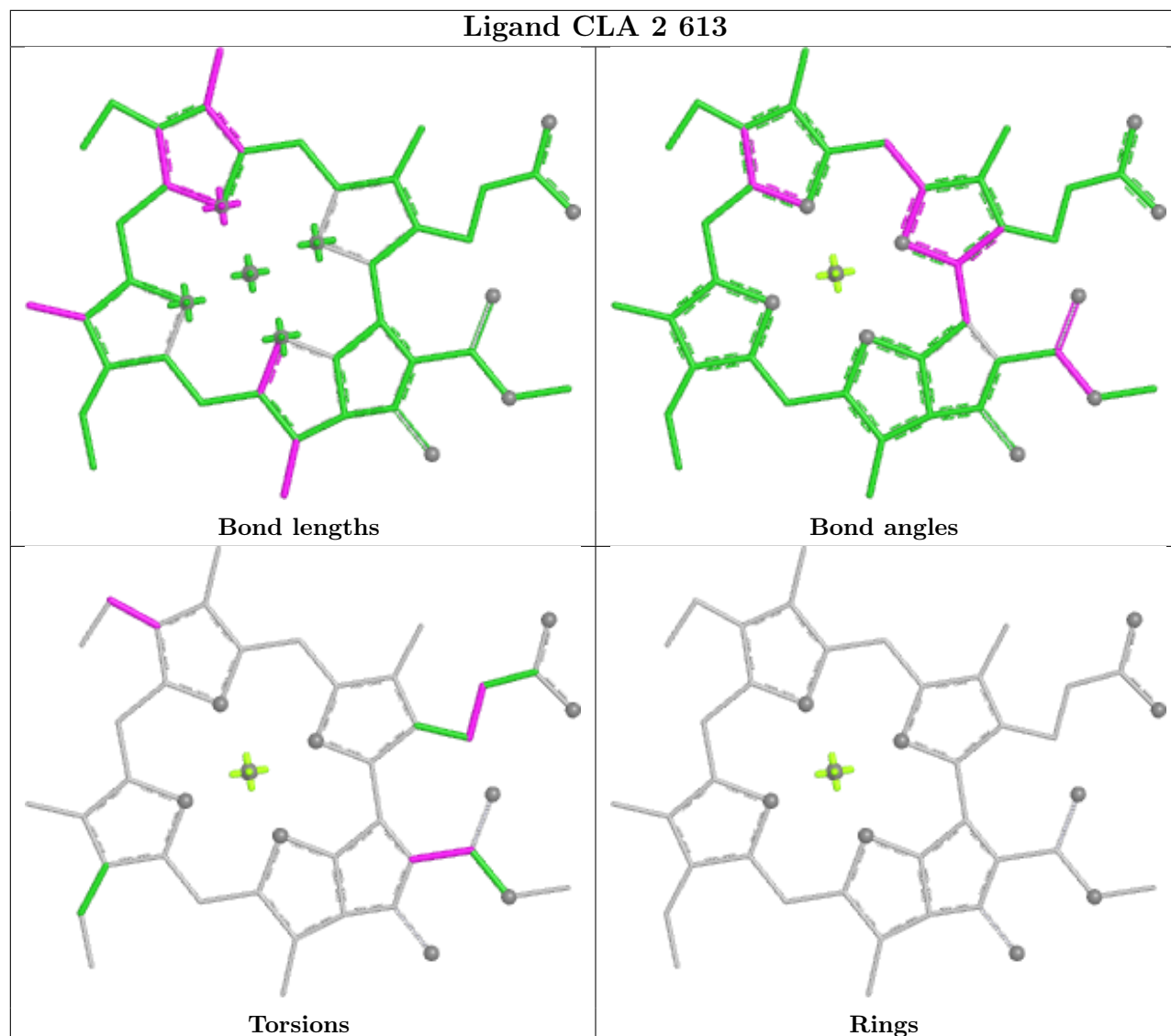
Ligand CLA 2 605



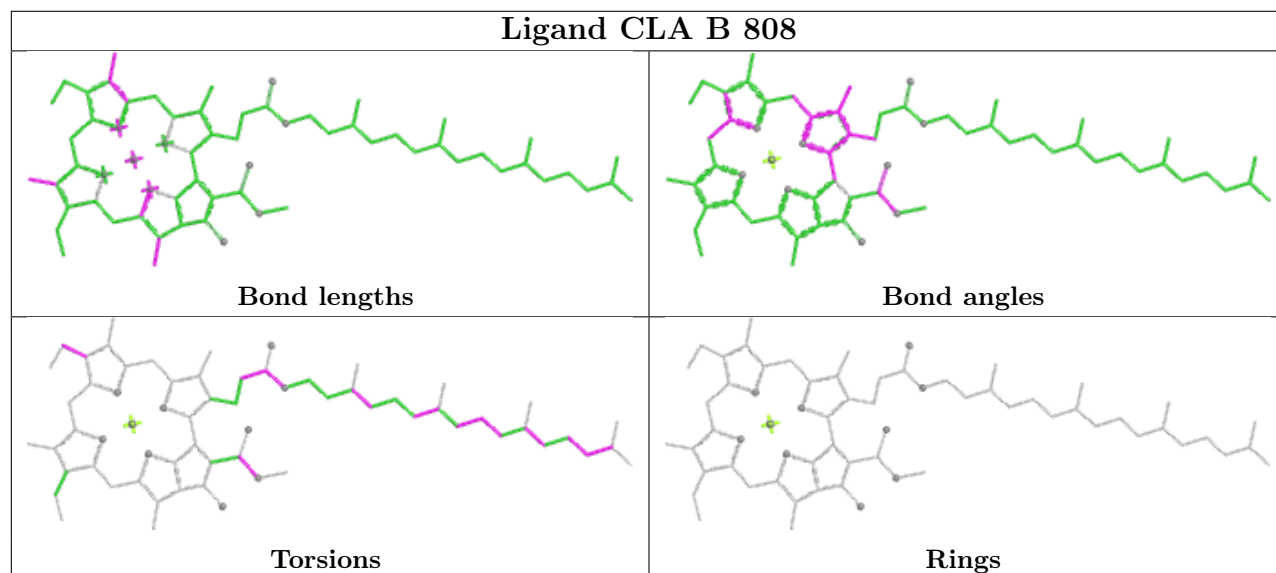
Ligand PQN B 843

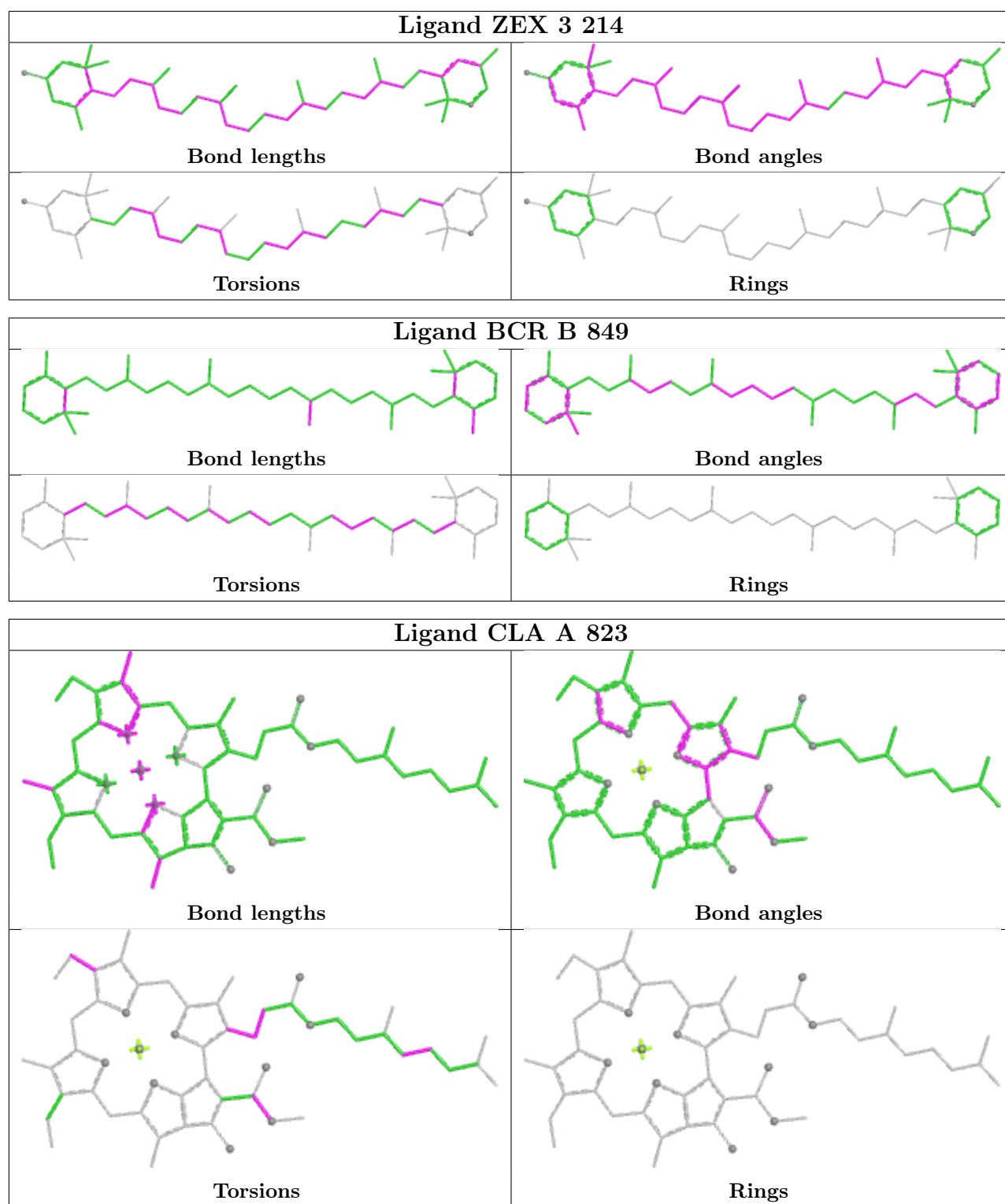


Ligand CLA 2 613

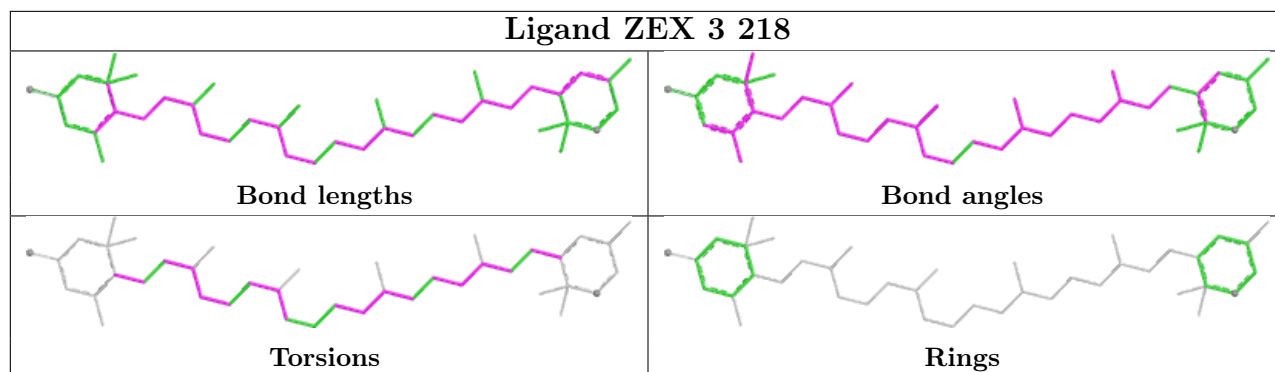


Ligand CLA B 808

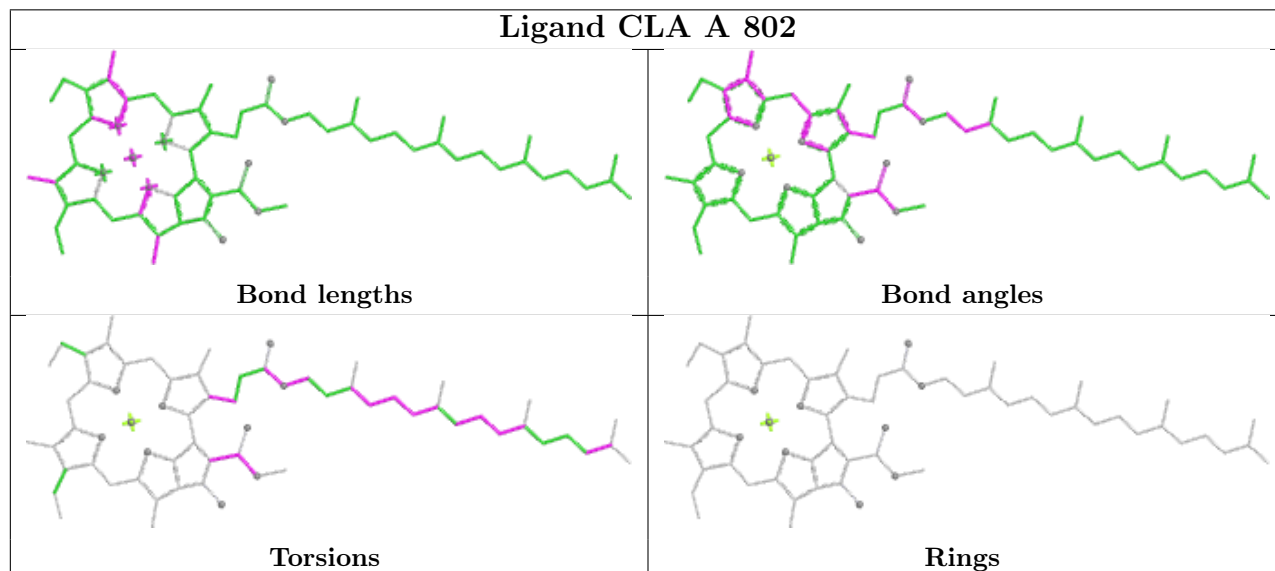




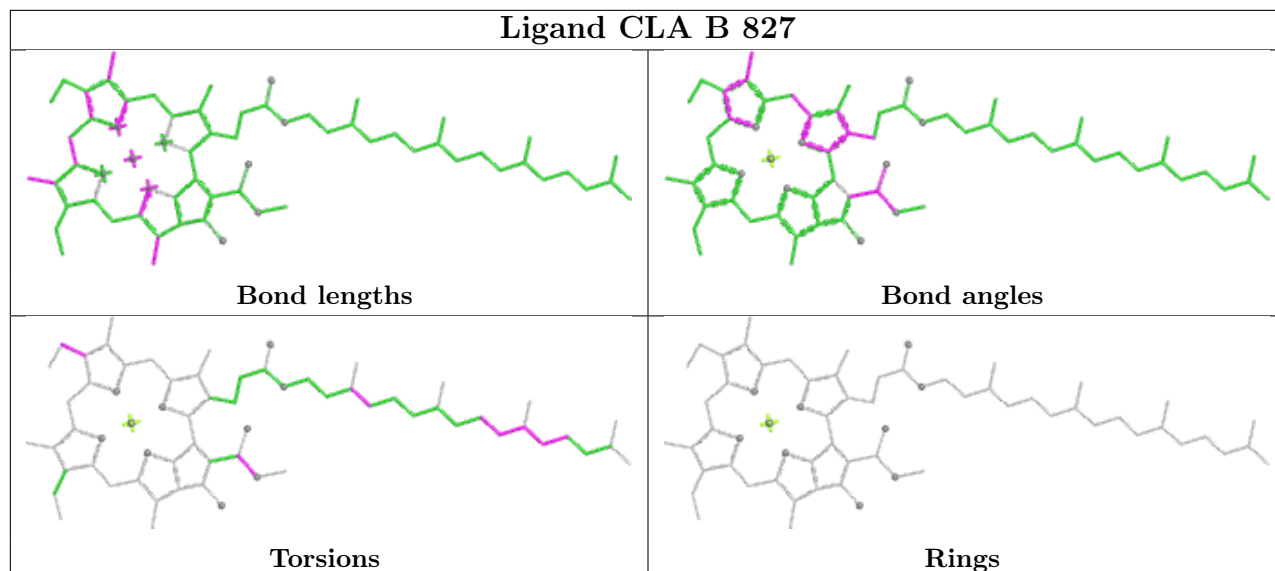
Ligand ZEX 3 218

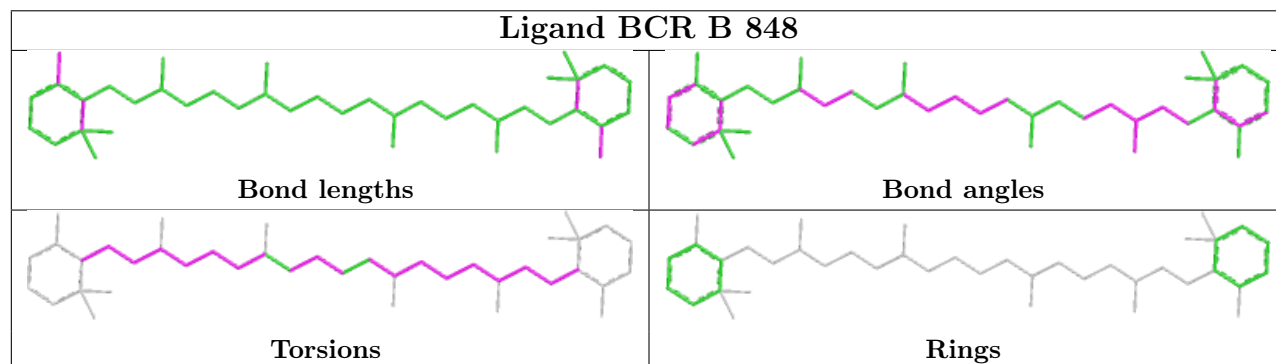
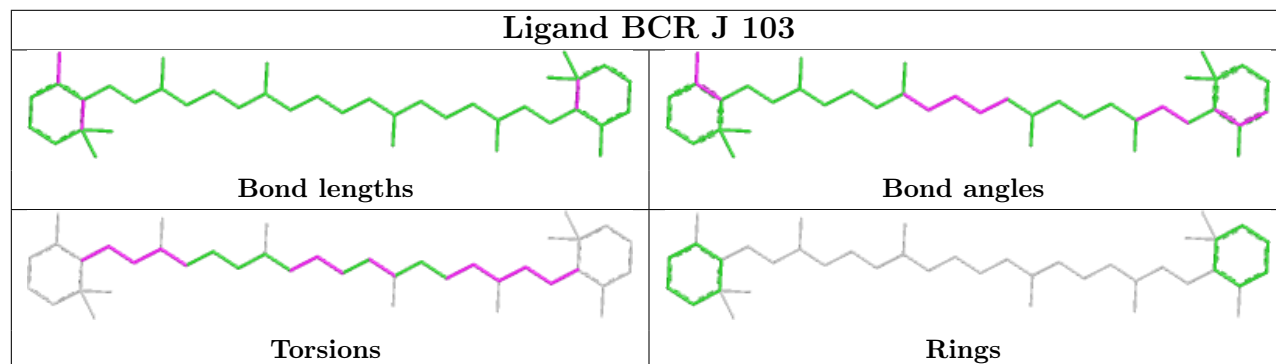
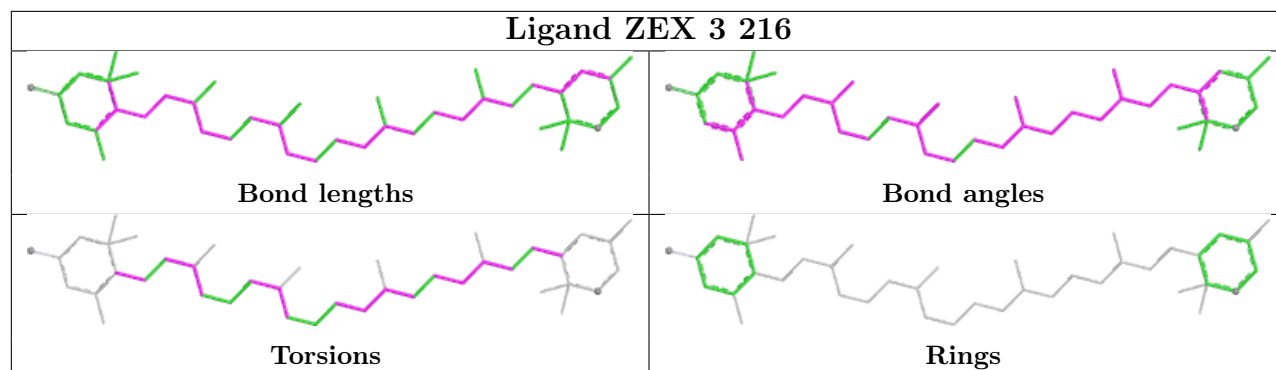


Ligand CLA A 802

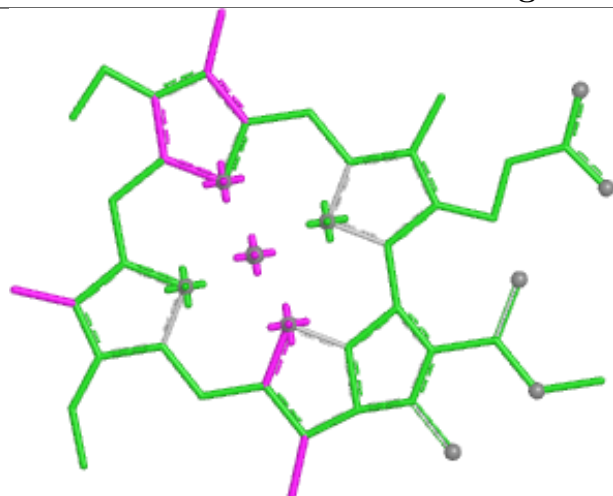


Ligand CLA B 827

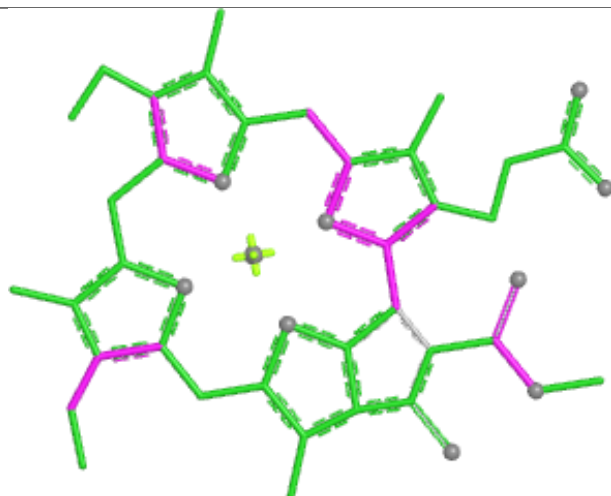




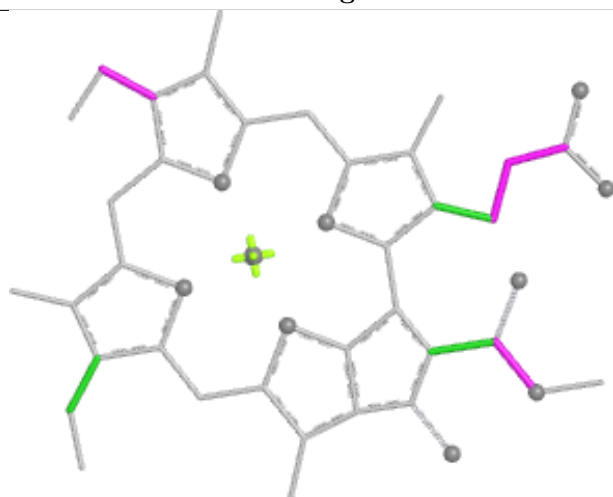
Ligand CLA 1 606



Bond lengths



Bond angles

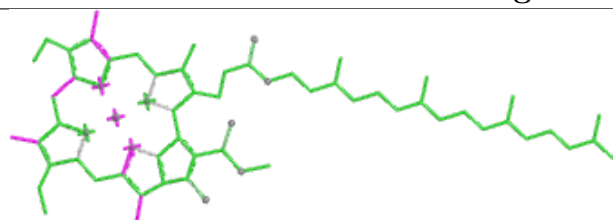


Torsions

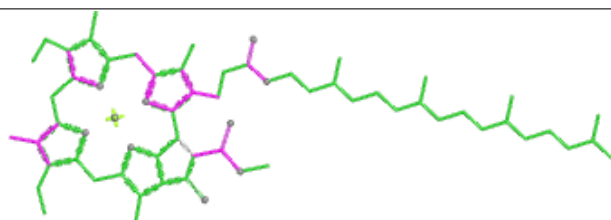


Rings

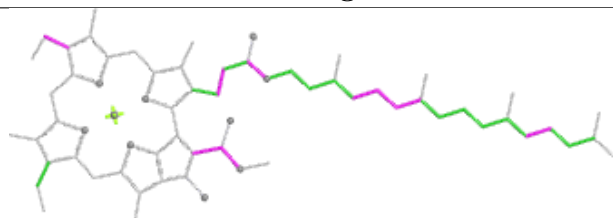
Ligand CLA A 832



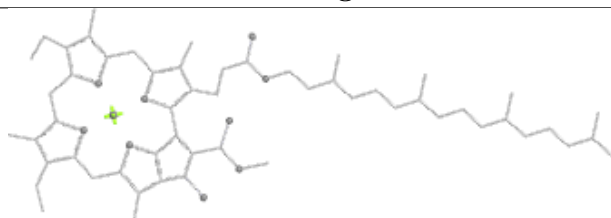
Bond lengths



Bond angles

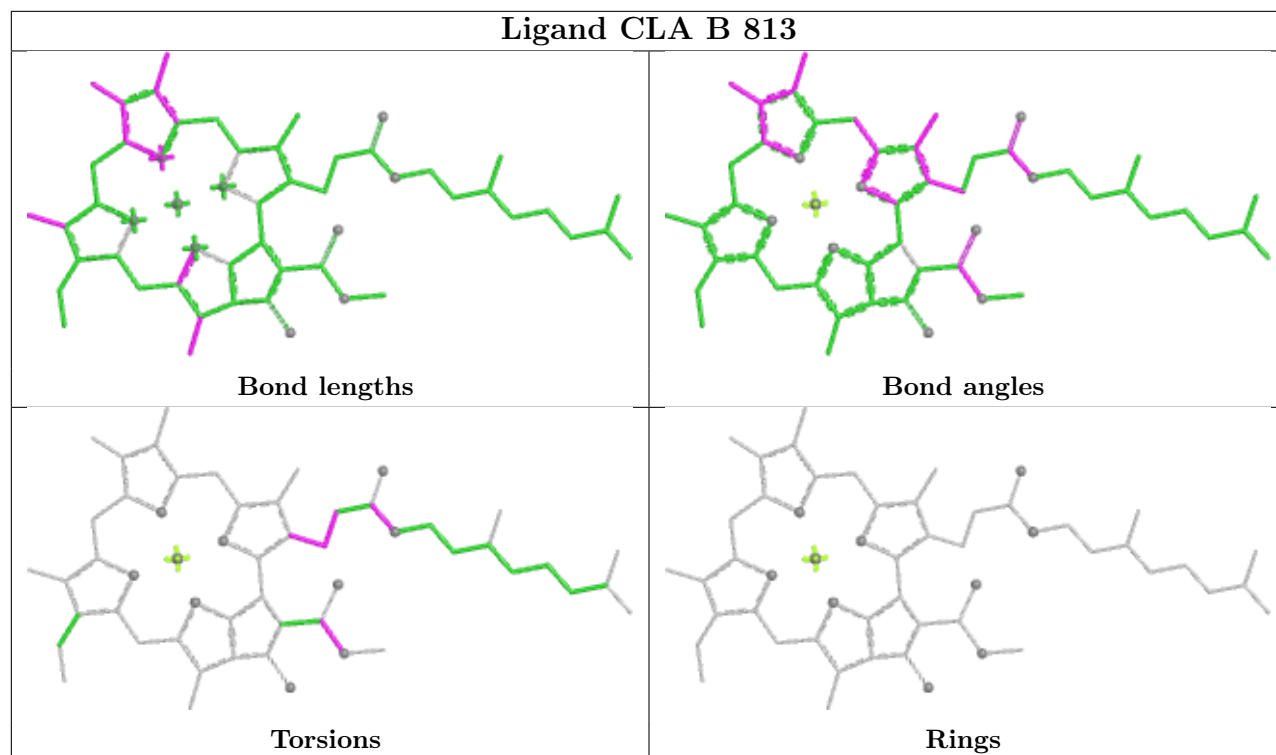


Torsions

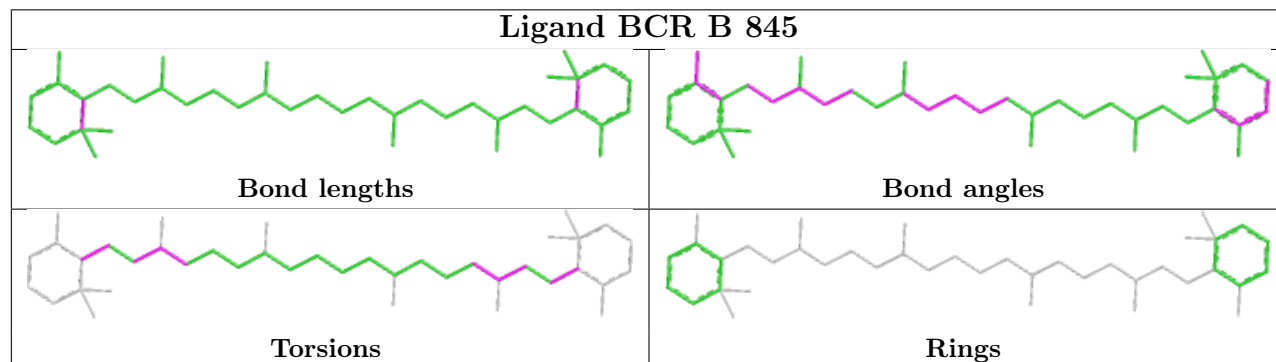


Rings

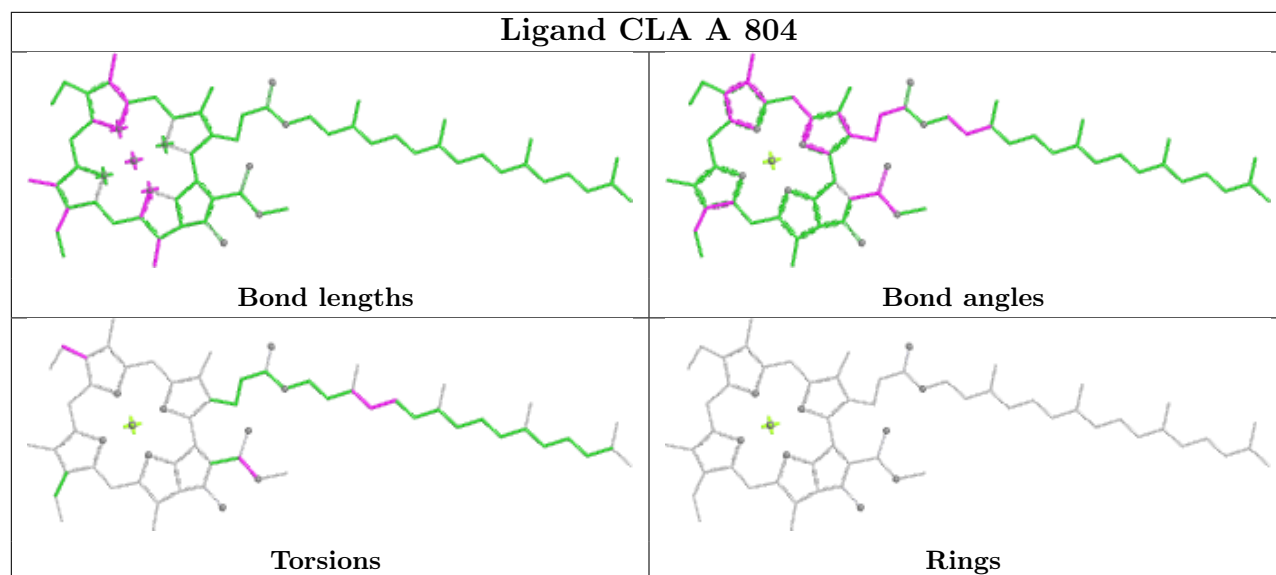
Ligand CLA B 813



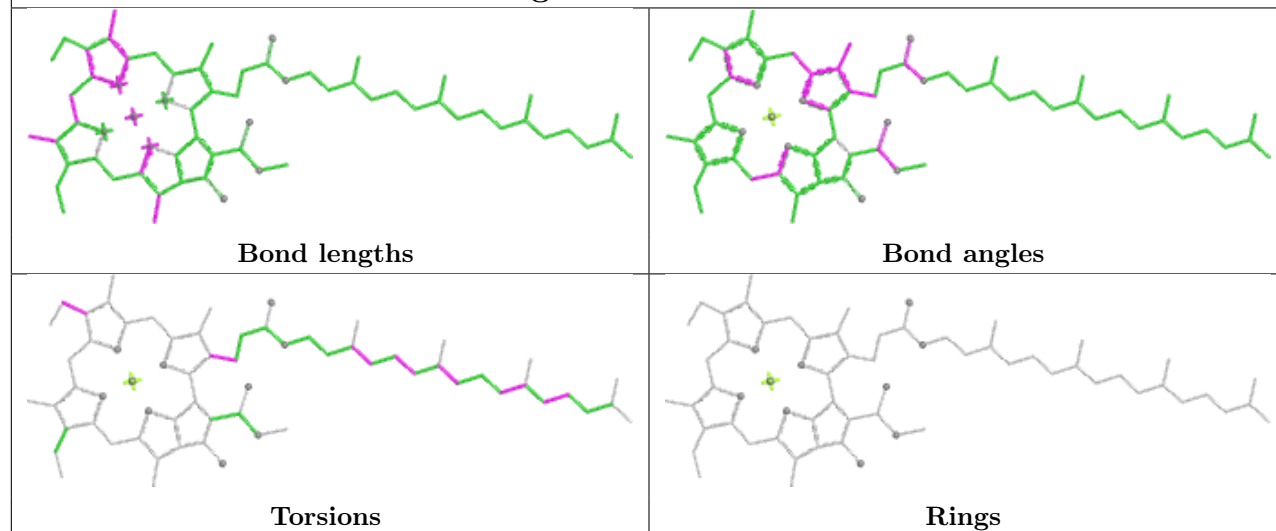
Ligand BCR B 845



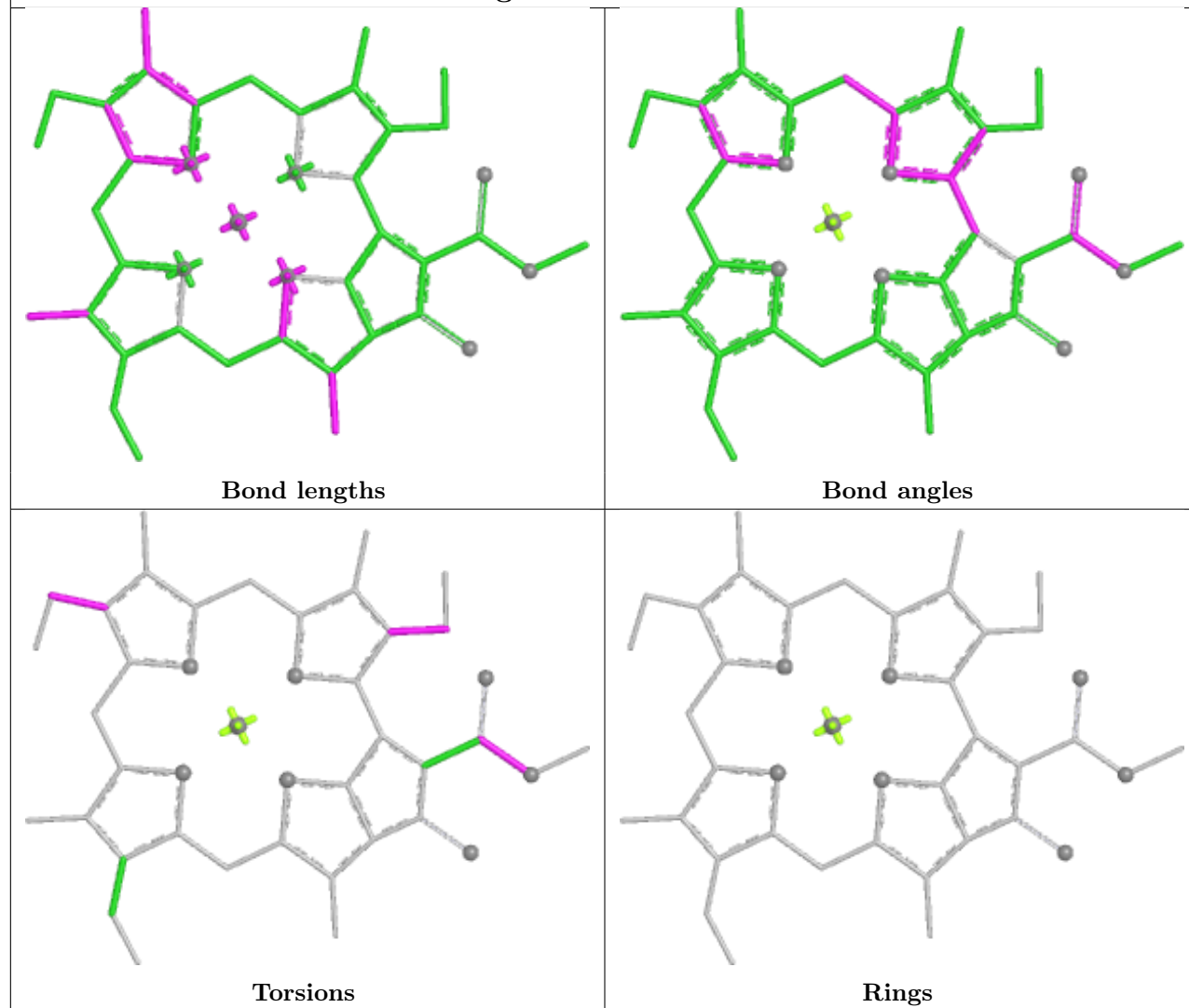
Ligand CLA A 804

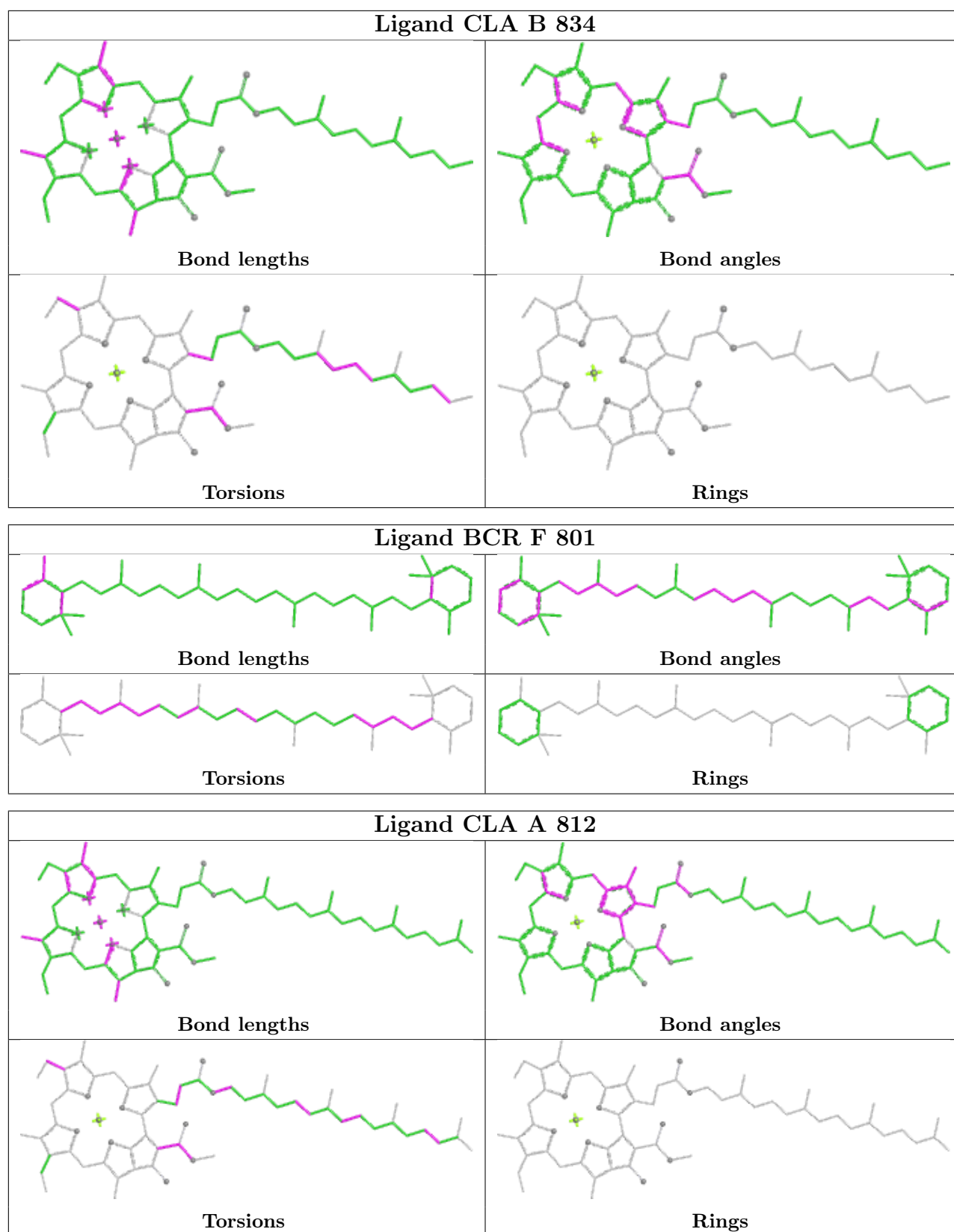


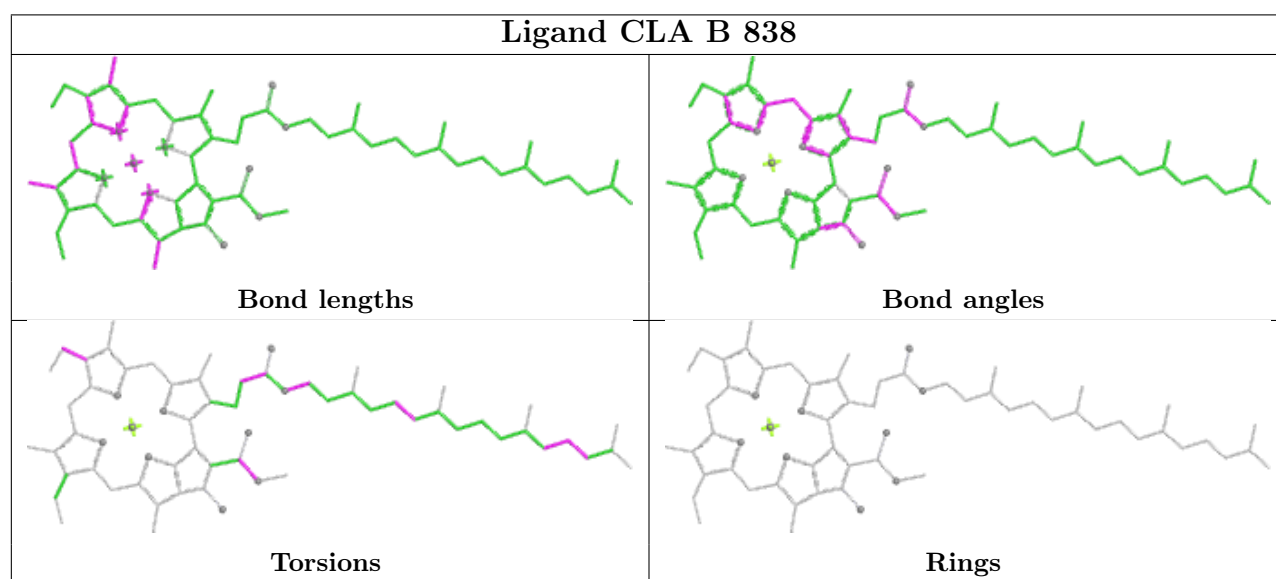
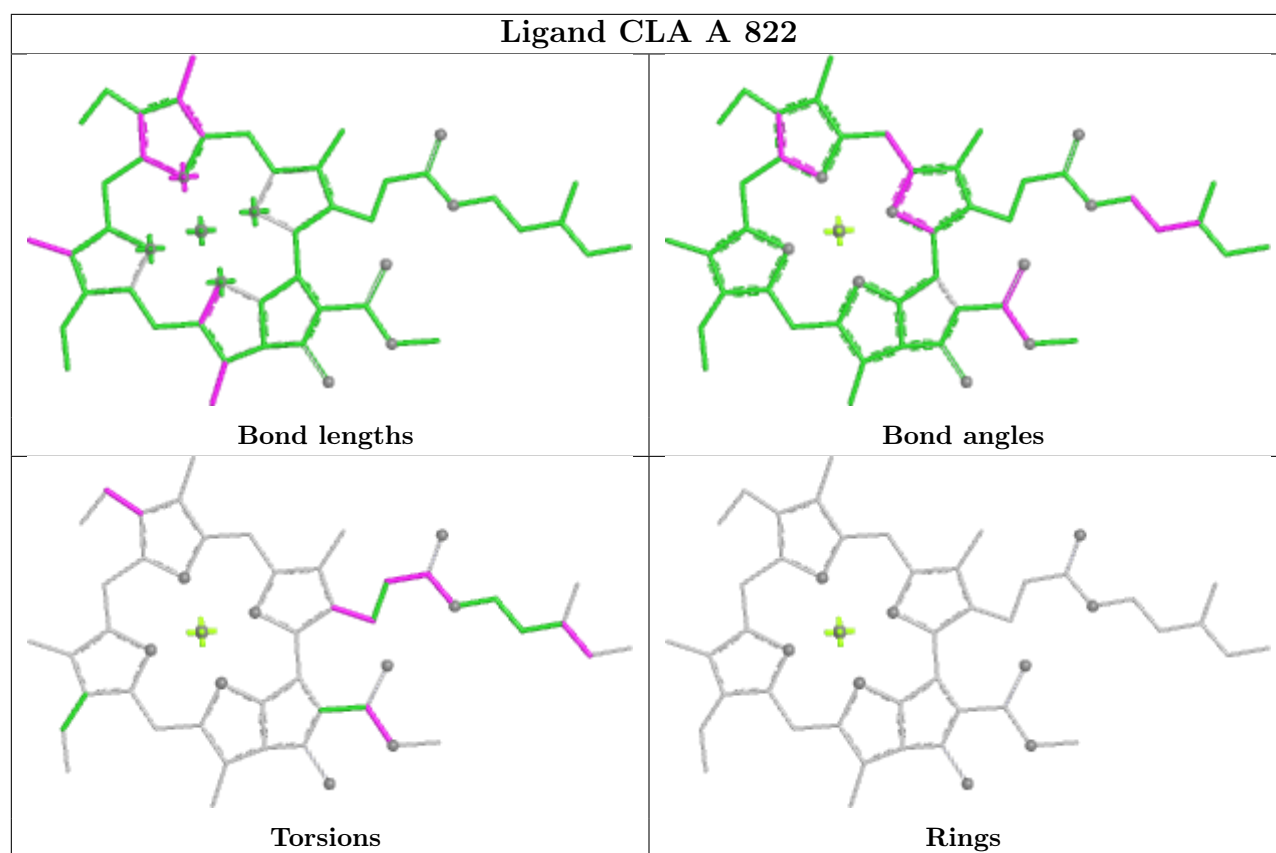
Ligand CLA A 833

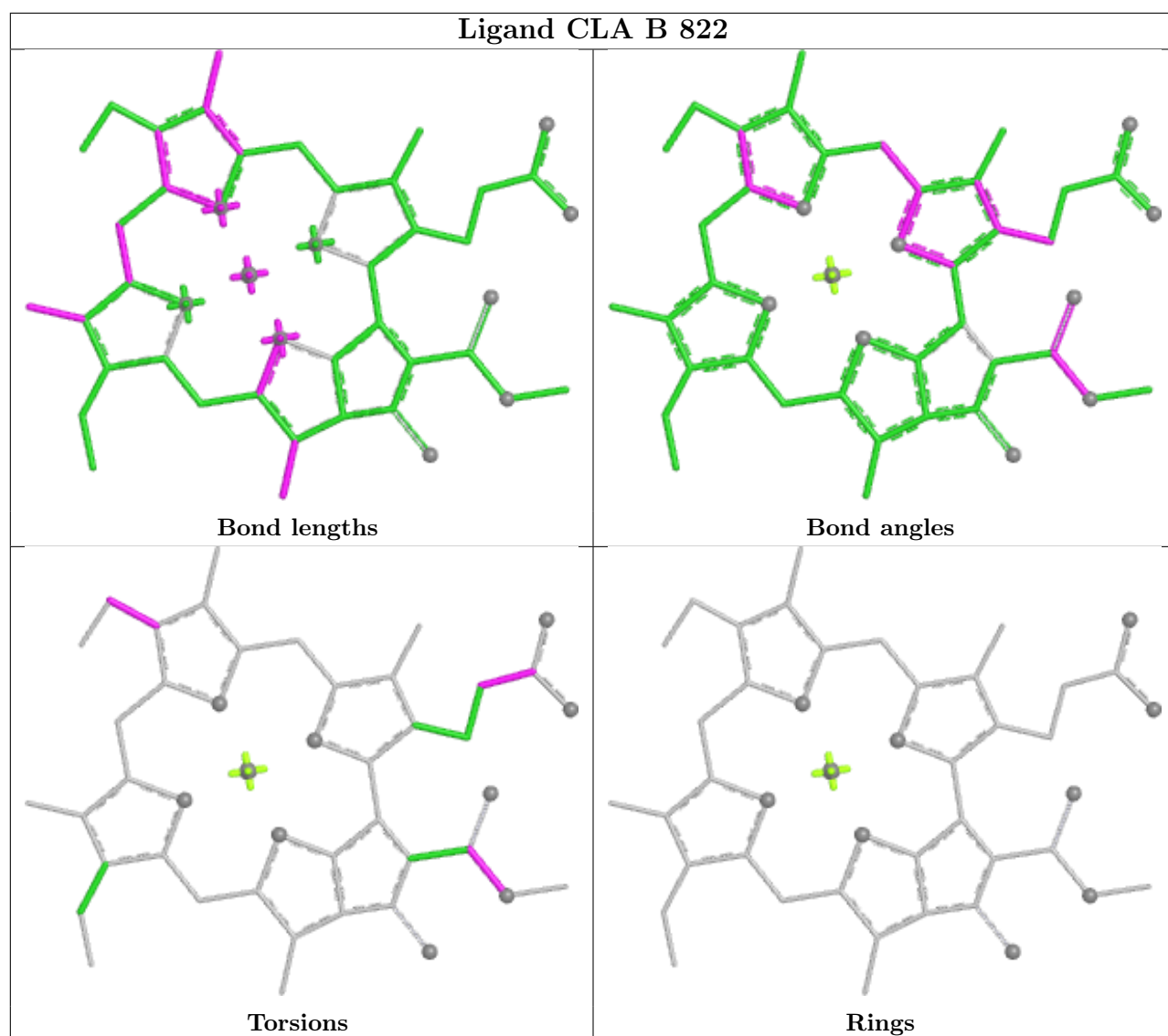


Ligand CLA B 817

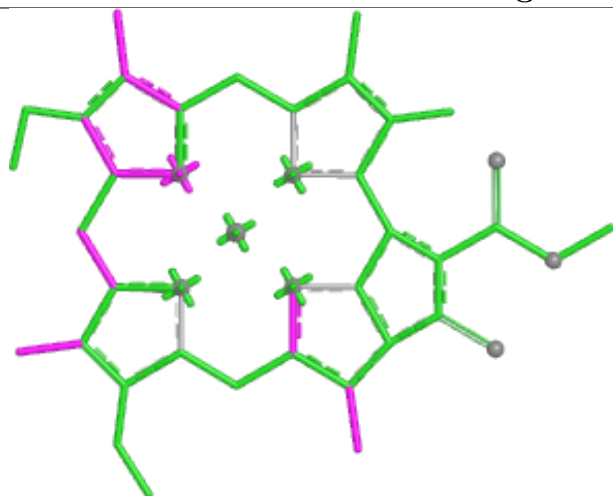




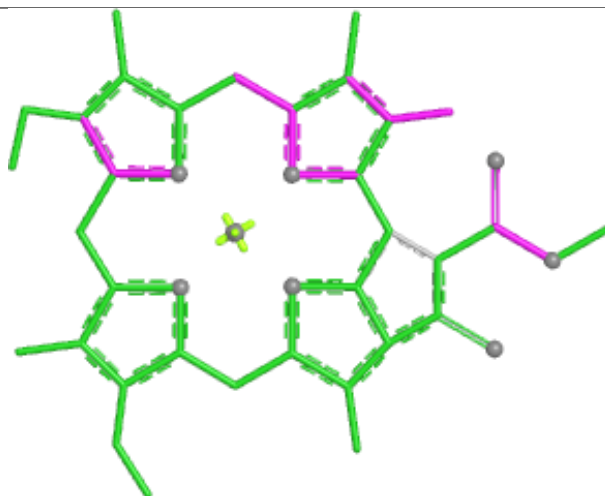




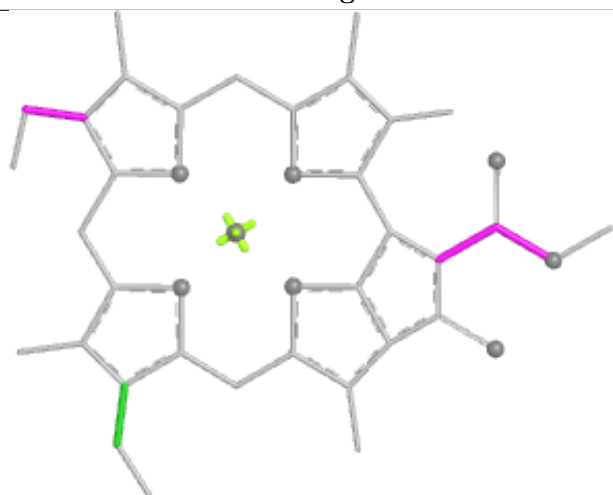
Ligand CLA F 803



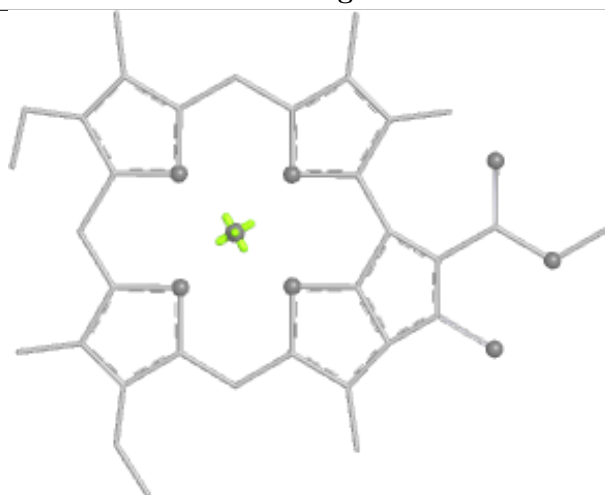
Bond lengths



Bond angles

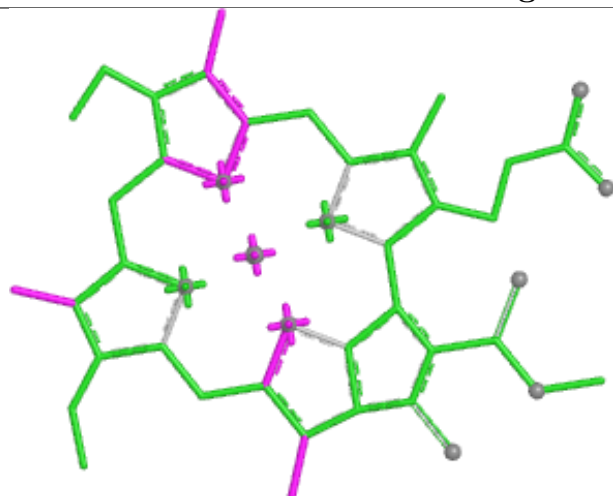


Torsions

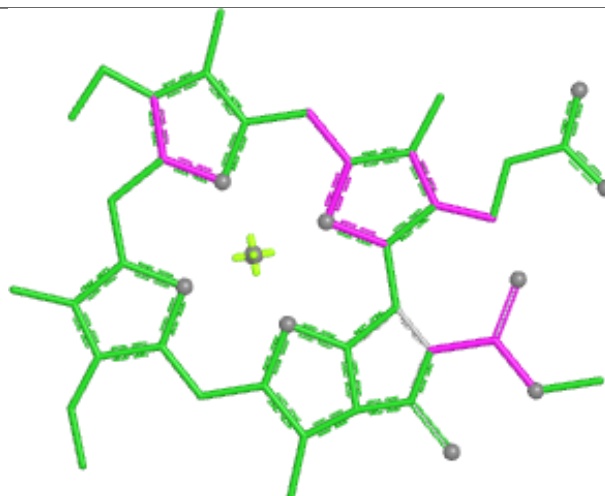


Rings

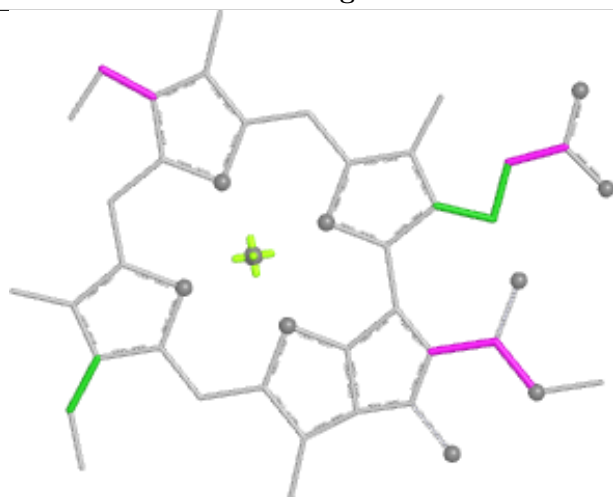
Ligand CLA 1 603



Bond lengths



Bond angles

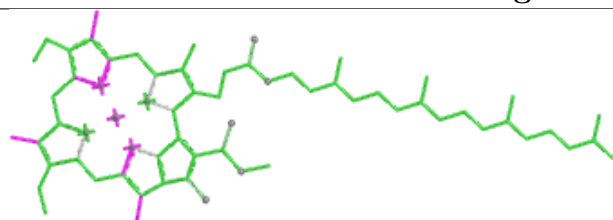


Torsions

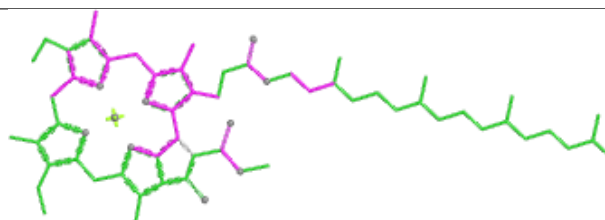


Rings

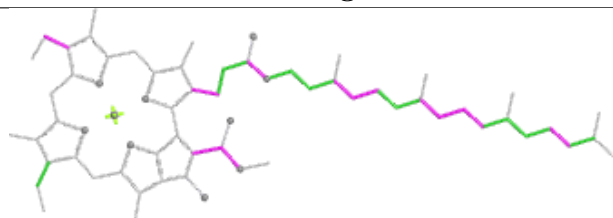
Ligand CLA A 808



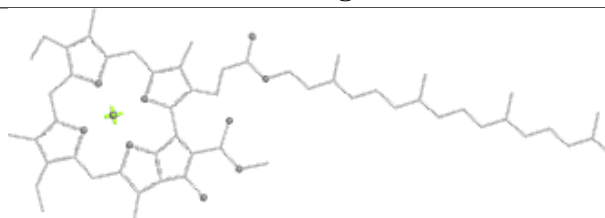
Bond lengths



Bond angles

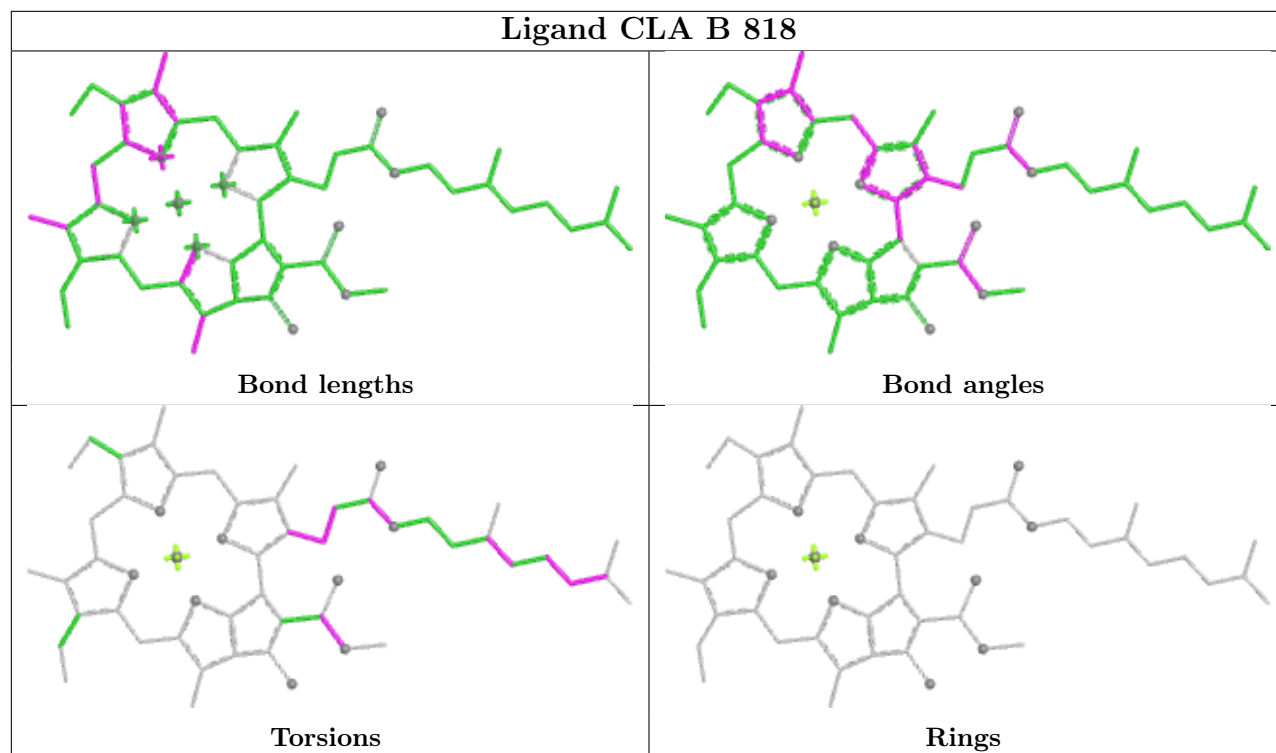


Torsions

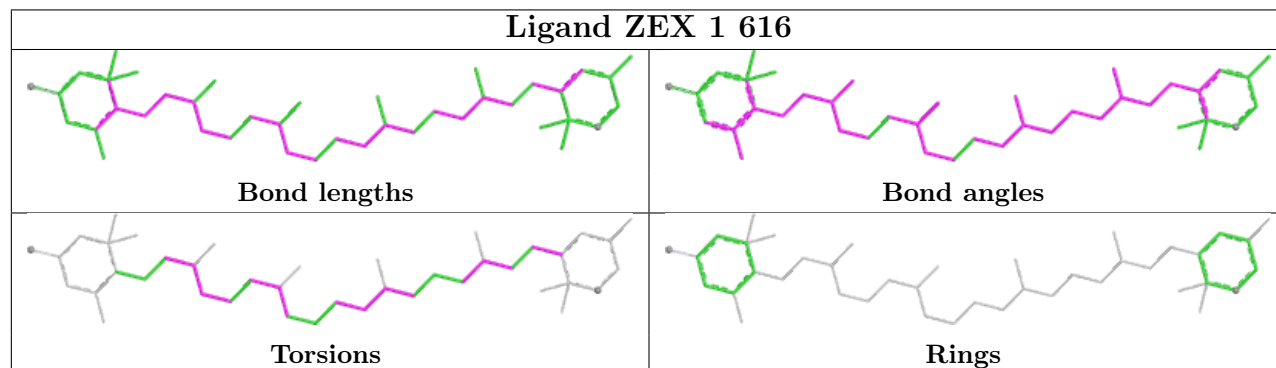


Rings

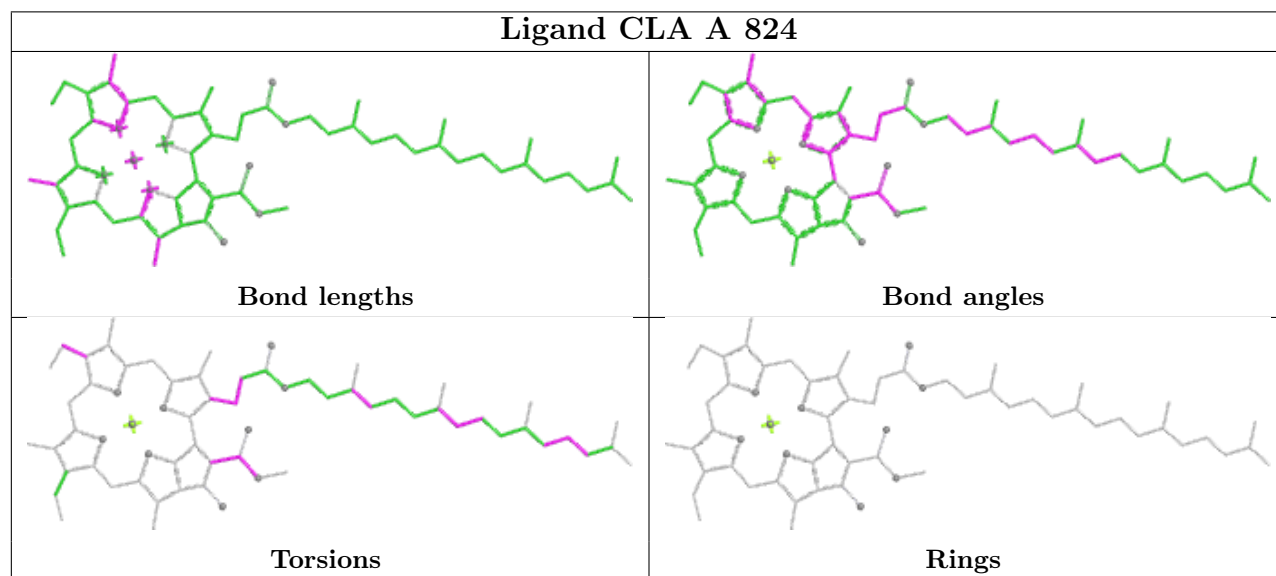
Ligand CLA B 818



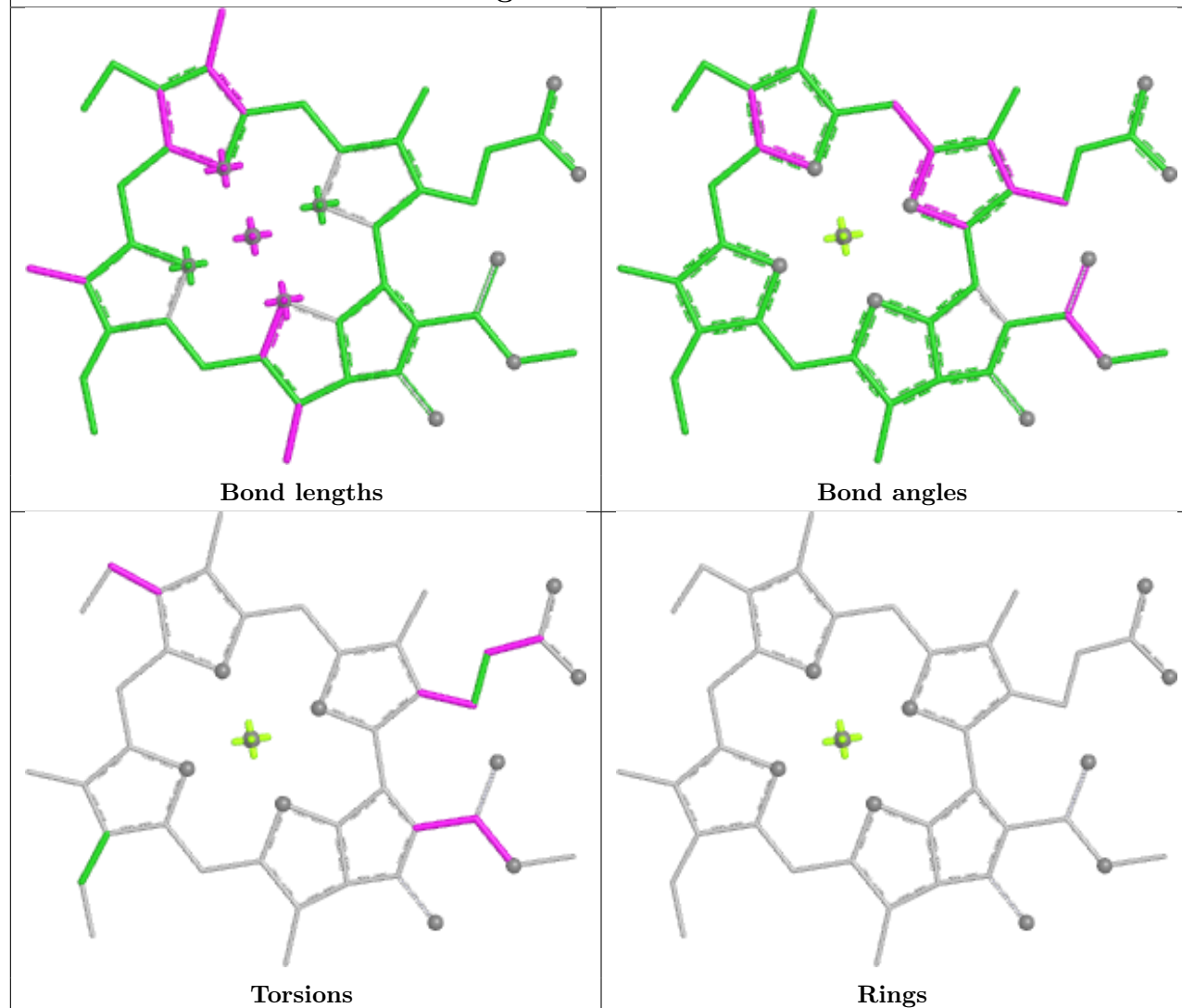
Ligand ZEX 1 616



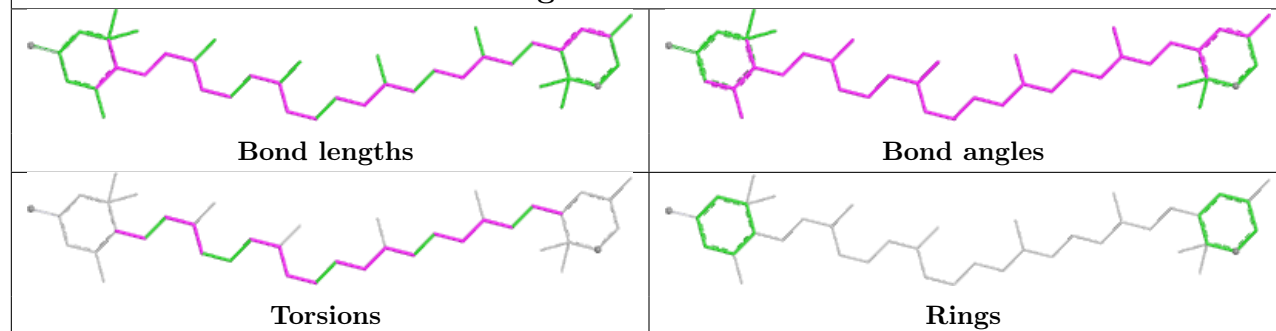
Ligand CLA A 824



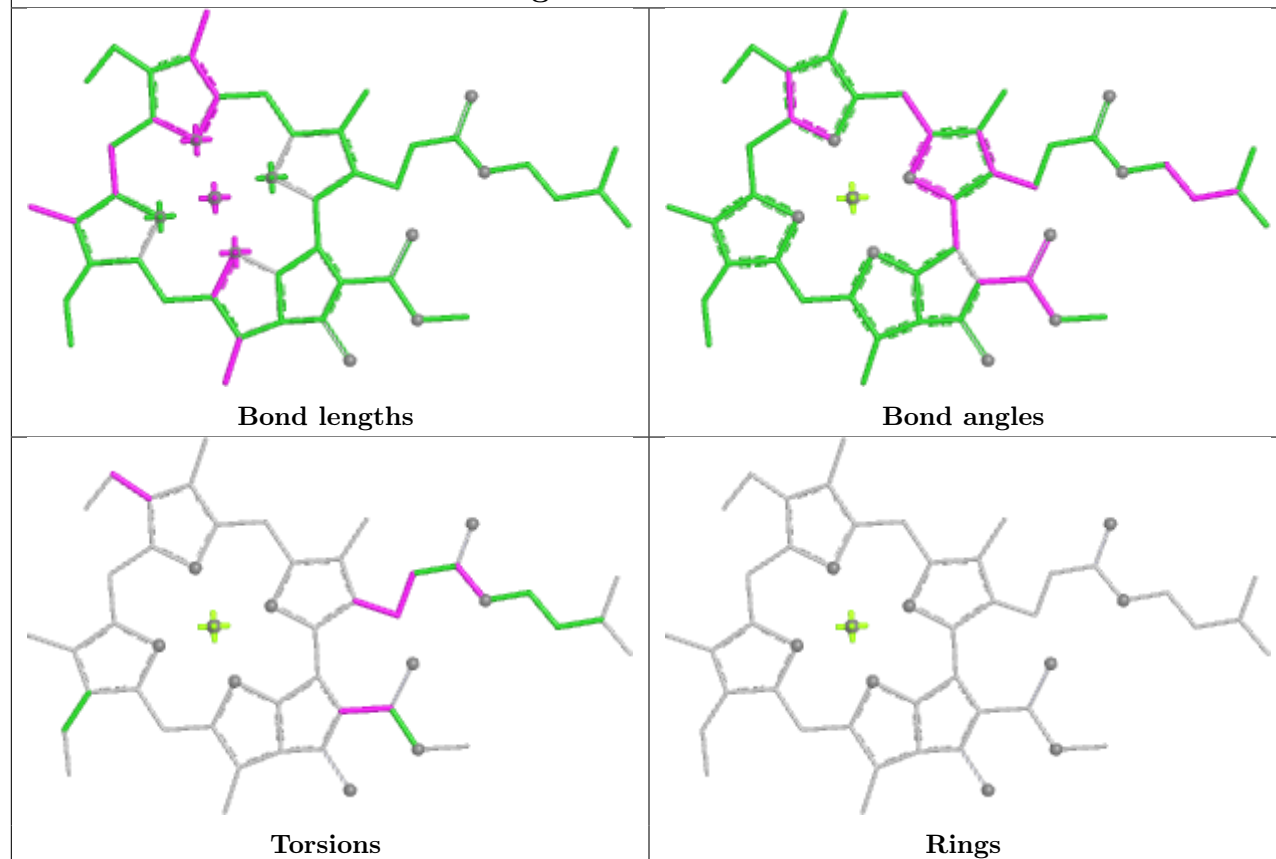
Ligand CLA 3 204



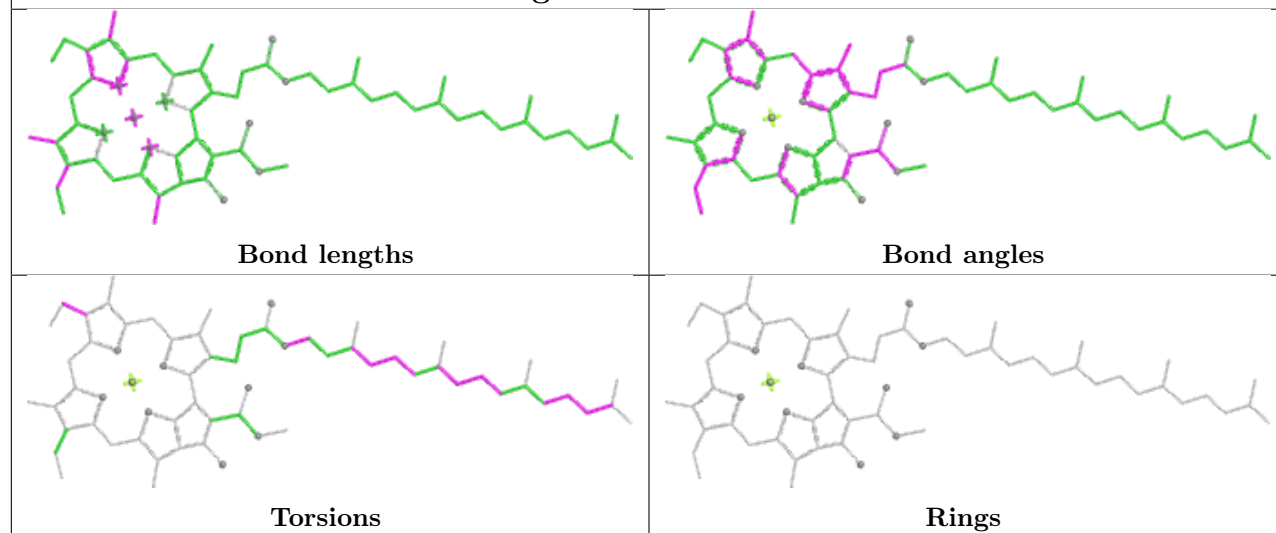
Ligand ZEX 1 614



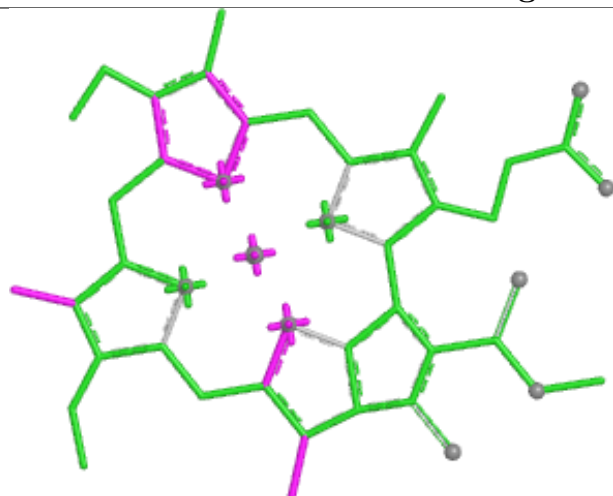
Ligand CLA A 830



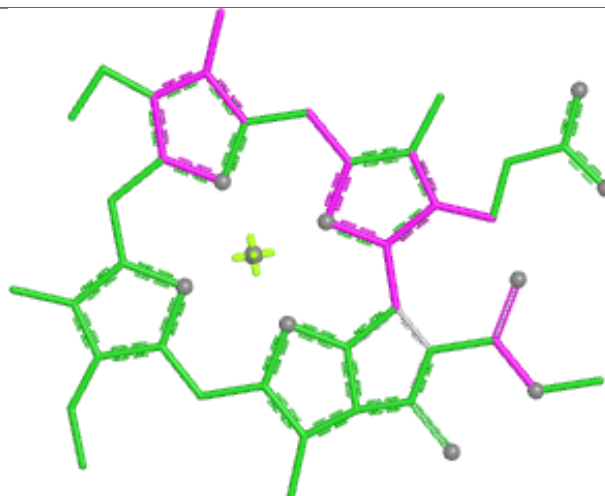
Ligand CLA B 801



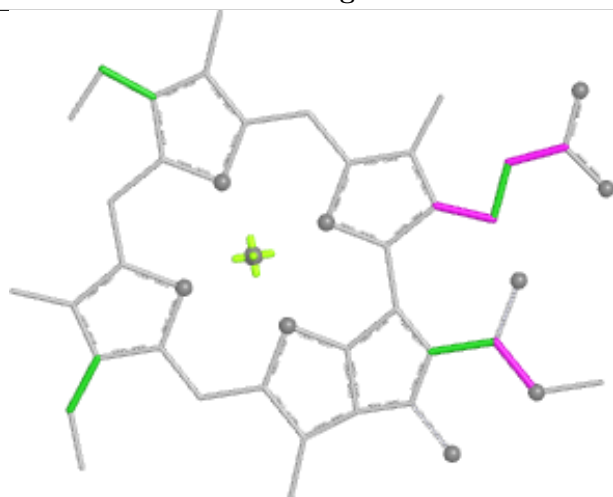
Ligand CLA 1 604



Bond lengths



Bond angles

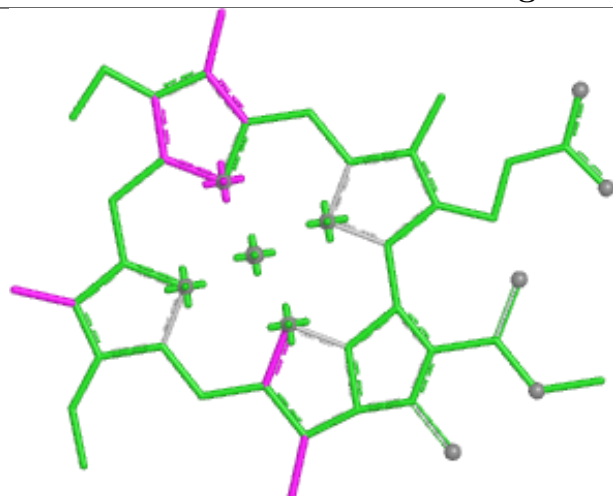


Torsions

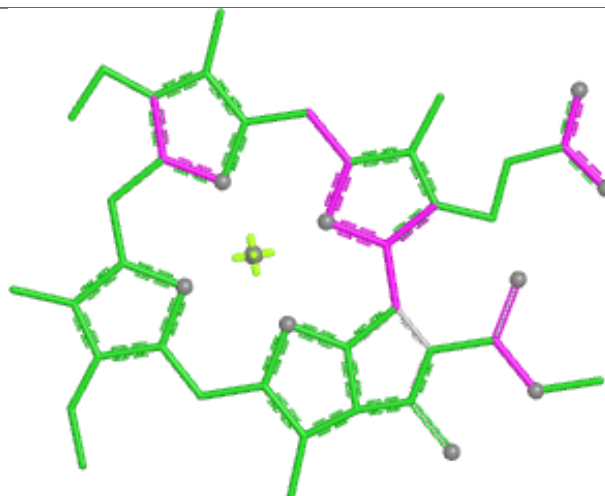


Rings

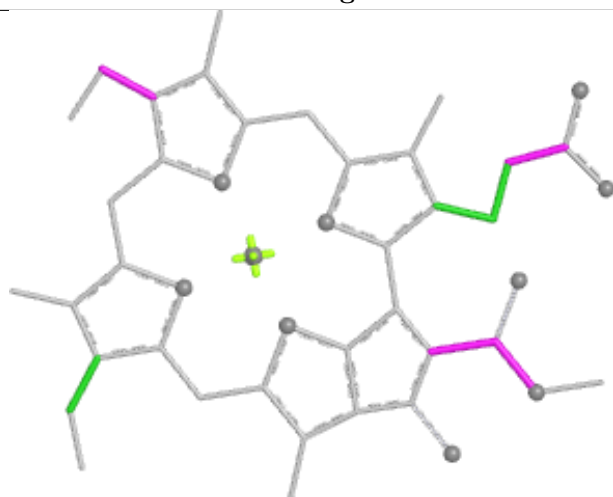
Ligand CLA 1 612



Bond lengths



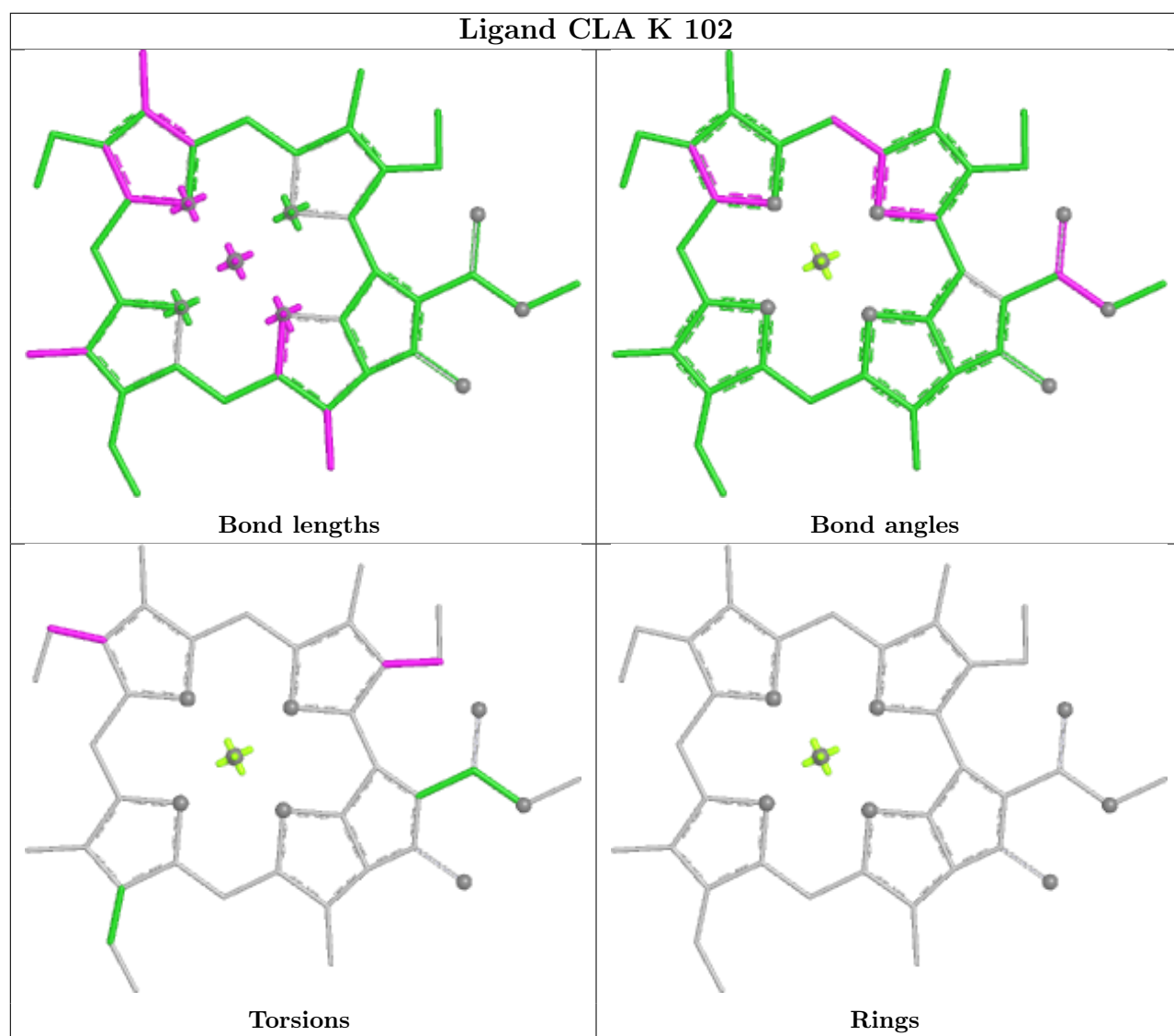
Bond angles



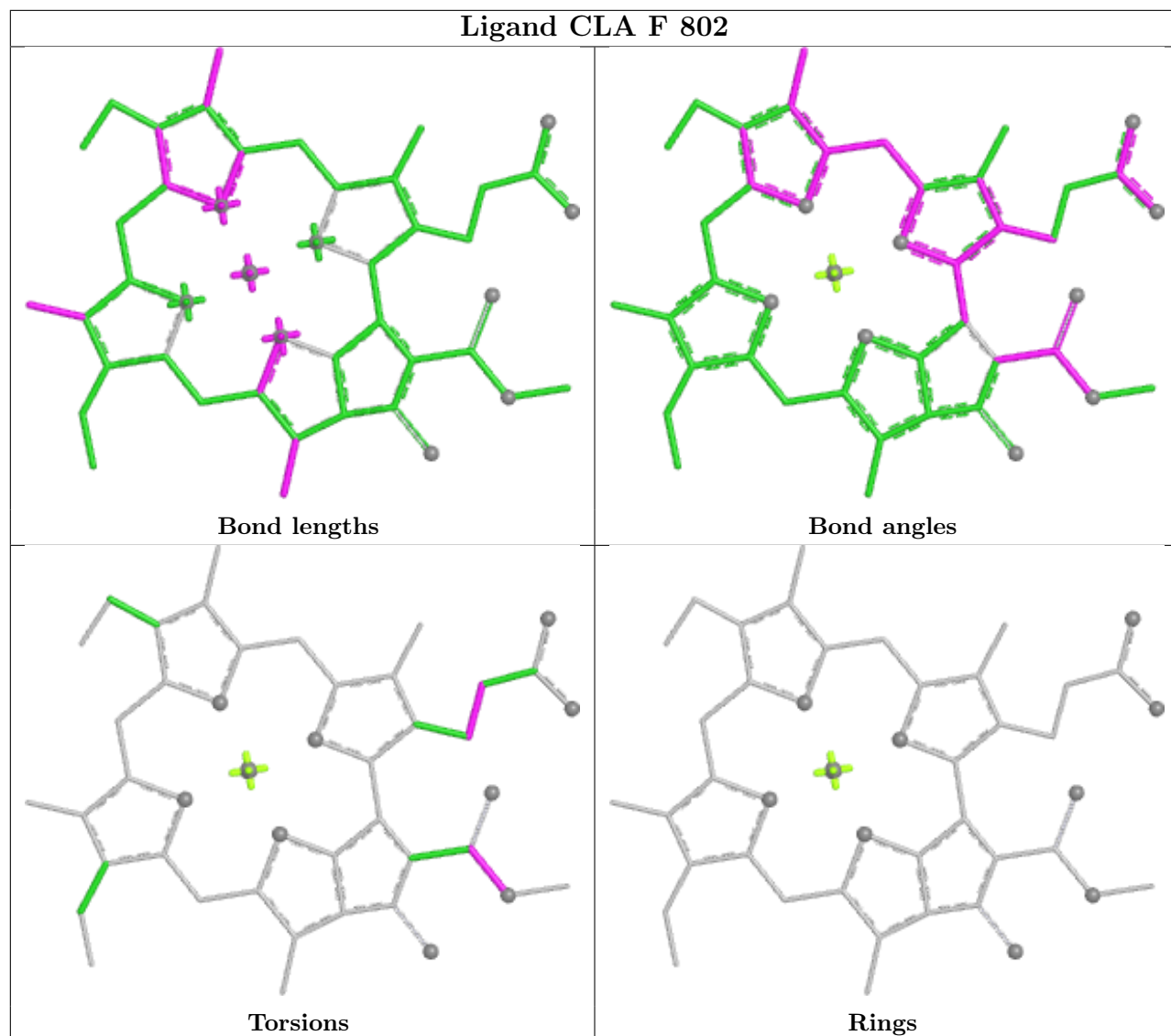
Torsions

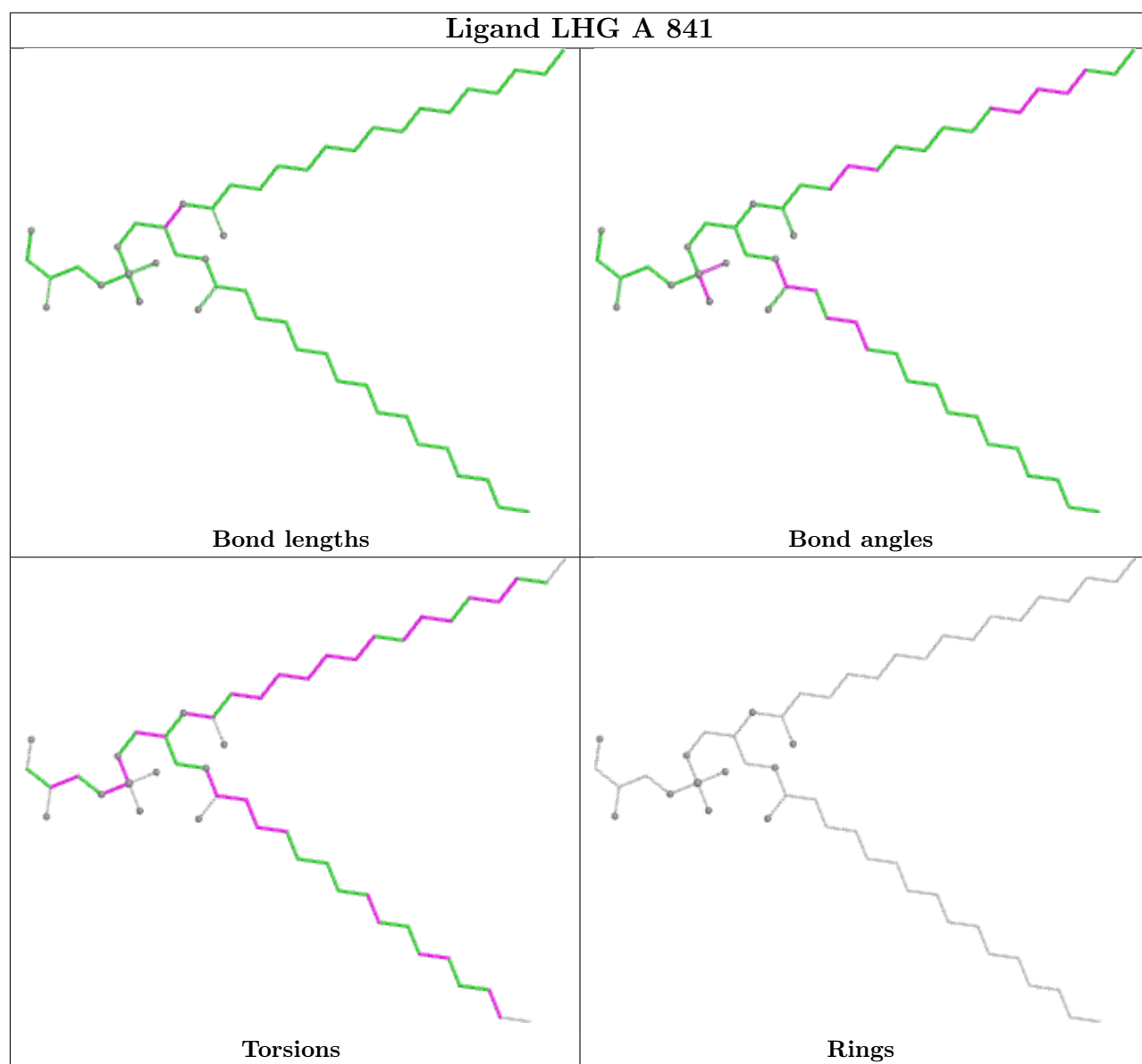


Rings

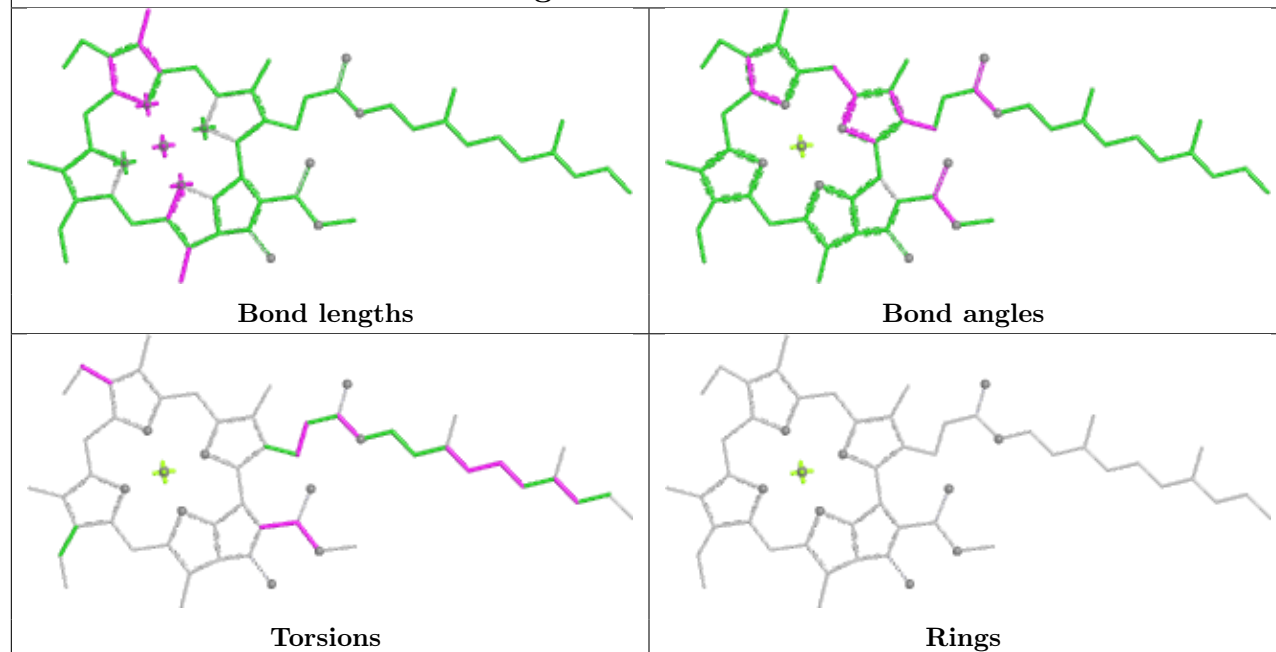


Ligand CLA F 802

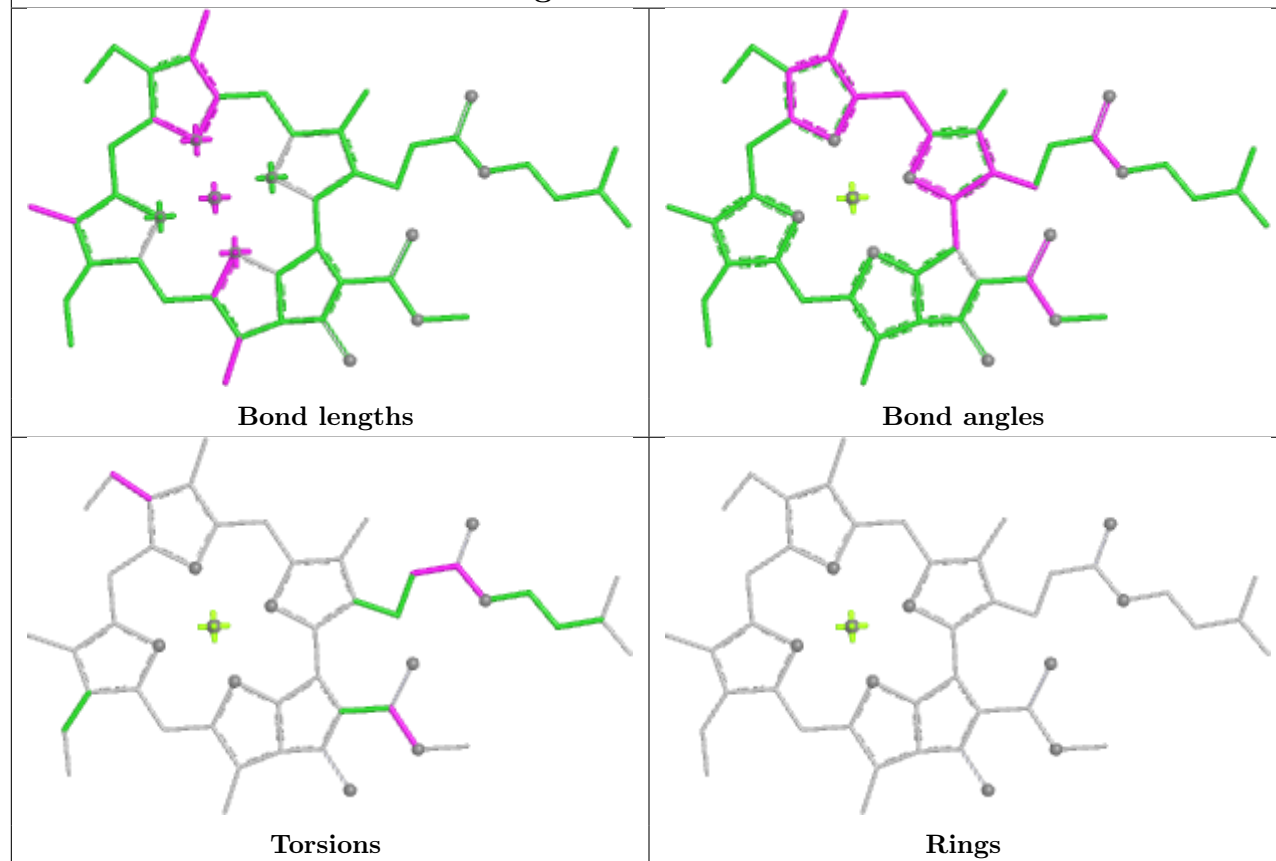


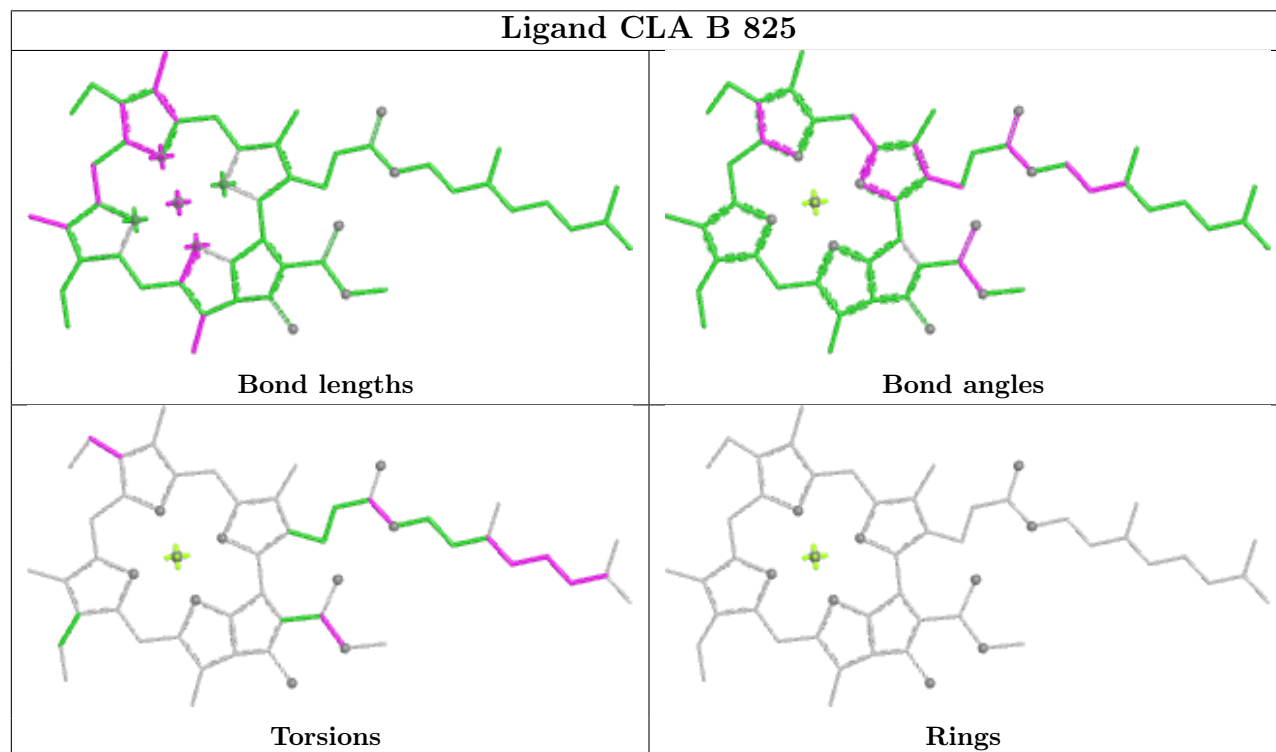
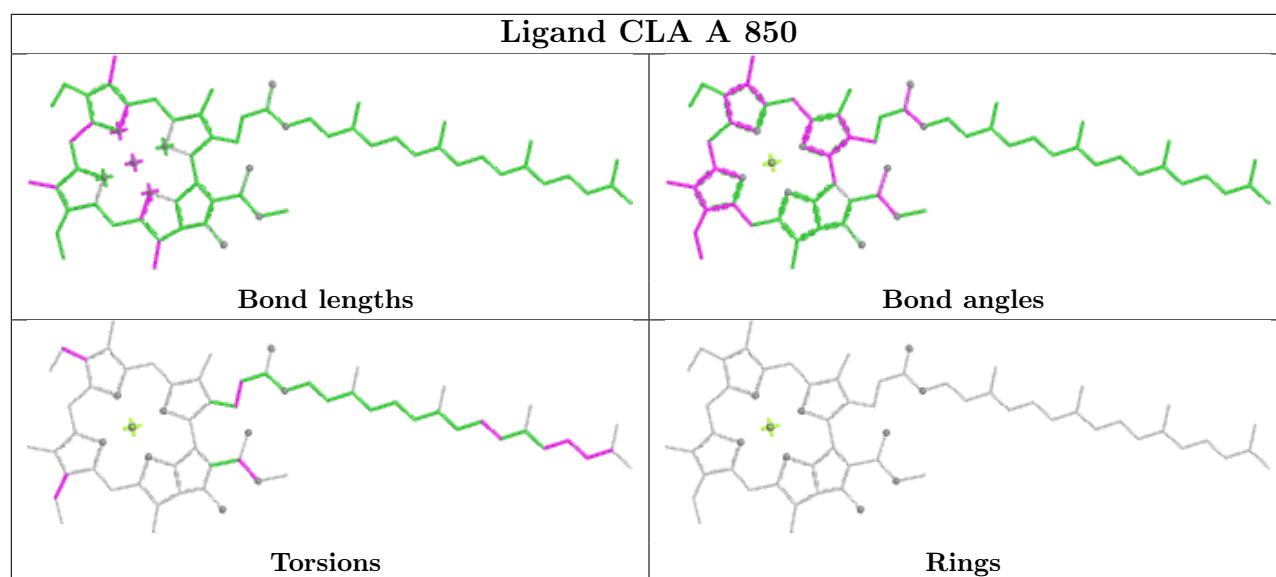


Ligand CLA L 203

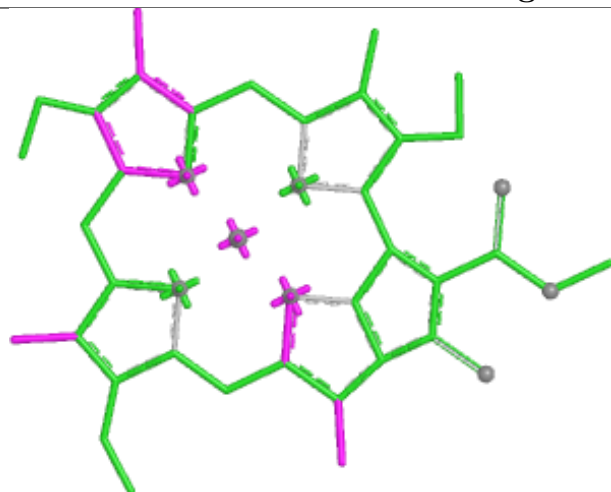


Ligand CLA L 205





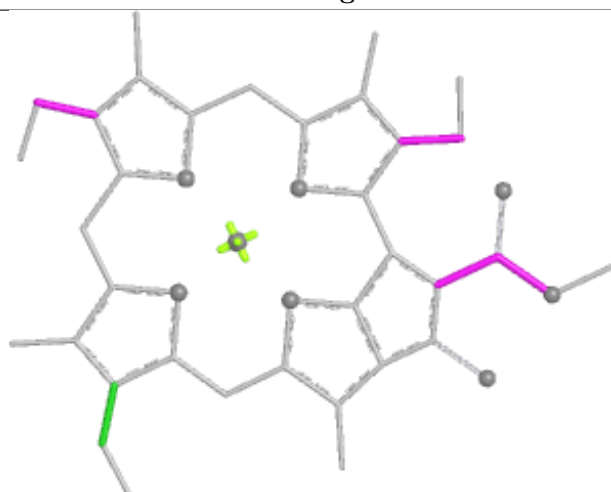
Ligand CLA J 101



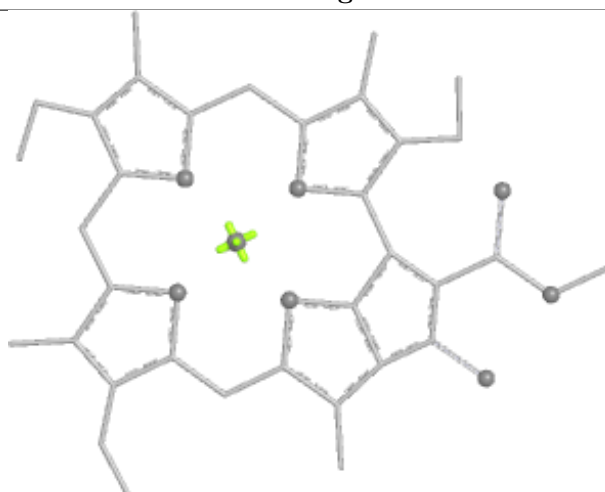
Bond lengths



Bond angles

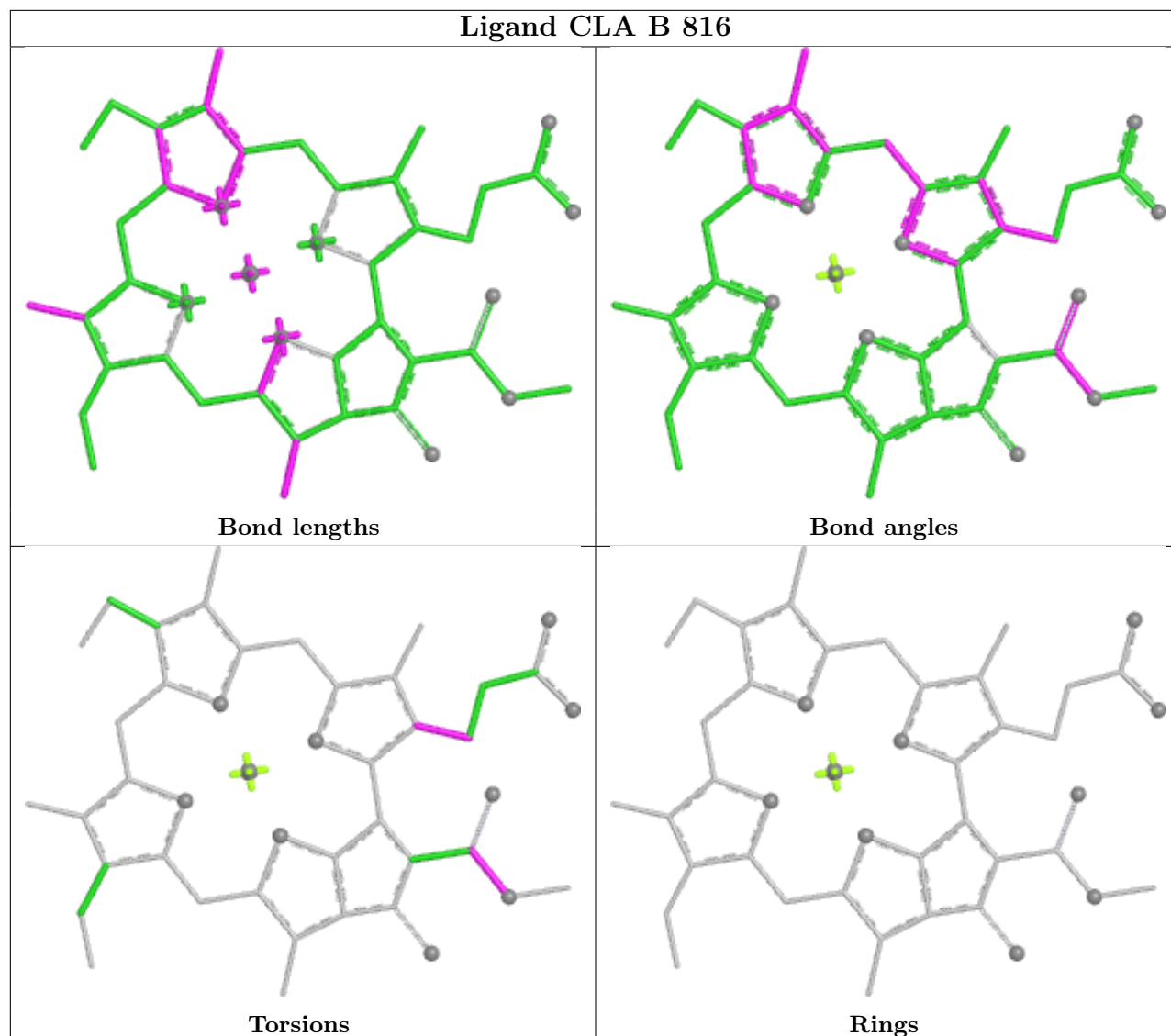


Torsions

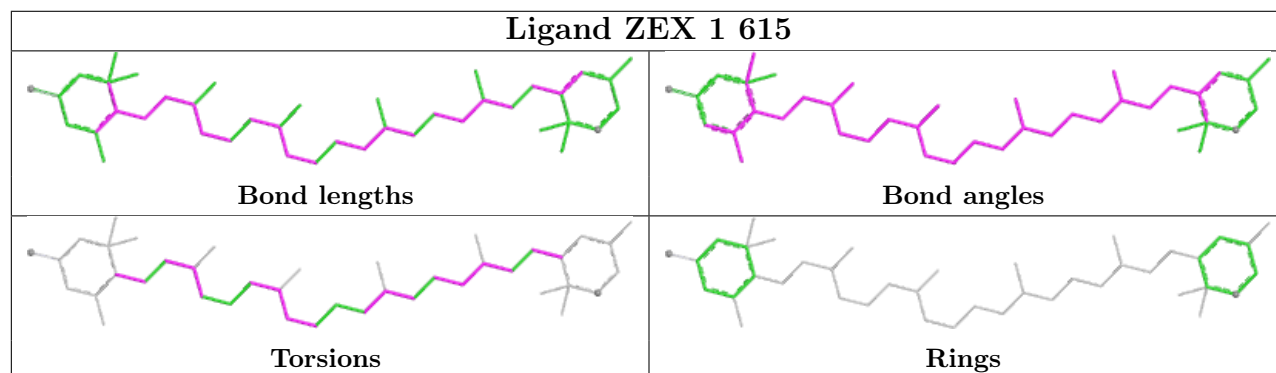


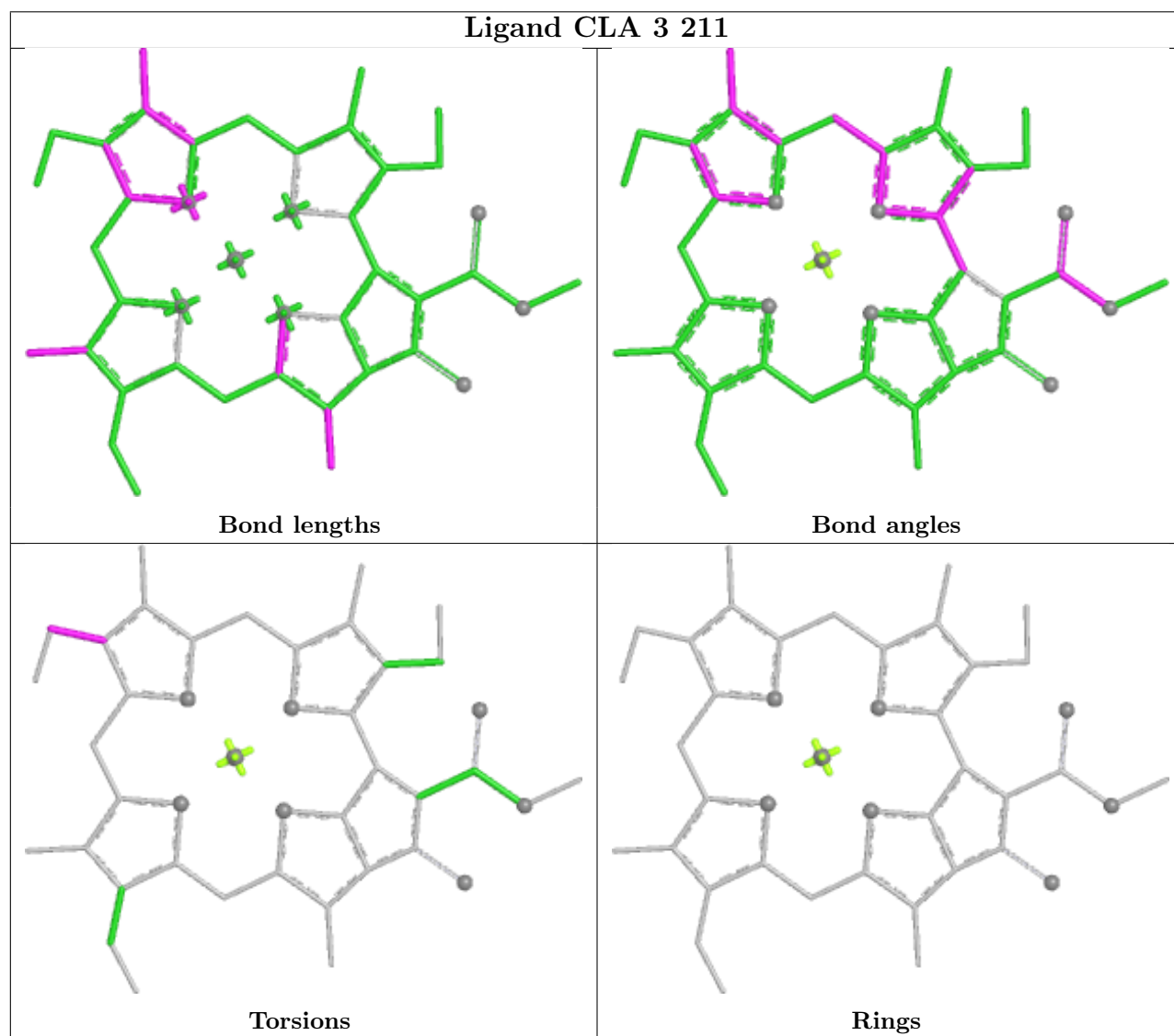
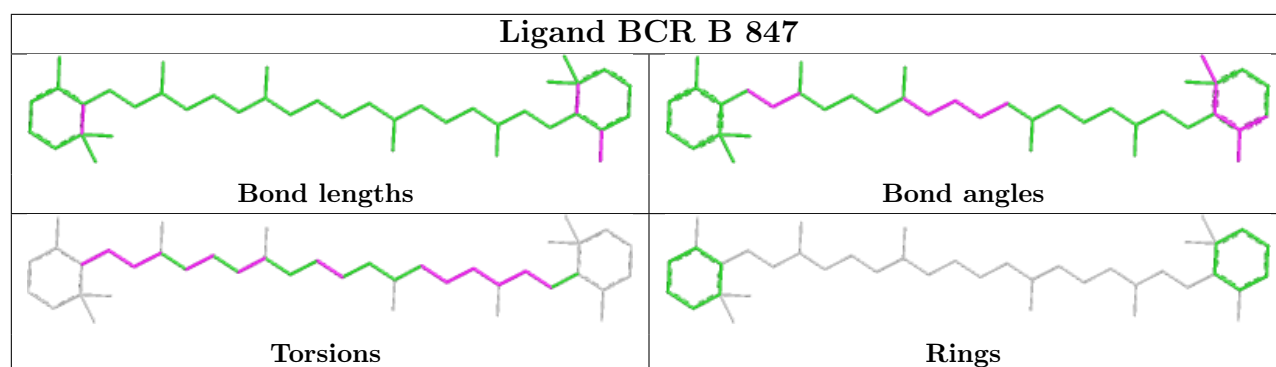
Rings

Ligand CLA B 816

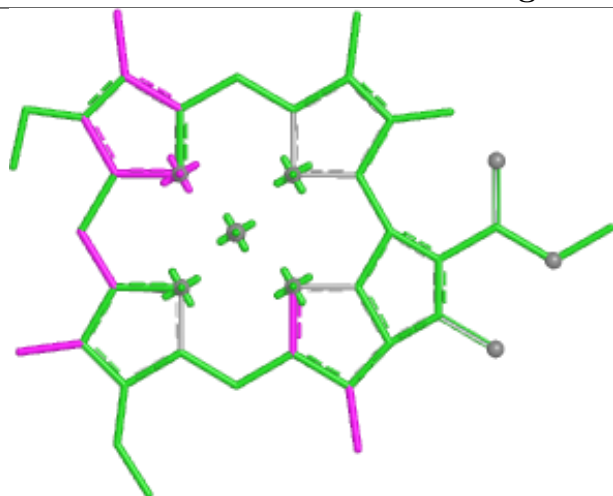


Ligand ZEX 1 615

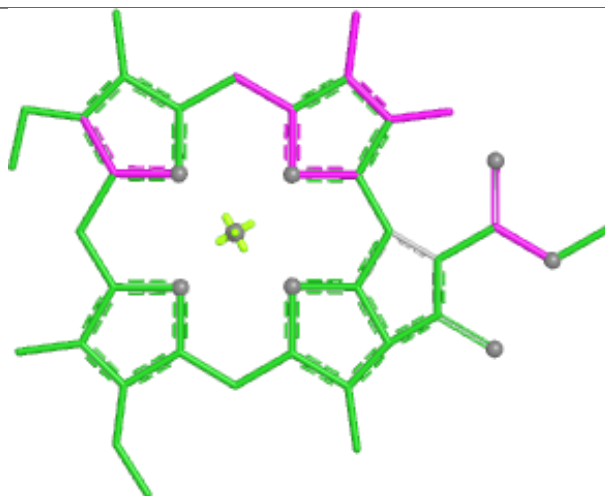




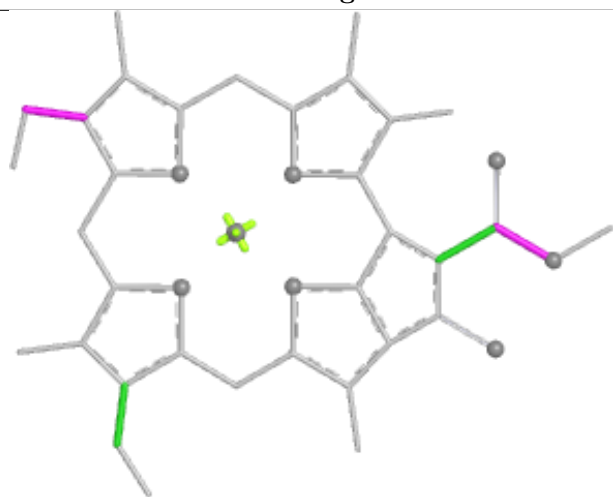
Ligand CLA 3 210



Bond lengths



Bond angles

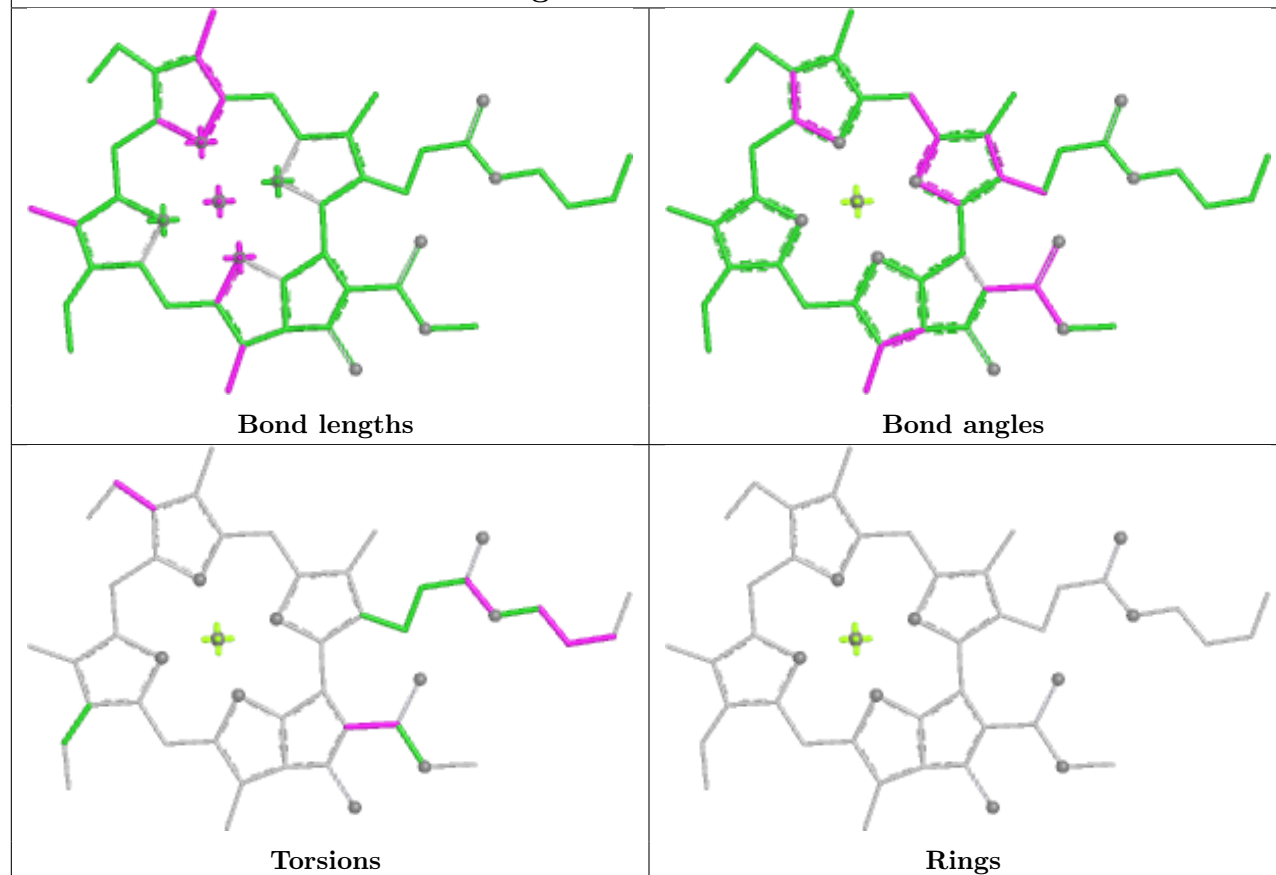


Torsions

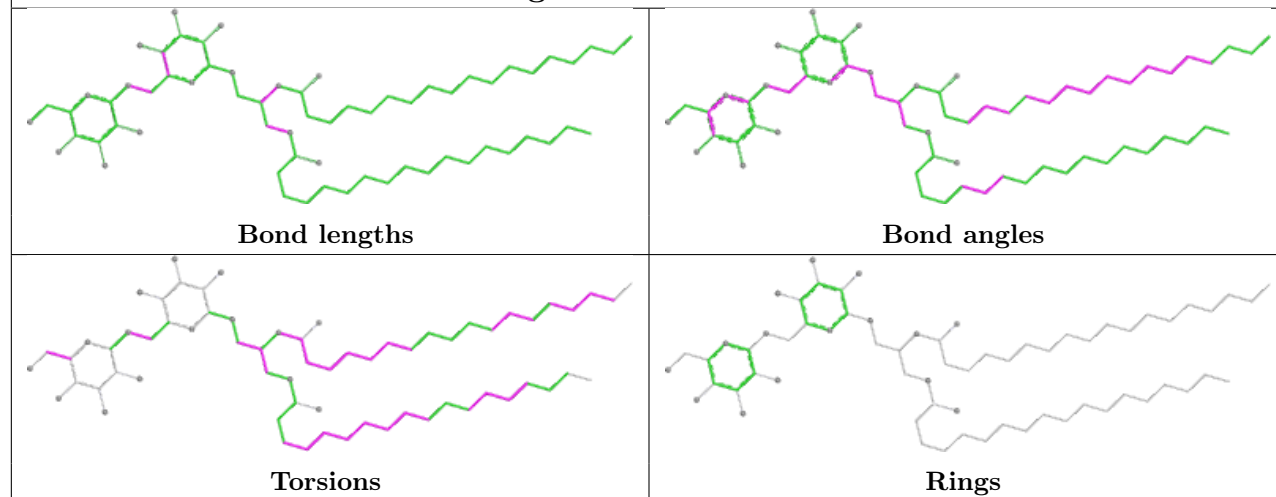


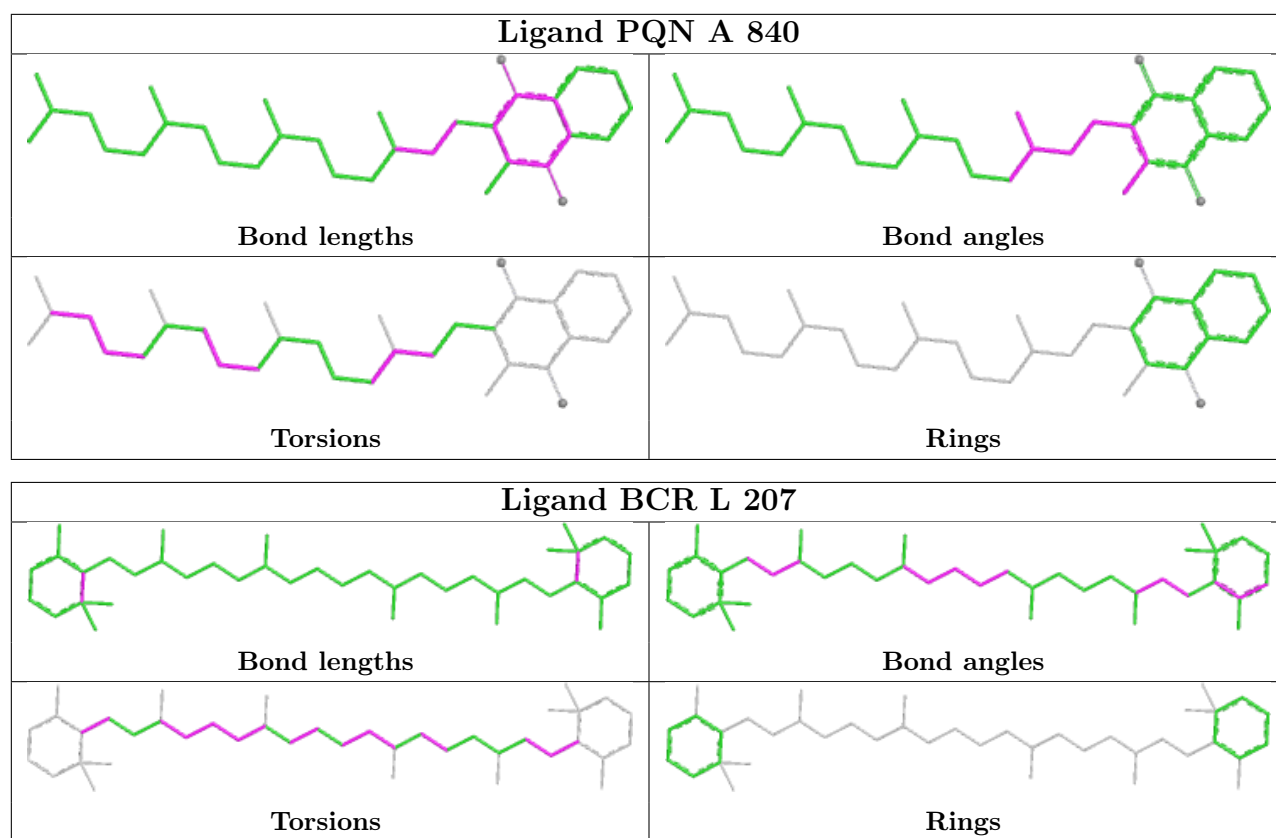
Rings

Ligand CLA A 821

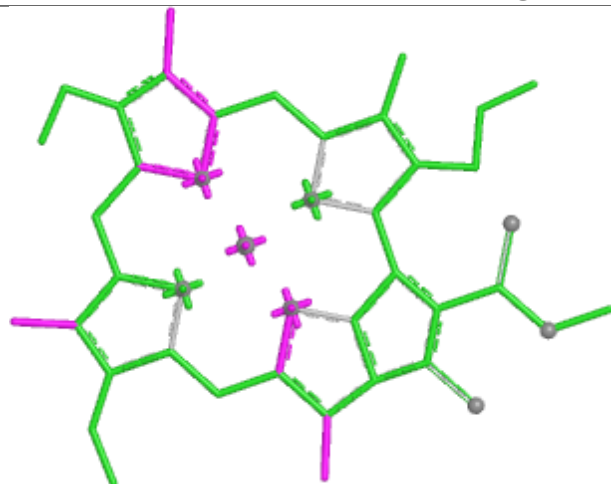


Ligand DGD B 850

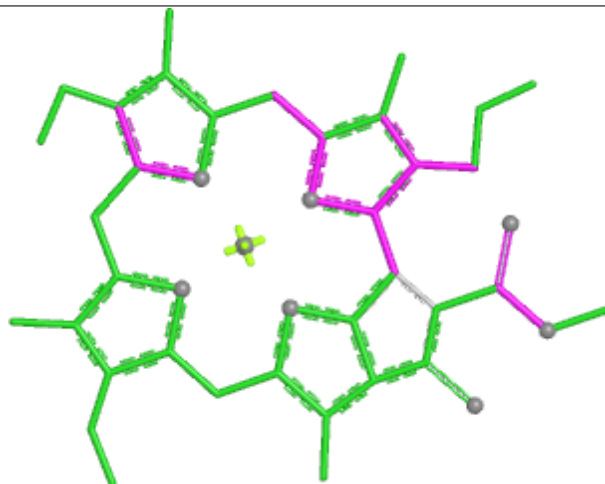




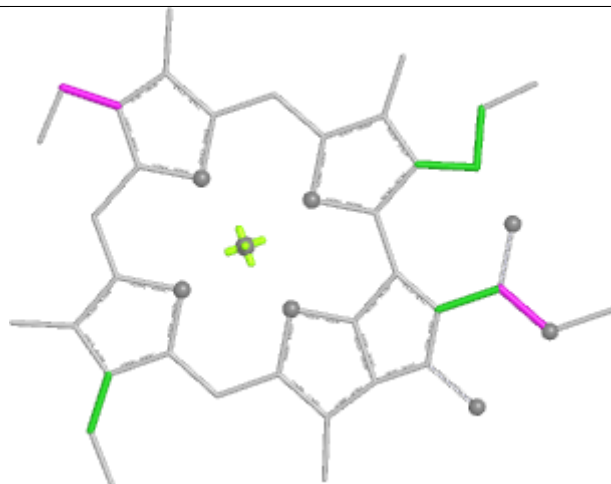
Ligand CLA B 824



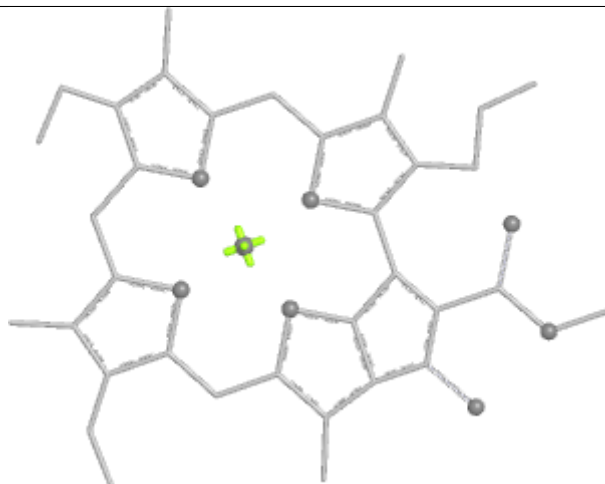
Bond lengths



Bond angles

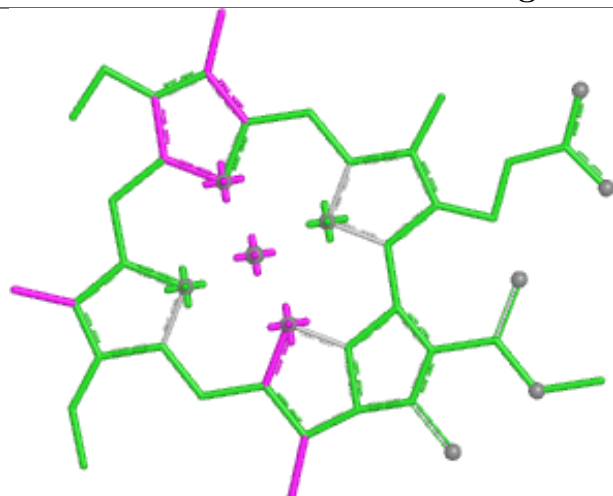


Torsions

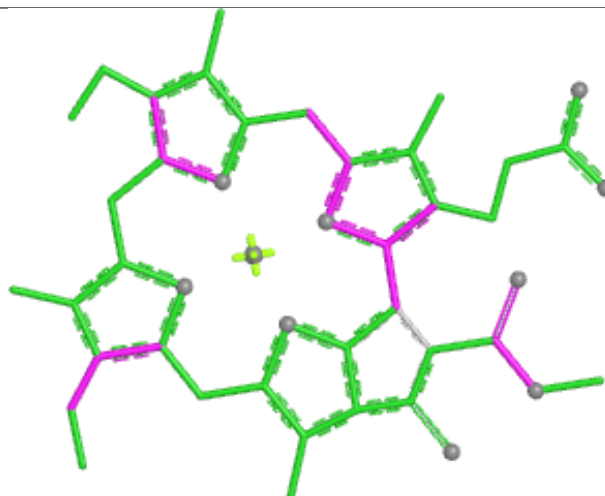


Rings

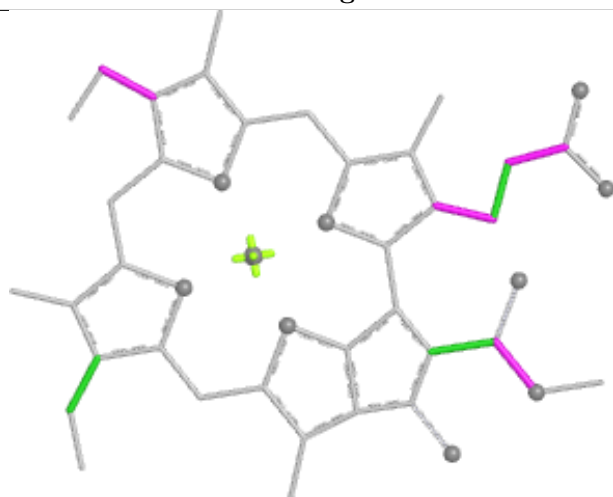
Ligand CLA 1 611



Bond lengths



Bond angles

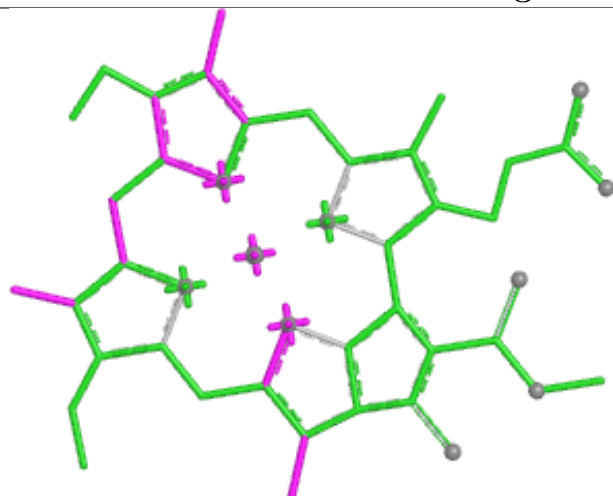


Torsions

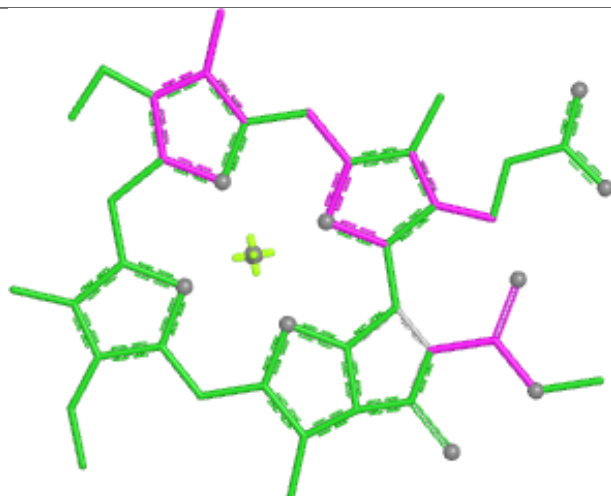


Rings

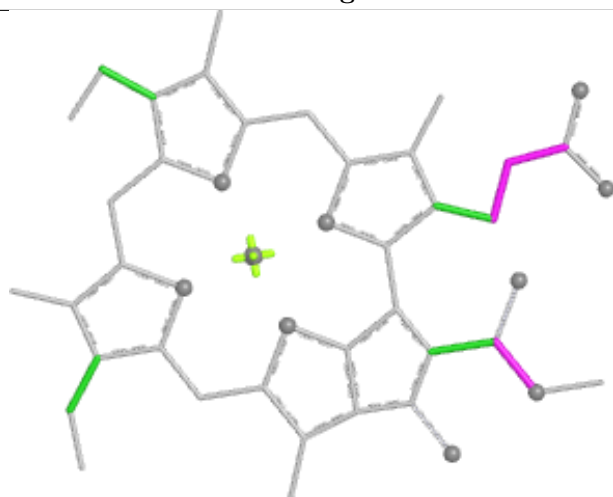
Ligand CLA B 806



Bond lengths



Bond angles

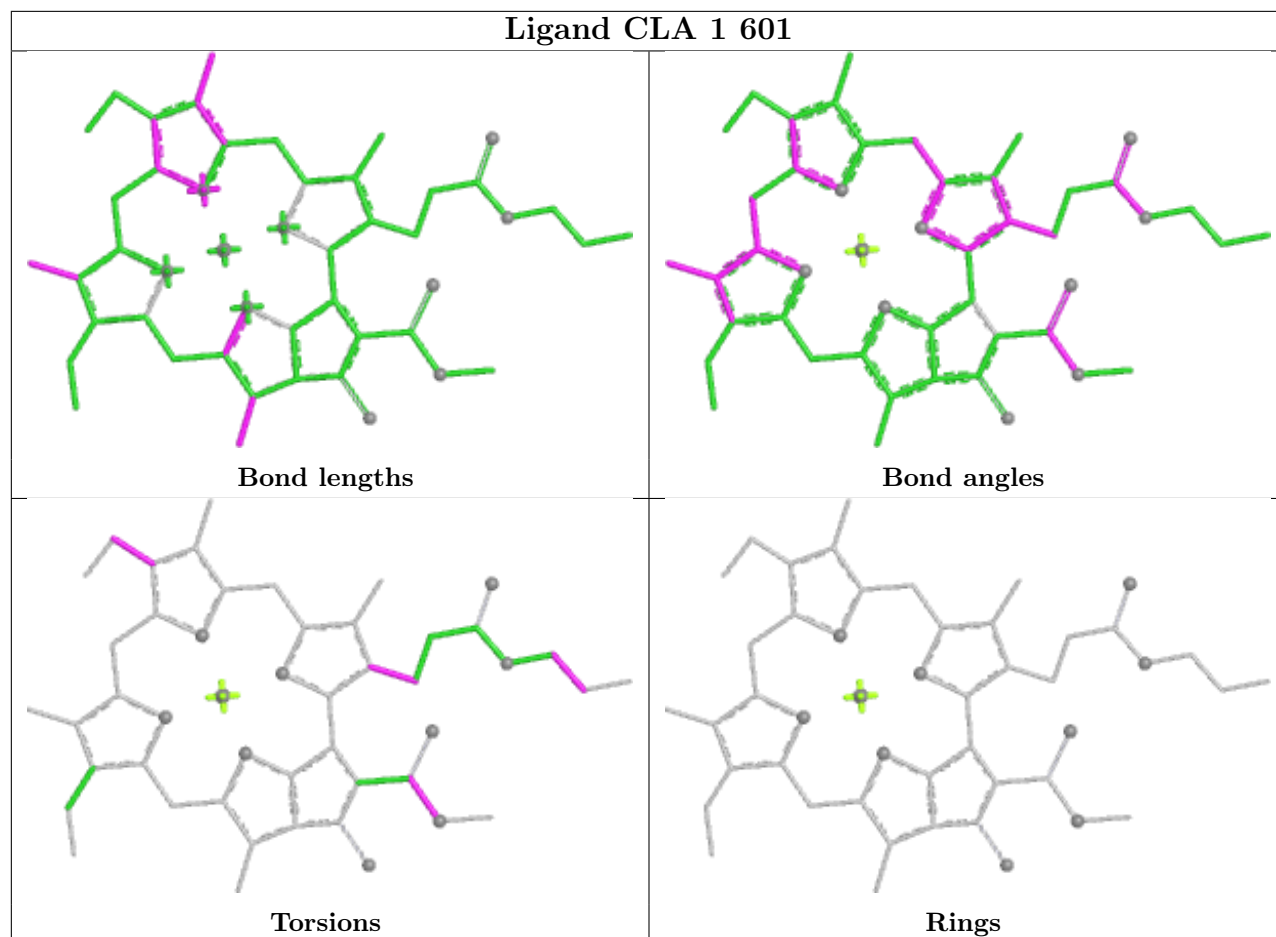


Torsions

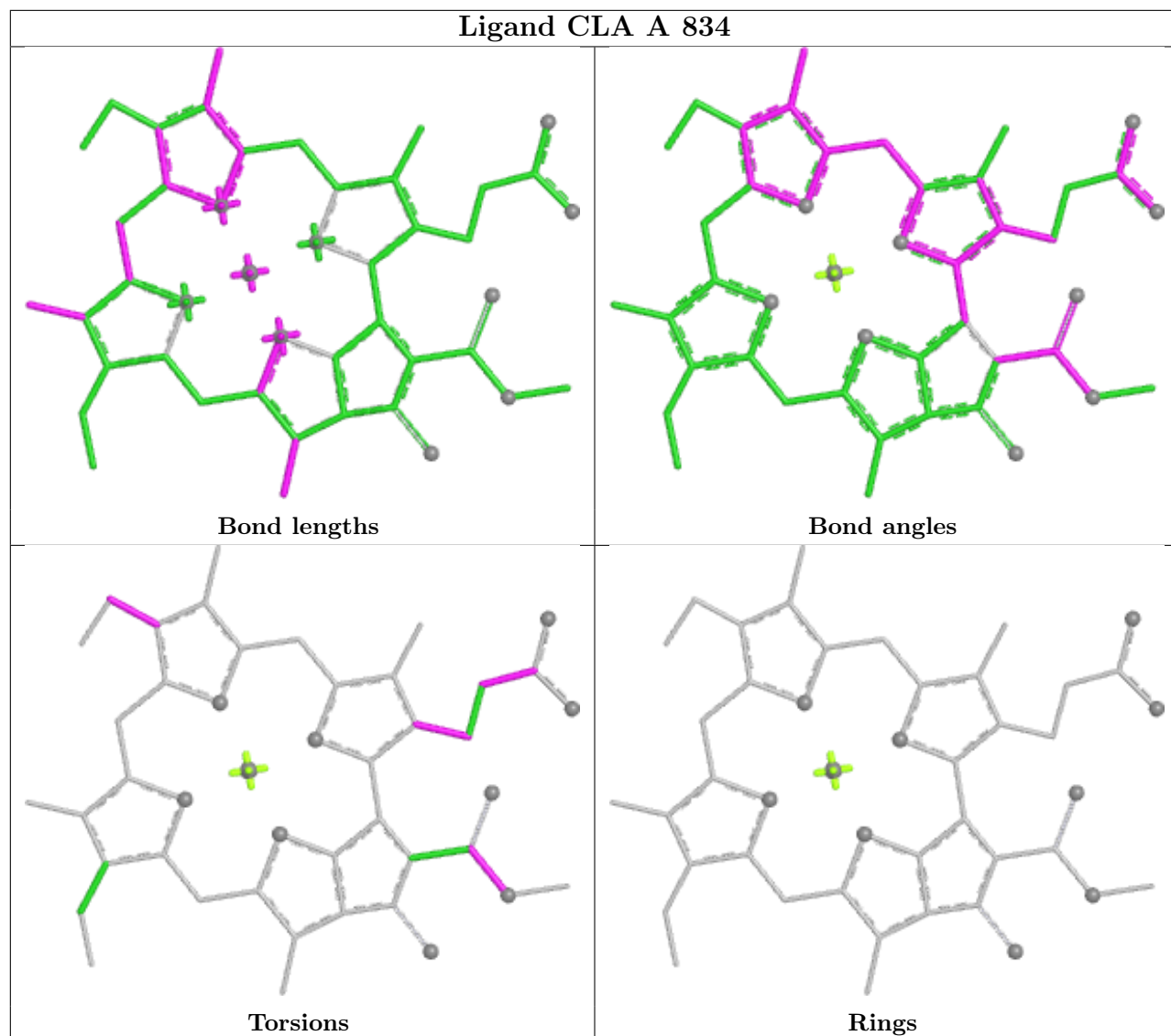


Rings

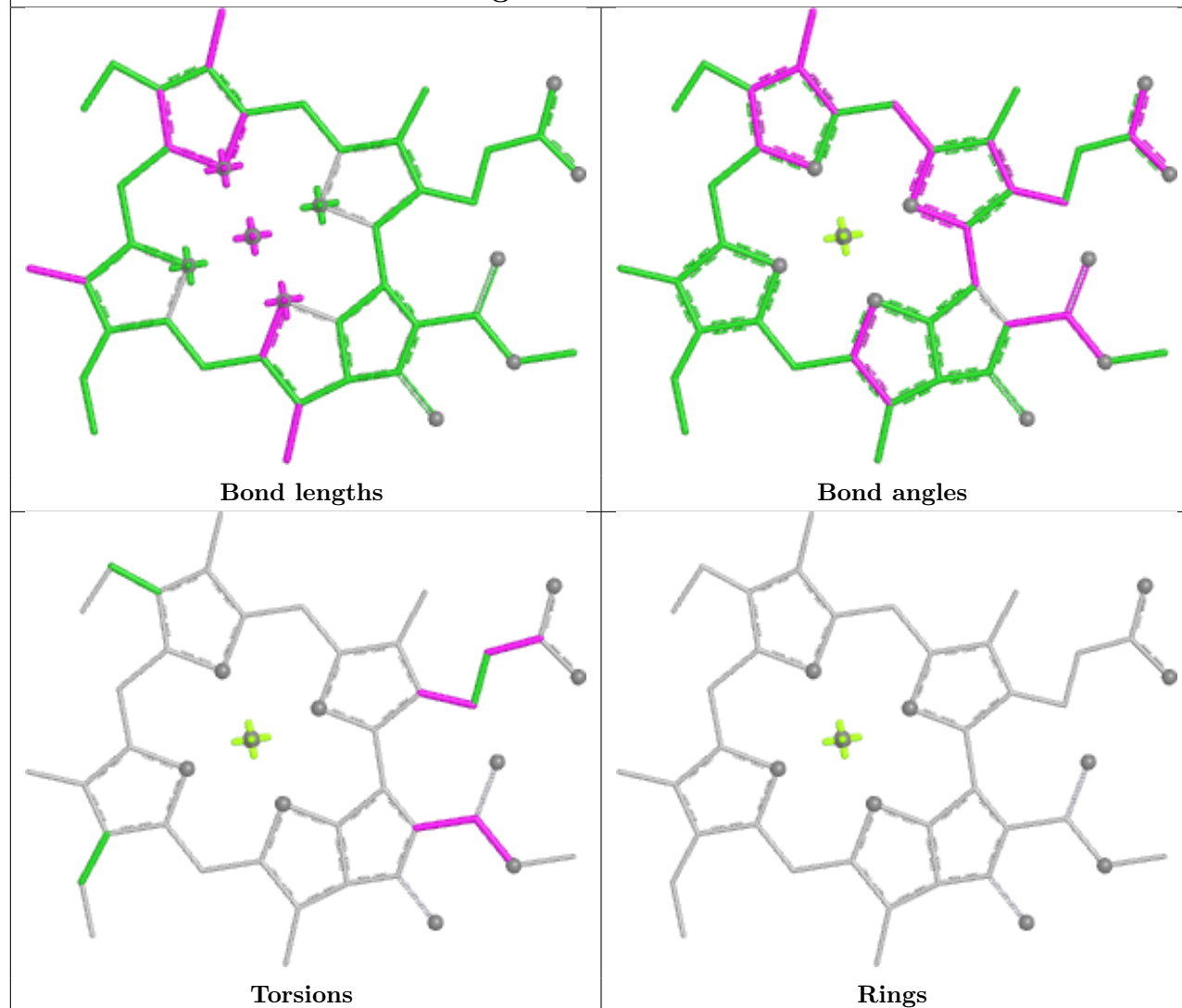
Ligand CLA 1 601



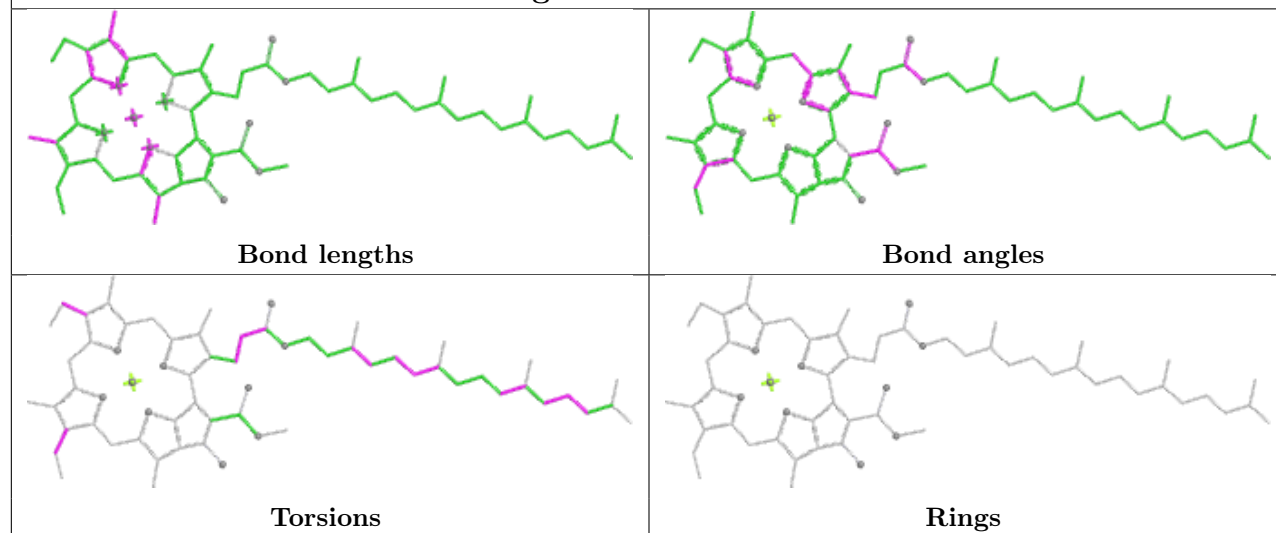
Ligand CLA A 834

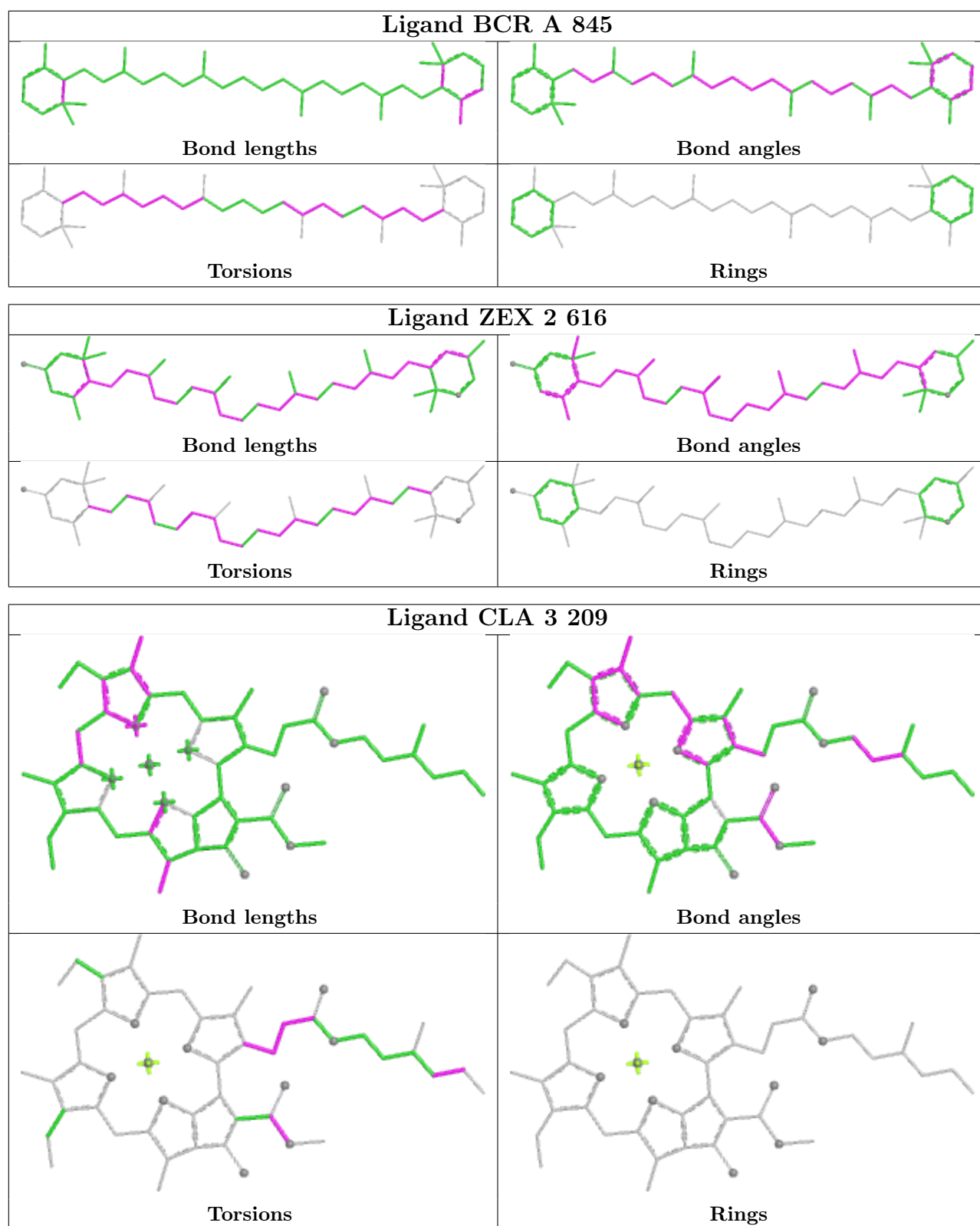


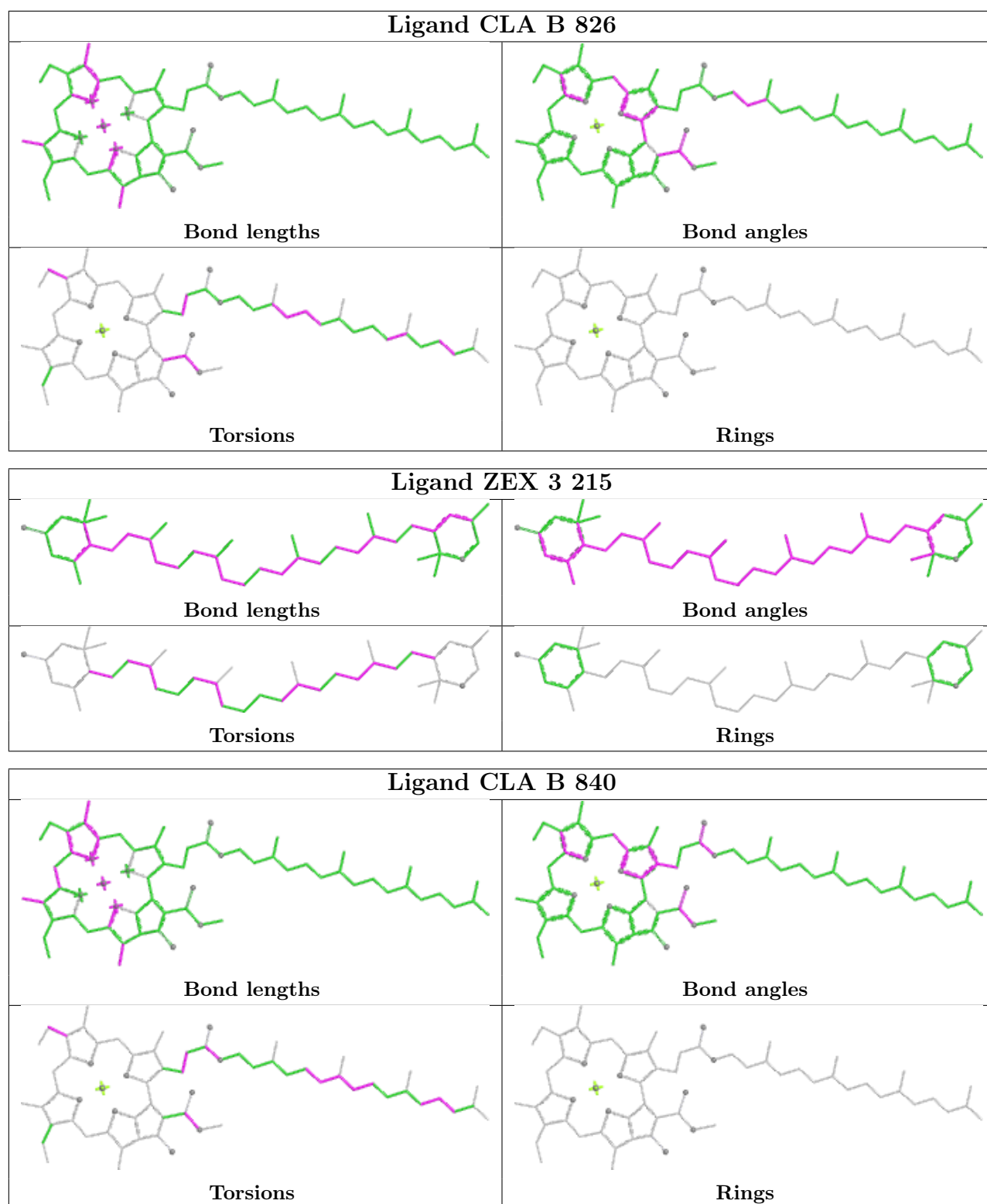
Ligand CLA A 813

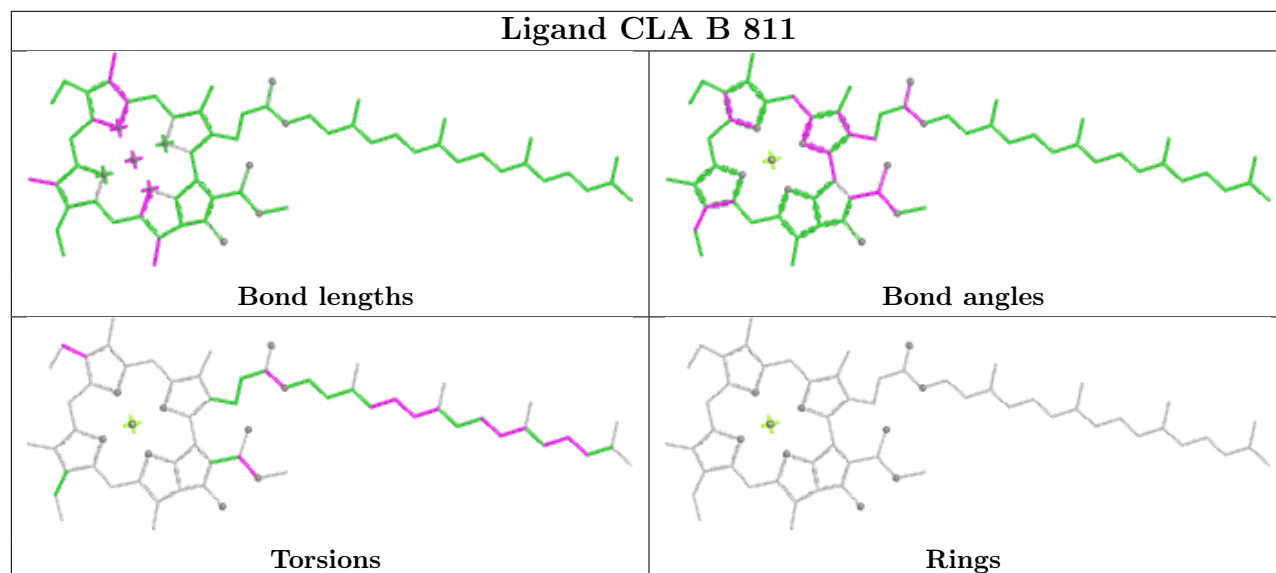
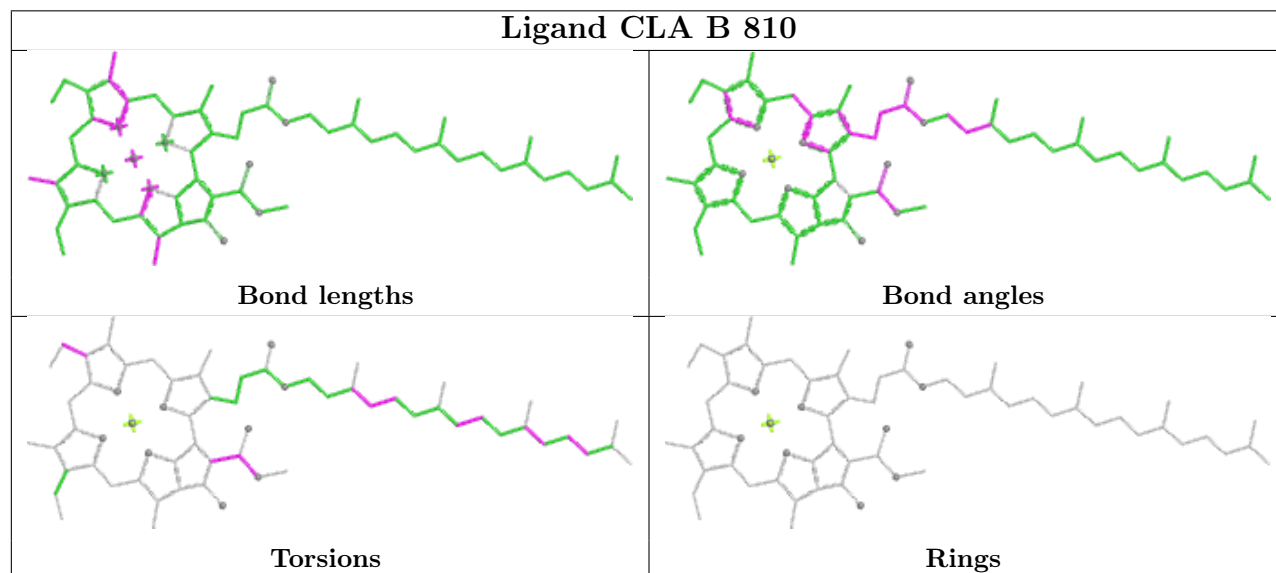
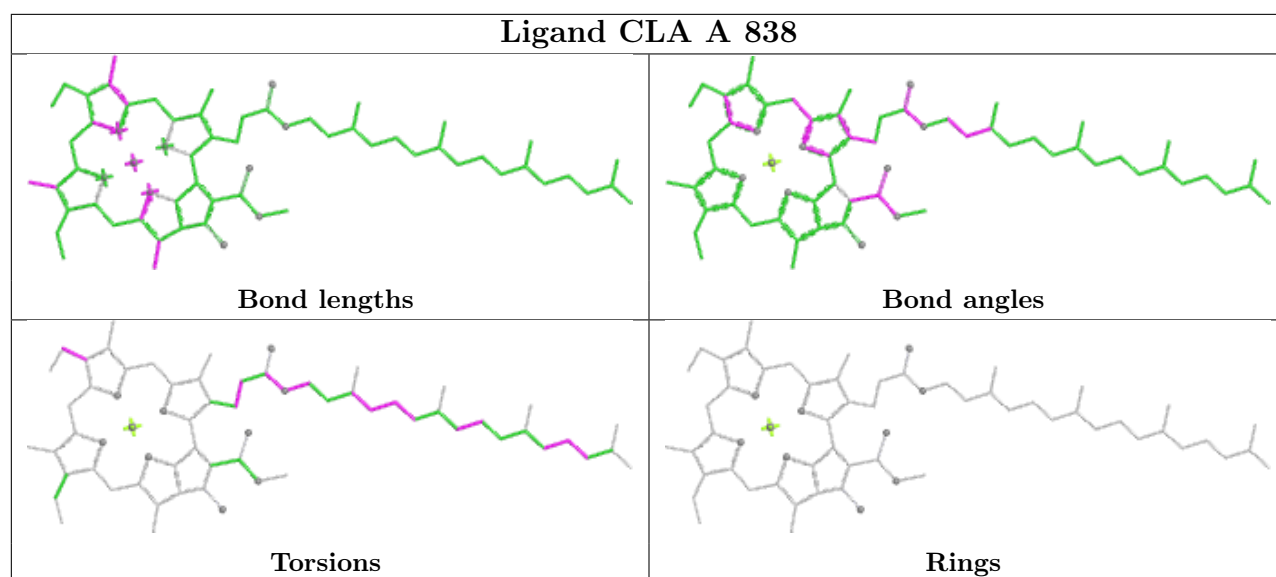


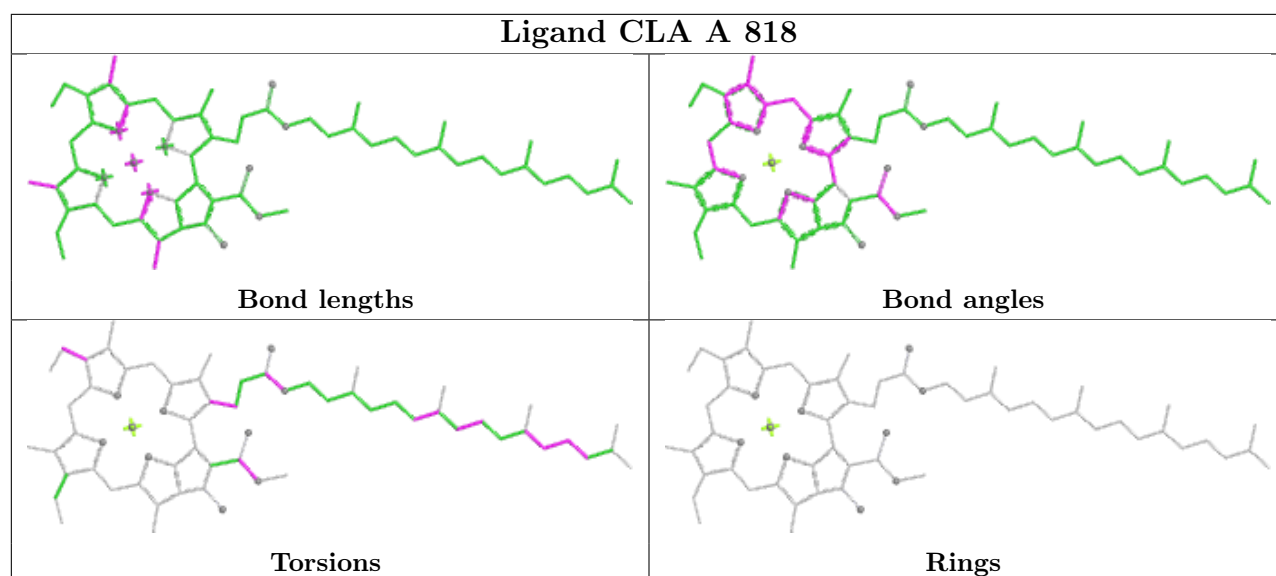
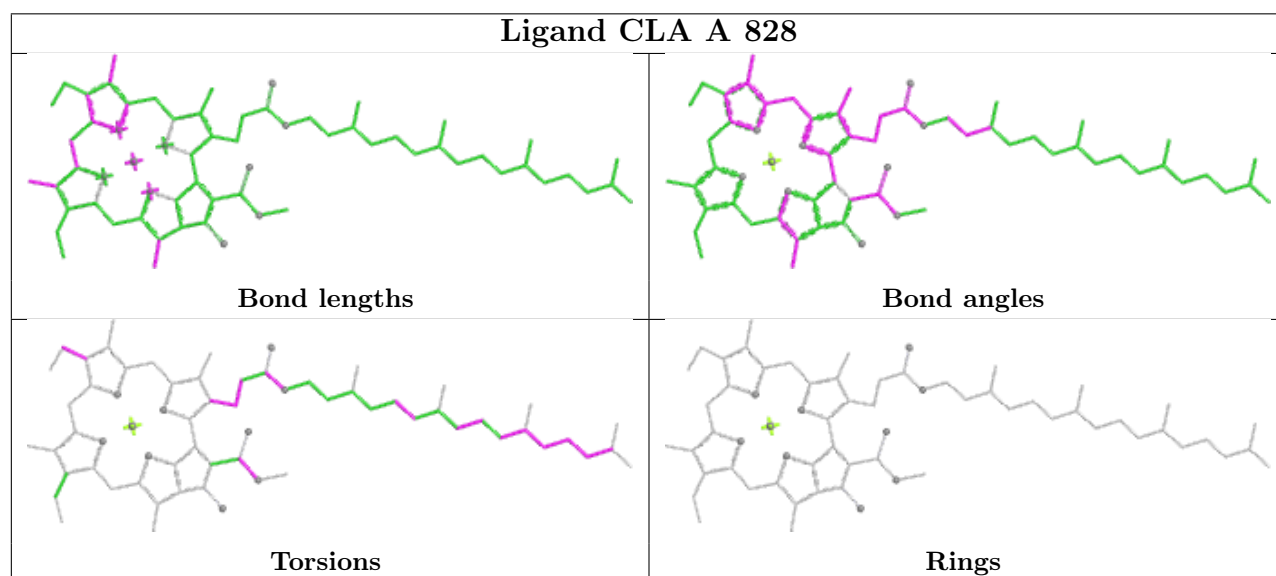
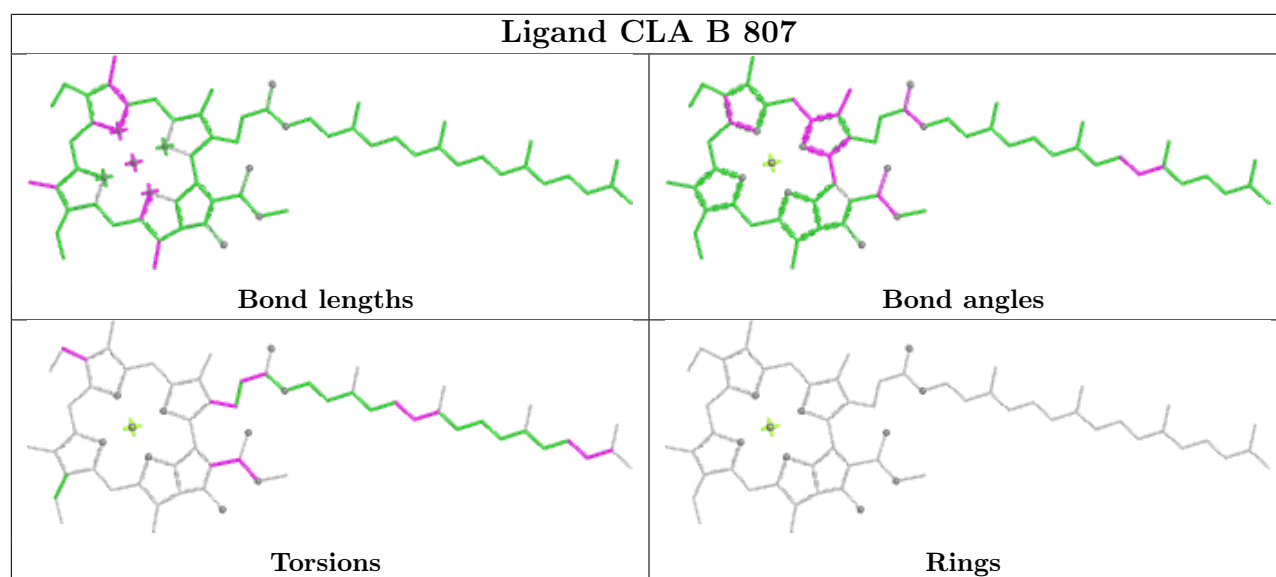
Ligand CLA B 809



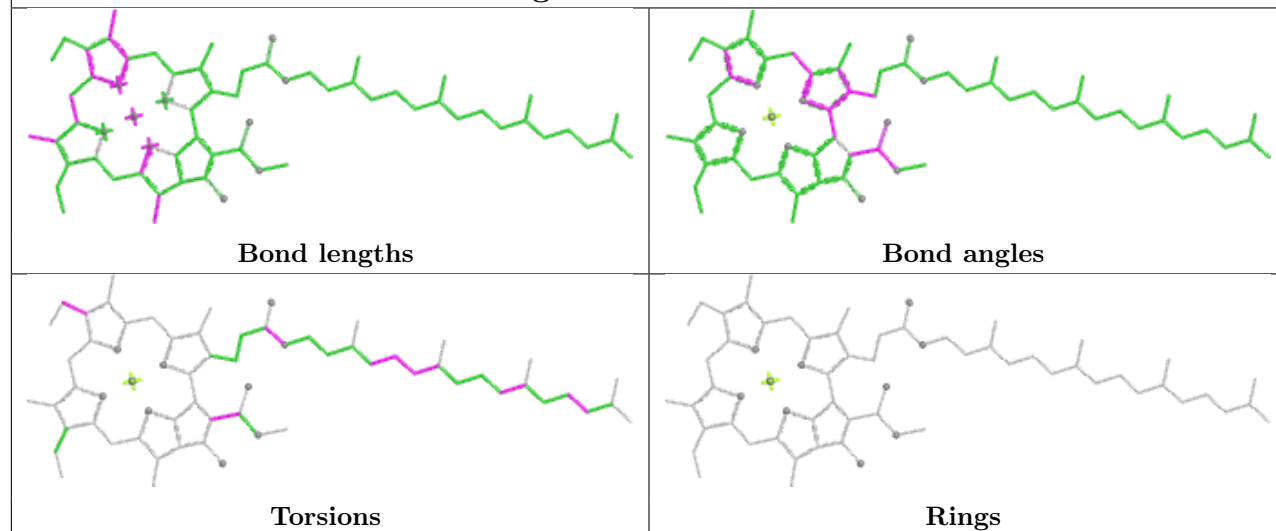




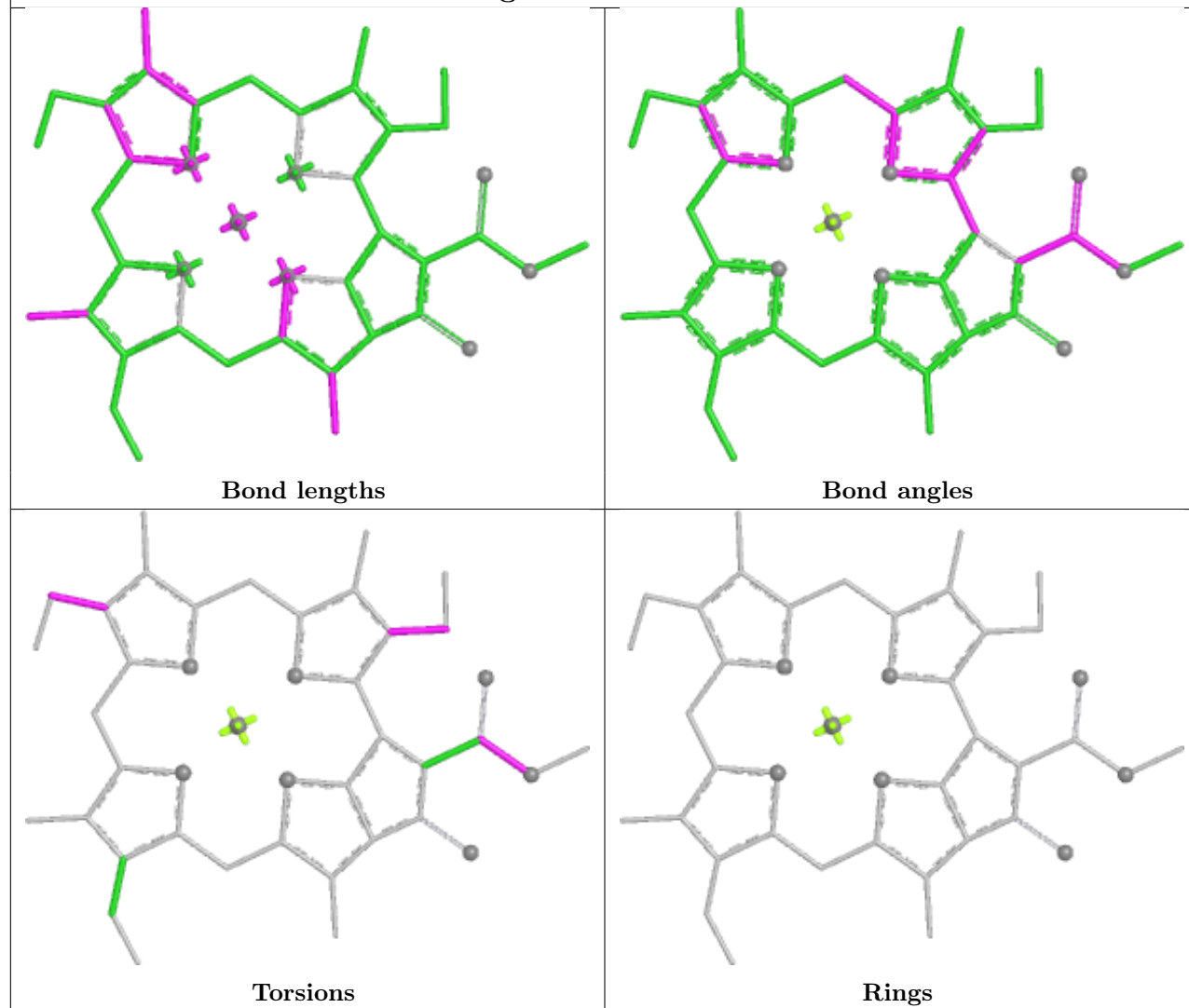


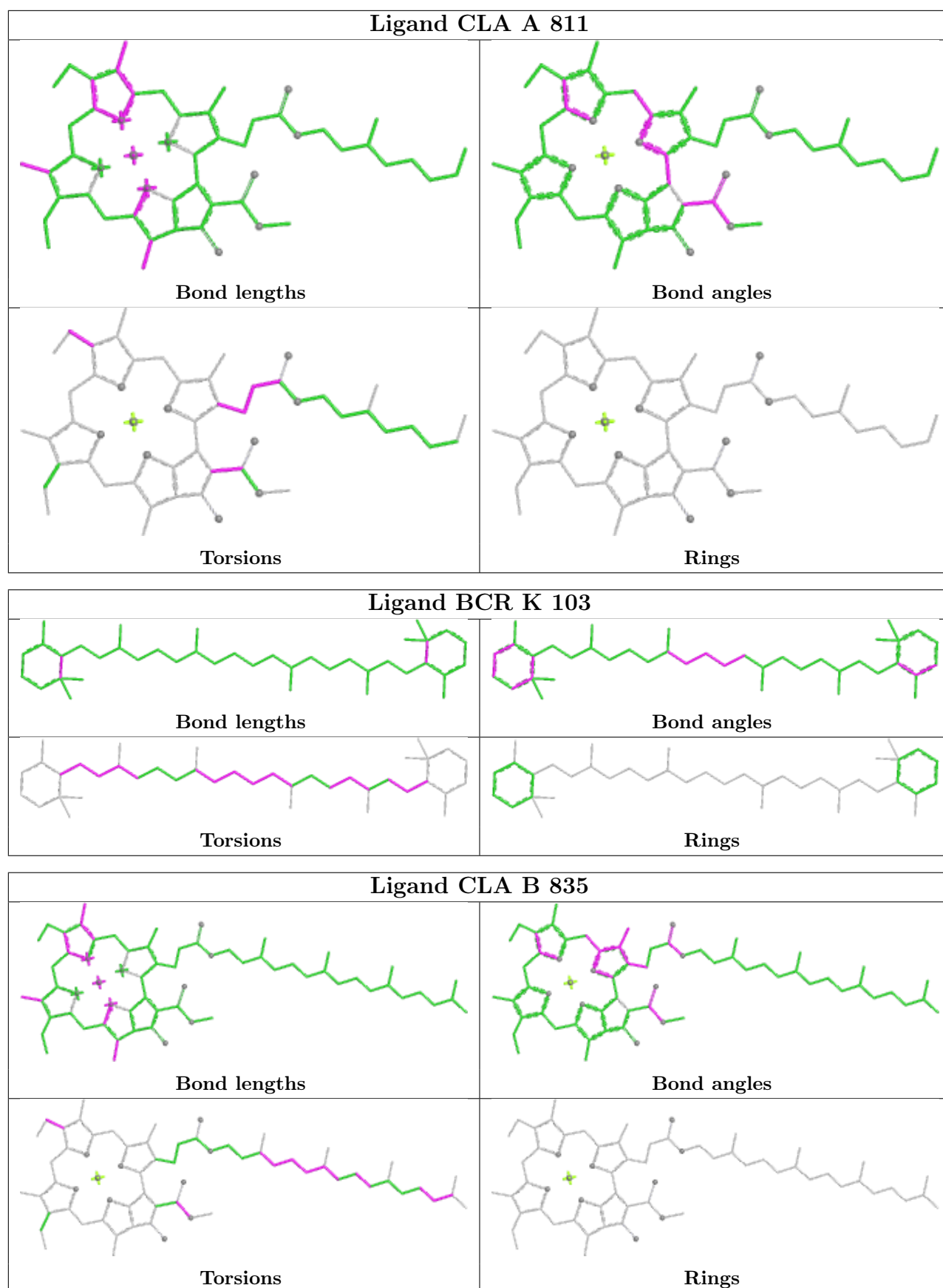


Ligand CLA B 828

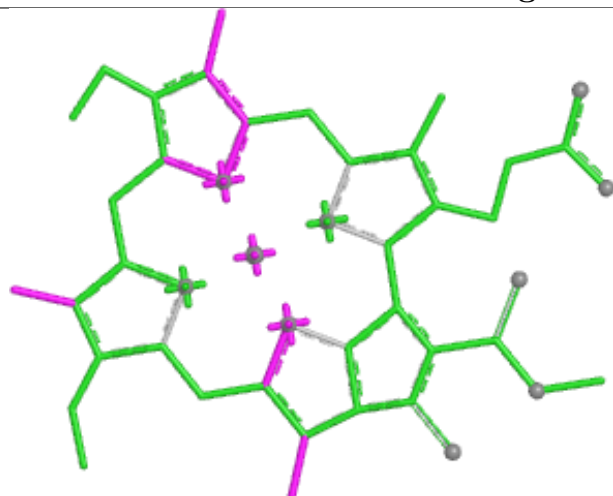


Ligand CLA 2 604

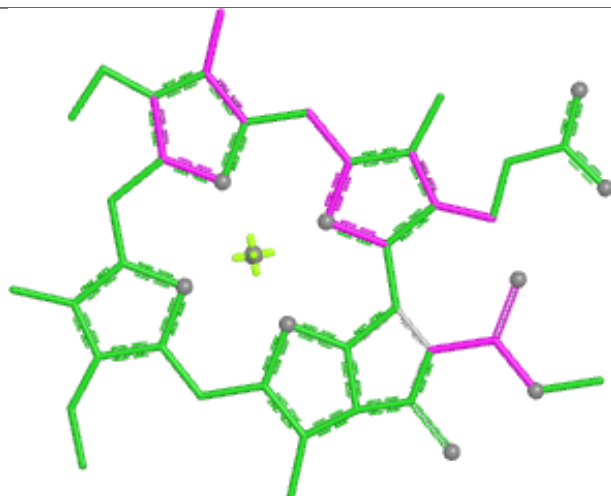




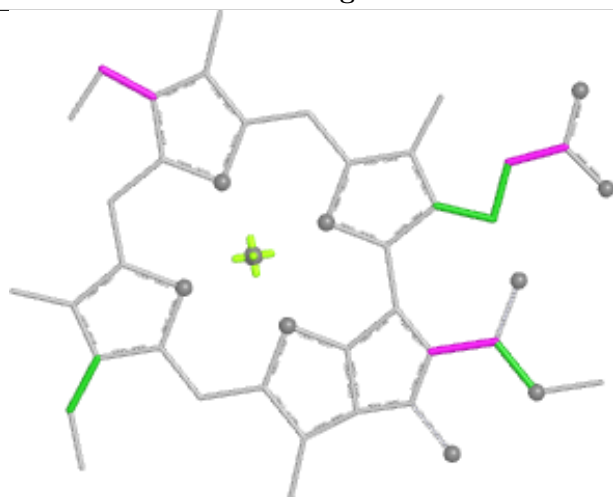
Ligand CLA 2 603



Bond lengths



Bond angles

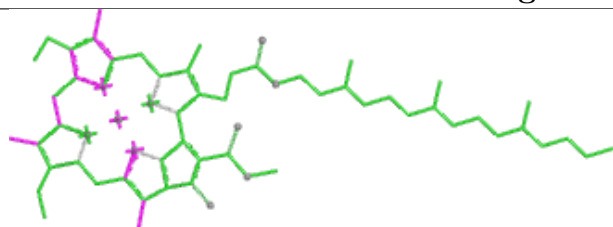


Torsions

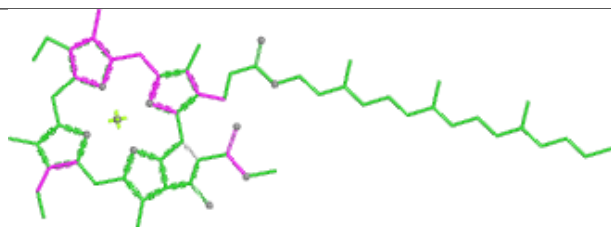


Rings

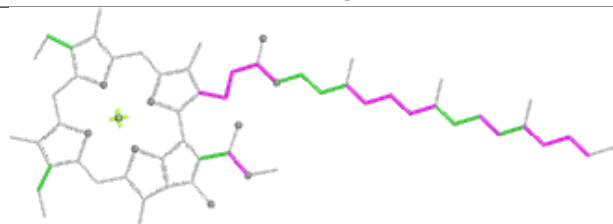
Ligand CLA 3 203



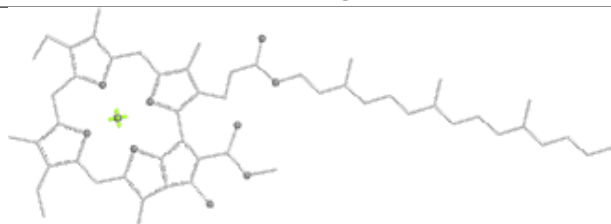
Bond lengths



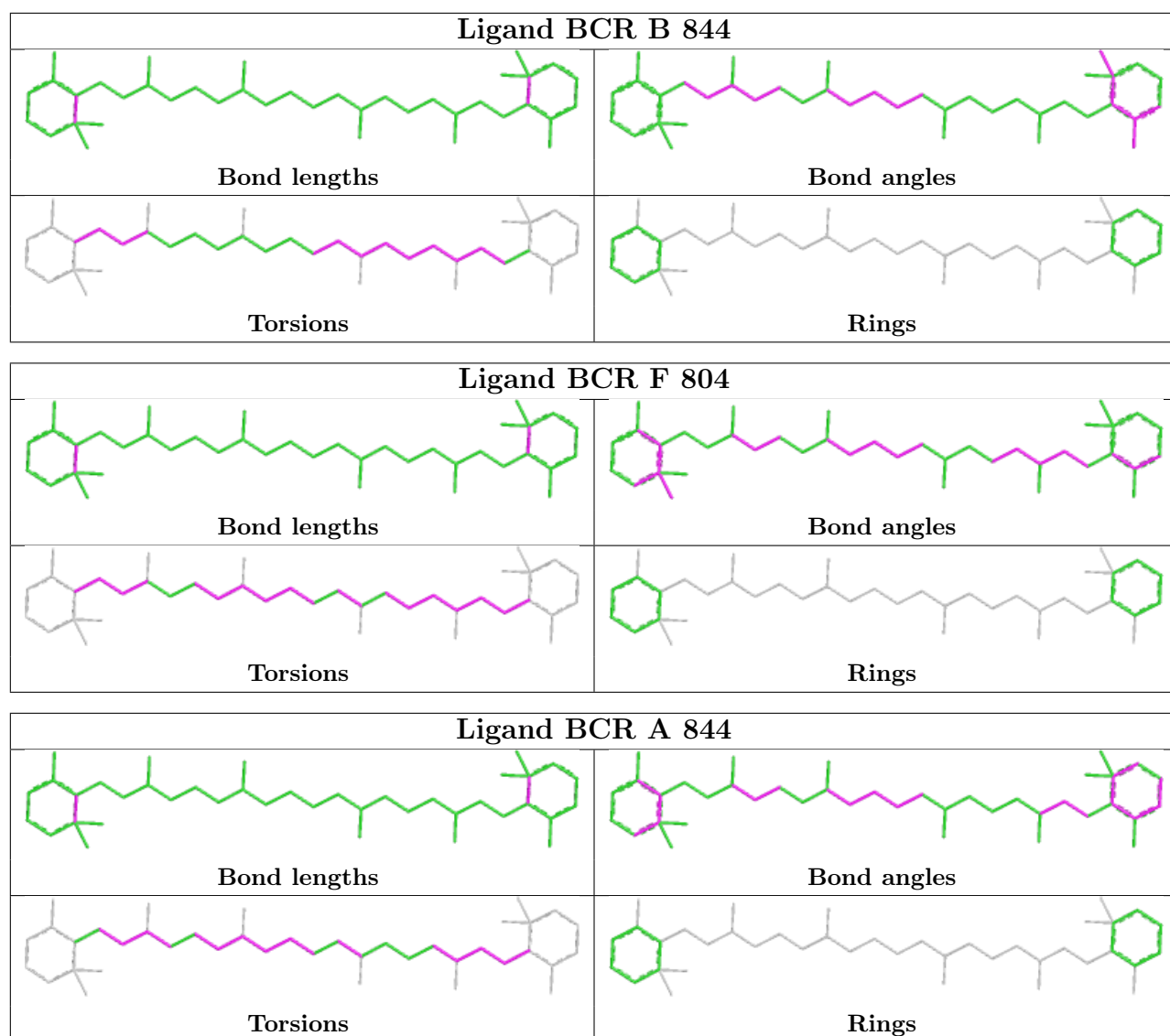
Bond angles

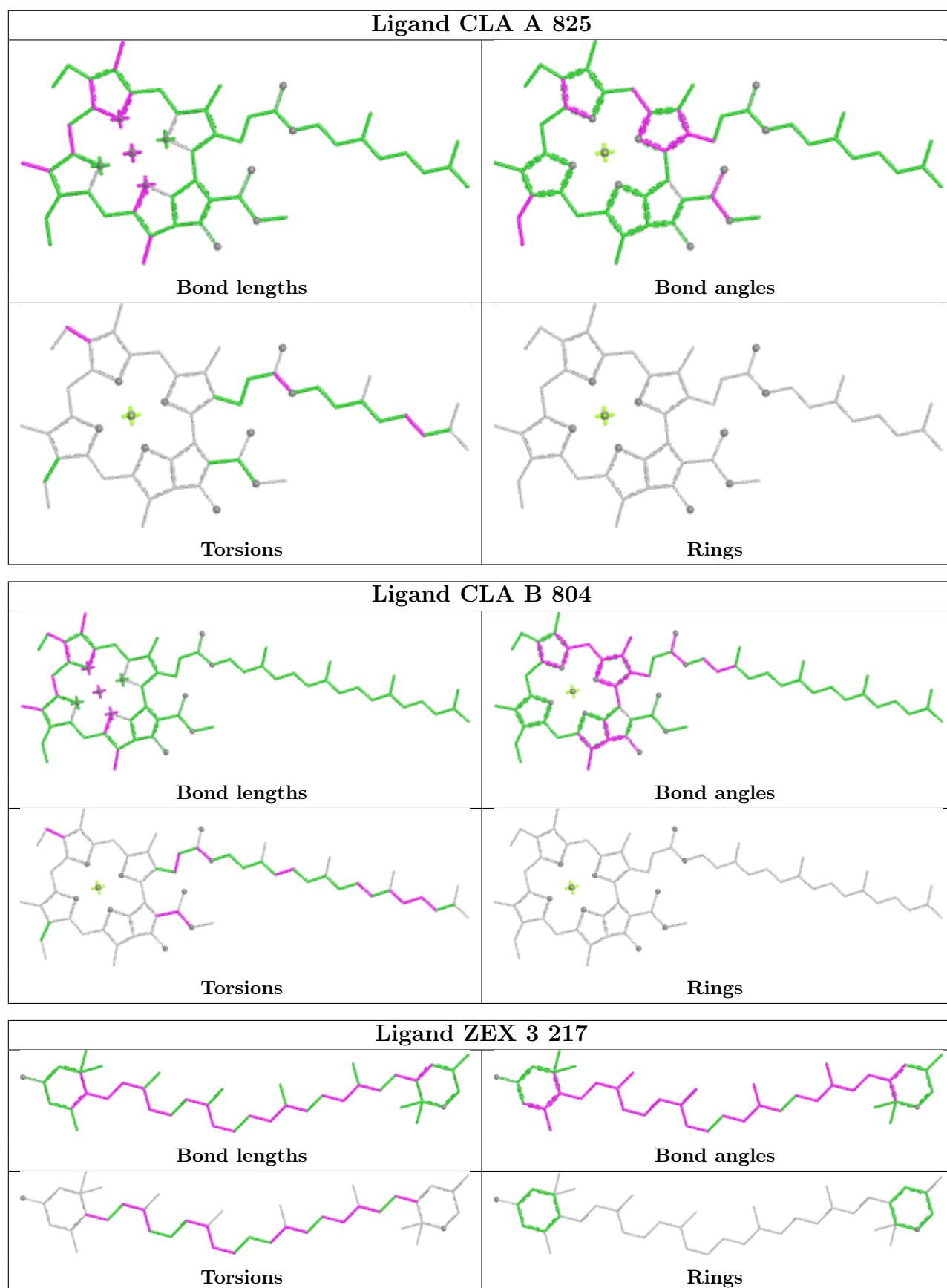


Torsions

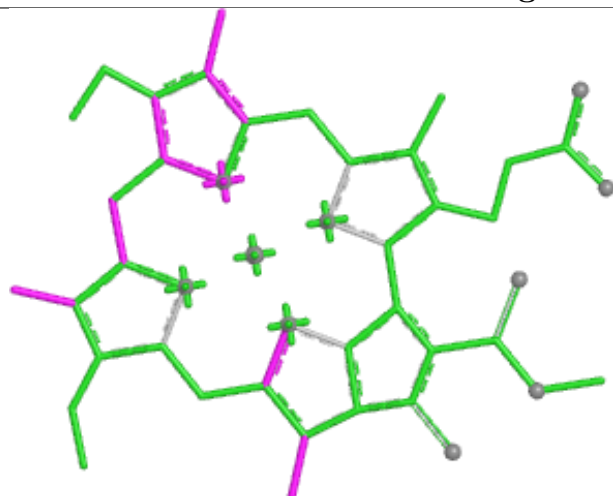


Rings

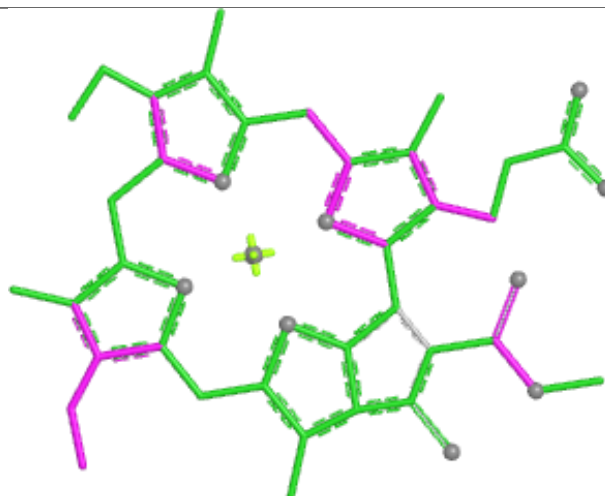




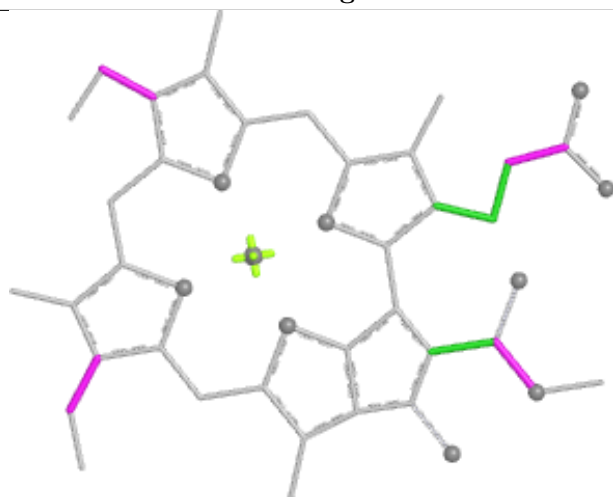
Ligand CLA 2 611



Bond lengths



Bond angles

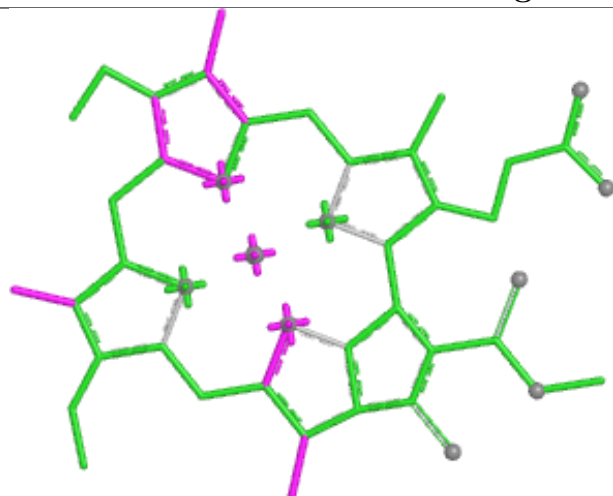


Torsions

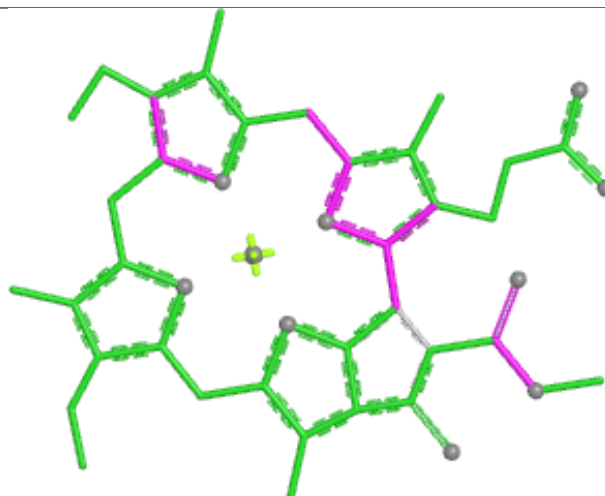


Rings

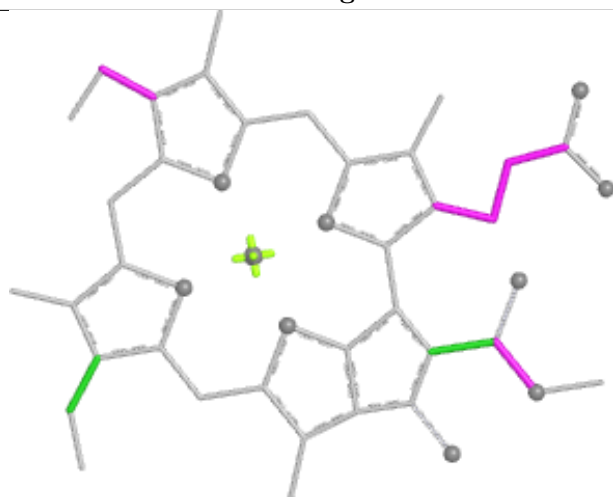
Ligand CLA B 836



Bond lengths



Bond angles

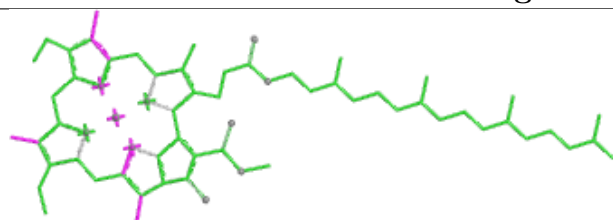


Torsions

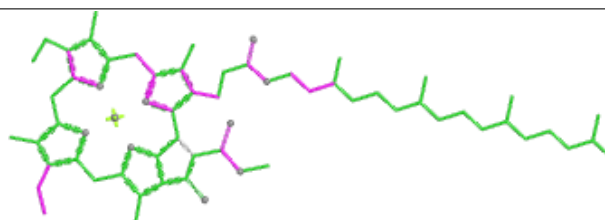


Rings

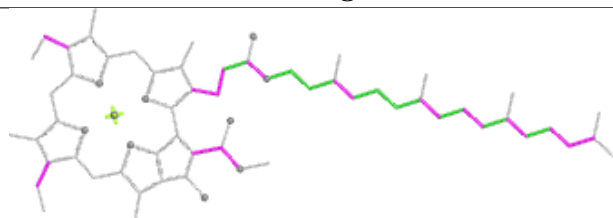
Ligand CLA B 815



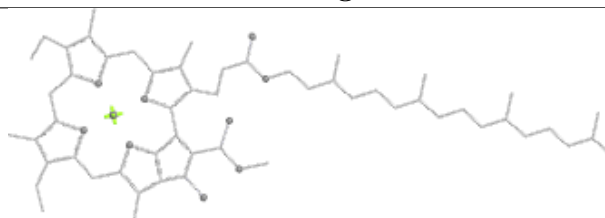
Bond lengths



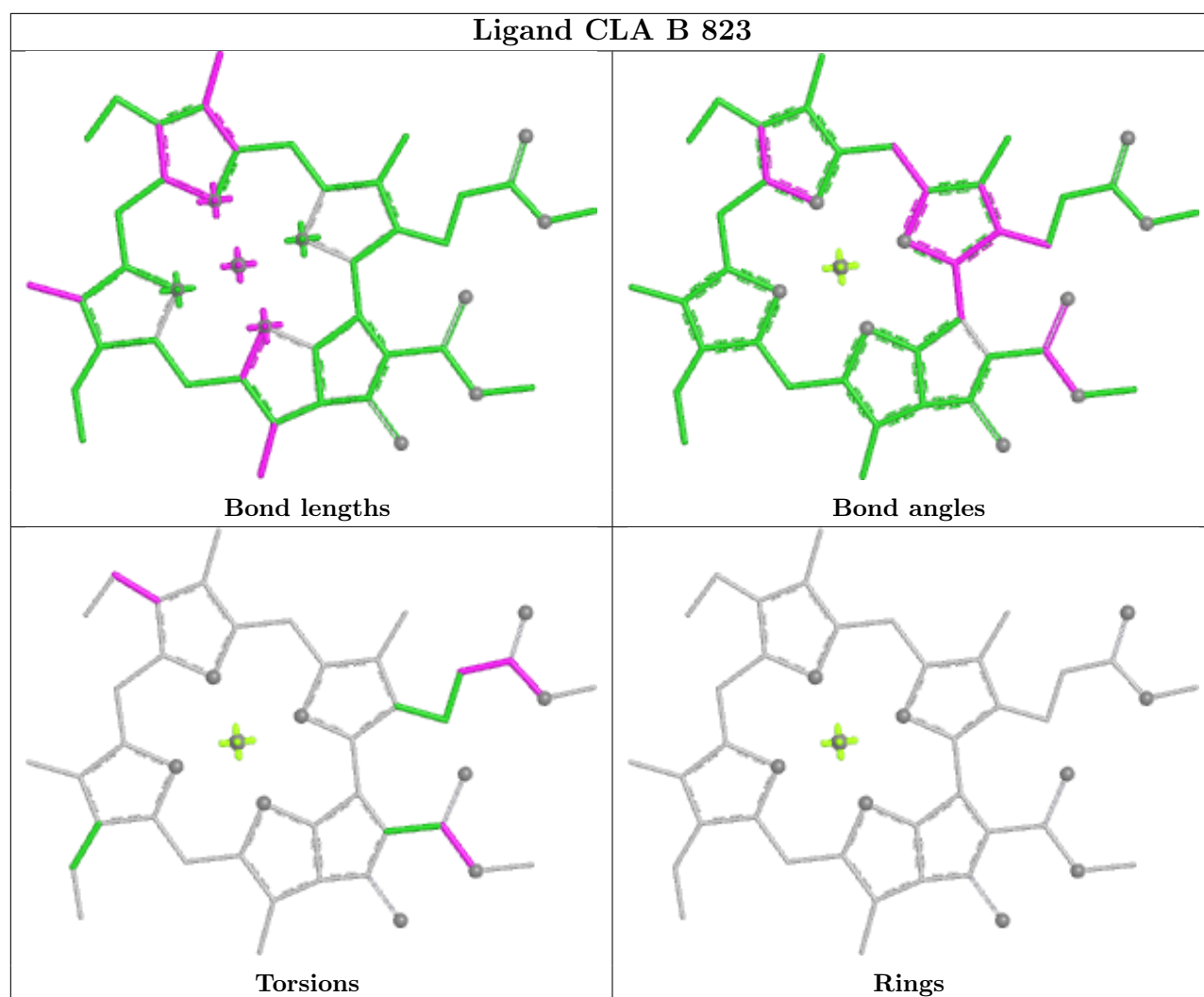
Bond angles



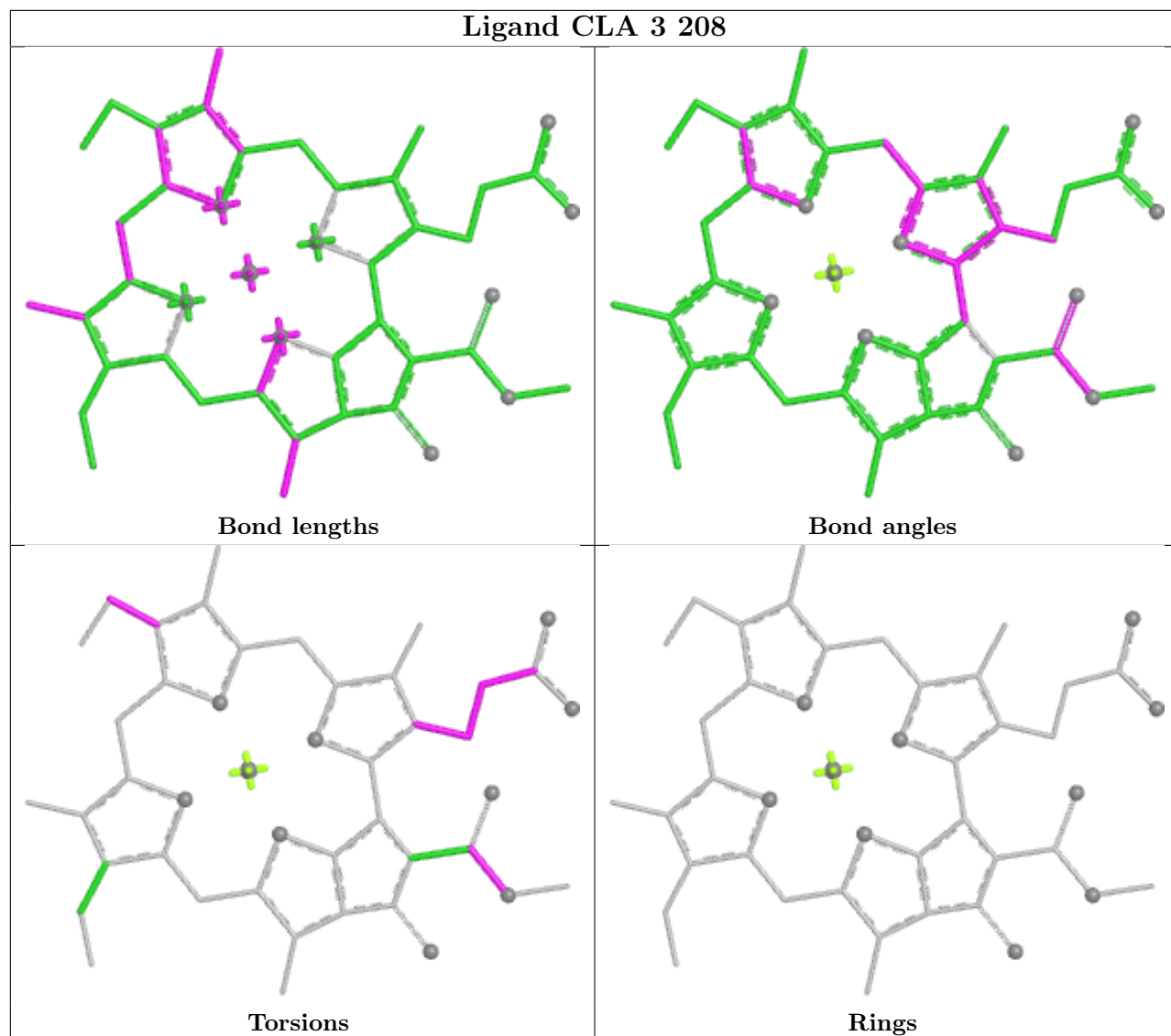
Torsions



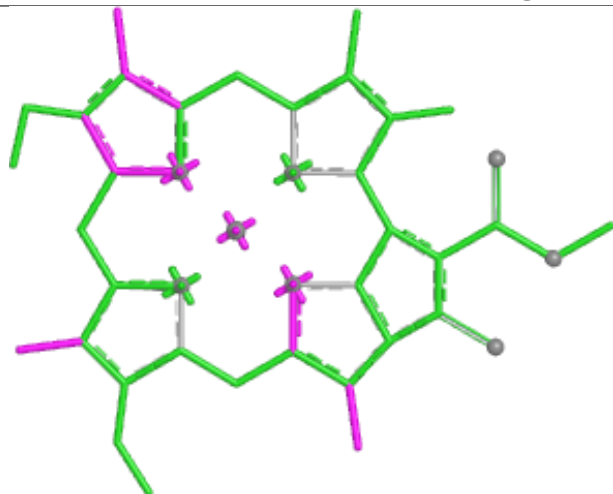
Rings



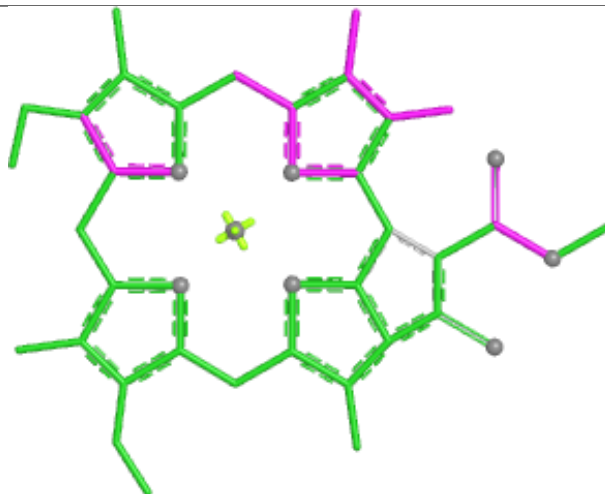
Ligand CLA 3 208



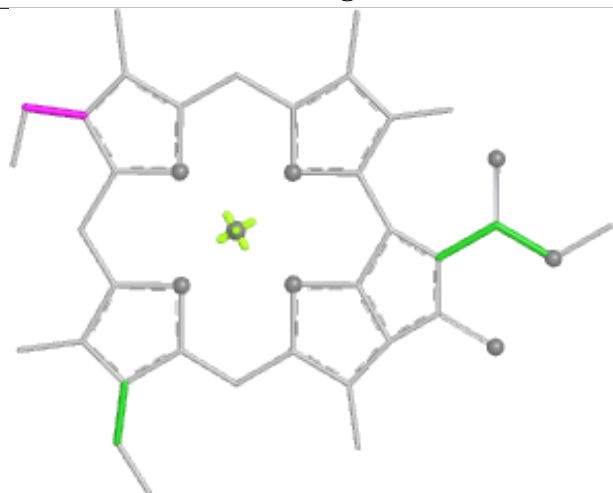
Ligand CLA 1 609



Bond lengths



Bond angles

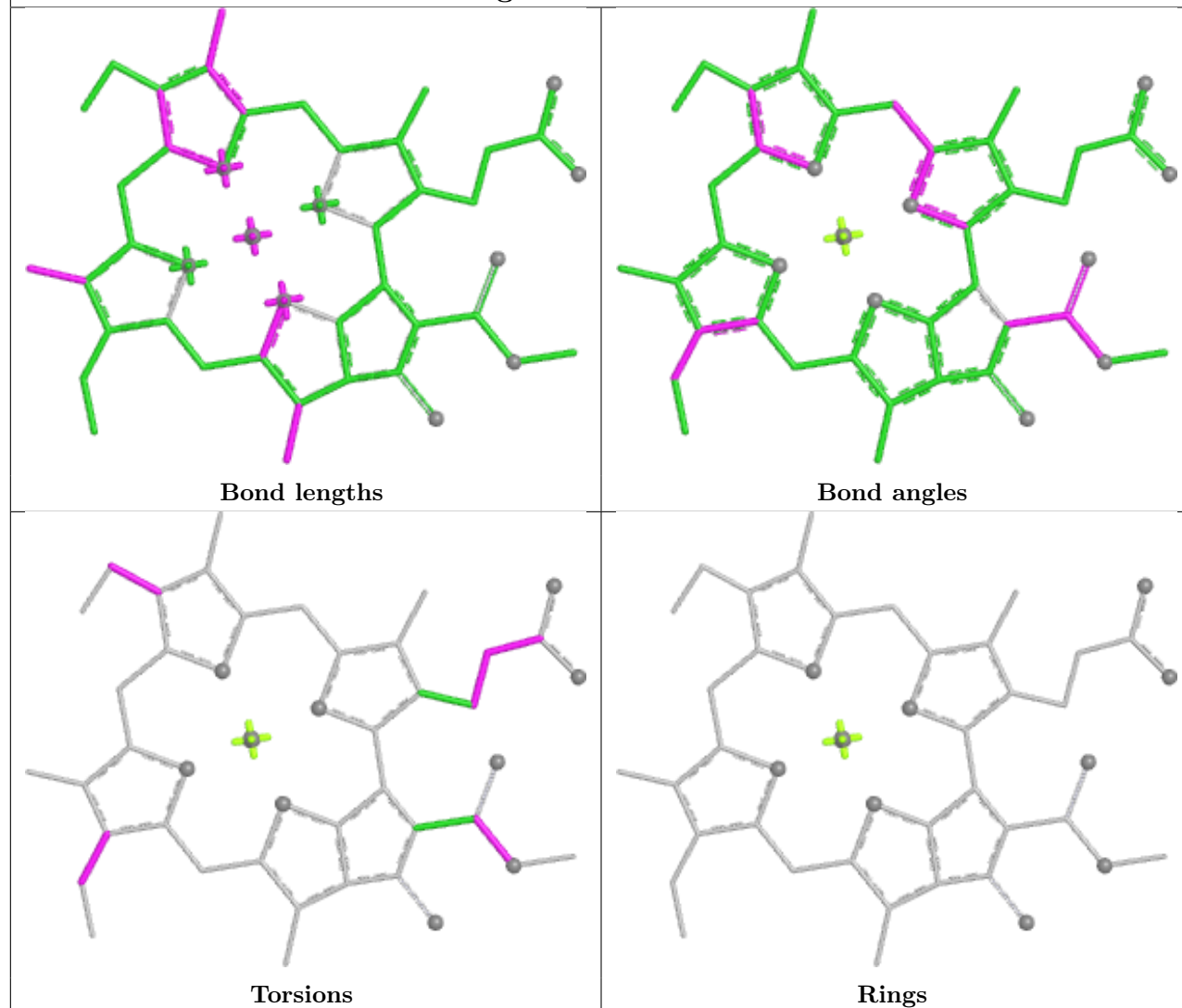


Torsions

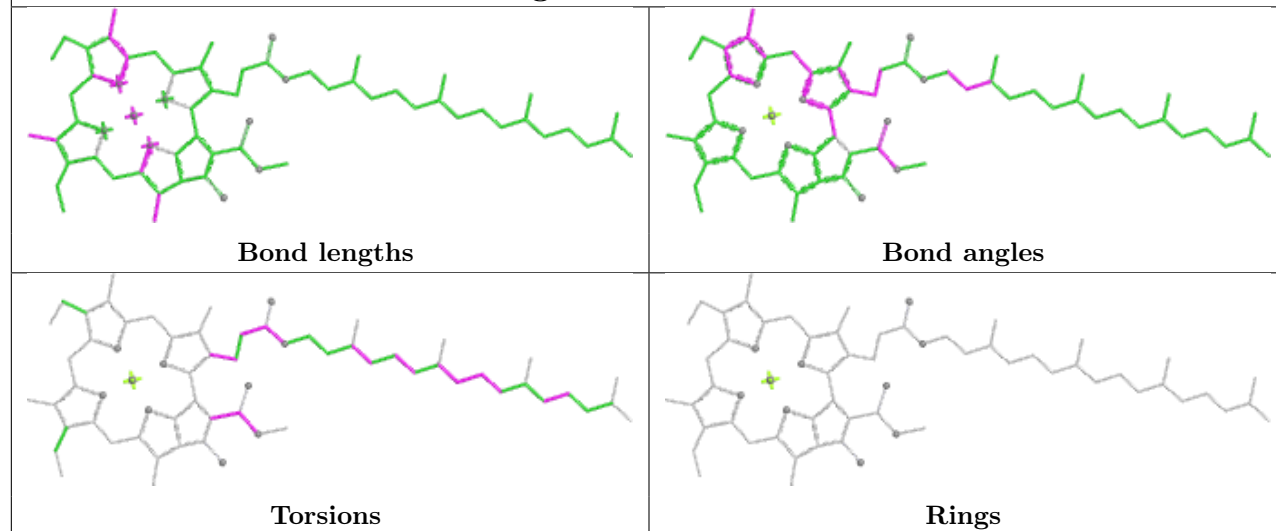


Rings

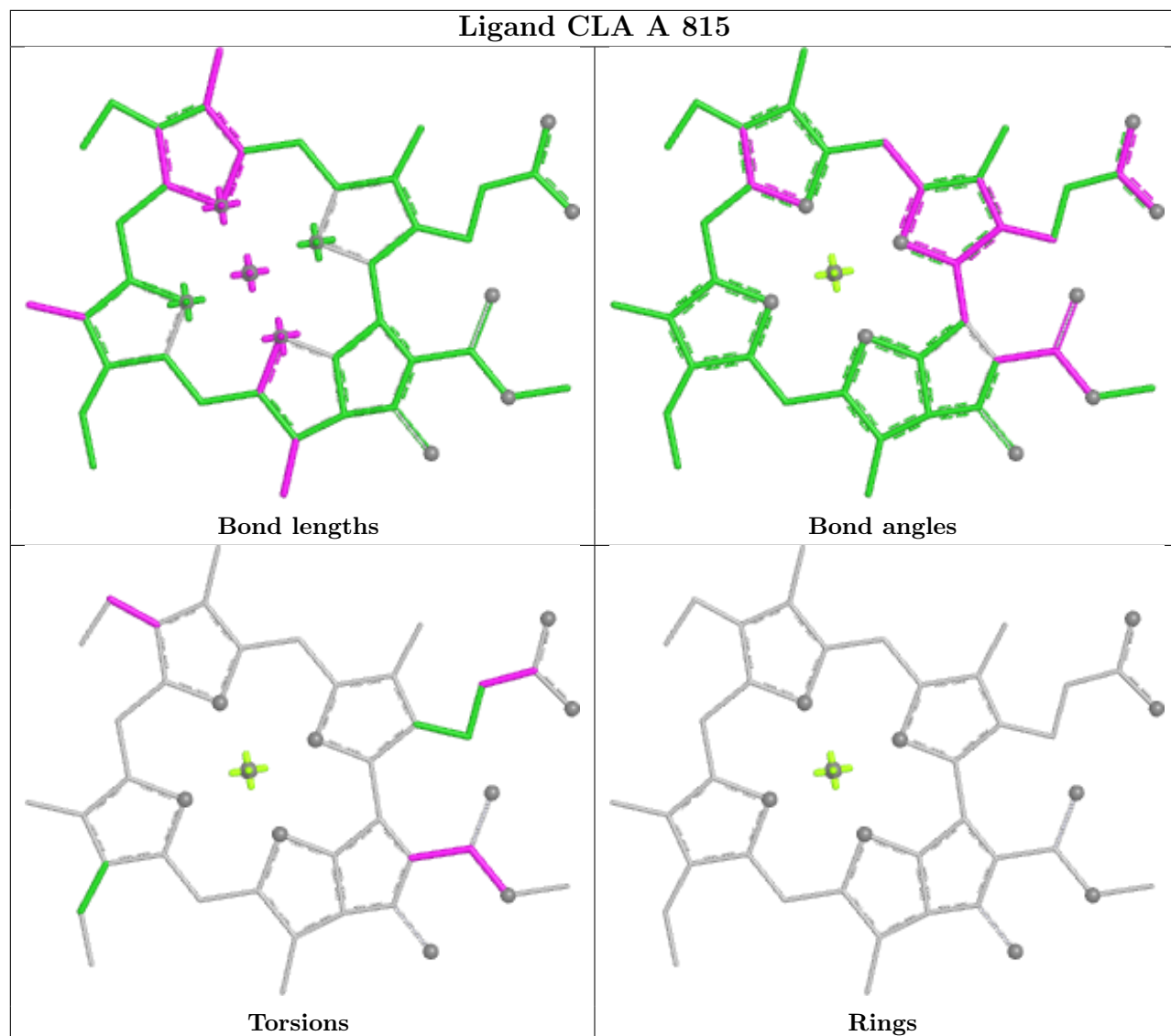
Ligand CLA 2 601



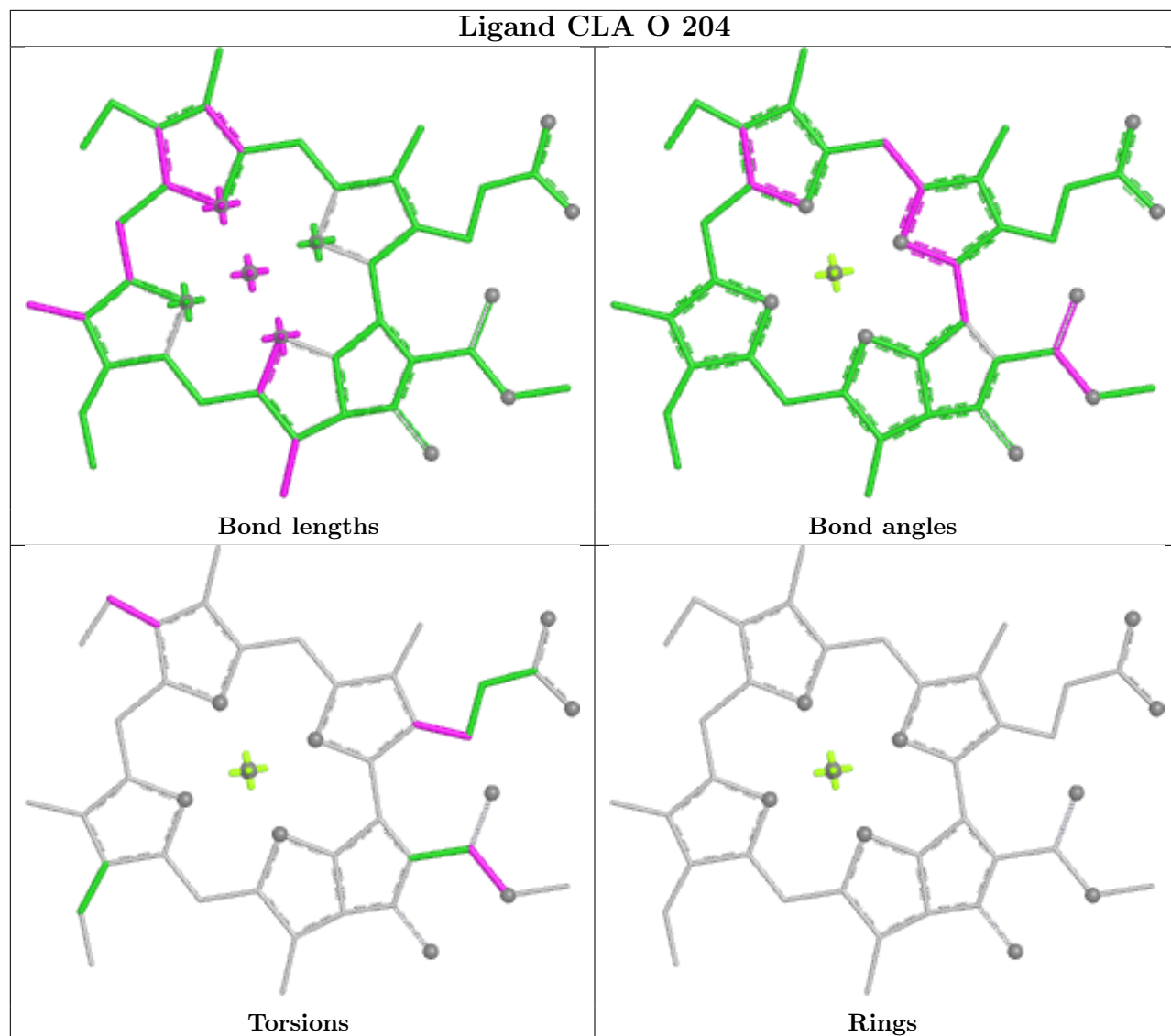
Ligand CLA A 805



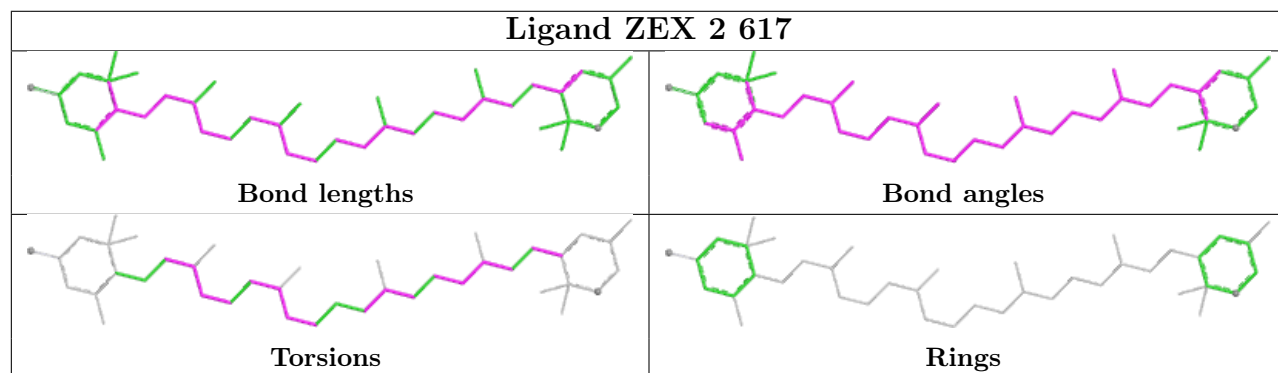
Ligand CLA A 815



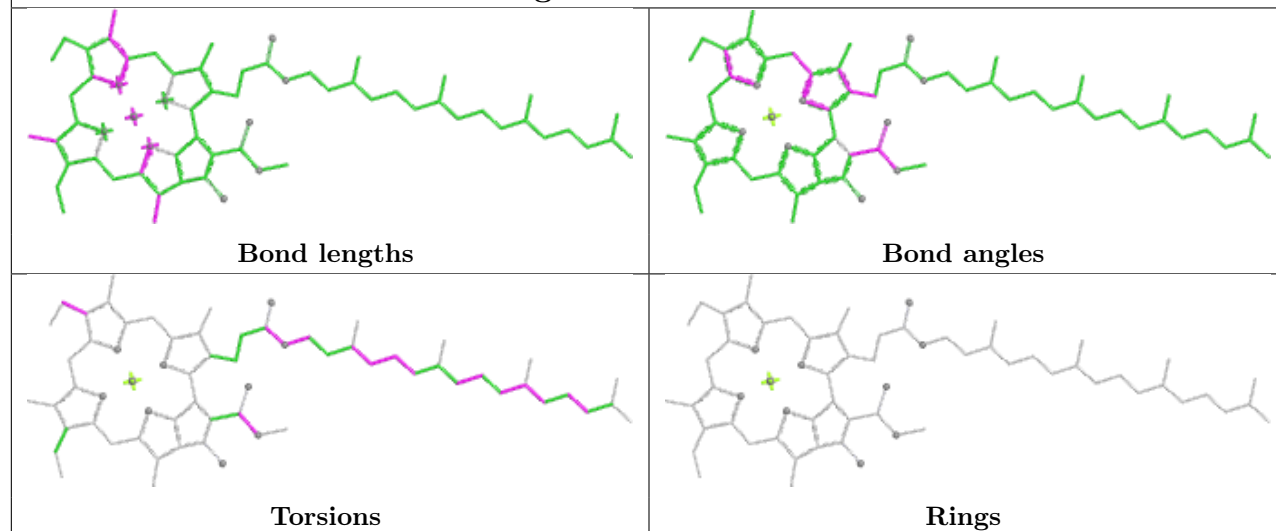
Ligand CLA O 204



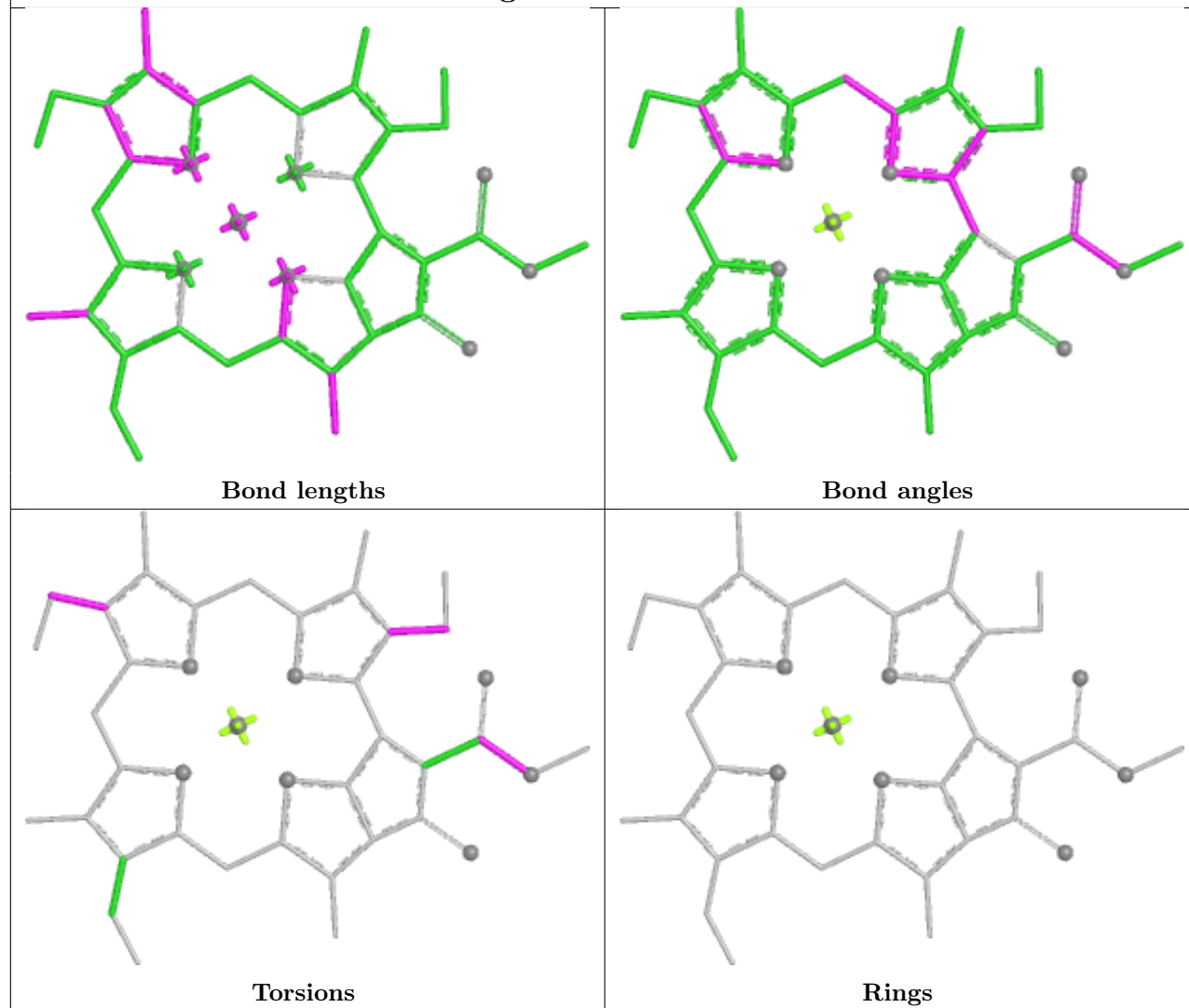
Ligand ZEX 2 617

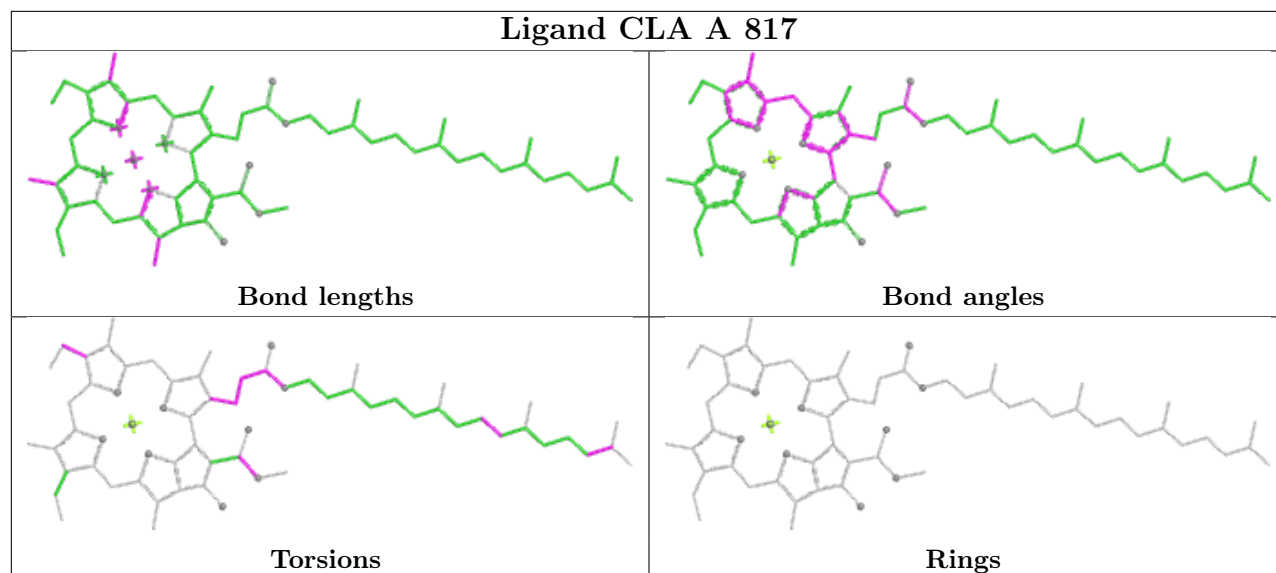
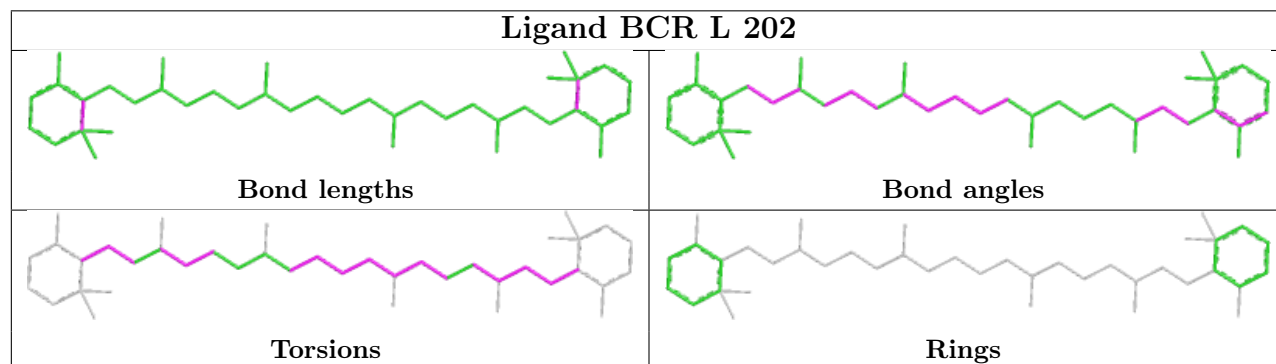
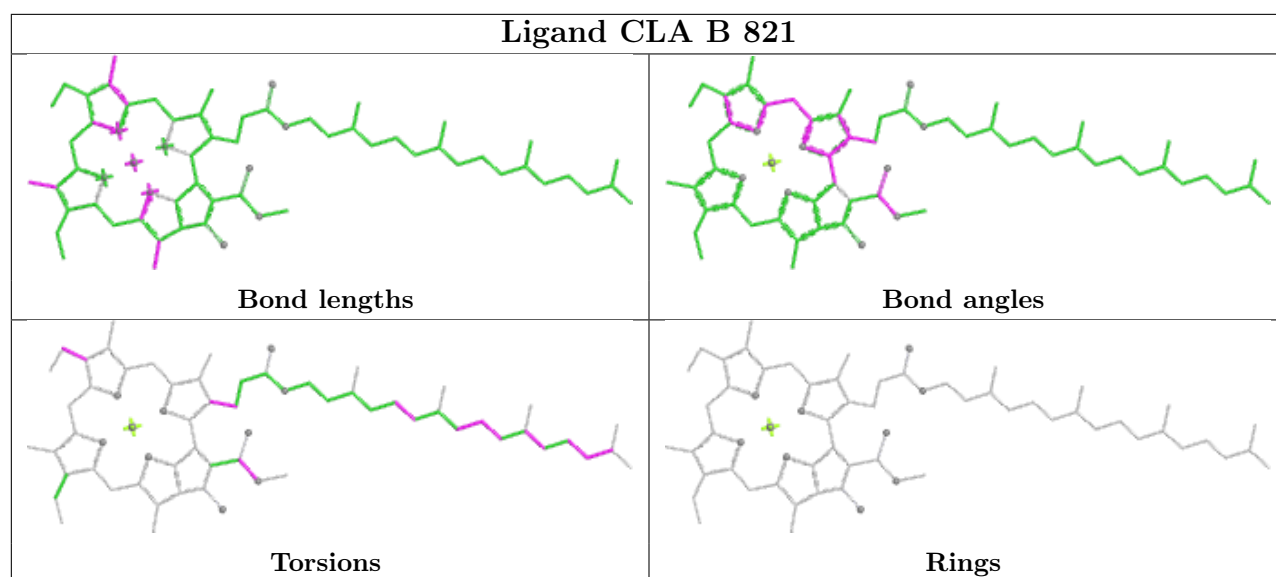


Ligand CLA L 204

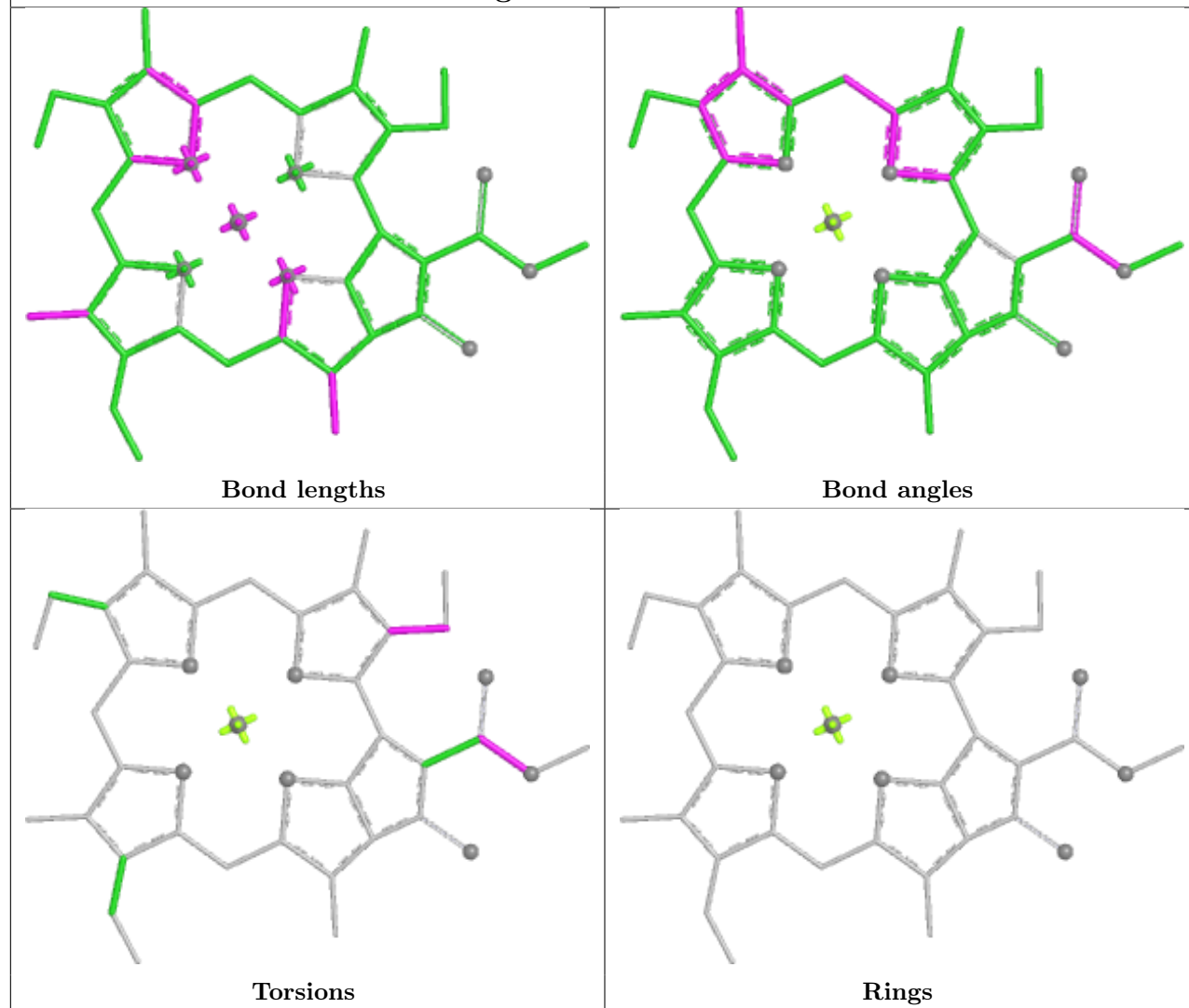


Ligand CLA 2 610

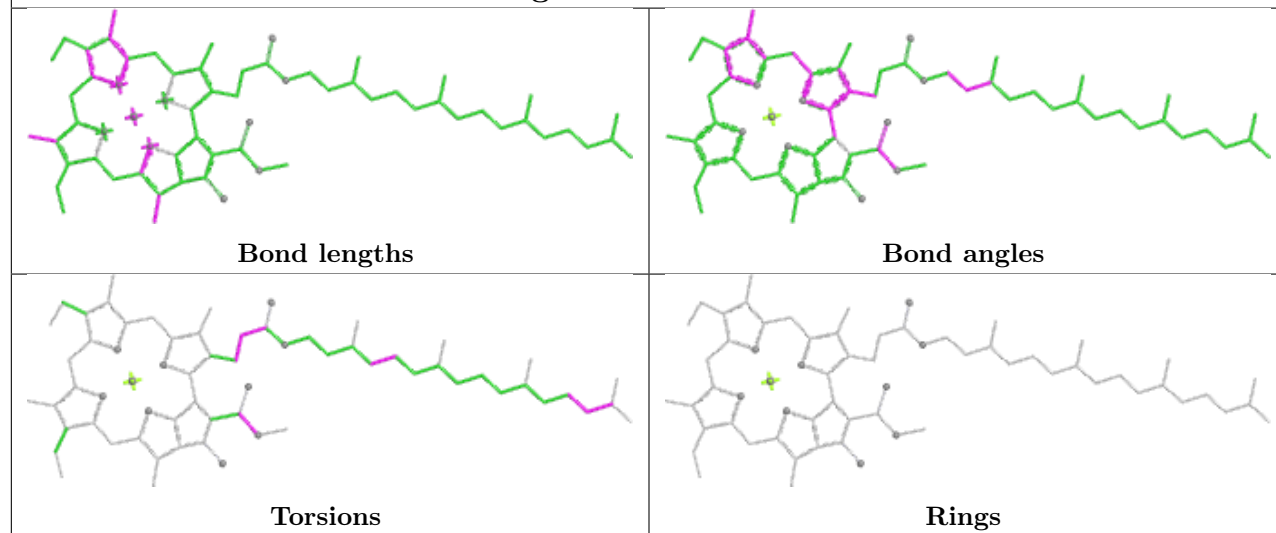




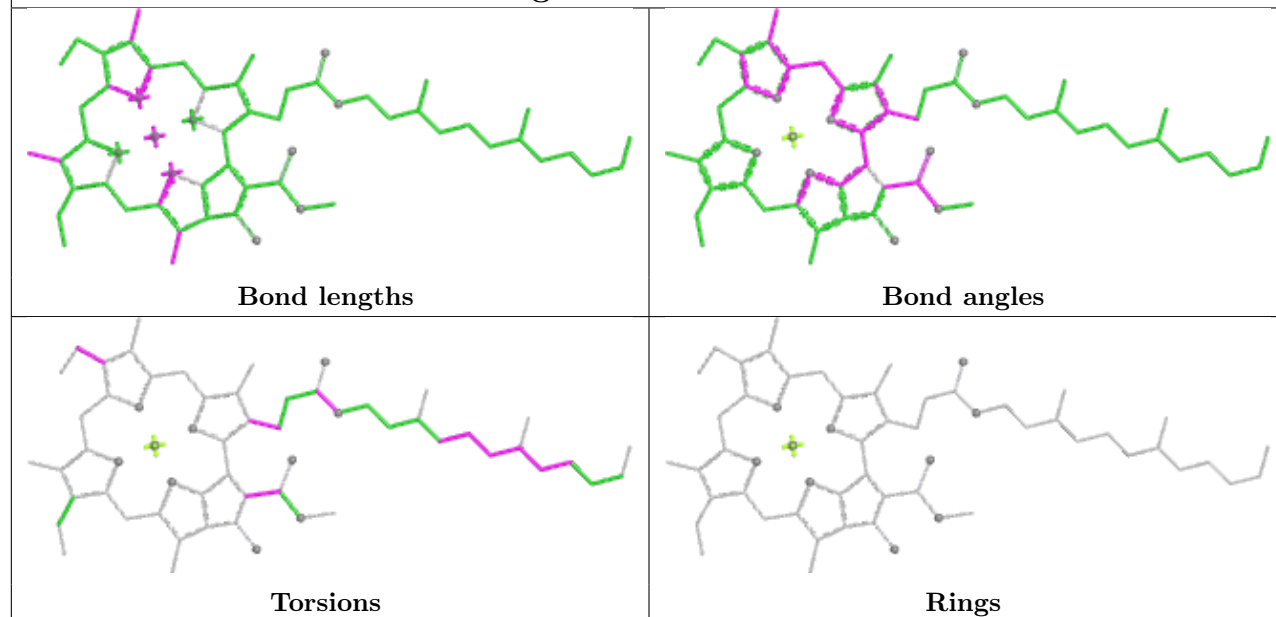
Ligand CLA A 814



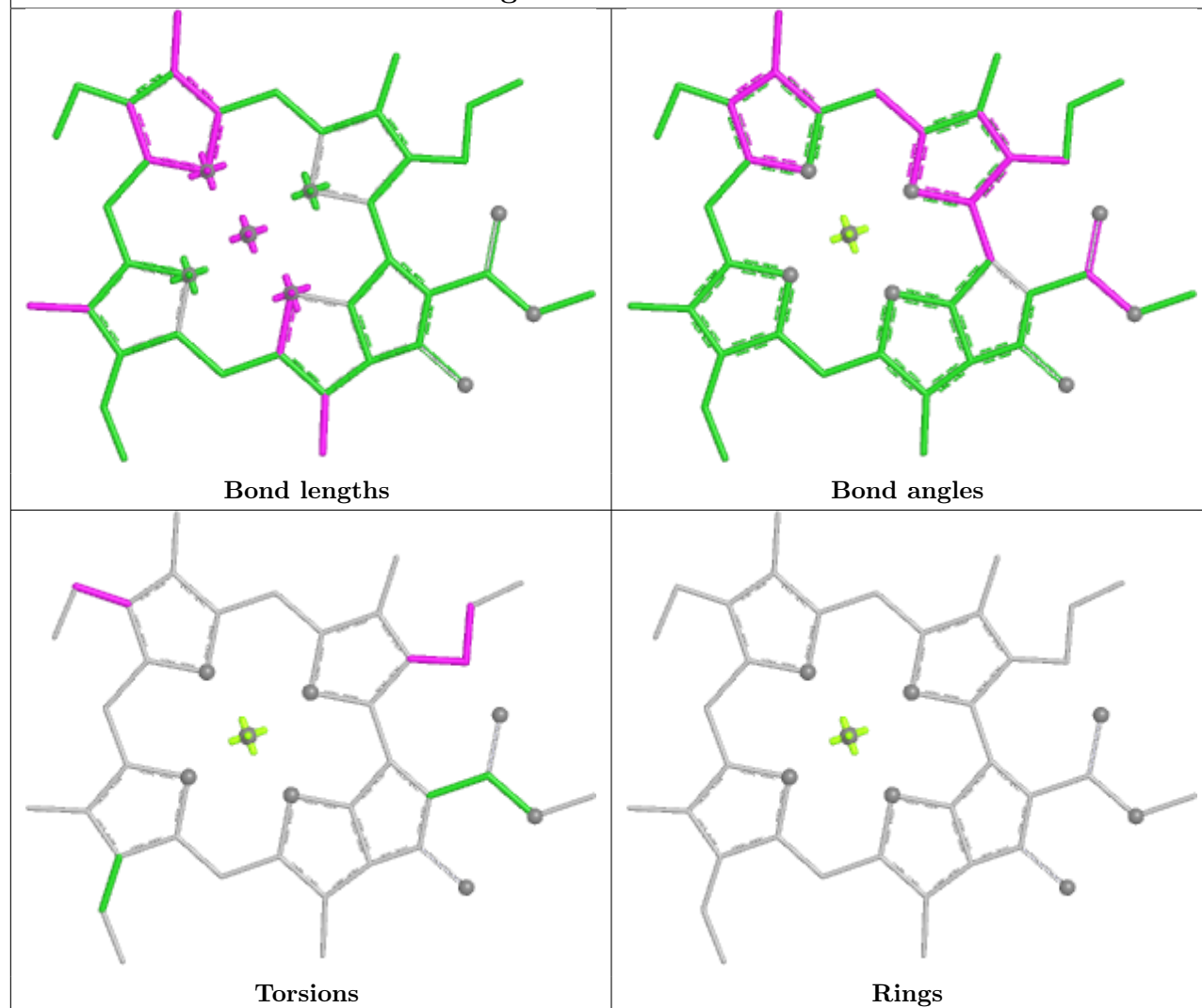
Ligand CLA A 837

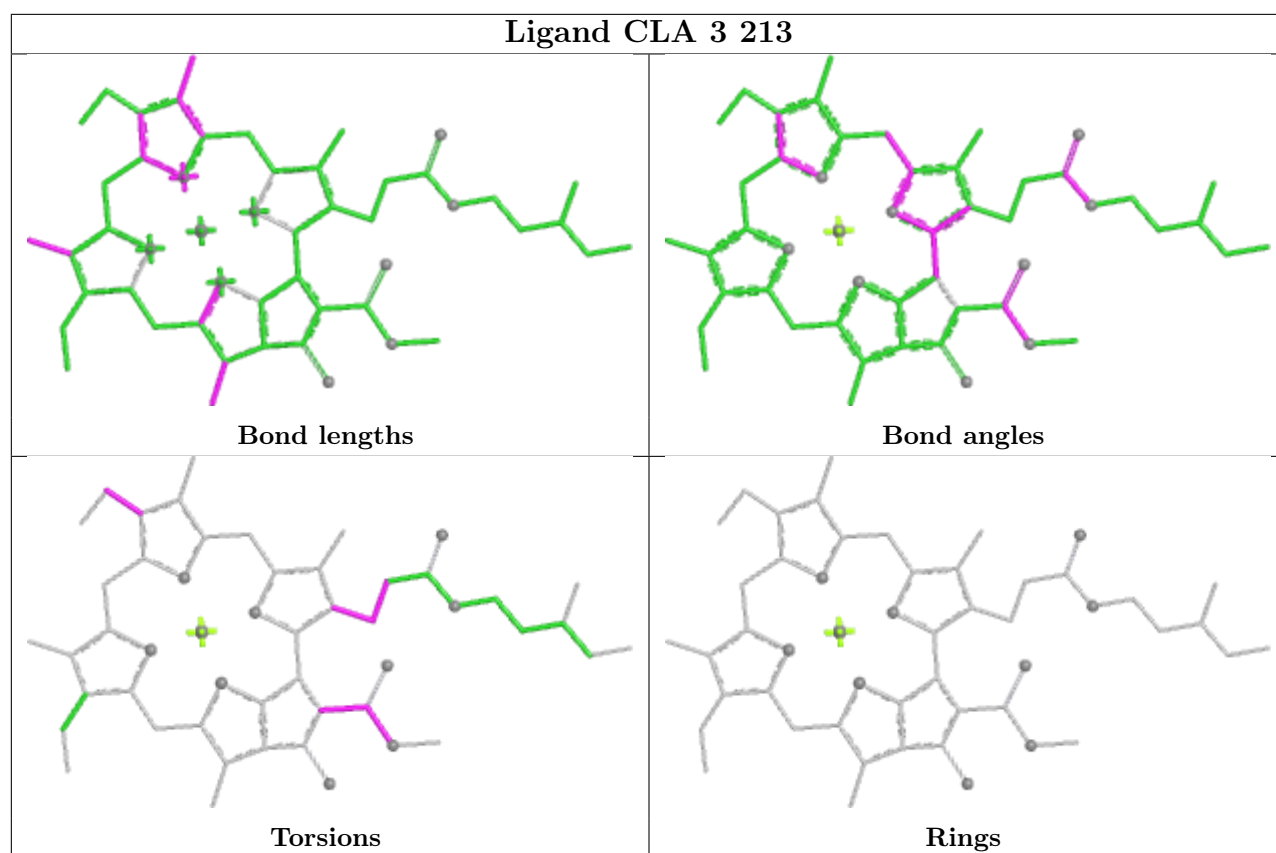


Ligand CLA B 819

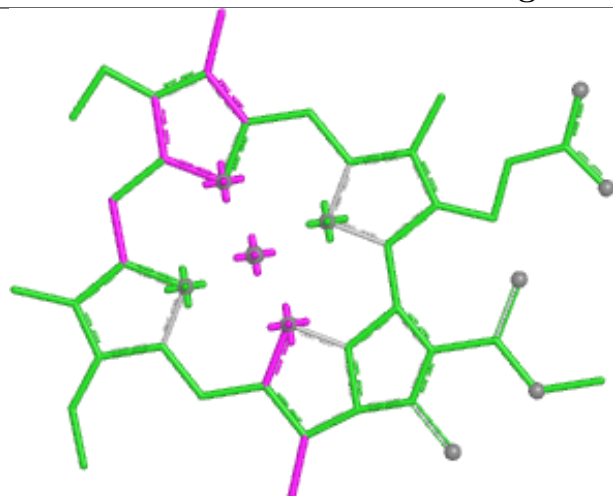


Ligand CLA A 851

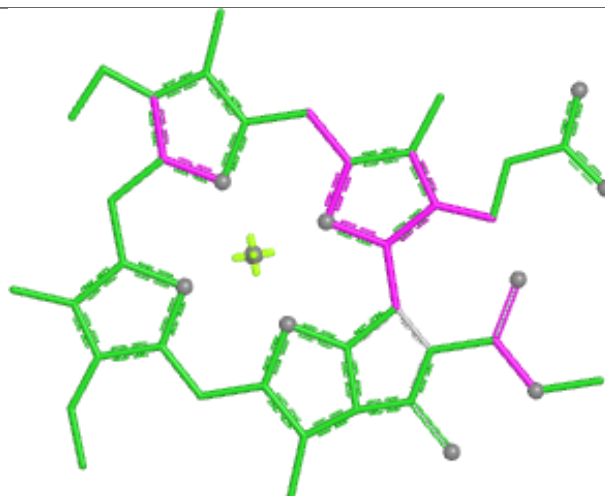




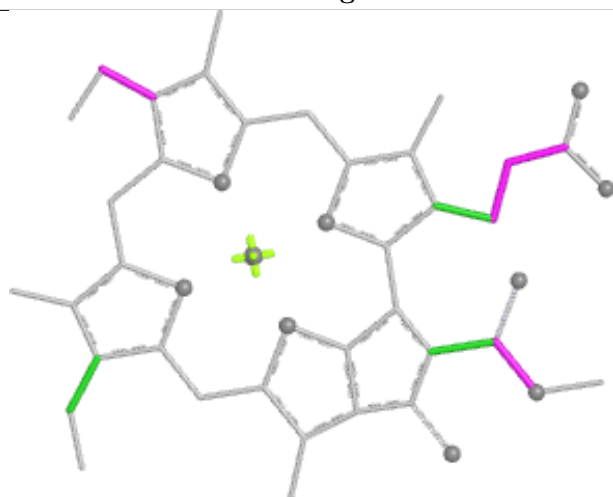
Ligand CLA 3 202



Bond lengths



Bond angles

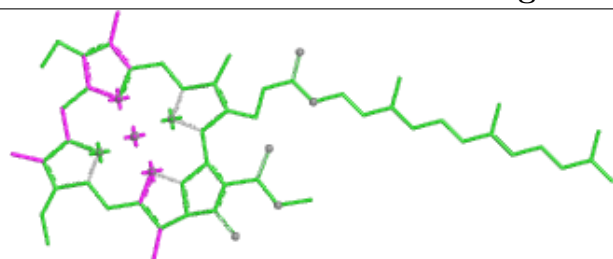


Torsions

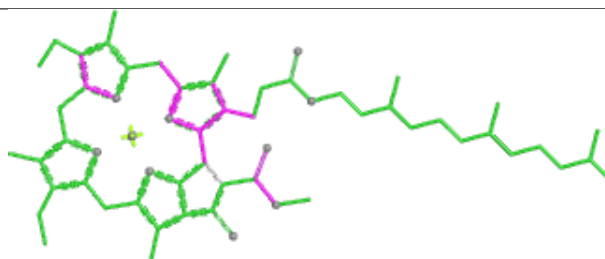


Rings

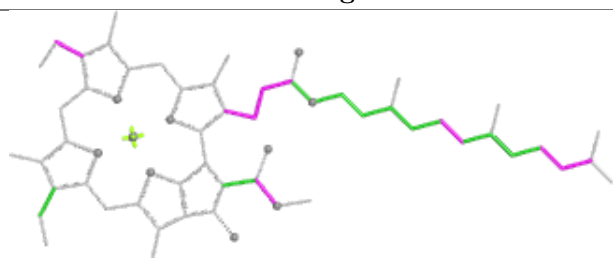
Ligand CLA 1 608



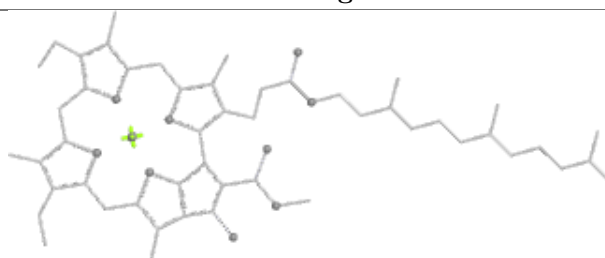
Bond lengths



Bond angles

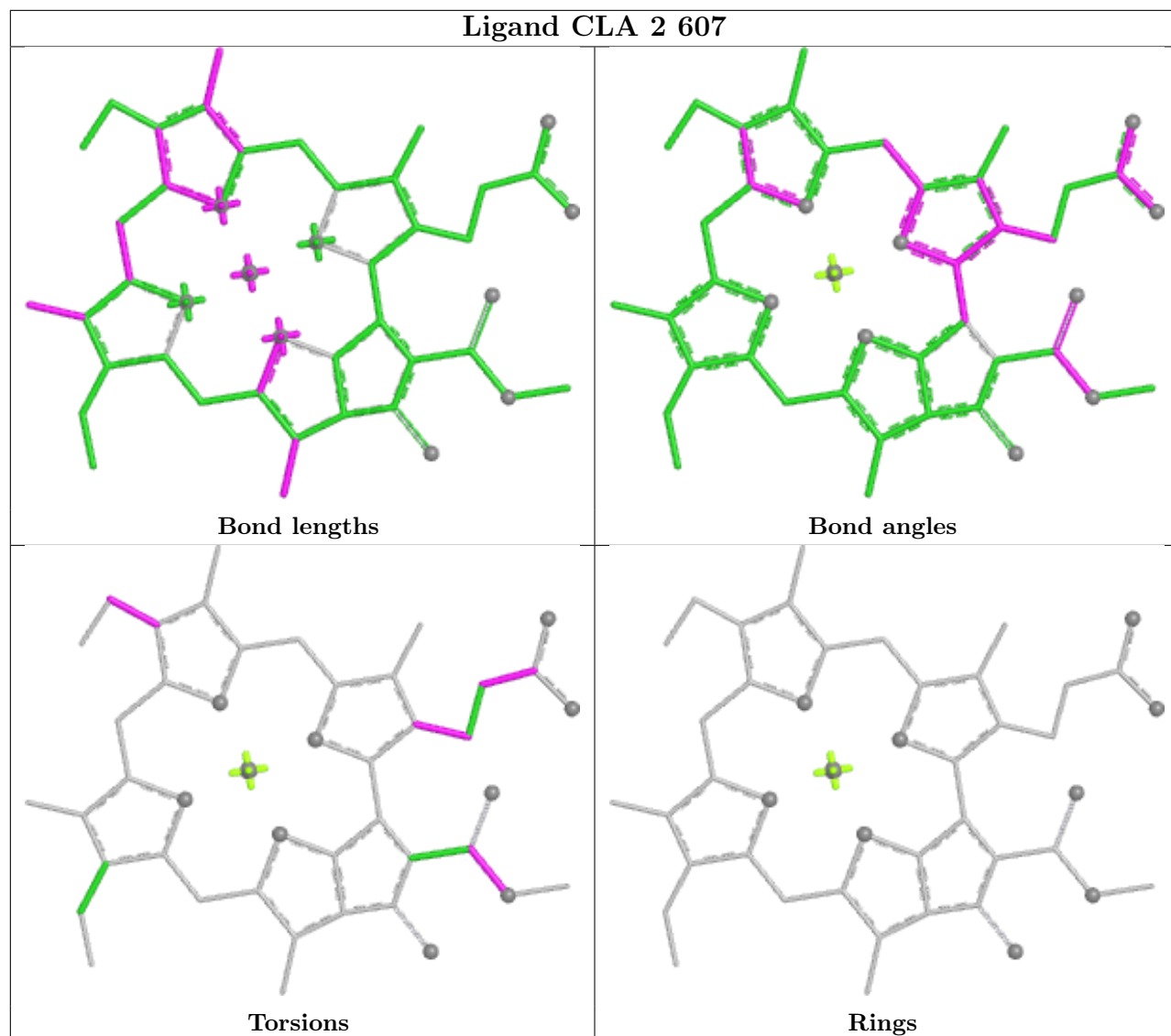


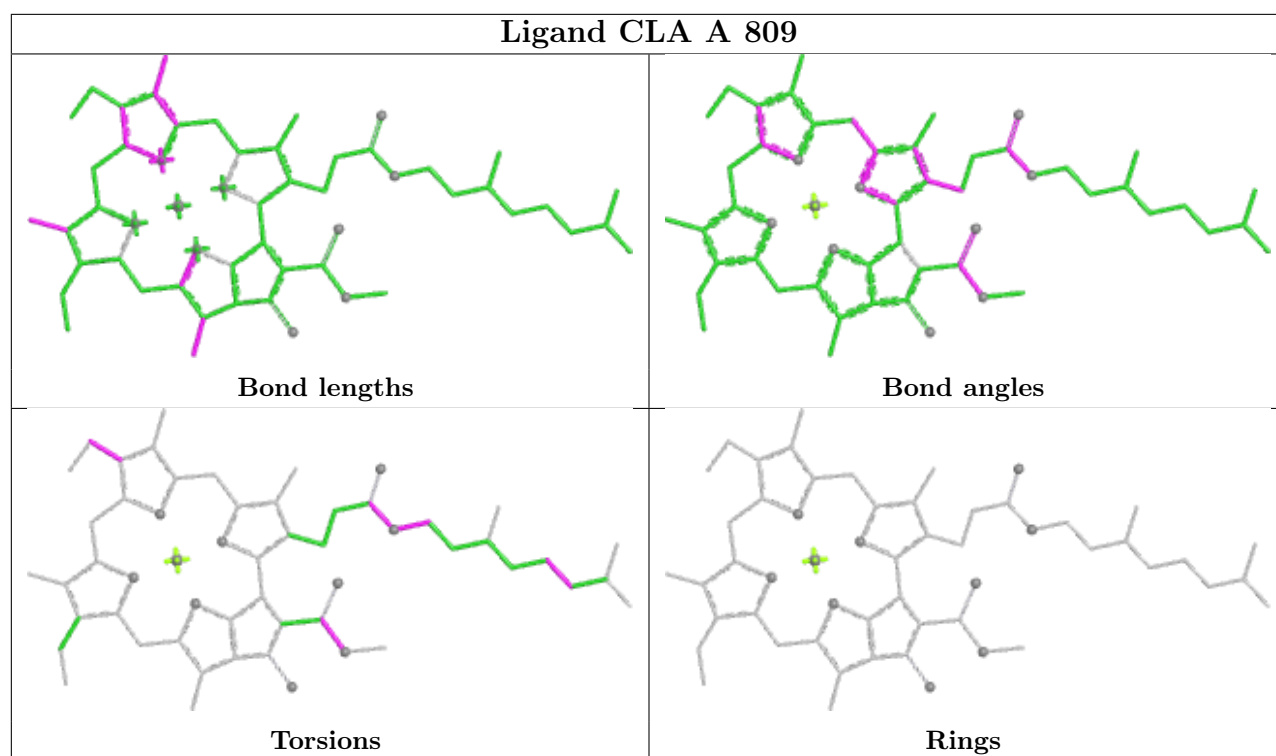
Torsions



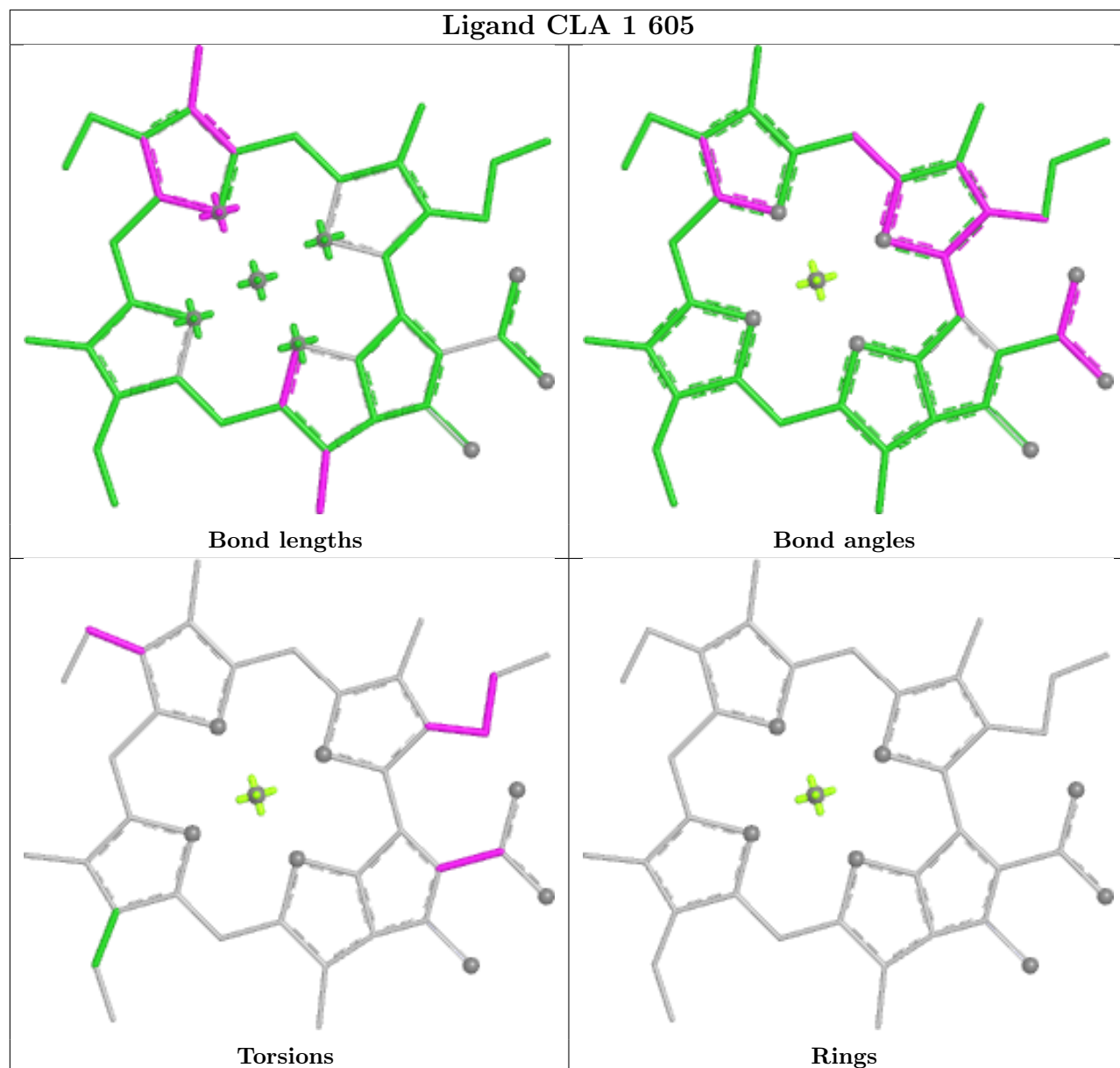
Rings

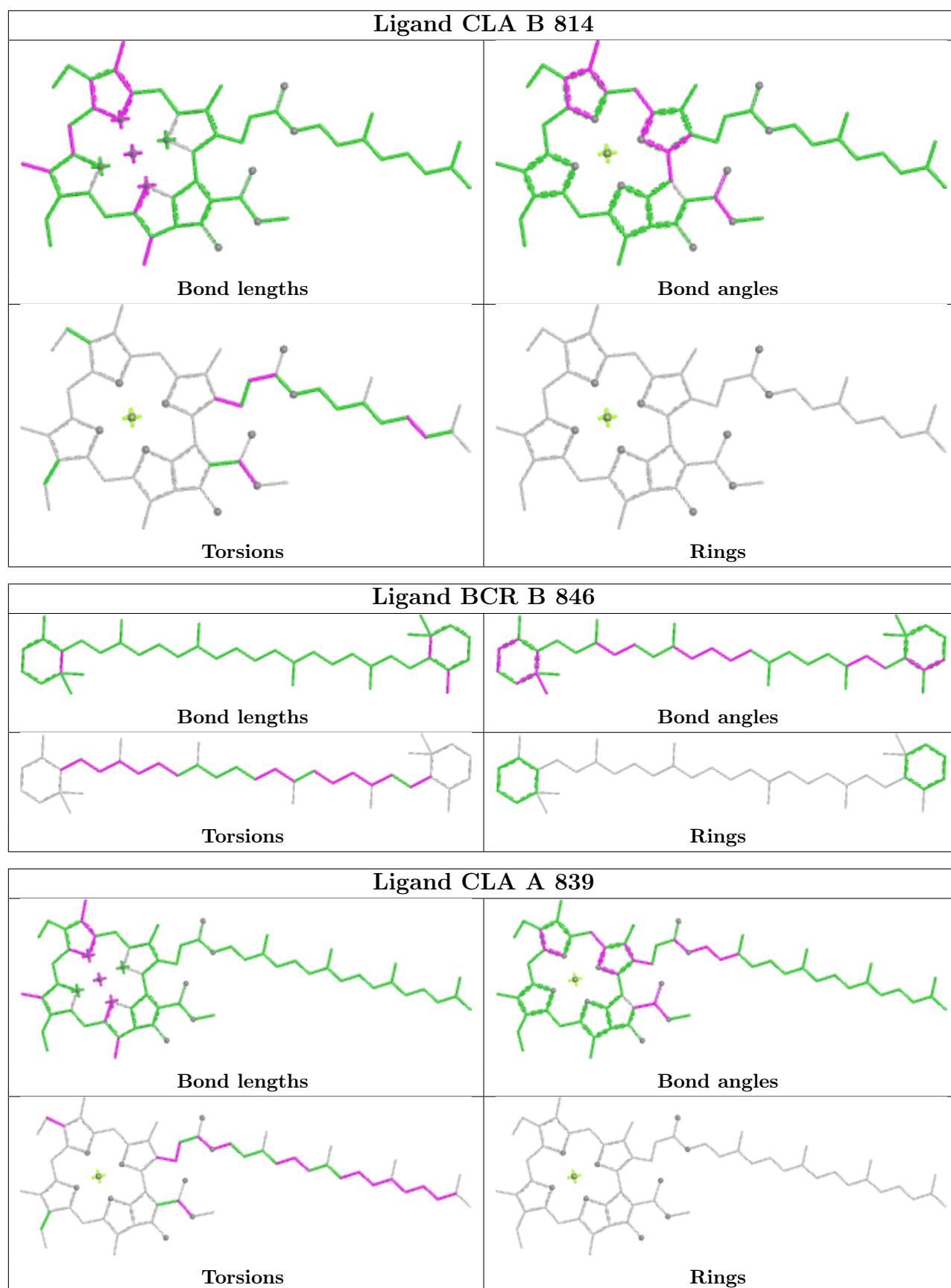
Ligand CLA 2 607

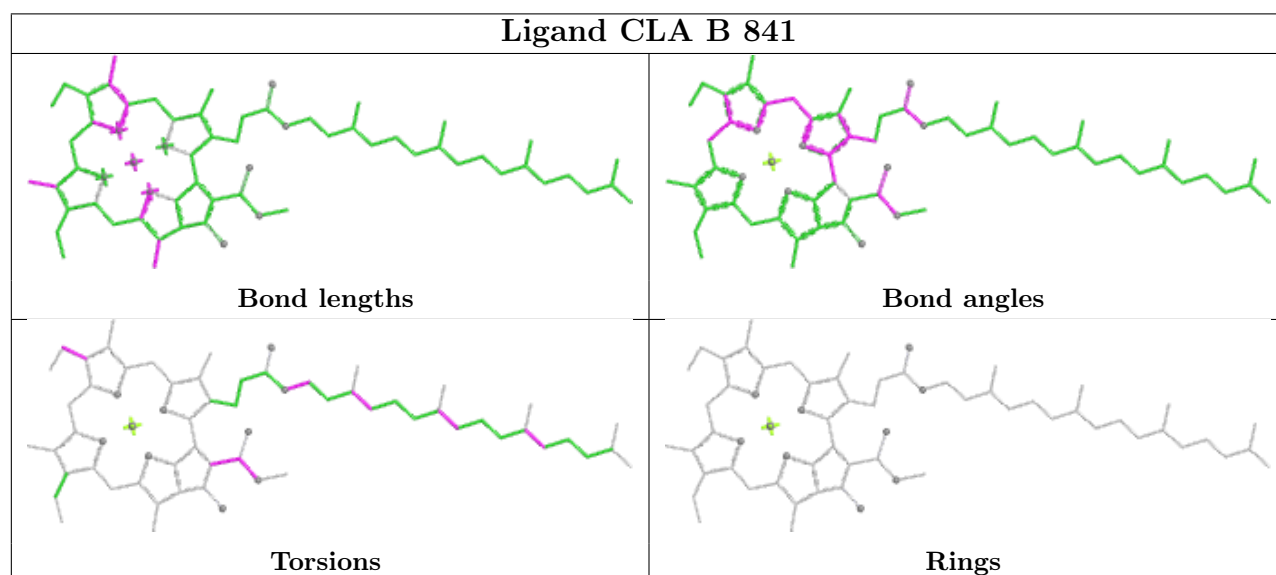
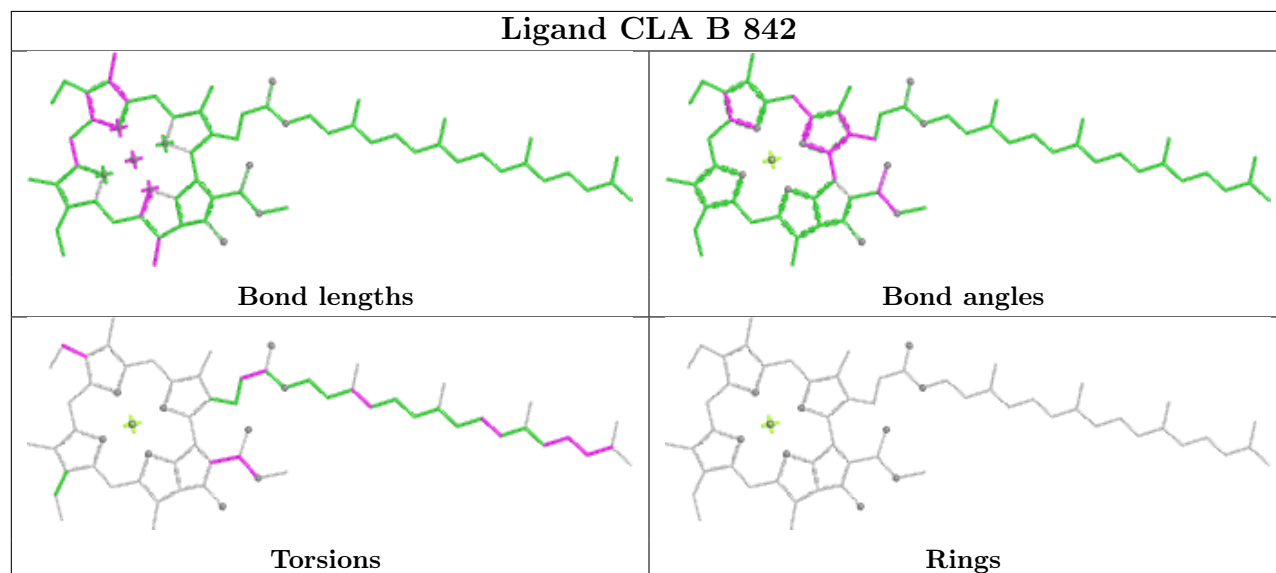
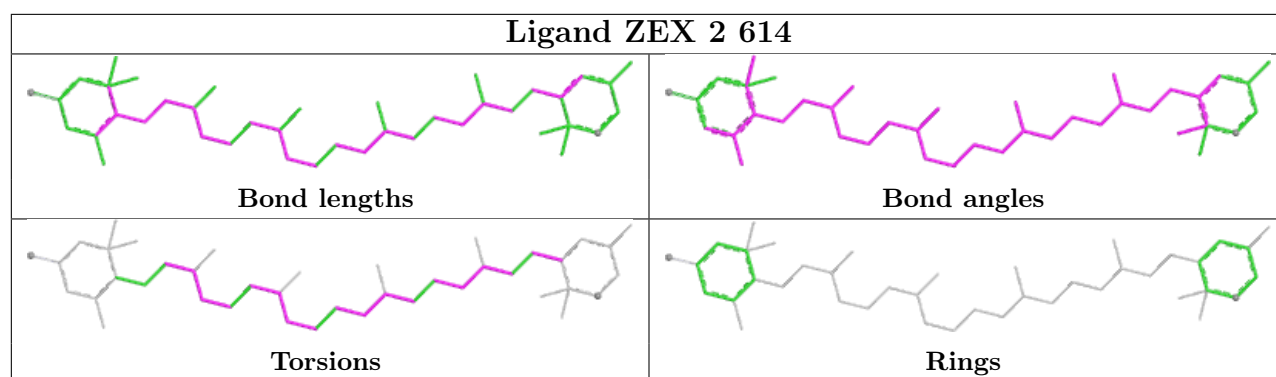


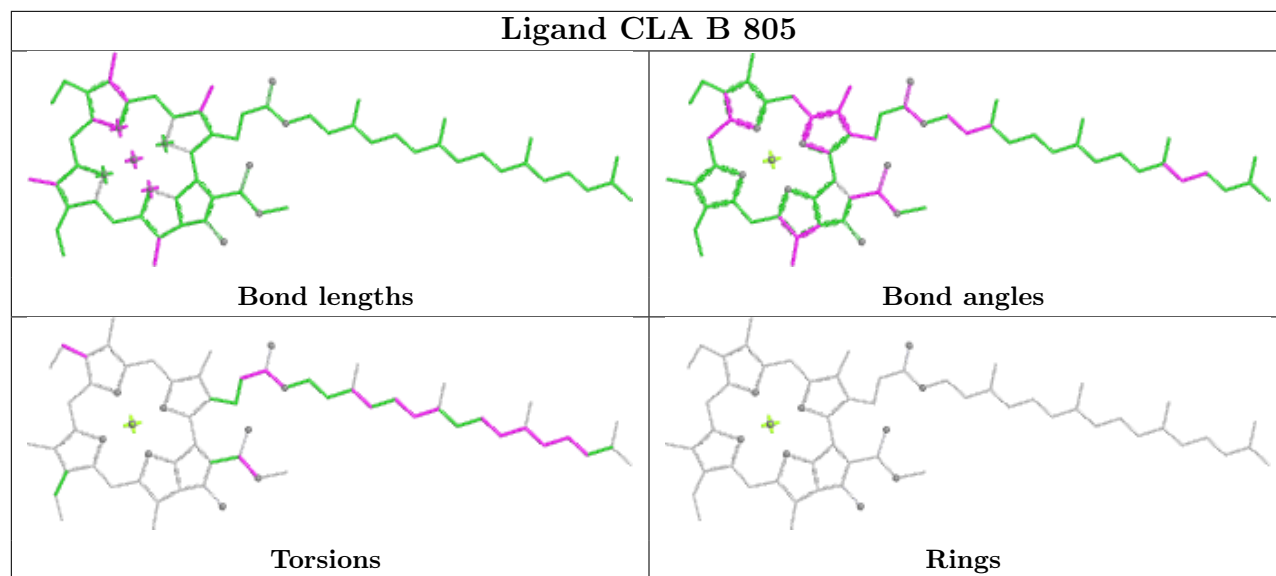


Ligand CLA 1 605









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.

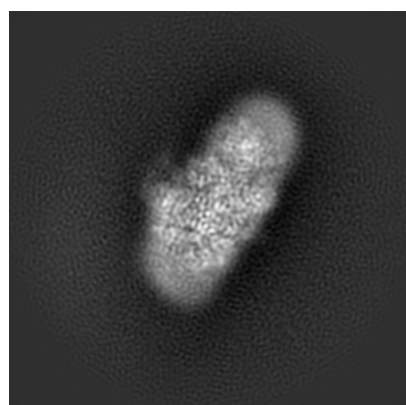
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6930. These allow visual inspection of the internal detail of the map and identification of artifacts.

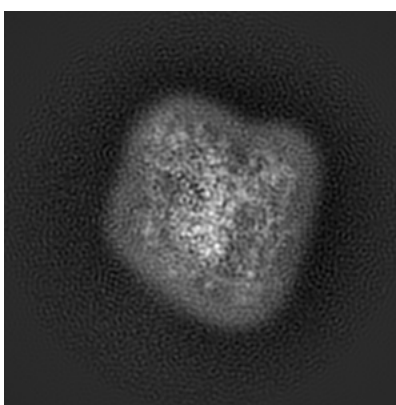
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

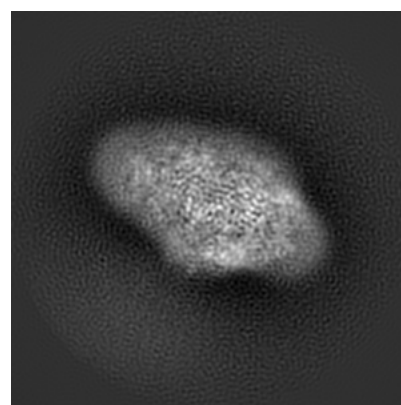
6.1.1 Primary map



X



Y

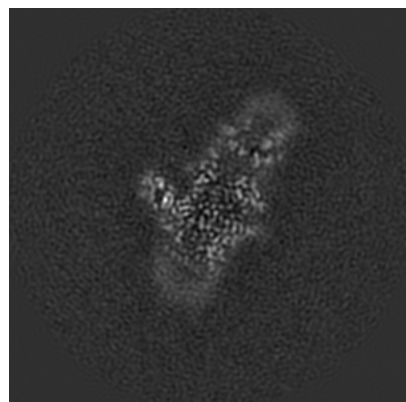


Z

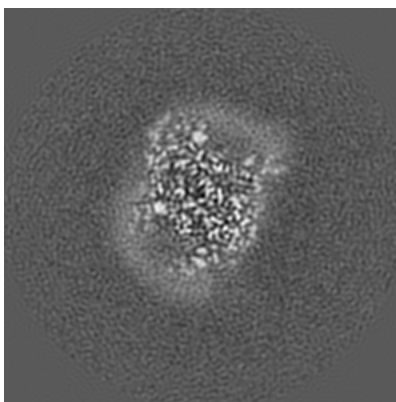
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

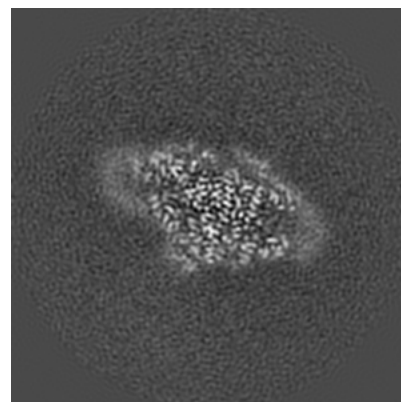
6.2.1 Primary map



X Index: 140



Y Index: 140

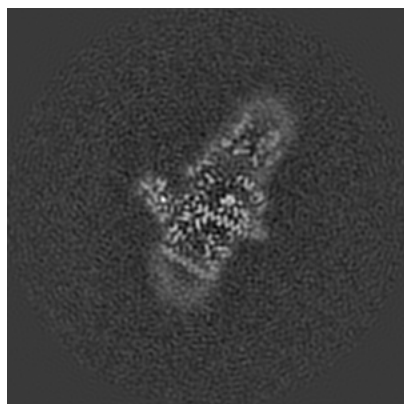


Z Index: 140

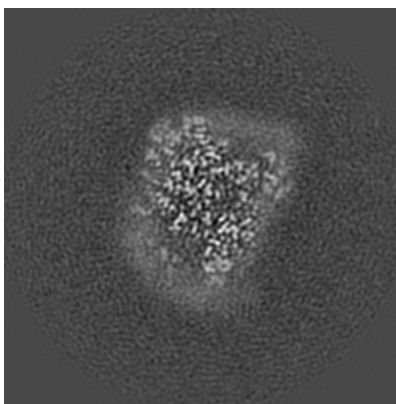
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

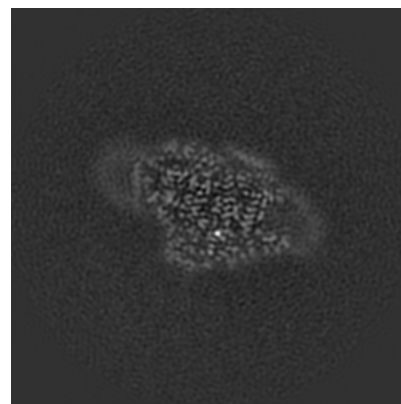
6.3.1 Primary map



X Index: 137



Y Index: 145

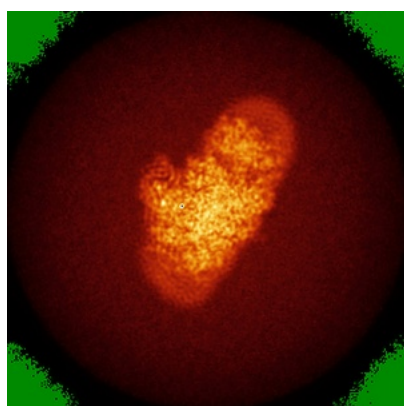


Z Index: 143

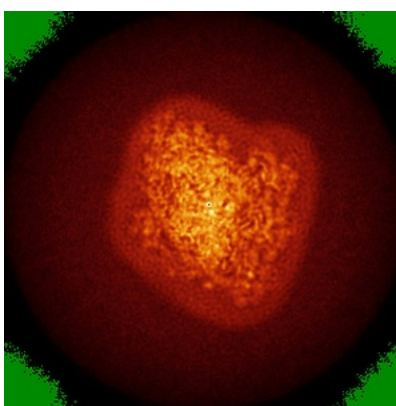
The images above show the largest variance slices of the map in three orthogonal directions.

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

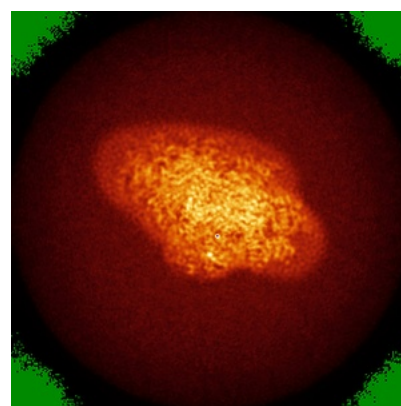
6.4.1 Primary map



X



Y

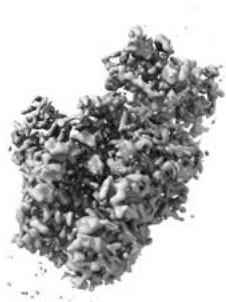


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.087. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

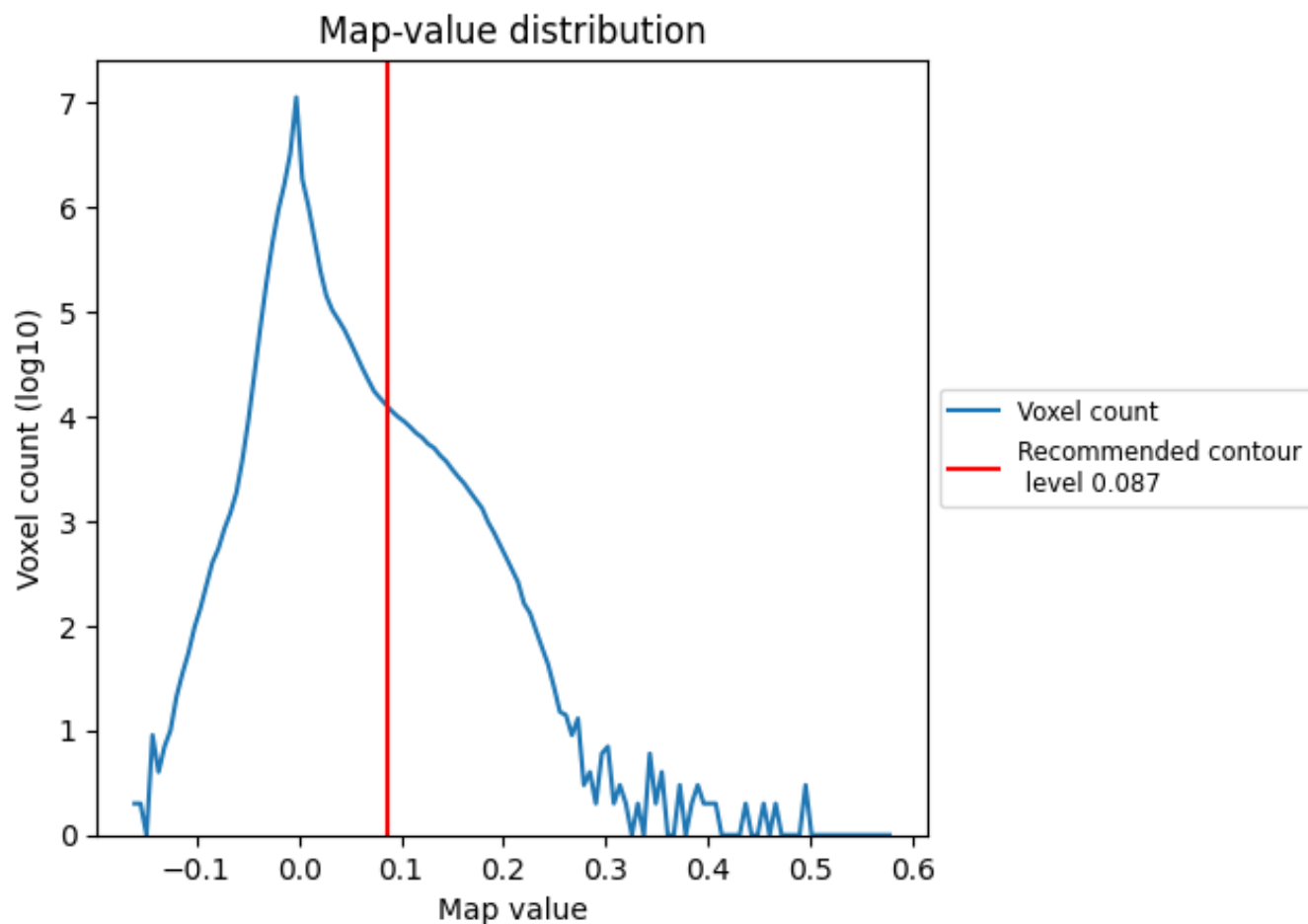
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

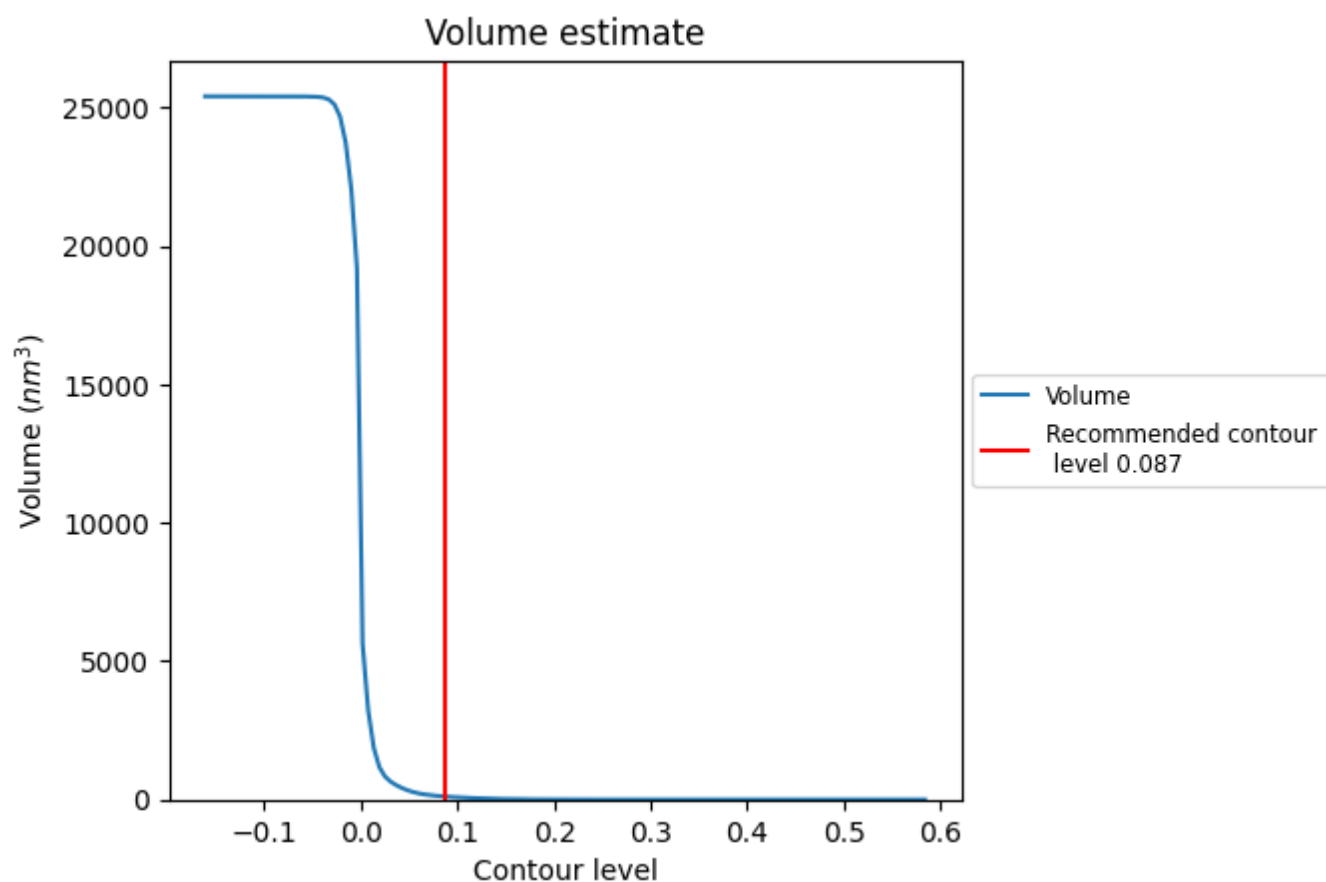
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

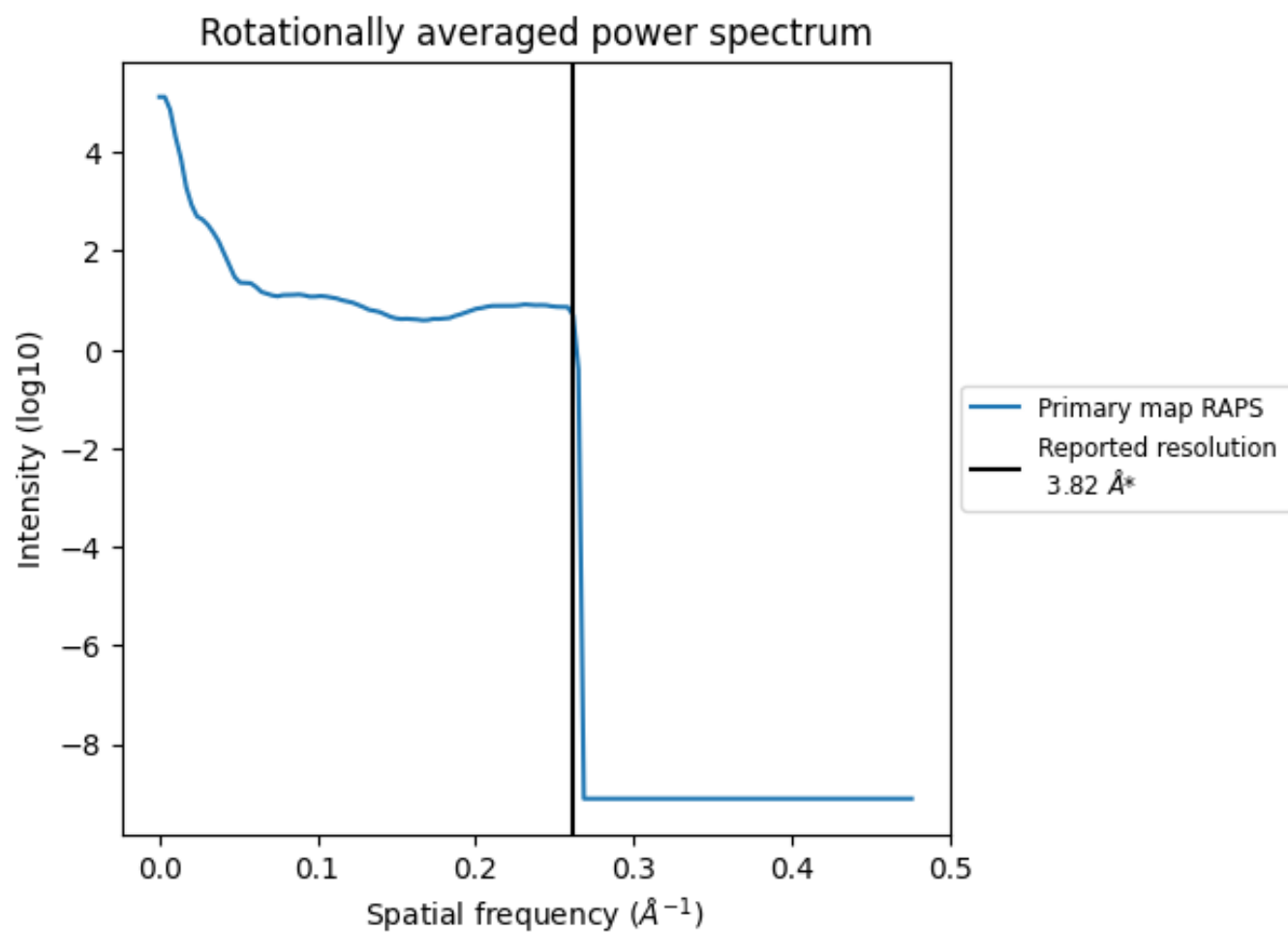
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm³; this corresponds to an approximate mass of 100 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 0.262 Å⁻¹

8 Fourier-Shell correlation

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

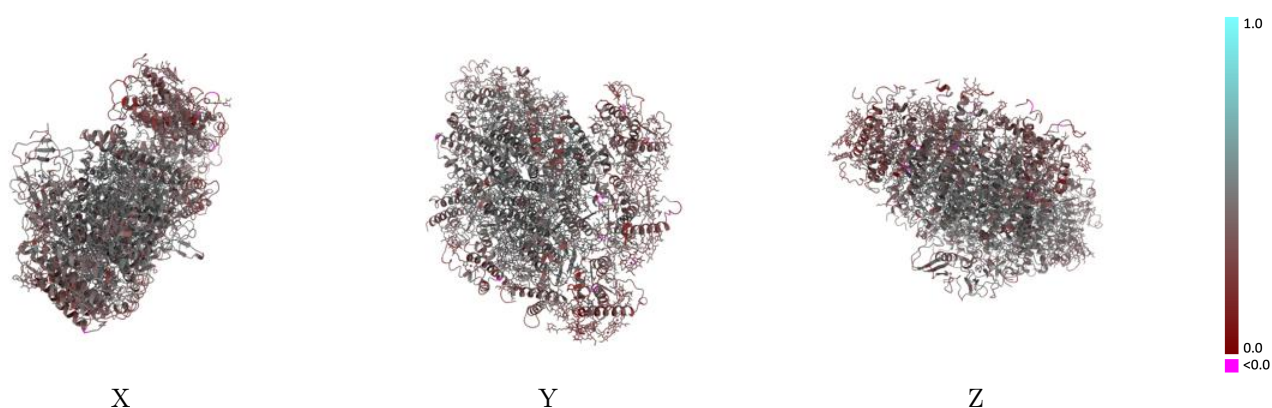
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6930 and PDB model 5ZGH. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)

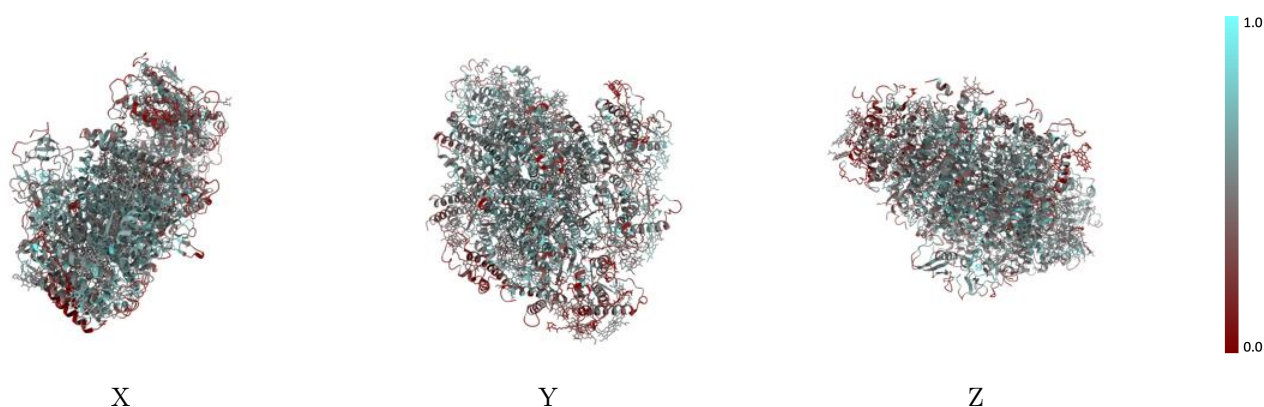
This section was not generated.

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



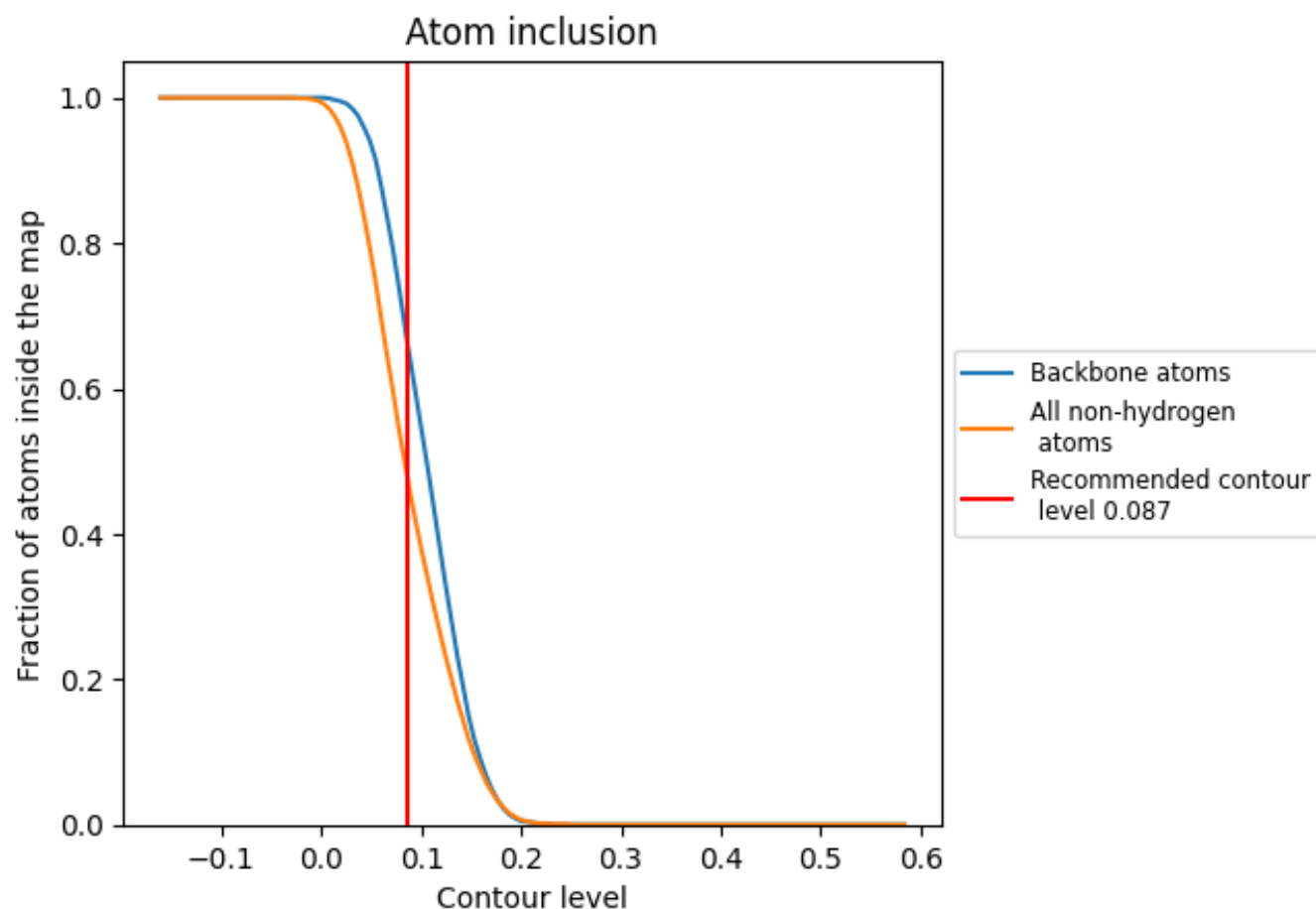
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.087).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 47% 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 (0.087) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4720	0.4070
1	0.3970	0.3350
2	0.4380	0.3490
3	0.3080	0.3220
A	0.5530	0.4540
B	0.5330	0.4330
C	0.5690	0.4290
D	0.4150	0.3880
E	0.4450	0.3930
F	0.4480	0.3970
I	0.3420	0.3860
J	0.4420	0.4570
K	0.3350	0.3470
L	0.3460	0.3750
M	0.0440	0.2930
O	0.1860	0.3230

