



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 10:02 AM JST

PDB ID : 5ZGB
EMDB ID : EMD-6929
Title : Cryo-EM structure of the red algal PSI-LHCR
Authors : Pi, X.
Deposited on : 2018-03-08
Resolution : 3.63 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:

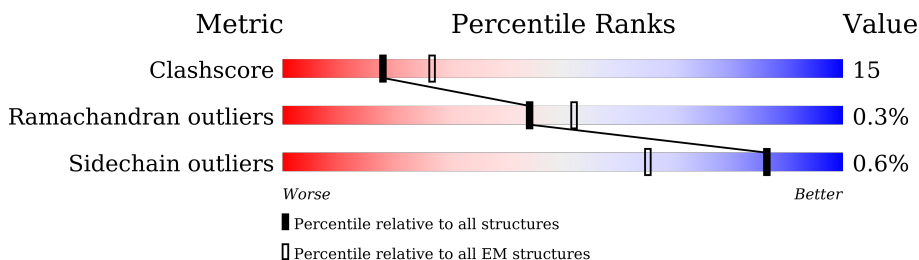
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.63 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	748	
2	B	732	
3	C	81	
4	D	139	
5	E	94	
6	F	185	
7	I	32	
8	J	38	

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Mol	Chain	Length	Quality of chain
9	K	60	
10	L	140	
11	M	29	
12	O	155	
13	1	175	
13	4	175	
14	2	199	
14	5	199	
15	3	188	

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	CL0	A	801	X	-	X	-
17	CLA	1	601	X	-	-	-
17	CLA	1	602	X	-	-	-
17	CLA	1	603	X	-	-	-
17	CLA	1	604	X	-	-	-
17	CLA	1	605	X	-	-	-
17	CLA	1	606	X	-	-	-
17	CLA	1	607	X	-	-	-
17	CLA	1	608	X	-	-	-
17	CLA	1	609	X	-	-	-
17	CLA	1	610	X	-	-	-
17	CLA	1	611	X	-	-	-
17	CLA	1	612	X	-	-	-
17	CLA	2	601	X	-	-	-
17	CLA	2	602	X	-	-	-
17	CLA	2	603	X	-	-	-
17	CLA	2	604	X	-	-	-
17	CLA	2	605	X	-	-	-
17	CLA	2	606	X	-	-	-
17	CLA	2	607	X	-	-	-
17	CLA	2	608	X	-	-	-
17	CLA	2	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	2	610	X	-	-	-
17	CLA	2	611	X	-	-	-
17	CLA	2	612	X	-	-	-
17	CLA	2	613	X	-	-	-
17	CLA	3	202	X	-	-	-
17	CLA	3	203	X	-	-	-
17	CLA	3	204	X	-	-	-
17	CLA	3	205	X	-	-	-
17	CLA	3	206	X	-	-	-
17	CLA	3	207	X	-	-	-
17	CLA	3	208	X	-	-	-
17	CLA	3	209	X	-	-	-
17	CLA	3	210	X	-	-	-
17	CLA	3	211	X	-	-	-
17	CLA	3	212	X	-	-	-
17	CLA	3	213	X	-	-	-
17	CLA	4	601	X	-	-	-
17	CLA	4	602	X	-	-	-
17	CLA	4	603	X	-	-	-
17	CLA	4	604	X	-	-	-
17	CLA	4	605	X	-	-	-
17	CLA	4	606	X	-	-	-
17	CLA	4	607	X	-	-	-
17	CLA	4	608	X	-	-	-
17	CLA	4	609	X	-	-	-
17	CLA	4	610	X	-	-	-
17	CLA	4	611	X	-	-	-
17	CLA	5	601	X	-	-	-
17	CLA	5	602	X	-	-	-
17	CLA	5	603	X	-	-	-
17	CLA	5	604	X	-	-	-
17	CLA	5	605	X	-	-	-
17	CLA	5	606	X	-	-	-
17	CLA	5	607	X	-	-	-
17	CLA	5	608	X	-	-	-
17	CLA	5	609	X	-	-	-
17	CLA	5	610	X	-	-	-
17	CLA	5	611	X	-	-	-
17	CLA	5	612	X	-	-	-
17	CLA	5	613	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	848	X	-	-	-
17	CLA	B	801	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	B	842	X	-	-	-
17	CLA	B	843	X	-	-	-
17	CLA	F	301	X	-	-	-
17	CLA	F	302	X	-	-	-
17	CLA	F	303	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	J	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	J	103	X	-	-	-
17	CLA	K	102	X	-	-	-
17	CLA	K	103	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
17	CLA	L	204	X	-	-	-
17	CLA	O	201	X	-	-	-
17	CLA	O	203	X	-	-	-
17	CLA	O	204	X	-	-	-
17	CLA	O	205	X	-	-	-
25	ZEX	1	615	-	X	-	-
25	ZEX	1	616	-	X	-	-
25	ZEX	2	614	-	X	-	-
25	ZEX	3	216	-	X	-	-
25	ZEX	3	218	-	X	-	-
25	ZEX	4	612	-	X	-	-
25	ZEX	5	614	-	X	-	-
25	ZEX	5	615	-	X	-	-

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 35011 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PsaA.

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

- Molecule 2 is a protein called PsaB.

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

- Molecule 3 is a protein called PsaC.

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

- Molecule 4 is a protein called PsaD.

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

- Molecule 5 is a protein called PsaE.

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

- Molecule 6 is a protein called PsaF.

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

- Molecule 7 is a protein called PsaI.

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

- Molecule 8 is a protein called PsaJ.

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

- Molecule 9 is a protein called PsaK.

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

- Molecule 10 is a protein called PsaL.

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

- Molecule 11 is a protein called PsaM.

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

- Molecule 12 is a protein called PsaO.

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

- Molecule 13 is a protein called Lhcr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	1	169	1351	887	227	229	8	0	0
13	4	170	1358	892	228	230	8	0	0

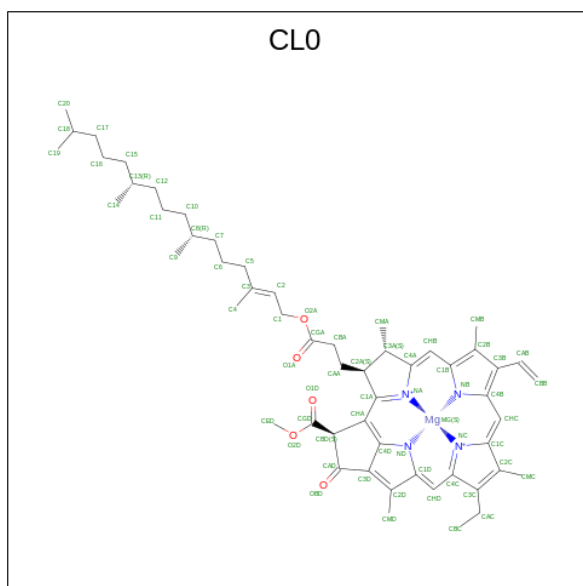
- Molecule 14 is a protein called Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	2	175	Total	C	N	O	S	0	0
			1371	892	233	239	7		
14	5	175	Total	C	N	O	S	0	0
			1371	892	233	239	7		

- Molecule 15 is a protein called Lhcr3.

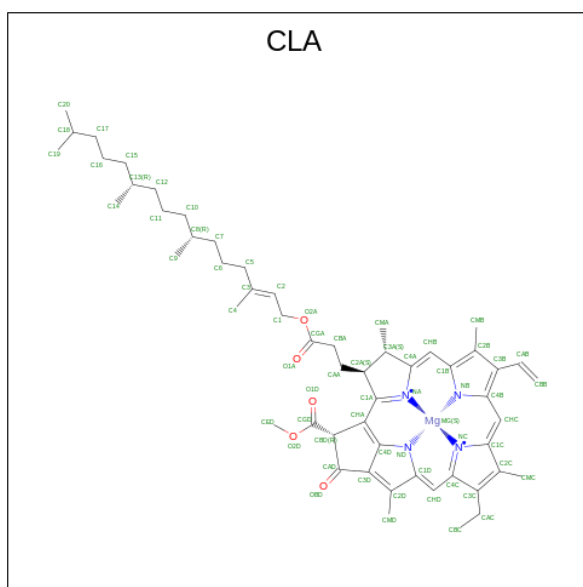
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	3	170	Total	C	N	O	S	0	0
			1303	845	219	232	7		

- Molecule 16 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	
17	A	1	Total	C	Mg	N	O	0
			2310	1922	39	156	193	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0
17	A	1	2310	1922	39	156	193	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	A	1	Total 2310	C 1922	Mg 39	N 156	O 193	0
17	A	1	Total 2310	C 1922	Mg 39	N 156	O 193	0
17	A	1	Total 2310	C 1922	Mg 39	N 156	O 193	0
17	A	1	Total 2310	C 1922	Mg 39	N 156	O 193	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0
17	B	1	Total 2469	C 2055	Mg 42	N 168	O 204	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	B	1	2469	2055	42	168	204	0
17	F	1	147	119	3	12	13	0
17	F	1	147	119	3	12	13	0
17	F	1	147	119	3	12	13	0
17	J	1	165	137	3	12	13	0
17	J	1	165	137	3	12	13	0
17	J	1	165	137	3	12	13	0
17	K	1	87	69	2	8	8	0
17	K	1	87	69	2	8	8	0
17	L	1	172	142	3	12	15	0
17	L	1	172	142	3	12	15	0
17	L	1	172	142	3	12	15	0
17	O	1	188	150	4	16	18	0
17	O	1	188	150	4	16	18	0
17	O	1	188	150	4	16	18	0
17	O	1	188	150	4	16	18	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	1	1	565	449	12	48	56	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0

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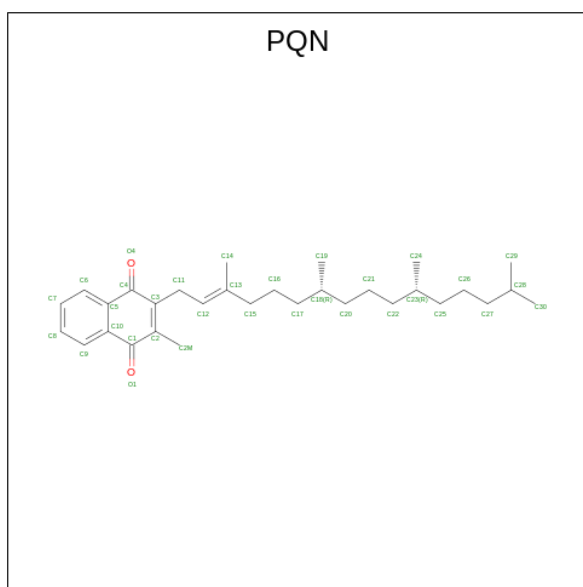
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	2	1	600	476	13	52	59	0
17	2	1	600	476	13	52	59	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	3	1	565	449	12	48	56	0
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0

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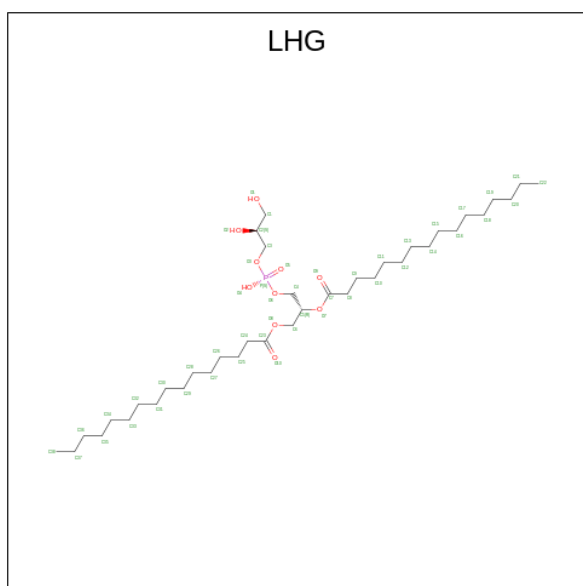
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0
17	4	1	505	399	11	44	51	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0
17	5	1	600	474	13	52	61	0

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



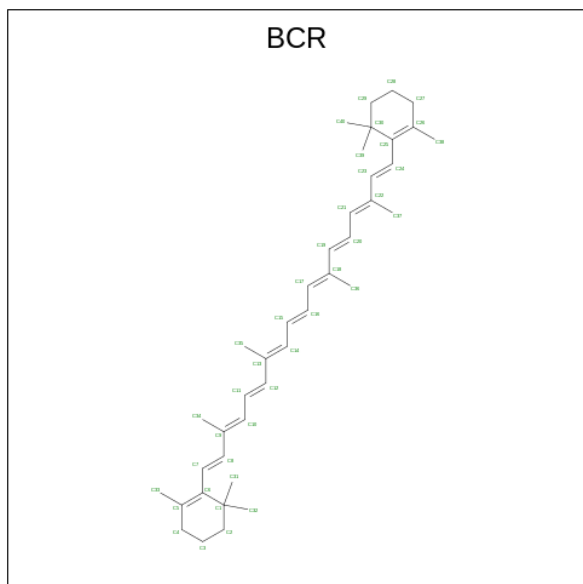
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			89	67	20	2	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	A	1	89	67	20	2	0

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



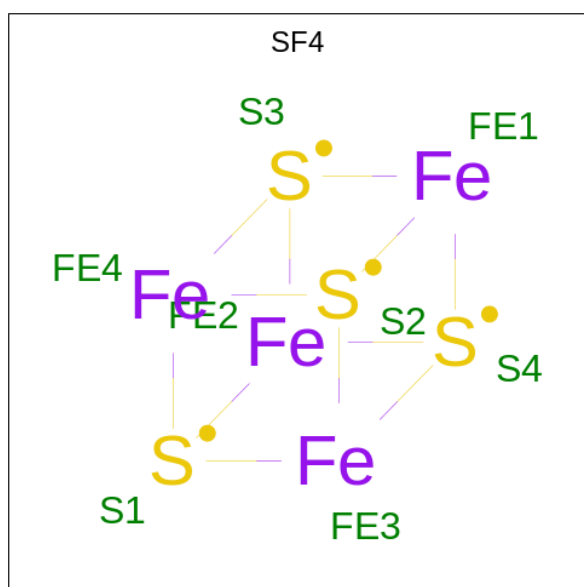
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			160	160	
20	A	1	Total	C	0
			160	160	
20	A	1	Total	C	0
			160	160	
20	A	1	Total	C	0
			160	160	
20	B	1	Total	C	0
			280	280	
20	B	1	Total	C	0
			280	280	
20	B	1	Total	C	0
			280	280	
20	B	1	Total	C	0
			280	280	
20	B	1	Total	C	0
			280	280	

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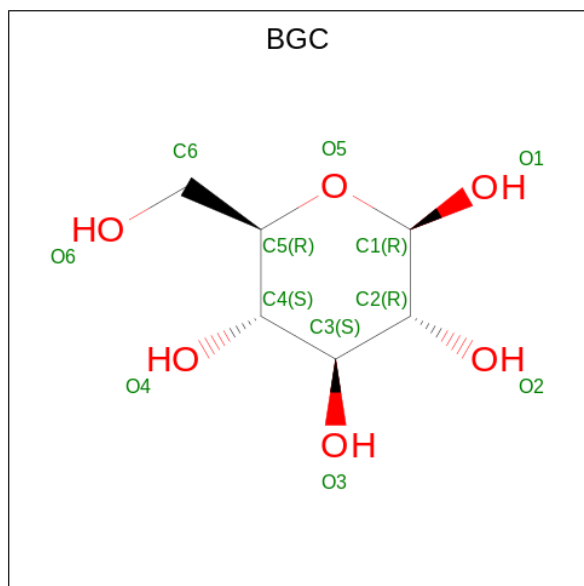
Mol	Chain	Residues	Atoms		AltConf
20	B	1	Total	C	0
			280	280	
20	F	1	Total	C	0
			40	40	
20	I	1	Total	C	0
			40	40	
20	J	1	Total	C	0
			80	80	
20	J	1	Total	C	0
			80	80	
20	K	1	Total	C	0
			80	80	
20	K	1	Total	C	0
			80	80	
20	L	1	Total	C	0
			120	120	
20	L	1	Total	C	0
			120	120	
20	L	1	Total	C	0
			120	120	
20	O	1	Total	C	0
			40	40	

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



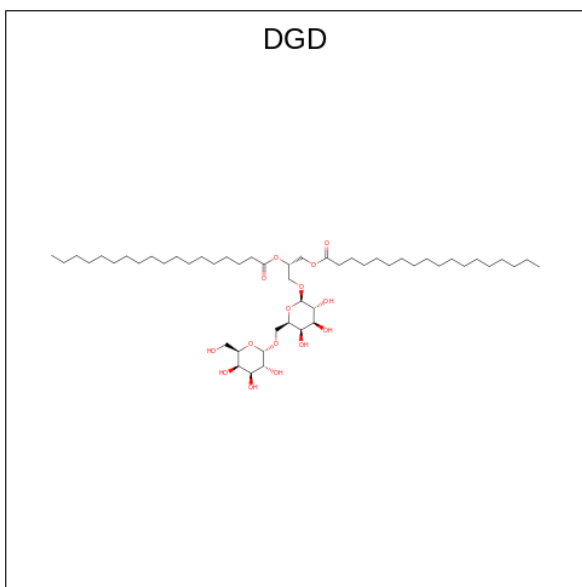
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			16	8	8	
21	C	1	Total	Fe	S	0
			16	8	8	

- Molecule 22 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



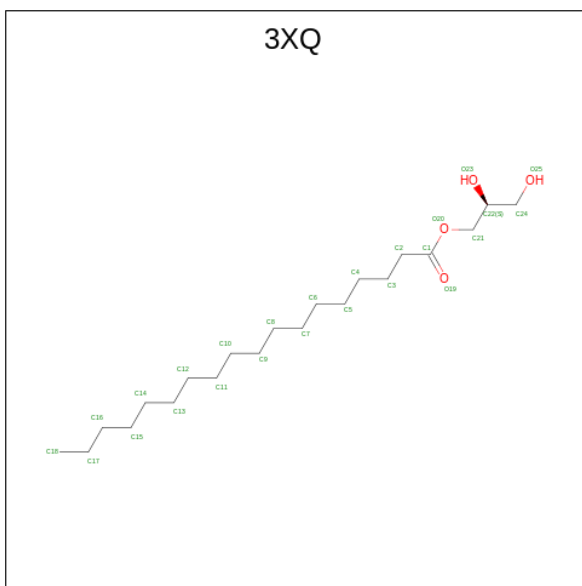
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			11	6	5	

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



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

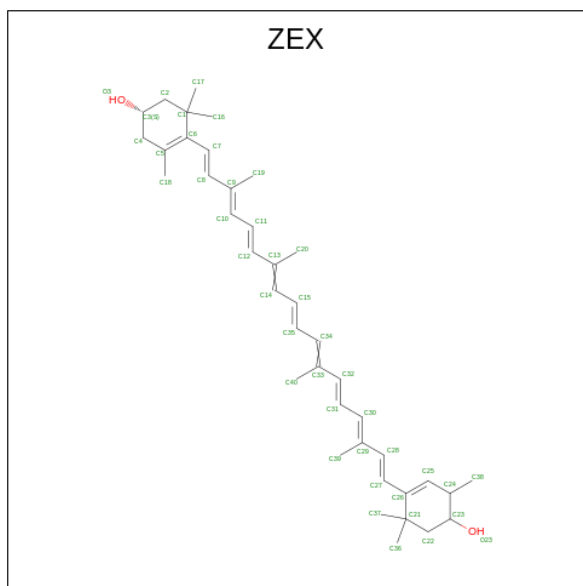
- Molecule 24 is (2S)-2,3-dihydroxypropyl octadecanoate (three-letter code: 3XQ) (formula: $C_{21}H_{42}O_4$).



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

- Molecule 25 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 (three-letter code: ZEX) (formula: C₄₀H₅₆O₂).



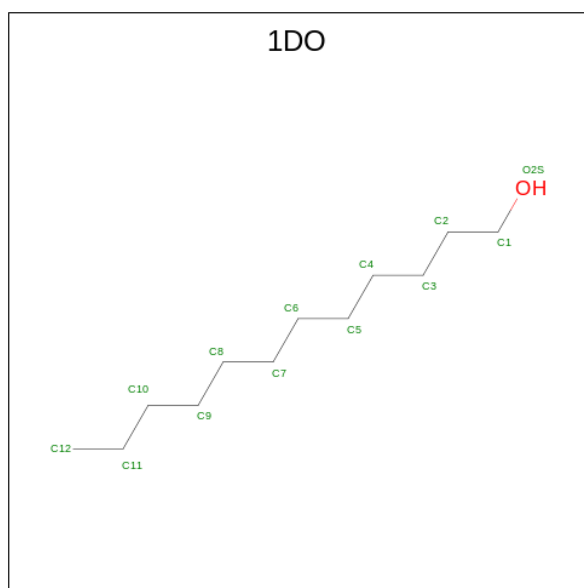
Mol	Chain	Residues	Atoms			AltConf
25	1	1	Total	C	O	0
			210	200	10	
25	1	1	Total	C	O	0
			210	200	10	
25	1	1	Total	C	O	0
			210	200	10	
25	1	1	Total	C	O	0
			210	200	10	
25	1	1	Total	C	O	0
			210	200	10	
25	2	1	Total	C	O	0
			168	160	8	
25	2	1	Total	C	O	0
			168	160	8	
25	2	1	Total	C	O	0
			168	160	8	
25	2	1	Total	C	O	0
			168	160	8	
25	3	1	Total	C	O	0
			252	240	12	
25	3	1	Total	C	O	0
			252	240	12	
25	3	1	Total	C	O	0
			252	240	12	
25	3	1	Total	C	O	0
			252	240	12	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	3	1	252	240	12	0
25	3	1	252	240	12	0
25	4	1	252	240	12	0
25	4	1	252	240	12	0
25	4	1	252	240	12	0
25	4	1	252	240	12	0
25	4	1	252	240	12	0
25	4	1	252	240	12	0
25	4	1	252	240	12	0
25	5	1	168	160	8	0
25	5	1	168	160	8	0
25	5	1	168	160	8	0
25	5	1	168	160	8	0

- Molecule 26 is 1-DODECANOL (three-letter code: 1DO) (formula: C₁₂H₂₆O).

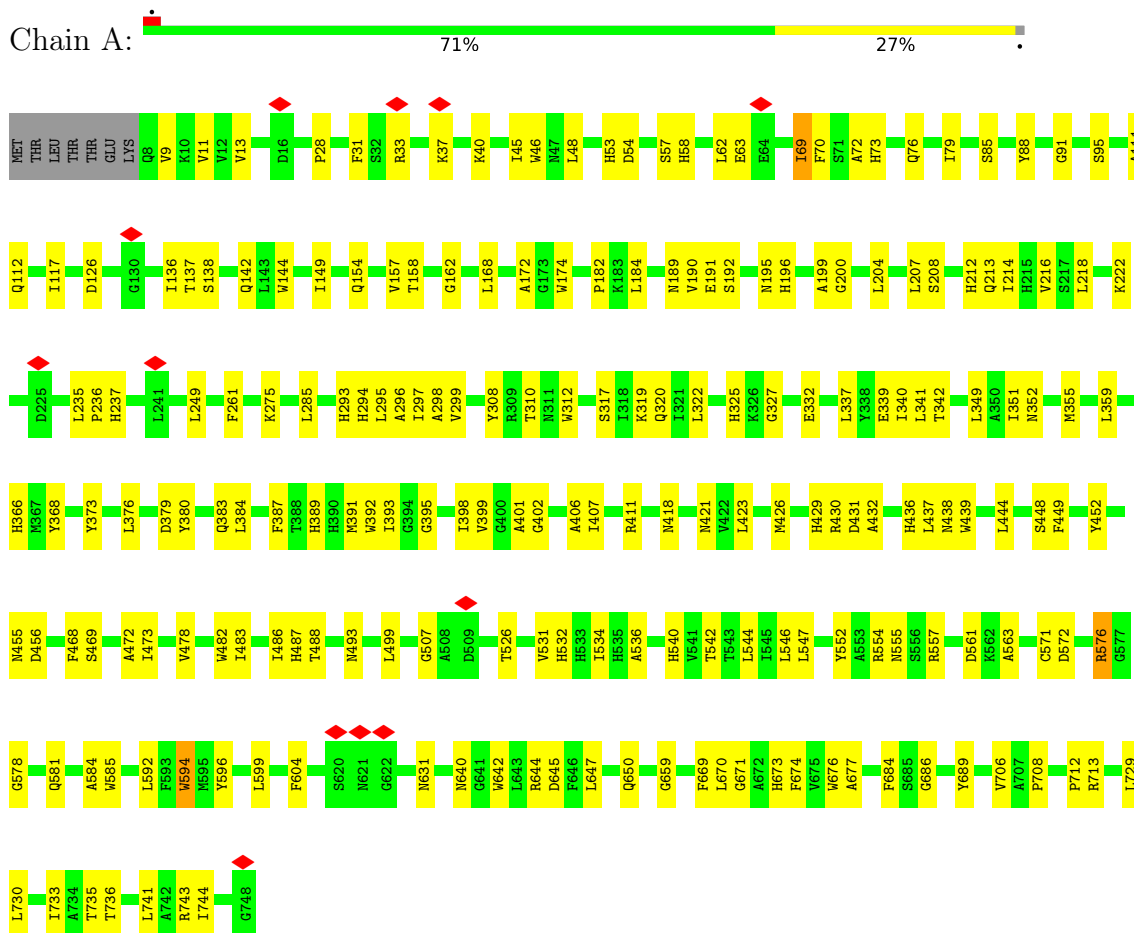


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	3	1	13	12	1	0

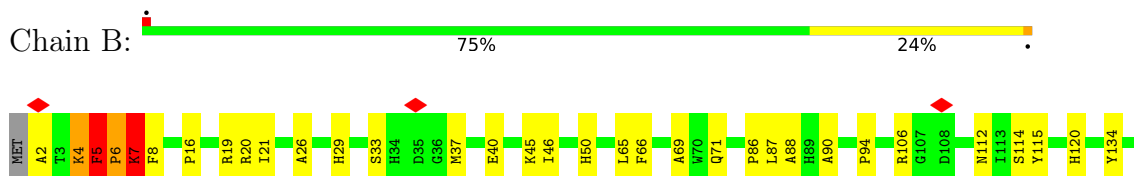
3 Residue-property plots [i](#)

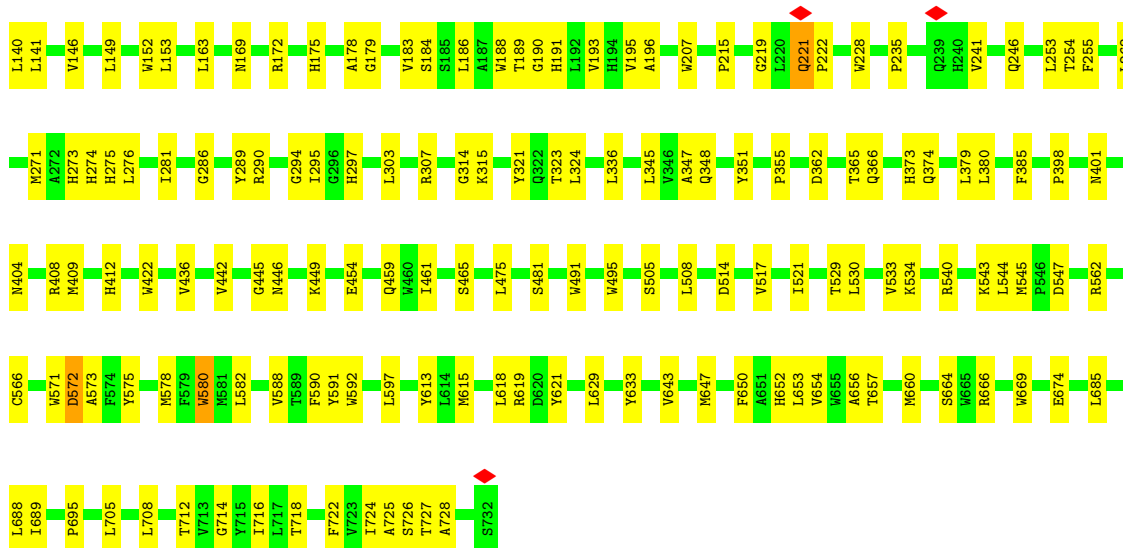
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PsaA



- Molecule 2: PsaB

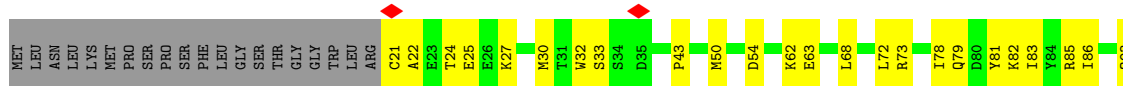




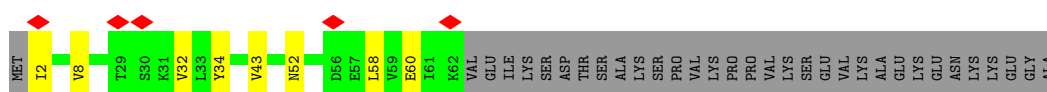
• Molecule 3: PsaC



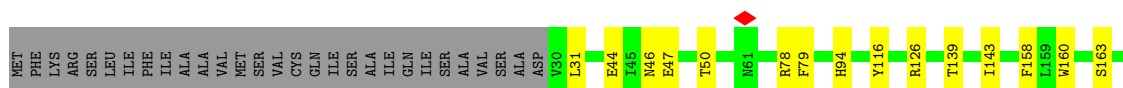
• Molecule 4: PsaD



• Molecule 5: PsaE



• Molecule 6: PsaF

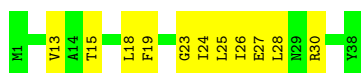




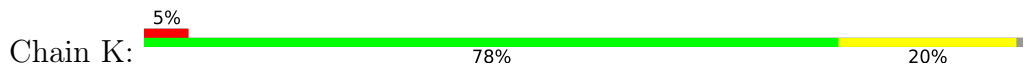
• Molecule 7: Psal



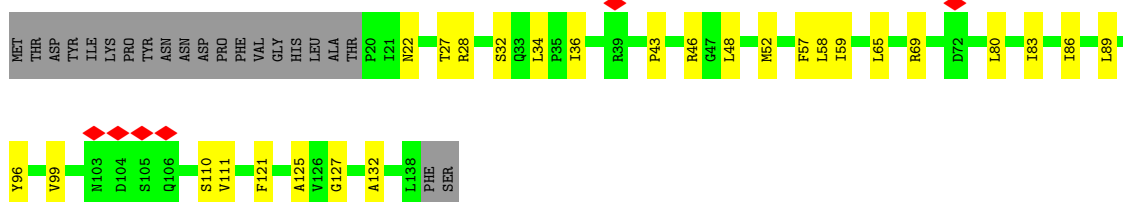
• Molecule 8: Psaj



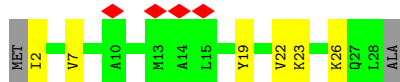
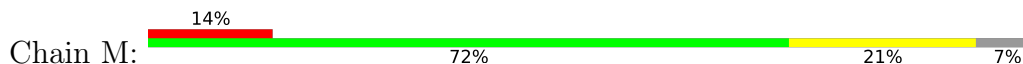
• Molecule 9: PsaK



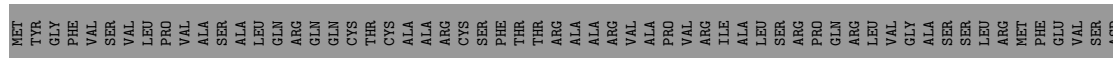
• Molecule 10: PsaL

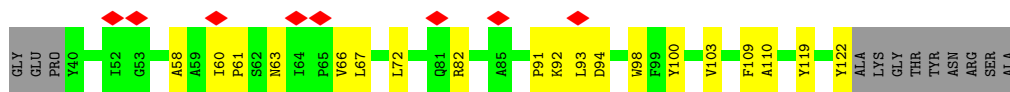


• Molecule 11: PsaM

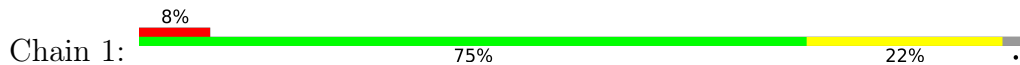


• Molecule 12: PsaO

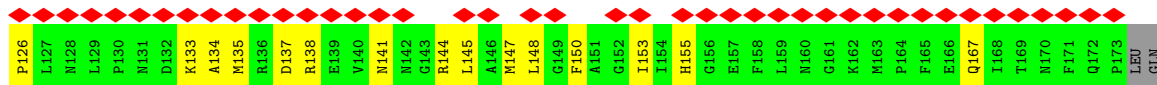
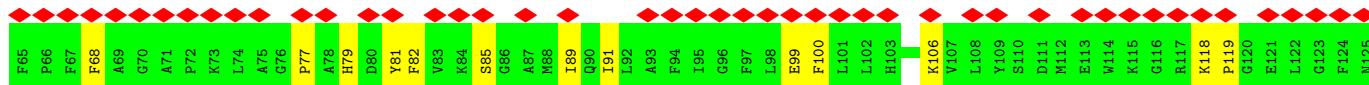
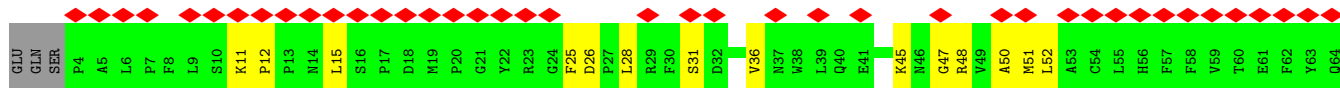
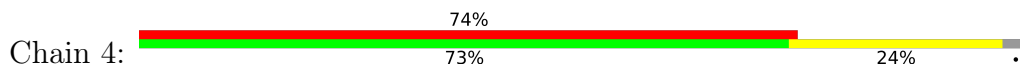




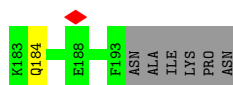
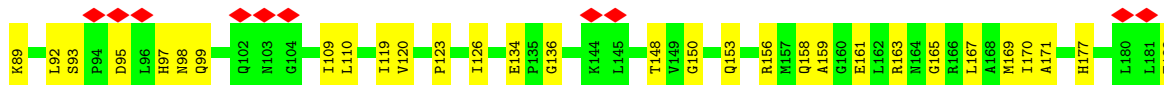
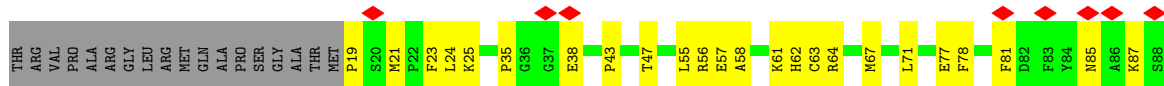
• Molecule 13: Lhcr1



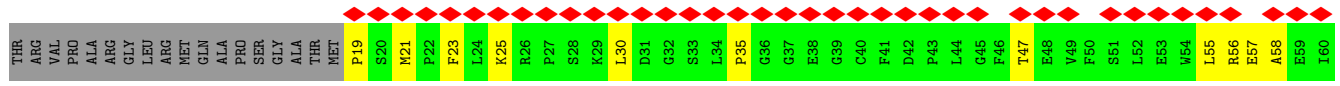
• Molecule 13: Lhcr1

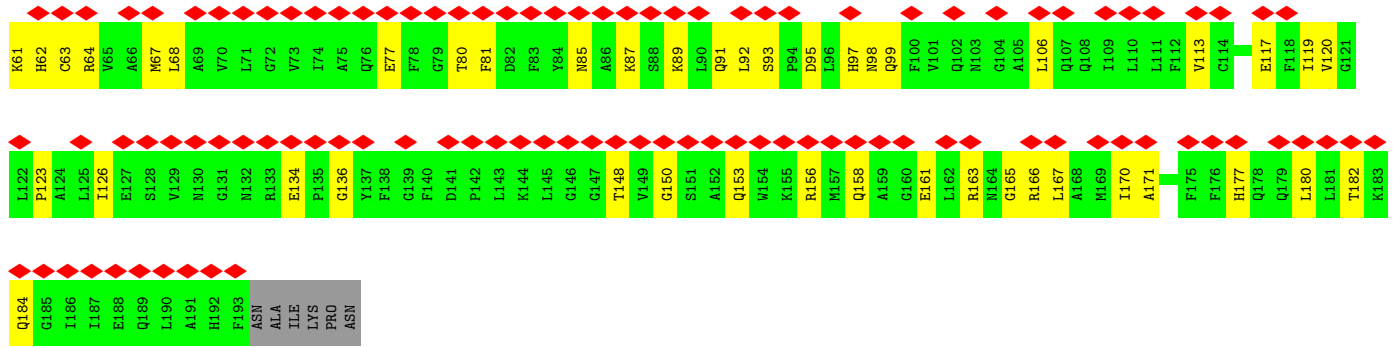


• Molecule 14: Lhcr2

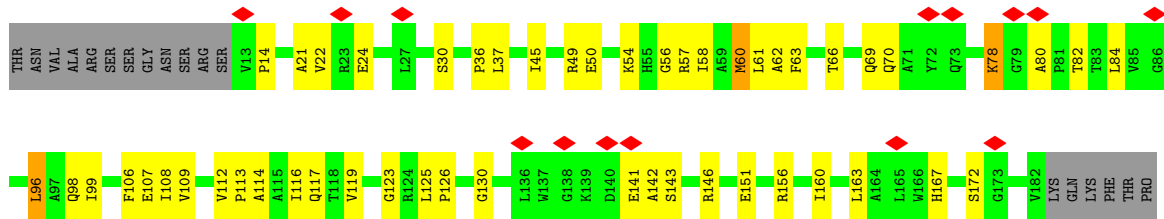


• Molecule 14: Lhcr2





• Molecule 15: Lhcr3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124279	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	0.653	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0562	Depositor
Map size (\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 (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	1/5985 (0.0%)	0.64	1/8158 (0.0%)
2	B	0.56	1/6028 (0.0%)	0.66	3/8236 (0.0%)
3	C	0.54	0/607	0.60	0/822
4	D	0.40	0/969	0.59	0/1307
5	E	0.49	0/502	0.56	0/680
6	F	0.44	0/1296	0.63	0/1760
7	I	0.40	0/235	0.73	1/321 (0.3%)
8	J	0.48	0/321	0.62	0/437
9	K	0.35	0/433	0.63	0/588
10	L	0.36	0/919	0.57	0/1247
11	M	0.29	0/205	0.60	0/277
12	O	0.36	0/664	0.66	0/913
13	1	0.36	0/1395	0.65	0/1884
13	4	0.36	0/1403	0.65	0/1895
14	2	0.38	0/1407	0.67	0/1898
14	5	0.38	0/1407	0.67	0/1898
15	3	0.41	1/1337 (0.1%)	0.69	2/1817 (0.1%)
All	All	0.49	3/25113 (0.0%)	0.64	7/34138 (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
14	2	0	2
14	5	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	594	TRP	CB-CG	-6.51	1.38	1.50
2	B	580	TRP	CB-CG	-5.68	1.40	1.50
15	3	80	ALA	C-N	5.42	1.44	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	572	ASP	CB-CG-OD1	8.16	125.64	118.30
2	B	514	ASP	CB-CG-OD1	7.40	124.96	118.30
1	A	571	CYS	CA-CB-SG	-6.53	102.25	114.00
7	I	16	LEU	CA-CB-CG	5.66	128.31	115.30
15	3	96	LEU	CA-CB-CG	5.59	128.16	115.30
2	B	221	GLN	CA-CB-CG	5.08	124.58	113.40
15	3	60	MET	CA-CB-CG	5.03	121.85	113.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	2	136	GLY	Peptide
14	2	98	ASN	Peptide
14	5	136	GLY	Peptide
14	5	98	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5798	0	5727	206	0
2	B	5819	0	5648	166	0
3	C	597	0	584	21	0
4	D	950	0	943	91	0
5	E	493	0	509	5	0
6	F	1263	0	1236	13	0
7	I	230	0	253	8	0
8	J	312	0	327	15	0
9	K	428	0	464	11	0
10	L	900	0	931	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	204	0	226	5	0
12	O	641	0	650	12	0
13	1	1351	0	1322	28	0
13	4	1358	0	1330	33	0
14	2	1371	0	1362	43	0
14	5	1371	0	1362	41	0
15	3	1303	0	1305	46	0
16	A	65	0	71	59	0
17	1	565	0	443	19	0
17	2	600	0	466	26	0
17	3	565	0	440	27	0
17	4	505	0	384	23	0
17	5	600	0	463	26	0
17	A	2310	0	2337	152	0
17	B	2469	0	2499	158	0
17	F	147	0	123	4	0
17	J	165	0	158	11	0
17	K	87	0	64	2	0
17	L	172	0	164	6	0
17	O	188	0	144	4	0
18	A	33	0	46	4	0
18	B	33	0	46	3	0
19	A	89	0	127	6	0
20	A	160	0	224	15	0
20	B	280	0	392	24	0
20	F	40	0	56	2	0
20	I	40	0	56	4	0
20	J	80	0	112	6	0
20	K	80	0	112	10	0
20	L	120	0	168	11	0
20	O	40	0	56	5	0
21	A	8	0	0	0	0
21	C	16	0	0	2	0
22	A	11	0	9	0	0
23	B	66	0	96	5	0
24	J	25	0	0	0	0
25	1	210	0	280	19	0
25	2	168	0	224	11	0
25	3	252	0	336	20	0
25	4	252	0	336	18	0
25	5	168	0	224	16	0
26	3	13	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35011	0	34860	1041	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 15.

All (1041) 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)
1:A:642:TRP:CD2	16:A:801:CL0:H56	1.25	1.63
4:D:82:LYS:HE3	4:D:95:LEU:CA	1.36	1.50
1:A:642:TRP:CE2	16:A:801:CL0:H56	1.50	1.45
4:D:82:LYS:NZ	4:D:95:LEU:HB2	1.26	1.44
4:D:82:LYS:CE	4:D:95:LEU:C	1.87	1.43
4:D:96:HIS:HB3	4:D:97:PRO:CD	1.44	1.37
1:A:647:LEU:CD1	16:A:801:CL0:H47	1.52	1.35
4:D:82:LYS:CE	4:D:95:LEU:CB	2.06	1.32
4:D:82:LYS:HE3	4:D:95:LEU:C	0.94	1.31
1:A:642:TRP:CD2	16:A:801:CL0:C14	2.13	1.30
4:D:82:LYS:CE	4:D:95:LEU:CA	2.07	1.29
4:D:82:LYS:CE	4:D:95:LEU:HB2	1.62	1.26
4:D:82:LYS:NZ	4:D:95:LEU:CB	1.99	1.25
4:D:82:LYS:HZ1	4:D:95:LEU:N	1.34	1.23
2:B:6:PRO:O	2:B:8:PHE:N	1.70	1.21
2:B:5:PHE:HB3	2:B:6:PRO:CD	1.67	1.21
4:D:96:HIS:CB	4:D:97:PRO:HD2	1.63	1.19
4:D:82:LYS:NZ	4:D:95:LEU:H	1.42	1.18
4:D:62:LYS:HE3	4:D:95:LEU:HD12	1.27	1.12
1:A:642:TRP:NE1	16:A:801:CL0:H52	1.65	1.12
4:D:62:LYS:HE3	4:D:95:LEU:CD1	1.79	1.12
2:B:5:PHE:HB3	2:B:6:PRO:HD3	1.31	1.09
4:D:96:HIS:CB	4:D:97:PRO:CD	2.19	1.09
1:A:642:TRP:CE3	16:A:801:CL0:H56	1.88	1.08
1:A:647:LEU:HD12	16:A:801:CL0:C9	1.83	1.07
4:D:82:LYS:HB2	4:D:97:PRO:HG2	1.37	1.05
2:B:5:PHE:CB	2:B:6:PRO:HD3	1.89	1.03
2:B:6:PRO:C	2:B:8:PHE:H	1.58	1.02
1:A:642:TRP:CE2	16:A:801:CL0:C14	2.39	1.01
2:B:5:PHE:CB	2:B:6:PRO:CD	2.38	1.00
1:A:647:LEU:HD12	16:A:801:CL0:H47	1.00	1.00
1:A:642:TRP:CE2	16:A:801:CL0:H52	1.97	0.99
4:D:82:LYS:HE3	4:D:95:LEU:O	1.60	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:THR:HG22	16:A:801:CL0:OBD	1.64	0.98
2:B:5:PHE:HB3	2:B:6:PRO:HD2	1.47	0.96
1:A:596:TYR:OH	16:A:801:CL0:O2D	1.84	0.95
2:B:134:TYR:HH	11:M:2:ILE:N	1.64	0.95
4:D:99:ASP:O	4:D:101:VAL:HG22	1.66	0.94
4:D:82:LYS:HE2	4:D:95:LEU:CB	1.95	0.94
1:A:647:LEU:CD1	16:A:801:CL0:C9	2.43	0.94
4:D:82:LYS:HZ1	4:D:95:LEU:CA	1.80	0.93
1:A:642:TRP:CE3	16:A:801:CL0:C14	2.48	0.92
4:D:81:TYR:CE2	4:D:96:HIS:CD2	2.58	0.92
2:B:5:PHE:CG	2:B:6:PRO:HD3	2.04	0.92
2:B:5:PHE:O	2:B:7:LYS:N	2.03	0.91
4:D:82:LYS:NZ	4:D:95:LEU:CA	2.28	0.91
4:D:62:LYS:CE	4:D:95:LEU:CD1	2.49	0.90
1:A:647:LEU:HD11	16:A:801:CL0:H47	1.53	0.89
1:A:596:TYR:CZ	16:A:801:CL0:H29	2.07	0.89
4:D:82:LYS:NZ	4:D:95:LEU:N	2.04	0.89
4:D:82:LYS:HE3	4:D:96:HIS:N	1.88	0.88
4:D:82:LYS:HE2	4:D:95:LEU:HB2	1.54	0.88
4:D:96:HIS:CG	4:D:97:PRO:HD3	2.10	0.87
4:D:81:TYR:CE2	4:D:96:HIS:HD2	1.94	0.86
4:D:98:LYS:O	4:D:98:LYS:NZ	2.10	0.85
4:D:62:LYS:CE	4:D:95:LEU:HD12	2.07	0.84
4:D:82:LYS:HZ3	4:D:95:LEU:HB2	1.05	0.84
1:A:642:TRP:NE1	16:A:801:CL0:C12	2.39	0.84
4:D:82:LYS:CD	4:D:95:LEU:O	2.25	0.83
4:D:82:LYS:HG2	4:D:95:LEU:O	1.79	0.81
1:A:596:TYR:OH	16:A:801:CL0:CED	2.28	0.81
4:D:82:LYS:HD3	4:D:96:HIS:HB3	1.62	0.81
4:D:82:LYS:HZ1	4:D:95:LEU:H	0.87	0.81
4:D:82:LYS:HD3	4:D:96:HIS:CB	2.11	0.81
2:B:5:PHE:O	2:B:7:LYS:HG2	1.80	0.80
1:A:735:THR:OG1	16:A:801:CL0:H28	1.80	0.80
14:2:95:ASP:O	14:2:99:GLN:HB2	1.81	0.80
8:J:24:ILE:O	8:J:28:LEU:HB2	1.82	0.79
4:D:96:HIS:CG	4:D:97:PRO:CD	2.66	0.79
1:A:642:TRP:CG	16:A:801:CL0:H56	2.14	0.79
1:A:642:TRP:CD1	16:A:801:CL0:H51	2.17	0.79
1:A:647:LEU:HD22	16:A:801:CL0:H26	1.64	0.79
14:5:95:ASP:O	14:5:99:GLN:HB2	1.81	0.79
13:4:47:GLY:O	13:4:51:MET:HB2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:42:PHE:HB2	20:K:101:BCR:H24C	1.64	0.78
4:D:62:LYS:HE3	4:D:95:LEU:HD13	1.65	0.77
13:1:47:GLY:O	13:1:51:MET:HB2	1.84	0.77
1:A:191:GLU:O	1:A:195:ASN:HB2	1.83	0.77
2:B:6:PRO:C	2:B:8:PHE:N	2.20	0.77
16:A:801:CL0:H42	17:B:806:CLA:HBB2	1.64	0.77
2:B:149:LEU:O	2:B:153:LEU:HB2	1.85	0.76
4:D:82:LYS:CE	4:D:95:LEU:N	2.48	0.75
4:D:81:TYR:HE2	4:D:96:HIS:CD2	2.05	0.74
4:D:97:PRO:O	4:D:99:ASP:N	2.21	0.74
4:D:62:LYS:NZ	4:D:95:LEU:HD13	2.03	0.73
1:A:393:ILE:HD13	17:A:827:CLA:HHC	1.70	0.73
4:D:82:LYS:HZ1	4:D:95:LEU:CB	1.80	0.73
4:D:96:HIS:CD2	4:D:97:PRO:HD3	2.22	0.72
4:D:62:LYS:CE	4:D:95:LEU:HD13	2.17	0.72
4:D:82:LYS:CG	4:D:95:LEU:O	2.38	0.72
4:D:82:LYS:HD3	4:D:97:PRO:HD2	1.71	0.71
16:A:801:CL0:H13	17:B:804:CLA:OBD	1.90	0.71
4:D:82:LYS:CD	4:D:95:LEU:C	2.58	0.71
13:1:147:MET:O	13:1:150:PHE:HB3	1.91	0.71
13:4:147:MET:O	13:4:150:PHE:HB3	1.91	0.71
16:A:801:CL0:H46	17:B:806:CLA:CBB	2.21	0.70
17:B:842:CLA:HBB1	20:B:850:BCR:H363	1.72	0.70
25:1:615:ZEX:H34	17:2:605:CLA:HBC3	1.73	0.70
17:B:831:CLA:H52	20:B:846:BCR:H23C	1.74	0.70
4:D:82:LYS:CE	4:D:95:LEU:O	2.25	0.69
4:D:82:LYS:CE	4:D:96:HIS:N	2.53	0.69
17:A:802:CLA:HMA2	17:A:809:CLA:HMD2	1.73	0.69
2:B:521:ILE:HG21	17:B:838:CLA:HAB	1.76	0.68
1:A:642:TRP:CD1	16:A:801:CL0:C11	2.77	0.68
17:O:204:CLA:HED2	17:O:204:CLA:H2A	1.74	0.68
17:3:204:CLA:HAC1	17:3:207:CLA:HAB	1.75	0.68
17:F:302:CLA:HAB	8:J:25:LEU:HD11	1.74	0.68
2:B:545:MET:SD	3:C:66:ARG:NH2	2.67	0.68
2:B:654:VAL:HG22	17:B:842:CLA:HMB3	1.76	0.68
2:B:530:LEU:O	2:B:534:LYS:HB2	1.94	0.67
1:A:642:TRP:CZ2	16:A:801:CL0:H56	2.25	0.67
4:D:27:LYS:O	4:D:86:ILE:HB	1.94	0.67
1:A:729:LEU:O	1:A:733:ILE:HB	1.95	0.67
17:A:831:CLA:HMC2	17:L:204:CLA:HBB2	1.76	0.67
14:2:177:HIS:HE1	25:2:617:ZEX:H14	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:TRP:CD1	16:A:801:CL0:C12	2.78	0.67
1:A:642:TRP:CG	16:A:801:CL0:C14	2.76	0.67
17:B:843:CLA:H2A	17:B:843:CLA:HED2	1.77	0.67
2:B:615:MET:O	2:B:619:ARG:HB3	1.95	0.66
14:2:93:SER:O	14:2:97:HIS:HB3	1.96	0.66
2:B:491:TRP:HE1	17:B:836:CLA:HED1	1.61	0.66
1:A:384:LEU:HD22	1:A:744:ILE:HD12	1.78	0.65
2:B:374:GLN:HE21	2:B:588:VAL:HG11	1.61	0.65
4:D:82:LYS:HE3	4:D:95:LEU:N	2.08	0.65
8:J:23:GLY:HA3	17:J:103:CLA:HAB	1.77	0.65
17:F:301:CLA:H2	8:J:13:VAL:HG12	1.78	0.65
15:3:113:PRO:O	15:3:117:GLN:HB2	1.97	0.65
14:5:93:SER:O	14:5:97:HIS:HB3	1.96	0.65
1:A:45:ILE:O	1:A:48:LEU:HB3	1.97	0.65
16:A:801:CL0:H42	17:B:806:CLA:CBB	2.27	0.65
1:A:398:ILE:O	1:A:401:ALA:HB3	1.98	0.64
1:A:54:ASP:HB3	1:A:57:SER:HB3	1.80	0.64
1:A:349:LEU:HD11	17:A:828:CLA:HBB1	1.80	0.64
4:D:99:ASP:O	4:D:101:VAL:CG2	2.41	0.64
13:4:155:HIS:HB3	17:4:611:CLA:HMD3	1.80	0.64
1:A:483:ILE:O	1:A:487:HIS:ND1	2.30	0.64
2:B:46:ILE:O	2:B:50:HIS:ND1	2.29	0.64
17:B:809:CLA:H162	17:B:831:CLA:HBB2	1.80	0.64
4:D:43:PRO:HD3	4:D:68:LEU:HD12	1.80	0.64
13:1:133:LYS:HG3	13:1:135:MET:H	1.62	0.64
1:A:112:GLN:NE2	17:A:807:CLA:OBD	2.31	0.64
17:A:806:CLA:HMC2	17:A:826:CLA:H121	1.80	0.63
17:3:203:CLA:HAB	25:3:215:ZEX:H12	1.80	0.63
13:4:133:LYS:HG3	13:4:135:MET:H	1.63	0.63
17:J:102:CLA:H2A	17:J:102:CLA:HED2	1.80	0.63
16:A:801:CL0:C7	17:B:806:CLA:HBB2	2.27	0.63
2:B:582:LEU:HD11	2:B:712:THR:HG22	1.80	0.63
20:A:846:BCR:H21C	17:B:801:CLA:H93	1.80	0.63
17:5:603:CLA:HMC2	25:5:615:ZEX:H403	1.80	0.63
17:A:831:CLA:H143	17:B:842:CLA:H2	1.80	0.62
2:B:235:PRO:HB3	2:B:254:THR:HG21	1.81	0.62
1:A:327:GLY:HA3	19:A:842:LHG:HC32	1.81	0.62
14:2:95:ASP:O	14:2:99:GLN:CB	2.46	0.62
2:B:179:GLY:HA3	17:B:816:CLA:HBB1	1.81	0.62
3:C:64:SER:OG	21:C:102:SF4:S3	2.57	0.62
1:A:488:THR:HG22	1:A:507:GLY:HA2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:89:LEU:HB3	20:L:205:BCR:H401	1.81	0.62
14:5:95:ASP:O	14:5:99:GLN:CB	2.46	0.62
1:A:452:TYR:HE2	1:A:534:ILE:HD11	1.64	0.62
1:A:576:ARG:NH1	4:D:63:GLU:OE1	2.33	0.62
1:A:168:LEU:O	1:A:172:ALA:HB2	2.00	0.61
15:3:113:PRO:O	15:3:117:GLN:CB	2.48	0.61
17:A:839:CLA:H151	20:L:201:BCR:H15C	1.81	0.61
20:B:805:BCR:H12C	17:F:302:CLA:HBB1	1.81	0.61
15:3:54:LYS:NZ	15:3:107:GLU:OE2	2.33	0.61
17:5:606:CLA:HBB2	25:5:617:ZEX:H193	1.82	0.61
1:A:449:PHE:CD1	16:A:801:CL0:H69	2.36	0.61
14:2:63:CYS:HB2	14:2:165:GLY:HA3	1.82	0.61
1:A:174:TRP:HB2	17:A:809:CLA:HMC3	1.82	0.61
4:D:96:HIS:HB3	4:D:97:PRO:HD2	0.68	0.61
17:4:601:CLA:HED3	17:4:609:CLA:HAB	1.81	0.61
1:A:395:GLY:HA3	1:A:599:LEU:HD11	1.82	0.61
1:A:642:TRP:CE3	16:A:801:CL0:H55	2.34	0.61
1:A:642:TRP:HE1	16:A:801:CL0:H48	1.65	0.61
17:A:848:CLA:H152	20:B:850:BCR:H16C	1.81	0.61
2:B:545:MET:HG2	2:B:547:ASP:H	1.65	0.61
2:B:221:GLN:HG2	2:B:222:PRO:HD3	1.83	0.60
14:5:63:CYS:HB2	14:5:165:GLY:HA3	1.82	0.60
3:C:24:ASP:O	3:C:44:ARG:NH2	2.34	0.60
17:A:807:CLA:H111	20:J:104:BCR:H332	1.82	0.60
2:B:140:LEU:HD21	20:B:847:BCR:H24C	1.82	0.60
17:B:802:CLA:H193	17:B:812:CLA:H2	1.83	0.60
1:A:392:TRP:CD1	17:A:826:CLA:HAB	2.37	0.60
1:A:596:TYR:CZ	16:A:801:CL0:CED	2.81	0.60
2:B:544:LEU:O	2:B:562:ARG:NH1	2.35	0.60
2:B:652:HIS:HB3	17:B:802:CLA:HBD	1.83	0.60
17:2:610:CLA:HMC3	25:2:614:ZEX:H402	1.83	0.60
17:5:603:CLA:HBC1	17:5:606:CLA:HMC2	1.83	0.60
1:A:11:VAL:HG11	17:A:808:CLA:HAA2	1.83	0.60
4:D:82:LYS:HE2	4:D:95:LEU:HB3	1.83	0.60
2:B:289:TYR:HA	2:B:297:HIS:H	1.66	0.60
1:A:578:GLY:O	2:B:666:ARG:NH2	2.32	0.60
15:3:167:HIS:HB3	17:3:212:CLA:HMD3	1.83	0.60
25:4:617:ZEX:H8	17:5:605:CLA:HAA2	1.84	0.59
14:5:19:PRO:HG3	14:5:25:LYS:HA	1.83	0.59
17:B:825:CLA:HAB	17:B:843:CLA:HED1	1.84	0.59
14:5:21:MET:HB3	14:5:23:PHE:HD2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:64:ARG:NH1	14:2:161:GLU:OE2	2.36	0.59
14:2:19:PRO:HG3	14:2:25:LYS:HA	1.83	0.59
17:A:805:CLA:HMC3	17:A:806:CLA:HHB	1.84	0.59
17:A:836:CLA:H191	17:L:203:CLA:H92	1.84	0.59
8:J:27:GLU:OE1	8:J:30:ARG:NH2	2.35	0.59
1:A:642:TRP:CE2	16:A:801:CL0:C12	2.80	0.59
4:D:123:ASN:OD1	4:D:139:ARG:NH1	2.36	0.59
1:A:200:GLY:HA3	17:A:811:CLA:HBB1	1.85	0.58
14:5:89:LYS:HD2	14:5:92:LEU:HB2	1.85	0.58
17:A:805:CLA:H142	17:A:805:CLA:H61	1.84	0.58
2:B:529:THR:O	2:B:533:VAL:HB	2.03	0.58
2:B:689:ILE:HD11	20:L:205:BCR:H382	1.84	0.58
4:D:98:LYS:HZ1	4:D:98:LYS:C	2.04	0.58
1:A:213:GLN:NE2	17:A:817:CLA:O1D	2.36	0.58
16:A:801:CL0:CMB	17:B:804:CLA:HMD1	2.34	0.58
15:3:141:GLU:HG3	15:3:143:SER:H	1.68	0.58
1:A:79:ILE:HG21	17:A:804:CLA:HMD2	1.83	0.58
1:A:142:GLN:NE2	1:A:379:ASP:OD2	2.37	0.58
17:B:835:CLA:H201	17:B:839:CLA:H111	1.85	0.58
14:2:21:MET:HB3	14:2:23:PHE:HD2	1.67	0.58
1:A:319:LYS:NZ	1:A:339:GLU:OE2	2.37	0.58
1:A:452:TYR:O	1:A:456:ASP:HB2	2.03	0.58
5:E:2:ILE:N	5:E:60:GLU:OE2	2.36	0.58
14:5:106:LEU:HB2	17:5:606:CLA:HMD3	1.86	0.58
1:A:669:PHE:O	1:A:673:HIS:ND1	2.29	0.57
13:4:141:ASN:ND2	17:4:609:CLA:O1D	2.37	0.57
1:A:456:ASP:OD1	2:B:633:TYR:OH	2.16	0.57
17:B:810:CLA:HAA1	7:I:11:VAL:HG22	1.86	0.57
14:2:89:LYS:HD2	14:2:92:LEU:HB2	1.85	0.57
1:A:671:GLY:O	1:A:674:PHE:HB3	2.04	0.57
17:A:819:CLA:HMB2	17:A:823:CLA:HMA3	1.87	0.57
17:A:824:CLA:HAB	20:A:845:BCR:HC7	1.84	0.57
19:A:841:LHG:H161	17:J:101:CLA:HMB2	1.86	0.57
17:1:606:CLA:HBB1	25:1:617:ZEX:H162	1.86	0.57
13:1:29:ARG:HH12	14:2:126:ILE:HG21	1.69	0.57
17:B:824:CLA:HMD2	20:B:845:BCR:HC7	1.87	0.57
14:5:64:ARG:NH1	14:5:161:GLU:OE2	2.36	0.57
17:A:831:CLA:H201	23:B:851:DGD:HA91	1.87	0.57
17:B:839:CLA:H152	20:F:304:BCR:H24C	1.85	0.57
17:2:601:CLA:HMC1	15:3:130:GLY:HA2	1.87	0.57
1:A:63:GLU:HG2	1:A:184:LEU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLN:HB2	17:A:803:CLA:HMB2	1.87	0.57
1:A:261:PHE:HA	17:K:103:CLA:HBC3	1.87	0.57
1:A:713:ARG:NH2	5:E:43:VAL:O	2.38	0.57
14:5:113:VAL:HG11	17:5:607:CLA:HBC2	1.86	0.57
17:B:822:CLA:H71	17:B:827:CLA:H122	1.87	0.56
4:D:21:CYS:SG	4:D:22:ALA:N	2.77	0.56
17:2:601:CLA:HMA1	25:2:617:ZEX:H221	1.86	0.56
15:3:70:GLN:NE2	15:3:82:THR:O	2.38	0.56
20:A:843:BCR:H383	20:K:101:BCR:H10C	1.86	0.56
2:B:314:GLY:HA2	2:B:408:ARG:HH21	1.70	0.56
7:I:31:GLU:HG3	10:L:99:VAL:HG13	1.86	0.56
9:K:8:THR:HG23	9:K:10:PRO:HD2	1.87	0.56
13:4:45:LYS:HE3	25:4:615:ZEX:H21	1.87	0.56
1:A:366:HIS:ND1	17:A:816:CLA:OBD	2.38	0.56
17:A:829:CLA:HBB2	17:A:837:CLA:HHC	1.87	0.56
2:B:653:LEU:HG	17:B:842:CLA:HAB	1.87	0.56
13:4:153:ILE:HD11	25:4:612:ZEX:H7	1.88	0.56
14:5:55:LEU:HB3	17:5:602:CLA:HHB	1.87	0.56
1:A:355:MET:HG3	17:A:823:CLA:HHB	1.87	0.56
1:A:439:TRP:NE1	17:A:831:CLA:OBD	2.32	0.56
1:A:592:LEU:HD21	17:A:828:CLA:HBC1	1.86	0.56
17:4:611:CLA:HBC2	25:4:614:ZEX:H31	1.86	0.56
12:O:109:PHE:HE1	17:O:204:CLA:HAC2	1.70	0.56
17:B:826:CLA:HBA1	20:B:848:BCR:H16C	1.86	0.56
3:C:27:GLU:OE2	3:C:44:ARG:NH2	2.37	0.56
17:A:817:CLA:HAB	17:A:817:CLA:H8	1.88	0.56
17:A:834:CLA:HAC2	12:O:66:VAL:HG11	1.87	0.56
2:B:461:ILE:HD13	17:B:836:CLA:HAB	1.88	0.56
14:2:25:LYS:NZ	15:3:123:GLY:O	2.38	0.56
15:3:78:LYS:HG3	17:3:205:CLA:HED2	1.87	0.56
1:A:536:ALA:HB1	17:A:836:CLA:HMB3	1.87	0.56
17:B:802:CLA:H201	17:B:812:CLA:H3A	1.88	0.56
14:5:68:LEU:HB3	17:5:604:CLA:HBB2	1.87	0.56
1:A:642:TRP:CD1	16:A:801:CL0:C13	2.89	0.56
2:B:5:PHE:HB2	2:B:20:ARG:NH2	2.21	0.55
15:3:142:ALA:O	15:3:146:ARG:N	2.39	0.55
1:A:391:MET:O	1:A:395:GLY:N	2.39	0.55
1:A:431:ASP:OD2	1:A:557:ARG:NH2	2.38	0.55
17:A:806:CLA:H2	17:A:826:CLA:H52	1.89	0.55
1:A:351:ILE:HG12	20:O:202:BCR:H371	1.89	0.55
1:A:642:TRP:CG	16:A:801:CL0:C13	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:85:ARG:HB2	4:D:93:GLN:HB2	1.89	0.55
14:2:170:ILE:HG21	25:3:201:ZEX:H32	1.88	0.55
1:A:670:LEU:HD11	2:B:615:MET:HB2	1.88	0.55
2:B:196:ALA:HB1	2:B:268:LEU:HD13	1.89	0.55
17:B:829:CLA:H191	17:B:843:CLA:H152	1.89	0.55
14:2:78:PHE:CD1	17:2:613:CLA:H3A	2.42	0.55
1:A:733:ILE:HG21	17:A:826:CLA:HMC2	1.89	0.54
2:B:351:TYR:O	2:B:505:SER:OG	2.26	0.54
4:D:98:LYS:CE	4:D:98:LYS:CA	2.85	0.54
9:K:35:GLN:O	9:K:39:SER:HB3	2.07	0.54
13:4:148:LEU:HD13	25:4:614:ZEX:H12	1.89	0.54
14:5:35:PRO:HD2	14:5:56:ARG:HH12	1.73	0.54
8:J:25:LEU:HD12	20:J:104:BCR:H371	1.89	0.54
14:5:163:ARG:NH1	17:5:609:CLA:O1D	2.41	0.54
17:A:838:CLA:H203	17:J:101:CLA:H152	1.90	0.54
2:B:120:HIS:NE2	2:B:362:ASP:OD2	2.39	0.54
4:D:30:MET:HA	4:D:83:ILE:HA	1.90	0.54
15:3:58:ILE:O	15:3:62:ALA:HB3	2.07	0.54
2:B:543:LYS:HG3	6:F:181:THR:HG22	1.89	0.54
17:A:815:CLA:C1D	17:A:816:CLA:HBB2	2.37	0.54
17:A:828:CLA:H172	20:A:846:BCR:H342	1.89	0.54
9:K:20:GLY:O	9:K:39:SER:OG	2.26	0.54
14:5:97:HIS:HB2	25:5:617:ZEX:H171	1.89	0.54
1:A:572:ASP:OD2	1:A:576:ARG:NH2	2.41	0.54
12:O:100:TYR:HA	12:O:103:VAL:HG12	1.89	0.54
17:1:606:CLA:HMB3	25:1:617:ZEX:H41	1.90	0.54
14:2:35:PRO:HD2	14:2:56:ARG:HH12	1.73	0.54
17:A:848:CLA:CGA	17:A:848:CLA:H3A	2.38	0.54
2:B:590:PHE:HD1	2:B:621:TYR:HE2	1.56	0.54
17:B:841:CLA:HAB	18:B:844:PQN:H151	1.89	0.54
13:1:45:LYS:NZ	13:1:99:GLU:OE2	2.41	0.54
15:3:112:VAL:HG13	15:3:116:ILE:HD12	1.89	0.54
17:5:603:CLA:HMA3	17:5:603:CLA:H71	1.90	0.54
1:A:596:TYR:CE2	16:A:801:CL0:H29	2.42	0.54
2:B:724:ILE:O	2:B:728:ALA:HB3	2.08	0.54
17:B:842:CLA:H171	20:L:205:BCR:H351	1.90	0.54
2:B:436:VAL:HG22	17:B:804:CLA:H12	1.90	0.54
2:B:615:MET:O	2:B:619:ARG:CB	2.56	0.54
2:B:716:ILE:HD13	17:B:830:CLA:HMC2	1.89	0.54
13:1:127:LEU:HD12	25:1:613:ZEX:H382	1.90	0.54
14:2:169:MET:HB3	25:2:615:ZEX:H403	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:110:ALA:HB2	20:O:202:BCR:HC22	1.89	0.53
14:2:57:GLU:OE2	14:2:61:LYS:NZ	2.40	0.53
4:D:94:TYR:CE2	4:D:97:PRO:HB2	2.43	0.53
17:3:204:CLA:HMC1	17:3:207:CLA:HAB	1.91	0.53
17:B:816:CLA:H151	17:B:831:CLA:HMD2	1.90	0.53
7:I:19:PRO:HG3	20:I:101:BCR:H14C	1.91	0.53
14:5:57:GLU:OE2	14:5:61:LYS:NZ	2.40	0.53
1:A:432:ALA:O	1:A:436:HIS:ND1	2.36	0.53
1:A:642:TRP:CG	16:A:801:CL0:H54	2.44	0.53
18:A:840:PQN:H301	17:J:101:CLA:H52	1.90	0.53
2:B:66:PHE:HZ	11:M:7:VAL:HG13	1.73	0.53
15:3:45:ILE:O	15:3:49:ARG:HB2	2.09	0.53
1:A:275:LYS:HG2	1:A:499:LEU:HD12	1.90	0.53
1:A:295:LEU:HD11	17:A:813:CLA:HMC1	1.91	0.53
1:A:557:ARG:HD2	2:B:674:GLU:HB3	1.90	0.53
2:B:385:PHE:HZ	17:B:828:CLA:HAB	1.71	0.53
17:4:606:CLA:HBC2	25:4:613:ZEX:H172	1.90	0.53
1:A:88:TYR:HE2	20:A:843:BCR:HC42	1.74	0.53
2:B:290:ARG:HE	2:B:294:GLY:HA2	1.74	0.53
2:B:517:VAL:HG11	2:B:591:TYR:CG	2.44	0.53
10:L:28:ARG:O	10:L:32:SER:HB3	2.09	0.53
1:A:449:PHE:HD1	16:A:801:CL0:H69	1.73	0.52
2:B:172:ARG:HG3	17:B:816:CLA:HBC2	1.91	0.52
6:F:158:PHE:CZ	17:1:607:CLA:H3A	2.44	0.52
17:A:809:CLA:H102	17:J:101:CLA:HBB2	1.92	0.52
17:B:817:CLA:HMA1	20:B:847:BCR:H402	1.90	0.52
1:A:437:LEU:HD11	1:A:547:LEU:HD12	1.91	0.52
17:B:821:CLA:HMD2	17:B:831:CLA:H71	1.91	0.52
17:2:608:CLA:HHC	25:2:614:ZEX:H12	1.92	0.52
15:3:61:LEU:HD23	17:3:205:CLA:HHC	1.91	0.52
13:4:45:LYS:NZ	13:4:99:GLU:OE2	2.41	0.52
3:C:8:TYR:HE2	4:D:120:ILE:HG13	1.74	0.52
13:1:45:LYS:HE3	25:1:616:ZEX:H21	1.92	0.52
1:A:437:LEU:HD13	1:A:544:LEU:HA	1.92	0.52
10:L:121:PHE:O	10:L:125:ALA:CB	2.57	0.52
1:A:659:GLY:HA2	2:B:445:GLY:HA2	1.91	0.52
17:B:831:CLA:H201	17:5:603:CLA:H143	1.90	0.52
1:A:13:VAL:HA	1:A:182:PRO:HA	1.92	0.52
7:I:25:ILE:O	7:I:29:ALA:HB2	2.10	0.52
8:J:15:THR:O	8:J:19:PHE:CB	2.57	0.52
10:L:127:GLY:HA3	20:L:206:BCR:H312	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:43:PRO:HD2	25:2:615:ZEX:H23	1.92	0.52
1:A:28:PRO:HG3	6:F:143:ILE:HG21	1.92	0.52
17:A:803:CLA:H41	17:A:827:CLA:H152	1.91	0.52
20:A:846:BCR:H403	20:A:846:BCR:H371	1.92	0.52
2:B:190:GLY:HA3	17:B:818:CLA:HAB	1.92	0.52
13:4:167:GLN:HG2	17:4:611:CLA:H2A	1.92	0.52
1:A:216:VAL:HG13	1:A:236:PRO:HB3	1.92	0.52
2:B:475:LEU:O	2:B:481:SER:OG	2.26	0.52
12:O:58:ALA:HB1	12:O:72:LEU:HB2	1.92	0.52
13:4:145:LEU:HD13	17:4:609:CLA:HBC1	1.91	0.52
1:A:406:ALA:HB1	1:A:584:ALA:HB1	1.92	0.52
17:A:831:CLA:H151	18:B:844:PQN:H193	1.91	0.52
17:A:839:CLA:H171	17:L:203:CLA:HMC3	1.92	0.52
2:B:5:PHE:HE2	2:B:21:ILE:HA	1.75	0.52
14:5:148:THR:HB	14:5:153:GLN:HB3	1.91	0.52
16:A:801:CL0:H18	17:B:806:CLA:C4C	2.40	0.51
17:A:804:CLA:HMA2	17:A:804:CLA:H2	1.91	0.51
17:B:803:CLA:H43	17:B:835:CLA:HED1	1.92	0.51
17:B:808:CLA:H43	17:B:809:CLA:HBB1	1.92	0.51
7:I:10:LEU:HA	7:I:13:THR:HG22	1.92	0.51
14:2:81:PHE:HZ	14:2:87:LYS:HB3	1.75	0.51
14:2:109:ILE:HD12	17:2:605:CLA:H3A	1.92	0.51
4:D:82:LYS:NZ	4:D:83:ILE:O	2.35	0.51
1:A:455:ASN:OD1	1:A:468:PHE:N	2.43	0.51
14:2:148:THR:HB	14:2:153:GLN:HB3	1.91	0.51
15:3:45:ILE:O	15:3:49:ARG:CB	2.58	0.51
1:A:337:LEU:HD23	1:A:340:ILE:HD12	1.91	0.51
17:3:206:CLA:H2A	17:3:206:CLA:HED2	1.91	0.51
2:B:4:LYS:NZ	2:B:4:LYS:CB	2.73	0.51
2:B:705:LEU:HD11	23:B:851:DGD:HB82	1.93	0.51
2:B:4:LYS:NZ	2:B:4:LYS:HB2	2.26	0.51
15:3:172:SER:OG	17:3:212:CLA:O1D	2.28	0.51
17:2:607:CLA:HBC3	25:2:616:ZEX:H381	1.92	0.51
1:A:192:SER:O	1:A:196:HIS:ND1	2.27	0.51
1:A:478:VAL:H	17:A:836:CLA:HMD1	1.76	0.51
17:A:822:CLA:HAC1	20:O:202:BCR:H23C	1.92	0.51
2:B:398:PRO:HG3	2:B:540:ARG:HH12	1.76	0.51
1:A:469:SER:H	1:A:472:ALA:HB3	1.75	0.51
17:A:838:CLA:H202	8:J:18:LEU:HD22	1.93	0.51
8:J:25:LEU:HD13	20:J:104:BCR:H402	1.92	0.51
14:5:153:GLN:HA	14:5:156:ARG:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ALA:HB3	17:B:801:CLA:HBB2	1.92	0.50
17:A:835:CLA:H3A	17:A:836:CLA:HAA2	1.93	0.50
17:B:841:CLA:HED3	7:I:27:PHE:HZ	1.76	0.50
14:5:177:HIS:HE1	25:5:617:ZEX:H35	1.75	0.50
1:A:325:HIS:O	19:A:842:LHG:O1	2.28	0.50
4:D:82:LYS:HD3	4:D:96:HIS:HB2	1.92	0.50
2:B:303:LEU:HD12	2:B:321:TYR:HB2	1.94	0.50
2:B:436:VAL:HG12	17:J:102:CLA:HAC1	1.92	0.50
3:C:17:CYS:SG	3:C:18:VAL:N	2.85	0.50
1:A:296:ALA:HA	17:A:815:CLA:HMC3	1.94	0.50
20:K:104:BCR:H371	20:K:104:BCR:H403	1.94	0.50
17:1:602:CLA:H72	25:1:614:ZEX:H28	1.92	0.50
17:5:608:CLA:HBB2	25:5:614:ZEX:H14	1.92	0.50
17:B:839:CLA:H92	20:F:304:BCR:H19C	1.94	0.50
4:D:85:ARG:HD2	4:D:95:LEU:HD11	1.93	0.50
1:A:293:HIS:CE1	1:A:297:ILE:HD11	2.47	0.50
1:A:473:ILE:HG12	10:L:69:ARG:HH12	1.76	0.50
17:A:804:CLA:HBD	17:A:804:CLA:HBA2	1.94	0.50
4:D:73:ARG:NH1	4:D:81:TYR:OH	2.41	0.50
10:L:36:ILE:O	10:L:46:ARG:NH1	2.45	0.50
15:3:50:GLU:O	15:3:54:LYS:HB2	2.11	0.50
17:3:209:CLA:HAB	25:3:214:ZEX:H12	1.93	0.50
13:4:28:LEU:HD21	14:5:119:ILE:HG12	1.93	0.50
13:4:48:ARG:HD2	17:4:608:CLA:C4C	2.42	0.50
14:5:81:PHE:HZ	14:5:87:LYS:HB3	1.75	0.50
2:B:186:LEU:O	2:B:189:THR:OG1	2.24	0.50
17:B:811:CLA:H171	17:B:830:CLA:H161	1.93	0.50
17:2:602:CLA:H2A	17:2:602:CLA:HED2	1.93	0.50
17:3:209:CLA:H61	25:3:214:ZEX:H10	1.94	0.50
9:K:34:THR:O	9:K:38:ALA:HB3	2.12	0.50
17:A:831:CLA:H13	20:B:850:BCR:H17C	1.94	0.49
17:B:801:CLA:H152	17:B:804:CLA:H161	1.93	0.49
17:B:802:CLA:H143	17:B:813:CLA:HBC3	1.94	0.49
10:L:43:PRO:HA	10:L:46:ARG:HB3	1.94	0.49
13:1:51:MET:HG2	25:1:613:ZEX:H403	1.94	0.49
13:1:55:LEU:HD23	17:1:604:CLA:HMC1	1.93	0.49
16:A:801:CL0:H13	17:B:804:CLA:CAD	2.42	0.49
2:B:618:LEU:HD12	17:B:804:CLA:HED2	1.94	0.49
17:A:816:CLA:H93	17:A:816:CLA:HMC2	1.95	0.49
2:B:5:PHE:CE2	2:B:21:ILE:HA	2.47	0.49
20:B:805:BCR:HC41	17:J:102:CLA:HBA1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:50:ALA:HB2	25:1:614:ZEX:H202	1.94	0.49
14:2:24:LEU:HD11	15:3:114:ALA:HB2	1.94	0.49
17:A:810:CLA:HAB	17:A:818:CLA:C4C	2.43	0.49
17:A:838:CLA:H162	8:J:18:LEU:HD22	1.95	0.49
2:B:454:GLU:OE1	2:B:459:GLN:NE2	2.40	0.49
20:B:848:BCR:H24C	20:B:849:BCR:H402	1.93	0.49
14:2:153:GLN:HA	14:2:156:ARG:HG2	1.93	0.49
1:A:531:VAL:HA	1:A:534:ILE:HD12	1.95	0.49
1:A:642:TRP:NE1	16:A:801:CL0:C11	2.75	0.49
17:A:832:CLA:HAC2	17:B:812:CLA:HBB2	1.94	0.49
17:A:848:CLA:HBB2	2:B:656:ALA:HB3	1.95	0.49
3:C:7:ILE:HG12	3:C:65:ILE:HG12	1.94	0.49
20:L:206:BCR:H403	20:L:206:BCR:H371	1.94	0.49
14:2:55:LEU:HD22	17:2:602:CLA:H43	1.95	0.49
4:D:62:LYS:NZ	4:D:95:LEU:CD1	2.72	0.49
4:D:72:LEU:HB3	4:D:78:ILE:HG21	1.93	0.49
17:2:610:CLA:HBB2	25:2:614:ZEX:H393	1.94	0.49
1:A:359:LEU:HG	17:A:825:CLA:H41	1.94	0.49
2:B:2:ALA:N	2:B:7:LYS:HA	2.28	0.49
2:B:355:PRO:HG3	17:B:821:CLA:HBA1	1.95	0.49
2:B:695:PRO:O	3:C:81:TYR:OH	2.31	0.49
13:4:126:PRO:HD2	25:4:612:ZEX:H221	1.94	0.49
17:5:611:CLA:HMC1	25:5:617:ZEX:H30	1.94	0.49
1:A:650:GLN:OE1	1:A:743:ARG:NE	2.46	0.49
17:B:841:CLA:H112	17:B:842:CLA:H121	1.95	0.49
17:B:841:CLA:H201	17:B:842:CLA:H172	1.95	0.49
14:2:77:GLU:HA	14:2:87:LYS:HE3	1.95	0.49
10:L:57:PHE:CE2	17:L:203:CLA:HBB1	2.47	0.49
25:3:216:ZEX:H30	25:3:218:ZEX:H362	1.95	0.49
1:A:207:LEU:HD12	1:A:298:ALA:HB1	1.94	0.48
14:2:55:LEU:HD13	17:2:602:CLA:H12	1.94	0.48
15:3:108:ILE:HG13	15:3:109:VAL:HG13	1.95	0.48
1:A:373:TYR:OH	17:A:827:CLA:OBD	2.24	0.48
2:B:71:GLN:NE2	17:B:810:CLA:O1D	2.43	0.48
2:B:86:PRO:O	2:B:114:SER:N	2.43	0.48
2:B:219:GLY:HA3	17:B:818:CLA:HMD1	1.95	0.48
2:B:454:GLU:HG2	6:F:94:HIS:HB3	1.96	0.48
17:B:812:CLA:H151	17:B:842:CLA:H11	1.95	0.48
14:5:77:GLU:HA	14:5:87:LYS:HE3	1.95	0.48
1:A:554:ARG:HG3	1:A:563:ALA:HB2	1.94	0.48
2:B:374:GLN:HE22	17:B:828:CLA:HMD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:826:CLA:HAB	17:B:833:CLA:HMD2	1.95	0.48
15:3:60:MET:HB3	25:3:214:ZEX:H202	1.95	0.48
15:3:125:LEU:HD12	15:3:126:PRO:HD2	1.96	0.48
15:3:99:ILE:HD11	17:3:206:CLA:HMD3	1.95	0.48
1:A:730:LEU:HD13	17:A:838:CLA:HMA1	1.95	0.48
16:A:801:CL0:CMB	17:B:804:CLA:OBD	2.60	0.48
17:A:807:CLA:HMA1	8:J:26:ILE:HD13	1.95	0.48
17:A:839:CLA:H121	17:B:841:CLA:H102	1.94	0.48
17:B:811:CLA:H122	17:B:830:CLA:H93	1.96	0.48
13:1:154:ILE:HG21	25:1:617:ZEX:H8	1.95	0.48
2:B:19:ARG:NH1	3:C:77:MET:SD	2.69	0.48
9:K:44:HIS:HD2	20:K:104:BCR:HC8	1.79	0.48
13:4:15:LEU:HA	13:4:36:VAL:HG11	1.96	0.48
17:4:608:CLA:HBB2	25:4:612:ZEX:H34	1.96	0.48
14:5:91:GLN:HG3	25:5:617:ZEX:H8	1.93	0.48
1:A:686:GLY:HA3	2:B:566:CYS:HB2	1.95	0.48
2:B:685:LEU:HD21	10:L:34:LEU:HD13	1.95	0.48
2:B:175:HIS:CG	17:B:816:CLA:HMC2	2.48	0.48
14:2:148:THR:HG22	14:2:150:GLY:H	1.78	0.48
25:4:614:ZEX:H201	17:5:605:CLA:HMB1	1.96	0.48
14:5:148:THR:HG22	14:5:150:GLY:H	1.78	0.48
14:5:167:LEU:O	14:5:171:ALA:HB3	2.14	0.48
16:A:801:CL0:H53	16:A:801:CL0:H61	1.56	0.48
17:A:822:CLA:HMA1	17:O:201:CLA:HAB	1.95	0.48
2:B:271:MET:O	2:B:275:HIS:ND1	2.37	0.48
10:L:48:LEU:O	10:L:52:MET:HB2	2.14	0.48
12:O:119:TYR:HA	12:O:122:TYR:HD2	1.78	0.48
17:3:206:CLA:HAA2	25:3:217:ZEX:H25	1.95	0.48
20:B:805:BCR:H323	17:B:835:CLA:HBB1	1.96	0.47
17:B:820:CLA:HBA1	17:B:820:CLA:H3A	1.74	0.47
4:D:33:SER:OG	4:D:54:ASP:OD1	2.31	0.47
7:I:25:ILE:O	7:I:29:ALA:CB	2.62	0.47
20:I:101:BCR:H372	20:L:201:BCR:H403	1.96	0.47
14:2:58:ALA:O	14:2:62:HIS:ND1	2.36	0.47
17:5:603:CLA:HMA2	17:5:603:CLA:H11	1.96	0.47
17:B:816:CLA:H203	17:B:831:CLA:H2	1.95	0.47
17:L:202:CLA:H3A	17:L:202:CLA:HBA2	1.53	0.47
13:4:100:PHE:HD1	13:4:106:LYS:HE2	1.79	0.47
1:A:359:LEU:HD22	17:A:817:CLA:H72	1.96	0.47
1:A:642:TRP:CZ2	16:A:801:CL0:C14	2.94	0.47
17:A:828:CLA:H121	19:A:841:LHG:H372	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:836:CLA:H11	17:A:837:CLA:HMD1	1.96	0.47
2:B:255:PHE:HZ	17:B:820:CLA:H2	1.79	0.47
14:2:67:MET:HB3	25:2:614:ZEX:H202	1.95	0.47
17:3:212:CLA:H3A	17:3:212:CLA:HBA2	1.54	0.47
17:5:612:CLA:HBC3	25:5:617:ZEX:H183	1.97	0.47
1:A:640:ASN:O	1:A:644:ARG:HB3	2.14	0.47
17:A:826:CLA:H3A	17:A:826:CLA:HBA2	1.58	0.47
17:A:831:CLA:HAB	17:A:832:CLA:HBB	1.95	0.47
17:B:837:CLA:H3A	17:B:837:CLA:HBA2	1.47	0.47
17:1:606:CLA:HBB2	25:1:614:ZEX:H192	1.95	0.47
1:A:40:LYS:HD2	6:F:139:THR:HG21	1.96	0.47
1:A:536:ALA:HB2	17:A:836:CLA:HMA1	1.95	0.47
13:1:15:LEU:HA	13:1:36:VAL:HG11	1.96	0.47
15:3:14:PRO:HD3	15:3:21:ALA:HA	1.96	0.47
17:4:607:CLA:H3A	17:4:607:CLA:HBA2	1.30	0.47
1:A:9:VAL:HG21	1:A:310:THR:HB	1.97	0.47
1:A:312:TRP:HB3	9:K:34:THR:HG21	1.96	0.47
1:A:576:ARG:O	2:B:666:ARG:NH2	2.44	0.47
17:A:831:CLA:H51	17:B:841:CLA:H71	1.97	0.47
2:B:184:SER:O	2:B:188:TRP:N	2.47	0.47
14:2:167:LEU:O	14:2:171:ALA:HB3	2.14	0.47
1:A:31:PHE:HB2	1:A:58:HIS:CD2	2.50	0.47
1:A:676:TRP:CG	16:A:801:CL0:H5	2.50	0.47
17:A:804:CLA:H101	17:A:804:CLA:H13	1.68	0.47
17:A:825:CLA:H143	17:A:833:CLA:H121	1.96	0.47
2:B:26:ALA:HA	17:B:832:CLA:H43	1.96	0.47
2:B:134:TYR:OH	11:M:2:ILE:N	2.40	0.47
2:B:191:HIS:O	2:B:195:VAL:N	2.45	0.47
17:B:841:CLA:H152	17:B:842:CLA:H91	1.97	0.47
4:D:85:ARG:HG3	4:D:95:LEU:HG	1.96	0.47
20:K:104:BCR:H342	20:K:104:BCR:H331	1.96	0.47
20:L:201:BCR:H331	20:L:201:BCR:H343	1.96	0.47
13:1:82:PHE:HA	13:1:85:SER:HB3	1.97	0.47
17:1:611:CLA:H3A	17:1:611:CLA:HBA2	1.46	0.47
26:3:219:1DO:H5C2	26:3:219:1DO:H2C1	1.73	0.47
1:A:294:HIS:HA	1:A:297:ILE:HD12	1.97	0.47
1:A:332:GLU:HB3	1:A:421:ASN:HA	1.97	0.47
2:B:660:MET:O	2:B:664:SER:OG	2.32	0.47
17:B:809:CLA:H191	23:B:851:DGD:HAG3	1.96	0.47
17:3:203:CLA:HBB2	25:3:215:ZEX:H14	1.96	0.47
1:A:392:TRP:HB3	17:A:826:CLA:HMC3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:834:CLA:HHC	17:A:834:CLA:HBB1	1.97	0.47
3:C:29:VAL:HG11	4:D:112:GLN:HB2	1.95	0.47
4:D:24:THR:HG23	4:D:25:GLU:HG2	1.96	0.47
25:5:614:ZEX:H25	25:5:614:ZEX:H28	1.69	0.47
2:B:307:ARG:HE	2:B:315:LYS:HA	1.80	0.47
17:B:816:CLA:H111	17:B:816:CLA:H152	1.45	0.47
10:L:121:PHE:O	10:L:125:ALA:HB2	2.15	0.47
11:M:22:VAL:HG22	11:M:26:LYS:HE2	1.97	0.47
1:A:455:ASN:HD21	1:A:468:PHE:HB2	1.80	0.46
17:A:848:CLA:H192	17:B:802:CLA:H152	1.97	0.46
2:B:178:ALA:HB2	2:B:286:GLY:HA3	1.97	0.46
10:L:59:ILE:HG13	10:L:132:ALA:HB3	1.97	0.46
17:4:611:CLA:HBC1	25:4:616:ZEX:H403	1.96	0.46
1:A:561:ASP:OD1	1:A:561:ASP:N	2.48	0.46
17:A:819:CLA:H193	20:O:202:BCR:H272	1.95	0.46
25:1:614:ZEX:H191	25:1:614:ZEX:H11	1.69	0.46
17:2:609:CLA:H2A	17:2:609:CLA:HED2	1.96	0.46
13:4:25:PHE:N	17:4:602:CLA:OBD	2.48	0.46
2:B:578:MET:HG2	2:B:708:LEU:HD21	1.96	0.46
17:B:822:CLA:HMD3	17:B:824:CLA:HMC3	1.97	0.46
17:B:832:CLA:H112	17:B:832:CLA:H142	1.82	0.46
4:D:82:LYS:HD3	4:D:95:LEU:O	2.13	0.46
17:5:601:CLA:HMC2	25:5:616:ZEX:H361	1.97	0.46
1:A:214:ILE:HA	1:A:218:LEU:HD12	1.96	0.46
17:A:810:CLA:HMC1	20:A:844:BCR:H371	1.97	0.46
17:A:836:CLA:H41	17:A:836:CLA:H62	1.66	0.46
2:B:115:TYR:HA	2:B:365:THR:HG22	1.98	0.46
17:B:814:CLA:H2A	17:B:814:CLA:HED3	1.97	0.46
17:B:841:CLA:H18	17:B:842:CLA:H112	1.98	0.46
17:4:601:CLA:HBA2	17:4:601:CLA:H3A	1.68	0.46
17:5:601:CLA:HBB2	17:5:602:CLA:HBC1	1.96	0.46
17:A:817:CLA:H43	17:A:817:CLA:HMB2	1.96	0.46
17:A:833:CLA:HBC2	17:A:834:CLA:HBB2	1.98	0.46
17:B:801:CLA:H3A	17:B:801:CLA:CGA	2.45	0.46
13:1:95:ILE:HD11	25:1:616:ZEX:H193	1.98	0.46
13:1:158:PHE:CG	17:1:612:CLA:HAA1	2.50	0.46
13:4:77:PRO:O	13:4:81:TYR:N	2.49	0.46
17:A:826:CLA:H18	20:J:104:BCR:H17C	1.97	0.46
2:B:592:TRP:HB2	17:B:838:CLA:HMC1	1.97	0.46
17:B:808:CLA:HBA1	17:B:808:CLA:H3A	1.59	0.46
13:1:53:ALA:HB1	25:1:614:ZEX:H182	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:135:MET:HA	13:1:138:ARG:HG2	1.98	0.46
25:3:201:ZEX:H403	17:3:206:CLA:HBB2	1.96	0.46
13:4:82:PHE:HA	13:4:85:SER:HB3	1.97	0.46
14:5:58:ALA:O	14:5:62:HIS:ND1	2.36	0.46
17:A:804:CLA:H151	17:A:827:CLA:HBB2	1.98	0.46
17:A:838:CLA:H11	17:B:801:CLA:H202	1.97	0.46
4:D:98:LYS:C	4:D:98:LYS:HE3	2.36	0.46
1:A:431:ASP:OD1	1:A:552:TYR:OH	2.33	0.46
1:A:708:PRO:HG2	1:A:712:PRO:HD3	1.97	0.46
2:B:183:VAL:O	2:B:186:LEU:HB3	2.16	0.46
2:B:643:VAL:HG22	17:B:812:CLA:HAC1	1.98	0.46
17:B:839:CLA:H3A	17:B:840:CLA:OBD	2.14	0.46
1:A:111:ALA:HB2	1:A:136:ILE:HD11	1.98	0.46
2:B:6:PRO:O	2:B:7:LYS:C	2.42	0.46
2:B:207:TRP:HZ2	17:B:817:CLA:HBA2	1.81	0.46
14:2:119:ILE:HG22	14:2:120:VAL:HG13	1.98	0.46
14:2:134:GLU:OE2	14:2:158:GLN:NE2	2.39	0.46
13:4:52:LEU:HB3	17:4:604:CLA:HMC3	1.96	0.46
1:A:642:TRP:CZ3	16:A:801:CL0:C14	2.97	0.46
15:3:116:ILE:HA	15:3:119:VAL:HG12	1.98	0.46
13:4:135:MET:HA	13:4:138:ARG:HG2	1.98	0.46
1:A:493:ASN:HB3	12:O:67:LEU:HD12	1.97	0.45
1:A:542:THR:HG22	1:A:594:TRP:HB3	1.98	0.45
1:A:642:TRP:CD1	16:A:801:CL0:H54	2.51	0.45
13:1:100:PHE:HD1	13:1:106:LYS:HE2	1.79	0.45
15:3:112:VAL:O	15:3:116:ILE:HB	2.16	0.45
17:B:812:CLA:H203	20:L:205:BCR:HC7	1.98	0.45
9:K:35:GLN:O	9:K:39:SER:CB	2.65	0.45
14:5:134:GLU:OE2	14:5:158:GLN:NE2	2.39	0.45
14:5:180:LEU:HB2	17:5:612:CLA:HED1	1.98	0.45
17:5:603:CLA:H41	17:5:603:CLA:H62	1.63	0.45
1:A:9:VAL:HG22	1:A:189:ASN:HD21	1.81	0.45
2:B:16:PRO:HG3	3:C:74:THR:HG22	1.97	0.45
2:B:40:GLU:HG2	2:B:163:LEU:HB2	1.97	0.45
2:B:193:VAL:HG12	2:B:215:PRO:HG2	1.98	0.45
13:1:77:PRO:O	13:1:81:TYR:N	2.49	0.45
15:3:22:VAL:HG12	15:3:24:GLU:H	1.81	0.45
1:A:581:GLN:HE22	2:B:664:SER:HA	1.82	0.45
17:A:821:CLA:HBA2	17:A:821:CLA:H3A	1.57	0.45
17:A:824:CLA:H3A	17:A:824:CLA:HBA2	1.68	0.45
3:C:73:THR:N	3:C:76:SER:OG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:50:ALA:HB2	25:4:613:ZEX:H202	1.98	0.45
1:A:126:ASP:OD1	1:A:126:ASP:N	2.50	0.45
1:A:407:ILE:HG23	1:A:411:ARG:HH11	1.82	0.45
1:A:532:HIS:CG	17:A:836:CLA:HED2	2.51	0.45
17:A:826:CLA:H151	17:A:826:CLA:H111	1.86	0.45
17:A:832:CLA:H203	17:A:832:CLA:H162	1.84	0.45
2:B:141:LEU:HD21	17:B:810:CLA:HMC1	1.99	0.45
2:B:253:LEU:HB3	2:B:273:HIS:HD2	1.81	0.45
17:B:827:CLA:H71	17:B:829:CLA:H42	1.99	0.45
3:C:8:TYR:CE2	4:D:120:ILE:HG13	2.51	0.45
12:O:91:PRO:HG2	12:O:93:LEU:HG	1.99	0.45
17:2:603:CLA:HAC1	17:2:606:CLA:HAB	1.98	0.45
15:3:163:LEU:HB2	25:3:218:ZEX:C15	2.46	0.45
1:A:585:TRP:NE1	17:A:828:CLA:HMD1	2.32	0.45
17:A:803:CLA:HBA1	17:A:803:CLA:H3A	1.74	0.45
17:A:839:CLA:H193	10:L:58:LEU:HD11	1.99	0.45
2:B:87:LEU:HD21	2:B:106:ARG:HD2	1.98	0.45
17:B:830:CLA:H141	23:B:851:DGD:HAS1	1.98	0.45
17:B:835:CLA:H202	17:B:835:CLA:H161	1.85	0.45
12:O:60:ILE:HG13	12:O:61:PRO:HD3	1.98	0.45
1:A:72:ALA:HB1	17:A:803:CLA:HBB1	1.98	0.45
1:A:154:GLN:O	1:A:158:THR:OG1	2.28	0.45
1:A:673:HIS:O	1:A:676:TRP:HB3	2.17	0.45
17:B:806:CLA:H152	17:B:806:CLA:H112	1.69	0.45
17:B:833:CLA:H3A	17:B:834:CLA:OBD	2.16	0.45
17:1:601:CLA:HMA2	25:1:615:ZEX:H161	1.99	0.45
17:4:611:CLA:H3A	17:4:611:CLA:HBA2	1.39	0.45
14:5:117:GLU:HG2	17:5:607:CLA:NA	2.32	0.45
17:A:806:CLA:H172	17:J:101:CLA:H91	1.99	0.45
17:A:825:CLA:H2	17:A:825:CLA:H61	1.61	0.45
17:B:809:CLA:H42	17:B:809:CLA:HMA2	1.99	0.45
20:B:847:BCR:H371	20:B:847:BCR:H392	1.99	0.45
17:1:601:CLA:HMB1	14:2:120:VAL:HG11	1.99	0.45
17:1:603:CLA:HAB	25:1:614:ZEX:H35	1.99	0.45
1:A:594:TRP:HE1	17:A:848:CLA:CHD	2.30	0.44
2:B:401:ASN:OD1	2:B:404:ASN:ND2	2.41	0.44
2:B:505:SER:HA	2:B:508:LEU:HD21	1.98	0.44
2:B:613:TYR:OH	2:B:619:ARG:NH2	2.36	0.44
17:B:818:CLA:HMB3	20:B:847:BCR:H11C	1.97	0.44
17:B:819:CLA:CHD	17:B:820:CLA:HBB2	2.47	0.44
17:2:603:CLA:HMC1	17:2:606:CLA:HAB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:813:CLA:H71	10:L:80:LEU:HB3	1.99	0.44
1:A:483:ILE:HA	1:A:486:ILE:HD12	2.00	0.44
1:A:684:PHE:HB2	17:B:801:CLA:HBC1	1.99	0.44
4:D:79:GLN:HA	4:D:81:TYR:HD1	1.82	0.44
8:J:30:ARG:HD3	20:J:105:BCR:HC22	1.99	0.44
17:2:601:CLA:H2A	25:3:201:ZEX:H361	2.00	0.44
1:A:70:PHE:HA	1:A:73:HIS:HD2	1.82	0.44
1:A:399:VAL:HG22	1:A:546:LEU:HD11	1.99	0.44
17:A:819:CLA:H142	17:A:824:CLA:HBB2	2.00	0.44
18:A:840:PQN:H111	20:B:805:BCR:H281	2.00	0.44
2:B:544:LEU:HD23	2:B:562:ARG:HH12	1.82	0.44
17:B:803:CLA:C1B	17:B:835:CLA:H41	2.48	0.44
17:B:827:CLA:H141	17:B:827:CLA:H161	1.83	0.44
4:D:32:TRP:HH2	4:D:50:MET:HG3	1.83	0.44
1:A:138:SER:HA	17:A:826:CLA:HMA2	2.00	0.44
1:A:222:LYS:HD3	1:A:249:LEU:HB3	1.99	0.44
16:A:801:CL0:H46	17:B:806:CLA:HBB2	1.96	0.44
17:A:817:CLA:H3A	17:A:817:CLA:HBA2	1.53	0.44
17:A:838:CLA:H192	20:A:846:BCR:H272	1.99	0.44
2:B:398:PRO:HG3	2:B:540:ARG:HH22	1.82	0.44
14:5:119:ILE:HG22	14:5:120:VAL:HG13	1.98	0.44
1:A:137:THR:HG21	1:A:741:LEU:HD22	2.00	0.44
18:B:844:PQN:H111	18:B:844:PQN:H2M1	1.75	0.44
14:2:159:ALA:HB1	17:2:609:CLA:HED3	2.00	0.44
14:5:170:ILE:HG21	25:5:616:ZEX:H392	1.98	0.44
1:A:430:ARG:NH2	1:A:555:ASN:O	2.34	0.44
2:B:348:GLN:HE21	17:B:829:CLA:HMD2	1.82	0.44
17:B:829:CLA:H143	17:B:829:CLA:H161	1.92	0.44
3:C:66:ARG:HA	3:C:66:ARG:HD2	1.78	0.44
13:4:144:ARG:NH1	25:4:614:ZEX:O3	2.42	0.44
1:A:112:GLN:HE21	17:A:805:CLA:HBB2	1.82	0.44
1:A:444:LEU:O	1:A:448:SER:CB	2.65	0.44
17:A:834:CLA:HBA2	17:A:834:CLA:H3A	1.56	0.44
2:B:65:LEU:HD21	20:B:847:BCR:H271	2.00	0.44
2:B:666:ARG:O	2:B:669:TRP:N	2.51	0.44
15:3:37:LEU:HD12	25:3:215:ZEX:H21	2.00	0.44
17:3:207:CLA:HMB3	25:3:218:ZEX:H173	2.00	0.44
1:A:190:VAL:HG21	1:A:342:THR:HG22	2.00	0.44
2:B:722:PHE:O	2:B:726:SER:CB	2.66	0.44
20:B:805:BCR:H20C	20:B:805:BCR:H361	1.79	0.44
5:E:32:VAL:HG12	5:E:34:TYR:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:145:LEU:HD13	17:1:609:CLA:HBC1	1.99	0.44
17:3:210:CLA:H2A	17:3:210:CLA:HED3	2.00	0.44
17:A:806:CLA:HMC3	17:A:807:CLA:HMD2	1.99	0.43
17:A:831:CLA:HMA1	20:I:101:BCR:H272	2.00	0.43
2:B:5:PHE:CG	2:B:6:PRO:CD	2.88	0.43
2:B:65:LEU:O	2:B:69:ALA:HB2	2.18	0.43
2:B:572:ASP:OD1	2:B:573:ALA:N	2.50	0.43
17:B:812:CLA:H162	17:B:842:CLA:H42	1.99	0.43
8:J:15:THR:O	8:J:19:PHE:HB3	2.17	0.43
1:A:62:LEU:HD21	17:A:823:CLA:H201	2.00	0.43
1:A:322:LEU:HD13	1:A:337:LEU:HB2	2.00	0.43
3:C:16:GLN:O	3:C:20:ALA:CB	2.66	0.43
13:1:29:ARG:HH22	14:2:126:ILE:HD13	1.83	0.43
14:2:110:LEU:HD13	17:2:606:CLA:HMD2	2.00	0.43
17:3:208:CLA:H3A	17:3:208:CLA:HBA2	1.46	0.43
1:A:204:LEU:HD22	20:A:843:BCR:H361	2.00	0.43
1:A:402:GLY:HA3	1:A:546:LEU:HD22	2.01	0.43
17:A:808:CLA:HBA2	17:A:811:CLA:H192	2.00	0.43
14:5:80:THR:HG21	17:5:604:CLA:HMD1	2.01	0.43
19:A:842:LHG:H251	19:A:842:LHG:H111	2.00	0.43
3:C:7:ILE:HG23	3:C:65:ILE:HG12	2.00	0.43
17:1:603:CLA:H2A	17:1:603:CLA:HED2	2.00	0.43
15:3:66:THR:HA	15:3:69:GLN:HB2	1.99	0.43
15:3:156:ARG:HD3	17:3:203:CLA:HAC2	2.01	0.43
15:3:160:ILE:HA	25:3:218:ZEX:H403	2.00	0.43
13:4:134:ALA:O	13:4:137:ASP:HB2	2.18	0.43
14:5:182:THR:HG22	14:5:184:GLN:H	1.83	0.43
1:A:208:SER:HB3	20:A:843:BCR:H363	2.01	0.43
1:A:212:HIS:O	1:A:216:VAL:HB	2.18	0.43
17:A:819:CLA:H202	20:O:202:BCR:H381	2.00	0.43
17:A:838:CLA:H91	17:A:838:CLA:H112	1.84	0.43
2:B:647:MET:O	2:B:650:PHE:HB3	2.18	0.43
17:B:831:CLA:H3A	17:B:831:CLA:HBA2	1.65	0.43
17:B:833:CLA:HMC3	17:B:840:CLA:HBB1	2.01	0.43
6:F:47:GLU:OE1	6:F:78:ARG:NH2	2.50	0.43
8:J:15:THR:O	8:J:19:PHE:HB2	2.18	0.43
1:A:9:VAL:HG13	1:A:189:ASN:HD21	1.84	0.43
1:A:368:TYR:HA	1:A:383:GLN:NE2	2.33	0.43
1:A:426:MET:HA	1:A:429:HIS:CE1	2.54	0.43
1:A:631:ASN:ND2	1:A:645:ASP:OD1	2.51	0.43
2:B:65:LEU:HD11	20:B:847:BCR:H271	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:LEU:HD22	2:B:380:LEU:HD22	2.00	0.43
17:B:801:CLA:HMC2	17:B:804:CLA:HAC2	2.00	0.43
7:I:9:ILE:HD11	17:4:606:CLA:HBB	2.01	0.43
13:1:134:ALA:O	13:1:137:ASP:HB2	2.18	0.43
15:3:160:ILE:HA	25:3:218:ZEX:H35	2.01	0.43
20:A:843:BCR:H361	20:A:843:BCR:H20C	1.83	0.43
2:B:409:MET:HA	2:B:412:HIS:CE1	2.53	0.43
15:3:57:ARG:NH1	15:3:151:GLU:OE2	2.51	0.43
1:A:317:SER:H	1:A:320:GLN:HE21	1.67	0.43
1:A:389:HIS:HE1	17:A:827:CLA:HBB1	1.83	0.43
1:A:642:TRP:CZ3	16:A:801:CL0:H56	2.46	0.43
2:B:271:MET:HA	2:B:274:HIS:HB3	2.01	0.43
17:B:822:CLA:H152	17:B:822:CLA:H112	1.82	0.43
4:D:85:ARG:HD2	4:D:95:LEU:CG	2.49	0.43
25:2:615:ZEX:H10	25:2:615:ZEX:H7	1.75	0.43
1:A:676:TRP:CB	16:A:801:CL0:H5	2.49	0.43
17:A:817:CLA:H41	17:A:817:CLA:H191	2.01	0.43
17:A:838:CLA:H102	17:A:838:CLA:H61	1.76	0.43
4:D:98:LYS:HE3	4:D:98:LYS:HB3	1.60	0.43
4:D:120:ILE:HG23	4:D:123:ASN:HD22	1.84	0.43
11:M:19:TYR:O	11:M:23:LYS:HB2	2.19	0.43
17:3:203:CLA:H72	17:3:204:CLA:HBB	2.00	0.43
13:4:89:ILE:HG13	17:4:606:CLA:HMD1	1.99	0.43
17:4:601:CLA:HMA2	25:4:614:ZEX:H161	2.01	0.43
1:A:199:ALA:HB1	17:A:818:CLA:HBC3	2.00	0.43
1:A:536:ALA:O	1:A:540:HIS:ND1	2.29	0.43
2:B:152:TRP:HH2	14:5:126:ILE:HD11	1.84	0.43
2:B:345:LEU:HD22	17:B:821:CLA:H62	2.00	0.43
2:B:571:TRP:HZ2	2:B:705:LEU:HD13	1.83	0.43
2:B:643:VAL:HG11	17:B:811:CLA:HAC1	2.00	0.43
2:B:724:ILE:O	2:B:728:ALA:CB	2.66	0.43
17:B:801:CLA:H62	17:B:801:CLA:H41	1.82	0.43
17:B:821:CLA:H93	17:B:821:CLA:H61	1.85	0.43
14:2:71:LEU:HD23	17:2:604:CLA:HMC1	2.00	0.43
14:2:167:LEU:O	14:2:171:ALA:CB	2.67	0.43
1:A:398:ILE:HD12	20:A:845:BCR:H343	2.00	0.42
1:A:482:TRP:HB2	12:O:92:LYS:HD3	2.01	0.42
17:A:831:CLA:HBB2	10:L:65:LEU:HD22	2.00	0.42
2:B:323:THR:HG21	2:B:401:ASN:HD21	1.84	0.42
17:B:841:CLA:H151	17:B:842:CLA:H121	2.01	0.42
4:D:62:LYS:HZ1	4:D:95:LEU:HD13	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:33:LEU:HD13	15:3:37:LEU:HB3	2.00	0.42
15:3:96:LEU:HA	15:3:99:ILE:HG12	2.00	0.42
13:4:79:HIS:CG	25:4:616:ZEX:H21	2.54	0.42
1:A:91:GLY:O	1:A:95:SER:OG	2.30	0.42
2:B:295:ILE:HG22	17:B:824:CLA:HMD1	2.00	0.42
2:B:597:LEU:HD21	2:B:727:THR:HG22	2.01	0.42
3:C:12:ILE:HG21	5:E:52:ASN:HD21	1.84	0.42
14:5:166:ARG:HB3	25:5:616:ZEX:H383	2.00	0.42
1:A:200:GLY:HA2	17:A:818:CLA:HBC1	2.00	0.42
2:B:33:SER:O	23:B:851:DGD:O5E	2.37	0.42
2:B:629:LEU:HD12	2:B:725:ALA:HB3	2.00	0.42
20:J:105:BCR:H20C	20:J:105:BCR:H361	1.84	0.42
13:1:89:ILE:HG13	17:1:606:CLA:HMD1	2.02	0.42
14:5:167:LEU:O	14:5:171:ALA:CB	2.67	0.42
1:A:418:ASN:HD21	1:A:423:LEU:HD22	1.85	0.42
17:A:806:CLA:H171	17:A:806:CLA:H13	1.86	0.42
17:A:834:CLA:HMD2	12:O:63:ASN:HD21	1.84	0.42
2:B:572:ASP:HA	2:B:575:TYR:HB3	2.02	0.42
2:B:714:GLY:O	2:B:718:THR:OG1	2.23	0.42
17:B:806:CLA:H111	17:B:806:CLA:H72	1.73	0.42
17:B:828:CLA:HBA2	17:B:828:CLA:H3A	1.70	0.42
17:B:843:CLA:H41	17:B:843:CLA:H61	1.82	0.42
3:C:26:LEU:HA	3:C:41:SER:O	2.19	0.42
20:I:101:BCR:H20C	20:I:101:BCR:H361	1.85	0.42
17:2:612:CLA:H3A	17:2:612:CLA:HBA2	1.65	0.42
1:A:392:TRP:NE1	17:A:826:CLA:HAB	2.34	0.42
2:B:207:TRP:HB3	17:5:606:CLA:HED2	2.01	0.42
2:B:654:VAL:O	2:B:657:THR:OG1	2.27	0.42
20:B:805:BCR:H12C	17:F:302:CLA:CBB	2.47	0.42
17:B:836:CLA:H2	17:B:837:CLA:HMB2	2.01	0.42
4:D:95:LEU:N	4:D:95:LEU:HD23	2.34	0.42
20:K:101:BCR:H20C	20:K:101:BCR:H361	1.82	0.42
10:L:83:ILE:HA	10:L:86:ILE:HB	2.00	0.42
15:3:113:PRO:O	15:3:117:GLN:HB3	2.20	0.42
1:A:53:HIS:CD2	17:A:803:CLA:HBB2	2.53	0.42
17:A:808:CLA:HBB2	17:A:811:CLA:HMA3	2.01	0.42
2:B:37:MET:SD	2:B:45:LYS:NZ	2.88	0.42
20:B:848:BCR:H342	20:B:848:BCR:H331	2.01	0.42
17:1:601:CLA:H3A	17:1:601:CLA:HBA2	1.75	0.42
14:5:67:MET:HB3	25:5:614:ZEX:H202	2.02	0.42
1:A:384:LEU:O	1:A:387:PHE:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:818:CLA:HHD	17:A:818:CLA:HAC1	1.88	0.42
17:A:830:CLA:H43	10:L:27:THR:HG23	2.02	0.42
17:A:848:CLA:HAC1	17:A:848:CLA:HMC1	1.90	0.42
2:B:146:VAL:HG13	17:B:814:CLA:HAC2	2.01	0.42
17:B:802:CLA:H18	17:B:813:CLA:HMC2	2.00	0.42
14:2:71:LEU:HG	17:2:604:CLA:HAC1	2.02	0.42
14:2:123:PRO:HA	14:2:126:ILE:HD12	2.01	0.42
17:2:602:CLA:H2	25:2:615:ZEX:H382	2.02	0.42
25:3:218:ZEX:H15	25:3:218:ZEX:H201	1.73	0.42
13:4:147:MET:HB3	25:4:613:ZEX:H403	2.01	0.42
17:A:806:CLA:H3A	17:A:806:CLA:HBA2	1.44	0.42
17:A:823:CLA:H193	17:A:823:CLA:H161	1.86	0.42
2:B:94:PRO:HB2	17:B:813:CLA:HAA1	2.00	0.42
2:B:442:VAL:HG11	2:B:613:TYR:CZ	2.54	0.42
12:O:94:ASP:HB3	12:O:98:TRP:HD1	1.84	0.42
17:1:602:CLA:HMC2	25:1:614:ZEX:H32	2.01	0.42
14:2:182:THR:HG22	14:2:184:GLN:H	1.83	0.42
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.90	0.42
17:A:811:CLA:H141	17:A:811:CLA:H162	1.89	0.42
17:A:825:CLA:H162	17:A:825:CLA:H121	1.76	0.42
17:A:831:CLA:C3B	17:A:832:CLA:HMB2	2.50	0.42
17:B:830:CLA:H142	17:B:832:CLA:H192	2.00	0.42
17:B:838:CLA:HMB2	17:B:840:CLA:HED1	2.02	0.42
13:4:51:MET:SD	17:4:608:CLA:HAB	2.60	0.42
17:5:603:CLA:H62	17:5:603:CLA:H102	1.61	0.42
1:A:46:TRP:HB3	19:A:841:LHG:HC81	2.01	0.42
1:A:157:VAL:HG21	17:A:814:CLA:HAA2	2.01	0.42
17:A:823:CLA:H93	17:A:823:CLA:H61	1.87	0.42
20:A:846:BCR:H24C	17:J:102:CLA:HMC2	2.01	0.42
2:B:71:GLN:OE1	2:B:90:ALA:N	2.40	0.42
17:B:820:CLA:H43	17:B:836:CLA:HED2	2.01	0.42
20:B:848:BCR:H15C	20:B:848:BCR:H351	1.85	0.42
13:1:147:MET:HB3	25:1:614:ZEX:H403	2.01	0.42
14:2:67:MET:HB2	17:2:608:CLA:HMC3	2.02	0.42
14:5:97:HIS:CD2	25:5:617:ZEX:H21	2.54	0.42
17:A:812:CLA:H3A	17:A:812:CLA:HBA1	1.69	0.41
17:A:817:CLA:H203	17:A:825:CLA:HAA1	2.01	0.41
17:A:848:CLA:HED3	17:A:848:CLA:HBD	1.93	0.41
2:B:5:PHE:CD2	2:B:6:PRO:HD3	2.49	0.41
17:B:821:CLA:H3A	17:B:821:CLA:HBA2	1.43	0.41
6:F:163:SER:HA	6:F:166:GLN:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HD13	17:A:816:CLA:HMA2	2.02	0.41
1:A:534:ILE:HG21	1:A:534:ILE:HD13	1.88	0.41
1:A:676:TRP:CD1	16:A:801:CL0:H8	2.55	0.41
1:A:689:TYR:CE1	2:B:534:LYS:HD2	2.55	0.41
17:A:805:CLA:H8	17:A:805:CLA:H121	1.85	0.41
17:A:805:CLA:HMB1	17:A:807:CLA:HED2	2.03	0.41
17:A:816:CLA:HBA2	17:A:816:CLA:H3A	1.43	0.41
17:A:833:CLA:H61	17:A:833:CLA:H41	1.90	0.41
17:A:834:CLA:HAB	20:A:845:BCR:H282	2.03	0.41
6:F:44:GLU:HA	6:F:79:PHE:CE2	2.55	0.41
9:K:50:ILE:HG13	17:K:102:CLA:HMC3	2.02	0.41
25:3:201:ZEX:H362	25:3:201:ZEX:H27	1.85	0.41
17:4:608:CLA:HAC2	25:4:615:ZEX:H42	2.01	0.41
17:5:608:CLA:CBB	25:5:614:ZEX:H12	2.50	0.41
1:A:293:HIS:NE2	1:A:297:ILE:HD11	2.36	0.41
1:A:373:TYR:HD2	1:A:376:LEU:HD22	1.85	0.41
1:A:647:LEU:HD22	16:A:801:CL0:CMD	2.41	0.41
17:A:815:CLA:HBB2	20:K:104:BCR:HC31	2.02	0.41
17:A:819:CLA:H62	17:A:819:CLA:H2	1.79	0.41
17:A:833:CLA:H18	17:A:837:CLA:H91	2.02	0.41
2:B:688:LEU:HD21	10:L:36:ILE:HG21	2.00	0.41
17:B:810:CLA:H161	17:B:810:CLA:H122	1.77	0.41
3:C:41:SER:HB2	4:D:112:GLN:HG3	2.01	0.41
10:L:110:SER:OG	10:L:111:VAL:N	2.53	0.41
15:3:36:PRO:HD2	25:3:215:ZEX:H3	2.03	0.41
25:4:613:ZEX:H25	25:4:613:ZEX:H28	1.78	0.41
14:5:123:PRO:HA	14:5:126:ILE:HD12	2.01	0.41
1:A:33:ARG:O	1:A:37:LYS:NZ	2.45	0.41
1:A:73:HIS:ND1	17:A:803:CLA:HAA1	2.36	0.41
1:A:149:ILE:HG23	1:A:154:GLN:HB2	2.02	0.41
17:A:848:CLA:H92	17:A:848:CLA:H62	1.89	0.41
17:B:829:CLA:H141	17:B:829:CLA:H203	2.01	0.41
17:B:836:CLA:H2	17:B:836:CLA:H61	1.78	0.41
6:F:44:GLU:HA	6:F:79:PHE:HE2	1.85	0.41
17:O:205:CLA:H3A	17:O:205:CLA:HBA1	1.37	0.41
15:3:107:GLU:HG2	17:3:208:CLA:NB	2.35	0.41
17:4:602:CLA:HAC2	25:4:614:ZEX:H22	2.03	0.41
16:A:801:CL0:C9	17:B:806:CLA:HBB2	2.50	0.41
17:A:813:CLA:HED2	17:A:813:CLA:HBD	1.89	0.41
17:A:820:CLA:HBA1	17:A:820:CLA:H3A	1.84	0.41
18:A:840:PQN:H292	18:A:840:PQN:H261	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:ILE:HG22	17:B:822:CLA:HMC1	2.02	0.41
2:B:351:TYR:HA	2:B:366:GLN:HE21	1.85	0.41
2:B:580:TRP:HE1	17:B:801:CLA:C1D	2.33	0.41
17:B:802:CLA:OBD	17:B:806:CLA:HMB3	2.21	0.41
17:B:835:CLA:H62	17:B:835:CLA:H2	1.69	0.41
17:B:842:CLA:HBC3	20:B:850:BCR:H21C	2.01	0.41
17:1:610:CLA:HMC2	25:1:613:ZEX:H11	2.01	0.41
13:4:68:PHE:HZ	17:4:604:CLA:HBD	1.85	0.41
1:A:191:GLU:HB3	1:A:308:TYR:HB3	2.01	0.41
1:A:604:PHE:HE2	16:A:801:CL0:H43	1.85	0.41
17:A:806:CLA:H161	17:B:801:CLA:H191	2.02	0.41
17:A:830:CLA:H2	17:L:203:CLA:H72	2.03	0.41
2:B:29:HIS:HD1	17:B:832:CLA:H12	1.85	0.41
2:B:276:LEU:HD21	17:B:819:CLA:C3B	2.50	0.41
17:B:809:CLA:H152	17:B:809:CLA:H111	1.80	0.41
3:C:53:ARG:N	21:C:101:SF4:S4	2.93	0.41
17:J:101:CLA:H92	17:J:101:CLA:H62	1.77	0.41
17:5:607:CLA:H3A	17:5:607:CLA:O2A	2.20	0.41
2:B:169:ASN:OD1	17:B:827:CLA:HHD	2.21	0.41
4:D:85:ARG:CG	4:D:95:LEU:HG	2.50	0.41
6:F:46:ASN:O	6:F:50:THR:CB	2.69	0.41
17:2:602:CLA:H171	17:2:602:CLA:H13	1.81	0.41
15:3:30:SER:OG	17:3:203:CLA:O1D	2.38	0.41
17:3:203:CLA:H13	25:3:215:ZEX:H193	2.01	0.41
13:4:68:PHE:CZ	17:4:604:CLA:HBD	2.56	0.41
17:A:829:CLA:HMC3	17:A:837:CLA:HBB1	2.02	0.41
2:B:422:TRP:NE1	17:B:835:CLA:OBD	2.48	0.41
14:5:30:LEU:HB3	14:5:47:THR:HG22	2.03	0.41
1:A:235:LEU:HB3	1:A:237:HIS:HB3	2.03	0.41
17:A:830:CLA:HMB1	17:A:839:CLA:HAA2	2.02	0.41
20:A:846:BCR:H382	17:B:804:CLA:H142	2.02	0.41
2:B:4:LYS:HB2	2:B:4:LYS:HZ2	1.86	0.41
2:B:88:ALA:HB3	2:B:112:ASN:HB2	2.03	0.41
2:B:241:VAL:HG12	2:B:246:GLN:HE21	1.85	0.41
2:B:324:LEU:HD22	17:B:827:CLA:HBC2	2.02	0.41
2:B:347:ALA:HB2	2:B:373:HIS:HB2	2.02	0.41
2:B:408:ARG:O	2:B:412:HIS:ND1	2.53	0.41
2:B:461:ILE:HD11	17:B:838:CLA:H43	2.03	0.41
2:B:465:SER:HB2	2:B:495:TRP:HH2	1.85	0.41
2:B:722:PHE:O	2:B:726:SER:HB3	2.21	0.41
17:B:802:CLA:H3A	17:B:802:CLA:O1A	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:811:CLA:H121	17:B:830:CLA:H162	2.02	0.41
17:B:831:CLA:H2A	17:B:831:CLA:HED3	2.03	0.41
17:B:839:CLA:H142	17:B:839:CLA:H112	1.90	0.41
4:D:78:ILE:H	4:D:78:ILE:HG13	1.82	0.41
8:J:18:LEU:HA	8:J:18:LEU:HD23	1.85	0.41
9:K:40:MET:O	9:K:44:HIS:HB2	2.21	0.41
20:K:101:BCR:H15C	20:K:101:BCR:H351	1.80	0.41
20:L:205:BCR:H24C	20:L:205:BCR:H371	1.85	0.41
17:2:601:CLA:HAB	15:3:106:PHE:CE1	2.56	0.41
15:3:56:GLY:O	15:3:60:MET:HG2	2.20	0.41
17:3:203:CLA:H2	25:3:215:ZEX:H183	2.02	0.41
13:4:26:ASP:OD2	13:4:31:SER:N	2.45	0.41
13:4:118:LYS:HD2	13:4:119:PRO:HD2	2.02	0.41
1:A:69:ILE:HD11	1:A:73:HIS:HE2	1.86	0.41
1:A:85:SER:HB3	1:A:162:GLY:HA3	2.03	0.41
1:A:299:VAL:HA	20:K:101:BCR:H352	2.03	0.41
1:A:380:TYR:O	1:A:384:LEU:N	2.52	0.41
17:A:838:CLA:HAB	17:B:801:CLA:H151	2.03	0.41
17:A:848:CLA:H111	17:A:848:CLA:H143	1.88	0.41
2:B:228:TRP:HB3	17:B:819:CLA:H3A	2.01	0.41
6:F:116:TYR:HA	6:F:160:TRP:HZ2	1.85	0.41
20:K:101:BCR:H353	20:K:104:BCR:HC32	2.03	0.41
15:3:98:GLN:HE22	17:3:206:CLA:C1A	2.34	0.41
1:A:352:ASN:ND2	17:A:803:CLA:OBD	2.53	0.40
1:A:706:VAL:HG22	6:F:126:ARG:HG3	2.03	0.40
17:A:810:CLA:H3A	17:A:810:CLA:HBA2	1.35	0.40
17:A:817:CLA:HAB	17:A:817:CLA:H121	2.03	0.40
17:B:829:CLA:H93	20:B:849:BCR:H17C	2.03	0.40
17:B:831:CLA:H171	20:B:846:BCR:H352	2.03	0.40
10:L:96:TYR:HB2	20:L:205:BCR:H361	2.03	0.40
14:5:177:HIS:CE1	25:5:617:ZEX:H35	2.56	0.40
17:A:815:CLA:H62	17:A:815:CLA:H41	1.52	0.40
18:A:840:PQN:H292	18:A:840:PQN:H243	2.03	0.40
2:B:446:ASN:ND2	2:B:449:LYS:HE3	2.36	0.40
4:D:81:TYR:OH	4:D:96:HIS:NE2	2.47	0.40
4:D:85:ARG:HD2	4:D:95:LEU:CD1	2.50	0.40
13:1:26:ASP:OD2	13:1:31:SER:N	2.45	0.40
13:1:49:VAL:HG11	17:1:607:CLA:HMD3	2.02	0.40
15:3:63:PHE:O	15:3:66:THR:OG1	2.29	0.40
2:B:385:PHE:CZ	17:B:828:CLA:HAB	2.54	0.40
17:B:816:CLA:H162	17:B:816:CLA:H192	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:832:CLA:H171	17:B:842:CLA:HMA2	2.03	0.40
17:1:612:CLA:HMC1	25:1:617:ZEX:H402	2.03	0.40
14:2:38:GLU:H	14:2:163:ARG:HH22	1.70	0.40
14:2:47:THR:OG1	17:2:602:CLA:O1A	2.39	0.40
1:A:117:ILE:HG21	1:A:117:ILE:HD13	1.89	0.40
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.90	0.40
1:A:676:TRP:NE1	16:A:801:CL0:O1A	2.54	0.40
2:B:149:LEU:O	2:B:153:LEU:CB	2.62	0.40
2:B:379:LEU:HD13	17:B:809:CLA:H122	2.03	0.40
2:B:454:GLU:HG3	6:F:31:LEU:HD11	2.03	0.40
17:B:808:CLA:H142	17:B:827:CLA:HBD	2.03	0.40
3:C:30:PRO:HG3	4:D:108:LYS:HG2	2.03	0.40
13:1:118:LYS:HD2	13:1:119:PRO:HD2	2.02	0.40
13:4:91:ILE:HD12	13:4:91:ILE:HA	1.98	0.40
1:A:88:TYR:HE1	1:A:144:TRP:HE1	1.69	0.40
1:A:531:VAL:HG13	1:A:534:ILE:HD12	2.02	0.40
17:B:806:CLA:H192	17:B:806:CLA:H162	1.89	0.40
17:B:830:CLA:CGA	17:B:830:CLA:H3A	2.48	0.40
5:E:8:VAL:HG11	5:E:58:LEU:HD12	2.02	0.40
13:1:21:GLY:O	13:1:144:ARG:NH2	2.54	0.40
15:3:58:ILE:O	15:3:62:ALA:CB	2.69	0.40
15:3:84:LEU:HA	15:3:84:LEU:HD12	1.90	0.40
15:3:96:LEU:HD21	17:3:207:CLA:HBC3	2.04	0.40
17:3:203:CLA:H122	17:3:203:CLA:H8	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	739/748 (99%)	681 (92%)	57 (8%)	1 (0%)	51 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	729/732 (100%)	654 (90%)	72 (10%)	3 (0%)	34	70
3	C	78/81 (96%)	68 (87%)	10 (13%)	0	100	100
4	D	117/139 (84%)	102 (87%)	12 (10%)	3 (3%)	5	34
5	E	59/94 (63%)	52 (88%)	7 (12%)	0	100	100
6	F	152/185 (82%)	134 (88%)	18 (12%)	0	100	100
7	I	29/32 (91%)	26 (90%)	3 (10%)	0	100	100
8	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	K	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
10	L	117/140 (84%)	106 (91%)	11 (9%)	0	100	100
11	M	25/29 (86%)	23 (92%)	2 (8%)	0	100	100
12	O	81/155 (52%)	67 (83%)	14 (17%)	0	100	100
13	1	167/175 (95%)	130 (78%)	36 (22%)	1 (1%)	25	63
13	4	168/175 (96%)	131 (78%)	36 (21%)	1 (1%)	25	63
14	2	173/199 (87%)	130 (75%)	43 (25%)	0	100	100
14	5	173/199 (87%)	130 (75%)	43 (25%)	0	100	100
15	3	168/188 (89%)	143 (85%)	25 (15%)	0	100	100
All	All	3068/3369 (91%)	2663 (87%)	396 (13%)	9 (0%)	44	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	PHE
2	B	7	LYS
4	D	96	HIS
4	D	100	GLY
2	B	6	PRO
4	D	98	LYS
13	1	12	PRO
13	4	12	PRO
1	A	526	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	598/605 (99%)	595 (100%)	3 (0%)	88	95
2	B	598/599 (100%)	595 (100%)	3 (0%)	88	95
3	C	66/67 (98%)	66 (100%)	0	100	100
4	D	101/118 (86%)	99 (98%)	2 (2%)	55	78
5	E	58/87 (67%)	58 (100%)	0	100	100
6	F	136/162 (84%)	136 (100%)	0	100	100
7	I	26/27 (96%)	26 (100%)	0	100	100
8	J	34/34 (100%)	34 (100%)	0	100	100
9	K	48/49 (98%)	48 (100%)	0	100	100
10	L	94/113 (83%)	93 (99%)	1 (1%)	73	87
11	M	22/23 (96%)	22 (100%)	0	100	100
12	O	64/121 (53%)	63 (98%)	1 (2%)	62	82
13	1	139/145 (96%)	138 (99%)	1 (1%)	84	92
13	4	140/145 (97%)	139 (99%)	1 (1%)	84	92
14	2	142/160 (89%)	141 (99%)	1 (1%)	84	92
14	5	142/160 (89%)	141 (99%)	1 (1%)	84	92
15	3	132/148 (89%)	131 (99%)	1 (1%)	81	91
All	All	2540/2763 (92%)	2525 (99%)	15 (1%)	86	94

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ILE
1	A	438	ASN
1	A	576	ARG
2	B	4	LYS
2	B	5	PHE
2	B	7	LYS
4	D	95	LEU
4	D	98	LYS
10	L	22	ASN
12	O	82	ARG
13	1	11	LYS
14	2	85	ASN

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Mol	Chain	Res	Type
15	3	78	LYS
13	4	11	LYS
14	5	85	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	189	ASN
1	A	320	GLN
2	B	374	GLN
10	L	22	ASN
12	O	86	GLN
13	1	167	GLN
14	2	85	ASN
15	3	98	GLN
14	5	85	ASN
14	5	164	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

215 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
17	CLA	3	210	-	41,49,73	1.77	7 (17%)	47,84,113	1.87	10 (21%)
17	CLA	2	606	-	45,53,73	1.72	10 (22%)	52,89,113	1.68	9 (17%)
17	CLA	B	810	-	65,73,73	1.41	10 (15%)	76,113,113	1.50	10 (13%)
16	CL0	A	801	-	65,73,73	2.87	24 (36%)	76,113,113	3.22	39 (51%)
17	CLA	1	612	-	45,53,73	1.75	9 (20%)	52,89,113	1.73	9 (17%)
17	CLA	2	610	-	42,50,73	1.77	10 (23%)	48,85,113	1.84	8 (16%)
17	CLA	A	813	-	42,50,73	1.74	9 (21%)	48,85,113	1.93	7 (14%)
17	CLA	B	841	-	65,73,73	1.44	10 (15%)	76,113,113	1.56	9 (11%)
17	CLA	A	822	-	55,63,73	1.58	11 (20%)	64,101,113	1.65	9 (14%)
17	CLA	2	601	-	45,53,73	1.72	8 (17%)	52,89,113	1.81	9 (17%)
17	CLA	J	102	-	58,66,73	1.52	11 (18%)	67,104,113	1.61	8 (11%)
17	CLA	2	605	-	45,53,73	1.73	10 (22%)	52,89,113	1.83	10 (19%)
17	CLA	B	828	-	65,73,73	1.45	10 (15%)	76,113,113	1.62	10 (13%)
17	CLA	2	612	-	45,53,73	1.74	10 (22%)	52,89,113	1.74	7 (13%)
17	CLA	A	838	-	65,73,73	1.43	10 (15%)	76,113,113	1.55	9 (11%)
17	CLA	A	804	-	65,73,73	1.44	9 (13%)	76,113,113	1.68	9 (11%)
25	ZEX	4	613	-	42,43,43	5.05	20 (47%)	55,60,60	5.08	31 (56%)
17	CLA	4	607	-	45,53,73	1.71	7 (15%)	52,89,113	1.83	10 (19%)
17	CLA	3	209	-	52,60,73	1.56	8 (15%)	60,97,113	1.70	9 (15%)
17	CLA	A	810	-	54,62,73	1.58	10 (18%)	62,99,113	1.53	7 (11%)
17	CLA	5	607	-	45,53,73	1.96	9 (20%)	52,89,113	1.74	12 (23%)
17	CLA	5	603	-	65,73,73	1.47	10 (15%)	76,113,113	1.59	13 (17%)
26	IDO	3	219	22	12,12,12	0.26	0	11,11,11	0.85	0
17	CLA	B	827	-	65,73,73	1.47	11 (16%)	76,113,113	1.66	12 (15%)
17	CLA	1	605	-	41,50,73	1.83	6 (14%)	46,85,113	1.67	8 (17%)
17	CLA	1	607	-	45,53,73	1.69	8 (17%)	52,89,113	1.97	10 (19%)
20	BCR	L	206	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	6 (10%)
17	CLA	B	820	-	59,67,73	1.57	10 (16%)	68,105,113	1.60	11 (16%)
17	CLA	1	602	-	59,67,73	1.45	10 (16%)	68,105,113	1.70	8 (11%)
20	BCR	A	846	-	41,41,41	1.33	2 (4%)	56,56,56	1.39	9 (16%)
17	CLA	B	831	-	65,73,73	1.56	9 (13%)	76,113,113	1.52	10 (13%)
20	BCR	J	105	-	41,41,41	1.32	3 (7%)	56,56,56	1.33	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	842	-	65,73,73	1.47	11 (16%)	76,113,113	1.52	7 (9%)
17	CLA	3	207	-	45,53,73	1.70	9 (20%)	52,89,113	1.79	9 (17%)
17	CLA	B	812	-	65,73,73	1.50	12 (18%)	76,113,113	1.55	12 (15%)
17	CLA	B	824	-	46,54,73	1.70	10 (21%)	53,90,113	1.68	8 (15%)
17	CLA	2	602	-	65,73,73	1.50	10 (15%)	76,113,113	1.53	8 (10%)
17	CLA	A	820	-	49,57,73	1.64	11 (22%)	55,93,113	1.77	9 (16%)
17	CLA	B	801	-	65,73,73	1.41	9 (13%)	76,113,113	2.03	14 (18%)
17	CLA	A	835	-	51,59,73	1.56	9 (17%)	59,96,113	1.81	9 (15%)
17	CLA	4	609	-	41,49,73	1.83	5 (12%)	47,84,113	1.79	8 (17%)
20	BCR	A	844	-	41,41,41	1.18	2 (4%)	56,56,56	1.42	10 (17%)
17	CLA	A	807	1	65,73,73	1.48	12 (18%)	76,113,113	1.68	15 (19%)
17	CLA	4	605	-	41,50,73	1.83	5 (12%)	46,85,113	1.77	7 (15%)
17	CLA	A	817	-	65,73,73	1.51	11 (16%)	76,113,113	1.56	11 (14%)
17	CLA	B	815	-	55,63,73	1.56	9 (16%)	64,101,113	1.56	8 (12%)
17	CLA	O	205	-	45,53,73	1.76	8 (17%)	52,89,113	1.62	9 (17%)
25	ZEX	3	214	-	42,43,43	5.06	19 (45%)	55,60,60	5.27	30 (54%)
17	CLA	B	808	-	65,73,73	1.46	10 (15%)	76,113,113	1.64	17 (22%)
17	CLA	1	603	-	45,53,73	1.77	10 (22%)	52,89,113	1.65	8 (15%)
17	CLA	O	203	-	41,49,73	1.80	6 (14%)	47,84,113	1.79	9 (19%)
17	CLA	3	212	-	46,54,73	1.68	7 (15%)	53,90,113	1.65	7 (13%)
17	CLA	B	832	-	65,73,73	1.54	12 (18%)	76,113,113	1.91	14 (18%)
17	CLA	A	836	-	65,73,73	1.48	11 (16%)	76,113,113	1.64	13 (17%)
17	CLA	B	818	-	42,50,73	1.81	10 (23%)	48,85,113	1.83	9 (18%)
17	CLA	5	612	-	45,53,73	1.74	6 (13%)	52,89,113	1.84	9 (17%)
17	CLA	A	823	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	14 (18%)
17	CLA	J	103	-	42,50,73	1.73	10 (23%)	48,85,113	1.77	8 (16%)
17	CLA	A	848	-	65,73,73	1.46	11 (16%)	76,113,113	2.11	18 (23%)
17	CLA	2	613	-	45,53,73	1.75	9 (20%)	52,89,113	1.66	9 (17%)
17	CLA	3	204	-	45,53,73	1.73	8 (17%)	52,89,113	1.71	9 (17%)
17	CLA	B	811	-	65,73,73	1.43	12 (18%)	76,113,113	1.83	15 (19%)
17	CLA	F	302	-	45,53,73	1.72	9 (20%)	52,89,113	1.75	8 (15%)
17	CLA	L	204	-	50,58,73	1.63	10 (20%)	58,95,113	1.63	9 (15%)
17	CLA	B	809	-	65,73,73	1.50	11 (16%)	76,113,113	1.55	10 (13%)
25	ZEX	3	217	-	42,43,43	5.10	20 (47%)	55,60,60	4.94	27 (49%)
20	BCR	B	849	-	41,41,41	1.27	3 (7%)	56,56,56	1.57	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	830	-	56,64,73	1.52	9 (16%)	65,102,113	1.61	8 (12%)
17	CLA	4	611	-	45,53,73	1.81	7 (15%)	52,89,113	1.65	9 (17%)
17	CLA	B	839	-	65,73,73	1.53	11 (16%)	76,113,113	1.51	9 (11%)
17	CLA	3	205	-	45,53,73	1.78	10 (22%)	52,89,113	1.79	9 (17%)
25	ZEX	1	613	-	42,43,43	4.99	18 (42%)	55,60,60	5.22	32 (58%)
25	ZEX	1	615	-	42,43,43	4.86	19 (45%)	55,60,60	5.26	33 (60%)
17	CLA	1	601	-	48,56,73	1.67	10 (20%)	55,92,113	2.27	13 (23%)
17	CLA	3	213	-	51,59,73	1.61	9 (17%)	59,96,113	1.61	8 (13%)
17	CLA	J	101	-	65,73,73	1.44	10 (15%)	76,113,113	1.64	10 (13%)
17	CLA	3	203	-	63,71,73	1.45	9 (14%)	73,110,113	1.74	9 (12%)
17	CLA	B	804	-	65,73,73	1.55	10 (15%)	76,113,113	1.69	19 (25%)
17	CLA	A	833	-	65,73,73	1.44	10 (15%)	76,113,113	1.58	10 (13%)
25	ZEX	3	201	-	42,43,43	5.19	19 (45%)	55,60,60	5.28	30 (54%)
17	CLA	B	816	-	65,73,73	1.41	10 (15%)	76,113,113	1.56	12 (15%)
19	LHG	A	842	-	39,39,48	0.76	1 (2%)	42,45,54	1.32	6 (14%)
17	CLA	F	301	-	61,69,73	1.48	10 (16%)	71,108,113	1.53	8 (11%)
17	CLA	L	202	10	57,65,73	1.58	10 (17%)	66,103,113	1.47	6 (9%)
17	CLA	B	834	-	43,51,73	1.77	10 (23%)	49,86,113	1.80	10 (20%)
17	CLA	A	802	-	55,63,73	1.55	10 (18%)	64,101,113	1.86	10 (15%)
20	BCR	B	845	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	8 (14%)
20	BCR	B	848	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	9 (16%)
17	CLA	3	206	-	45,53,73	1.84	9 (20%)	52,89,113	1.81	12 (23%)
17	CLA	4	601	-	48,56,73	1.68	7 (14%)	55,92,113	1.84	11 (20%)
20	BCR	A	845	-	41,41,41	1.34	3 (7%)	56,56,56	1.43	9 (16%)
22	BGC	A	849	26	11,11,12	1.66	3 (27%)	15,15,17	1.04	0
17	CLA	A	803	-	65,73,73	1.49	12 (18%)	76,113,113	1.77	13 (17%)
17	CLA	F	303	-	41,49,73	1.74	9 (21%)	47,84,113	1.82	8 (17%)
17	CLA	5	601	-	45,53,73	1.76	6 (13%)	52,89,113	1.71	8 (15%)
25	ZEX	1	617	-	42,43,43	4.91	18 (42%)	55,60,60	5.13	29 (52%)
17	CLA	A	816	-	65,73,73	1.48	11 (16%)	76,113,113	1.56	10 (13%)
17	CLA	L	203	-	65,73,73	1.43	10 (15%)	76,113,113	1.45	7 (9%)
17	CLA	5	611	-	45,53,73	1.76	5 (11%)	52,89,113	1.68	8 (15%)
17	CLA	A	819	-	65,73,73	1.51	11 (16%)	76,113,113	1.71	9 (11%)
17	CLA	4	608	-	45,53,73	1.79	9 (20%)	52,89,113	1.80	9 (17%)
25	ZEX	2	617	-	42,43,43	4.80	19 (45%)	55,60,60	5.29	29 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	5	613	-	43,52,73	1.77	5 (11%)	51,87,113	1.67	9 (17%)
20	BCR	B	846	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	6 (10%)
17	CLA	A	827	-	65,73,73	1.57	10 (15%)	76,113,113	1.58	14 (18%)
17	CLA	5	608	-	45,53,73	1.74	9 (20%)	52,89,113	1.88	10 (19%)
25	ZEX	5	617	-	42,43,43	4.98	19 (45%)	55,60,60	5.31	26 (47%)
17	CLA	B	803	-	65,73,73	1.44	10 (15%)	76,113,113	1.64	10 (13%)
25	ZEX	4	614	-	42,43,43	5.17	19 (45%)	55,60,60	4.78	29 (52%)
17	CLA	A	806	1	65,73,73	1.41	11 (16%)	76,113,113	1.56	10 (13%)
18	PQN	A	840	-	34,34,34	2.77	10 (29%)	42,45,45	2.16	5 (11%)
17	CLA	K	102	-	45,53,73	1.69	10 (22%)	52,89,113	1.70	9 (17%)
17	CLA	5	605	-	45,53,73	1.75	6 (13%)	52,89,113	1.69	8 (15%)
25	ZEX	4	612	-	42,43,43	5.10	19 (45%)	55,60,60	5.09	31 (56%)
17	CLA	4	602	-	59,67,73	1.51	9 (15%)	68,105,113	1.70	10 (14%)
25	ZEX	5	615	-	42,43,43	5.32	20 (47%)	55,60,60	4.94	31 (56%)
25	ZEX	5	614	-	42,43,43	5.17	20 (47%)	55,60,60	5.13	32 (58%)
20	BCR	O	202	-	41,41,41	1.34	3 (7%)	56,56,56	1.53	11 (19%)
17	CLA	B	813	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	11 (14%)
17	CLA	A	831	-	65,73,73	1.44	10 (15%)	76,113,113	1.59	10 (13%)
17	CLA	A	811	-	65,73,73	1.46	11 (16%)	76,113,113	1.53	10 (13%)
17	CLA	B	835	-	65,73,73	1.54	10 (15%)	76,113,113	1.54	8 (10%)
23	DGD	B	851	-	67,67,67	1.03	3 (4%)	81,81,81	1.47	11 (13%)
17	CLA	B	830	-	65,73,73	1.43	11 (16%)	76,113,113	1.49	11 (14%)
17	CLA	5	604	-	45,53,73	1.74	7 (15%)	52,89,113	1.72	8 (15%)
17	CLA	B	825	-	43,51,73	1.77	11 (25%)	49,86,113	1.67	9 (18%)
17	CLA	B	838	-	60,68,73	1.56	10 (16%)	70,107,113	1.62	11 (15%)
25	ZEX	1	614	-	42,43,43	5.03	19 (45%)	55,60,60	5.77	30 (54%)
17	CLA	K	103	-	42,50,73	1.77	9 (21%)	48,85,113	1.81	8 (16%)
17	CLA	B	814	-	54,62,73	1.66	9 (16%)	67,100,113	1.90	12 (17%)
24	3XQ	J	106	-	24,24,24	0.60	1 (4%)	25,25,25	1.13	0
17	CLA	1	604	-	45,53,73	1.66	8 (17%)	52,89,113	1.72	8 (15%)
17	CLA	4	604	-	45,53,73	1.77	7 (15%)	52,89,113	1.63	9 (17%)
17	CLA	A	825	-	65,73,73	1.48	10 (15%)	76,113,113	1.62	10 (13%)
25	ZEX	2	614	-	42,43,43	4.94	19 (45%)	55,60,60	5.25	33 (60%)
17	CLA	A	837	-	65,73,73	1.41	8 (12%)	76,113,113	1.56	9 (11%)
17	CLA	B	833	-	45,53,73	1.77	10 (22%)	52,89,113	1.71	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	808	-	55,63,73	1.57	11 (20%)	64,101,113	1.58	10 (15%)
20	BCR	B	850	-	41,41,41	1.26	3 (7%)	56,56,56	1.53	9 (16%)
17	CLA	5	606	-	45,53,73	1.81	10 (22%)	52,89,113	2.45	22 (42%)
21	SF4	A	847	-	0,12,12	-	-	-	-	-
17	CLA	B	826	-	55,63,73	1.60	10 (18%)	64,101,113	1.50	9 (14%)
17	CLA	1	606	-	45,53,73	1.72	10 (22%)	52,89,113	1.67	9 (17%)
17	CLA	2	604	-	42,50,73	1.71	10 (23%)	48,85,113	1.90	7 (14%)
17	CLA	A	839	-	65,73,73	1.46	12 (18%)	76,113,113	1.59	9 (11%)
17	CLA	2	603	-	45,53,73	1.67	9 (20%)	52,89,113	1.80	7 (13%)
18	PQN	B	844	-	34,34,34	2.78	9 (26%)	42,45,45	2.32	7 (16%)
25	ZEX	3	216	-	42,43,43	5.09	19 (45%)	55,60,60	5.10	31 (56%)
17	CLA	B	821	-	60,68,73	1.47	11 (18%)	70,107,113	1.71	10 (14%)
17	CLA	1	611	-	45,53,73	1.70	10 (22%)	52,89,113	2.13	10 (19%)
20	BCR	K	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.35	7 (12%)
17	CLA	1	610	-	45,53,73	1.76	8 (17%)	52,89,113	1.74	10 (19%)
20	BCR	B	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.34	8 (14%)
17	CLA	B	823	-	45,53,73	1.74	10 (22%)	52,89,113	1.70	8 (15%)
20	BCR	L	201	-	41,41,41	1.30	3 (7%)	56,56,56	1.35	9 (16%)
17	CLA	2	611	-	45,53,73	1.72	10 (22%)	52,89,113	1.88	10 (19%)
17	CLA	A	821	-	51,59,73	1.65	9 (17%)	59,96,113	1.60	8 (13%)
20	BCR	L	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.56	9 (16%)
17	CLA	B	807	-	45,53,73	1.70	10 (22%)	52,89,113	1.81	8 (15%)
17	CLA	A	826	-	65,73,73	1.46	10 (15%)	76,113,113	1.70	10 (13%)
20	BCR	I	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.40	8 (14%)
25	ZEX	4	615	-	42,43,43	5.16	19 (45%)	55,60,60	4.81	28 (50%)
17	CLA	2	609	-	41,49,73	1.78	9 (21%)	47,84,113	1.81	9 (19%)
17	CLA	A	812	-	45,53,73	1.65	9 (20%)	52,89,113	1.88	10 (19%)
17	CLA	B	840	-	47,55,73	1.62	9 (19%)	54,91,113	1.81	8 (14%)
17	CLA	B	829	-	65,73,73	1.46	10 (15%)	76,113,113	1.54	9 (11%)
21	SF4	C	102	-	0,12,12	-	-	-	-	-
17	CLA	B	819	-	55,63,73	1.50	9 (16%)	64,101,113	1.65	8 (12%)
17	CLA	B	836	-	65,73,73	1.48	10 (15%)	76,113,113	1.54	11 (14%)
17	CLA	B	843	-	65,73,73	1.44	8 (12%)	76,113,113	1.47	11 (14%)
17	CLA	O	201	-	52,60,73	1.59	8 (15%)	60,97,113	1.67	9 (15%)
17	CLA	1	609	-	41,49,73	1.75	8 (19%)	47,84,113	1.88	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	2	607	-	45,53,73	1.71	10 (22%)	52,89,113	1.77	9 (17%)
20	BCR	K	101	-	41,41,41	1.23	3 (7%)	56,56,56	1.36	9 (16%)
17	CLA	3	208	-	45,53,73	1.78	10 (22%)	52,89,113	1.67	8 (15%)
17	CLA	B	802	-	65,73,73	1.57	11 (16%)	76,113,113	1.75	24 (31%)
25	ZEX	4	616	-	42,43,43	5.04	19 (45%)	55,60,60	5.19	32 (58%)
25	ZEX	1	616	-	42,43,43	5.05	19 (45%)	55,60,60	5.10	32 (58%)
25	ZEX	5	616	-	42,43,43	5.23	20 (47%)	55,60,60	5.04	28 (50%)
17	CLA	A	805	-	65,73,73	1.44	9 (13%)	76,113,113	1.70	13 (17%)
17	CLA	B	817	-	45,53,73	1.67	10 (22%)	52,89,113	1.78	7 (13%)
17	CLA	A	824	-	55,63,73	1.55	11 (20%)	64,101,113	1.76	12 (18%)
25	ZEX	2	616	-	42,43,43	5.27	20 (47%)	55,60,60	4.77	29 (52%)
17	CLA	4	606	-	45,53,73	1.74	8 (17%)	52,89,113	1.76	6 (11%)
17	CLA	A	832	-	65,73,73	1.40	10 (15%)	76,113,113	1.73	13 (17%)
17	CLA	4	603	-	45,53,73	1.69	8 (17%)	52,89,113	1.79	9 (17%)
17	CLA	A	818	-	45,53,73	1.73	10 (22%)	52,89,113	1.98	12 (23%)
25	ZEX	2	615	-	42,43,43	4.79	18 (42%)	55,60,60	5.10	31 (56%)
17	CLA	A	828	-	65,73,73	1.62	13 (20%)	76,113,113	1.86	19 (25%)
17	CLA	A	815	-	62,70,73	1.46	10 (16%)	72,109,113	1.55	8 (11%)
17	CLA	4	610	-	45,53,73	1.78	6 (13%)	52,89,113	1.72	8 (15%)
17	CLA	O	204	-	50,58,73	1.65	7 (14%)	58,95,113	1.61	10 (17%)
20	BCR	A	843	-	41,41,41	1.23	3 (7%)	56,56,56	1.35	7 (12%)
17	CLA	1	608	-	60,68,73	1.51	10 (16%)	70,107,113	1.54	9 (12%)
17	CLA	B	822	-	65,73,73	1.49	11 (16%)	76,113,113	1.49	7 (9%)
17	CLA	A	814	-	45,53,73	1.75	8 (17%)	52,89,113	1.79	12 (23%)
17	CLA	B	806	-	65,73,73	1.52	12 (18%)	76,113,113	1.87	14 (18%)
17	CLA	A	829	-	50,58,73	1.70	10 (20%)	58,95,113	1.53	10 (17%)
25	ZEX	3	215	-	42,43,43	4.97	19 (45%)	55,60,60	5.27	33 (60%)
17	CLA	A	809	-	65,73,73	1.43	11 (16%)	76,113,113	1.60	11 (14%)
17	CLA	5	609	-	41,49,73	1.88	8 (19%)	47,84,113	2.11	16 (34%)
17	CLA	3	211	-	42,50,73	1.78	9 (21%)	48,85,113	1.76	9 (18%)
17	CLA	5	610	-	45,53,73	1.71	7 (15%)	52,89,113	1.75	7 (13%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
17	CLA	A	834	-	45,53,73	1.77	9 (20%)	52,89,113	1.72	8 (15%)
19	LHG	A	841	-	48,48,48	0.69	1 (2%)	51,54,54	1.27	6 (11%)
17	CLA	2	608	-	50,58,73	1.64	8 (16%)	58,95,113	1.90	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	3	202	-	45,53,73	1.71	7 (15%)	52,89,113	1.70	9 (17%)
20	BCR	F	304	-	41,41,41	1.18	2 (4%)	56,56,56	1.39	10 (17%)
20	BCR	J	104	-	41,41,41	1.28	3 (7%)	56,56,56	1.42	9 (16%)
25	ZEX	4	617	-	42,43,43	5.16	19 (45%)	55,60,60	5.04	30 (54%)
17	CLA	5	602	-	45,53,73	1.78	6 (13%)	52,89,113	1.82	10 (19%)
25	ZEX	3	218	-	42,43,43	5.43	20 (47%)	55,60,60	4.52	33 (60%)
20	BCR	B	805	-	41,41,41	1.27	3 (7%)	56,56,56	1.48	10 (17%)
17	CLA	B	837	-	45,53,73	1.78	10 (22%)	52,89,113	1.69	7 (13%)

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
17	CLA	3	210	-	1/1/10/20	5/8/86/115	-
17	CLA	2	606	-	1/1/11/20	7/13/91/115	-
17	CLA	B	810	-	1/1/15/20	17/37/115/115	-
16	CLO	A	801	-	3/3/20/25	10/37/135/135	-
17	CLA	1	612	-	1/1/11/20	7/13/91/115	-
17	CLA	2	610	-	1/1/10/20	5/10/88/115	-
17	CLA	A	813	-	1/1/10/20	5/10/88/115	-
17	CLA	B	841	-	1/1/15/20	14/37/115/115	-
17	CLA	A	822	-	1/1/13/20	7/25/103/115	-
17	CLA	2	601	-	1/1/11/20	6/13/91/115	-
17	CLA	J	102	-	1/1/13/20	8/29/107/115	-
17	CLA	2	605	-	1/1/11/20	7/13/91/115	-
17	CLA	B	828	-	1/1/15/20	4/37/115/115	-
17	CLA	2	612	-	1/1/11/20	3/13/91/115	-
17	CLA	A	838	-	1/1/15/20	11/37/115/115	-
17	CLA	A	804	-	1/1/15/20	14/37/115/115	-
25	ZEX	4	613	-	-	16/29/67/67	0/2/2/2
17	CLA	4	607	-	1/1/11/20	7/13/91/115	-
17	CLA	3	209	-	1/1/12/20	7/22/100/115	-
17	CLA	A	810	-	1/1/12/20	8/24/102/115	-
17	CLA	5	607	-	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	5	603	-	1/1/15/20	20/37/115/115	-
26	1DO	3	219	22	-	3/10/10/10	-
17	CLA	B	827	-	1/1/15/20	11/37/115/115	-
17	CLA	1	605	-	1/1/10/20	3/9/87/115	-
17	CLA	1	607	-	1/1/11/20	7/13/91/115	-
20	BCR	L	206	-	-	15/29/63/63	0/2/2/2
17	CLA	B	820	-	1/1/13/20	16/30/108/115	-
17	CLA	1	602	-	1/1/13/20	10/30/108/115	-
20	BCR	A	846	-	-	18/29/63/63	0/2/2/2
17	CLA	B	831	-	1/1/15/20	14/37/115/115	-
20	BCR	J	105	-	-	14/29/63/63	0/2/2/2
17	CLA	B	842	-	1/1/15/20	14/37/115/115	-
17	CLA	3	207	-	1/1/11/20	5/13/91/115	-
17	CLA	B	812	-	1/1/15/20	18/37/115/115	-
17	CLA	B	824	-	1/1/11/20	6/15/93/115	-
17	CLA	2	602	-	1/1/15/20	12/37/115/115	-
17	CLA	A	820	-	1/1/11/20	5/18/96/115	-
17	CLA	B	801	-	1/1/15/20	14/37/115/115	-
17	CLA	A	835	-	1/1/12/20	10/21/99/115	-
17	CLA	4	609	-	1/1/10/20	5/8/86/115	-
20	BCR	A	844	-	-	17/29/63/63	0/2/2/2
17	CLA	A	807	1	1/1/15/20	19/37/115/115	-
17	CLA	4	605	-	1/1/10/20	2/9/87/115	-
17	CLA	A	817	-	1/1/15/20	15/37/115/115	-
17	CLA	B	815	-	1/1/13/20	6/25/103/115	-
17	CLA	O	205	-	1/1/11/20	6/13/91/115	-
25	ZEX	3	214	-	-	14/29/67/67	0/2/2/2
17	CLA	B	808	-	1/1/15/20	16/37/115/115	-
17	CLA	1	603	-	1/1/11/20	7/13/91/115	-
17	CLA	O	203	-	1/1/10/20	3/8/86/115	-
17	CLA	3	212	-	1/1/11/20	8/15/93/115	-
17	CLA	B	832	-	1/1/15/20	10/37/115/115	-
17	CLA	A	836	-	1/1/15/20	13/37/115/115	-
17	CLA	B	818	-	1/1/10/20	4/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	5	612	-	1/1/11/20	5/13/91/115	-
17	CLA	A	823	-	1/1/15/20	16/37/115/115	-
17	CLA	J	103	-	1/1/10/20	6/10/88/115	-
17	CLA	A	848	-	1/1/15/20	9/37/115/115	-
17	CLA	2	613	-	1/1/11/20	5/13/91/115	-
17	CLA	3	204	-	1/1/11/20	6/13/91/115	-
17	CLA	B	811	-	1/1/15/20	6/37/115/115	-
17	CLA	F	302	-	1/1/11/20	4/13/91/115	-
17	CLA	L	204	-	1/1/12/20	6/19/97/115	-
17	CLA	B	809	-	1/1/15/20	15/37/115/115	-
25	ZEX	3	217	-	-	15/29/67/67	0/2/2/2
20	BCR	B	849	-	-	23/29/63/63	0/2/2/2
17	CLA	A	830	-	1/1/13/20	6/27/105/115	-
17	CLA	4	611	-	1/1/11/20	8/13/91/115	-
17	CLA	B	839	-	1/1/15/20	10/37/115/115	-
17	CLA	3	205	-	1/1/11/20	7/13/91/115	-
25	ZEX	1	613	-	-	16/29/67/67	0/2/2/2
25	ZEX	1	615	-	-	20/29/67/67	0/2/2/2
17	CLA	1	601	-	1/1/11/20	6/17/95/115	-
17	CLA	3	213	-	1/1/12/20	8/21/99/115	-
17	CLA	J	101	-	1/1/15/20	18/37/115/115	-
17	CLA	3	203	-	1/1/14/20	20/35/113/115	-
17	CLA	B	804	-	1/1/15/20	17/37/115/115	-
17	CLA	A	833	-	1/1/15/20	16/37/115/115	-
25	ZEX	3	201	-	-	16/29/67/67	0/2/2/2
17	CLA	B	816	-	1/1/15/20	19/37/115/115	-
19	LHG	A	842	-	-	19/44/44/53	-
17	CLA	F	301	-	1/1/14/20	14/33/111/115	-
17	CLA	L	202	10	1/1/13/20	14/28/106/115	-
17	CLA	B	834	-	1/1/10/20	3/11/89/115	-
17	CLA	A	802	-	1/1/13/20	7/25/103/115	-
20	BCR	B	845	-	-	16/29/63/63	0/2/2/2
20	BCR	B	848	-	-	19/29/63/63	0/2/2/2
17	CLA	3	206	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	601	-	1/1/11/20	7/17/95/115	-
20	BCR	A	845	-	-	18/29/63/63	0/2/2/2
22	BGC	A	849	26	-	2/2/19/22	0/1/1/1
17	CLA	A	803	-	1/1/15/20	2/37/115/115	-
17	CLA	F	303	-	1/1/10/20	3/8/86/115	-
17	CLA	5	601	-	1/1/11/20	6/13/91/115	-
25	ZEX	1	617	-	-	18/29/67/67	0/2/2/2
17	CLA	A	816	-	1/1/15/20	11/37/115/115	-
17	CLA	L	203	-	1/1/15/20	14/37/115/115	-
17	CLA	5	611	-	1/1/11/20	7/13/91/115	-
17	CLA	A	819	-	1/1/15/20	13/37/115/115	-
17	CLA	4	608	-	1/1/11/20	6/13/91/115	-
25	ZEX	2	617	-	-	19/29/67/67	0/2/2/2
17	CLA	5	613	-	1/1/10/20	4/10/88/115	-
20	BCR	B	846	-	-	11/29/63/63	0/2/2/2
17	CLA	A	827	-	1/1/15/20	18/37/115/115	-
17	CLA	5	608	-	1/1/11/20	5/13/91/115	-
25	ZEX	5	617	-	-	18/29/67/67	0/2/2/2
17	CLA	B	803	-	1/1/15/20	22/37/115/115	-
25	ZEX	4	614	-	-	17/29/67/67	0/2/2/2
17	CLA	A	806	1	1/1/15/20	16/37/115/115	-
18	PQN	A	840	-	-	11/23/43/43	0/2/2/2
17	CLA	K	102	-	1/1/11/20	5/13/91/115	-
17	CLA	5	605	-	1/1/11/20	8/13/91/115	-
25	ZEX	4	612	-	-	19/29/67/67	0/2/2/2
17	CLA	4	602	-	1/1/13/20	14/30/108/115	-
25	ZEX	5	615	-	-	19/29/67/67	0/2/2/2
25	ZEX	5	614	-	-	18/29/67/67	0/2/2/2
20	BCR	O	202	-	-	14/29/63/63	0/2/2/2
17	CLA	B	813	-	1/1/15/20	15/37/115/115	-
17	CLA	A	831	-	1/1/15/20	18/37/115/115	-
17	CLA	A	811	-	1/1/15/20	13/37/115/115	-
17	CLA	B	835	-	1/1/15/20	17/37/115/115	-
23	DGD	B	851	-	-	30/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	830	-	1/1/15/20	21/37/115/115	-
17	CLA	5	604	-	1/1/11/20	6/13/91/115	-
17	CLA	B	825	-	1/1/10/20	5/11/89/115	-
17	CLA	B	838	-	1/1/14/20	18/31/109/115	-
25	ZEX	1	614	-	-	16/29/67/67	0/2/2/2
17	CLA	K	103	-	1/1/10/20	5/10/88/115	-
17	CLA	B	814	-	1/1/13/20	10/25/101/115	-
24	3XQ	J	106	-	-	17/24/24/24	-
17	CLA	1	604	-	1/1/11/20	7/13/91/115	-
17	CLA	4	604	-	1/1/11/20	7/13/91/115	-
17	CLA	A	825	-	1/1/15/20	9/37/115/115	-
25	ZEX	2	614	-	-	18/29/67/67	0/2/2/2
17	CLA	A	837	-	1/1/15/20	12/37/115/115	-
17	CLA	B	833	-	1/1/11/20	5/13/91/115	-
17	CLA	A	808	-	1/1/13/20	8/25/103/115	-
20	BCR	B	850	-	-	15/29/63/63	0/2/2/2
17	CLA	5	606	-	1/1/11/20	3/13/91/115	-
25	ZEX	3	216	-	-	19/29/67/67	0/2/2/2
17	CLA	B	826	-	1/1/13/20	7/25/103/115	-
17	CLA	1	606	-	1/1/11/20	6/13/91/115	-
17	CLA	2	604	-	1/1/10/20	3/10/88/115	-
17	CLA	A	839	-	1/1/15/20	17/37/115/115	-
17	CLA	2	603	-	1/1/11/20	2/13/91/115	-
18	PQN	B	844	-	-	7/23/43/43	0/2/2/2
21	SF4	A	847	-	-	-	0/6/5/5
17	CLA	B	821	-	1/1/14/20	16/31/109/115	-
17	CLA	1	611	-	1/1/11/20	10/13/91/115	-
20	BCR	K	104	-	-	19/29/63/63	0/2/2/2
17	CLA	1	610	-	1/1/11/20	4/13/91/115	-
20	BCR	B	847	-	-	23/29/63/63	0/2/2/2
17	CLA	B	823	-	1/1/11/20	2/13/91/115	-
20	BCR	L	201	-	-	18/29/63/63	0/2/2/2
17	CLA	2	611	-	1/1/11/20	5/13/91/115	-
17	CLA	A	821	-	1/1/12/20	12/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	L	205	-	-	15/29/63/63	0/2/2/2
17	CLA	B	807	-	1/1/11/20	7/13/91/115	-
17	CLA	A	826	-	1/1/15/20	12/37/115/115	-
20	BCR	I	101	-	-	18/29/63/63	0/2/2/2
25	ZEX	4	615	-	-	16/29/67/67	0/2/2/2
17	CLA	2	609	-	1/1/10/20	3/8/86/115	-
17	CLA	A	812	-	1/1/11/20	6/13/91/115	-
17	CLA	B	840	-	1/1/11/20	4/16/94/115	-
17	CLA	B	829	-	1/1/15/20	17/37/115/115	-
21	SF4	C	102	-	-	-	0/6/5/5
17	CLA	B	819	-	1/1/13/20	12/25/103/115	-
17	CLA	B	836	-	1/1/15/20	16/37/115/115	-
17	CLA	B	843	-	1/1/15/20	16/37/115/115	-
17	CLA	O	201	-	1/1/12/20	7/22/100/115	-
17	CLA	1	609	-	1/1/10/20	0/8/86/115	-
17	CLA	2	607	-	1/1/11/20	3/13/91/115	-
20	BCR	K	101	-	-	11/29/63/63	0/2/2/2
17	CLA	3	208	-	1/1/11/20	8/13/91/115	-
17	CLA	B	802	-	1/1/15/20	12/37/115/115	-
25	ZEX	4	616	-	-	17/29/67/67	0/2/2/2
25	ZEX	1	616	-	-	20/29/67/67	0/2/2/2
25	ZEX	5	616	-	-	16/29/67/67	0/2/2/2
17	CLA	A	805	-	1/1/15/20	16/37/115/115	-
17	CLA	B	817	-	1/1/11/20	3/13/91/115	-
17	CLA	A	824	-	1/1/13/20	5/25/103/115	-
25	ZEX	2	616	-	-	19/29/67/67	0/2/2/2
17	CLA	4	606	-	1/1/11/20	4/13/91/115	-
17	CLA	A	832	-	1/1/15/20	18/37/115/115	-
17	CLA	4	603	-	1/1/11/20	10/13/91/115	-
17	CLA	A	818	-	1/1/11/20	7/13/91/115	-
25	ZEX	2	615	-	-	16/29/67/67	0/2/2/2
17	CLA	A	828	-	1/1/15/20	10/37/115/115	-
17	CLA	A	815	-	1/1/14/20	13/34/112/115	-
17	CLA	4	610	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	O	204	-	1/1/12/20	6/19/97/115	-
20	BCR	A	843	-	-	16/29/63/63	0/2/2/2
17	CLA	1	608	-	1/1/14/20	9/31/109/115	-
17	CLA	B	822	-	1/1/15/20	17/37/115/115	-
17	CLA	A	814	-	1/1/11/20	4/13/91/115	-
17	CLA	B	806	-	1/1/15/20	16/37/115/115	-
17	CLA	A	829	-	1/1/12/20	4/19/97/115	-
25	ZEX	3	215	-	-	16/29/67/67	0/2/2/2
17	CLA	A	809	-	1/1/15/20	13/37/115/115	-
17	CLA	5	609	-	1/1/10/20	5/8/86/115	-
17	CLA	3	211	-	1/1/10/20	1/10/88/115	-
17	CLA	5	610	-	1/1/11/20	8/13/91/115	-
21	SF4	C	101	3	-	-	0/6/5/5
17	CLA	A	834	-	1/1/11/20	8/13/91/115	-
19	LHG	A	841	-	-	27/53/53/53	-
17	CLA	2	608	-	1/1/12/20	8/19/97/115	-
17	CLA	3	202	-	1/1/11/20	5/13/91/115	-
20	BCR	F	304	-	-	18/29/63/63	0/2/2/2
20	BCR	J	104	-	-	16/29/63/63	0/2/2/2
25	ZEX	4	617	-	-	18/29/67/67	0/2/2/2
17	CLA	5	602	-	1/1/11/20	7/13/91/115	-
25	ZEX	3	218	-	-	17/29/67/67	0/2/2/2
20	BCR	B	805	-	-	15/29/63/63	0/2/2/2
17	CLA	B	837	-	1/1/11/20	6/13/91/115	-

All (2053) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	218	ZEX	C14-C13	15.85	1.56	1.35
25	2	616	ZEX	C14-C13	14.96	1.55	1.35
25	1	616	ZEX	C14-C13	14.67	1.55	1.35
25	3	201	ZEX	C14-C13	14.51	1.55	1.35
25	3	216	ZEX	C14-C13	14.50	1.55	1.35
25	4	614	ZEX	C14-C13	14.49	1.55	1.35
25	4	615	ZEX	C14-C13	14.46	1.54	1.35
25	5	615	ZEX	C14-C13	14.45	1.54	1.35
25	1	617	ZEX	C14-C13	14.44	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	614	ZEX	C14-C13	14.40	1.54	1.35
25	4	616	ZEX	C14-C13	14.35	1.54	1.35
25	4	613	ZEX	C14-C13	14.35	1.54	1.35
25	4	617	ZEX	C14-C13	14.35	1.54	1.35
25	5	616	ZEX	C14-C13	14.34	1.54	1.35
25	3	217	ZEX	C14-C13	14.33	1.54	1.35
25	5	614	ZEX	C14-C13	14.21	1.54	1.35
25	3	218	ZEX	C10-C9	14.20	1.54	1.35
25	4	612	ZEX	C14-C13	14.20	1.54	1.35
25	2	614	ZEX	C14-C13	14.16	1.54	1.35
25	3	201	ZEX	C10-C9	14.10	1.54	1.35
25	1	613	ZEX	C14-C13	14.05	1.54	1.35
25	3	215	ZEX	C14-C13	13.98	1.54	1.35
25	1	613	ZEX	C10-C9	13.86	1.54	1.35
25	5	617	ZEX	C14-C13	13.83	1.54	1.35
25	5	615	ZEX	C10-C9	13.81	1.54	1.35
25	3	214	ZEX	C14-C13	13.81	1.54	1.35
25	2	615	ZEX	C14-C13	13.72	1.54	1.35
25	4	614	ZEX	C10-C9	13.68	1.53	1.35
25	1	615	ZEX	C14-C13	13.59	1.53	1.35
25	4	613	ZEX	C10-C9	13.50	1.53	1.35
25	4	615	ZEX	C10-C9	13.47	1.53	1.35
25	5	614	ZEX	C10-C9	13.42	1.53	1.35
25	4	612	ZEX	C10-C9	13.37	1.53	1.35
25	5	615	ZEX	C30-C29	13.36	1.53	1.35
25	2	617	ZEX	C14-C13	13.32	1.53	1.35
25	5	616	ZEX	C10-C9	13.31	1.53	1.35
25	3	217	ZEX	C10-C9	13.23	1.53	1.35
25	2	616	ZEX	C10-C9	13.18	1.53	1.35
25	3	216	ZEX	C10-C9	13.17	1.53	1.35
25	3	215	ZEX	C10-C9	13.16	1.53	1.35
25	3	218	ZEX	C34-C33	13.16	1.53	1.35
25	2	616	ZEX	C30-C29	13.13	1.53	1.35
25	4	616	ZEX	C10-C9	13.10	1.53	1.35
25	1	614	ZEX	C10-C9	13.07	1.53	1.35
25	4	617	ZEX	C10-C9	13.07	1.53	1.35
25	1	615	ZEX	C10-C9	13.04	1.53	1.35
25	4	617	ZEX	C30-C29	13.01	1.53	1.35
25	4	615	ZEX	C30-C29	12.99	1.53	1.35
25	1	616	ZEX	C10-C9	12.95	1.52	1.35
25	3	217	ZEX	C30-C29	12.94	1.52	1.35
25	3	214	ZEX	C10-C9	12.92	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	614	ZEX	C10-C9	12.90	1.52	1.35
25	4	614	ZEX	C30-C29	12.89	1.52	1.35
25	5	616	ZEX	C30-C29	12.83	1.52	1.35
25	5	615	ZEX	C34-C33	12.80	1.52	1.35
25	2	617	ZEX	C10-C9	12.80	1.52	1.35
25	3	218	ZEX	C30-C29	12.79	1.52	1.35
25	5	617	ZEX	C10-C9	12.77	1.52	1.35
25	5	614	ZEX	C30-C29	12.76	1.52	1.35
25	5	617	ZEX	C30-C29	12.73	1.52	1.35
25	4	613	ZEX	C30-C29	12.66	1.52	1.35
25	2	615	ZEX	C10-C9	12.64	1.52	1.35
25	1	617	ZEX	C10-C9	12.60	1.52	1.35
25	4	612	ZEX	C34-C33	12.52	1.52	1.35
25	3	214	ZEX	C30-C29	12.51	1.52	1.35
25	1	616	ZEX	C30-C29	12.45	1.52	1.35
25	3	201	ZEX	C30-C29	12.40	1.52	1.35
25	5	616	ZEX	C34-C33	12.36	1.52	1.35
25	4	615	ZEX	C34-C33	12.33	1.52	1.35
25	3	216	ZEX	C30-C29	12.32	1.52	1.35
25	2	616	ZEX	C34-C33	12.31	1.52	1.35
25	1	615	ZEX	C30-C29	12.31	1.52	1.35
25	5	614	ZEX	C34-C33	12.27	1.52	1.35
25	4	616	ZEX	C30-C29	12.24	1.52	1.35
25	4	617	ZEX	C34-C33	12.24	1.52	1.35
25	3	217	ZEX	C34-C33	12.23	1.52	1.35
25	3	214	ZEX	C34-C33	12.22	1.52	1.35
25	4	612	ZEX	C30-C29	12.21	1.52	1.35
25	4	614	ZEX	C5-C6	12.19	1.55	1.34
25	5	617	ZEX	C34-C33	12.15	1.51	1.35
25	3	215	ZEX	C5-C6	12.15	1.55	1.34
25	5	614	ZEX	C5-C6	12.14	1.55	1.34
25	2	615	ZEX	C5-C6	12.12	1.55	1.34
25	3	201	ZEX	C34-C33	12.11	1.51	1.35
25	3	215	ZEX	C30-C29	12.09	1.51	1.35
25	3	214	ZEX	C5-C6	12.09	1.55	1.34
25	1	617	ZEX	C30-C29	12.07	1.51	1.35
25	1	614	ZEX	C30-C29	12.03	1.51	1.35
25	1	613	ZEX	C30-C29	12.03	1.51	1.35
25	3	218	ZEX	C5-C6	12.03	1.55	1.34
25	4	616	ZEX	C34-C33	12.01	1.51	1.35
25	2	614	ZEX	C34-C33	12.00	1.51	1.35
25	3	216	ZEX	C34-C33	12.00	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	616	ZEX	C34-C33	11.98	1.51	1.35
25	4	614	ZEX	C34-C33	11.96	1.51	1.35
25	4	612	ZEX	C5-C6	11.95	1.55	1.34
25	5	615	ZEX	C5-C6	11.94	1.55	1.34
25	4	613	ZEX	C34-C33	11.94	1.51	1.35
25	2	614	ZEX	C5-C6	11.93	1.55	1.34
25	4	617	ZEX	C5-C6	11.92	1.55	1.34
25	1	613	ZEX	C34-C33	11.91	1.51	1.35
25	1	614	ZEX	C34-C33	11.91	1.51	1.35
25	2	614	ZEX	C30-C29	11.89	1.51	1.35
25	1	614	ZEX	C5-C6	11.88	1.55	1.34
25	5	616	ZEX	C5-C6	11.88	1.55	1.34
25	1	617	ZEX	C34-C33	11.86	1.51	1.35
25	4	615	ZEX	C5-C6	11.82	1.54	1.34
25	3	217	ZEX	C5-C6	11.82	1.54	1.34
25	2	617	ZEX	C30-C29	11.80	1.51	1.35
25	4	616	ZEX	C5-C6	11.80	1.54	1.34
25	3	216	ZEX	C5-C6	11.74	1.54	1.34
25	2	616	ZEX	C5-C6	11.65	1.54	1.34
25	2	617	ZEX	C5-C6	11.59	1.54	1.34
25	2	617	ZEX	C34-C33	11.56	1.51	1.35
25	1	616	ZEX	C5-C6	11.56	1.54	1.34
25	2	615	ZEX	C34-C33	11.53	1.51	1.35
25	3	201	ZEX	C5-C6	11.43	1.54	1.34
25	1	615	ZEX	C34-C33	11.43	1.50	1.35
25	3	215	ZEX	C34-C33	11.36	1.50	1.35
25	1	615	ZEX	C5-C6	11.35	1.54	1.34
25	1	617	ZEX	C5-C6	11.31	1.54	1.34
25	5	617	ZEX	C5-C6	11.20	1.53	1.34
25	4	613	ZEX	C5-C6	11.12	1.53	1.34
25	2	615	ZEX	C30-C29	11.09	1.50	1.35
25	1	613	ZEX	C5-C6	11.05	1.53	1.34
25	5	616	ZEX	C25-C26	10.79	1.53	1.33
25	5	615	ZEX	C25-C26	10.62	1.53	1.33
25	4	617	ZEX	C25-C26	10.55	1.53	1.33
25	3	201	ZEX	C25-C26	10.50	1.53	1.33
25	3	216	ZEX	C25-C26	10.39	1.53	1.33
25	4	612	ZEX	C25-C26	10.22	1.52	1.33
25	2	616	ZEX	C25-C26	10.21	1.52	1.33
25	3	214	ZEX	C25-C26	10.11	1.52	1.33
25	5	614	ZEX	C25-C26	10.10	1.52	1.33
25	4	614	ZEX	C25-C26	10.05	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	218	ZEX	C25-C26	10.02	1.52	1.33
25	1	614	ZEX	C25-C26	10.01	1.52	1.33
25	4	616	ZEX	C25-C26	10.01	1.52	1.33
25	4	613	ZEX	C25-C26	9.95	1.52	1.33
25	4	615	ZEX	C25-C26	9.94	1.52	1.33
25	3	215	ZEX	C25-C26	9.92	1.52	1.33
25	5	617	ZEX	C25-C26	9.91	1.52	1.33
25	1	613	ZEX	C25-C26	9.86	1.52	1.33
25	1	616	ZEX	C25-C26	9.86	1.52	1.33
25	3	217	ZEX	C25-C26	9.82	1.52	1.33
25	1	617	ZEX	C25-C26	9.74	1.51	1.33
25	1	615	ZEX	C25-C26	9.67	1.51	1.33
25	2	617	ZEX	C25-C26	9.66	1.51	1.33
25	2	614	ZEX	C25-C26	9.48	1.51	1.33
25	2	615	ZEX	C25-C26	9.35	1.51	1.33
16	A	801	CL0	C1B-NB	-9.16	1.27	1.35
16	A	801	CL0	C1D-ND	-8.30	1.27	1.37
18	A	840	PQN	C12-C13	8.16	1.52	1.33
18	B	844	PQN	C12-C13	8.06	1.52	1.33
18	B	844	PQN	O4-C4	7.98	1.40	1.23
18	A	840	PQN	O4-C4	7.91	1.40	1.23
17	5	607	CLA	C4B-NB	7.78	1.42	1.35
16	A	801	CL0	C4B-NB	-7.58	1.28	1.35
18	A	840	PQN	O1-C1	7.56	1.39	1.23
17	4	605	CLA	C4B-NB	7.52	1.41	1.35
18	B	844	PQN	O1-C1	7.49	1.39	1.23
17	5	602	CLA	C4B-NB	7.42	1.41	1.35
17	5	611	CLA	C4B-NB	7.40	1.41	1.35
17	4	610	CLA	C4B-NB	7.39	1.41	1.35
17	A	834	CLA	C4B-NB	7.37	1.41	1.35
17	1	605	CLA	C4B-NB	7.35	1.41	1.35
17	4	609	CLA	C4B-NB	7.34	1.41	1.35
17	4	611	CLA	C4B-NB	7.31	1.41	1.35
17	5	613	CLA	C4B-NB	7.29	1.41	1.35
17	B	835	CLA	C4B-NB	7.26	1.41	1.35
17	5	609	CLA	C4B-NB	7.24	1.41	1.35
17	3	206	CLA	C4B-NB	7.22	1.41	1.35
17	4	606	CLA	C4B-NB	7.15	1.41	1.35
17	5	605	CLA	C4B-NB	7.15	1.41	1.35
17	5	612	CLA	C4B-NB	7.15	1.41	1.35
17	5	601	CLA	C4B-NB	7.11	1.41	1.35
17	4	604	CLA	C4B-NB	7.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	613	CLA	C4B-NB	7.09	1.41	1.35
17	O	205	CLA	C4B-NB	7.07	1.41	1.35
17	4	608	CLA	C4B-NB	7.06	1.41	1.35
17	2	602	CLA	C4B-NB	7.05	1.41	1.35
17	O	203	CLA	C4B-NB	7.04	1.41	1.35
17	1	610	CLA	C4B-NB	7.02	1.41	1.35
17	L	202	CLA	C4B-NB	7.01	1.41	1.35
17	4	602	CLA	C4B-NB	7.00	1.41	1.35
17	A	821	CLA	C4B-NB	6.98	1.41	1.35
17	4	607	CLA	C4B-NB	6.95	1.41	1.35
17	4	601	CLA	C4B-NB	6.94	1.41	1.35
17	O	204	CLA	C4B-NB	6.93	1.41	1.35
17	3	210	CLA	C4B-NB	6.90	1.41	1.35
17	3	211	CLA	C4B-NB	6.90	1.41	1.35
17	3	212	CLA	C4B-NB	6.88	1.41	1.35
17	3	205	CLA	C4B-NB	6.87	1.41	1.35
17	5	604	CLA	C4B-NB	6.87	1.41	1.35
17	B	813	CLA	C4B-NB	6.85	1.41	1.35
17	B	818	CLA	C4B-NB	6.84	1.41	1.35
17	B	837	CLA	C4B-NB	6.83	1.41	1.35
17	3	202	CLA	C4B-NB	6.79	1.41	1.35
17	2	610	CLA	C4B-NB	6.76	1.41	1.35
17	2	612	CLA	C4B-NB	6.76	1.41	1.35
17	1	612	CLA	C4B-NB	6.75	1.41	1.35
17	5	610	CLA	C4B-NB	6.73	1.41	1.35
17	1	609	CLA	C4B-NB	6.73	1.41	1.35
17	3	204	CLA	C4B-NB	6.72	1.41	1.35
17	B	824	CLA	C4B-NB	6.70	1.41	1.35
17	5	603	CLA	C4B-NB	6.70	1.41	1.35
17	5	608	CLA	C4B-NB	6.68	1.41	1.35
17	2	609	CLA	C4B-NB	6.68	1.41	1.35
17	A	820	CLA	C4B-NB	6.68	1.41	1.35
17	2	606	CLA	C4B-NB	6.67	1.41	1.35
17	4	603	CLA	C4B-NB	6.65	1.41	1.35
17	B	843	CLA	C4B-NB	6.63	1.41	1.35
17	1	608	CLA	C4B-NB	6.63	1.41	1.35
17	B	831	CLA	C4B-NB	6.62	1.41	1.35
17	B	823	CLA	C4B-NB	6.61	1.41	1.35
17	F	302	CLA	C4B-NB	6.58	1.41	1.35
17	3	209	CLA	C4B-NB	6.57	1.41	1.35
17	2	611	CLA	C4B-NB	6.57	1.41	1.35
17	B	815	CLA	C4B-NB	6.56	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	826	CLA	C4B-NB	6.53	1.41	1.35
17	A	808	CLA	C4B-NB	6.52	1.41	1.35
17	B	829	CLA	C4B-NB	6.52	1.41	1.35
17	3	213	CLA	C4B-NB	6.51	1.41	1.35
17	B	825	CLA	C4B-NB	6.48	1.41	1.35
17	3	208	CLA	C4B-NB	6.47	1.41	1.35
17	A	818	CLA	C4B-NB	6.47	1.41	1.35
17	A	814	CLA	C4B-NB	6.47	1.41	1.35
17	O	201	CLA	C4B-NB	6.46	1.41	1.35
17	A	829	CLA	C4B-NB	6.43	1.40	1.35
17	A	833	CLA	C4B-NB	6.42	1.40	1.35
17	F	303	CLA	C4B-NB	6.39	1.40	1.35
17	K	102	CLA	C4B-NB	6.39	1.40	1.35
17	3	207	CLA	C4B-NB	6.38	1.40	1.35
17	J	103	CLA	C4B-NB	6.37	1.40	1.35
17	A	810	CLA	C4B-NB	6.37	1.40	1.35
17	A	819	CLA	C4B-NB	6.37	1.40	1.35
17	2	601	CLA	C4B-NB	6.37	1.40	1.35
17	B	814	CLA	C4B-NB	6.35	1.40	1.35
17	K	103	CLA	C4B-NB	6.34	1.40	1.35
17	3	203	CLA	C4B-NB	6.34	1.40	1.35
17	1	603	CLA	C4B-NB	6.33	1.40	1.35
17	B	807	CLA	C4B-NB	6.32	1.40	1.35
17	B	820	CLA	C4B-NB	6.30	1.40	1.35
17	B	836	CLA	C4B-NB	6.29	1.40	1.35
17	A	827	CLA	C4B-NB	6.29	1.40	1.35
17	B	833	CLA	C4B-NB	6.28	1.40	1.35
17	B	834	CLA	C4B-NB	6.27	1.40	1.35
17	2	608	CLA	C4B-NB	6.27	1.40	1.35
17	B	812	CLA	C4B-NB	6.25	1.40	1.35
17	A	830	CLA	C4B-NB	6.25	1.40	1.35
17	B	808	CLA	C4B-NB	6.25	1.40	1.35
17	L	203	CLA	C4B-NB	6.25	1.40	1.35
17	2	605	CLA	C4B-NB	6.24	1.40	1.35
17	B	839	CLA	C4B-NB	6.23	1.40	1.35
17	B	842	CLA	C4B-NB	6.23	1.40	1.35
16	A	801	CL0	C1C-NC	-6.22	1.28	1.37
17	L	204	CLA	C4B-NB	6.22	1.40	1.35
17	A	836	CLA	C4B-NB	6.21	1.40	1.35
17	A	813	CLA	C4B-NB	6.20	1.40	1.35
17	1	606	CLA	C4B-NB	6.19	1.40	1.35
17	A	815	CLA	C4B-NB	6.19	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	819	CLA	C4B-NB	6.18	1.40	1.35
17	A	809	CLA	C4B-NB	6.18	1.40	1.35
17	A	828	CLA	C4B-NB	6.16	1.40	1.35
17	A	839	CLA	C4B-NB	6.16	1.40	1.35
17	A	831	CLA	C4B-NB	6.15	1.40	1.35
17	1	611	CLA	C4B-NB	6.15	1.40	1.35
17	2	607	CLA	C4B-NB	6.15	1.40	1.35
17	1	601	CLA	C4B-NB	6.13	1.40	1.35
17	A	805	CLA	C4B-NB	6.12	1.40	1.35
17	B	841	CLA	C4B-NB	6.12	1.40	1.35
17	B	810	CLA	C4B-NB	6.11	1.40	1.35
17	B	803	CLA	C4B-NB	6.11	1.40	1.35
17	J	101	CLA	C4B-NB	6.11	1.40	1.35
17	B	822	CLA	C4B-NB	6.09	1.40	1.35
17	B	811	CLA	C4B-NB	6.09	1.40	1.35
17	2	603	CLA	C4B-NB	6.09	1.40	1.35
17	A	802	CLA	C4B-NB	6.08	1.40	1.35
25	5	614	ZEX	C27-C26	6.07	1.52	1.46
17	F	301	CLA	C4B-NB	6.04	1.40	1.35
16	A	801	CL0	CMA-C3A	-6.04	1.40	1.53
17	1	604	CLA	C4B-NB	6.04	1.40	1.35
17	B	817	CLA	C4B-NB	6.03	1.40	1.35
17	A	803	CLA	C4B-NB	5.99	1.40	1.35
17	A	817	CLA	C4B-NB	5.99	1.40	1.35
17	B	827	CLA	C4B-NB	5.99	1.40	1.35
17	A	823	CLA	C4B-NB	5.98	1.40	1.35
17	A	838	CLA	C4B-NB	5.96	1.40	1.35
17	1	607	CLA	C4B-NB	5.96	1.40	1.35
17	B	832	CLA	C4B-NB	5.96	1.40	1.35
17	A	825	CLA	C4B-NB	5.95	1.40	1.35
17	B	821	CLA	C4B-NB	5.94	1.40	1.35
17	A	804	CLA	C4B-NB	5.93	1.40	1.35
17	5	606	CLA	C4B-NB	5.87	1.40	1.35
17	1	602	CLA	C4B-NB	5.80	1.40	1.35
17	B	840	CLA	C4B-NB	5.79	1.40	1.35
17	2	604	CLA	C4B-NB	5.77	1.40	1.35
17	A	807	CLA	C4B-NB	5.76	1.40	1.35
17	A	806	CLA	C4B-NB	5.75	1.40	1.35
17	A	837	CLA	C4B-NB	5.72	1.40	1.35
17	B	809	CLA	C4B-NB	5.71	1.40	1.35
17	A	824	CLA	C4B-NB	5.71	1.40	1.35
17	J	102	CLA	C4B-NB	5.71	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	201	ZEX	C27-C26	5.70	1.52	1.46
17	A	812	CLA	C4B-NB	5.69	1.40	1.35
17	A	822	CLA	C4B-NB	5.68	1.40	1.35
25	2	616	ZEX	C27-C26	5.67	1.52	1.46
25	3	218	ZEX	C27-C26	5.61	1.52	1.46
17	B	806	CLA	C4B-NB	5.60	1.40	1.35
25	5	616	ZEX	C27-C26	5.60	1.52	1.46
17	B	828	CLA	C4B-NB	5.59	1.40	1.35
17	A	811	CLA	C4B-NB	5.58	1.40	1.35
17	B	804	CLA	C4B-NB	5.57	1.40	1.35
17	A	835	CLA	C4B-NB	5.54	1.40	1.35
17	B	838	CLA	C4B-NB	5.40	1.40	1.35
17	B	816	CLA	C4B-NB	5.40	1.40	1.35
17	B	801	CLA	C4B-NB	5.39	1.40	1.35
17	A	848	CLA	C4B-NB	5.37	1.40	1.35
17	A	826	CLA	C4B-NB	5.36	1.40	1.35
17	A	816	CLA	C4B-NB	5.31	1.39	1.35
25	4	617	ZEX	C27-C26	5.19	1.51	1.46
25	4	612	ZEX	C27-C26	5.15	1.51	1.46
17	A	832	CLA	C4B-NB	5.06	1.39	1.35
25	5	615	ZEX	C27-C26	5.05	1.51	1.46
16	A	801	CL0	C3D-C4D	-5.02	1.32	1.44
25	5	617	ZEX	C27-C26	5.00	1.51	1.46
25	4	614	ZEX	C27-C26	4.95	1.51	1.46
17	B	830	CLA	C4B-NB	4.93	1.39	1.35
25	4	615	ZEX	C27-C26	4.90	1.51	1.46
25	1	616	ZEX	C27-C26	4.83	1.51	1.46
25	3	217	ZEX	C27-C26	4.83	1.51	1.46
17	A	828	CLA	CMB-C2B	-4.82	1.41	1.51
25	3	216	ZEX	C27-C26	4.79	1.51	1.46
25	4	616	ZEX	C27-C26	4.76	1.51	1.46
25	1	614	ZEX	C27-C26	4.66	1.51	1.46
16	A	801	CL0	C2A-C1A	-4.55	1.42	1.52
25	4	613	ZEX	C27-C26	4.54	1.51	1.46
25	2	616	ZEX	C28-C29	4.51	1.55	1.45
17	B	838	CLA	C4D-ND	-4.50	1.31	1.37
16	A	801	CL0	C3A-C2A	-4.48	1.41	1.54
25	1	613	ZEX	C27-C26	4.48	1.51	1.46
16	A	801	CL0	MG-ND	-4.46	1.96	2.05
25	3	214	ZEX	C27-C26	4.46	1.51	1.46
25	1	615	ZEX	C27-C26	4.44	1.51	1.46
17	B	832	CLA	CMB-C2B	-4.41	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	616	ZEX	C24-C25	4.33	1.54	1.50
17	5	609	CLA	C1D-ND	4.33	1.43	1.37
17	B	802	CLA	C4B-NB	4.33	1.39	1.35
25	3	215	ZEX	C27-C26	4.32	1.50	1.46
17	A	825	CLA	C4D-ND	-4.32	1.31	1.37
17	5	606	CLA	CMD-C2D	-4.32	1.41	1.50
25	3	218	ZEX	C28-C29	4.31	1.55	1.45
17	B	802	CLA	C4D-ND	-4.26	1.31	1.37
25	3	214	ZEX	C24-C25	4.23	1.54	1.50
25	5	615	ZEX	C24-C25	4.22	1.54	1.50
17	A	824	CLA	C4D-ND	-4.19	1.31	1.37
25	2	615	ZEX	C27-C26	4.18	1.50	1.46
17	B	830	CLA	C4D-ND	-4.14	1.32	1.37
25	1	617	ZEX	C27-C26	4.12	1.50	1.46
16	A	801	CL0	CMD-C2D	-4.11	1.42	1.50
25	4	614	ZEX	C7-C6	4.11	1.59	1.45
25	3	201	ZEX	C7-C6	4.10	1.59	1.45
25	3	218	ZEX	C7-C6	4.09	1.59	1.45
25	5	615	ZEX	C35-C34	4.09	1.56	1.43
25	1	613	ZEX	C24-C25	4.08	1.54	1.50
18	A	840	PQN	C2-C1	-4.08	1.39	1.48
17	4	611	CLA	C1D-ND	4.06	1.42	1.37
17	2	608	CLA	C4D-ND	-4.06	1.32	1.37
17	B	802	CLA	C3B-C2B	-4.05	1.34	1.40
18	B	844	PQN	C2-C1	-4.05	1.39	1.48
17	A	807	CLA	C4D-ND	-4.05	1.32	1.37
17	A	803	CLA	C4D-ND	-4.04	1.32	1.37
17	B	840	CLA	C4D-ND	-4.04	1.32	1.37
25	4	612	ZEX	C7-C6	4.04	1.59	1.45
17	A	828	CLA	C4D-ND	-4.03	1.32	1.37
17	B	802	CLA	C3B-CAB	-4.03	1.39	1.47
17	B	839	CLA	C4D-ND	-4.03	1.32	1.37
17	B	831	CLA	CMB-C2B	-4.03	1.43	1.51
17	A	816	CLA	C4D-ND	-4.02	1.32	1.37
25	5	616	ZEX	C28-C29	4.02	1.54	1.45
25	4	615	ZEX	C28-C29	4.01	1.54	1.45
25	1	617	ZEX	C7-C6	4.00	1.59	1.45
17	K	103	CLA	C4D-ND	-4.00	1.32	1.37
25	3	218	ZEX	C35-C34	3.99	1.55	1.43
17	A	822	CLA	C4D-ND	-3.98	1.32	1.37
25	2	617	ZEX	C27-C26	3.98	1.50	1.46
17	B	822	CLA	C4D-ND	-3.97	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	617	ZEX	C28-C29	3.97	1.54	1.45
25	4	615	ZEX	C7-C6	3.97	1.59	1.45
25	5	616	ZEX	C7-C6	3.97	1.59	1.45
20	A	845	BCR	C30-C25	-3.96	1.48	1.53
17	A	811	CLA	C4D-ND	-3.96	1.32	1.37
25	5	615	ZEX	C7-C6	3.95	1.59	1.45
17	A	848	CLA	C4D-ND	-3.94	1.32	1.37
17	A	817	CLA	CMB-C2B	-3.94	1.43	1.51
17	4	605	CLA	C1D-ND	3.93	1.42	1.37
17	B	816	CLA	C4D-ND	-3.93	1.32	1.37
25	2	616	ZEX	C7-C6	3.92	1.59	1.45
17	4	610	CLA	C1D-ND	3.92	1.42	1.37
17	B	814	CLA	C4D-ND	-3.92	1.32	1.37
25	4	613	ZEX	C7-C6	3.92	1.59	1.45
17	A	826	CLA	C4D-ND	-3.91	1.32	1.37
17	A	819	CLA	C4D-ND	-3.91	1.32	1.37
25	5	614	ZEX	C7-C6	3.91	1.59	1.45
17	A	831	CLA	C4D-ND	-3.90	1.32	1.37
17	B	809	CLA	C4D-ND	-3.90	1.32	1.37
17	B	834	CLA	C4D-ND	-3.90	1.32	1.37
25	1	614	ZEX	C24-C25	3.90	1.54	1.50
17	B	804	CLA	C4D-ND	-3.90	1.32	1.37
25	4	616	ZEX	C7-C6	3.90	1.58	1.45
25	5	617	ZEX	C7-C6	3.89	1.58	1.45
17	B	814	CLA	CAB-C3B	-3.89	1.43	1.51
17	B	827	CLA	C4D-ND	-3.89	1.32	1.37
17	A	835	CLA	C4D-ND	-3.89	1.32	1.37
25	1	614	ZEX	C7-C6	3.88	1.58	1.45
25	3	215	ZEX	C7-C6	3.88	1.58	1.45
25	2	616	ZEX	C35-C34	3.88	1.55	1.43
25	5	614	ZEX	C28-C29	3.88	1.54	1.45
17	5	601	CLA	C1D-ND	3.87	1.42	1.37
25	2	615	ZEX	C7-C6	3.86	1.58	1.45
25	3	214	ZEX	C7-C6	3.86	1.58	1.45
17	L	203	CLA	C4D-ND	-3.86	1.32	1.37
25	2	614	ZEX	C7-C6	3.86	1.58	1.45
25	1	616	ZEX	C7-C6	3.86	1.58	1.45
25	5	616	ZEX	C24-C25	3.84	1.54	1.50
17	A	830	CLA	C4D-ND	-3.84	1.32	1.37
25	4	617	ZEX	C7-C6	3.84	1.58	1.45
17	A	837	CLA	C4D-ND	-3.84	1.32	1.37
17	B	835	CLA	C4D-ND	-3.84	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	216	ZEX	C7-C6	3.83	1.58	1.45
17	1	602	CLA	C4D-ND	-3.83	1.32	1.37
20	J	105	BCR	C30-C25	-3.83	1.48	1.53
25	2	616	ZEX	C31-C30	3.83	1.55	1.43
25	2	614	ZEX	C35-C34	3.83	1.55	1.43
17	3	208	CLA	C1D-ND	3.83	1.42	1.37
17	2	602	CLA	C4D-ND	-3.82	1.32	1.37
17	B	841	CLA	C4D-ND	-3.82	1.32	1.37
16	A	801	CL0	CAA-C2A	-3.82	1.47	1.54
25	3	217	ZEX	C7-C6	3.82	1.58	1.45
17	B	836	CLA	C4D-ND	-3.82	1.32	1.37
17	4	601	CLA	C1D-ND	3.81	1.42	1.37
17	5	607	CLA	C3B-C2B	-3.81	1.35	1.40
25	4	617	ZEX	C24-C25	3.81	1.54	1.50
25	5	615	ZEX	C28-C29	3.80	1.54	1.45
17	A	804	CLA	C4D-ND	-3.80	1.32	1.37
17	B	806	CLA	C4D-ND	-3.79	1.32	1.37
17	J	101	CLA	C4D-ND	-3.79	1.32	1.37
25	5	616	ZEX	C35-C34	3.79	1.55	1.43
17	B	804	CLA	C3B-C2B	-3.79	1.35	1.40
25	1	613	ZEX	C7-C6	3.78	1.58	1.45
17	A	827	CLA	CMB-C2B	-3.78	1.43	1.51
17	3	204	CLA	C4D-ND	-3.78	1.32	1.37
17	5	613	CLA	C1D-ND	3.78	1.42	1.37
25	1	616	ZEX	C28-C29	3.78	1.54	1.45
20	J	105	BCR	C1-C6	-3.78	1.48	1.53
17	O	203	CLA	C1D-ND	3.78	1.42	1.37
25	3	216	ZEX	C28-C29	3.77	1.54	1.45
17	5	610	CLA	C1D-ND	3.77	1.42	1.37
17	A	813	CLA	C4D-ND	-3.77	1.32	1.37
25	3	201	ZEX	C35-C34	3.77	1.55	1.43
17	B	810	CLA	C4D-ND	-3.76	1.32	1.37
25	3	217	ZEX	C28-C29	3.75	1.54	1.45
17	O	204	CLA	C1D-ND	3.75	1.42	1.37
17	A	836	CLA	C4D-ND	-3.75	1.32	1.37
17	4	604	CLA	C1D-ND	3.74	1.42	1.37
17	2	604	CLA	C4D-ND	-3.74	1.32	1.37
20	O	202	BCR	C30-C25	-3.74	1.48	1.53
25	4	614	ZEX	C28-C29	3.74	1.54	1.45
17	4	609	CLA	C1D-ND	3.74	1.42	1.37
25	1	615	ZEX	C7-C6	3.73	1.58	1.45
17	O	201	CLA	C4D-ND	-3.73	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	826	CLA	C4D-ND	-3.72	1.32	1.37
17	3	205	CLA	C4D-ND	-3.72	1.32	1.37
20	A	846	BCR	C30-C25	-3.72	1.48	1.53
25	4	617	ZEX	C35-C34	3.72	1.55	1.43
25	2	614	ZEX	C27-C26	3.72	1.50	1.46
17	B	831	CLA	C4D-ND	-3.72	1.32	1.37
17	5	608	CLA	C1D-ND	3.72	1.42	1.37
17	1	612	CLA	C1D-ND	3.72	1.42	1.37
17	B	812	CLA	C4D-ND	-3.71	1.32	1.37
17	3	203	CLA	C4D-ND	-3.70	1.32	1.37
17	1	603	CLA	C4D-ND	-3.70	1.32	1.37
17	1	608	CLA	C4D-ND	-3.70	1.32	1.37
17	B	829	CLA	C4D-ND	-3.69	1.32	1.37
25	4	613	ZEX	C8-C9	3.69	1.53	1.45
17	B	818	CLA	C4D-ND	-3.69	1.32	1.37
25	5	614	ZEX	C35-C34	3.69	1.54	1.43
17	1	605	CLA	C1D-ND	3.68	1.42	1.37
17	2	609	CLA	C1D-ND	3.68	1.42	1.37
17	J	102	CLA	C4D-ND	-3.68	1.32	1.37
17	2	601	CLA	C4D-ND	-3.68	1.32	1.37
17	A	833	CLA	C4D-ND	-3.68	1.32	1.37
25	3	216	ZEX	C35-C34	3.67	1.54	1.43
17	B	842	CLA	CMB-C2B	-3.67	1.44	1.51
17	A	806	CLA	C4D-ND	-3.67	1.32	1.37
17	B	814	CLA	CMB-C2B	-3.66	1.44	1.51
17	B	833	CLA	C4D-ND	-3.66	1.32	1.37
25	4	614	ZEX	C35-C34	3.66	1.54	1.43
17	A	838	CLA	C4D-ND	-3.66	1.32	1.37
25	1	613	ZEX	C35-C34	3.65	1.54	1.43
17	B	812	CLA	CMB-C2B	-3.65	1.44	1.51
17	B	825	CLA	C4D-ND	-3.65	1.32	1.37
25	4	615	ZEX	C35-C34	3.65	1.54	1.43
17	4	608	CLA	C1D-ND	3.65	1.42	1.37
17	B	828	CLA	C4D-ND	-3.65	1.32	1.37
17	3	208	CLA	C4D-ND	-3.64	1.32	1.37
25	4	612	ZEX	C35-C34	3.64	1.54	1.43
25	4	613	ZEX	C28-C29	3.64	1.53	1.45
20	L	201	BCR	C1-C6	-3.64	1.48	1.53
20	K	101	BCR	C1-C6	-3.63	1.48	1.53
25	1	617	ZEX	C35-C34	3.63	1.54	1.43
17	2	603	CLA	C4D-ND	-3.63	1.32	1.37
25	1	616	ZEX	C35-C34	3.63	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	611	CLA	C1D-ND	3.63	1.42	1.37
17	B	815	CLA	C4D-ND	-3.63	1.32	1.37
17	5	612	CLA	C1D-ND	3.63	1.42	1.37
17	L	204	CLA	C4D-ND	-3.63	1.32	1.37
17	A	808	CLA	C4D-ND	-3.62	1.32	1.37
17	A	815	CLA	C4D-ND	-3.62	1.32	1.37
25	3	217	ZEX	C35-C34	3.62	1.54	1.43
17	B	806	CLA	C3B-C2B	-3.61	1.35	1.40
17	A	814	CLA	C4D-ND	-3.61	1.32	1.37
17	A	818	CLA	C4D-ND	-3.61	1.32	1.37
18	B	844	PQN	C10-C1	-3.61	1.41	1.48
17	3	206	CLA	CMB-C2B	-3.61	1.44	1.51
17	A	829	CLA	C4D-ND	-3.61	1.32	1.37
25	4	615	ZEX	C8-C9	3.61	1.53	1.45
25	4	616	ZEX	C35-C34	3.61	1.54	1.43
17	F	301	CLA	C4D-ND	-3.61	1.32	1.37
17	A	810	CLA	C4D-ND	-3.61	1.32	1.37
17	A	809	CLA	C4D-ND	-3.60	1.32	1.37
20	B	847	BCR	C30-C25	-3.60	1.48	1.53
17	B	823	CLA	C4D-ND	-3.60	1.32	1.37
20	A	845	BCR	C1-C6	-3.59	1.48	1.53
25	3	218	ZEX	C24-C25	3.59	1.54	1.50
17	B	832	CLA	C4D-ND	-3.59	1.32	1.37
17	1	611	CLA	C4D-ND	-3.59	1.32	1.37
17	4	607	CLA	C1D-ND	3.59	1.42	1.37
17	B	808	CLA	C4D-ND	-3.59	1.32	1.37
25	3	218	ZEX	C8-C9	3.59	1.53	1.45
17	A	823	CLA	C4D-ND	-3.59	1.32	1.37
17	B	843	CLA	C4D-ND	-3.58	1.32	1.37
17	A	814	CLA	C1D-ND	3.58	1.42	1.37
25	3	214	ZEX	C28-C29	3.58	1.53	1.45
20	A	846	BCR	C1-C6	-3.58	1.48	1.53
25	1	613	ZEX	C28-C29	3.58	1.53	1.45
17	A	836	CLA	CMB-C2B	-3.58	1.44	1.51
17	A	827	CLA	C4D-ND	-3.57	1.32	1.37
17	B	813	CLA	C4D-ND	-3.57	1.32	1.37
25	5	616	ZEX	C31-C30	3.57	1.54	1.43
25	3	214	ZEX	C35-C34	3.57	1.54	1.43
17	2	607	CLA	C1D-ND	3.56	1.42	1.37
25	5	615	ZEX	C31-C30	3.56	1.54	1.43
25	4	617	ZEX	C28-C29	3.55	1.53	1.45
17	B	842	CLA	C4D-ND	-3.55	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	606	CLA	C4D-ND	-3.55	1.32	1.37
25	4	613	ZEX	C35-C34	3.55	1.54	1.43
17	B	801	CLA	C4D-ND	-3.55	1.32	1.37
17	5	605	CLA	C1D-ND	3.55	1.42	1.37
16	A	801	CL0	C3A-C4A	-3.55	1.40	1.51
25	2	617	ZEX	C35-C34	3.54	1.54	1.43
25	5	617	ZEX	C35-C34	3.54	1.54	1.43
20	B	805	BCR	C30-C25	-3.53	1.48	1.53
17	F	302	CLA	C4D-ND	-3.52	1.32	1.37
17	A	817	CLA	C3B-C2B	-3.52	1.35	1.40
17	3	209	CLA	C4D-ND	-3.52	1.32	1.37
17	1	604	CLA	C4D-ND	-3.52	1.32	1.37
17	A	848	CLA	CMC-C2C	-3.52	1.43	1.50
17	B	824	CLA	C4D-ND	-3.51	1.32	1.37
17	1	607	CLA	CMD-C2D	-3.51	1.43	1.50
25	3	216	ZEX	C24-C25	3.51	1.53	1.50
18	B	844	PQN	C3-C4	-3.51	1.38	1.47
17	A	827	CLA	C3B-C2B	-3.51	1.35	1.40
25	3	201	ZEX	C24-C25	3.51	1.53	1.50
25	4	612	ZEX	C28-C29	3.50	1.53	1.45
25	3	218	ZEX	C15-C14	3.50	1.54	1.43
25	2	617	ZEX	C7-C6	3.50	1.57	1.45
17	4	603	CLA	C1D-ND	3.49	1.42	1.37
17	2	607	CLA	C4D-ND	-3.49	1.32	1.37
17	B	835	CLA	C3B-C2B	-3.49	1.35	1.40
17	B	828	CLA	CMD-C2D	-3.49	1.43	1.50
25	3	215	ZEX	C24-C25	3.49	1.53	1.50
17	B	843	CLA	C1D-ND	3.49	1.42	1.37
17	4	602	CLA	C4D-ND	-3.48	1.32	1.37
25	4	616	ZEX	C28-C29	3.48	1.53	1.45
25	3	214	ZEX	C31-C30	3.48	1.54	1.43
17	A	812	CLA	C4D-ND	-3.48	1.32	1.37
17	5	607	CLA	CHC-C1C	3.48	1.43	1.35
17	3	207	CLA	C4D-ND	-3.48	1.32	1.37
25	3	218	ZEX	C31-C30	3.47	1.54	1.43
17	B	807	CLA	C4D-ND	-3.47	1.32	1.37
17	B	803	CLA	C4D-ND	-3.47	1.32	1.37
17	5	608	CLA	C4D-ND	-3.47	1.32	1.37
17	K	102	CLA	C4D-ND	-3.47	1.32	1.37
25	4	614	ZEX	C8-C9	3.47	1.53	1.45
25	3	218	ZEX	C11-C10	3.47	1.54	1.43
17	B	820	CLA	C4D-ND	-3.47	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	828	CLA	C3B-C2B	-3.46	1.35	1.40
17	A	834	CLA	C4D-ND	-3.46	1.32	1.37
17	A	820	CLA	C4D-ND	-3.46	1.32	1.37
17	B	821	CLA	C4D-ND	-3.46	1.32	1.37
17	B	836	CLA	C1D-ND	3.46	1.42	1.37
17	A	817	CLA	C4D-ND	-3.46	1.32	1.37
25	3	201	ZEX	C28-C29	3.45	1.53	1.45
17	A	832	CLA	C4D-ND	-3.45	1.32	1.37
25	1	614	ZEX	C31-C30	3.45	1.54	1.43
25	1	614	ZEX	C35-C34	3.45	1.54	1.43
25	3	217	ZEX	C31-C30	3.45	1.54	1.43
20	L	201	BCR	C30-C25	-3.45	1.49	1.53
20	J	104	BCR	C1-C6	-3.44	1.49	1.53
17	2	612	CLA	C4D-ND	-3.44	1.33	1.37
17	B	817	CLA	C4D-ND	-3.44	1.33	1.37
17	3	213	CLA	C1D-ND	3.44	1.42	1.37
17	A	805	CLA	C4D-ND	-3.44	1.33	1.37
17	B	802	CLA	CMB-C2B	-3.44	1.44	1.51
17	J	102	CLA	C1D-ND	3.44	1.42	1.37
25	1	615	ZEX	C28-C29	3.44	1.53	1.45
17	5	607	CLA	C1D-ND	3.44	1.42	1.37
17	A	839	CLA	C4D-ND	-3.43	1.33	1.37
17	3	210	CLA	C1D-ND	3.43	1.42	1.37
17	3	211	CLA	C1D-ND	3.43	1.42	1.37
20	B	849	BCR	C30-C25	-3.42	1.49	1.53
25	3	215	ZEX	C35-C34	3.42	1.54	1.43
17	J	103	CLA	C4D-ND	-3.42	1.33	1.37
20	F	304	BCR	C30-C25	-3.42	1.49	1.53
17	B	839	CLA	C3B-C2B	-3.42	1.35	1.40
17	F	303	CLA	C4D-ND	-3.42	1.33	1.37
25	4	613	ZEX	C31-C30	3.41	1.54	1.43
25	4	614	ZEX	C31-C30	3.41	1.54	1.43
17	5	603	CLA	C1D-ND	3.41	1.42	1.37
17	2	613	CLA	C1D-ND	3.41	1.42	1.37
17	B	811	CLA	C4D-ND	-3.41	1.33	1.37
17	B	819	CLA	C4D-ND	-3.41	1.33	1.37
17	B	820	CLA	CMB-C2B	-3.40	1.44	1.51
17	O	205	CLA	C1D-ND	3.40	1.42	1.37
17	B	822	CLA	CMB-C2B	-3.40	1.44	1.51
17	5	603	CLA	C4D-ND	-3.40	1.33	1.37
18	A	840	PQN	C3-C4	-3.39	1.38	1.47
17	2	610	CLA	C1D-ND	3.39	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	609	CLA	C4D-ND	-3.39	1.33	1.37
17	B	804	CLA	CHC-C1C	3.39	1.43	1.35
17	1	606	CLA	C4D-ND	-3.39	1.33	1.37
16	A	801	CL0	CMB-C2B	-3.39	1.44	1.51
25	4	615	ZEX	C31-C30	3.39	1.53	1.43
17	3	202	CLA	C1D-ND	3.38	1.41	1.37
25	5	614	ZEX	C31-C30	3.38	1.53	1.43
25	5	616	ZEX	C8-C9	3.38	1.53	1.45
20	A	843	BCR	C1-C6	-3.38	1.49	1.53
17	O	203	CLA	C4D-ND	-3.38	1.33	1.37
25	2	615	ZEX	C35-C34	3.38	1.53	1.43
25	4	617	ZEX	C31-C30	3.38	1.53	1.43
17	A	834	CLA	C1D-ND	3.38	1.41	1.37
25	1	615	ZEX	C31-C30	3.37	1.53	1.43
17	1	610	CLA	C4D-ND	-3.36	1.33	1.37
25	3	216	ZEX	C31-C30	3.36	1.53	1.43
25	3	201	ZEX	C11-C10	3.36	1.53	1.43
17	B	839	CLA	CMB-C2B	-3.36	1.44	1.51
25	1	614	ZEX	C8-C9	3.36	1.53	1.45
17	L	202	CLA	C4D-ND	-3.35	1.33	1.37
17	A	821	CLA	C4D-ND	-3.35	1.33	1.37
17	1	607	CLA	C4D-ND	-3.35	1.33	1.37
25	3	201	ZEX	C31-C30	3.34	1.53	1.43
17	2	611	CLA	C4D-ND	-3.34	1.33	1.37
17	A	821	CLA	C1D-ND	3.33	1.41	1.37
17	2	608	CLA	C1D-ND	3.33	1.41	1.37
17	3	212	CLA	C1D-ND	3.33	1.41	1.37
17	2	612	CLA	C1D-ND	3.33	1.41	1.37
25	1	616	ZEX	C31-C30	3.33	1.53	1.43
25	4	616	ZEX	C31-C30	3.32	1.53	1.43
17	1	601	CLA	C1D-ND	3.32	1.41	1.37
20	L	206	BCR	C1-C6	-3.32	1.49	1.53
17	K	103	CLA	C1D-ND	3.32	1.41	1.37
17	L	202	CLA	C1D-ND	3.31	1.41	1.37
17	B	837	CLA	C4D-ND	-3.31	1.33	1.37
25	2	617	ZEX	C28-C29	3.31	1.53	1.45
17	2	605	CLA	C4D-ND	-3.31	1.33	1.37
25	3	201	ZEX	C8-C9	3.31	1.53	1.45
25	5	617	ZEX	C31-C30	3.31	1.53	1.43
17	2	604	CLA	C1D-ND	3.31	1.41	1.37
25	1	615	ZEX	C35-C34	3.31	1.53	1.43
17	B	825	CLA	CMB-C2B	-3.29	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	840	PQN	C10-C1	-3.29	1.41	1.48
17	A	839	CLA	CMB-C2B	-3.29	1.44	1.51
17	3	211	CLA	C4D-ND	-3.29	1.33	1.37
25	5	616	ZEX	C11-C10	3.28	1.53	1.43
25	4	613	ZEX	C11-C10	3.28	1.53	1.43
25	2	614	ZEX	C28-C29	3.28	1.53	1.45
25	5	615	ZEX	C8-C9	3.28	1.53	1.45
20	O	202	BCR	C1-C6	-3.28	1.49	1.53
17	B	816	CLA	C1D-ND	3.28	1.41	1.37
17	4	611	CLA	CHC-C1C	3.28	1.43	1.35
25	1	613	ZEX	C31-C30	3.27	1.53	1.43
17	B	838	CLA	C3B-C2B	-3.27	1.35	1.40
17	A	802	CLA	C4D-ND	-3.27	1.33	1.37
25	5	615	ZEX	C32-C33	3.26	1.53	1.45
25	1	617	ZEX	C28-C29	3.26	1.52	1.45
25	2	616	ZEX	C32-C33	3.26	1.52	1.45
17	2	613	CLA	C4D-ND	-3.26	1.33	1.37
17	3	213	CLA	C4D-ND	-3.25	1.33	1.37
25	1	613	ZEX	C11-C10	3.25	1.53	1.43
17	3	205	CLA	C1D-ND	3.25	1.41	1.37
17	5	602	CLA	C4D-ND	-3.25	1.33	1.37
25	3	201	ZEX	C15-C14	3.24	1.53	1.43
17	A	810	CLA	C1D-ND	3.24	1.41	1.37
25	2	616	ZEX	C15-C14	3.24	1.53	1.43
17	1	603	CLA	CMB-C2B	-3.24	1.44	1.51
25	4	612	ZEX	C31-C30	3.24	1.53	1.43
17	5	604	CLA	C4D-ND	-3.24	1.33	1.37
17	5	606	CLA	C1D-ND	3.24	1.41	1.37
17	B	831	CLA	C3B-C2B	-3.24	1.35	1.40
20	B	850	BCR	C30-C25	-3.24	1.49	1.53
17	A	805	CLA	C1D-ND	3.23	1.41	1.37
25	2	617	ZEX	C31-C30	3.23	1.53	1.43
17	5	602	CLA	C1D-ND	3.23	1.41	1.37
25	2	616	ZEX	C11-C10	3.23	1.53	1.43
25	4	612	ZEX	C11-C10	3.22	1.53	1.43
25	4	615	ZEX	C11-C10	3.22	1.53	1.43
16	A	801	CL0	CBD-CGD	-3.22	1.42	1.52
25	2	615	ZEX	C28-C29	3.22	1.52	1.45
17	2	610	CLA	C4D-ND	-3.21	1.33	1.37
17	A	804	CLA	C1D-ND	3.21	1.41	1.37
17	A	832	CLA	C1D-ND	3.21	1.41	1.37
25	5	615	ZEX	C11-C10	3.21	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	614	ZEX	C15-C14	3.21	1.53	1.43
17	B	832	CLA	CMD-C2D	-3.21	1.44	1.50
20	I	101	BCR	C30-C25	-3.21	1.49	1.53
17	3	202	CLA	C4D-ND	-3.20	1.33	1.37
17	1	610	CLA	C1D-ND	3.20	1.41	1.37
17	4	609	CLA	C4D-ND	-3.20	1.33	1.37
17	3	203	CLA	CHC-C1C	3.20	1.43	1.35
17	A	819	CLA	CMB-C2B	-3.20	1.45	1.51
17	A	827	CLA	CMD-C2D	-3.20	1.44	1.50
17	4	605	CLA	CHC-C1C	3.20	1.43	1.35
17	1	601	CLA	C4D-ND	-3.19	1.33	1.37
25	1	617	ZEX	C8-C9	3.19	1.52	1.45
25	3	218	ZEX	C1-C6	3.19	1.58	1.53
17	4	602	CLA	CHC-C1C	3.19	1.43	1.35
25	2	615	ZEX	C8-C9	3.19	1.52	1.45
17	B	837	CLA	C1D-ND	3.19	1.41	1.37
25	3	215	ZEX	C31-C30	3.19	1.53	1.43
17	4	604	CLA	C4D-ND	-3.18	1.33	1.37
17	A	836	CLA	C3B-C2B	-3.18	1.36	1.40
17	A	822	CLA	C1D-ND	3.18	1.41	1.37
16	A	801	CL0	MG-NC	-3.18	1.98	2.06
17	2	608	CLA	CHC-C1C	3.18	1.43	1.35
25	3	218	ZEX	C12-C13	3.18	1.52	1.45
25	5	617	ZEX	C8-C9	3.18	1.52	1.45
17	A	827	CLA	CHC-C1C	3.18	1.43	1.35
25	3	217	ZEX	C8-C9	3.17	1.52	1.45
17	5	611	CLA	C4D-ND	-3.16	1.33	1.37
17	3	207	CLA	C1D-ND	3.16	1.41	1.37
17	1	604	CLA	C1D-ND	3.16	1.41	1.37
17	2	601	CLA	C1D-ND	3.16	1.41	1.37
17	4	608	CLA	CHC-C1C	3.16	1.43	1.35
25	3	217	ZEX	C11-C10	3.16	1.53	1.43
25	1	617	ZEX	C31-C30	3.16	1.53	1.43
17	B	802	CLA	MG-ND	-3.15	1.99	2.05
17	5	611	CLA	CHC-C1C	3.15	1.43	1.35
17	F	303	CLA	C1D-ND	3.15	1.41	1.37
25	3	218	ZEX	C32-C33	3.15	1.52	1.45
25	3	214	ZEX	C32-C33	3.15	1.52	1.45
17	4	603	CLA	C4D-ND	-3.14	1.33	1.37
25	1	616	ZEX	C11-C10	3.14	1.53	1.43
17	B	808	CLA	C3B-C2B	-3.14	1.36	1.40
25	5	615	ZEX	C15-C14	3.14	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	827	CLA	CMB-C2B	-3.13	1.45	1.51
17	A	803	CLA	CMB-C2B	-3.13	1.45	1.51
17	3	205	CLA	CHC-C1C	3.13	1.43	1.35
17	4	609	CLA	CHC-C1C	3.13	1.43	1.35
25	4	612	ZEX	C8-C9	3.13	1.52	1.45
17	A	832	CLA	C3B-C2B	-3.13	1.36	1.40
17	4	606	CLA	C1D-ND	3.13	1.41	1.37
17	B	822	CLA	C3B-C2B	-3.12	1.36	1.40
17	3	206	CLA	C4D-ND	-3.12	1.33	1.37
17	A	816	CLA	MG-ND	-3.12	1.99	2.05
17	5	606	CLA	C4D-ND	-3.12	1.33	1.37
25	2	616	ZEX	C8-C9	3.12	1.52	1.45
17	B	824	CLA	C1D-ND	3.12	1.41	1.37
17	1	609	CLA	C1D-ND	3.11	1.41	1.37
25	1	616	ZEX	C8-C9	3.11	1.52	1.45
25	1	614	ZEX	C11-C10	3.11	1.53	1.43
17	B	813	CLA	C1D-ND	3.11	1.41	1.37
25	5	614	ZEX	C15-C14	3.11	1.53	1.43
17	B	804	CLA	CMB-C2B	-3.11	1.45	1.51
25	4	614	ZEX	C11-C10	3.11	1.53	1.43
20	B	846	BCR	C1-C6	-3.10	1.49	1.53
25	2	614	ZEX	C31-C30	3.10	1.53	1.43
25	4	617	ZEX	C8-C9	3.10	1.52	1.45
17	A	819	CLA	C1D-ND	3.10	1.41	1.37
25	4	616	ZEX	C8-C9	3.10	1.52	1.45
25	5	616	ZEX	C32-C33	3.10	1.52	1.45
25	4	612	ZEX	C15-C14	3.10	1.53	1.43
17	A	807	CLA	C1D-ND	3.10	1.41	1.37
17	A	828	CLA	MG-ND	-3.09	1.99	2.05
20	B	849	BCR	C1-C6	-3.09	1.49	1.53
17	3	209	CLA	C1D-ND	3.09	1.41	1.37
17	3	210	CLA	C4D-ND	-3.09	1.33	1.37
17	A	823	CLA	C1D-ND	3.09	1.41	1.37
17	2	605	CLA	C1D-ND	3.09	1.41	1.37
25	5	615	ZEX	C1-C6	3.09	1.58	1.53
25	4	616	ZEX	C24-C25	3.08	1.53	1.50
16	A	801	CL0	CBB-CAB	3.08	1.49	1.29
17	4	606	CLA	C4D-ND	-3.08	1.33	1.37
17	3	206	CLA	C1D-ND	3.08	1.41	1.37
25	5	616	ZEX	C15-C14	3.08	1.53	1.43
25	4	617	ZEX	C11-C10	3.08	1.53	1.43
17	4	601	CLA	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	606	CLA	C1D-ND	3.07	1.41	1.37
17	B	809	CLA	C1D-ND	3.07	1.41	1.37
17	A	802	CLA	C1D-ND	3.07	1.41	1.37
17	B	823	CLA	C1D-ND	3.07	1.41	1.37
17	B	834	CLA	CMB-C2B	-3.07	1.45	1.51
20	A	844	BCR	C1-C6	-3.07	1.49	1.53
25	3	216	ZEX	C8-C9	3.07	1.52	1.45
20	B	848	BCR	C30-C25	-3.07	1.49	1.53
17	B	842	CLA	C3B-C2B	-3.06	1.36	1.40
17	A	825	CLA	C1D-ND	3.06	1.41	1.37
20	K	104	BCR	C1-C6	-3.06	1.49	1.53
17	A	812	CLA	C1D-ND	3.06	1.41	1.37
17	B	802	CLA	C1D-ND	3.06	1.41	1.37
17	O	201	CLA	C1D-ND	3.06	1.41	1.37
17	A	813	CLA	C1D-ND	3.06	1.41	1.37
17	5	601	CLA	CHC-C1C	3.06	1.42	1.35
25	3	215	ZEX	C8-C9	3.06	1.52	1.45
25	3	217	ZEX	C32-C33	3.06	1.52	1.45
17	B	815	CLA	C1D-ND	3.06	1.41	1.37
17	B	831	CLA	CMD-C2D	-3.06	1.44	1.50
25	4	616	ZEX	C15-C14	3.06	1.52	1.43
25	3	215	ZEX	C11-C10	3.06	1.52	1.43
25	3	216	ZEX	C11-C10	3.05	1.52	1.43
25	5	614	ZEX	C1-C6	3.05	1.58	1.53
17	A	811	CLA	C1D-ND	3.05	1.41	1.37
17	A	815	CLA	CHC-C1C	3.05	1.42	1.35
25	4	614	ZEX	C15-C14	3.05	1.52	1.43
20	A	843	BCR	C30-C25	-3.05	1.49	1.53
17	O	204	CLA	C4D-ND	-3.05	1.33	1.37
17	5	604	CLA	C1D-ND	3.05	1.41	1.37
17	B	804	CLA	C3B-CAB	-3.05	1.41	1.47
17	O	204	CLA	CHC-C1C	3.05	1.42	1.35
25	2	614	ZEX	C32-C33	3.05	1.52	1.45
25	4	615	ZEX	C15-C14	3.05	1.52	1.43
17	B	820	CLA	C3B-C2B	-3.04	1.36	1.40
17	A	829	CLA	CHC-C1C	3.04	1.42	1.35
25	5	614	ZEX	C32-C33	3.04	1.52	1.45
25	5	614	ZEX	C11-C10	3.04	1.52	1.43
25	3	214	ZEX	C15-C14	3.04	1.52	1.43
17	B	801	CLA	CMD-C2D	-3.04	1.44	1.50
17	3	209	CLA	CHC-C1C	3.04	1.42	1.35
17	B	812	CLA	C1D-ND	3.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	837	CLA	CMB-C2B	-3.04	1.45	1.51
17	3	212	CLA	C4D-ND	-3.04	1.33	1.37
25	3	218	ZEX	C8-C7	3.04	1.42	1.33
17	A	802	CLA	CHC-C1C	3.03	1.42	1.35
25	4	616	ZEX	C11-C10	3.03	1.52	1.43
17	4	604	CLA	CHC-C1C	3.03	1.42	1.35
17	5	612	CLA	C4D-ND	-3.03	1.33	1.37
17	B	822	CLA	C1D-ND	3.03	1.41	1.37
17	1	601	CLA	CMC-C2C	-3.03	1.44	1.50
17	B	838	CLA	CMB-C2B	-3.03	1.45	1.51
17	3	208	CLA	CHC-C1C	3.03	1.42	1.35
17	A	807	CLA	CMB-C2B	-3.03	1.45	1.51
25	5	616	ZEX	C1-C6	3.03	1.57	1.53
25	5	614	ZEX	C8-C9	3.02	1.52	1.45
17	1	604	CLA	CHC-C1C	3.02	1.42	1.35
17	B	808	CLA	CMB-C2B	-3.02	1.45	1.51
25	4	613	ZEX	C15-C14	3.02	1.52	1.43
17	O	203	CLA	CHC-C1C	3.02	1.42	1.35
17	4	610	CLA	CHC-C1C	3.01	1.42	1.35
17	2	609	CLA	C4D-ND	-3.00	1.33	1.37
17	B	830	CLA	C3B-CAB	-3.00	1.41	1.47
17	B	833	CLA	CMB-C2B	-3.00	1.45	1.51
25	3	216	ZEX	C15-C14	3.00	1.52	1.43
17	A	816	CLA	C3B-CAB	-3.00	1.41	1.47
17	B	832	CLA	MG-ND	-3.00	1.99	2.05
25	2	614	ZEX	C11-C10	3.00	1.52	1.43
17	A	819	CLA	CMC-C2C	-3.00	1.44	1.50
17	B	828	CLA	CHC-C1C	3.00	1.42	1.35
17	L	202	CLA	CMB-C2B	-3.00	1.45	1.51
25	1	617	ZEX	C15-C14	3.00	1.52	1.43
17	A	818	CLA	C1D-ND	3.00	1.41	1.37
23	B	851	DGD	O2G-C2G	-3.00	1.39	1.46
17	O	205	CLA	C4D-ND	-3.00	1.33	1.37
17	B	838	CLA	C3B-CAB	-3.00	1.41	1.47
17	B	821	CLA	CMB-C2B	-3.00	1.45	1.51
17	A	826	CLA	C3B-CAB	-3.00	1.41	1.47
17	B	826	CLA	C1D-ND	3.00	1.41	1.37
17	A	816	CLA	C3B-C2B	-3.00	1.36	1.40
25	1	616	ZEX	C15-C14	2.99	1.52	1.43
25	3	217	ZEX	C15-C14	2.99	1.52	1.43
17	3	210	CLA	CHC-C1C	2.99	1.42	1.35
17	4	602	CLA	C1D-ND	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	610	CLA	C4D-ND	-2.99	1.33	1.37
25	5	617	ZEX	C15-C14	2.99	1.52	1.43
25	3	214	ZEX	C8-C9	2.99	1.52	1.45
17	1	612	CLA	C4D-ND	-2.99	1.33	1.37
17	2	602	CLA	C1D-ND	2.99	1.41	1.37
17	A	829	CLA	CMB-C2B	-2.99	1.45	1.51
17	5	601	CLA	C4D-ND	-2.98	1.33	1.37
17	B	819	CLA	C1D-ND	2.98	1.41	1.37
17	A	837	CLA	CMB-C2B	-2.98	1.45	1.51
17	1	610	CLA	CHC-C1C	2.98	1.42	1.35
17	O	205	CLA	CHC-C1C	2.98	1.42	1.35
25	1	614	ZEX	C15-C14	2.98	1.52	1.43
17	O	201	CLA	CHC-C1C	2.98	1.42	1.35
17	L	204	CLA	C1D-ND	2.98	1.41	1.37
17	B	801	CLA	CHC-C1C	2.98	1.42	1.35
20	J	104	BCR	C30-C25	-2.98	1.49	1.53
25	4	617	ZEX	C15-C14	2.98	1.52	1.43
17	J	103	CLA	C1D-ND	2.98	1.41	1.37
17	B	834	CLA	C1D-ND	2.98	1.41	1.37
25	2	615	ZEX	C11-C10	2.97	1.52	1.43
18	B	844	PQN	C5-C4	-2.97	1.42	1.48
17	B	826	CLA	CHC-C1C	2.97	1.42	1.35
17	A	808	CLA	C1D-ND	2.97	1.41	1.37
25	2	617	ZEX	C11-C10	2.97	1.52	1.43
17	A	816	CLA	CMB-C2B	-2.97	1.45	1.51
17	A	832	CLA	CMB-C2B	-2.97	1.45	1.51
17	B	839	CLA	CHC-C1C	2.97	1.42	1.35
17	2	605	CLA	CHC-C1C	2.97	1.42	1.35
18	B	844	PQN	C10-C5	-2.97	1.35	1.40
25	4	616	ZEX	C32-C33	2.97	1.52	1.45
17	A	819	CLA	CHC-C1C	2.96	1.42	1.35
17	1	605	CLA	C4D-ND	-2.96	1.33	1.37
17	4	611	CLA	C4D-ND	-2.96	1.33	1.37
17	B	806	CLA	CMD-C2D	-2.96	1.44	1.50
25	1	613	ZEX	C15-C14	2.96	1.52	1.43
17	5	607	CLA	C4D-ND	-2.96	1.33	1.37
17	A	836	CLA	C1D-ND	2.96	1.41	1.37
17	A	823	CLA	CMB-C2B	-2.96	1.45	1.51
17	4	608	CLA	C4D-ND	-2.96	1.33	1.37
17	5	613	CLA	CHC-C1C	2.96	1.42	1.35
17	B	837	CLA	C3B-C2B	-2.95	1.36	1.40
20	B	850	BCR	C1-C6	-2.95	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	805	CLA	CHC-C1C	2.95	1.42	1.35
17	2	609	CLA	CHC-C1C	2.95	1.42	1.35
25	1	616	ZEX	C32-C33	2.95	1.52	1.45
17	A	826	CLA	CHC-C1C	2.95	1.42	1.35
17	1	607	CLA	C1D-ND	2.95	1.41	1.37
17	2	612	CLA	CHC-C1C	2.95	1.42	1.35
17	1	607	CLA	CHC-C1C	2.94	1.42	1.35
17	A	831	CLA	CMB-C2B	-2.94	1.45	1.51
17	B	832	CLA	C3B-C2B	-2.94	1.36	1.40
17	A	833	CLA	CMB-C2B	-2.94	1.45	1.51
17	B	807	CLA	CHC-C1C	2.94	1.42	1.35
17	2	606	CLA	C1D-ND	2.94	1.41	1.37
17	B	818	CLA	C1D-ND	2.94	1.41	1.37
25	3	215	ZEX	C28-C29	2.94	1.52	1.45
25	2	615	ZEX	C31-C30	2.94	1.52	1.43
20	B	848	BCR	C1-C6	-2.93	1.49	1.53
17	5	602	CLA	CHC-C1C	2.93	1.42	1.35
17	B	803	CLA	CMB-C2B	-2.93	1.45	1.51
17	A	811	CLA	C3B-C2B	-2.93	1.36	1.40
17	B	807	CLA	C1D-ND	2.93	1.41	1.37
17	A	809	CLA	CMB-C2B	-2.93	1.45	1.51
17	1	601	CLA	CHC-C1C	2.93	1.42	1.35
17	B	808	CLA	C1D-ND	2.92	1.41	1.37
17	A	839	CLA	C1D-ND	2.92	1.41	1.37
25	5	617	ZEX	C32-C33	2.92	1.52	1.45
25	5	617	ZEX	C11-C10	2.92	1.52	1.43
17	L	204	CLA	CHC-C1C	2.92	1.42	1.35
17	B	809	CLA	CMB-C2B	-2.92	1.45	1.51
17	A	806	CLA	CMB-C2B	-2.92	1.45	1.51
22	A	849	BGC	O2-C2	-2.92	1.37	1.43
25	1	614	ZEX	C1-C6	2.92	1.57	1.53
17	2	611	CLA	CHC-C1C	2.91	1.42	1.35
20	B	845	BCR	C1-C6	-2.91	1.49	1.53
25	3	215	ZEX	C15-C14	2.91	1.52	1.43
17	B	815	CLA	CHC-C1C	2.91	1.42	1.35
17	A	838	CLA	CMB-C2B	-2.91	1.45	1.51
17	A	837	CLA	C1D-ND	2.91	1.41	1.37
17	B	812	CLA	C3B-C2B	-2.91	1.36	1.40
17	5	604	CLA	CHC-C1C	2.91	1.42	1.35
25	4	617	ZEX	C32-C33	2.91	1.52	1.45
17	B	806	CLA	C3B-CAB	-2.91	1.42	1.47
17	B	818	CLA	CHC-C1C	2.90	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	203	CLA	C1D-ND	2.90	1.41	1.37
17	B	819	CLA	CHC-C1C	2.90	1.42	1.35
17	B	836	CLA	CHC-C1C	2.90	1.42	1.35
17	B	827	CLA	CMD-C2D	-2.90	1.44	1.50
17	A	808	CLA	CMB-C2B	-2.90	1.45	1.51
18	A	840	PQN	C10-C5	-2.90	1.35	1.40
17	B	830	CLA	CMB-C2B	-2.90	1.45	1.51
17	B	835	CLA	CHC-C1C	2.90	1.42	1.35
17	B	837	CLA	CHC-C1C	2.90	1.42	1.35
17	B	833	CLA	CHC-C1C	2.90	1.42	1.35
17	B	809	CLA	C3B-CAB	-2.90	1.42	1.47
25	1	617	ZEX	C11-C10	2.90	1.52	1.43
17	F	301	CLA	C1D-ND	2.90	1.41	1.37
17	5	609	CLA	CHC-C1C	2.90	1.42	1.35
17	B	833	CLA	C1D-ND	2.90	1.41	1.37
17	B	813	CLA	CMB-C2B	-2.90	1.45	1.51
17	2	603	CLA	C1D-ND	2.89	1.41	1.37
25	1	613	ZEX	C8-C9	2.89	1.52	1.45
17	B	809	CLA	C3B-C2B	-2.89	1.36	1.40
17	A	818	CLA	CMB-C2B	-2.89	1.45	1.51
17	K	102	CLA	CHC-C1C	2.89	1.42	1.35
17	2	602	CLA	CHC-C1C	2.89	1.42	1.35
17	J	101	CLA	C1D-ND	2.89	1.41	1.37
17	3	212	CLA	CHC-C1C	2.89	1.42	1.35
17	2	611	CLA	C1D-ND	2.89	1.41	1.37
17	A	810	CLA	CHC-C1C	2.89	1.42	1.35
17	5	610	CLA	CHC-C1C	2.89	1.42	1.35
17	1	603	CLA	C3B-C2B	-2.89	1.36	1.40
17	F	302	CLA	C1D-ND	2.89	1.41	1.37
17	B	835	CLA	CMB-C2B	-2.89	1.45	1.51
17	A	830	CLA	CHC-C1C	2.88	1.42	1.35
17	4	610	CLA	C4D-ND	-2.88	1.33	1.37
17	B	811	CLA	CMD-C2D	-2.88	1.44	1.50
17	B	838	CLA	MG-ND	-2.88	2.00	2.05
17	1	608	CLA	CHC-C1C	2.88	1.42	1.35
17	A	838	CLA	CHC-C1C	2.88	1.42	1.35
17	A	822	CLA	CHC-C1C	2.88	1.42	1.35
17	A	827	CLA	MG-ND	-2.88	2.00	2.05
17	1	609	CLA	CHC-C1C	2.87	1.42	1.35
17	5	605	CLA	CHC-C1C	2.87	1.42	1.35
17	5	605	CLA	C4D-ND	-2.87	1.33	1.37
17	2	607	CLA	CHC-C1C	2.87	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	829	CLA	C3B-C2B	-2.87	1.36	1.40
20	K	101	BCR	C30-C25	-2.87	1.49	1.53
17	1	605	CLA	CHC-C1C	2.87	1.42	1.35
17	B	829	CLA	CHC-C1C	2.87	1.42	1.35
17	B	833	CLA	C3B-C2B	-2.87	1.36	1.40
17	B	817	CLA	CHC-C1C	2.86	1.42	1.35
17	1	608	CLA	C1D-ND	2.86	1.41	1.37
17	A	811	CLA	CMB-C2B	-2.86	1.45	1.51
17	F	303	CLA	CHC-C1C	2.86	1.42	1.35
17	B	840	CLA	CHC-C1C	2.86	1.42	1.35
17	1	602	CLA	CMB-C2B	-2.86	1.45	1.51
17	3	202	CLA	CHC-C1C	2.86	1.42	1.35
25	4	617	ZEX	C1-C6	2.86	1.57	1.53
17	A	829	CLA	CMD-C2D	-2.86	1.44	1.50
17	A	806	CLA	C3B-C2B	-2.86	1.36	1.40
17	A	825	CLA	CHC-C1C	2.86	1.42	1.35
17	A	809	CLA	C1D-ND	2.85	1.41	1.37
17	5	606	CLA	CHC-C1C	2.85	1.42	1.35
25	4	613	ZEX	C24-C25	2.85	1.53	1.50
17	5	602	CLA	CMB-C2B	-2.85	1.45	1.51
17	3	205	CLA	CMB-C2B	-2.85	1.45	1.51
25	2	614	ZEX	C8-C9	2.85	1.52	1.45
17	2	613	CLA	CHC-C1C	2.85	1.42	1.35
25	3	201	ZEX	C8-C7	2.85	1.41	1.33
17	2	606	CLA	CHC-C1C	2.85	1.42	1.35
17	B	828	CLA	CMB-C2B	-2.85	1.45	1.51
17	2	610	CLA	CHC-C1C	2.85	1.42	1.35
18	B	844	PQN	C3-C2	2.84	1.40	1.35
25	4	612	ZEX	C8-C7	2.84	1.41	1.33
17	B	801	CLA	CMB-C2B	-2.84	1.45	1.51
17	K	103	CLA	CHC-C1C	2.84	1.42	1.35
17	A	810	CLA	CMB-C2B	-2.84	1.45	1.51
25	3	214	ZEX	C11-C10	2.84	1.52	1.43
17	5	607	CLA	CMB-C2B	-2.84	1.45	1.51
17	B	825	CLA	C1D-ND	2.84	1.41	1.37
17	4	605	CLA	C4D-ND	-2.84	1.33	1.37
17	4	607	CLA	CHC-C1C	2.84	1.42	1.35
25	1	617	ZEX	C24-C25	2.83	1.53	1.50
17	A	848	CLA	CHC-C1C	2.83	1.42	1.35
17	A	820	CLA	CMB-C2B	-2.83	1.45	1.51
17	A	804	CLA	CHC-C1C	2.83	1.42	1.35
17	5	613	CLA	C4D-ND	-2.83	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	834	CLA	CHC-C1C	2.83	1.42	1.35
17	A	833	CLA	CHC-C1C	2.83	1.42	1.35
25	4	615	ZEX	C1-C6	2.83	1.57	1.53
17	B	820	CLA	MG-ND	-2.83	2.00	2.05
17	A	839	CLA	C3B-C2B	-2.83	1.36	1.40
20	F	304	BCR	C1-C6	-2.83	1.49	1.53
25	2	614	ZEX	C1-C6	2.83	1.57	1.53
19	A	841	LHG	O7-C5	-2.83	1.39	1.46
17	K	102	CLA	C1D-ND	2.83	1.41	1.37
17	F	301	CLA	CHC-C1C	2.83	1.42	1.35
17	L	202	CLA	CHC-C1C	2.82	1.42	1.35
17	A	825	CLA	CMC-C2C	-2.82	1.44	1.50
17	2	608	CLA	CMC-C2C	-2.82	1.44	1.50
25	1	615	ZEX	C8-C9	2.82	1.52	1.45
25	4	615	ZEX	C32-C33	2.82	1.52	1.45
25	4	614	ZEX	C24-C25	2.82	1.53	1.50
17	B	843	CLA	CHC-C1C	2.81	1.42	1.35
17	A	813	CLA	CHC-C1C	2.81	1.42	1.35
17	2	604	CLA	CHC-C1C	2.81	1.42	1.35
17	A	829	CLA	C1D-ND	2.81	1.41	1.37
25	4	614	ZEX	C8-C7	2.81	1.41	1.33
17	5	603	CLA	CHC-C1C	2.81	1.42	1.35
17	B	839	CLA	C3B-CAB	-2.81	1.42	1.47
25	2	616	ZEX	C12-C13	2.81	1.52	1.45
17	3	211	CLA	CHC-C1C	2.81	1.42	1.35
17	3	213	CLA	CHC-C1C	2.81	1.42	1.35
17	1	601	CLA	CMB-C2B	-2.81	1.45	1.51
17	5	612	CLA	CHC-C1C	2.80	1.42	1.35
17	A	803	CLA	CMC-C2C	-2.80	1.44	1.50
25	3	201	ZEX	C32-C33	2.80	1.52	1.45
17	1	612	CLA	CHC-C1C	2.80	1.42	1.35
17	3	207	CLA	CHC-C1C	2.80	1.42	1.35
17	4	603	CLA	CHC-C1C	2.80	1.42	1.35
17	B	803	CLA	CHC-C1C	2.80	1.42	1.35
17	A	817	CLA	C1D-ND	2.80	1.41	1.37
17	3	206	CLA	CHC-C1C	2.80	1.42	1.35
17	B	821	CLA	C1D-ND	2.80	1.41	1.37
17	3	204	CLA	C1D-ND	2.80	1.41	1.37
25	4	614	ZEX	C32-C33	2.80	1.52	1.45
17	A	834	CLA	CHC-C1C	2.79	1.42	1.35
25	3	214	ZEX	C1-C6	2.79	1.57	1.53
17	J	103	CLA	CHC-C1C	2.79	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	608	CLA	CHC-C1C	2.79	1.42	1.35
17	B	833	CLA	CMD-C2D	-2.79	1.44	1.50
25	1	616	ZEX	C24-C25	2.79	1.53	1.50
17	A	809	CLA	CHC-C1C	2.79	1.42	1.35
17	A	822	CLA	CMC-C2C	-2.79	1.44	1.50
17	B	841	CLA	CMB-C2B	-2.79	1.45	1.51
17	5	604	CLA	CMB-C2B	-2.79	1.45	1.51
25	4	615	ZEX	C8-C7	2.79	1.41	1.33
17	A	816	CLA	CMD-C2D	-2.79	1.44	1.50
17	A	823	CLA	CMD-C2D	-2.78	1.44	1.50
17	B	816	CLA	CHC-C1C	2.78	1.42	1.35
17	B	830	CLA	C3B-C2B	-2.78	1.36	1.40
17	A	826	CLA	C3B-C2B	-2.78	1.36	1.40
17	B	838	CLA	C1D-ND	2.78	1.41	1.37
25	2	615	ZEX	C15-C14	2.78	1.52	1.43
17	A	822	CLA	CMB-C2B	-2.78	1.45	1.51
17	B	803	CLA	C3B-C2B	-2.78	1.36	1.40
17	F	302	CLA	CMB-C2B	-2.77	1.45	1.51
17	B	816	CLA	CMB-C2B	-2.77	1.45	1.51
17	A	832	CLA	C3B-CAB	-2.77	1.42	1.47
17	A	848	CLA	MG-ND	-2.77	2.00	2.05
17	A	822	CLA	C3B-C2B	-2.77	1.36	1.40
17	A	830	CLA	CMB-C2B	-2.77	1.45	1.51
17	2	601	CLA	CHC-C1C	2.77	1.42	1.35
25	1	615	ZEX	C11-C10	2.77	1.52	1.43
25	4	612	ZEX	C32-C33	2.77	1.51	1.45
17	B	836	CLA	CMB-C2B	-2.77	1.45	1.51
17	A	826	CLA	CMB-C2B	-2.77	1.45	1.51
17	B	811	CLA	C3B-C2B	-2.77	1.36	1.40
17	B	814	CLA	MG-ND	-2.77	2.00	2.05
17	J	101	CLA	CMC-C2C	-2.76	1.44	1.50
17	A	812	CLA	CHC-C1C	2.76	1.42	1.35
18	A	840	PQN	C3-C2	2.76	1.40	1.35
17	1	611	CLA	CHC-C1C	2.76	1.42	1.35
17	B	830	CLA	CMC-C2C	-2.76	1.44	1.50
17	3	203	CLA	CMC-C2C	-2.76	1.44	1.50
17	A	823	CLA	C3B-C2B	-2.76	1.36	1.40
17	B	829	CLA	C1D-ND	2.76	1.41	1.37
17	B	841	CLA	CHC-C1C	2.75	1.42	1.35
17	B	823	CLA	CHC-C1C	2.75	1.42	1.35
17	3	204	CLA	CHC-C1C	2.75	1.42	1.35
17	A	826	CLA	CMC-C2C	-2.75	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	828	CLA	CMC-C2C	-2.75	1.45	1.50
17	B	820	CLA	C1D-ND	2.75	1.41	1.37
17	B	839	CLA	C1D-ND	2.75	1.41	1.37
17	B	813	CLA	C3B-C2B	-2.74	1.36	1.40
17	B	820	CLA	C3B-CAB	-2.74	1.42	1.47
25	4	613	ZEX	C8-C7	2.74	1.41	1.33
17	A	835	CLA	CHC-C1C	2.74	1.42	1.35
25	5	616	ZEX	C8-C7	2.74	1.41	1.33
17	B	830	CLA	MG-ND	-2.74	2.00	2.05
17	A	824	CLA	CHC-C1C	2.74	1.42	1.35
17	4	608	CLA	CMB-C2B	-2.74	1.45	1.51
17	B	841	CLA	CMC-C2C	-2.74	1.45	1.50
25	1	613	ZEX	C32-C33	2.74	1.51	1.45
17	A	824	CLA	CMB-C2B	-2.74	1.45	1.51
25	1	614	ZEX	C8-C7	2.74	1.41	1.33
25	1	615	ZEX	C15-C14	2.74	1.51	1.43
17	B	841	CLA	C1D-ND	2.74	1.41	1.37
17	B	809	CLA	CMC-C2C	-2.74	1.45	1.50
20	B	846	BCR	C30-C25	-2.73	1.50	1.53
17	A	814	CLA	CMB-C2B	-2.73	1.46	1.51
17	A	816	CLA	C1D-ND	2.73	1.41	1.37
17	A	802	CLA	CMB-C2B	-2.73	1.46	1.51
17	B	806	CLA	CMB-C2B	-2.73	1.46	1.51
17	B	803	CLA	C1D-ND	2.73	1.41	1.37
17	4	607	CLA	C4D-ND	-2.73	1.33	1.37
17	A	805	CLA	CMB-C2B	-2.73	1.46	1.51
17	B	810	CLA	CHC-C1C	2.73	1.42	1.35
17	2	603	CLA	CHC-C1C	2.73	1.42	1.35
17	1	603	CLA	CHC-C1C	2.73	1.42	1.35
17	A	814	CLA	CHC-C1C	2.73	1.42	1.35
17	A	826	CLA	C1D-ND	2.72	1.41	1.37
17	2	602	CLA	CMB-C2B	-2.72	1.46	1.51
17	5	607	CLA	C3B-CAB	-2.72	1.42	1.47
17	B	828	CLA	MG-ND	-2.72	2.00	2.05
17	A	829	CLA	C3B-CAB	-2.72	1.42	1.47
17	B	809	CLA	CHC-C1C	2.72	1.41	1.35
25	1	614	ZEX	C28-C29	2.72	1.51	1.45
17	A	820	CLA	CHC-C1C	2.72	1.41	1.35
17	A	834	CLA	CMB-C2B	-2.72	1.46	1.51
17	B	806	CLA	MG-ND	-2.71	2.00	2.05
17	2	603	CLA	CMB-C2B	-2.71	1.46	1.51
17	1	606	CLA	C3B-CAB	-2.71	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	817	CLA	C1D-ND	2.71	1.41	1.37
20	B	805	BCR	C1-C6	-2.71	1.50	1.53
17	B	824	CLA	CHC-C1C	2.71	1.41	1.35
17	1	610	CLA	CMB-C2B	-2.71	1.46	1.51
25	2	617	ZEX	C15-C14	2.71	1.51	1.43
17	1	602	CLA	C1D-ND	2.71	1.41	1.37
20	L	206	BCR	C30-C25	-2.71	1.50	1.53
17	B	827	CLA	CHC-C1C	2.71	1.41	1.35
17	A	825	CLA	MG-ND	-2.70	2.00	2.05
17	5	606	CLA	MG-ND	-2.70	2.00	2.05
17	A	821	CLA	CMB-C2B	-2.70	1.46	1.51
17	3	208	CLA	CMB-C2B	-2.70	1.46	1.51
17	B	840	CLA	CMB-C2B	-2.70	1.46	1.51
17	B	827	CLA	C1D-ND	2.70	1.41	1.37
25	2	616	ZEX	C1-C6	2.70	1.57	1.53
17	B	810	CLA	C1D-ND	2.70	1.41	1.37
17	F	302	CLA	CHC-C1C	2.70	1.41	1.35
17	A	837	CLA	CHC-C1C	2.70	1.41	1.35
17	B	818	CLA	CMC-C2C	-2.69	1.45	1.50
17	J	101	CLA	CHC-C1C	2.69	1.41	1.35
17	B	811	CLA	CMB-C2B	-2.69	1.46	1.51
17	B	822	CLA	CMC-C2C	-2.69	1.45	1.50
17	F	303	CLA	CMB-C2B	-2.69	1.46	1.51
17	B	811	CLA	C1D-ND	2.69	1.41	1.37
17	B	842	CLA	C1D-ND	2.69	1.41	1.37
17	A	828	CLA	CMD-C2D	-2.69	1.45	1.50
25	3	201	ZEX	C12-C13	2.69	1.51	1.45
25	4	614	ZEX	C1-C6	2.68	1.57	1.53
25	4	613	ZEX	C32-C33	2.68	1.51	1.45
17	F	301	CLA	CMB-C2B	-2.68	1.46	1.51
17	L	203	CLA	CMB-C2B	-2.68	1.46	1.51
17	2	605	CLA	CMD-C2D	-2.68	1.45	1.50
17	B	818	CLA	CMB-C2B	-2.68	1.46	1.51
17	5	606	CLA	CMB-C2B	-2.68	1.46	1.51
17	B	826	CLA	CMB-C2B	-2.68	1.46	1.51
17	J	102	CLA	CHC-C1C	2.68	1.41	1.35
17	L	203	CLA	CHC-C1C	2.68	1.41	1.35
20	K	104	BCR	C30-C25	-2.68	1.50	1.53
17	1	606	CLA	CMB-C2B	-2.68	1.46	1.51
17	1	603	CLA	CMD-C2D	-2.68	1.45	1.50
17	B	820	CLA	CHC-C1C	2.68	1.41	1.35
25	4	615	ZEX	C24-C25	2.67	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	616	ZEX	C12-C13	2.67	1.51	1.45
17	A	803	CLA	CHC-C1C	2.67	1.41	1.35
17	A	815	CLA	CMB-C2B	-2.67	1.46	1.51
17	A	806	CLA	CHC-C1C	2.67	1.41	1.35
17	1	608	CLA	CMB-C2B	-2.67	1.46	1.51
17	3	207	CLA	CMB-C2B	-2.67	1.46	1.51
17	B	817	CLA	CMB-C2B	-2.66	1.46	1.51
17	L	203	CLA	C1D-ND	2.66	1.41	1.37
17	B	815	CLA	CMB-C2B	-2.66	1.46	1.51
17	A	838	CLA	C1D-ND	2.66	1.41	1.37
22	A	849	BGC	O3-C3	-2.66	1.36	1.43
25	3	216	ZEX	C32-C33	2.66	1.51	1.45
17	2	611	CLA	CMB-C2B	-2.66	1.46	1.51
17	B	831	CLA	MG-ND	-2.66	2.00	2.05
17	B	825	CLA	C3B-C2B	-2.66	1.36	1.40
17	J	103	CLA	CMB-C2B	-2.66	1.46	1.51
17	A	821	CLA	CHC-C1C	2.66	1.41	1.35
17	A	807	CLA	CMD-C2D	-2.66	1.45	1.50
17	J	101	CLA	CMB-C2B	-2.65	1.46	1.51
17	A	836	CLA	CHC-C1C	2.65	1.41	1.35
17	2	606	CLA	CMB-C2B	-2.65	1.46	1.51
17	2	612	CLA	CMB-C2B	-2.65	1.46	1.51
17	B	825	CLA	CHC-C1C	2.65	1.41	1.35
25	1	617	ZEX	C8-C7	2.65	1.41	1.33
17	A	824	CLA	C3B-CAB	-2.65	1.42	1.47
25	1	615	ZEX	C32-C33	2.65	1.51	1.45
17	A	803	CLA	C3B-C2B	-2.65	1.36	1.40
17	A	822	CLA	C3B-CAB	-2.65	1.42	1.47
17	L	204	CLA	C3B-CAB	-2.64	1.42	1.47
17	A	811	CLA	CHC-C1C	2.64	1.41	1.35
17	B	826	CLA	C3B-C2B	-2.64	1.36	1.40
17	B	817	CLA	CMD-C2D	-2.64	1.45	1.50
17	O	205	CLA	CMD-C2D	-2.64	1.45	1.50
17	B	829	CLA	CMB-C2B	-2.64	1.46	1.51
17	4	601	CLA	CHC-C1C	2.64	1.41	1.35
17	3	211	CLA	CMB-C2B	-2.64	1.46	1.51
17	2	607	CLA	CMB-C2B	-2.64	1.46	1.51
17	3	206	CLA	C3B-C2B	-2.63	1.36	1.40
17	B	821	CLA	CMD-C2D	-2.63	1.45	1.50
17	A	825	CLA	CMB-C2B	-2.63	1.46	1.51
17	A	803	CLA	C1D-ND	2.63	1.41	1.37
17	A	804	CLA	CMB-C2B	-2.63	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	823	CLA	CHC-C1C	2.63	1.41	1.35
17	O	201	CLA	CMB-C2B	-2.63	1.46	1.51
25	3	217	ZEX	C1-C6	2.63	1.57	1.53
17	A	812	CLA	CMD-C2D	-2.63	1.45	1.50
17	A	824	CLA	C3B-C2B	-2.63	1.36	1.40
25	3	217	ZEX	C8-C7	2.63	1.41	1.33
17	4	601	CLA	CMB-C2B	-2.62	1.46	1.51
17	A	816	CLA	CHC-C1C	2.62	1.41	1.35
25	3	217	ZEX	C24-C25	2.62	1.53	1.50
17	5	606	CLA	C3B-CAB	-2.62	1.42	1.47
17	L	204	CLA	CMB-C2B	-2.62	1.46	1.51
17	1	605	CLA	CMB-C2B	-2.62	1.46	1.51
17	A	808	CLA	CHC-C1C	2.62	1.41	1.35
17	L	204	CLA	C3B-C2B	-2.62	1.36	1.40
17	A	831	CLA	MG-ND	-2.62	2.00	2.05
17	B	801	CLA	MG-ND	-2.62	2.00	2.05
25	2	616	ZEX	C8-C7	2.62	1.41	1.33
17	1	606	CLA	CHC-C1C	2.61	1.41	1.35
17	1	604	CLA	CMB-C2B	-2.61	1.46	1.51
17	B	810	CLA	CMB-C2B	-2.61	1.46	1.51
17	A	829	CLA	MG-ND	-2.61	2.00	2.05
17	A	818	CLA	CHC-C1C	2.61	1.41	1.35
17	B	808	CLA	MG-ND	-2.61	2.00	2.05
17	1	611	CLA	CMB-C2B	-2.61	1.46	1.51
17	5	608	CLA	CMB-C2B	-2.61	1.46	1.51
17	3	204	CLA	CMB-C2B	-2.61	1.46	1.51
17	B	842	CLA	CMD-C2D	-2.61	1.45	1.50
17	A	827	CLA	C3B-CAB	-2.61	1.42	1.47
25	5	617	ZEX	C8-C7	2.61	1.40	1.33
17	3	204	CLA	CMD-C2D	-2.61	1.45	1.50
20	L	205	BCR	C30-C25	-2.61	1.50	1.53
17	J	102	CLA	CMB-C2B	-2.60	1.46	1.51
25	3	216	ZEX	C1-C6	2.60	1.57	1.53
17	B	807	CLA	CMB-C2B	-2.60	1.46	1.51
17	B	814	CLA	CMC-C2C	-2.60	1.45	1.50
25	1	613	ZEX	C8-C7	2.60	1.40	1.33
17	1	611	CLA	CMD-C2D	-2.60	1.45	1.50
17	2	609	CLA	CMB-C2B	-2.60	1.46	1.51
17	B	825	CLA	MG-ND	-2.59	2.00	2.05
25	1	615	ZEX	C8-C7	2.59	1.40	1.33
17	5	609	CLA	C4D-ND	-2.59	1.34	1.37
17	B	823	CLA	CMB-C2B	-2.59	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	804	CLA	CMD-C2D	-2.59	1.45	1.50
17	A	835	CLA	MG-ND	-2.59	2.00	2.05
17	A	815	CLA	CMC-C2C	-2.59	1.45	1.50
17	4	606	CLA	CMD-C2D	-2.59	1.45	1.50
17	2	601	CLA	CMB-C2B	-2.59	1.46	1.51
17	B	813	CLA	CHC-C1C	2.59	1.41	1.35
25	1	616	ZEX	C1-C6	2.59	1.57	1.53
17	A	831	CLA	CHC-C1C	2.58	1.41	1.35
17	B	827	CLA	MG-ND	-2.58	2.00	2.05
20	L	205	BCR	C1-C6	-2.58	1.50	1.53
17	4	606	CLA	CMB-C2B	-2.58	1.46	1.51
17	A	848	CLA	CMD-C2D	-2.58	1.45	1.50
17	J	102	CLA	C3B-C2B	-2.58	1.36	1.40
17	K	102	CLA	CMB-C2B	-2.58	1.46	1.51
17	A	833	CLA	C1D-ND	2.58	1.41	1.37
17	B	824	CLA	CMB-C2B	-2.58	1.46	1.51
17	A	809	CLA	CMD-C2D	-2.58	1.45	1.50
17	2	605	CLA	CMB-C2B	-2.58	1.46	1.51
17	B	804	CLA	MG-ND	-2.58	2.00	2.05
17	A	811	CLA	CMC-C2C	-2.58	1.45	1.50
16	A	801	CL0	C5-C3	-2.57	1.45	1.51
17	B	830	CLA	CHC-C1C	2.57	1.41	1.35
25	5	615	ZEX	C12-C13	2.57	1.51	1.45
25	5	615	ZEX	C8-C7	2.57	1.40	1.33
17	1	606	CLA	C3B-C2B	-2.57	1.36	1.40
17	1	603	CLA	C1D-ND	2.57	1.40	1.37
17	B	831	CLA	CHC-C1C	2.57	1.41	1.35
17	A	838	CLA	CMC-C2C	-2.57	1.45	1.50
17	B	841	CLA	CMD-C2D	-2.57	1.45	1.50
25	1	616	ZEX	C12-C13	2.57	1.51	1.45
17	A	803	CLA	MG-ND	-2.56	2.00	2.05
17	A	835	CLA	CMB-C2B	-2.56	1.46	1.51
17	2	604	CLA	CMB-C2B	-2.56	1.46	1.51
17	B	809	CLA	MG-ND	-2.56	2.00	2.05
17	1	608	CLA	CMC-C2C	-2.56	1.45	1.50
17	A	805	CLA	C3B-CAB	-2.56	1.42	1.47
17	A	808	CLA	C3B-C2B	-2.56	1.36	1.40
17	L	202	CLA	C3B-C2B	-2.56	1.36	1.40
17	A	837	CLA	MG-ND	-2.56	2.00	2.05
17	A	807	CLA	CHC-C1C	2.56	1.41	1.35
17	A	812	CLA	CMB-C2B	-2.56	1.46	1.51
17	B	806	CLA	CMC-C2C	-2.55	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	831	CLA	C1D-ND	2.55	1.40	1.37
17	J	102	CLA	C3B-CAB	-2.55	1.42	1.47
25	4	617	ZEX	C8-C7	2.55	1.40	1.33
17	B	811	CLA	CHC-C1C	2.55	1.41	1.35
17	B	823	CLA	CMD-C2D	-2.55	1.45	1.50
17	A	803	CLA	CMD-C2D	-2.55	1.45	1.50
17	A	807	CLA	MG-ND	-2.55	2.00	2.05
17	1	608	CLA	C3B-C2B	-2.55	1.36	1.40
17	L	203	CLA	CMD-C2D	-2.55	1.45	1.50
25	4	612	ZEX	C24-C25	2.54	1.53	1.50
17	A	835	CLA	C3B-CAB	-2.54	1.42	1.47
25	2	617	ZEX	C8-C9	2.54	1.51	1.45
17	A	806	CLA	C1D-ND	2.54	1.40	1.37
25	3	216	ZEX	C8-C7	2.54	1.40	1.33
17	B	838	CLA	CMC-C2C	-2.54	1.45	1.50
17	A	839	CLA	CHC-C1C	2.54	1.41	1.35
17	A	813	CLA	CMB-C2B	-2.54	1.46	1.51
17	B	835	CLA	C1D-ND	2.54	1.40	1.37
17	1	602	CLA	CHC-C1C	2.54	1.41	1.35
17	2	610	CLA	CMB-C2B	-2.54	1.46	1.51
25	4	612	ZEX	C1-C6	2.54	1.57	1.53
25	5	614	ZEX	C8-C7	2.53	1.40	1.33
17	A	838	CLA	C3B-C2B	-2.53	1.36	1.40
17	A	828	CLA	C4B-CHC	-2.53	1.34	1.41
17	A	814	CLA	C3B-C2B	-2.53	1.36	1.40
25	3	215	ZEX	C12-C13	2.53	1.51	1.45
17	B	843	CLA	CMB-C2B	-2.53	1.46	1.51
17	K	103	CLA	CMB-C2B	-2.53	1.46	1.51
17	A	839	CLA	CMD-C2D	-2.53	1.45	1.50
17	B	802	CLA	CMD-C2D	-2.53	1.45	1.50
20	I	101	BCR	C1-C6	-2.53	1.50	1.53
17	1	607	CLA	CMB-C2B	-2.53	1.46	1.51
25	4	616	ZEX	C8-C7	2.53	1.40	1.33
17	A	807	CLA	C3B-CAB	-2.53	1.42	1.47
17	2	613	CLA	CMB-C2B	-2.53	1.46	1.51
17	A	848	CLA	CMB-C2B	-2.53	1.46	1.51
17	5	613	CLA	CMB-C2B	-2.53	1.46	1.51
17	A	830	CLA	C1D-ND	2.52	1.40	1.37
17	A	805	CLA	CMD-C2D	-2.52	1.45	1.50
25	1	616	ZEX	C8-C7	2.52	1.40	1.33
17	B	828	CLA	C3B-C2B	-2.52	1.36	1.40
17	A	803	CLA	C3B-CAB	-2.52	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	603	CLA	CMD-C2D	-2.52	1.45	1.50
17	B	838	CLA	CHC-C1C	2.52	1.41	1.35
25	4	613	ZEX	C12-C13	2.52	1.51	1.45
25	3	214	ZEX	C8-C7	2.52	1.40	1.33
17	A	818	CLA	CMD-C2D	-2.52	1.45	1.50
17	B	840	CLA	C1D-ND	2.52	1.40	1.37
17	B	812	CLA	MG-ND	-2.52	2.00	2.05
17	B	834	CLA	C3B-C2B	-2.52	1.36	1.40
25	1	617	ZEX	C32-C33	2.52	1.51	1.45
17	A	820	CLA	CMD-C2D	-2.52	1.45	1.50
17	3	202	CLA	CMB-C2B	-2.52	1.46	1.51
17	B	822	CLA	CHC-C1C	2.52	1.41	1.35
17	B	826	CLA	C3B-CAB	-2.51	1.42	1.47
17	B	819	CLA	CMB-C2B	-2.51	1.46	1.51
25	2	615	ZEX	C8-C7	2.51	1.40	1.33
17	1	611	CLA	MG-ND	-2.51	2.00	2.05
17	A	807	CLA	C3B-C2B	-2.51	1.36	1.40
17	B	821	CLA	CHC-C1C	2.51	1.41	1.35
17	A	815	CLA	C1D-ND	2.51	1.40	1.37
17	B	804	CLA	CMC-C2C	-2.51	1.45	1.50
17	4	611	CLA	CMB-C2B	-2.51	1.46	1.51
17	A	815	CLA	CMD-C2D	-2.51	1.45	1.50
17	3	205	CLA	CMC-C2C	-2.51	1.45	1.50
17	A	813	CLA	CMD-C2D	-2.50	1.45	1.50
17	1	603	CLA	MG-ND	-2.50	2.00	2.05
17	J	101	CLA	CMD-C2D	-2.50	1.45	1.50
17	B	801	CLA	CMC-C2C	-2.50	1.45	1.50
17	B	810	CLA	C3B-C2B	-2.50	1.36	1.40
17	F	302	CLA	CMD-C2D	-2.50	1.45	1.50
17	3	213	CLA	CMB-C2B	-2.50	1.46	1.51
25	3	215	ZEX	C32-C33	2.50	1.51	1.45
25	1	614	ZEX	C32-C33	2.49	1.51	1.45
17	A	817	CLA	MG-ND	-2.49	2.00	2.05
25	4	613	ZEX	C1-C6	2.49	1.57	1.53
17	B	834	CLA	CMC-C2C	-2.49	1.45	1.50
17	A	802	CLA	CMC-C2C	-2.49	1.45	1.50
17	B	829	CLA	CMC-C2C	-2.49	1.45	1.50
17	A	811	CLA	C3B-CAB	-2.49	1.42	1.47
25	4	614	ZEX	C12-C13	2.49	1.51	1.45
17	5	612	CLA	CMB-C2B	-2.49	1.46	1.51
17	A	826	CLA	CMD-C2D	-2.49	1.45	1.50
17	A	835	CLA	C1D-ND	2.49	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	611	CLA	C1D-ND	2.48	1.40	1.37
17	A	807	CLA	CMC-C2C	-2.48	1.45	1.50
17	A	817	CLA	CMD-C2D	-2.48	1.45	1.50
25	5	617	ZEX	C24-C25	2.48	1.52	1.50
17	K	103	CLA	CMC-C2C	-2.48	1.45	1.50
25	1	613	ZEX	C12-C13	2.48	1.51	1.45
25	2	617	ZEX	C32-C33	2.48	1.51	1.45
17	A	805	CLA	CMC-C2C	-2.48	1.45	1.50
17	A	826	CLA	MG-ND	-2.48	2.00	2.05
17	A	831	CLA	C3B-C2B	-2.48	1.36	1.40
25	3	217	ZEX	C12-C13	2.48	1.51	1.45
17	B	838	CLA	CMD-C2D	-2.48	1.45	1.50
23	B	851	DGD	O1G-C1G	-2.48	1.39	1.45
17	1	612	CLA	CMB-C2B	-2.48	1.46	1.51
17	4	610	CLA	CMB-C2B	-2.47	1.46	1.51
17	B	812	CLA	CMD-C2D	-2.47	1.45	1.50
17	B	839	CLA	CMD-C2D	-2.47	1.45	1.50
17	5	605	CLA	CMB-C2B	-2.47	1.46	1.51
17	A	830	CLA	MG-ND	-2.47	2.00	2.05
17	O	201	CLA	CMC-C2C	-2.47	1.45	1.50
25	3	216	ZEX	C12-C13	2.47	1.51	1.45
17	1	603	CLA	C3B-CAB	-2.47	1.42	1.47
17	J	103	CLA	C3B-C2B	-2.47	1.36	1.40
17	J	102	CLA	CMC-C2C	-2.47	1.45	1.50
17	B	833	CLA	C3B-CAB	-2.47	1.42	1.47
17	1	606	CLA	CMD-C2D	-2.47	1.45	1.50
17	F	301	CLA	C3B-C2B	-2.46	1.36	1.40
17	B	831	CLA	C1D-ND	2.46	1.40	1.37
25	2	614	ZEX	C8-C7	2.46	1.40	1.33
25	4	616	ZEX	C1-C6	2.46	1.57	1.53
17	B	814	CLA	CMD-C2D	-2.46	1.45	1.50
17	1	612	CLA	CMD-C2D	-2.46	1.45	1.50
17	O	205	CLA	CMB-C2B	-2.46	1.46	1.51
17	4	601	CLA	CMC-C2C	-2.46	1.45	1.50
17	B	829	CLA	MG-ND	-2.46	2.00	2.05
17	B	803	CLA	C3B-CAB	-2.46	1.42	1.47
17	A	809	CLA	CMC-C2C	-2.45	1.45	1.50
17	A	817	CLA	CHC-C1C	2.45	1.41	1.35
17	4	604	CLA	CMB-C2B	-2.45	1.46	1.51
17	A	825	CLA	CMD-C2D	-2.45	1.45	1.50
17	B	806	CLA	CHC-C1C	2.45	1.41	1.35
17	A	820	CLA	C1D-ND	2.45	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	849	BGC	C2-C3	2.45	1.56	1.52
25	3	215	ZEX	C8-C7	2.45	1.40	1.33
17	B	823	CLA	MG-ND	-2.45	2.00	2.05
17	B	808	CLA	C3B-CAB	-2.44	1.43	1.47
17	1	604	CLA	MG-ND	-2.44	2.00	2.05
17	B	829	CLA	C3B-CAB	-2.44	1.43	1.47
17	A	831	CLA	CMC-C2C	-2.44	1.45	1.50
17	4	607	CLA	CMB-C2B	-2.44	1.46	1.51
17	2	602	CLA	CMC-C2C	-2.44	1.45	1.50
17	1	606	CLA	MG-ND	-2.44	2.00	2.05
17	3	203	CLA	CMB-C2B	-2.44	1.46	1.51
17	A	832	CLA	CHC-C1C	2.44	1.41	1.35
17	B	842	CLA	CHC-C1C	2.44	1.41	1.35
17	A	820	CLA	MG-ND	-2.43	2.01	2.05
25	4	612	ZEX	C12-C13	2.43	1.51	1.45
17	B	822	CLA	C3B-CAB	-2.43	1.43	1.47
25	4	615	ZEX	C12-C13	2.43	1.51	1.45
17	B	830	CLA	C1D-ND	2.43	1.40	1.37
17	3	212	CLA	CMB-C2B	-2.43	1.46	1.51
17	3	208	CLA	CMC-C2C	-2.43	1.45	1.50
17	A	833	CLA	CMD-C2D	-2.43	1.45	1.50
17	B	834	CLA	MG-ND	-2.43	2.01	2.05
17	4	606	CLA	CHC-C1C	2.43	1.41	1.35
17	B	812	CLA	CHC-C1C	2.43	1.41	1.35
17	3	206	CLA	CMD-C2D	-2.43	1.45	1.50
17	B	822	CLA	MG-ND	-2.43	2.01	2.05
17	F	301	CLA	CMD-C2D	-2.43	1.45	1.50
17	K	102	CLA	CMD-C2D	-2.43	1.45	1.50
17	B	808	CLA	CHC-C1C	2.42	1.41	1.35
17	4	609	CLA	CMB-C2B	-2.42	1.46	1.51
17	5	603	CLA	CMB-C2B	-2.42	1.46	1.51
25	4	616	ZEX	C12-C13	2.42	1.51	1.45
17	1	609	CLA	CMB-C2B	-2.42	1.46	1.51
17	A	810	CLA	CMD-C2D	-2.42	1.45	1.50
17	A	813	CLA	CMC-C2C	-2.42	1.45	1.50
17	5	601	CLA	CMB-C2B	-2.42	1.46	1.51
17	B	813	CLA	CMC-C2C	-2.42	1.45	1.50
17	A	823	CLA	MG-ND	-2.42	2.01	2.05
17	F	301	CLA	CMC-C2C	-2.42	1.45	1.50
17	A	805	CLA	MG-ND	-2.42	2.01	2.05
17	B	801	CLA	CAC-C3C	-2.42	1.44	1.51
17	A	827	CLA	CMC-C2C	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	814	CLA	CHC-C1C	2.41	1.41	1.35
17	B	825	CLA	CMD-C2D	-2.41	1.45	1.50
25	1	615	ZEX	C24-C25	2.41	1.52	1.50
17	A	811	CLA	CMD-C2D	-2.41	1.45	1.50
17	A	810	CLA	C3B-C2B	-2.41	1.37	1.40
17	B	832	CLA	CHC-C1C	2.41	1.41	1.35
17	3	206	CLA	MG-ND	-2.41	2.01	2.05
18	A	840	PQN	C5-C4	-2.41	1.43	1.48
17	B	803	CLA	CMC-C2C	-2.41	1.45	1.50
17	5	604	CLA	CMD-C2D	-2.41	1.45	1.50
17	A	806	CLA	CMD-C2D	-2.41	1.45	1.50
17	B	840	CLA	CMD-C2D	-2.41	1.45	1.50
16	A	801	CL0	CHD-C4C	-2.41	1.33	1.39
17	A	802	CLA	C3B-CAB	-2.40	1.43	1.47
16	A	801	CL0	OBD-CAD	-2.40	1.18	1.22
17	A	815	CLA	MG-ND	-2.40	2.01	2.05
17	A	804	CLA	CMC-C2C	-2.40	1.45	1.50
17	A	815	CLA	C3B-CAB	-2.40	1.43	1.47
17	2	611	CLA	CMC-C2C	-2.40	1.45	1.50
17	J	101	CLA	MG-ND	-2.40	2.01	2.05
17	1	602	CLA	CMD-C2D	-2.40	1.45	1.50
17	A	848	CLA	C3B-CAB	-2.40	1.43	1.47
17	3	205	CLA	C3B-C2B	-2.40	1.37	1.40
17	1	610	CLA	CMD-C2D	-2.40	1.45	1.50
16	A	801	CL0	C3B-C2B	2.40	1.43	1.40
17	B	829	CLA	CMD-C2D	-2.40	1.45	1.50
17	B	816	CLA	MG-ND	-2.40	2.01	2.05
17	A	836	CLA	CMC-C2C	-2.39	1.45	1.50
17	B	811	CLA	CMC-C2C	-2.39	1.45	1.50
17	A	833	CLA	MG-ND	-2.39	2.01	2.05
17	A	824	CLA	MG-ND	-2.39	2.01	2.05
17	A	802	CLA	C3B-C2B	-2.39	1.37	1.40
17	1	604	CLA	CMD-C2D	-2.39	1.45	1.50
17	A	819	CLA	C3B-C2B	-2.39	1.37	1.40
17	3	210	CLA	CMB-C2B	-2.39	1.46	1.51
17	4	603	CLA	CMB-C2B	-2.39	1.46	1.51
17	B	836	CLA	CMC-C2C	-2.39	1.45	1.50
17	B	840	CLA	MG-ND	-2.39	2.01	2.05
20	J	104	BCR	C38-C26	-2.39	1.47	1.50
17	A	821	CLA	C3B-C2B	-2.39	1.37	1.40
17	A	806	CLA	C3B-CAB	-2.39	1.43	1.47
17	B	841	CLA	MG-ND	-2.39	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	209	CLA	CMB-C2B	-2.39	1.46	1.51
17	B	836	CLA	C3B-C2B	-2.39	1.37	1.40
17	5	609	CLA	CMB-C2B	-2.39	1.46	1.51
17	A	831	CLA	CMD-C2D	-2.38	1.45	1.50
17	B	831	CLA	CMC-C2C	-2.38	1.45	1.50
17	5	603	CLA	C3B-CAB	-2.38	1.43	1.47
17	B	817	CLA	MG-ND	-2.38	2.01	2.05
17	A	802	CLA	CMD-C2D	-2.38	1.45	1.50
17	A	804	CLA	CMD-C2D	-2.37	1.45	1.50
17	B	841	CLA	C3B-C2B	-2.37	1.37	1.40
17	3	207	CLA	C3B-CAB	-2.37	1.43	1.47
17	2	611	CLA	C3B-C2B	-2.37	1.37	1.40
17	B	839	CLA	CMC-C2C	-2.37	1.45	1.50
17	A	836	CLA	C3B-CAB	-2.37	1.43	1.47
17	F	303	CLA	C3B-C2B	-2.37	1.37	1.40
17	B	832	CLA	C1B-NB	-2.37	1.33	1.35
25	3	214	ZEX	C12-C13	2.36	1.51	1.45
17	3	208	CLA	C3B-C2B	-2.36	1.37	1.40
17	A	839	CLA	MG-ND	-2.36	2.01	2.05
17	B	807	CLA	CMC-C2C	-2.36	1.45	1.50
17	B	818	CLA	MG-ND	-2.36	2.01	2.05
19	A	842	LHG	O7-C5	-2.36	1.40	1.46
17	J	102	CLA	CMD-C2D	-2.36	1.45	1.50
17	A	833	CLA	C3B-C2B	-2.35	1.37	1.40
17	A	821	CLA	CMD-C2D	-2.35	1.45	1.50
17	B	835	CLA	CMD-C2D	-2.35	1.45	1.50
17	A	836	CLA	MG-ND	-2.35	2.01	2.05
17	3	208	CLA	C3B-CAB	-2.35	1.43	1.47
17	B	832	CLA	CMC-C2C	-2.35	1.45	1.50
17	2	606	CLA	CMC-C2C	-2.35	1.45	1.50
25	4	617	ZEX	C12-C13	2.35	1.51	1.45
17	A	817	CLA	CMC-C2C	-2.35	1.45	1.50
17	2	602	CLA	MG-ND	-2.35	2.01	2.05
17	2	611	CLA	C3B-CAB	-2.35	1.43	1.47
17	A	812	CLA	CMC-C2C	-2.35	1.45	1.50
17	2	608	CLA	MG-ND	-2.35	2.01	2.05
17	A	839	CLA	CMC-C2C	-2.35	1.45	1.50
17	B	810	CLA	CMC-C2C	-2.35	1.45	1.50
17	A	828	CLA	C1D-ND	2.35	1.40	1.37
17	B	832	CLA	C4B-CHC	-2.34	1.34	1.41
17	A	809	CLA	C3B-C2B	-2.34	1.37	1.40
17	B	818	CLA	CMD-C2D	-2.34	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	609	CLA	C3C-C2C	2.34	1.41	1.36
17	B	803	CLA	CMD-C2D	-2.34	1.45	1.50
17	1	602	CLA	MG-ND	-2.34	2.01	2.05
17	F	302	CLA	C3B-C2B	-2.34	1.37	1.40
17	O	203	CLA	CMB-C2B	-2.34	1.46	1.51
17	A	835	CLA	CMD-C2D	-2.34	1.45	1.50
17	B	826	CLA	CMD-C2D	-2.34	1.45	1.50
17	2	608	CLA	CMB-C2B	-2.34	1.46	1.51
17	5	610	CLA	CMB-C2B	-2.33	1.46	1.51
17	O	201	CLA	CMD-C2D	-2.33	1.45	1.50
17	B	842	CLA	MG-ND	-2.33	2.01	2.05
17	B	813	CLA	CMD-C2D	-2.33	1.45	1.50
17	B	815	CLA	CMC-C2C	-2.33	1.45	1.50
17	2	604	CLA	CMC-C2C	-2.33	1.45	1.50
17	B	815	CLA	CMD-C2D	-2.33	1.45	1.50
17	B	810	CLA	MG-ND	-2.33	2.01	2.05
17	B	820	CLA	CMD-C2D	-2.33	1.45	1.50
17	2	605	CLA	CAA-C2A	-2.33	1.49	1.54
17	B	828	CLA	C3B-CAB	-2.33	1.43	1.47
17	F	301	CLA	MG-ND	-2.32	2.01	2.05
17	1	610	CLA	MG-ND	-2.32	2.01	2.05
17	4	602	CLA	CMB-C2B	-2.32	1.46	1.51
17	2	610	CLA	CMC-C2C	-2.32	1.45	1.50
20	A	844	BCR	C30-C25	-2.32	1.50	1.53
17	A	828	CLA	CAC-C3C	-2.32	1.45	1.51
17	A	814	CLA	C3B-CAB	-2.31	1.43	1.47
17	B	841	CLA	C3B-CAB	-2.31	1.43	1.47
17	B	817	CLA	CMC-C2C	-2.31	1.45	1.50
20	B	845	BCR	C30-C25	-2.31	1.50	1.53
17	A	806	CLA	MG-ND	-2.31	2.01	2.05
17	F	302	CLA	MG-ND	-2.31	2.01	2.05
17	J	103	CLA	C3B-CAB	-2.31	1.43	1.47
17	B	830	CLA	CMD-C2D	-2.31	1.45	1.50
17	B	836	CLA	CMD-C2D	-2.31	1.45	1.50
17	2	612	CLA	CMC-C2C	-2.31	1.45	1.50
17	B	820	CLA	CMC-C2C	-2.31	1.45	1.50
17	B	816	CLA	CMD-C2D	-2.31	1.45	1.50
17	5	606	CLA	C3B-C2B	-2.31	1.37	1.40
17	A	806	CLA	CMC-C2C	-2.31	1.45	1.50
17	A	838	CLA	C3B-CAB	-2.31	1.43	1.47
17	A	837	CLA	CMD-C2D	-2.31	1.45	1.50
17	B	834	CLA	CMD-C2D	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	102	CLA	MG-ND	-2.31	2.01	2.05
17	2	602	CLA	CMD-C2D	-2.30	1.45	1.50
17	O	204	CLA	CMB-C2B	-2.30	1.46	1.51
17	5	606	CLA	C3C-C2C	2.30	1.41	1.36
17	B	839	CLA	MG-ND	-2.30	2.01	2.05
17	L	203	CLA	MG-ND	-2.30	2.01	2.05
17	L	203	CLA	C3B-CAB	-2.30	1.43	1.47
17	L	204	CLA	CMD-C2D	-2.30	1.45	1.50
20	B	847	BCR	C1-C6	-2.30	1.50	1.53
17	B	829	CLA	C3B-C2B	-2.30	1.37	1.40
17	2	607	CLA	CMD-C2D	-2.30	1.45	1.50
17	A	804	CLA	MG-ND	-2.30	2.01	2.05
17	A	832	CLA	MG-ND	-2.30	2.01	2.05
17	A	838	CLA	CMD-C2D	-2.30	1.45	1.50
17	A	822	CLA	MG-ND	-2.30	2.01	2.05
17	A	834	CLA	C3B-C2B	-2.30	1.37	1.40
17	B	813	CLA	MG-ND	-2.30	2.01	2.05
17	3	213	CLA	C3B-CAB	-2.30	1.43	1.47
17	3	204	CLA	MG-ND	-2.30	2.01	2.05
17	A	836	CLA	CMD-C2D	-2.30	1.45	1.50
17	2	602	CLA	C3B-C2B	-2.29	1.37	1.40
17	B	807	CLA	CMD-C2D	-2.29	1.45	1.50
17	B	809	CLA	CMD-C2D	-2.29	1.45	1.50
17	4	604	CLA	CMC-C2C	-2.29	1.45	1.50
17	5	603	CLA	CMC-C2C	-2.29	1.45	1.50
17	B	802	CLA	CMC-C2C	-2.29	1.45	1.50
17	B	842	CLA	CMC-C2C	-2.29	1.45	1.50
17	5	603	CLA	CMD-C2D	-2.29	1.45	1.50
17	K	103	CLA	MG-ND	-2.29	2.01	2.05
17	F	301	CLA	C3B-CAB	-2.29	1.43	1.47
17	5	607	CLA	CMC-C2C	-2.29	1.45	1.50
17	B	834	CLA	C3B-CAB	-2.29	1.43	1.47
17	A	812	CLA	MG-ND	-2.29	2.01	2.05
17	A	815	CLA	C3B-C2B	-2.29	1.37	1.40
17	A	810	CLA	MG-ND	-2.29	2.01	2.05
17	A	822	CLA	CMD-C2D	-2.28	1.46	1.50
17	1	602	CLA	CMC-C2C	-2.28	1.46	1.50
17	A	830	CLA	CMC-C2C	-2.28	1.46	1.50
17	A	832	CLA	CMD-C2D	-2.28	1.46	1.50
17	1	611	CLA	CMC-C2C	-2.28	1.46	1.50
17	B	810	CLA	CMD-C2D	-2.28	1.46	1.50
17	4	608	CLA	C3B-C2B	-2.28	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	603	CLA	C3B-C2B	-2.28	1.37	1.40
17	5	608	CLA	CMC-C2C	-2.28	1.46	1.50
17	A	828	CLA	C1B-NB	-2.27	1.33	1.35
17	B	833	CLA	CMC-C2C	-2.27	1.46	1.50
17	B	811	CLA	CAC-C3C	-2.27	1.45	1.51
17	B	802	CLA	CHC-C1C	2.27	1.40	1.35
17	A	811	CLA	MG-ND	-2.27	2.01	2.05
17	2	603	CLA	CMC-C2C	-2.27	1.46	1.50
17	A	817	CLA	C3B-CAB	-2.27	1.43	1.47
17	A	838	CLA	MG-ND	-2.27	2.01	2.05
17	B	821	CLA	MG-ND	-2.27	2.01	2.05
17	A	828	CLA	C3B-CAB	-2.27	1.43	1.47
17	L	203	CLA	CMC-C2C	-2.27	1.46	1.50
25	5	614	ZEX	C12-C13	2.27	1.50	1.45
25	2	617	ZEX	C8-C7	2.27	1.39	1.33
17	B	828	CLA	C1D-ND	2.27	1.40	1.37
17	B	827	CLA	CMC-C2C	-2.27	1.46	1.50
17	3	210	CLA	CMD-C2D	-2.27	1.46	1.50
17	2	612	CLA	CMD-C2D	-2.27	1.46	1.50
17	5	611	CLA	CMB-C2B	-2.26	1.46	1.51
17	B	815	CLA	MG-ND	-2.26	2.01	2.05
17	B	823	CLA	CMC-C2C	-2.26	1.46	1.50
17	B	836	CLA	C3B-CAB	-2.26	1.43	1.47
17	A	830	CLA	CMD-C2D	-2.26	1.46	1.50
17	B	826	CLA	CMC-C2C	-2.26	1.46	1.50
17	2	605	CLA	C3B-C2B	-2.26	1.37	1.40
17	A	817	CLA	C4B-CHC	-2.26	1.34	1.41
17	B	818	CLA	C3B-C2B	-2.25	1.37	1.40
17	B	811	CLA	C3B-CAB	-2.25	1.43	1.47
17	B	832	CLA	C1D-ND	2.25	1.40	1.37
17	4	605	CLA	CMB-C2B	-2.25	1.47	1.51
17	A	831	CLA	C3B-CAB	-2.25	1.43	1.47
17	A	818	CLA	MG-ND	-2.25	2.01	2.05
17	B	826	CLA	MG-ND	-2.25	2.01	2.05
17	B	816	CLA	CMC-C2C	-2.25	1.46	1.50
17	2	604	CLA	C3B-C2B	-2.25	1.37	1.40
17	L	204	CLA	MG-ND	-2.25	2.01	2.05
17	2	606	CLA	C3B-C2B	-2.25	1.37	1.40
17	3	204	CLA	CMC-C2C	-2.25	1.46	1.50
23	B	851	DGD	O5D-C6D	-2.25	1.39	1.43
17	3	211	CLA	CMC-C2C	-2.24	1.46	1.50
25	2	616	ZEX	C27-C28	2.24	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	833	CLA	MG-ND	-2.24	2.01	2.05
17	3	206	CLA	C3B-CAB	-2.24	1.43	1.47
25	5	614	ZEX	C27-C28	2.24	1.39	1.33
17	B	804	CLA	C1D-ND	2.24	1.40	1.37
17	A	809	CLA	C3B-CAB	-2.24	1.43	1.47
17	3	203	CLA	CMD-C2D	-2.24	1.46	1.50
17	A	829	CLA	CMC-C2C	-2.24	1.46	1.50
18	A	840	PQN	C11-C12	2.24	1.53	1.50
17	A	819	CLA	CMD-C2D	-2.24	1.46	1.50
17	1	608	CLA	C3B-CAB	-2.24	1.43	1.47
17	B	807	CLA	MG-ND	-2.24	2.01	2.05
17	A	837	CLA	CMC-C2C	-2.24	1.46	1.50
17	B	803	CLA	MG-ND	-2.23	2.01	2.05
17	A	819	CLA	MG-ND	-2.23	2.01	2.05
17	B	807	CLA	C3B-CAB	-2.23	1.43	1.47
17	B	837	CLA	C3B-CAB	-2.23	1.43	1.47
17	A	823	CLA	C3B-CAB	-2.23	1.43	1.47
17	B	818	CLA	C3B-CAB	-2.23	1.43	1.47
17	3	213	CLA	C3B-C2B	-2.23	1.37	1.40
17	B	825	CLA	C3B-CAB	-2.23	1.43	1.47
17	2	608	CLA	CMD-C2D	-2.23	1.46	1.50
17	B	806	CLA	C1D-ND	2.23	1.40	1.37
17	B	824	CLA	C3B-C2B	-2.23	1.37	1.40
17	B	816	CLA	C3B-CAB	-2.23	1.43	1.47
17	A	820	CLA	CMC-C2C	-2.23	1.46	1.50
17	1	604	CLA	CMC-C2C	-2.23	1.46	1.50
17	1	610	CLA	CMC-C2C	-2.23	1.46	1.50
25	5	617	ZEX	C12-C13	2.22	1.50	1.45
17	B	819	CLA	CMC-C2C	-2.22	1.46	1.50
17	1	611	CLA	C3B-CAB	-2.22	1.43	1.47
17	J	102	CLA	MG-ND	-2.22	2.01	2.05
17	B	802	CLA	C4B-CHC	-2.22	1.34	1.41
25	2	617	ZEX	C24-C25	2.22	1.52	1.50
24	J	106	3XQ	O20-C21	-2.22	1.40	1.45
25	5	616	ZEX	C27-C28	2.22	1.39	1.33
17	2	609	CLA	C3B-C2B	-2.22	1.37	1.40
17	A	828	CLA	CHC-C1C	2.22	1.40	1.35
17	A	833	CLA	CMC-C2C	-2.22	1.46	1.50
17	A	808	CLA	MG-ND	-2.22	2.01	2.05
17	A	818	CLA	C3B-C2B	-2.22	1.37	1.40
17	B	836	CLA	MG-ND	-2.21	2.01	2.05
17	K	103	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	824	CLA	CMD-C2D	-2.21	1.46	1.50
17	2	602	CLA	C3B-CAB	-2.21	1.43	1.47
17	A	808	CLA	CMD-C2D	-2.21	1.46	1.50
17	B	821	CLA	CAC-C3C	-2.21	1.45	1.51
17	B	837	CLA	MG-ND	-2.21	2.01	2.05
17	2	609	CLA	CMD-C2D	-2.21	1.46	1.50
17	A	825	CLA	C3B-CAB	-2.21	1.43	1.47
17	B	810	CLA	C3B-CAB	-2.21	1.43	1.47
17	A	823	CLA	CMC-C2C	-2.21	1.46	1.50
17	3	203	CLA	C3B-CAB	-2.21	1.43	1.47
17	B	808	CLA	CMD-C2D	-2.21	1.46	1.50
17	A	810	CLA	CMC-C2C	-2.21	1.46	1.50
17	3	205	CLA	CMD-C2D	-2.21	1.46	1.50
17	J	103	CLA	CMC-C2C	-2.21	1.46	1.50
17	A	832	CLA	C4B-CHC	-2.21	1.34	1.41
17	B	808	CLA	CMC-C2C	-2.21	1.46	1.50
17	2	611	CLA	CMD-C2D	-2.20	1.46	1.50
17	2	601	CLA	C3B-C2B	-2.20	1.37	1.40
17	1	608	CLA	MG-ND	-2.20	2.01	2.05
25	2	615	ZEX	C1-C6	2.20	1.56	1.53
17	A	848	CLA	C4B-CHC	-2.20	1.34	1.41
17	5	605	CLA	CMD-C2D	-2.20	1.46	1.50
17	2	606	CLA	C3B-CAB	-2.20	1.43	1.47
25	3	218	ZEX	C27-C28	2.20	1.39	1.33
17	A	825	CLA	C3B-C2B	-2.20	1.37	1.40
17	B	812	CLA	CMC-C2C	-2.20	1.46	1.50
17	2	601	CLA	CMC-C2C	-2.20	1.46	1.50
17	3	208	CLA	CMD-C2D	-2.20	1.46	1.50
17	B	821	CLA	CMC-C2C	-2.20	1.46	1.50
17	B	843	CLA	MG-ND	-2.20	2.01	2.05
17	B	837	CLA	CMD-C2D	-2.20	1.46	1.50
17	4	602	CLA	CMC-C2C	-2.19	1.46	1.50
17	B	828	CLA	CMC-C2C	-2.19	1.46	1.50
17	1	612	CLA	MG-ND	-2.19	2.01	2.05
17	J	101	CLA	C3B-CAB	-2.19	1.43	1.47
17	2	606	CLA	CMD-C2D	-2.19	1.46	1.50
17	A	821	CLA	CMC-C2C	-2.19	1.46	1.50
17	J	103	CLA	CMD-C2D	-2.19	1.46	1.50
17	A	813	CLA	MG-ND	-2.19	2.01	2.05
17	4	602	CLA	CMD-C2D	-2.19	1.46	1.50
17	3	205	CLA	MG-ND	-2.19	2.01	2.05
17	B	812	CLA	C4B-CHC	-2.19	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	835	CLA	CMC-C2C	-2.19	1.46	1.50
17	B	827	CLA	C3B-C2B	-2.19	1.37	1.40
16	A	801	CL0	C4B-CHC	-2.18	1.34	1.41
17	3	212	CLA	CMC-C2C	-2.18	1.46	1.50
17	A	808	CLA	C3B-CAB	-2.18	1.43	1.47
25	2	614	ZEX	C12-C13	2.18	1.50	1.45
17	A	821	CLA	MG-ND	-2.18	2.01	2.05
17	A	839	CLA	C3B-CAB	-2.18	1.43	1.47
17	B	840	CLA	CMC-C2C	-2.18	1.46	1.50
17	3	209	CLA	CMC-C2C	-2.18	1.46	1.50
17	A	820	CLA	C3B-C2B	-2.18	1.37	1.40
17	A	816	CLA	CMC-C2C	-2.18	1.46	1.50
17	4	608	CLA	CMD-C2D	-2.18	1.46	1.50
17	3	202	CLA	CMD-C2D	-2.17	1.46	1.50
17	A	818	CLA	C3B-CAB	-2.17	1.43	1.47
25	1	614	ZEX	C12-C13	2.17	1.50	1.45
16	A	801	CL0	C3C-C2C	-2.17	1.32	1.36
17	B	814	CLA	C4B-CHC	-2.17	1.35	1.41
25	2	615	ZEX	C12-C13	2.17	1.50	1.45
16	A	801	CL0	C3D-C2D	-2.17	1.33	1.39
17	2	601	CLA	C3B-CAB	-2.17	1.43	1.47
17	5	609	CLA	CMD-C2D	-2.17	1.46	1.50
17	A	848	CLA	C3B-C2B	-2.17	1.37	1.40
17	2	610	CLA	C3B-C2B	-2.17	1.37	1.40
17	2	604	CLA	C3B-CAB	-2.17	1.43	1.47
17	A	816	CLA	C4B-CHC	-2.17	1.35	1.41
17	K	102	CLA	CMC-C2C	-2.16	1.46	1.50
17	1	601	CLA	C3B-C2B	-2.16	1.37	1.40
17	B	824	CLA	CMD-C2D	-2.16	1.46	1.50
16	A	801	CL0	C1B-CHB	-2.16	1.35	1.41
17	B	842	CLA	C3B-CAB	-2.16	1.43	1.47
17	4	606	CLA	CMC-C2C	-2.16	1.46	1.50
25	3	215	ZEX	C1-C6	2.16	1.56	1.53
17	4	608	CLA	CMC-C2C	-2.16	1.46	1.50
17	3	207	CLA	CMD-C2D	-2.16	1.46	1.50
17	B	821	CLA	C3B-C2B	-2.16	1.37	1.40
17	A	834	CLA	CMC-C2C	-2.16	1.46	1.50
17	B	819	CLA	CMD-C2D	-2.16	1.46	1.50
17	2	607	CLA	C3B-C2B	-2.16	1.37	1.40
20	K	101	BCR	C33-C5	-2.16	1.47	1.50
17	L	203	CLA	C3B-C2B	-2.16	1.37	1.40
17	B	824	CLA	MG-ND	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	202	CLA	C3B-CAB	-2.15	1.43	1.47
17	4	611	CLA	CMD-C2D	-2.15	1.46	1.50
17	2	612	CLA	MG-ND	-2.15	2.01	2.05
17	5	604	CLA	MG-ND	-2.15	2.01	2.05
17	B	806	CLA	CMA-C3A	-2.15	1.48	1.53
17	A	824	CLA	C1D-ND	2.15	1.40	1.37
20	A	843	BCR	C33-C5	-2.15	1.47	1.50
17	B	811	CLA	C4B-CHC	-2.15	1.35	1.41
17	1	611	CLA	C3B-C2B	-2.15	1.37	1.40
17	2	607	CLA	CMC-C2C	-2.15	1.46	1.50
17	A	813	CLA	C3B-CAB	-2.15	1.43	1.47
17	1	607	CLA	C3B-C2B	-2.15	1.37	1.40
17	3	212	CLA	CMD-C2D	-2.15	1.46	1.50
17	B	843	CLA	CMD-C2D	-2.14	1.46	1.50
25	2	617	ZEX	C1-C6	2.14	1.56	1.53
17	B	832	CLA	C3B-CAB	-2.14	1.43	1.47
17	J	103	CLA	MG-ND	-2.14	2.01	2.05
17	4	603	CLA	CMD-C2D	-2.14	1.46	1.50
17	A	803	CLA	CAC-C3C	-2.14	1.45	1.51
17	A	802	CLA	MG-ND	-2.14	2.01	2.05
17	1	607	CLA	MG-ND	-2.14	2.01	2.05
17	F	302	CLA	CMC-C2C	-2.14	1.46	1.50
17	1	601	CLA	MG-ND	-2.14	2.01	2.05
17	3	208	CLA	MG-ND	-2.14	2.01	2.05
17	3	207	CLA	C3B-C2B	-2.13	1.37	1.40
17	A	810	CLA	C3B-CAB	-2.13	1.43	1.47
17	2	603	CLA	MG-ND	-2.13	2.01	2.05
17	1	603	CLA	CMC-C2C	-2.13	1.46	1.50
17	1	612	CLA	CMC-C2C	-2.13	1.46	1.50
17	A	839	CLA	C4B-CHC	-2.13	1.35	1.41
17	2	607	CLA	MG-ND	-2.13	2.01	2.05
17	2	604	CLA	MG-ND	-2.13	2.01	2.05
25	2	615	ZEX	C32-C33	2.13	1.50	1.45
17	A	834	CLA	CMD-C2D	-2.13	1.46	1.50
17	B	822	CLA	CMD-C2D	-2.13	1.46	1.50
17	2	606	CLA	MG-ND	-2.13	2.01	2.05
17	5	608	CLA	C3B-CAB	-2.13	1.43	1.47
17	3	209	CLA	MG-ND	-2.13	2.01	2.05
17	B	824	CLA	C3B-CAB	-2.13	1.43	1.47
20	B	847	BCR	C38-C26	-2.13	1.47	1.50
17	5	609	CLA	C1D-C2D	2.12	1.49	1.45
17	A	803	CLA	C4B-CHC	-2.12	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	610	CLA	CMC-C2C	-2.12	1.46	1.50
17	3	211	CLA	MG-ND	-2.12	2.01	2.05
17	1	601	CLA	C3B-CAB	-2.12	1.43	1.47
17	B	837	CLA	CMC-C2C	-2.12	1.46	1.50
25	5	614	ZEX	C24-C25	2.12	1.52	1.50
17	1	609	CLA	MG-ND	-2.12	2.01	2.05
25	2	617	ZEX	C12-C13	2.12	1.50	1.45
17	5	612	CLA	CMD-C2D	-2.12	1.46	1.50
17	1	609	CLA	CMD-C2D	-2.12	1.46	1.50
17	L	202	CLA	MG-ND	-2.12	2.01	2.05
17	J	101	CLA	C3B-C2B	-2.12	1.37	1.40
17	A	830	CLA	C3B-CAB	-2.11	1.43	1.47
17	3	210	CLA	MG-ND	-2.11	2.01	2.05
17	3	209	CLA	CMD-C2D	-2.11	1.46	1.50
17	2	610	CLA	CMD-C2D	-2.11	1.46	1.50
17	B	842	CLA	C4B-CHC	-2.11	1.35	1.41
17	B	807	CLA	C3B-C2B	-2.11	1.37	1.40
17	A	809	CLA	MG-ND	-2.11	2.01	2.05
20	A	845	BCR	C33-C5	-2.11	1.47	1.50
17	4	607	CLA	CMD-C2D	-2.11	1.46	1.50
25	1	615	ZEX	C12-C13	2.11	1.50	1.45
25	5	617	ZEX	C27-C28	2.11	1.39	1.33
17	L	202	CLA	CMD-C2D	-2.11	1.46	1.50
17	A	835	CLA	CMC-C2C	-2.10	1.46	1.50
17	3	205	CLA	C3B-CAB	-2.10	1.43	1.47
17	1	608	CLA	CMD-C2D	-2.10	1.46	1.50
17	B	811	CLA	MG-ND	-2.10	2.01	2.05
17	O	205	CLA	MG-ND	-2.10	2.01	2.05
17	F	303	CLA	CMC-C2C	-2.10	1.46	1.50
17	2	605	CLA	C3B-CAB	-2.10	1.43	1.47
17	A	820	CLA	C3B-CAB	-2.10	1.43	1.47
17	2	611	CLA	MG-ND	-2.10	2.01	2.05
17	A	808	CLA	CMC-C2C	-2.10	1.46	1.50
17	2	607	CLA	C3B-CAB	-2.10	1.43	1.47
17	2	603	CLA	C3B-CAB	-2.09	1.43	1.47
17	5	603	CLA	MG-ND	-2.09	2.01	2.05
17	2	610	CLA	C3B-CAB	-2.09	1.43	1.47
20	B	805	BCR	C38-C26	-2.09	1.47	1.50
17	B	825	CLA	CMC-C2C	-2.09	1.46	1.50
20	J	105	BCR	C33-C5	-2.09	1.47	1.50
17	A	819	CLA	C3B-CAB	-2.09	1.43	1.47
17	2	604	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	814	CLA	CMD-C2D	-2.08	1.46	1.50
17	B	819	CLA	MG-ND	-2.08	2.01	2.05
17	A	836	CLA	C4B-CHC	-2.08	1.35	1.41
17	A	824	CLA	CMC-C2C	-2.08	1.46	1.50
20	B	850	BCR	C38-C26	-2.08	1.47	1.50
17	O	205	CLA	C3B-CAB	-2.08	1.43	1.47
17	O	201	CLA	MG-ND	-2.08	2.01	2.05
17	F	303	CLA	CMD-C2D	-2.08	1.46	1.50
17	3	207	CLA	CMC-C2C	-2.08	1.46	1.50
17	2	613	CLA	CMC-C2C	-2.08	1.46	1.50
17	A	833	CLA	C3B-CAB	-2.08	1.43	1.47
17	A	818	CLA	C4B-CHC	-2.08	1.35	1.41
17	B	815	CLA	C3B-C2B	-2.08	1.37	1.40
17	4	608	CLA	C3B-CAB	-2.08	1.43	1.47
17	1	606	CLA	CMC-C2C	-2.08	1.46	1.50
17	B	823	CLA	C3B-C2B	-2.08	1.37	1.40
17	2	612	CLA	C3B-CAB	-2.08	1.43	1.47
17	1	602	CLA	CAC-C3C	-2.07	1.45	1.51
17	2	610	CLA	MG-ND	-2.07	2.01	2.05
17	B	835	CLA	MG-ND	-2.07	2.01	2.05
17	O	203	CLA	CMD-C2D	-2.07	1.46	1.50
17	A	807	CLA	CAC-C3C	-2.07	1.45	1.51
17	J	102	CLA	C4B-CHC	-2.07	1.35	1.41
17	K	102	CLA	C3B-C2B	-2.07	1.37	1.40
25	1	615	ZEX	C1-C6	2.07	1.56	1.53
17	B	824	CLA	CMC-C2C	-2.06	1.46	1.50
17	1	601	CLA	CMD-C2D	-2.06	1.46	1.50
17	B	817	CLA	C3B-CAB	-2.06	1.43	1.47
17	4	601	CLA	C3B-C2B	-2.06	1.37	1.40
17	4	603	CLA	CMC-C2C	-2.06	1.46	1.50
17	B	812	CLA	C3B-CAB	-2.06	1.43	1.47
17	2	612	CLA	C3B-C2B	-2.06	1.37	1.40
17	A	804	CLA	C3B-CAB	-2.06	1.43	1.47
17	5	607	CLA	CMD-C2D	-2.06	1.46	1.50
25	3	217	ZEX	C27-C28	2.05	1.39	1.33
17	A	848	CLA	C1D-ND	2.05	1.40	1.37
17	B	827	CLA	C3B-CAB	-2.05	1.43	1.47
17	B	806	CLA	C4B-CHC	-2.05	1.35	1.41
17	4	604	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	806	CLA	C4B-CHC	-2.05	1.35	1.41
17	1	612	CLA	C4B-CHC	-2.05	1.35	1.41
17	3	211	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	204	CLA	CMC-C2C	-2.05	1.46	1.50
17	5	601	CLA	C3B-CAB	-2.05	1.43	1.47
17	L	202	CLA	CMC-C2C	-2.05	1.46	1.50
17	5	610	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	807	CLA	C4B-CHC	-2.05	1.35	1.41
17	4	607	CLA	CMC-C2C	-2.05	1.46	1.50
17	A	827	CLA	C1D-ND	2.05	1.40	1.37
17	5	608	CLA	CMD-C2D	-2.05	1.46	1.50
17	2	605	CLA	CMC-C2C	-2.05	1.46	1.50
25	3	201	ZEX	C1-C6	2.05	1.56	1.53
17	A	819	CLA	CMA-C3A	-2.05	1.48	1.53
17	B	821	CLA	C4B-CHC	-2.04	1.35	1.41
17	3	213	CLA	MG-ND	-2.04	2.01	2.05
17	B	835	CLA	C3B-CAB	-2.04	1.43	1.47
17	3	203	CLA	MG-ND	-2.04	2.01	2.05
17	4	603	CLA	MG-ND	-2.04	2.01	2.05
17	A	811	CLA	C4B-CHC	-2.04	1.35	1.41
25	1	617	ZEX	C12-C13	2.04	1.50	1.45
17	2	613	CLA	C3B-CAB	-2.04	1.43	1.47
17	2	613	CLA	MG-ND	-2.04	2.01	2.05
17	B	823	CLA	C3B-CAB	-2.04	1.43	1.47
17	F	303	CLA	C3B-CAB	-2.03	1.43	1.47
17	B	816	CLA	C3B-C2B	-2.03	1.37	1.40
17	B	813	CLA	CAC-C3C	-2.03	1.45	1.51
17	B	825	CLA	C4B-CHC	-2.03	1.35	1.41
17	A	820	CLA	CAC-C3C	-2.03	1.45	1.51
17	B	843	CLA	C3B-CAB	-2.03	1.43	1.47
25	2	614	ZEX	C24-C25	2.03	1.52	1.50
20	L	201	BCR	C33-C5	-2.03	1.47	1.50
17	4	611	CLA	C3B-C2B	-2.03	1.37	1.40
17	K	103	CLA	C3B-CAB	-2.03	1.43	1.47
17	3	202	CLA	MG-ND	-2.03	2.01	2.05
17	A	822	CLA	CAC-C3C	-2.03	1.45	1.51
17	B	839	CLA	CAC-C3C	-2.03	1.45	1.51
17	A	812	CLA	C3B-CAB	-2.03	1.43	1.47
17	4	602	CLA	MG-ND	-2.03	2.01	2.05
17	B	817	CLA	C3B-C2B	-2.03	1.37	1.40
17	4	606	CLA	MG-ND	-2.03	2.01	2.05
17	A	824	CLA	CAC-C3C	-2.02	1.45	1.51
17	2	609	CLA	C3B-CAB	-2.02	1.43	1.47
17	A	839	CLA	CMA-C3A	-2.02	1.48	1.53
17	B	809	CLA	C4B-CHC	-2.02	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	602	CLA	C4B-CHC	-2.02	1.35	1.41
17	O	204	CLA	CMC-C2C	-2.02	1.46	1.50
17	2	613	CLA	C3B-C2B	-2.02	1.37	1.40
25	5	615	ZEX	C27-C28	2.02	1.39	1.33
17	1	609	CLA	CMC-C2C	-2.02	1.46	1.50
20	B	849	BCR	C38-C26	-2.02	1.47	1.50
20	O	202	BCR	C38-C26	-2.01	1.47	1.50
17	5	608	CLA	MG-ND	-2.01	2.01	2.05
17	B	801	CLA	C3B-CAB	-2.01	1.43	1.47
17	B	840	CLA	C3B-CAB	-2.01	1.43	1.47
17	A	809	CLA	CAC-C3C	-2.01	1.45	1.51
17	3	211	CLA	C3B-C2B	-2.01	1.37	1.40
17	O	204	CLA	CMD-C2D	-2.01	1.46	1.50
17	1	605	CLA	CMC-C2C	-2.01	1.46	1.50
17	K	102	CLA	C3B-CAB	-2.01	1.43	1.47
17	5	602	CLA	C3B-CAB	-2.01	1.43	1.47
17	2	609	CLA	MG-ND	-2.01	2.01	2.05
17	4	610	CLA	CMD-C2D	-2.01	1.46	1.50
17	B	827	CLA	C4B-CHC	-2.01	1.35	1.41
17	4	602	CLA	CMA-C3A	-2.01	1.48	1.53
17	B	812	CLA	CAC-C3C	-2.01	1.46	1.51
17	A	834	CLA	MG-ND	-2.01	2.01	2.05
17	B	822	CLA	C4B-CHC	-2.00	1.35	1.41
17	B	819	CLA	C3B-CAB	-2.00	1.43	1.47
17	A	808	CLA	C4B-CHC	-2.00	1.35	1.41
25	4	613	ZEX	C27-C28	2.00	1.39	1.33
17	B	830	CLA	C4B-CHC	-2.00	1.35	1.41
17	3	213	CLA	CMC-C2C	-2.00	1.46	1.50

All (2576) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	614	ZEX	C31-C30-C29	-16.44	103.84	127.31
25	1	614	ZEX	C39-C29-C28	-14.08	95.90	118.08
25	5	617	ZEX	C15-C14-C13	-13.48	108.07	127.31
25	3	201	ZEX	C31-C30-C29	-13.33	108.28	127.31
16	A	801	CL0	C4A-NA-C1A	13.29	112.68	106.71
25	1	614	ZEX	C28-C27-C26	-13.08	104.74	127.09
25	4	616	ZEX	C18-C5-C6	-12.92	110.02	124.53
25	4	616	ZEX	C11-C10-C9	-12.84	108.99	127.31
25	1	615	ZEX	C18-C5-C6	-12.72	110.25	124.53
25	1	613	ZEX	C18-C5-C6	-12.70	110.27	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	614	ZEX	C11-C10-C9	-12.67	109.22	127.31
25	5	617	ZEX	C18-C5-C6	-12.55	110.44	124.53
25	2	616	ZEX	C35-C34-C33	-12.53	109.43	127.31
25	5	617	ZEX	C11-C10-C9	-12.48	109.50	127.31
25	4	615	ZEX	C11-C10-C9	-12.47	109.51	127.31
25	3	216	ZEX	C18-C5-C6	-12.44	110.56	124.53
25	1	613	ZEX	C31-C30-C29	-12.32	109.72	127.31
25	4	614	ZEX	C18-C5-C6	-12.29	110.73	124.53
25	2	615	ZEX	C31-C30-C29	-12.28	109.78	127.31
25	2	616	ZEX	C18-C5-C6	-12.27	110.75	124.53
25	4	617	ZEX	C18-C5-C6	-12.20	110.83	124.53
25	1	615	ZEX	C15-C14-C13	-12.15	109.97	127.31
25	5	615	ZEX	C18-C5-C6	-12.13	110.91	124.53
25	5	616	ZEX	C18-C5-C6	-12.08	110.97	124.53
25	2	614	ZEX	C11-C10-C9	-12.03	110.14	127.31
25	1	617	ZEX	C31-C30-C29	-12.02	110.16	127.31
25	4	612	ZEX	C35-C34-C33	-11.89	110.34	127.31
25	3	201	ZEX	C18-C5-C6	-11.85	111.22	124.53
25	4	612	ZEX	C18-C5-C6	-11.81	111.27	124.53
25	4	613	ZEX	C11-C10-C9	-11.81	110.46	127.31
25	1	617	ZEX	C18-C5-C6	-11.78	111.31	124.53
25	4	613	ZEX	C18-C5-C6	-11.77	111.31	124.53
25	1	616	ZEX	C31-C30-C29	-11.72	110.58	127.31
25	4	613	ZEX	C31-C30-C29	-11.69	110.62	127.31
25	5	617	ZEX	C20-C13-C14	-11.66	106.58	122.92
25	3	214	ZEX	C18-C5-C6	-11.66	111.43	124.53
25	3	215	ZEX	C18-C5-C6	-11.65	111.44	124.53
25	4	612	ZEX	C31-C30-C29	-11.59	110.77	127.31
25	2	617	ZEX	C18-C5-C6	-11.52	111.59	124.53
25	2	615	ZEX	C18-C5-C6	-11.51	111.60	124.53
25	3	214	ZEX	C11-C10-C9	-11.47	110.94	127.31
25	1	616	ZEX	C18-C5-C6	-11.44	111.68	124.53
25	4	615	ZEX	C18-C5-C6	-11.40	111.73	124.53
25	5	614	ZEX	C35-C34-C33	-11.38	111.06	127.31
25	2	614	ZEX	C18-C5-C6	-11.37	111.76	124.53
25	3	201	ZEX	C35-C34-C33	-11.32	111.16	127.31
25	1	614	ZEX	C39-C29-C30	-11.32	107.07	122.92
25	1	616	ZEX	C11-C10-C9	-11.30	111.18	127.31
25	3	214	ZEX	C35-C34-C33	-11.30	111.18	127.31
25	5	614	ZEX	C18-C5-C6	-11.30	111.84	124.53
25	1	614	ZEX	C18-C5-C6	-11.28	111.86	124.53
25	3	217	ZEX	C18-C5-C6	-11.24	111.91	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	614	ZEX	C15-C14-C13	-11.20	111.32	127.31
25	2	615	ZEX	C15-C14-C13	-11.13	111.43	127.31
25	3	214	ZEX	C20-C13-C14	-11.12	107.34	122.92
25	3	214	ZEX	C31-C30-C29	-11.07	111.51	127.31
25	1	617	ZEX	C11-C10-C9	-11.04	111.56	127.31
25	3	215	ZEX	C20-C13-C14	-11.01	107.49	122.92
25	3	215	ZEX	C31-C30-C29	-10.94	111.70	127.31
25	5	617	ZEX	C19-C9-C10	-10.82	107.77	122.92
25	1	615	ZEX	C11-C10-C9	-10.80	111.90	127.31
25	3	215	ZEX	C15-C14-C13	-10.79	111.90	127.31
25	5	616	ZEX	C35-C34-C33	-10.75	111.97	127.31
25	2	617	ZEX	C15-C14-C13	-10.72	112.00	127.31
25	5	614	ZEX	C20-C13-C14	-10.70	107.93	122.92
25	3	217	ZEX	C11-C10-C9	-10.69	112.05	127.31
25	5	616	ZEX	C11-C10-C9	-10.67	112.08	127.31
25	4	616	ZEX	C35-C34-C33	-10.63	112.14	127.31
25	2	615	ZEX	C39-C29-C30	-10.58	108.10	122.92
25	1	616	ZEX	C35-C34-C33	-10.56	112.25	127.31
25	1	613	ZEX	C15-C14-C13	-10.50	112.33	127.31
25	4	617	ZEX	C35-C34-C33	-10.47	112.36	127.31
25	3	217	ZEX	C15-C14-C13	-10.46	112.39	127.31
25	2	617	ZEX	C35-C34-C33	-10.45	112.39	127.31
25	2	614	ZEX	C31-C30-C29	-10.43	112.42	127.31
25	3	218	ZEX	C39-C29-C30	-10.41	108.34	122.92
25	3	216	ZEX	C35-C34-C33	-10.39	112.48	127.31
25	3	201	ZEX	C20-C13-C14	-10.33	108.45	122.92
17	B	811	CLA	C4A-NA-C1A	10.33	111.35	106.71
25	2	616	ZEX	C40-C33-C34	-10.30	108.49	122.92
25	2	614	ZEX	C19-C9-C10	-10.30	108.50	122.92
25	4	617	ZEX	C15-C14-C13	-10.27	112.66	127.31
25	3	217	ZEX	C35-C34-C33	-10.20	112.75	127.31
25	3	216	ZEX	C11-C10-C9	-10.15	112.82	127.31
25	3	215	ZEX	C11-C10-C9	-10.12	112.87	127.31
25	3	201	ZEX	C15-C14-C13	-10.12	112.87	127.31
25	3	214	ZEX	C15-C14-C13	-10.10	112.89	127.31
25	5	616	ZEX	C19-C9-C10	-10.10	108.78	122.92
25	4	616	ZEX	C31-C30-C29	-10.09	112.92	127.31
25	1	616	ZEX	C15-C14-C13	-10.06	112.95	127.31
25	4	617	ZEX	C11-C10-C9	-10.02	113.01	127.31
25	4	616	ZEX	C15-C14-C13	-10.02	113.01	127.31
25	4	614	ZEX	C15-C14-C13	-10.00	113.04	127.31
25	2	617	ZEX	C20-C13-C14	-9.99	108.93	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	614	ZEX	C35-C34-C33	-9.97	113.09	127.31
25	4	617	ZEX	C40-C33-C34	-9.96	108.97	122.92
25	3	217	ZEX	C40-C33-C34	-9.95	108.99	122.92
25	1	615	ZEX	C20-C13-C14	-9.94	108.99	122.92
25	5	614	ZEX	C31-C30-C29	-9.94	113.12	127.31
25	1	616	ZEX	C40-C33-C34	-9.93	109.01	122.92
25	1	613	ZEX	C11-C10-C9	-9.93	113.14	127.31
25	2	617	ZEX	C31-C30-C29	-9.92	113.15	127.31
25	2	614	ZEX	C39-C29-C30	-9.90	109.06	122.92
25	5	615	ZEX	C31-C30-C29	-9.89	113.19	127.31
25	1	616	ZEX	C39-C29-C30	-9.89	109.07	122.92
25	1	613	ZEX	C39-C29-C30	-9.88	109.08	122.92
25	2	617	ZEX	C40-C33-C34	-9.88	109.08	122.92
25	3	218	ZEX	C31-C30-C29	-9.86	113.23	127.31
25	3	201	ZEX	C39-C29-C30	-9.85	109.12	122.92
25	5	616	ZEX	C40-C33-C34	-9.84	109.13	122.92
25	3	217	ZEX	C19-C9-C10	-9.84	109.14	122.92
25	1	615	ZEX	C27-C26-C25	-9.83	106.94	122.84
25	5	615	ZEX	C35-C34-C33	-9.83	113.29	127.31
25	1	614	ZEX	C19-C9-C10	-9.81	109.19	122.92
25	4	615	ZEX	C15-C14-C13	-9.80	113.33	127.31
25	5	616	ZEX	C20-C13-C14	-9.79	109.20	122.92
25	4	612	ZEX	C39-C29-C30	-9.77	109.24	122.92
25	4	614	ZEX	C11-C10-C9	-9.75	113.39	127.31
25	5	616	ZEX	C31-C30-C29	-9.74	113.40	127.31
25	3	218	ZEX	C18-C5-C6	-9.74	113.59	124.53
18	B	844	PQN	C11-C12-C13	-9.74	110.58	126.79
17	B	806	CLA	C4A-NA-C1A	9.73	111.08	106.71
25	3	214	ZEX	C19-C9-C10	-9.72	109.31	122.92
25	2	617	ZEX	C39-C29-C30	-9.70	109.34	122.92
25	2	614	ZEX	C27-C26-C25	-9.68	107.18	122.84
25	4	615	ZEX	C19-C9-C10	-9.68	109.37	122.92
25	2	615	ZEX	C19-C9-C10	-9.67	109.38	122.92
25	5	615	ZEX	C27-C26-C25	-9.66	107.23	122.84
25	3	216	ZEX	C40-C33-C34	-9.63	109.43	122.92
25	1	617	ZEX	C15-C14-C13	-9.63	113.56	127.31
25	1	616	ZEX	C19-C9-C10	-9.61	109.45	122.92
17	1	601	CLA	C4A-NA-C1A	9.60	111.02	106.71
25	4	615	ZEX	C35-C34-C33	-9.57	113.65	127.31
25	5	615	ZEX	C40-C33-C34	-9.53	109.58	122.92
25	5	616	ZEX	C39-C29-C30	-9.52	109.58	122.92
25	3	217	ZEX	C20-C13-C14	-9.49	109.62	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	615	ZEX	C20-C13-C14	-9.47	109.66	122.92
25	3	216	ZEX	C19-C9-C10	-9.46	109.67	122.92
25	5	616	ZEX	C15-C14-C13	-9.46	113.81	127.31
25	5	617	ZEX	C39-C29-C30	-9.44	109.70	122.92
25	4	616	ZEX	C39-C29-C30	-9.44	109.70	122.92
25	3	215	ZEX	C40-C33-C34	-9.43	109.71	122.92
25	3	218	ZEX	C15-C14-C13	-9.38	113.93	127.31
25	1	613	ZEX	C19-C9-C8	-9.37	103.31	118.08
25	4	613	ZEX	C19-C9-C10	-9.37	109.80	122.92
25	4	616	ZEX	C40-C33-C34	-9.36	109.81	122.92
25	5	617	ZEX	C1-C6-C5	-9.35	109.44	122.61
25	4	616	ZEX	C19-C9-C10	-9.34	109.84	122.92
25	5	617	ZEX	C35-C34-C33	-9.34	113.98	127.31
25	4	613	ZEX	C15-C14-C13	-9.32	114.00	127.31
25	4	617	ZEX	C20-C13-C14	-9.30	109.89	122.92
25	4	617	ZEX	C19-C9-C10	-9.30	109.90	122.92
25	5	615	ZEX	C20-C13-C14	-9.24	109.98	122.92
25	2	616	ZEX	C19-C9-C10	-9.24	109.98	122.92
25	5	614	ZEX	C40-C33-C34	-9.23	109.99	122.92
25	1	617	ZEX	C39-C29-C30	-9.22	110.01	122.92
25	3	201	ZEX	C40-C33-C34	-9.21	110.02	122.92
25	5	617	ZEX	C27-C26-C25	-9.20	107.97	122.84
25	3	215	ZEX	C39-C29-C30	-9.18	110.06	122.92
25	3	216	ZEX	C31-C30-C29	-9.18	114.21	127.31
25	2	616	ZEX	C31-C30-C29	-9.17	114.23	127.31
25	2	614	ZEX	C20-C13-C14	-9.15	110.10	122.92
25	4	612	ZEX	C20-C13-C14	-9.14	110.11	122.92
25	3	214	ZEX	C40-C33-C34	-9.11	110.16	122.92
25	3	214	ZEX	C39-C29-C30	-9.09	110.19	122.92
25	2	614	ZEX	C40-C33-C34	-9.08	110.20	122.92
25	4	613	ZEX	C1-C6-C5	-9.08	109.82	122.61
25	2	616	ZEX	C11-C10-C9	-9.04	114.41	127.31
25	5	614	ZEX	C27-C26-C25	-9.04	108.23	122.84
25	4	616	ZEX	C20-C13-C14	-9.03	110.28	122.92
25	3	216	ZEX	C39-C29-C30	-8.98	110.34	122.92
25	1	615	ZEX	C40-C33-C34	-8.95	110.38	122.92
25	4	613	ZEX	C39-C29-C30	-8.94	110.39	122.92
25	4	613	ZEX	C20-C13-C14	-8.94	110.40	122.92
25	4	614	ZEX	C19-C9-C10	-8.93	110.41	122.92
25	1	613	ZEX	C20-C13-C14	-8.93	110.42	122.92
25	2	615	ZEX	C11-C10-C9	-8.92	114.58	127.31
25	2	617	ZEX	C27-C26-C25	-8.92	108.42	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	216	ZEX	C15-C14-C13	-8.88	114.64	127.31
25	4	613	ZEX	C35-C34-C33	-8.87	114.64	127.31
25	1	615	ZEX	C19-C9-C10	-8.86	110.51	122.92
25	3	215	ZEX	C35-C34-C33	-8.84	114.70	127.31
25	2	617	ZEX	C11-C10-C9	-8.84	114.70	127.31
25	5	614	ZEX	C19-C9-C10	-8.83	110.56	122.92
25	3	217	ZEX	C27-C26-C25	-8.83	108.57	122.84
17	B	835	CLA	C4A-NA-C1A	8.82	110.67	106.71
17	4	601	CLA	C4A-NA-C1A	8.79	110.66	106.71
25	3	201	ZEX	C27-C26-C25	-8.76	108.68	122.84
25	5	615	ZEX	C11-C10-C9	-8.75	114.82	127.31
25	3	216	ZEX	C27-C26-C25	-8.75	108.70	122.84
25	4	614	ZEX	C20-C13-C14	-8.74	110.67	122.92
25	5	614	ZEX	C20-C13-C12	-8.74	104.30	118.08
25	5	617	ZEX	C31-C30-C29	-8.74	114.83	127.31
25	4	613	ZEX	C40-C33-C34	-8.74	110.69	122.92
17	5	612	CLA	C4A-NA-C1A	8.72	110.63	106.71
25	5	615	ZEX	C15-C14-C13	-8.71	114.88	127.31
25	1	617	ZEX	C19-C9-C10	-8.71	110.72	122.92
25	1	613	ZEX	C1-C6-C5	-8.69	110.37	122.61
25	4	612	ZEX	C19-C9-C10	-8.69	110.75	122.92
25	3	215	ZEX	C19-C9-C10	-8.69	110.76	122.92
25	1	616	ZEX	C20-C13-C14	-8.66	110.80	122.92
25	2	614	ZEX	C35-C34-C33	-8.64	114.98	127.31
25	3	215	ZEX	C39-C29-C28	-8.63	104.47	118.08
25	1	614	ZEX	C15-C14-C13	-8.63	115.00	127.31
25	3	218	ZEX	C20-C13-C14	-8.60	110.88	122.92
25	2	615	ZEX	C32-C33-C34	-8.56	105.81	118.94
25	5	614	ZEX	C39-C29-C30	-8.55	110.95	122.92
18	A	840	PQN	C11-C12-C13	-8.55	112.56	126.79
25	4	614	ZEX	C35-C34-C33	-8.53	115.14	127.31
17	A	848	CLA	C4A-NA-C1A	8.52	110.53	106.71
25	1	617	ZEX	C1-C6-C5	-8.49	110.65	122.61
25	2	616	ZEX	C39-C29-C30	-8.46	111.07	122.92
25	1	613	ZEX	C40-C33-C34	-8.41	111.14	122.92
17	B	814	CLA	C4A-NA-C1A	8.41	110.49	106.71
25	4	614	ZEX	C40-C33-C34	-8.40	111.16	122.92
25	4	615	ZEX	C20-C13-C14	-8.39	111.17	122.92
25	3	216	ZEX	C20-C13-C14	-8.39	111.17	122.92
17	A	839	CLA	C4A-NA-C1A	8.37	110.47	106.71
17	B	842	CLA	C4A-NA-C1A	8.36	110.46	106.71
17	A	813	CLA	C4A-NA-C1A	8.35	110.46	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	201	ZEX	C1-C6-C5	-8.34	110.86	122.61
25	1	615	ZEX	C32-C33-C34	-8.33	106.16	118.94
25	3	218	ZEX	C40-C33-C34	-8.30	111.29	122.92
25	4	617	ZEX	C27-C26-C25	-8.30	109.41	122.84
25	1	613	ZEX	C35-C34-C33	-8.30	115.47	127.31
17	A	818	CLA	C4A-NA-C1A	8.27	110.42	106.71
25	2	615	ZEX	C28-C29-C30	-8.26	106.27	118.94
25	1	615	ZEX	C31-C30-C29	-8.22	115.57	127.31
17	B	832	CLA	CMB-C2B-C1B	-8.21	115.85	128.46
25	4	612	ZEX	C40-C33-C34	-8.20	111.43	122.92
25	3	217	ZEX	C39-C29-C30	-8.19	111.44	122.92
25	2	617	ZEX	C19-C9-C10	-8.19	111.45	122.92
25	4	615	ZEX	C27-C26-C25	-8.18	109.61	122.84
25	5	615	ZEX	C39-C29-C30	-8.15	111.50	122.92
25	4	615	ZEX	C40-C33-C34	-8.15	111.51	122.92
25	2	615	ZEX	C35-C34-C33	-8.13	115.71	127.31
17	2	602	CLA	C4A-NA-C1A	8.12	110.36	106.71
25	3	218	ZEX	C19-C9-C10	-8.11	111.56	122.92
25	1	614	ZEX	C40-C33-C34	-8.10	111.57	122.92
17	A	802	CLA	C4A-NA-C1A	8.09	110.34	106.71
25	3	201	ZEX	C11-C10-C9	-8.07	115.79	127.31
25	5	617	ZEX	C40-C33-C34	-8.06	111.63	122.92
25	1	613	ZEX	C27-C26-C25	-8.06	109.81	122.84
17	A	820	CLA	C4A-NA-C1A	8.05	110.33	106.71
25	5	616	ZEX	C27-C26-C25	-8.04	109.85	122.84
17	B	841	CLA	C4A-NA-C1A	8.02	110.31	106.71
25	4	613	ZEX	C32-C33-C34	-7.99	106.68	118.94
25	2	616	ZEX	C20-C13-C14	-7.98	111.74	122.92
25	5	614	ZEX	C11-C10-C9	-7.98	115.92	127.31
17	2	604	CLA	C4A-NA-C1A	7.98	110.29	106.71
17	2	601	CLA	C4A-NA-C1A	7.96	110.28	106.71
25	3	215	ZEX	C27-C26-C25	-7.95	109.98	122.84
17	4	610	CLA	C4A-NA-C1A	7.95	110.28	106.71
25	4	612	ZEX	C15-C14-C13	-7.95	115.97	127.31
25	3	215	ZEX	C32-C33-C34	-7.92	106.78	118.94
17	A	826	CLA	C4A-NA-C1A	7.92	110.27	106.71
17	A	806	CLA	C4A-NA-C1A	7.92	110.27	106.71
25	1	617	ZEX	C35-C34-C33	-7.90	116.04	127.31
25	2	617	ZEX	C19-C9-C8	-7.89	105.64	118.08
25	4	614	ZEX	C39-C29-C30	-7.89	111.87	122.92
17	A	832	CLA	C4A-NA-C1A	7.88	110.25	106.71
17	2	605	CLA	C4A-NA-C1A	7.87	110.24	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	606	CLA	C4A-NA-C1A	7.87	110.24	106.71
25	4	614	ZEX	C27-C26-C25	-7.85	110.14	122.84
25	1	617	ZEX	C20-C13-C14	-7.83	111.96	122.92
17	B	818	CLA	C4A-NA-C1A	7.82	110.22	106.71
17	A	831	CLA	C4A-NA-C1A	7.82	110.22	106.71
17	1	611	CLA	CAC-C3C-C4C	7.80	134.93	124.81
25	5	615	ZEX	C19-C9-C10	-7.80	112.00	122.92
25	4	612	ZEX	C11-C10-C9	-7.78	116.20	127.31
17	B	821	CLA	C4A-NA-C1A	7.77	110.20	106.71
25	4	616	ZEX	C27-C26-C25	-7.77	110.28	122.84
25	4	612	ZEX	C12-C13-C14	-7.77	107.03	118.94
25	5	614	ZEX	C8-C9-C10	-7.76	107.03	118.94
17	B	808	CLA	C4A-NA-C1A	7.75	110.19	106.71
17	A	819	CLA	C4A-NA-C1A	7.75	110.19	106.71
25	2	614	ZEX	C15-C14-C13	-7.74	116.26	127.31
25	3	218	ZEX	C11-C10-C9	-7.74	116.26	127.31
17	B	810	CLA	C4A-NA-C1A	7.73	110.18	106.71
17	5	608	CLA	C4A-NA-C1A	7.73	110.18	106.71
17	1	608	CLA	C4A-NA-C1A	7.72	110.18	106.71
25	1	613	ZEX	C19-C9-C10	-7.72	112.11	122.92
25	1	616	ZEX	C27-C26-C25	-7.72	110.36	122.84
17	B	822	CLA	C4A-NA-C1A	7.70	110.17	106.71
25	3	217	ZEX	C31-C30-C29	-7.70	116.33	127.31
25	1	617	ZEX	C40-C33-C34	-7.69	112.15	122.92
25	1	615	ZEX	C39-C29-C30	-7.69	112.15	122.92
25	1	615	ZEX	C8-C9-C10	-7.68	107.15	118.94
17	5	603	CLA	C4A-NA-C1A	7.68	110.16	106.71
17	B	801	CLA	C4A-NA-C1A	7.67	110.16	106.71
17	3	207	CLA	C4A-NA-C1A	7.67	110.15	106.71
25	2	617	ZEX	C28-C29-C30	-7.66	107.19	118.94
25	4	615	ZEX	C31-C30-C29	-7.65	116.39	127.31
25	1	617	ZEX	C27-C26-C25	-7.64	110.48	122.84
17	2	610	CLA	C4A-NA-C1A	7.63	110.14	106.71
25	4	617	ZEX	C31-C30-C29	-7.61	116.45	127.31
17	K	103	CLA	C4A-NA-C1A	7.61	110.13	106.71
25	1	615	ZEX	C35-C34-C33	-7.61	116.45	127.31
25	3	217	ZEX	C28-C29-C30	-7.60	107.28	118.94
17	B	819	CLA	C4A-NA-C1A	7.58	110.11	106.71
17	B	807	CLA	C4A-NA-C1A	7.58	110.11	106.71
25	4	614	ZEX	C32-C33-C34	-7.58	107.32	118.94
25	2	617	ZEX	C8-C9-C10	-7.57	107.32	118.94
17	3	213	CLA	C4A-NA-C1A	7.56	110.10	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	612	ZEX	C27-C26-C25	-7.56	110.62	122.84
17	A	814	CLA	C4A-NA-C1A	7.56	110.10	106.71
17	L	203	CLA	C4A-NA-C1A	7.55	110.10	106.71
17	2	608	CLA	C4A-NA-C1A	7.54	110.10	106.71
17	5	604	CLA	C4A-NA-C1A	7.49	110.07	106.71
17	3	204	CLA	C4A-NA-C1A	7.47	110.06	106.71
25	4	616	ZEX	C28-C29-C30	-7.47	107.48	118.94
25	2	614	ZEX	C28-C29-C30	-7.47	107.48	118.94
17	A	808	CLA	C4A-NA-C1A	7.46	110.06	106.71
17	A	825	CLA	C4A-NA-C1A	7.42	110.04	106.71
17	B	803	CLA	C4A-NA-C1A	7.42	110.04	106.71
16	A	801	CL0	CBA-CAA-C2A	-7.42	91.96	113.86
25	4	612	ZEX	C8-C9-C10	-7.41	107.58	118.94
17	1	602	CLA	C4A-NA-C1A	7.39	110.03	106.71
17	B	837	CLA	C4A-NA-C1A	7.38	110.02	106.71
25	4	614	ZEX	C28-C29-C30	-7.37	107.64	118.94
17	B	824	CLA	C4A-NA-C1A	7.36	110.02	106.71
25	5	615	ZEX	C39-C29-C28	-7.36	106.48	118.08
17	4	607	CLA	C4A-NA-C1A	7.36	110.01	106.71
17	A	803	CLA	C4A-NA-C1A	7.32	110.00	106.71
17	A	838	CLA	C4A-NA-C1A	7.31	109.99	106.71
17	A	834	CLA	C4A-NA-C1A	7.30	109.99	106.71
25	5	615	ZEX	C40-C33-C32	-7.29	106.59	118.08
17	B	829	CLA	C4A-NA-C1A	7.29	109.98	106.71
17	J	102	CLA	C4A-NA-C1A	7.29	109.98	106.71
17	F	303	CLA	C4A-NA-C1A	7.28	109.98	106.71
17	5	605	CLA	C4A-NA-C1A	7.28	109.98	106.71
25	2	616	ZEX	C8-C9-C10	-7.28	107.77	118.94
16	A	801	CL0	CHB-C4A-NA	7.28	134.58	124.51
25	3	216	ZEX	C8-C9-C10	-7.28	107.78	118.94
17	A	837	CLA	C4A-NA-C1A	7.27	109.97	106.71
17	J	103	CLA	C4A-NA-C1A	7.26	109.97	106.71
17	A	822	CLA	C4A-NA-C1A	7.25	109.97	106.71
17	A	836	CLA	C4A-NA-C1A	7.25	109.96	106.71
17	A	823	CLA	C4A-NA-C1A	7.24	109.96	106.71
17	J	101	CLA	C4A-NA-C1A	7.24	109.96	106.71
25	3	201	ZEX	C19-C9-C10	-7.24	112.78	122.92
17	3	212	CLA	C4A-NA-C1A	7.24	109.96	106.71
25	4	617	ZEX	C28-C29-C30	-7.23	107.84	118.94
17	B	840	CLA	C4A-NA-C1A	7.23	109.95	106.71
25	3	218	ZEX	C35-C34-C33	-7.21	117.02	127.31
17	B	823	CLA	C4A-NA-C1A	7.21	109.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	809	CLA	C4A-NA-C1A	7.20	109.94	106.71
17	A	815	CLA	C4A-NA-C1A	7.20	109.94	106.71
25	1	613	ZEX	C32-C33-C34	-7.20	107.90	118.94
25	4	613	ZEX	C27-C26-C25	-7.19	111.22	122.84
17	2	603	CLA	C4A-NA-C1A	7.18	109.93	106.71
17	2	607	CLA	C4A-NA-C1A	7.17	109.93	106.71
25	3	214	ZEX	C39-C29-C28	-7.16	106.80	118.08
17	B	825	CLA	C4A-NA-C1A	7.16	109.92	106.71
25	3	215	ZEX	C20-C13-C12	-7.16	106.80	118.08
25	4	612	ZEX	C28-C29-C30	-7.15	107.97	118.94
25	3	214	ZEX	C8-C9-C10	-7.15	107.98	118.94
25	1	617	ZEX	C8-C9-C10	-7.14	107.99	118.94
17	B	836	CLA	C4A-NA-C1A	7.13	109.91	106.71
25	1	615	ZEX	C39-C29-C28	-7.12	106.86	118.08
17	3	202	CLA	C4A-NA-C1A	7.12	109.91	106.71
25	4	615	ZEX	C28-C29-C30	-7.12	108.02	118.94
17	B	801	CLA	CMB-C2B-C1B	-7.09	117.56	128.46
17	F	302	CLA	C4A-NA-C1A	7.09	109.89	106.71
25	3	201	ZEX	C39-C29-C28	-7.08	106.92	118.08
25	4	614	ZEX	C31-C30-C29	-7.07	117.22	127.31
17	4	603	CLA	C4A-NA-C1A	7.07	109.89	106.71
17	B	815	CLA	C4A-NA-C1A	7.06	109.88	106.71
25	1	614	ZEX	C12-C13-C14	-7.03	108.15	118.94
17	5	610	CLA	C4A-NA-C1A	7.03	109.87	106.71
17	L	202	CLA	C4A-NA-C1A	7.03	109.86	106.71
17	5	602	CLA	C4A-NA-C1A	7.02	109.86	106.71
17	A	828	CLA	C4A-NA-C1A	7.02	109.86	106.71
17	A	828	CLA	CMB-C2B-C1B	-7.02	117.68	128.46
17	3	203	CLA	C4A-NA-C1A	7.02	109.86	106.71
25	1	615	ZEX	C12-C13-C14	-7.00	108.20	118.94
25	3	201	ZEX	C7-C8-C9	-6.99	115.67	126.23
17	K	102	CLA	C4A-NA-C1A	6.98	109.84	106.71
25	4	615	ZEX	C32-C33-C34	-6.98	108.23	118.94
17	A	833	CLA	C4A-NA-C1A	6.98	109.84	106.71
25	1	614	ZEX	C20-C13-C14	-6.98	113.15	122.92
17	B	838	CLA	C4A-NA-C1A	6.92	109.82	106.71
25	3	216	ZEX	C12-C13-C14	-6.92	108.32	118.94
17	4	604	CLA	C4A-NA-C1A	6.92	109.82	106.71
25	3	201	ZEX	C19-C9-C8	-6.91	107.18	118.08
17	4	605	CLA	C4A-NA-C1A	6.91	109.81	106.71
17	3	209	CLA	C4A-NA-C1A	6.90	109.81	106.71
17	5	601	CLA	C4A-NA-C1A	6.90	109.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	614	ZEX	C32-C33-C34	-6.89	108.36	118.94
17	B	827	CLA	C4A-NA-C1A	6.89	109.80	106.71
17	B	817	CLA	C4A-NA-C1A	6.88	109.80	106.71
17	1	606	CLA	C4A-NA-C1A	6.88	109.80	106.71
25	4	616	ZEX	C32-C33-C34	-6.87	108.40	118.94
17	A	811	CLA	C4A-NA-C1A	6.87	109.79	106.71
25	4	615	ZEX	C39-C29-C30	-6.86	113.31	122.92
17	2	612	CLA	C4A-NA-C1A	6.86	109.79	106.71
17	A	817	CLA	C4A-NA-C1A	6.86	109.79	106.71
17	A	821	CLA	C4A-NA-C1A	6.86	109.79	106.71
25	2	616	ZEX	C15-C14-C13	-6.85	117.53	127.31
25	3	214	ZEX	C27-C26-C25	-6.85	111.76	122.84
25	4	612	ZEX	C40-C33-C32	-6.84	107.29	118.08
25	4	617	ZEX	C12-C13-C14	-6.84	108.45	118.94
17	4	609	CLA	C4A-NA-C1A	6.84	109.78	106.71
25	4	617	ZEX	C39-C29-C30	-6.83	113.35	122.92
17	3	211	CLA	C4A-NA-C1A	6.82	109.77	106.71
25	1	617	ZEX	C32-C33-C34	-6.82	108.48	118.94
25	2	615	ZEX	C27-C26-C25	-6.80	111.84	122.84
17	2	606	CLA	C4A-NA-C1A	6.80	109.77	106.71
25	3	214	ZEX	C20-C13-C12	-6.80	107.36	118.08
17	L	204	CLA	C4A-NA-C1A	6.79	109.76	106.71
17	A	824	CLA	C4A-NA-C1A	6.79	109.76	106.71
25	4	612	ZEX	C1-C6-C5	-6.78	113.06	122.61
17	5	611	CLA	C4A-NA-C1A	6.78	109.75	106.71
18	B	844	PQN	C15-C13-C12	-6.77	107.42	121.12
25	2	614	ZEX	C27-C28-C29	-6.77	116.01	126.23
17	A	804	CLA	C4A-NA-C1A	6.76	109.75	106.71
25	3	216	ZEX	C32-C33-C34	-6.76	108.57	118.94
17	A	807	CLA	C4A-NA-C1A	6.76	109.74	106.71
25	4	617	ZEX	C8-C9-C10	-6.75	108.59	118.94
25	4	615	ZEX	C12-C13-C14	-6.74	108.60	118.94
25	2	615	ZEX	C12-C13-C14	-6.72	108.62	118.94
25	2	617	ZEX	C12-C13-C14	-6.71	108.65	118.94
25	2	614	ZEX	C20-C13-C12	-6.71	107.51	118.08
17	1	609	CLA	C4A-NA-C1A	6.68	109.71	106.71
25	5	617	ZEX	C32-C33-C34	-6.68	108.69	118.94
17	1	605	CLA	C4A-NA-C1A	6.67	109.71	106.71
25	3	218	ZEX	C19-C9-C8	-6.67	107.58	118.08
25	1	615	ZEX	C28-C29-C30	-6.66	108.72	118.94
25	2	617	ZEX	C40-C33-C32	-6.65	107.59	118.08
17	O	203	CLA	C4A-NA-C1A	6.65	109.70	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	613	CLA	C4A-NA-C1A	6.62	109.68	106.71
17	1	604	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	A	840	PQN	C15-C13-C12	-6.61	107.74	121.12
17	B	813	CLA	C4A-NA-C1A	6.61	109.68	106.71
25	1	617	ZEX	C40-C33-C32	-6.61	107.67	118.08
17	O	201	CLA	C4A-NA-C1A	6.61	109.68	106.71
25	3	217	ZEX	C32-C33-C34	-6.60	108.81	118.94
25	1	617	ZEX	C39-C29-C28	-6.58	107.71	118.08
17	3	205	CLA	C4A-NA-C1A	6.58	109.66	106.71
25	2	617	ZEX	C32-C33-C34	-6.58	108.85	118.94
17	B	832	CLA	C4A-NA-C1A	6.58	109.66	106.71
25	3	215	ZEX	C28-C27-C26	-6.58	115.85	127.09
17	B	830	CLA	C4A-NA-C1A	6.57	109.66	106.71
25	2	616	ZEX	C40-C33-C32	-6.56	107.74	118.08
17	1	611	CLA	C4A-NA-C1A	6.56	109.66	106.71
17	B	809	CLA	C4A-NA-C1A	6.55	109.65	106.71
17	B	812	CLA	C4A-NA-C1A	6.54	109.65	106.71
17	A	816	CLA	C4A-NA-C1A	6.54	109.65	106.71
17	B	820	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	A	812	CLA	C4A-NA-C1A	6.51	109.64	106.71
17	4	611	CLA	C4A-NA-C1A	6.51	109.64	106.71
17	2	609	CLA	C4A-NA-C1A	6.51	109.63	106.71
25	3	215	ZEX	C19-C9-C8	-6.51	107.82	118.08
25	2	614	ZEX	C39-C29-C28	-6.50	107.84	118.08
17	4	602	CLA	C4A-NA-C1A	6.48	109.62	106.71
17	5	609	CLA	C4A-NA-C1A	6.44	109.60	106.71
17	A	810	CLA	C4A-NA-C1A	6.43	109.60	106.71
17	1	612	CLA	C4A-NA-C1A	6.43	109.59	106.71
17	1	610	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	1	617	ZEX	C28-C27-C26	-6.42	116.13	127.09
17	3	210	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	4	608	CLA	C4A-NA-C1A	6.38	109.58	106.71
25	5	615	ZEX	C12-C13-C14	-6.37	109.16	118.94
17	F	301	CLA	C4A-NA-C1A	6.35	109.56	106.71
25	3	216	ZEX	C28-C29-C30	-6.35	109.20	118.94
17	2	613	CLA	C4A-NA-C1A	6.34	109.56	106.71
17	B	801	CLA	CMB-C2B-C3B	6.34	136.53	124.68
25	3	201	ZEX	C20-C13-C12	-6.32	108.12	118.08
17	1	603	CLA	C4A-NA-C1A	6.29	109.54	106.71
25	5	616	ZEX	C12-C13-C14	-6.29	109.28	118.94
25	4	612	ZEX	C19-C9-C8	-6.28	108.19	118.08
25	4	613	ZEX	C12-C13-C14	-6.27	109.31	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	615	ZEX	C8-C9-C10	-6.26	109.33	118.94
25	3	201	ZEX	C40-C33-C32	-6.26	108.21	118.08
25	5	617	ZEX	C20-C13-C12	-6.25	108.22	118.08
17	5	606	CLA	C2D-C1D-ND	-6.25	105.50	110.10
17	A	835	CLA	C4A-NA-C1A	6.25	109.51	106.71
17	A	830	CLA	C4A-NA-C1A	6.23	109.51	106.71
17	B	826	CLA	C4A-NA-C1A	6.23	109.51	106.71
25	3	218	ZEX	C20-C13-C12	-6.22	108.27	118.08
17	2	611	CLA	C4A-NA-C1A	6.22	109.50	106.71
25	2	614	ZEX	C12-C13-C14	-6.22	109.40	118.94
25	3	218	ZEX	C27-C26-C25	-6.21	112.80	122.84
25	3	217	ZEX	C12-C13-C14	-6.21	109.41	118.94
25	3	218	ZEX	C40-C33-C32	-6.18	108.33	118.08
17	O	205	CLA	C4A-NA-C1A	6.18	109.49	106.71
17	5	606	CLA	C4A-NA-C1A	6.17	109.48	106.71
25	1	617	ZEX	C28-C29-C30	-6.15	109.51	118.94
17	A	848	CLA	CAC-C3C-C4C	6.14	132.77	124.81
25	4	617	ZEX	C39-C29-C28	-6.13	108.41	118.08
25	2	614	ZEX	C8-C9-C10	-6.13	109.53	118.94
17	B	843	CLA	C4A-NA-C1A	6.13	109.46	106.71
17	B	831	CLA	C4A-NA-C1A	6.11	109.45	106.71
17	A	805	CLA	C4A-NA-C1A	6.10	109.45	106.71
25	1	614	ZEX	C20-C13-C12	-6.09	108.48	118.08
17	B	816	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	2	615	ZEX	C40-C33-C34	-6.08	114.41	122.92
25	5	614	ZEX	C19-C9-C8	-6.06	108.53	118.08
25	1	613	ZEX	C20-C13-C12	-6.05	108.54	118.08
16	A	801	CL0	O2D-CGD-CBD	6.05	122.02	111.27
17	3	208	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	4	616	ZEX	C20-C13-C12	-6.04	108.56	118.08
25	3	214	ZEX	C28-C27-C26	-6.04	116.77	127.09
17	B	839	CLA	C4A-NA-C1A	6.03	109.42	106.71
25	3	217	ZEX	C8-C9-C10	-6.02	109.70	118.94
17	O	204	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	1	617	ZEX	C20-C13-C12	-5.98	108.65	118.08
25	5	617	ZEX	C19-C9-C8	-5.98	108.65	118.08
16	A	801	CL0	C2A-C3A-C4A	5.98	111.53	101.87
25	2	617	ZEX	C39-C29-C28	-5.97	108.67	118.08
25	1	615	ZEX	C19-C9-C8	-5.96	108.69	118.08
25	3	215	ZEX	C28-C29-C30	-5.95	109.81	118.94
25	2	614	ZEX	C7-C8-C9	-5.95	117.25	126.23
25	3	216	ZEX	C40-C33-C32	-5.91	108.77	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	206	CLA	CMB-C2B-C1B	-5.90	119.39	128.46
25	1	616	ZEX	C12-C13-C14	-5.89	109.90	118.94
17	1	607	CLA	C4A-NA-C1A	5.89	109.35	106.71
25	5	614	ZEX	C39-C29-C28	-5.88	108.81	118.08
17	B	834	CLA	C4A-NA-C1A	5.85	109.33	106.71
25	2	614	ZEX	C19-C9-C8	-5.83	108.89	118.08
25	2	616	ZEX	C12-C13-C14	-5.83	109.99	118.94
25	5	615	ZEX	C19-C9-C8	-5.80	108.94	118.08
17	A	805	CLA	CMB-C2B-C1B	-5.80	119.55	128.46
17	A	829	CLA	C4A-NA-C1A	5.80	109.31	106.71
16	A	801	CL0	CAA-C2A-C1A	5.79	130.94	111.97
25	4	613	ZEX	C28-C29-C30	-5.79	110.06	118.94
25	3	216	ZEX	C28-C27-C26	-5.77	117.23	127.09
25	1	616	ZEX	C32-C33-C34	-5.77	110.09	118.94
25	1	616	ZEX	C20-C13-C12	-5.74	109.03	118.08
25	2	614	ZEX	C40-C33-C32	-5.74	109.03	118.08
25	4	617	ZEX	C32-C33-C34	-5.73	110.15	118.94
17	1	607	CLA	CAA-CBA-CGA	5.73	127.70	112.51
25	3	215	ZEX	C8-C9-C10	-5.69	110.20	118.94
25	4	615	ZEX	C40-C33-C32	-5.69	109.11	118.08
25	3	216	ZEX	C20-C13-C12	-5.66	109.15	118.08
25	5	615	ZEX	C20-C13-C12	-5.66	109.16	118.08
25	2	617	ZEX	C20-C13-C12	-5.64	109.19	118.08
25	4	614	ZEX	C39-C29-C28	-5.63	109.20	118.08
17	B	827	CLA	CMB-C2B-C1B	-5.63	119.81	128.46
17	A	835	CLA	CMB-C2B-C1B	-5.62	119.83	128.46
25	4	615	ZEX	C20-C13-C12	-5.62	109.22	118.08
25	3	216	ZEX	C39-C29-C28	-5.60	109.25	118.08
17	2	608	CLA	CMB-C2B-C1B	-5.60	119.86	128.46
16	A	801	CL0	C4D-CHA-C1A	-5.60	114.44	121.25
25	1	613	ZEX	C40-C33-C32	-5.58	109.28	118.08
25	5	616	ZEX	C19-C9-C8	-5.58	109.29	118.08
25	5	616	ZEX	C39-C29-C28	-5.57	109.30	118.08
17	3	203	CLA	CMB-C2B-C1B	-5.57	119.91	128.46
25	1	616	ZEX	C39-C29-C28	-5.54	109.34	118.08
25	3	201	ZEX	C23-C24-C25	5.54	117.22	109.33
25	4	617	ZEX	C20-C13-C12	-5.51	109.39	118.08
25	1	614	ZEX	C1-C6-C5	-5.49	114.88	122.61
25	3	215	ZEX	C40-C33-C32	-5.49	109.42	118.08
25	3	217	ZEX	C1-C6-C5	-5.49	114.88	122.61
17	1	602	CLA	CMB-C2B-C1B	-5.49	120.03	128.46
25	5	616	ZEX	C32-C33-C34	-5.49	110.52	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	824	CLA	CAA-C2A-C3A	-5.48	97.78	112.78
17	B	832	CLA	CMB-C2B-C3B	5.46	134.90	124.68
25	5	615	ZEX	C27-C28-C29	-5.46	117.99	126.23
25	1	616	ZEX	C40-C33-C32	-5.45	109.48	118.08
25	1	613	ZEX	C28-C29-C30	-5.45	110.58	118.94
25	4	614	ZEX	C8-C9-C10	-5.44	110.59	118.94
25	4	614	ZEX	C40-C33-C32	-5.44	109.50	118.08
25	1	617	ZEX	C12-C13-C14	-5.43	110.60	118.94
25	4	616	ZEX	C27-C28-C29	-5.43	118.03	126.23
17	B	833	CLA	C4A-NA-C1A	5.41	109.14	106.71
25	1	615	ZEX	C20-C13-C12	-5.39	109.58	118.08
17	A	827	CLA	CMB-C2B-C1B	-5.39	120.19	128.46
25	4	616	ZEX	C8-C9-C10	-5.39	110.68	118.94
17	A	830	CLA	CMB-C2B-C1B	-5.39	120.19	128.46
25	5	615	ZEX	C8-C9-C10	-5.38	110.69	118.94
25	1	616	ZEX	C19-C9-C8	-5.37	109.61	118.08
16	A	801	CL0	C1D-ND-C4D	-5.37	102.52	106.33
25	4	616	ZEX	C12-C13-C14	-5.36	110.71	118.94
17	A	848	CLA	CMB-C2B-C1B	-5.36	120.23	128.46
25	2	616	ZEX	C1-C6-C5	-5.35	115.08	122.61
25	5	614	ZEX	C28-C29-C30	-5.35	110.74	118.94
25	4	613	ZEX	C39-C29-C28	-5.34	109.66	118.08
25	4	615	ZEX	C1-C6-C5	-5.34	115.09	122.61
25	4	616	ZEX	C39-C29-C28	-5.34	109.67	118.08
25	5	616	ZEX	C20-C13-C12	-5.34	109.67	118.08
25	3	217	ZEX	C20-C13-C12	-5.33	109.68	118.08
17	A	819	CLA	CMB-C2B-C1B	-5.32	120.28	128.46
17	1	601	CLA	CMB-C2B-C1B	-5.32	120.29	128.46
17	B	828	CLA	CAA-C2A-C3A	-5.32	98.21	112.78
25	2	616	ZEX	C27-C26-C25	-5.32	114.24	122.84
25	1	615	ZEX	C7-C8-C9	-5.32	118.20	126.23
25	3	217	ZEX	C39-C29-C28	-5.31	109.70	118.08
17	A	812	CLA	CMB-C2B-C1B	-5.31	120.30	128.46
25	5	614	ZEX	C40-C33-C32	-5.30	109.72	118.08
25	2	616	ZEX	C19-C9-C8	-5.30	109.73	118.08
17	3	206	CLA	C4A-NA-C1A	5.29	109.08	106.71
25	4	617	ZEX	C19-C9-C8	-5.29	109.75	118.08
25	5	617	ZEX	C39-C29-C28	-5.24	109.82	118.08
25	4	612	ZEX	C39-C29-C28	-5.24	109.83	118.08
17	B	828	CLA	C4A-NA-C1A	5.23	109.06	106.71
25	3	214	ZEX	C32-C33-C34	-5.23	110.92	118.94
17	A	837	CLA	CMB-C2B-C1B	-5.23	120.43	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	614	ZEX	C12-C13-C14	-5.22	110.94	118.94
25	2	615	ZEX	C20-C13-C12	-5.21	109.86	118.08
17	3	209	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
25	5	616	ZEX	C1-C6-C5	-5.19	115.30	122.61
25	1	613	ZEX	C39-C29-C28	-5.18	109.91	118.08
25	4	614	ZEX	C20-C13-C12	-5.18	109.91	118.08
17	A	835	CLA	CMB-C2B-C3B	5.18	134.37	124.68
25	2	615	ZEX	C19-C9-C8	-5.17	109.94	118.08
25	1	616	ZEX	C1-C6-C5	-5.16	115.34	122.61
17	B	831	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
25	3	214	ZEX	C12-C13-C14	-5.14	111.05	118.94
17	B	840	CLA	CMB-C2B-C1B	-5.14	120.57	128.46
25	1	615	ZEX	C1-C6-C5	-5.14	115.38	122.61
25	2	616	ZEX	C20-C13-C12	-5.13	109.99	118.08
25	4	615	ZEX	C28-C27-C26	-5.13	118.32	127.09
25	5	616	ZEX	C40-C33-C32	-5.13	110.00	118.08
17	B	834	CLA	CMB-C2B-C1B	-5.13	120.58	128.46
25	4	612	ZEX	C20-C13-C12	-5.12	110.01	118.08
25	4	614	ZEX	C19-C9-C8	-5.12	110.01	118.08
18	A	840	PQN	C14-C13-C12	-5.11	110.57	123.68
25	5	615	ZEX	C7-C8-C9	-5.10	118.52	126.23
18	B	844	PQN	C14-C13-C12	-5.10	110.59	123.68
25	3	216	ZEX	C1-C6-C5	-5.10	115.43	122.61
25	4	617	ZEX	C1-C6-C5	-5.10	115.43	122.61
25	3	214	ZEX	C7-C8-C9	-5.10	118.53	126.23
17	B	821	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
17	A	804	CLA	CAA-C2A-C3A	-5.08	98.86	112.78
25	2	617	ZEX	C27-C28-C29	-5.07	118.58	126.23
25	5	616	ZEX	C7-C8-C9	-5.06	118.58	126.23
25	5	617	ZEX	C28-C29-C30	-5.06	111.17	118.94
25	1	616	ZEX	C28-C29-C30	-5.05	111.19	118.94
25	3	216	ZEX	C19-C9-C8	-5.05	110.12	118.08
25	4	612	ZEX	C32-C33-C34	-5.04	111.20	118.94
25	1	614	ZEX	C27-C26-C25	-5.04	114.69	122.84
17	2	608	CLA	CMB-C2B-C3B	5.03	134.09	124.68
17	2	611	CLA	CAC-C3C-C4C	5.02	131.32	124.81
25	2	614	ZEX	C32-C33-C34	-5.01	111.25	118.94
25	4	613	ZEX	C20-C13-C12	-5.01	110.18	118.08
17	B	828	CLA	CMB-C2B-C1B	-5.01	120.77	128.46
17	3	203	CLA	CMB-C2B-C3B	5.00	134.03	124.68
25	3	214	ZEX	C28-C29-C30	-4.98	111.30	118.94
25	3	214	ZEX	C19-C9-C8	-4.98	110.24	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	805	CLA	CMB-C2B-C3B	4.98	133.99	124.68
17	A	848	CLA	CHB-C4A-NA	4.97	131.39	124.51
17	4	605	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
17	1	610	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
25	1	614	ZEX	C27-C28-C29	4.95	133.72	126.23
25	1	616	ZEX	C8-C9-C10	-4.93	111.37	118.94
25	3	218	ZEX	C28-C29-C30	-4.92	111.39	118.94
17	A	848	CLA	CMB-C2B-C3B	4.90	133.85	124.68
25	1	614	ZEX	C19-C9-C8	-4.90	110.36	118.08
25	2	617	ZEX	C1-C6-C5	-4.90	115.72	122.61
25	1	613	ZEX	C12-C13-C14	-4.89	111.43	118.94
25	4	614	ZEX	C1-C6-C5	-4.89	115.73	122.61
25	5	616	ZEX	C8-C9-C10	-4.89	111.44	118.94
17	A	804	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
25	4	616	ZEX	C19-C9-C8	-4.88	110.39	118.08
25	2	616	ZEX	C39-C29-C28	-4.87	110.40	118.08
25	1	615	ZEX	C28-C27-C26	-4.87	118.77	127.09
17	A	802	CLA	CMB-C2B-C1B	-4.86	120.99	128.46
25	4	617	ZEX	C40-C33-C32	-4.86	110.42	118.08
16	A	801	CL0	CBC-CAC-C3C	-4.84	99.10	112.43
17	A	817	CLA	CMB-C2B-C1B	-4.83	121.04	128.46
25	4	616	ZEX	C1-C6-C5	-4.83	115.81	122.61
25	5	614	ZEX	C32-C33-C34	-4.83	111.53	118.94
17	2	603	CLA	CMB-C2B-C1B	-4.82	121.05	128.46
17	A	813	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
25	2	615	ZEX	C40-C33-C32	-4.80	110.52	118.08
17	A	803	CLA	CMB-C2B-C1B	-4.80	121.09	128.46
25	5	614	ZEX	C7-C8-C9	-4.78	119.02	126.23
17	5	607	CLA	CAC-C3C-C4C	4.77	131.00	124.81
17	1	604	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
17	1	609	CLA	CAA-C2A-C3A	-4.76	105.00	116.10
17	5	606	CLA	CMC-C2C-C1C	-4.74	117.81	125.04
25	1	616	ZEX	C28-C27-C26	-4.74	118.99	127.09
25	4	614	ZEX	C27-C28-C29	-4.74	119.07	126.23
25	1	617	ZEX	C8-C7-C6	-4.74	113.89	127.20
17	A	807	CLA	CMB-C2B-C1B	-4.74	121.19	128.46
17	1	601	CLA	CMB-C2B-C3B	4.73	133.53	124.68
25	2	617	ZEX	C28-C27-C26	-4.73	119.00	127.09
25	4	613	ZEX	C40-C33-C32	-4.72	110.64	118.08
17	A	812	CLA	CMB-C2B-C3B	4.72	133.50	124.68
25	3	217	ZEX	C19-C9-C8	-4.71	110.66	118.08
16	A	801	CL0	C6-C5-C3	-4.70	101.14	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	617	ZEX	C18-C5-C4	-4.69	105.66	114.36
17	O	201	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
25	5	616	ZEX	C28-C29-C30	-4.68	111.75	118.94
25	5	615	ZEX	C1-C6-C5	-4.67	116.04	122.61
17	B	817	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
25	3	201	ZEX	C27-C28-C29	-4.66	119.20	126.23
25	4	617	ZEX	C27-C28-C29	-4.65	119.20	126.23
25	2	615	ZEX	C18-C5-C4	-4.65	105.74	114.36
17	B	801	CLA	CHB-C4A-NA	4.64	130.93	124.51
17	5	608	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
25	4	617	ZEX	C23-C24-C25	4.64	115.93	109.33
25	2	617	ZEX	C7-C6-C5	-4.64	110.23	121.46
17	4	603	CLA	CMB-C2B-C1B	-4.59	121.40	128.46
17	5	607	CLA	C4A-NA-C1A	4.57	108.76	106.71
17	B	807	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
25	3	215	ZEX	C1-C6-C5	-4.57	116.18	122.61
17	B	814	CLA	CMD-C2D-C1D	-4.57	116.67	124.71
25	4	617	ZEX	C28-C27-C26	-4.55	119.32	127.09
25	1	614	ZEX	C23-C24-C25	4.55	115.81	109.33
17	1	601	CLA	CHB-C4A-NA	4.55	130.80	124.51
17	2	609	CLA	CAA-C2A-C3A	-4.54	105.50	116.10
25	3	218	ZEX	C2-C3-C4	4.54	116.52	110.30
25	1	613	ZEX	C23-C24-C25	4.54	115.79	109.33
17	A	802	CLA	CMB-C2B-C3B	4.53	133.15	124.68
17	1	611	CLA	CAC-C3C-C2C	-4.53	119.79	127.53
17	5	602	CLA	CMB-C2B-C1B	-4.52	121.51	128.46
17	3	210	CLA	CAA-C2A-C3A	-4.52	105.55	116.10
17	5	609	CLA	CBC-CAC-C3C	4.51	124.87	112.43
25	3	201	ZEX	C28-C27-C26	-4.50	119.39	127.09
17	5	611	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
25	3	201	ZEX	C32-C33-C34	-4.49	112.05	118.94
25	4	613	ZEX	C19-C9-C8	-4.49	111.00	118.08
17	5	610	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
17	B	816	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
25	4	613	ZEX	C4-C5-C6	-4.49	110.85	120.85
17	5	606	CLA	CMB-C2B-C1B	-4.49	121.57	128.46
17	B	804	CLA	C4A-NA-C1A	4.48	108.72	106.71
17	O	203	CLA	CAA-C2A-C3A	-4.47	105.66	116.10
25	1	613	ZEX	C27-C28-C29	-4.46	119.50	126.23
17	B	840	CLA	CMB-C2B-C3B	4.46	133.02	124.68
17	F	302	CLA	CMB-C2B-C1B	-4.44	121.63	128.46
25	3	214	ZEX	C40-C33-C32	-4.44	111.08	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	615	ZEX	C28-C29-C30	-4.44	112.13	118.94
25	2	616	ZEX	C23-C24-C25	4.43	115.64	109.33
17	1	602	CLA	CMB-C2B-C3B	4.41	132.94	124.68
17	3	209	CLA	CMB-C2B-C3B	4.41	132.93	124.68
17	A	830	CLA	CMB-C2B-C3B	4.41	132.93	124.68
17	B	814	CLA	CMB-C2B-C1B	-4.40	121.69	128.46
17	3	205	CLA	CMB-C2B-C1B	-4.40	121.71	128.46
17	F	303	CLA	CAA-C2A-C3A	-4.39	105.86	116.10
17	4	608	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
17	A	836	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
17	B	827	CLA	CMB-C2B-C3B	4.38	132.87	124.68
25	3	218	ZEX	C39-C29-C28	-4.38	111.18	118.08
25	2	615	ZEX	C27-C28-C29	-4.37	119.64	126.23
17	A	802	CLA	CHB-C4A-NA	4.37	130.55	124.51
25	1	613	ZEX	C8-C9-C10	-4.36	112.25	118.94
16	A	801	CL0	C2C-C1C-NC	4.36	114.06	109.97
23	B	851	DGD	O5D-C6D-C5D	-4.35	101.00	109.05
25	2	615	ZEX	C1-C6-C5	-4.34	116.50	122.61
25	3	218	ZEX	C8-C9-C10	-4.34	112.28	118.94
20	B	850	BCR	C24-C23-C22	-4.33	119.69	126.23
17	A	815	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
17	4	602	CLA	CAA-C2A-C3A	-4.32	100.95	112.78
25	3	214	ZEX	C7-C6-C5	-4.32	111.00	121.46
25	2	615	ZEX	C39-C29-C28	-4.31	111.29	118.08
25	1	616	ZEX	C7-C6-C5	-4.30	111.04	121.46
25	3	218	ZEX	C16-C1-C6	4.29	117.26	110.30
17	B	820	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
25	2	614	ZEX	C1-C6-C5	-4.29	116.57	122.61
25	2	616	ZEX	C28-C27-C26	-4.28	119.78	127.09
17	B	828	CLA	CMB-C2B-C3B	4.27	132.66	124.68
25	3	217	ZEX	C40-C33-C32	-4.27	111.35	118.08
17	B	806	CLA	CHB-C4A-NA	4.27	130.41	124.51
17	A	809	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
25	4	615	ZEX	C39-C29-C28	-4.25	111.37	118.08
17	A	837	CLA	CMB-C2B-C3B	4.25	132.63	124.68
25	5	616	ZEX	C27-C28-C29	-4.24	119.83	126.23
17	B	838	CLA	CAC-C3C-C4C	4.24	130.31	124.81
17	4	602	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
25	4	612	ZEX	C18-C5-C4	-4.23	106.51	114.36
17	A	833	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
25	3	214	ZEX	C1-C6-C5	-4.22	116.67	122.61
17	A	825	CLA	CMB-C2B-C1B	-4.22	121.98	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	841	LHG	O4-P-O5	4.22	133.09	112.24
20	B	849	BCR	C24-C23-C22	-4.21	119.87	126.23
17	5	606	CLA	CMB-C2B-C3B	4.21	132.56	124.68
25	4	617	ZEX	C7-C8-C9	-4.21	119.88	126.23
20	K	104	BCR	C2-C1-C6	4.20	116.95	110.48
25	5	617	ZEX	C12-C13-C14	-4.19	112.51	118.94
17	1	611	CLA	CBC-CAC-C3C	4.19	123.97	112.43
17	A	819	CLA	CMB-C2B-C3B	4.19	132.51	124.68
25	1	614	ZEX	C40-C33-C32	-4.19	111.48	118.08
25	3	201	ZEX	C8-C9-C10	-4.18	112.53	118.94
17	4	605	CLA	CMB-C2B-C3B	4.18	132.49	124.68
17	B	812	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
17	A	834	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
17	J	101	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
19	A	842	LHG	O4-P-O5	4.17	132.84	112.24
17	A	813	CLA	CMB-C2B-C3B	4.16	132.46	124.68
17	2	603	CLA	CMB-C2B-C3B	4.15	132.44	124.68
17	B	829	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
25	2	614	ZEX	C7-C6-C5	-4.14	111.43	121.46
17	A	828	CLA	CMB-C2B-C3B	4.13	132.40	124.68
17	B	804	CLA	CMD-C2D-C1D	-4.13	117.44	124.71
25	5	614	ZEX	C1-C6-C5	-4.12	116.81	122.61
25	3	215	ZEX	C23-C24-C25	4.12	115.19	109.33
17	B	817	CLA	CMB-C2B-C3B	4.11	132.37	124.68
25	2	617	ZEX	C7-C8-C9	-4.11	120.02	126.23
17	B	803	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
17	2	604	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
17	4	603	CLA	CMB-C2B-C3B	4.11	132.37	124.68
25	3	216	ZEX	C7-C6-C5	-4.11	111.52	121.46
17	A	804	CLA	CMB-C2B-C3B	4.10	132.35	124.68
25	4	615	ZEX	C8-C9-C10	-4.10	112.65	118.94
25	5	617	ZEX	C40-C33-C32	-4.09	111.64	118.08
17	B	802	CLA	C2D-C1D-ND	-4.08	107.09	110.10
16	A	801	CL0	C11-C10-C8	-4.08	102.72	115.92
17	A	818	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
17	A	827	CLA	C4A-NA-C1A	4.08	108.54	106.71
25	5	615	ZEX	C7-C6-C5	-4.08	111.59	121.46
17	B	819	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
17	3	206	CLA	CMB-C2B-C3B	4.07	132.29	124.68
18	A	840	PQN	C14-C13-C15	-4.07	108.43	115.27
25	1	615	ZEX	C40-C33-C32	-4.07	111.67	118.08
25	3	215	ZEX	C18-C5-C4	-4.06	106.83	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	604	CLA	CMB-C2B-C3B	4.06	132.27	124.68
17	5	609	CLA	CAA-C2A-C3A	-4.05	106.64	116.10
17	B	834	CLA	CMB-C2B-C3B	4.05	132.26	124.68
17	2	610	CLA	CAA-C2A-C3A	-4.04	104.16	114.26
17	B	814	CLA	CMD-C2D-C3D	4.03	136.90	127.61
25	4	616	ZEX	C40-C33-C32	-4.03	111.73	118.08
25	3	215	ZEX	C27-C28-C29	-4.03	120.15	126.23
17	1	612	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
25	4	615	ZEX	C19-C9-C8	-4.03	111.73	118.08
16	A	801	CL0	CMB-C2B-C3B	4.02	132.20	124.68
25	3	218	ZEX	C8-C7-C6	-4.02	115.91	127.20
17	B	832	CLA	C2D-C1D-ND	-4.02	107.14	110.10
25	1	613	ZEX	C28-C27-C26	-4.02	120.22	127.09
17	5	613	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
17	5	601	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
25	5	616	ZEX	C7-C6-C5	-4.01	111.74	121.46
17	A	838	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
17	A	831	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
25	2	614	ZEX	C28-C27-C26	-4.00	120.26	127.09
17	O	201	CLA	CMB-C2B-C3B	3.99	132.15	124.68
25	3	218	ZEX	C1-C6-C5	-3.99	116.99	122.61
17	A	826	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
17	A	826	CLA	CMB-C2B-C3B	3.97	132.11	124.68
17	3	208	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
17	3	211	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
25	3	201	ZEX	C28-C29-C30	-3.96	112.86	118.94
17	B	821	CLA	CMB-C2B-C3B	3.96	132.09	124.68
17	B	806	CLA	CMA-C3A-C4A	-3.95	101.16	111.77
17	A	803	CLA	CAA-CBA-CGA	-3.95	101.72	113.25
25	4	614	ZEX	C7-C6-C5	-3.94	111.92	121.46
25	3	216	ZEX	C23-C24-C25	3.94	114.94	109.33
25	3	216	ZEX	C38-C24-C23	-3.94	106.11	112.20
20	L	205	BCR	C24-C23-C22	-3.94	120.28	126.23
25	2	617	ZEX	C8-C7-C6	-3.94	116.15	127.20
17	L	203	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
17	B	841	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
17	A	803	CLA	CMB-C2B-C3B	3.93	132.03	124.68
17	B	811	CLA	CHB-C4A-NA	3.93	129.94	124.51
17	B	815	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
17	A	848	CLA	CAA-C2A-C3A	-3.91	102.07	112.78
17	B	816	CLA	CMB-C2B-C3B	3.91	131.99	124.68
16	A	801	CL0	CGD-CBD-CAD	-3.91	98.08	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	801	CL0	O1D-CGD-CBD	-3.90	116.50	124.48
25	2	615	ZEX	C7-C6-C5	-3.90	112.01	121.46
17	B	807	CLA	CMB-C2B-C3B	3.90	131.98	124.68
25	3	214	ZEX	C18-C5-C4	-3.90	107.13	114.36
17	4	607	CLA	CHB-C4A-NA	3.89	129.90	124.51
17	1	609	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
17	3	204	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
17	1	610	CLA	CMB-C2B-C3B	3.89	131.96	124.68
25	3	214	ZEX	C38-C24-C23	-3.88	106.20	112.20
25	1	614	ZEX	C18-C5-C4	-3.87	107.18	114.36
17	2	612	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
17	5	608	CLA	CMB-C2B-C3B	3.87	131.92	124.68
25	1	615	ZEX	C7-C6-C5	-3.87	112.09	121.46
25	4	613	ZEX	C2-C3-C4	3.86	115.58	110.30
25	3	218	ZEX	C32-C33-C34	-3.85	113.03	118.94
17	4	609	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
17	A	807	CLA	CMB-C2B-C3B	3.84	131.86	124.68
25	1	613	ZEX	C4-C5-C6	-3.83	112.31	120.85
17	F	301	CLA	CAA-C2A-C3A	-3.83	102.28	112.78
17	5	610	CLA	CMB-C2B-C3B	3.83	131.84	124.68
25	4	617	ZEX	C7-C6-C5	-3.82	112.20	121.46
25	1	617	ZEX	C27-C28-C29	-3.82	120.47	126.23
17	1	607	CLA	C2D-C1D-ND	-3.81	107.29	110.10
25	4	616	ZEX	C7-C6-C5	-3.81	112.23	121.46
17	B	813	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
25	2	614	ZEX	C18-C5-C4	-3.81	107.30	114.36
17	3	203	CLA	CAA-C2A-C3A	-3.80	102.36	112.78
25	3	214	ZEX	C23-C24-C25	3.79	114.73	109.33
17	A	826	CLA	CHB-C4A-NA	3.79	129.75	124.51
25	2	615	ZEX	C28-C27-C26	-3.78	120.62	127.09
17	5	611	CLA	CMB-C2B-C3B	3.78	131.76	124.68
17	4	602	CLA	CMB-C2B-C3B	3.78	131.74	124.68
17	A	827	CLA	CMB-C2B-C3B	3.78	131.74	124.68
25	4	612	ZEX	C35-C15-C14	-3.77	115.75	123.47
17	B	839	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
25	4	612	ZEX	C28-C27-C26	-3.77	120.65	127.09
17	B	806	CLA	CMA-C3A-C2A	-3.77	98.64	113.83
25	2	616	ZEX	C7-C6-C5	-3.76	112.35	121.46
17	A	819	CLA	CHB-C4A-NA	3.76	129.71	124.51
17	B	814	CLA	CAB-C3B-C4B	-3.75	122.70	128.46
25	3	217	ZEX	C7-C6-C5	-3.75	112.38	121.46
20	I	101	BCR	C15-C16-C17	-3.75	115.80	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	614	ZEX	C7-C6-C5	-3.75	112.38	121.46
17	A	816	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
25	1	615	ZEX	C27-C28-C29	-3.75	120.58	126.23
17	3	210	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
17	A	832	CLA	CHB-C4A-NA	3.74	129.69	124.51
17	B	843	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
17	B	808	CLA	CHB-C4A-NA	3.74	129.68	124.51
17	O	203	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
17	4	609	CLA	CAA-C2A-C3A	-3.73	107.40	116.10
25	5	615	ZEX	C31-C32-C33	-3.73	115.95	126.42
17	A	820	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
17	A	832	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
17	4	607	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
17	B	818	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
25	4	616	ZEX	C28-C27-C26	-3.71	120.75	127.09
17	A	825	CLA	CMB-C2B-C3B	3.71	131.62	124.68
25	5	617	ZEX	C4-C5-C6	-3.70	112.60	120.85
17	1	603	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
17	A	802	CLA	CMA-C3A-C4A	-3.70	101.83	111.77
17	3	207	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
17	A	815	CLA	CMB-C2B-C3B	3.69	131.59	124.68
20	L	205	BCR	C2-C1-C6	3.69	116.16	110.48
25	5	615	ZEX	C28-C27-C26	-3.69	120.79	127.09
25	5	616	ZEX	C23-C24-C25	3.69	114.58	109.33
17	F	301	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
17	1	605	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
25	5	614	ZEX	C18-C5-C4	-3.68	107.54	114.36
25	2	616	ZEX	C38-C24-C23	-3.67	106.53	112.20
17	A	809	CLA	CAA-C2A-C3A	-3.67	102.73	112.78
25	1	613	ZEX	C8-C7-C6	-3.67	116.90	127.20
17	2	604	CLA	CMB-C2B-C3B	3.66	131.53	124.68
17	B	802	CLA	C1D-ND-C4D	3.66	108.94	106.33
17	K	103	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
17	B	829	CLA	CMB-C2B-C3B	3.66	131.52	124.68
17	B	803	CLA	CHB-C4A-NA	3.65	129.57	124.51
25	5	617	ZEX	C28-C27-C26	-3.65	120.85	127.09
17	4	608	CLA	CMB-C2B-C3B	3.65	131.51	124.68
25	1	615	ZEX	C15-C35-C34	-3.65	116.00	123.47
25	1	615	ZEX	C18-C5-C4	-3.64	107.61	114.36
17	B	804	CLA	CMD-C2D-C3D	3.64	135.99	127.61
17	2	607	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
17	B	819	CLA	CMB-C2B-C3B	3.63	131.48	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	836	CLA	CHB-C4A-NA	3.63	129.53	124.51
25	3	218	ZEX	C7-C6-C5	-3.62	112.69	121.46
17	B	823	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
17	B	833	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
17	5	602	CLA	CMB-C2B-C3B	3.60	131.41	124.68
16	A	801	CL0	CMD-C2D-C1D	3.60	131.05	124.71
25	3	215	ZEX	C8-C7-C6	-3.59	117.11	127.20
17	A	824	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
17	A	810	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
17	K	102	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
17	5	606	CLA	CHB-C4A-NA	3.58	129.46	124.51
23	B	851	DGD	O3G-C3G-C2G	-3.57	102.28	110.90
17	3	202	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
17	3	203	CLA	CHB-C4A-NA	3.57	129.45	124.51
17	4	601	CLA	CHB-C4A-NA	3.57	129.44	124.51
17	B	802	CLA	C1B-CHB-C4A	-3.56	123.06	130.12
17	A	822	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
25	1	617	ZEX	C11-C12-C13	-3.56	116.42	126.42
20	L	201	BCR	C15-C16-C17	-3.56	116.19	123.47
17	A	833	CLA	CMB-C2B-C3B	3.55	131.32	124.68
17	5	605	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
25	4	615	ZEX	C7-C6-C5	-3.55	112.87	121.46
17	A	805	CLA	CAA-C2A-C3A	-3.54	103.07	112.78
20	K	101	BCR	C15-C16-C17	-3.54	116.22	123.47
17	J	101	CLA	CMB-C2B-C3B	3.54	131.30	124.68
17	A	820	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
25	1	614	ZEX	C11-C12-C13	-3.54	116.48	126.42
17	5	601	CLA	CMB-C2B-C3B	3.53	131.29	124.68
20	B	849	BCR	C2-C1-C6	3.53	115.92	110.48
17	A	848	CLA	O2D-CGD-CBD	3.53	117.55	111.27
17	O	204	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
17	1	607	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
17	2	608	CLA	CHB-C4A-NA	3.53	129.39	124.51
17	2	601	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
25	5	617	ZEX	C11-C12-C13	-3.52	116.54	126.42
17	A	806	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
17	3	205	CLA	CMB-C2B-C3B	3.51	131.24	124.68
25	2	615	ZEX	C7-C8-C9	-3.51	120.94	126.23
17	3	212	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
17	5	609	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
17	1	607	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
17	B	806	CLA	C2A-C3A-C4A	3.49	107.50	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	821	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
17	B	806	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
17	4	604	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
17	B	803	CLA	CMB-C2B-C3B	3.47	131.18	124.68
17	B	835	CLA	CHB-C4A-NA	3.47	129.31	124.51
17	3	208	CLA	CMB-C2B-C3B	3.47	131.18	124.68
17	5	609	CLA	CMC-C2C-C1C	-3.47	119.75	125.04
17	2	605	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
25	1	614	ZEX	C38-C24-C23	-3.47	106.84	112.20
25	3	217	ZEX	C8-C7-C6	-3.47	117.47	127.20
17	2	613	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
20	A	845	BCR	C11-C10-C9	-3.46	122.36	127.31
17	5	613	CLA	CBD-CHA-C1A	3.46	132.97	127.43
20	J	105	BCR	C24-C23-C22	-3.46	121.01	126.23
17	A	832	CLA	CMC-C2C-C1C	-3.46	119.78	125.04
17	A	809	CLA	CMB-C2B-C3B	3.45	131.14	124.68
17	A	803	CLA	CHB-C4A-NA	3.45	129.29	124.51
25	4	613	ZEX	C8-C9-C10	-3.45	113.64	118.94
17	2	604	CLA	CAA-C2A-C3A	-3.45	105.64	114.26
17	A	848	CLA	CAC-C3C-C2C	-3.45	121.63	127.53
17	J	101	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
17	B	819	CLA	CHB-C4A-NA	3.44	129.27	124.51
17	B	829	CLA	CHB-C4A-NA	3.44	129.27	124.51
17	B	804	CLA	CMA-C3A-C4A	-3.44	102.52	111.77
17	1	611	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
17	A	839	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
20	O	202	BCR	C24-C23-C22	-3.43	121.05	126.23
17	1	612	CLA	CMB-C2B-C3B	3.43	131.10	124.68
17	B	825	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
17	5	606	CLA	CMC-C2C-C3C	3.42	135.41	126.12
25	3	201	ZEX	C4-C5-C6	-3.42	113.22	120.85
17	A	822	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
18	B	844	PQN	C14-C13-C15	-3.42	109.52	115.27
17	5	612	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
17	2	610	CLA	CHB-C4A-NA	3.42	129.24	124.51
17	2	606	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
17	B	804	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
17	A	807	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
25	4	614	ZEX	C7-C8-C9	-3.41	121.08	126.23
17	B	816	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
16	A	801	CL0	O2A-C1-C2	3.41	117.59	108.64
17	A	816	CLA	CHB-C4A-NA	3.41	129.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	603	CLA	CHB-C4A-NA	3.41	129.22	124.51
16	A	801	CL0	C3B-C4B-NB	3.41	113.62	109.21
17	2	611	CLA	CBC-CAC-C3C	3.41	121.83	112.43
17	2	602	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
17	2	604	CLA	CHB-C4A-NA	3.40	129.22	124.51
17	B	817	CLA	CHB-C4A-NA	3.40	129.21	124.51
17	J	103	CLA	CAA-C2A-C3A	-3.40	105.77	114.26
17	B	802	CLA	C4A-NA-C1A	3.39	108.23	106.71
17	B	832	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
17	2	611	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
17	B	837	CLA	CHB-C4A-NA	3.39	129.20	124.51
25	5	614	ZEX	C38-C24-C25	-3.39	105.48	110.87
25	1	616	ZEX	C27-C28-C29	-3.38	121.12	126.23
25	5	614	ZEX	C23-C24-C25	3.38	114.15	109.33
17	F	303	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
17	B	814	CLA	CAB-C3B-C2B	3.37	131.29	124.69
17	A	838	CLA	CMB-C2B-C3B	3.37	130.98	124.68
25	5	617	ZEX	C8-C9-C10	-3.37	113.77	118.94
17	2	609	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
25	2	615	ZEX	C37-C21-C26	-3.36	104.84	110.30
17	B	837	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
16	A	801	CL0	CAA-C2A-C3A	3.36	121.98	112.78
25	2	617	ZEX	C18-C5-C4	-3.36	108.13	114.36
17	L	204	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
17	2	605	CLA	CHB-C4A-NA	3.35	129.15	124.51
17	A	836	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
20	L	205	BCR	C39-C30-C25	3.35	115.74	110.30
17	A	833	CLA	CAA-C2A-C3A	-3.35	103.61	112.78
25	4	616	ZEX	C8-C7-C6	-3.35	117.80	127.20
17	B	820	CLA	CMB-C2B-C3B	3.34	130.93	124.68
25	3	217	ZEX	C18-C5-C4	-3.34	108.17	114.36
25	5	615	ZEX	C23-C24-C25	3.34	114.09	109.33
17	A	812	CLA	O2D-CGD-O1D	-3.34	117.32	123.84
25	1	614	ZEX	C31-C32-C33	-3.33	117.07	126.42
17	A	816	CLA	CMB-C2B-C3B	3.33	130.91	124.68
17	4	606	CLA	CAC-C3C-C4C	3.33	129.13	124.81
17	A	833	CLA	CHB-C4A-NA	3.33	129.11	124.51
17	O	205	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
17	J	103	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
17	J	103	CLA	CHB-C4A-NA	3.32	129.11	124.51
17	5	604	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
17	5	603	CLA	O2D-CGD-O1D	-3.32	117.34	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	824	CLA	CMB-C2B-C3B	3.32	130.89	124.68
17	F	302	CLA	CMB-C2B-C3B	3.32	130.88	124.68
17	B	804	CLA	CHB-C4A-NA	3.31	129.09	124.51
25	4	613	ZEX	C7-C8-C9	-3.31	121.23	126.23
17	1	609	CLA	CMB-C2B-C3B	3.31	130.87	124.68
17	5	607	CLA	CBC-CAC-C3C	3.31	121.55	112.43
17	B	827	CLA	CHB-C4A-NA	3.30	129.08	124.51
20	K	101	BCR	C15-C14-C13	-3.30	122.60	127.31
17	A	810	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
17	L	203	CLA	CMB-C2B-C3B	3.30	130.85	124.68
23	B	851	DGD	O6D-C1D-O3G	-3.30	102.16	109.97
17	B	815	CLA	CHB-C4A-NA	3.30	129.07	124.51
17	4	608	CLA	CHB-C4A-NA	3.29	129.07	124.51
17	B	810	CLA	CHB-C4A-NA	3.29	129.06	124.51
25	3	214	ZEX	C27-C28-C29	-3.29	121.26	126.23
17	5	612	CLA	CHB-C4A-NA	3.29	129.06	124.51
17	A	812	CLA	CHB-C4A-NA	3.29	129.06	124.51
17	B	841	CLA	CMB-C2B-C3B	3.29	130.83	124.68
17	B	807	CLA	CHB-C4A-NA	3.29	129.06	124.51
17	A	839	CLA	CHB-C4A-NA	3.28	129.05	124.51
17	A	805	CLA	CHB-C4A-NA	3.28	129.05	124.51
17	B	815	CLA	CMB-C2B-C3B	3.28	130.82	124.68
17	1	608	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
17	B	801	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
17	A	811	CLA	CHB-C4A-NA	3.28	129.04	124.51
17	B	836	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
20	B	848	BCR	C15-C16-C17	-3.27	116.77	123.47
17	2	612	CLA	CMB-C2B-C3B	3.27	130.80	124.68
17	B	820	CLA	CHB-C4A-NA	3.27	129.03	124.51
25	3	218	ZEX	C27-C28-C29	-3.27	121.30	126.23
17	K	103	CLA	CAA-C2A-C3A	-3.27	106.09	114.26
17	4	602	CLA	O2A-CGA-O1A	-3.27	115.35	123.59
17	B	824	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
17	A	805	CLA	C1B-CHB-C4A	-3.27	123.65	130.12
17	4	601	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
17	A	822	CLA	CHB-C4A-NA	3.26	129.02	124.51
17	B	808	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
17	5	609	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
17	A	807	CLA	CAA-C2A-C3A	-3.26	103.86	112.78
17	A	831	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
17	A	831	CLA	CMB-C2B-C3B	3.24	130.75	124.68
17	A	818	CLA	CHB-C4A-NA	3.24	128.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	827	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
17	A	825	CLA	CHB-C4A-NA	3.24	128.99	124.51
17	B	843	CLA	CMB-C2B-C3B	3.23	130.73	124.68
17	A	818	CLA	CMB-C2B-C3B	3.23	130.73	124.68
25	1	617	ZEX	C7-C6-C5	-3.23	113.63	121.46
17	B	830	CLA	CMB-C2B-C3B	3.23	130.72	124.68
17	2	612	CLA	CHB-C4A-NA	3.23	128.98	124.51
17	2	607	CLA	CMB-C2B-C3B	3.23	130.72	124.68
17	3	210	CLA	CMB-C2B-C3B	3.23	130.72	124.68
25	1	614	ZEX	C7-C8-C9	-3.23	121.36	126.23
17	A	829	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
17	5	613	CLA	CMB-C2B-C3B	3.23	130.71	124.68
17	B	809	CLA	CHB-C4A-NA	3.22	128.97	124.51
17	2	607	CLA	CHB-C4A-NA	3.22	128.97	124.51
20	L	205	BCR	C15-C14-C13	-3.22	122.72	127.31
17	A	808	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
17	5	603	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
25	4	614	ZEX	C18-C5-C4	-3.22	108.40	114.36
25	4	613	ZEX	C28-C27-C26	-3.21	121.60	127.09
17	3	202	CLA	CHB-C4A-NA	3.21	128.95	124.51
17	J	102	CLA	CHB-C4A-NA	3.21	128.95	124.51
17	B	804	CLA	CMB-C2B-C3B	3.21	130.68	124.68
17	1	608	CLA	CHB-C4A-NA	3.20	128.94	124.51
17	B	833	CLA	CHB-C4A-NA	3.20	128.94	124.51
17	4	609	CLA	CMB-C2B-C3B	3.20	130.66	124.68
25	4	612	ZEX	C31-C32-C33	-3.19	117.45	126.42
17	B	811	CLA	CAA-C2A-C3A	-3.19	104.04	112.78
17	B	838	CLA	CBC-CAC-C3C	3.19	121.22	112.43
17	B	842	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
17	A	822	CLA	CMB-C2B-C3B	3.19	130.64	124.68
25	3	215	ZEX	C7-C6-C5	-3.19	113.75	121.46
17	A	848	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
17	A	816	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
17	5	605	CLA	CHB-C4A-NA	3.18	128.91	124.51
25	3	214	ZEX	C11-C12-C13	-3.18	117.49	126.42
17	O	204	CLA	CMB-C2B-C3B	3.18	130.62	124.68
25	4	614	ZEX	C28-C27-C26	-3.18	121.66	127.09
17	3	213	CLA	CHB-C4A-NA	3.18	128.90	124.51
17	3	211	CLA	CMB-C2B-C3B	3.17	130.62	124.68
17	4	611	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
17	A	835	CLA	CHB-C4A-NA	3.17	128.90	124.51
17	3	203	CLA	CAC-C3C-C4C	3.17	128.93	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	608	CLA	CAA-C2A-C3A	-3.17	104.10	112.78
17	2	606	CLA	CAA-C2A-C3A	-3.17	104.10	112.78
17	F	301	CLA	CMB-C2B-C3B	3.17	130.60	124.68
17	3	210	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
17	O	203	CLA	CMB-C2B-C3B	3.16	130.59	124.68
20	A	845	BCR	C24-C23-C22	-3.16	121.46	126.23
25	5	616	ZEX	C18-C5-C4	-3.15	108.51	114.36
25	4	613	ZEX	C27-C28-C29	-3.15	121.47	126.23
17	4	607	CLA	CMB-C2B-C3B	3.15	130.57	124.68
17	2	601	CLA	CHB-C4A-NA	3.15	128.87	124.51
17	1	601	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
17	B	828	CLA	CAA-C2A-C1A	-3.15	101.66	111.97
25	4	612	ZEX	C27-C28-C29	-3.15	121.48	126.23
17	A	819	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
17	2	605	CLA	CMB-C2B-C3B	3.14	130.56	124.68
17	2	602	CLA	CHB-C4A-NA	3.14	128.86	124.51
25	3	215	ZEX	C37-C21-C26	-3.14	105.20	110.30
16	A	801	CL0	CHA-C4D-ND	3.13	139.06	132.50
17	B	822	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
25	3	216	ZEX	C7-C8-C9	-3.13	121.50	126.23
17	2	606	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
17	3	211	CLA	CAA-C2A-C3A	-3.13	106.44	114.26
17	1	601	CLA	CMC-C2C-C1C	-3.13	120.27	125.04
17	3	207	CLA	CMB-C2B-C3B	3.13	130.53	124.68
17	4	611	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
17	2	610	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
25	1	617	ZEX	C19-C9-C8	-3.13	113.15	118.08
17	K	103	CLA	CMB-C2B-C3B	3.13	130.53	124.68
17	F	303	CLA	CHB-C4A-NA	3.13	128.83	124.51
25	5	617	ZEX	C8-C7-C6	-3.13	118.42	127.20
17	5	606	CLA	CMD-C2D-C3D	-3.12	120.44	127.61
17	A	832	CLA	O2D-CGD-CBD	3.12	116.81	111.27
17	B	811	CLA	O2A-CGA-O1A	-3.12	115.72	123.59
17	A	815	CLA	CHB-C4A-NA	3.12	128.82	124.51
17	1	601	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
17	1	604	CLA	CAA-C2A-C3A	-3.12	104.25	112.78
17	A	806	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
17	1	607	CLA	CMB-C2B-C3B	3.11	130.49	124.68
16	A	801	CL0	C1-C2-C3	-3.11	120.67	126.04
17	B	801	CLA	CBC-CAC-C3C	-3.11	103.87	112.43
17	A	836	CLA	CMB-C2B-C3B	3.11	130.49	124.68
25	3	216	ZEX	C27-C28-C29	-3.10	121.55	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	616	ZEX	C28-C29-C30	-3.10	114.18	118.94
17	4	608	CLA	CAA-C2A-C3A	-3.10	104.28	112.78
17	B	830	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
17	5	612	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
17	5	606	CLA	CMA-C3A-C4A	-3.10	103.44	111.77
17	J	101	CLA	CAA-C2A-C3A	-3.10	104.29	112.78
17	A	835	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
25	1	614	ZEX	C8-C9-C10	-3.10	114.19	118.94
25	3	216	ZEX	C8-C7-C6	-3.10	118.51	127.20
25	1	613	ZEX	C11-C12-C13	-3.10	117.72	126.42
17	B	802	CLA	CHB-C4A-NA	3.09	128.79	124.51
17	4	610	CLA	CHB-C4A-NA	3.09	128.79	124.51
25	2	615	ZEX	C11-C12-C13	-3.09	117.74	126.42
17	A	811	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
17	B	822	CLA	CHB-C4A-NA	3.09	128.78	124.51
20	J	104	BCR	C15-C16-C17	-3.08	117.16	123.47
20	B	849	BCR	C11-C10-C9	-3.08	122.91	127.31
17	A	832	CLA	CAA-C2A-C3A	-3.08	104.33	112.78
20	B	805	BCR	C24-C23-C22	-3.08	121.58	126.23
17	B	804	CLA	OBD-CAD-C3D	3.08	135.94	128.52
17	A	814	CLA	CHB-C4A-NA	3.08	128.77	124.51
20	O	202	BCR	C39-C30-C25	-3.08	105.30	110.30
17	2	608	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
25	1	617	ZEX	C31-C32-C33	-3.08	117.77	126.42
17	A	818	CLA	CAC-C3C-C4C	-3.08	120.82	124.81
17	A	826	CLA	C1-C2-C3	-3.08	120.72	126.04
17	B	806	CLA	CED-O2D-CGD	-3.08	108.98	115.94
17	A	806	CLA	CHB-C4A-NA	3.08	128.77	124.51
17	B	818	CLA	CHB-C4A-NA	3.07	128.76	124.51
17	B	813	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
20	B	849	BCR	C3-C4-C5	-3.06	108.61	114.08
17	B	842	CLA	CHB-C4A-NA	3.06	128.75	124.51
17	A	837	CLA	CHB-C4A-NA	3.06	128.74	124.51
17	3	204	CLA	CMB-C2B-C3B	3.06	130.40	124.68
17	B	818	CLA	CMB-C2B-C3B	3.06	130.40	124.68
20	B	848	BCR	C15-C14-C13	-3.05	122.96	127.31
17	1	601	CLA	CHC-C1C-NC	3.05	128.83	124.20
17	A	834	CLA	CHB-C4A-NA	3.05	128.73	124.51
17	B	818	CLA	CAA-C2A-C3A	-3.05	106.65	114.26
25	1	616	ZEX	C8-C7-C6	-3.05	118.65	127.20
17	4	611	CLA	CHB-C4A-NA	3.05	128.72	124.51
25	2	617	ZEX	C31-C32-C33	-3.04	117.86	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	101	CLA	CHB-C4A-NA	3.04	128.72	124.51
20	B	849	BCR	C37-C22-C21	-3.04	118.66	122.92
17	1	612	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
17	3	213	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
25	3	201	ZEX	C11-C12-C13	-3.04	117.88	126.42
25	1	617	ZEX	C4-C5-C6	-3.04	114.08	120.85
20	B	849	BCR	C15-C14-C13	-3.04	122.98	127.31
17	A	814	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
17	A	831	CLA	CHB-C4A-NA	3.03	128.71	124.51
17	B	821	CLA	CHB-C4A-NA	3.03	128.71	124.51
17	2	613	CLA	CMB-C2B-C3B	3.03	130.34	124.68
17	F	302	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
17	2	613	CLA	CHB-C4A-NA	3.02	128.69	124.51
17	B	839	CLA	CMB-C2B-C3B	3.02	130.33	124.68
25	5	614	ZEX	C27-C28-C29	-3.02	121.67	126.23
17	A	804	CLA	CHB-C4A-NA	3.02	128.69	124.51
17	A	803	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
17	2	611	CLA	CAC-C3C-C2C	-3.02	122.37	127.53
17	B	823	CLA	CMB-C2B-C3B	3.01	130.32	124.68
25	2	616	ZEX	C8-C7-C6	-3.01	118.74	127.20
20	B	850	BCR	C15-C14-C13	-3.01	123.01	127.31
17	A	838	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
25	2	615	ZEX	C15-C35-C34	-3.01	117.30	123.47
17	B	839	CLA	CHB-C4A-NA	3.01	128.68	124.51
20	L	205	BCR	C11-C10-C9	-3.01	123.02	127.31
17	A	821	CLA	CHB-C4A-NA	3.00	128.67	124.51
17	1	611	CLA	CMB-C2B-C3B	3.00	130.29	124.68
17	2	611	CLA	CHB-C4A-NA	3.00	128.66	124.51
25	3	215	ZEX	C12-C13-C14	-3.00	114.34	118.94
17	4	603	CLA	CHB-C4A-NA	3.00	128.66	124.51
17	B	802	CLA	C7-C6-C5	-3.00	105.22	113.36
20	B	805	BCR	C2-C1-C6	3.00	115.09	110.48
17	5	604	CLA	CHB-C4A-NA	3.00	128.65	124.51
17	A	832	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
17	B	801	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
17	2	611	CLA	CMB-C2B-C3B	2.99	130.27	124.68
17	B	806	CLA	C1-C2-C3	-2.99	120.88	126.04
17	3	208	CLA	CHB-C4A-NA	2.99	128.64	124.51
17	A	848	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
17	3	212	CLA	CHB-C4A-NA	2.99	128.64	124.51
17	L	204	CLA	CMB-C2B-C3B	2.99	130.26	124.68
17	5	607	CLA	CAA-C2A-C3A	-2.98	104.61	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	838	CLA	CHB-C4A-NA	2.98	128.64	124.51
17	B	802	CLA	CMB-C2B-C3B	2.98	130.26	124.68
17	A	817	CLA	CMB-C2B-C3B	2.98	130.25	124.68
20	B	847	BCR	C24-C23-C22	-2.98	121.73	126.23
17	3	207	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	3	218	ZEX	C23-C24-C25	2.98	113.57	109.33
17	A	848	CLA	CHC-C1C-NC	2.98	128.72	124.20
17	5	601	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	4	617	ZEX	C18-C5-C4	-2.97	108.84	114.36
17	4	604	CLA	CMB-C2B-C3B	2.97	130.24	124.68
20	L	206	BCR	C7-C8-C9	-2.97	121.74	126.23
17	3	205	CLA	CHB-C4A-NA	2.97	128.62	124.51
17	3	202	CLA	CMB-C2B-C3B	2.97	130.24	124.68
20	A	843	BCR	C7-C8-C9	-2.97	121.75	126.23
17	K	102	CLA	CMB-C2B-C3B	2.97	130.24	124.68
17	B	828	CLA	C2D-C1D-ND	-2.97	107.92	110.10
17	L	202	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
17	B	823	CLA	CHB-C4A-NA	2.97	128.62	124.51
17	A	828	CLA	C1D-ND-C4D	2.97	108.44	106.33
17	3	212	CLA	CMB-C2B-C3B	2.96	130.22	124.68
17	B	804	CLA	C4D-C3D-CAD	-2.96	104.60	108.10
17	J	102	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
17	4	610	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
17	B	830	CLA	CHB-C4A-NA	2.96	128.61	124.51
17	5	609	CLA	C2D-C1D-ND	-2.96	107.92	110.10
17	A	820	CLA	O2D-CGD-CBD	2.96	116.53	111.27
17	5	606	CLA	CMD-C2D-C1D	2.96	129.93	124.71
17	4	606	CLA	CHB-C4A-NA	2.96	128.60	124.51
17	4	610	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
25	3	201	ZEX	C12-C13-C14	-2.96	114.41	118.94
20	L	206	BCR	C15-C14-C13	-2.96	123.09	127.31
17	A	824	CLA	CAA-C2A-C1A	-2.96	102.29	111.97
17	B	832	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
25	4	612	ZEX	C8-C7-C6	-2.95	118.91	127.20
17	B	801	CLA	CGD-CBD-CAD	2.95	120.30	110.73
17	A	808	CLA	CHB-C4A-NA	2.95	128.59	124.51
17	B	836	CLA	CMB-C2B-C3B	2.95	130.20	124.68
17	A	820	CLA	CHB-C4A-NA	2.95	128.59	124.51
17	5	605	CLA	CMB-C2B-C3B	2.95	130.19	124.68
25	3	201	ZEX	C31-C32-C33	-2.95	118.13	126.42
17	B	824	CLA	CHB-C4A-NA	2.95	128.59	124.51
17	A	803	CLA	C1B-CHB-C4A	-2.95	124.28	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	804	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
17	A	810	CLA	CMB-C2B-C3B	2.95	130.19	124.68
17	5	608	CLA	CHB-C4A-NA	2.94	128.58	124.51
17	A	832	CLA	CMC-C2C-C3C	2.94	134.11	126.12
17	B	803	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
17	2	601	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
17	3	203	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
17	A	814	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
17	A	832	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
20	B	846	BCR	C7-C8-C9	-2.93	121.80	126.23
17	L	202	CLA	CHB-C4A-NA	2.93	128.56	124.51
17	A	813	CLA	CHB-C4A-NA	2.93	128.56	124.51
17	A	823	CLA	CHB-C4A-NA	2.93	128.56	124.51
17	B	833	CLA	CMB-C2B-C3B	2.93	130.16	124.68
17	B	801	CLA	O1D-CGD-CBD	2.93	130.47	124.48
25	5	614	ZEX	C3-C4-C5	2.93	117.68	111.85
17	J	102	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
25	5	614	ZEX	C21-C22-C23	2.92	120.01	113.69
17	A	818	CLA	CAC-C3C-C2C	2.92	132.53	127.53
17	1	606	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
17	A	810	CLA	CHB-C4A-NA	2.92	128.55	124.51
25	1	616	ZEX	C18-C5-C4	-2.92	108.95	114.36
17	2	603	CLA	CHB-C4A-NA	2.92	128.55	124.51
17	5	603	CLA	CMB-C2B-C3B	2.92	130.14	124.68
20	B	805	BCR	C3-C4-C5	-2.92	108.87	114.08
20	F	304	BCR	C24-C23-C22	-2.92	121.83	126.23
17	J	103	CLA	CMB-C2B-C3B	2.92	130.13	124.68
17	1	607	CLA	O2A-CGA-O1A	-2.91	116.04	123.30
25	3	215	ZEX	C17-C1-C6	-2.91	105.57	110.30
20	L	206	BCR	C15-C16-C17	-2.91	117.51	123.47
17	4	602	CLA	CMA-C3A-C2A	-2.91	102.08	113.83
17	L	204	CLA	CHB-C4A-NA	2.91	128.54	124.51
17	B	807	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	3	206	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	5	601	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	B	820	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	B	826	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
20	L	205	BCR	C15-C16-C17	-2.91	117.52	123.47
20	B	848	BCR	C27-C26-C25	2.91	126.95	122.73
17	A	827	CLA	CMA-C3A-C2A	-2.91	102.10	113.83
17	O	204	CLA	CHB-C4A-NA	2.90	128.53	124.51
17	B	826	CLA	O2D-CGD-O1D	-2.90	118.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	605	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	4	612	ZEX	C7-C6-C5	-2.90	114.43	121.46
17	2	603	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
17	3	209	CLA	CHB-C4A-NA	2.90	128.52	124.51
17	B	822	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
17	O	205	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	3	216	ZEX	C18-C5-C4	-2.90	108.98	114.36
17	A	806	CLA	CMB-C2B-C3B	2.90	130.10	124.68
17	1	606	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	5	615	ZEX	C32-C33-C34	-2.90	114.50	118.94
17	B	802	CLA	C4D-CHA-C1A	2.90	124.77	121.25
17	1	607	CLA	CHB-C4A-NA	2.90	128.52	124.51
17	F	303	CLA	CMB-C2B-C3B	2.89	130.09	124.68
17	B	810	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
17	B	817	CLA	CAA-C2A-C3A	-2.89	104.86	112.78
20	B	848	BCR	C30-C25-C26	-2.89	118.54	122.61
17	K	102	CLA	CHB-C4A-NA	2.89	128.51	124.51
17	K	103	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	4	616	ZEX	C18-C5-C4	-2.89	109.00	114.36
17	B	809	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
17	5	606	CLA	CGD-CBD-CAD	-2.89	101.38	110.73
25	3	215	ZEX	C7-C8-C9	-2.88	121.88	126.23
17	2	612	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
17	2	611	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
17	5	608	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
17	B	829	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
17	O	205	CLA	CMB-C2B-C3B	2.88	130.06	124.68
17	B	821	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
17	1	603	CLA	CMB-C2B-C3B	2.88	130.06	124.68
17	F	302	CLA	CHB-C4A-NA	2.87	128.49	124.51
20	A	846	BCR	C15-C16-C17	-2.87	117.59	123.47
17	B	834	CLA	CHB-C4A-NA	2.87	128.49	124.51
17	5	610	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
17	A	834	CLA	CMB-C2B-C3B	2.87	130.05	124.68
17	A	830	CLA	CHB-C4A-NA	2.87	128.48	124.51
17	A	803	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
17	A	828	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
17	A	816	CLA	C2D-C1D-ND	-2.87	107.99	110.10
17	3	207	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
17	4	609	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
17	4	602	CLA	CHB-C4A-NA	2.86	128.47	124.51
17	3	204	CLA	CHB-C4A-NA	2.86	128.47	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	205	CLA	O2D-CGD-CBD	2.86	116.35	111.27
17	A	828	CLA	CHB-C4A-NA	2.86	128.47	124.51
17	2	609	CLA	CHB-C4A-NA	2.86	128.47	124.51
17	L	204	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	1	610	CLA	CHB-C4A-NA	2.85	128.46	124.51
17	1	611	CLA	CHB-C4A-NA	2.85	128.46	124.51
17	A	830	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
17	B	810	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
17	2	601	CLA	O1D-CGD-CBD	2.85	130.32	124.48
17	A	813	CLA	CAA-C2A-C3A	-2.85	107.14	114.26
17	O	205	CLA	CHB-C4A-NA	2.85	128.45	124.51
17	A	838	CLA	C1-C2-C3	-2.85	121.12	126.04
17	A	839	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
17	5	609	CLA	CMC-C2C-C3C	2.85	133.84	126.12
17	O	201	CLA	CAA-C2A-C3A	-2.85	104.98	112.78
17	A	828	CLA	CHC-C1C-NC	2.85	128.52	124.20
17	4	608	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
25	1	613	ZEX	C18-C5-C4	-2.84	109.09	114.36
17	A	829	CLA	CHB-C4A-NA	2.84	128.44	124.51
17	B	836	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
17	4	603	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
20	I	101	BCR	C15-C14-C13	-2.84	123.26	127.31
17	A	824	CLA	CHB-C4A-NA	2.83	128.43	124.51
17	1	609	CLA	CHB-C4A-NA	2.83	128.43	124.51
25	1	616	ZEX	C7-C8-C9	-2.83	121.95	126.23
17	3	207	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	B	841	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
17	2	606	CLA	CMB-C2B-C3B	2.83	129.97	124.68
17	A	809	CLA	CHB-C4A-NA	2.83	128.43	124.51
23	B	851	DGD	CDB-CCB-CBB	-2.83	100.06	114.42
17	3	211	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	B	806	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
20	B	849	BCR	C15-C16-C17	-2.83	117.69	123.47
17	2	609	CLA	CMB-C2B-C3B	2.83	129.96	124.68
25	3	201	ZEX	C38-C24-C23	-2.83	107.84	112.20
20	B	805	BCR	C11-C10-C9	-2.82	123.28	127.31
17	B	814	CLA	CHB-C4A-NA	2.82	128.42	124.51
17	5	607	CLA	CHB-C4A-NA	2.82	128.41	124.51
17	A	820	CLA	CMB-C2B-C3B	2.82	129.96	124.68
16	A	801	CL0	C2A-C1A-CHA	2.82	128.79	123.86
17	A	824	CLA	CBC-CAC-C3C	2.82	120.20	112.43
17	5	605	CLA	O2D-CGD-O1D	-2.82	118.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	206	BCR	C11-C10-C9	-2.82	123.29	127.31
17	B	843	CLA	CHB-C4A-NA	2.82	128.41	124.51
17	K	102	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	B	802	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
17	A	805	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	4	604	CLA	CHB-C4A-NA	2.81	128.40	124.51
17	B	802	CLA	CHA-C1A-NA	-2.81	119.96	126.40
20	O	202	BCR	C15-C16-C17	-2.81	117.72	123.47
17	4	608	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
20	B	848	BCR	C40-C30-C25	2.81	114.86	110.30
17	A	828	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
25	4	615	ZEX	C7-C8-C9	-2.81	121.99	126.23
17	F	301	CLA	CHB-C4A-NA	2.81	128.39	124.51
17	2	602	CLA	CMB-C2B-C3B	2.80	129.92	124.68
17	B	812	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
16	A	801	CL0	C2D-C1D-ND	2.80	112.17	110.10
25	4	614	ZEX	C11-C12-C13	-2.80	118.55	126.42
20	K	104	BCR	C15-C16-C17	-2.80	117.74	123.47
25	3	215	ZEX	C15-C35-C34	-2.80	117.74	123.47
25	1	615	ZEX	C31-C32-C33	-2.80	118.56	126.42
25	2	617	ZEX	C11-C12-C13	-2.80	118.56	126.42
17	4	601	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
20	L	205	BCR	C3-C4-C5	-2.80	109.08	114.08
25	5	615	ZEX	C18-C5-C4	-2.80	109.17	114.36
17	B	820	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
25	2	615	ZEX	C31-C32-C33	-2.79	118.56	126.42
17	B	841	CLA	CHB-C4A-NA	2.79	128.38	124.51
17	2	608	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
17	B	821	CLA	CAA-CBA-CGA	-2.79	105.10	113.25
17	O	203	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	4	602	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	1	617	ZEX	C7-C8-C9	2.79	130.45	126.23
17	5	606	CLA	C3D-C2D-C1D	2.79	109.64	105.83
20	B	850	BCR	C2-C1-C6	2.79	114.77	110.48
25	5	614	ZEX	C28-C27-C26	-2.79	122.33	127.09
17	A	822	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
17	J	102	CLA	CMB-C2B-C3B	2.78	129.89	124.68
17	5	602	CLA	CHD-C1D-ND	-2.78	121.90	124.45
20	A	846	BCR	C23-C22-C21	-2.78	114.68	118.94
17	B	834	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
17	A	803	CLA	CAC-C3C-C4C	2.78	128.41	124.81
17	1	608	CLA	CMB-C2B-C3B	2.78	129.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	103	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	3	213	CLA	CMB-C2B-C3B	2.78	129.88	124.68
25	3	215	ZEX	C11-C12-C13	-2.78	118.61	126.42
17	A	823	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
17	O	204	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	1	608	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	L	203	CLA	CHB-C4A-NA	2.77	128.35	124.51
17	3	210	CLA	CHB-C4A-NA	2.77	128.35	124.51
25	4	615	ZEX	C18-C5-C4	-2.77	109.22	114.36
20	L	201	BCR	C20-C21-C22	-2.77	123.35	127.31
20	J	104	BCR	C40-C30-C25	2.77	114.79	110.30
17	1	602	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
17	A	816	CLA	C1D-ND-C4D	2.77	108.30	106.33
17	B	806	CLA	O2D-CGD-CBD	2.77	116.19	111.27
17	A	811	CLA	CMB-C2B-C3B	2.77	129.85	124.68
17	5	610	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	1	613	ZEX	C15-C35-C34	-2.77	117.81	123.47
17	L	203	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
17	1	602	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	1	615	ZEX	C11-C12-C13	-2.76	118.66	126.42
20	B	805	BCR	C16-C15-C14	-2.76	117.82	123.47
17	5	606	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	3	211	CLA	CHB-C4A-NA	2.76	128.33	124.51
17	2	613	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	1	606	CLA	CMB-C2B-C3B	2.76	129.84	124.68
25	2	614	ZEX	C3-C4-C5	2.76	117.34	111.85
17	1	601	CLA	O2A-CGA-O1A	-2.76	116.64	123.59
17	B	815	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
17	5	602	CLA	CAA-C2A-C3A	-2.75	105.24	112.78
25	3	218	ZEX	C4-C5-C6	-2.75	114.71	120.85
17	5	606	CLA	CED-O2D-CGD	2.75	122.16	115.94
17	1	609	CLA	CAC-C3C-C4C	2.75	128.38	124.81
17	A	832	CLA	CMB-C2B-C3B	2.75	129.82	124.68
17	2	610	CLA	CMB-C2B-C3B	2.75	129.82	124.68
17	J	102	CLA	CAA-C2A-C3A	-2.75	105.25	112.78
20	B	850	BCR	C3-C4-C5	-2.75	109.17	114.08
17	B	832	CLA	CHB-C4A-NA	2.75	128.31	124.51
17	4	609	CLA	CHB-C4A-NA	2.75	128.31	124.51
17	2	610	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
17	4	604	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
20	A	844	BCR	C15-C16-C17	-2.75	117.85	123.47
17	B	813	CLA	CMB-C2B-C3B	2.75	129.81	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	836	CLA	CHB-C4A-NA	2.75	128.31	124.51
17	B	825	CLA	CHB-C4A-NA	2.75	128.31	124.51
17	B	808	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
17	A	822	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
17	O	201	CLA	CHB-C4A-NA	2.74	128.30	124.51
17	1	602	CLA	CHB-C4A-NA	2.74	128.30	124.51
17	B	831	CLA	CMB-C2B-C3B	2.74	129.80	124.68
17	A	826	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
17	F	303	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
17	A	829	CLA	CMB-C2B-C3B	2.74	129.80	124.68
17	2	606	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	B	802	CLA	CMA-C3A-C4A	-2.73	104.42	111.77
20	B	846	BCR	C15-C14-C13	-2.73	123.41	127.31
20	A	844	BCR	C15-C14-C13	-2.73	123.41	127.31
20	A	843	BCR	C27-C26-C25	2.73	126.69	122.73
20	B	847	BCR	C27-C26-C25	2.73	126.69	122.73
17	B	819	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
19	A	842	LHG	O8-C23-C24	2.73	120.46	111.91
17	A	818	CLA	CMC-C2C-C1C	-2.72	120.89	125.04
17	B	830	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
17	B	834	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
17	3	209	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
25	5	616	ZEX	C28-C27-C26	-2.72	122.44	127.09
20	F	304	BCR	C15-C14-C13	-2.72	123.42	127.31
20	F	304	BCR	C11-C10-C9	-2.72	123.43	127.31
25	2	616	ZEX	C7-C8-C9	-2.72	122.12	126.23
17	B	811	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
17	2	607	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	4	613	ZEX	C23-C24-C25	2.72	113.20	109.33
16	A	801	CL0	CHA-C1A-NA	-2.72	120.17	126.40
17	1	601	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
17	B	833	CLA	C2D-C1D-ND	-2.72	108.10	110.10
17	A	838	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
20	A	846	BCR	C20-C21-C22	-2.72	123.43	127.31
17	5	613	CLA	CHB-C4A-NA	2.71	128.27	124.51
17	5	602	CLA	CHB-C4A-NA	2.71	128.26	124.51
17	B	824	CLA	CMB-C2B-C3B	2.71	129.75	124.68
17	B	833	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
17	B	808	CLA	C11-C12-C13	-2.71	107.15	115.92
17	3	205	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
17	B	840	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
17	3	206	CLA	C2D-C1D-ND	-2.71	108.11	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	605	CLA	CHB-C4A-NA	2.71	128.26	124.51
17	B	809	CLA	CMB-C2B-C3B	2.71	129.74	124.68
17	3	210	CLA	CAC-C3C-C4C	2.71	128.32	124.81
20	J	105	BCR	C15-C16-C17	-2.71	117.93	123.47
17	5	607	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
17	A	838	CLA	CAA-C2A-C3A	-2.70	105.37	112.78
17	2	607	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
17	5	609	CLA	CMB-C2B-C3B	2.70	129.73	124.68
17	B	801	CLA	CAA-CBA-CGA	-2.70	105.37	113.25
17	B	839	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
20	I	101	BCR	C31-C1-C6	2.70	114.67	110.30
17	A	825	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
17	A	802	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
17	5	609	CLA	CHB-C4A-NA	2.69	128.24	124.51
17	5	606	CLA	CHA-C4D-ND	2.69	138.13	132.50
17	B	842	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
17	5	611	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
17	2	603	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
17	2	601	CLA	CMB-C2B-C3B	2.69	129.71	124.68
17	B	810	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
17	2	608	CLA	C1-C2-C3	-2.69	122.41	126.75
17	B	838	CLA	CHB-C4A-NA	2.69	128.22	124.51
17	A	802	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
17	B	824	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
17	1	612	CLA	C2A-C1A-CHA	2.68	128.55	123.86
17	F	302	CLA	O2D-CGD-CBD	2.68	116.03	111.27
25	1	615	ZEX	C23-C24-C25	2.68	113.14	109.33
17	B	833	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
17	A	835	CLA	C2A-C1A-CHA	2.68	128.54	123.86
17	A	834	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
17	B	803	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
20	A	846	BCR	C37-C22-C21	-2.67	119.18	122.92
17	1	601	CLA	C3A-C2A-C1A	2.67	105.34	101.34
17	2	611	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
17	2	604	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
25	5	617	ZEX	C15-C35-C34	-2.67	118.00	123.47
17	A	825	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	5	614	ZEX	C12-C13-C14	-2.67	114.84	118.94
17	B	801	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
25	4	617	ZEX	C8-C7-C6	-2.67	119.71	127.20
17	5	606	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
17	B	809	CLA	O2A-C1-C2	-2.66	101.63	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	837	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
25	4	617	ZEX	C37-C21-C26	-2.66	105.98	110.30
20	A	843	BCR	C15-C14-C13	-2.66	123.51	127.31
17	A	823	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
17	3	205	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
17	A	809	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
17	1	607	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
16	A	801	CL0	C3D-C4D-CHA	-2.66	106.64	112.72
17	4	611	CLA	CMB-C2B-C3B	2.66	129.65	124.68
17	B	816	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
17	A	828	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
17	A	806	CLA	O2D-CGD-CBD	2.66	115.99	111.27
17	3	213	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
17	B	811	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
17	B	839	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
20	L	205	BCR	C27-C26-C25	2.65	126.57	122.73
17	B	827	CLA	C2D-C1D-ND	-2.65	108.15	110.10
17	B	812	CLA	C2D-C1D-ND	-2.64	108.16	110.10
25	5	617	ZEX	C27-C28-C29	-2.64	122.24	126.23
20	A	845	BCR	C15-C16-C17	-2.64	118.06	123.47
25	3	218	ZEX	C31-C32-C33	-2.64	118.99	126.42
17	A	821	CLA	CMB-C2B-C3B	2.64	129.62	124.68
17	A	836	CLA	O2D-CGD-CBD	2.64	115.96	111.27
17	B	809	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
17	3	203	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
20	B	850	BCR	C11-C10-C9	-2.64	123.54	127.31
17	O	203	CLA	CHB-C4A-NA	2.64	128.16	124.51
20	F	304	BCR	C15-C16-C17	-2.64	118.07	123.47
17	B	809	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
17	1	604	CLA	CHB-C4A-NA	2.63	128.15	124.51
20	L	201	BCR	C15-C14-C13	-2.63	123.56	127.31
17	A	818	CLA	CMC-C2C-C3C	2.63	133.25	126.12
17	1	605	CLA	CHB-C4A-NA	2.63	128.14	124.51
17	A	837	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
17	B	811	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
17	3	208	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
25	3	218	ZEX	C37-C21-C26	-2.62	106.05	110.30
25	3	201	ZEX	C38-C24-C25	-2.61	106.71	110.87
17	B	816	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
17	1	612	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	2	605	CLA	CAA-CBA-CGA	-2.61	105.58	112.51
17	B	830	CLA	C1B-CHB-C4A	-2.61	124.95	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	801	CLA	C3C-C4C-NC	-2.61	107.64	110.57
17	A	815	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
20	B	845	BCR	C7-C8-C9	-2.60	122.30	126.23
25	5	614	ZEX	C11-C12-C13	-2.60	119.10	126.42
17	4	607	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
17	4	601	CLA	CMB-C2B-C3B	2.60	129.54	124.68
17	3	205	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
20	A	843	BCR	C15-C16-C17	-2.60	118.15	123.47
25	2	614	ZEX	C11-C12-C13	-2.60	119.12	126.42
17	3	212	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
17	B	813	CLA	CHB-C4A-NA	2.59	128.10	124.51
17	1	603	CLA	CHB-C4A-NA	2.59	128.10	124.51
25	2	615	ZEX	C3-C4-C5	2.59	117.02	111.85
17	B	843	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
17	B	802	CLA	C4D-C3D-CAD	-2.59	105.04	108.10
17	B	832	CLA	C1D-ND-C4D	2.59	108.18	106.33
17	5	606	CLA	CHD-C1D-C2D	2.59	130.91	125.48
17	3	209	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
18	B	844	PQN	C16-C17-C18	-2.59	107.55	115.92
25	5	615	ZEX	C3-C4-C5	2.59	117.01	111.85
20	B	845	BCR	C15-C16-C17	-2.59	118.17	123.47
17	A	818	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
17	A	807	CLA	O2A-CGA-O1A	-2.59	117.07	123.59
17	4	606	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
17	3	207	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
17	2	605	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
20	B	847	BCR	C31-C1-C6	2.58	114.49	110.30
17	B	811	CLA	CBA-CAA-C2A	2.58	121.48	113.86
17	A	826	CLA	O2D-CGD-CBD	2.58	115.85	111.27
25	2	614	ZEX	C23-C24-C25	2.58	113.00	109.33
17	1	603	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
17	A	805	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
17	2	612	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
20	O	202	BCR	C29-C30-C25	2.58	114.45	110.48
17	B	818	CLA	O1D-CGD-CBD	2.58	129.76	124.48
17	B	826	CLA	CHB-C4A-NA	2.58	128.07	124.51
17	A	833	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
17	F	302	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
17	B	843	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
17	A	835	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
17	A	838	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
17	B	827	CLA	C1B-CHB-C4A	-2.57	125.02	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	613	CLA	CHD-C1D-ND	-2.57	122.09	124.45
17	A	819	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
17	B	832	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
17	4	606	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
19	A	841	LHG	O8-C23-C24	2.57	119.97	111.91
23	B	851	DGD	C3G-C2G-C1G	-2.57	105.71	111.79
16	A	801	CL0	CHC-C1C-C2C	-2.57	119.62	126.72
17	B	812	CLA	CMB-C2B-C3B	2.57	129.48	124.68
17	A	833	CLA	CMA-C3A-C2A	-2.57	103.48	113.83
17	5	607	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
17	5	612	CLA	CMB-C2B-C3B	2.56	129.47	124.68
17	1	605	CLA	O2D-CGD-O1D	-2.56	118.27	124.09
17	A	809	CLA	O1D-CGD-CBD	2.56	129.73	124.48
17	A	812	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
17	J	101	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
19	A	842	LHG	C20-C19-C18	-2.56	101.42	114.42
17	B	826	CLA	CMB-C2B-C3B	2.56	129.47	124.68
20	B	848	BCR	C38-C26-C27	-2.56	108.70	113.62
20	O	202	BCR	C7-C8-C9	-2.56	122.37	126.23
17	A	812	CLA	C2D-C1D-ND	-2.56	108.22	110.10
17	1	603	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
20	K	104	BCR	C15-C14-C13	-2.56	123.66	127.31
19	A	841	LHG	C11-C10-C9	-2.56	101.44	114.42
17	J	102	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
17	B	840	CLA	CHB-C4A-NA	2.55	128.04	124.51
16	A	801	CL0	CMC-C2C-C3C	2.55	133.05	126.12
17	A	814	CLA	CMB-C2B-C3B	2.55	129.46	124.68
17	A	805	CLA	C2D-C1D-ND	-2.55	108.22	110.10
17	A	839	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
20	B	850	BCR	C15-C16-C17	-2.55	118.25	123.47
17	5	603	CLA	O1D-CGD-CBD	2.55	129.69	124.48
17	B	810	CLA	CMB-C2B-C3B	2.54	129.44	124.68
17	B	840	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
17	5	602	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
20	B	847	BCR	C2-C1-C6	2.54	114.39	110.48
17	B	804	CLA	CHA-C1A-NA	-2.54	120.58	126.40
17	B	810	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
17	A	809	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
17	B	814	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
20	A	844	BCR	C37-C22-C21	-2.54	119.37	122.92
20	A	845	BCR	C27-C26-C25	2.54	126.41	122.73
17	L	204	CLA	C1B-CHB-C4A	-2.54	125.09	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	104	BCR	C20-C21-C22	-2.54	123.69	127.31
17	3	206	CLA	CHB-C4A-NA	2.53	128.02	124.51
17	5	608	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
17	5	607	CLA	CAC-C3C-C2C	-2.53	123.20	127.53
20	B	849	BCR	C20-C21-C22	-2.53	123.70	127.31
17	4	601	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
17	A	817	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	I	101	BCR	C11-C10-C9	-2.53	123.70	127.31
20	B	805	BCR	C27-C26-C25	2.53	126.41	122.73
25	2	616	ZEX	C18-C5-C4	-2.53	109.67	114.36
17	L	204	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
25	1	613	ZEX	C17-C1-C6	-2.53	106.20	110.30
17	B	813	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
17	B	809	CLA	CMC-C2C-C1C	-2.53	121.19	125.04
17	5	603	CLA	C2A-C1A-CHA	2.53	128.28	123.86
20	B	847	BCR	C11-C10-C9	-2.52	123.71	127.31
17	B	822	CLA	CMB-C2B-C1B	-2.52	124.58	128.46
17	A	836	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
17	5	604	CLA	CMB-C2B-C3B	2.52	129.40	124.68
17	B	803	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
25	3	217	ZEX	C4-C5-C6	-2.52	115.23	120.85
17	1	610	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
17	B	839	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
17	A	815	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
17	B	816	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	4	610	CLA	CMB-C2B-C3B	2.51	129.38	124.68
17	B	814	CLA	CMB-C2B-C3B	2.51	129.61	124.69
20	A	844	BCR	C11-C10-C9	-2.51	123.73	127.31
17	3	206	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
17	A	816	CLA	C2A-C1A-CHA	2.51	128.25	123.86
17	A	848	CLA	CED-O2D-CGD	2.51	121.61	115.94
17	2	610	CLA	CMA-C3A-C4A	2.51	118.51	111.77
17	B	812	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	A	816	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
16	A	801	CL0	C3D-C4D-ND	2.51	114.29	110.24
20	J	104	BCR	C27-C26-C25	2.51	126.37	122.73
17	B	841	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
17	5	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
17	2	609	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
17	B	839	CLA	CHD-C1D-ND	-2.50	122.16	124.45
17	B	835	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
25	3	218	ZEX	C3-C4-C5	2.50	116.84	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	830	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
17	B	802	CLA	CAA-C2A-C1A	2.50	120.17	111.97
20	O	202	BCR	C40-C30-C25	2.50	114.35	110.30
17	A	824	CLA	C3A-C2A-C1A	2.50	105.08	101.34
20	F	304	BCR	C27-C26-C25	2.50	126.36	122.73
17	A	819	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
25	1	616	ZEX	C3-C4-C5	2.50	116.83	111.85
17	A	808	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
17	B	840	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
17	3	204	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
20	F	304	BCR	C31-C1-C6	2.49	114.34	110.30
17	A	834	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
17	B	804	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
20	A	845	BCR	C7-C8-C9	-2.49	122.47	126.23
17	A	811	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
17	A	827	CLA	C2D-C1D-ND	-2.49	108.27	110.10
25	1	614	ZEX	C7-C6-C5	-2.49	115.43	121.46
17	B	826	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
17	B	801	CLA	CMA-C3A-C4A	-2.49	105.09	111.77
25	2	614	ZEX	C38-C24-C23	-2.49	108.36	112.20
20	J	104	BCR	C37-C22-C21	-2.49	119.44	122.92
20	A	845	BCR	C34-C9-C10	-2.49	119.44	122.92
17	A	828	CLA	C2A-C1A-CHA	2.48	128.20	123.86
17	A	823	CLA	CAA-CBA-CGA	-2.48	105.99	113.25
17	B	843	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
17	A	804	CLA	C1-C2-C3	-2.48	121.75	126.04
17	B	837	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
17	A	817	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
17	1	610	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
17	2	611	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
20	O	202	BCR	C15-C14-C13	-2.48	123.77	127.31
17	A	833	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
17	2	608	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
25	4	613	ZEX	C7-C6-C5	-2.48	115.46	121.46
20	B	846	BCR	C15-C16-C17	-2.48	118.40	123.47
20	A	844	BCR	C24-C23-C22	-2.48	122.49	126.23
25	4	612	ZEX	C7-C8-C9	-2.48	122.50	126.23
20	K	101	BCR	C35-C13-C14	-2.47	119.46	122.92
17	A	830	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
17	L	202	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
17	A	826	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
17	B	837	CLA	CMB-C2B-C3B	2.47	129.30	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	104	BCR	C3-C4-C5	-2.47	109.67	114.08
17	B	803	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
17	B	808	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
16	A	801	CL0	CMA-C3A-C2A	-2.47	103.87	113.83
17	2	612	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
17	O	205	CLA	C2D-C1D-ND	-2.47	108.29	110.10
20	A	844	BCR	C1-C6-C5	-2.47	119.14	122.61
17	B	841	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
17	A	815	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
17	B	828	CLA	C3A-C2A-C1A	2.46	105.03	101.34
17	A	828	CLA	C2D-C1D-ND	-2.46	108.29	110.10
17	B	831	CLA	C2D-C1D-ND	-2.46	108.29	110.10
17	B	840	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
17	A	817	CLA	C2D-C1D-ND	-2.46	108.29	110.10
17	B	838	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
17	B	812	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
20	A	845	BCR	C37-C22-C21	-2.46	119.48	122.92
17	4	607	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
17	3	206	CLA	C2A-C1A-CHA	2.46	128.15	123.86
17	A	828	CLA	C16-C15-C13	-2.46	107.98	115.92
17	A	836	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
17	B	825	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
20	A	843	BCR	C11-C10-C9	-2.45	123.81	127.31
17	A	805	CLA	C3A-C2A-C1A	2.45	105.01	101.34
17	2	602	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
17	A	823	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
17	L	202	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
20	K	101	BCR	C27-C26-C25	2.45	126.29	122.73
17	B	809	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
16	A	801	CL0	CMB-C2B-C1B	-2.45	124.70	128.46
18	B	844	PQN	C2M-C2-C3	-2.45	120.41	124.40
17	2	602	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
16	A	801	CL0	C16-C17-C18	-2.44	104.47	115.98
17	2	604	CLA	C2A-C1A-CHA	2.44	128.13	123.86
17	A	823	CLA	C2D-C1D-ND	-2.44	108.31	110.10
17	A	823	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
17	A	836	CLA	C2A-C1A-CHA	2.44	128.12	123.86
17	B	819	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
20	K	101	BCR	C24-C23-C22	-2.44	122.55	126.23
25	1	615	ZEX	C38-C24-C23	-2.44	108.44	112.20
17	5	601	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
17	B	828	CLA	C1B-CHB-C4A	-2.43	125.30	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	807	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
17	5	612	CLA	C2A-C1A-CHA	2.43	128.11	123.86
20	A	846	BCR	C27-C26-C25	2.43	126.26	122.73
17	5	609	CLA	O2D-CGD-CBD	2.43	115.59	111.27
17	F	302	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
17	A	829	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
17	1	607	CLA	O1A-CGA-CBA	2.43	130.89	123.08
17	F	303	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
20	O	202	BCR	C16-C15-C14	-2.43	118.50	123.47
17	1	606	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
17	3	202	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
17	B	806	CLA	O2A-C1-C2	-2.43	102.25	108.64
17	2	601	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
17	4	603	CLA	O2A-CGA-O1A	-2.43	117.25	123.30
17	A	819	CLA	CHC-C1C-NC	2.43	127.88	124.20
17	B	842	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
17	A	828	CLA	CMC-C2C-C1C	-2.43	121.34	125.04
17	A	807	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	B	804	CLA	C4D-CHA-C1A	2.42	124.20	121.25
17	B	817	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
17	1	605	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
17	A	808	CLA	CMB-C2B-C3B	2.42	129.21	124.68
17	2	610	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
17	B	832	CLA	CHC-C1C-NC	2.42	127.87	124.20
17	B	831	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
20	L	201	BCR	C27-C26-C25	2.42	126.24	122.73
17	B	802	CLA	C1-C2-C3	-2.42	121.86	126.04
17	B	837	CLA	C2A-C1A-CHA	2.42	128.09	123.86
25	1	614	ZEX	C8-C7-C6	-2.42	120.42	127.20
17	3	211	CLA	O2D-CGD-CBD	2.42	115.56	111.27
17	B	814	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
17	B	820	CLA	C2A-C1A-CHA	2.42	128.08	123.86
17	1	612	CLA	CHA-C1A-NA	-2.42	120.87	126.40
17	A	831	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
25	5	614	ZEX	C8-C7-C6	-2.41	120.42	127.20
17	B	808	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
25	1	613	ZEX	C7-C6-C5	-2.41	115.62	121.46
17	B	836	CLA	CMA-C3A-C4A	-2.41	105.29	111.77
17	A	839	CLA	CMB-C2B-C3B	2.41	129.19	124.68
17	2	605	CLA	C3A-C2A-C1A	2.41	104.95	101.34
17	B	823	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
17	A	839	CLA	CAA-C2A-C3A	-2.41	106.19	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	827	CLA	CAA-CBA-CGA	-2.41	106.22	113.25
25	3	201	ZEX	C18-C5-C4	-2.40	109.90	114.36
17	A	814	CLA	O2D-CGD-CBD	2.40	115.54	111.27
17	B	811	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
17	2	607	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
20	B	846	BCR	C28-C27-C26	-2.40	109.79	114.08
25	3	217	ZEX	C23-C24-C25	2.40	112.75	109.33
17	A	811	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
25	4	615	ZEX	C8-C7-C6	-2.40	120.47	127.20
17	O	201	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
25	3	216	ZEX	C11-C12-C13	-2.39	119.69	126.42
17	B	811	CLA	C3A-C2A-C1A	2.39	104.92	101.34
25	3	214	ZEX	C3-C4-C5	2.39	116.62	111.85
17	B	802	CLA	C3B-C4B-NB	-2.39	106.12	109.21
25	3	214	ZEX	C35-C15-C14	-2.39	118.58	123.47
17	4	602	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
23	B	851	DGD	CBB-CAB-C9B	-2.39	102.31	114.42
17	B	807	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
20	A	844	BCR	C40-C30-C25	2.38	114.17	110.30
25	3	218	ZEX	C11-C12-C13	-2.38	119.72	126.42
25	2	615	ZEX	C8-C7-C6	-2.38	120.50	127.20
17	A	817	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
17	5	612	CLA	O2D-CGD-CBD	2.38	115.50	111.27
19	A	841	LHG	C20-C19-C18	-2.38	102.33	114.42
17	B	823	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
25	2	614	ZEX	C35-C15-C14	-2.38	118.60	123.47
17	A	806	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
17	A	803	CLA	O1D-CGD-CBD	2.38	129.36	124.48
17	1	603	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
25	1	616	ZEX	C4-C5-C6	-2.38	115.54	120.85
17	5	608	CLA	O2D-CGD-CBD	2.38	115.50	111.27
17	F	301	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
17	A	821	CLA	C1-C2-C3	-2.38	121.93	126.04
20	B	850	BCR	C28-C27-C26	-2.38	109.83	114.08
17	B	827	CLA	C1-C2-C3	-2.38	121.93	126.04
20	J	104	BCR	C7-C8-C9	-2.37	122.65	126.23
19	A	842	LHG	C11-C10-C9	-2.37	102.37	114.42
17	4	607	CLA	O2D-CGD-CBD	2.37	115.49	111.27
17	O	204	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
17	1	612	CLA	C2D-C1D-ND	-2.37	108.36	110.10
20	I	101	BCR	C27-C26-C25	2.37	126.17	122.73
17	4	605	CLA	O2D-CGD-O1D	-2.37	118.71	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	802	CLA	C2A-C1A-CHA	2.37	128.00	123.86
17	5	603	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
20	J	105	BCR	C27-C26-C25	2.37	126.17	122.73
17	A	810	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
20	K	104	BCR	C27-C26-C25	2.37	126.17	122.73
25	1	613	ZEX	C31-C32-C33	-2.37	119.77	126.42
17	B	819	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
17	B	823	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
17	F	301	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
17	2	603	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
17	B	808	CLA	O2D-CGD-CBD	2.36	115.47	111.27
25	4	616	ZEX	C23-C24-C25	2.36	112.70	109.33
20	O	202	BCR	C11-C10-C9	-2.36	123.94	127.31
20	J	104	BCR	C28-C27-C26	-2.36	109.86	114.08
20	L	201	BCR	C7-C8-C9	-2.36	122.67	126.23
17	B	802	CLA	CMA-C3A-C2A	-2.36	104.30	113.83
17	A	821	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
17	A	829	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
16	A	801	CL0	CAC-C3C-C4C	2.36	127.87	124.81
17	A	808	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
17	A	814	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
17	A	822	CLA	C2A-C1A-CHA	2.36	127.98	123.86
20	B	805	BCR	C20-C21-C22	-2.35	123.95	127.31
17	B	818	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
17	A	848	CLA	C3C-C4C-NC	-2.35	107.93	110.57
17	5	606	CLA	CHC-C1C-NC	2.35	127.77	124.20
17	5	604	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
20	A	843	BCR	C33-C5-C6	-2.35	121.89	124.53
17	A	821	CLA	C2D-C1D-ND	-2.35	108.37	110.10
17	5	606	CLA	C4D-C3D-CAD	2.35	110.86	108.10
17	B	833	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
17	B	834	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
17	B	816	CLA	CED-O2D-CGD	-2.35	110.63	115.94
17	J	103	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
17	A	825	CLA	C2A-C1A-CHA	2.35	127.96	123.86
17	1	611	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
17	B	808	CLA	C2A-C1A-CHA	2.34	127.96	123.86
25	3	216	ZEX	C35-C15-C14	-2.34	118.68	123.47
17	B	829	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	3	218	ZEX	C12-C13-C14	-2.34	115.35	118.94
17	K	103	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	4	616	ZEX	C21-C26-C27	-2.34	109.16	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	838	CLA	C2A-C1A-CHA	2.34	127.95	123.86
17	1	606	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
17	3	202	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
17	2	606	CLA	CHD-C1D-ND	-2.34	122.31	124.45
20	J	105	BCR	C15-C14-C13	-2.34	123.98	127.31
20	B	849	BCR	C27-C26-C25	2.33	126.12	122.73
17	B	815	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
17	B	803	CLA	C1-C2-C3	-2.33	122.01	126.04
17	O	204	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
17	O	203	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
17	5	605	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
20	L	206	BCR	C27-C26-C25	2.33	126.11	122.73
25	4	613	ZEX	C21-C26-C27	-2.33	109.19	115.78
17	B	828	CLA	O1D-CGD-CBD	2.33	129.25	124.48
17	1	608	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
17	3	204	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
17	5	605	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
17	B	831	CLA	CMA-C3A-C2A	-2.33	104.44	113.83
25	1	614	ZEX	C38-C24-C25	-2.33	107.17	110.87
17	A	829	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
17	B	821	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
17	A	814	CLA	CHD-C1D-ND	-2.33	122.32	124.45
23	B	851	DGD	C5B-C4B-C3B	-2.32	102.62	114.42
25	3	217	ZEX	C11-C12-C13	-2.32	119.89	126.42
17	A	827	CLA	O2A-C1-C2	-2.32	102.53	108.64
17	A	814	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
17	A	812	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
17	5	608	CLA	C2A-C1A-CHA	2.32	127.92	123.86
17	4	601	CLA	CMC-C2C-C1C	-2.32	121.50	125.04
25	4	616	ZEX	C7-C8-C9	-2.32	122.73	126.23
25	3	217	ZEX	C7-C8-C9	-2.32	122.73	126.23
25	2	617	ZEX	C35-C15-C14	-2.32	118.72	123.47
17	3	212	CLA	C2A-C1A-CHA	2.32	127.91	123.86
20	B	846	BCR	C24-C23-C22	-2.32	122.73	126.23
17	B	817	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
17	3	208	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
17	3	202	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
17	A	811	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
25	4	612	ZEX	C11-C12-C13	-2.31	119.92	126.42
17	B	835	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	A	841	LHG	C27-C26-C25	-2.31	102.69	114.42
17	B	836	CLA	O2D-CGD-O1D	-2.31	119.32	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	823	CLA	O1D-CGD-CBD	2.31	129.21	124.48
20	B	848	BCR	C37-C22-C21	-2.31	119.69	122.92
17	B	830	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
17	B	810	CLA	O2D-CGD-CBD	2.31	115.37	111.27
17	B	811	CLA	CMB-C2B-C3B	2.31	129.00	124.68
17	O	201	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
17	4	611	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
17	B	825	CLA	CMB-C2B-C3B	2.31	128.99	124.68
25	4	617	ZEX	C31-C32-C33	-2.31	119.94	126.42
25	3	214	ZEX	C8-C7-C6	-2.31	120.73	127.20
19	A	842	LHG	C18-C17-C16	-2.30	102.72	114.42
17	3	209	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
17	1	606	CLA	C2D-C1D-ND	-2.30	108.41	110.10
20	K	104	BCR	C24-C23-C22	-2.30	122.75	126.23
17	B	838	CLA	CHA-C1A-NA	-2.30	121.13	126.40
25	2	616	ZEX	C4-C5-C6	-2.30	115.72	120.85
17	A	827	CLA	O2D-CGD-CBD	2.30	115.36	111.27
17	B	802	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
17	B	827	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
17	B	814	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
20	A	845	BCR	C15-C14-C13	-2.30	124.03	127.31
17	A	806	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
17	2	605	CLA	CHD-C1D-ND	-2.30	122.34	124.45
17	3	209	CLA	C6-C5-C3	-2.30	110.86	114.62
17	B	811	CLA	C1-C2-C3	-2.30	122.07	126.04
25	4	616	ZEX	C11-C12-C13	-2.30	119.97	126.42
20	A	844	BCR	C27-C26-C25	2.30	126.06	122.73
17	3	206	CLA	C1D-ND-C4D	2.29	107.97	106.33
17	2	608	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
17	B	802	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
17	2	609	CLA	C2D-C1D-ND	-2.29	108.42	110.10
20	B	805	BCR	C37-C22-C21	-2.29	119.72	122.92
17	A	827	CLA	CMD-C2D-C1D	-2.29	120.68	124.71
17	A	813	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
17	4	603	CLA	C2A-C1A-CHA	2.29	127.86	123.86
17	1	606	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
17	B	812	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	B	851	DGD	CFB-CEB-CDB	-2.29	102.82	114.42
17	2	609	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
25	2	615	ZEX	C21-C26-C27	-2.28	109.32	115.78
17	A	835	CLA	CHA-C1A-NA	-2.28	121.17	126.40
17	A	814	CLA	C2A-C1A-CHA	2.28	127.85	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	602	CLA	CAA-CBA-CGA	2.28	119.92	113.25
25	4	616	ZEX	C17-C1-C6	-2.28	106.60	110.30
25	3	201	ZEX	C7-C6-C5	-2.28	115.94	121.46
17	5	607	CLA	O2A-CGA-O1A	-2.28	117.61	123.30
17	B	835	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
17	A	805	CLA	C2A-C1A-CHA	2.28	127.85	123.86
17	2	606	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	4	601	CLA	CHC-C1C-NC	2.28	127.66	124.20
17	1	602	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	K	103	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
17	A	821	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	A	824	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	3	208	CLA	C2A-C1A-CHA	2.28	127.84	123.86
17	5	611	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
25	1	616	ZEX	C38-C24-C23	-2.28	108.68	112.20
25	5	614	ZEX	C22-C23-C24	2.28	116.83	111.76
17	B	804	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
17	B	830	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
17	J	103	CLA	C2A-C1A-CHA	2.27	127.83	123.86
17	1	604	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
17	A	807	CLA	CED-O2D-CGD	-2.27	110.80	115.94
17	A	827	CLA	C3B-C4B-NB	-2.27	106.28	109.21
16	A	801	CL0	C14-C13-C12	-2.27	103.07	111.29
17	3	210	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
17	K	102	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	B	845	BCR	C27-C26-C25	2.27	126.02	122.73
17	A	826	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
17	1	610	CLA	C2A-C1A-CHA	2.27	127.82	123.86
17	5	609	CLA	CHD-C1D-ND	-2.26	122.37	124.45
17	B	812	CLA	CAC-C3C-C4C	2.26	127.75	124.81
17	3	206	CLA	CHA-C1A-NA	-2.26	121.21	126.40
17	B	802	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
17	A	816	CLA	CHA-C1A-NA	-2.26	121.22	126.40
17	A	823	CLA	CMB-C2B-C3B	2.26	128.91	124.68
20	B	845	BCR	C15-C14-C13	-2.26	124.08	127.31
17	B	824	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
17	B	822	CLA	C2A-C1A-CHA	2.26	127.81	123.86
17	A	833	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
17	5	601	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
17	3	213	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
20	B	847	BCR	C15-C16-C17	-2.26	118.85	123.47
19	A	842	LHG	C27-C26-C25	-2.26	102.96	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	612	CLA	C3A-C2A-C1A	2.26	104.72	101.34
17	4	607	CLA	CMA-C3A-C4A	-2.26	105.71	111.77
17	5	602	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
17	B	829	CLA	C2A-C1A-CHA	2.26	127.80	123.86
17	B	827	CLA	CMA-C3A-C4A	-2.26	105.71	111.77
17	A	815	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
17	O	204	CLA	C2A-C1A-CHA	2.25	127.80	123.86
17	A	806	CLA	CAA-C2A-C1A	-2.25	104.59	111.97
25	2	616	ZEX	C35-C15-C14	-2.25	118.86	123.47
25	1	615	ZEX	C17-C1-C6	-2.25	106.64	110.30
17	B	807	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
25	4	612	ZEX	C4-C5-C6	-2.25	115.83	120.85
17	2	601	CLA	CHD-C1D-ND	-2.25	122.39	124.45
17	2	605	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
17	B	830	CLA	C2A-C1A-CHA	2.25	127.80	123.86
17	B	836	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
17	B	839	CLA	CMA-C3A-C4A	-2.25	105.72	111.77
20	J	104	BCR	C15-C14-C13	-2.25	124.10	127.31
17	A	836	CLA	C4-C3-C5	2.25	119.05	115.27
17	4	609	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
17	L	203	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
25	5	614	ZEX	C31-C32-C33	-2.25	120.11	126.42
17	B	825	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
17	B	812	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
17	3	204	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
17	3	213	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
17	A	804	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
17	B	813	CLA	O2D-CGD-CBD	2.24	115.25	111.27
20	O	202	BCR	C28-C27-C26	-2.24	110.08	114.08
17	B	804	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
25	1	613	ZEX	C21-C26-C27	-2.24	109.45	115.78
17	A	824	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
17	A	837	CLA	C2A-C1A-CHA	2.24	127.77	123.86
17	B	826	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	B	851	DGD	CAB-C9B-C8B	-2.24	103.08	114.42
17	B	820	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
25	3	218	ZEX	C38-C24-C23	-2.23	108.75	112.20
17	B	824	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
17	5	609	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
17	A	811	CLA	C2A-C1A-CHA	2.23	127.76	123.86
17	B	808	CLA	CMB-C2B-C3B	2.23	128.85	124.68
25	2	617	ZEX	C4-C5-C6	-2.23	115.88	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	825	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
17	B	835	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
17	5	611	CLA	CHD-C1D-ND	-2.23	122.41	124.45
20	A	846	BCR	C38-C26-C27	-2.23	109.34	113.62
17	B	832	CLA	C6-C7-C8	-2.23	108.72	115.92
17	4	604	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
25	4	614	ZEX	C38-C24-C23	-2.22	108.76	112.20
17	3	213	CLA	C2A-C1A-CHA	2.22	127.75	123.86
17	B	806	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
17	B	809	CLA	CHC-C1C-NC	2.22	127.58	124.20
17	1	605	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
20	A	844	BCR	C2-C1-C6	2.22	113.90	110.48
17	5	606	CLA	C1D-ND-C4D	2.22	107.91	106.33
25	5	615	ZEX	C8-C7-C6	-2.22	120.96	127.20
17	B	826	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
17	A	803	CLA	CHC-C1C-NC	2.22	127.57	124.20
17	A	807	CLA	CMA-C3A-C4A	2.22	117.74	111.77
17	3	208	CLA	CHA-C1A-NA	-2.22	121.32	126.40
25	1	614	ZEX	C35-C15-C14	-2.22	118.94	123.47
17	B	843	CLA	C2A-C1A-CHA	2.21	127.73	123.86
25	1	616	ZEX	C23-C24-C25	2.21	112.48	109.33
17	A	824	CLA	CHD-C1D-ND	-2.21	122.42	124.45
17	4	610	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
17	B	810	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
25	4	613	ZEX	C11-C12-C13	-2.21	120.20	126.42
25	2	614	ZEX	C2-C3-C4	2.21	113.33	110.30
17	K	102	CLA	C2A-C1A-CHA	2.21	127.72	123.86
25	4	615	ZEX	C3-C4-C5	2.21	116.25	111.85
17	B	835	CLA	CHD-C1D-ND	-2.21	122.43	124.45
17	B	837	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
17	A	811	CLA	CHA-C1A-NA	-2.21	121.35	126.40
17	A	848	CLA	CHD-C4C-C3C	2.20	128.08	124.84
17	1	609	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
20	K	101	BCR	C11-C10-C9	-2.20	124.17	127.31
17	5	604	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
25	1	615	ZEX	C3-C4-C5	2.20	116.24	111.85
17	A	802	CLA	C2A-C1A-CHA	2.20	127.71	123.86
17	A	831	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
20	B	805	BCR	C35-C13-C14	-2.20	119.84	122.92
17	3	202	CLA	C2A-C1A-CHA	2.20	127.70	123.86
17	A	832	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
17	B	829	CLA	O2D-CGD-CBD	2.20	115.17	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	831	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
17	1	611	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
17	B	820	CLA	C1D-ND-C4D	2.19	107.89	106.33
17	3	202	CLA	O2A-CGA-O1A	-2.19	117.84	123.30
17	A	807	CLA	C2D-C1D-ND	-2.19	108.49	110.10
17	A	806	CLA	C3A-C2A-C1A	2.19	104.61	101.34
17	A	836	CLA	C3A-C2A-C1A	2.19	104.61	101.34
17	A	818	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
17	A	813	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
17	4	605	CLA	C2A-C1A-CHA	2.19	127.68	123.86
17	B	820	CLA	C2D-C1D-ND	-2.19	108.49	110.10
17	B	834	CLA	C2A-C1A-CHA	2.19	127.68	123.86
17	4	611	CLA	O2D-CGD-CBD	2.18	115.15	111.27
17	B	831	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
17	A	803	CLA	C2A-C1A-CHA	2.18	127.68	123.86
17	3	211	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
25	1	613	ZEX	C38-C24-C23	-2.18	108.83	112.20
17	A	833	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	A	828	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
17	A	831	CLA	CBA-CAA-C2A	-2.18	107.42	113.86
17	1	604	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
17	B	810	CLA	CHD-C1D-ND	-2.18	122.45	124.45
17	5	610	CLA	C2A-C1A-CHA	2.18	127.67	123.86
25	4	616	ZEX	C3-C4-C5	2.18	116.19	111.85
17	5	604	CLA	C2A-C1A-CHA	2.18	127.67	123.86
17	5	608	CLA	O2A-CGA-O1A	-2.18	117.87	123.30
20	B	846	BCR	C39-C30-C25	2.18	113.83	110.30
17	B	811	CLA	O2A-CGA-CBA	2.18	118.74	111.91
17	L	204	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
17	5	611	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
17	2	613	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
17	5	603	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
25	3	218	ZEX	C21-C26-C27	-2.17	109.63	115.78
17	A	802	CLA	O2D-CGD-CBD	2.17	115.13	111.27
17	B	816	CLA	C2A-C1A-CHA	2.17	127.66	123.86
17	2	606	CLA	O2A-CGA-O1A	-2.17	117.89	123.30
17	B	806	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
17	1	609	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
20	A	845	BCR	C33-C5-C6	-2.17	122.09	124.53
17	2	607	CLA	C2A-C1A-CHA	2.17	127.65	123.86
25	4	614	ZEX	C21-C26-C27	-2.17	109.65	115.78
17	A	811	CLA	CMA-C3A-C4A	-2.17	105.95	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	823	CLA	CAC-C3C-C4C	2.17	127.62	124.81
17	A	848	CLA	C2A-C1A-CHA	2.17	127.65	123.86
25	4	615	ZEX	C4-C5-C6	-2.17	116.02	120.85
20	K	101	BCR	C7-C8-C9	-2.17	122.96	126.23
20	J	104	BCR	C11-C10-C9	-2.17	124.22	127.31
17	L	202	CLA	CMB-C2B-C3B	2.17	128.73	124.68
25	2	614	ZEX	C21-C26-C27	-2.17	109.65	115.78
17	B	828	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	F	301	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
17	4	608	CLA	C2D-C1D-ND	-2.16	108.51	110.10
17	5	613	CLA	C2A-C1A-CHA	2.16	127.64	123.86
17	2	609	CLA	CMA-C3A-C2A	-2.16	111.05	116.10
17	A	823	CLA	C2A-C1A-CHA	2.16	127.64	123.86
17	B	838	CLA	CBA-CAA-C2A	-2.16	107.48	113.86
17	1	608	CLA	C2A-C1A-CHA	2.16	127.64	123.86
17	B	808	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
17	5	607	CLA	C3B-C4B-NB	-2.16	106.42	109.21
17	L	204	CLA	C2A-C1A-CHA	2.16	127.64	123.86
25	3	215	ZEX	C31-C32-C33	-2.16	120.35	126.42
17	B	818	CLA	C2A-C1A-CHA	2.16	127.63	123.86
20	O	202	BCR	C16-C17-C18	-2.16	124.23	127.31
17	O	204	CLA	CAC-C3C-C4C	2.16	127.61	124.81
17	4	605	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
20	L	201	BCR	C24-C23-C22	-2.16	122.98	126.23
17	1	601	CLA	C2A-C1A-CHA	2.16	127.63	123.86
25	2	614	ZEX	C37-C21-C26	-2.16	106.80	110.30
17	A	828	CLA	CMC-C2C-C3C	2.16	131.97	126.12
17	3	206	CLA	CAA-C2A-C3A	-2.16	106.88	112.78
17	4	608	CLA	C2A-C1A-CHA	2.15	127.63	123.86
17	A	834	CLA	C2A-C1A-CHA	2.15	127.63	123.86
17	5	602	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
17	O	203	CLA	C2A-C1A-CHA	2.15	127.61	123.85
25	5	615	ZEX	C11-C12-C13	-2.15	120.37	126.42
25	1	615	ZEX	C8-C7-C6	-2.15	121.16	127.20
17	A	828	CLA	CHA-C1A-NA	-2.15	121.47	126.40
17	A	820	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
17	B	831	CLA	CHB-C4A-NA	2.15	127.49	124.51
20	A	846	BCR	C16-C15-C14	-2.15	119.07	123.47
17	A	804	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
17	2	602	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
17	B	838	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
17	B	835	CLA	C2A-C1A-CHA	2.15	127.61	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	212	CLA	C1B-CHB-C4A	-2.15	125.87	130.12
17	B	831	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
17	B	818	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
17	1	606	CLA	C2A-C1A-CHA	2.14	127.61	123.86
20	L	201	BCR	C10-C11-C12	-2.14	116.53	123.22
20	B	845	BCR	C11-C10-C9	-2.14	124.25	127.31
17	A	827	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
17	B	827	CLA	C2A-C1A-CHA	2.14	127.60	123.86
17	2	613	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
25	4	613	ZEX	C35-C15-C14	-2.14	119.09	123.47
20	B	845	BCR	C33-C5-C6	-2.14	122.13	124.53
17	3	210	CLA	CMA-C3A-C2A	-2.14	111.11	116.10
17	5	610	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
25	4	612	ZEX	C21-C26-C27	-2.14	109.73	115.78
17	1	612	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
17	A	817	CLA	C2A-C1A-CHA	2.14	127.59	123.86
17	A	818	CLA	C2A-C1A-CHA	2.14	127.59	123.86
17	B	815	CLA	C2A-C1A-CHA	2.14	127.59	123.86
17	B	804	CLA	C6-C7-C8	-2.14	109.02	115.92
17	A	832	CLA	C2D-C1D-ND	-2.13	108.53	110.10
17	B	827	CLA	CAA-C2A-C3A	-2.13	106.93	112.78
17	A	827	CLA	CHA-C1A-NA	-2.13	121.51	126.40
17	A	819	CLA	C7-C6-C5	-2.13	107.57	113.36
16	A	801	CL0	CMD-C2D-C3D	-2.13	122.71	127.61
17	B	812	CLA	C1D-ND-C4D	2.13	107.85	106.33
17	B	842	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
25	2	616	ZEX	C3-C4-C5	2.13	116.10	111.85
17	3	207	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
17	3	203	CLA	CHD-C1D-ND	-2.13	122.50	124.45
17	4	610	CLA	C3A-C2A-C1A	2.13	104.53	101.34
23	B	851	DGD	C7A-C6A-C5A	-2.13	103.61	114.42
25	4	614	ZEX	C15-C35-C34	-2.13	119.11	123.47
25	4	617	ZEX	C4-C5-C6	-2.13	116.10	120.85
25	1	616	ZEX	C31-C32-C33	-2.13	120.43	126.42
17	3	207	CLA	CHD-C1D-ND	-2.13	122.50	124.45
25	4	612	ZEX	C38-C24-C23	-2.13	108.91	112.20
17	B	816	CLA	CHA-C1A-NA	-2.13	121.52	126.40
17	B	804	CLA	C3B-C4B-NB	-2.13	106.46	109.21
17	5	613	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
17	A	807	CLA	C2A-C1A-CHA	2.13	127.58	123.86
17	B	822	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
25	3	215	ZEX	C3-C4-C5	2.13	116.09	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	821	CLA	CMA-C3A-C2A	-2.13	105.25	113.83
17	B	808	CLA	C16-C17-C18	-2.13	105.96	115.98
20	I	101	BCR	C1-C6-C5	-2.12	119.62	122.61
25	4	615	ZEX	C31-C32-C33	-2.12	120.45	126.42
17	4	610	CLA	C2A-C1A-CHA	2.12	127.57	123.86
17	B	834	CLA	CHA-C1A-NA	-2.12	121.54	126.40
20	J	105	BCR	C11-C10-C9	-2.12	124.28	127.31
16	A	801	CL0	CMC-C2C-C1C	-2.12	121.81	125.04
17	B	841	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
16	A	801	CL0	C11-C12-C13	-2.12	109.06	115.92
17	B	823	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
17	B	836	CLA	CHD-C1D-ND	-2.12	122.51	124.45
20	B	845	BCR	C40-C30-C25	2.12	113.74	110.30
17	B	843	CLA	CHA-C1A-NA	-2.12	121.54	126.40
20	B	850	BCR	C31-C1-C6	2.12	113.74	110.30
20	B	849	BCR	C30-C25-C26	-2.12	119.63	122.61
16	A	801	CL0	C4C-C3C-C2C	-2.12	103.81	106.90
17	B	804	CLA	C2A-C1A-CHA	2.12	127.56	123.86
17	A	804	CLA	CHA-C1A-NA	-2.12	121.55	126.40
25	3	215	ZEX	C38-C24-C25	-2.12	107.50	110.87
17	B	830	CLA	C6-C7-C8	-2.12	109.08	115.92
17	B	814	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
20	B	847	BCR	C3-C4-C5	-2.11	110.30	114.08
17	A	808	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
17	5	609	CLA	CAC-C3C-C2C	2.11	131.14	127.53
17	A	839	CLA	O2D-CGD-CBD	2.11	115.02	111.27
17	A	848	CLA	C1C-C2C-C3C	2.11	109.18	106.96
20	J	105	BCR	C37-C22-C21	-2.11	119.97	122.92
17	3	211	CLA	C2A-C1A-CHA	2.11	127.55	123.86
17	5	601	CLA	C2A-C1A-CHA	2.11	127.55	123.86
20	B	848	BCR	C11-C10-C9	-2.11	124.30	127.31
17	A	809	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
17	A	831	CLA	C2A-C1A-CHA	2.11	127.54	123.86
17	5	603	CLA	C4-C3-C5	2.11	118.82	115.27
20	I	101	BCR	C2-C1-C6	2.11	113.72	110.48
17	4	601	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
17	A	839	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
17	A	807	CLA	O2D-CGD-CBD	2.11	115.01	111.27
17	B	832	CLA	C3C-C4C-NC	-2.11	108.21	110.57
17	B	836	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
17	4	601	CLA	C3A-C2A-C1A	2.10	104.49	101.34
17	K	102	CLA	O2A-CGA-O1A	-2.10	118.06	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	609	CLA	CMA-C3A-C2A	-2.10	111.19	116.10
17	A	805	CLA	CAC-C3C-C4C	2.10	127.54	124.81
20	F	304	BCR	C2-C1-C6	2.10	113.72	110.48
17	A	822	CLA	O1D-CGD-CBD	2.10	128.78	124.48
17	A	814	CLA	C3C-C4C-NC	-2.10	108.22	110.57
17	B	836	CLA	C2D-C1D-ND	-2.10	108.56	110.10
17	B	804	CLA	CMA-C3A-C2A	-2.10	105.36	113.83
17	4	603	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
17	B	843	CLA	C2D-C1D-ND	-2.10	108.56	110.10
20	L	206	BCR	C33-C5-C6	-2.10	122.17	124.53
17	1	604	CLA	C2A-C1A-CHA	2.10	127.52	123.86
20	L	201	BCR	C11-C10-C9	-2.10	124.32	127.31
20	B	847	BCR	C16-C15-C14	-2.10	119.18	123.47
17	A	835	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
20	J	105	BCR	C20-C21-C22	-2.10	124.32	127.31
17	B	808	CLA	CHA-C1A-NA	-2.09	121.60	126.40
17	J	101	CLA	C2A-C1A-CHA	2.09	127.52	123.86
17	B	802	CLA	OBD-CAD-C3D	2.09	133.56	128.52
17	2	601	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
25	3	216	ZEX	C4-C5-C6	-2.09	116.19	120.85
17	O	201	CLA	C1-C2-C3	-2.09	122.43	126.04
17	5	603	CLA	CMC-C2C-C1C	-2.09	121.86	125.04
17	B	811	CLA	C3C-C4C-NC	-2.09	108.23	110.57
20	B	850	BCR	C7-C8-C9	-2.09	123.08	126.23
17	O	205	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
17	B	842	CLA	C2A-C1A-CHA	2.09	127.51	123.86
17	K	103	CLA	C2A-C1A-CHA	2.09	127.51	123.86
17	B	827	CLA	CHA-C1A-NA	-2.09	121.61	126.40
17	2	613	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
17	5	603	CLA	CHA-C1A-NA	-2.09	121.62	126.40
17	2	605	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
17	B	825	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
17	A	809	CLA	C7-C6-C5	-2.09	107.69	113.36
18	A	840	PQN	C2M-C2-C3	-2.09	121.00	124.40
17	A	827	CLA	CHB-C4A-NA	2.09	127.40	124.51
17	A	817	CLA	CHC-C1C-NC	2.08	127.37	124.20
25	5	615	ZEX	C35-C15-C14	-2.08	119.20	123.47
17	B	825	CLA	C2A-C1A-CHA	2.08	127.50	123.86
17	B	803	CLA	C3C-C4C-NC	-2.08	108.23	110.57
17	B	807	CLA	C2A-C1A-CHA	2.08	127.50	123.86
17	4	601	CLA	C2A-C1A-CHA	2.08	127.50	123.86
25	1	616	ZEX	C11-C12-C13	-2.08	120.57	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	604	CLA	C2A-C1A-CHA	2.08	127.50	123.86
17	A	802	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
17	L	203	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
17	B	833	CLA	CHA-C1A-NA	-2.08	121.63	126.40
20	A	846	BCR	C15-C14-C13	-2.08	124.34	127.31
17	A	820	CLA	CMD-C2D-C3D	2.08	132.40	127.61
17	4	607	CLA	C2A-C1A-CHA	2.08	127.50	123.86
17	1	603	CLA	C2D-C1D-ND	-2.08	108.57	110.10
17	A	834	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
17	A	803	CLA	C3C-C4C-NC	-2.08	108.24	110.57
17	B	808	CLA	C1-C2-C3	-2.08	122.45	126.04
17	B	841	CLA	C4-C3-C5	2.08	118.77	115.27
20	K	101	BCR	C38-C26-C27	-2.08	109.63	113.62
25	4	613	ZEX	C17-C1-C6	-2.08	106.93	110.30
17	5	605	CLA	O2D-CGD-CBD	2.07	114.95	111.27
17	B	834	CLA	C2D-C1D-ND	-2.07	108.58	110.10
20	F	304	BCR	C20-C21-C22	-2.07	124.35	127.31
25	1	615	ZEX	C21-C26-C27	-2.07	109.91	115.78
17	B	832	CLA	C3A-C2A-C1A	2.07	104.44	101.34
20	F	304	BCR	C35-C13-C14	-2.07	120.02	122.92
17	B	808	CLA	C1D-ND-C4D	2.07	107.81	106.33
17	A	812	CLA	CHA-C1A-NA	-2.07	121.65	126.40
17	4	609	CLA	C2A-C1A-CHA	2.07	127.47	123.85
17	B	816	CLA	C1-C2-C3	-2.07	122.46	126.04
17	B	830	CLA	CHA-C1A-NA	-2.07	121.65	126.40
19	A	841	LHG	C18-C17-C16	-2.07	103.91	114.42
17	A	829	CLA	C2D-C1D-ND	-2.07	108.58	110.10
17	B	838	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
23	B	851	DGD	C8B-C7B-C6B	-2.07	103.92	114.42
17	A	808	CLA	CAA-CBA-CGA	-2.07	107.20	113.25
25	3	217	ZEX	C21-C26-C27	-2.07	109.92	115.78
20	I	101	BCR	C38-C26-C27	-2.07	109.64	113.62
17	B	808	CLA	O2A-C1-C2	-2.07	103.20	108.64
17	A	825	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
17	5	603	CLA	CHC-C1C-NC	2.07	127.34	124.20
25	4	614	ZEX	C37-C21-C26	-2.06	106.95	110.30
25	5	616	ZEX	C31-C32-C33	-2.06	120.62	126.42
17	B	821	CLA	C2A-C1A-CHA	2.06	127.47	123.86
17	3	204	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
17	B	832	CLA	CHA-C4D-ND	2.06	136.82	132.50
25	4	615	ZEX	C27-C28-C29	-2.06	123.12	126.23
25	5	617	ZEX	C7-C6-C5	-2.06	116.47	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	832	CLA	C3A-C2A-C1A	2.06	104.43	101.34
17	4	606	CLA	CAC-C3C-C2C	-2.06	124.00	127.53
17	B	816	CLA	CBC-CAC-C3C	2.06	118.11	112.43
25	2	616	ZEX	C32-C33-C34	-2.06	115.78	118.94
17	B	819	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
17	B	801	CLA	CMA-C3A-C2A	-2.06	105.52	113.83
17	A	814	CLA	CHA-C1A-NA	-2.06	121.68	126.40
17	1	610	CLA	CHA-C1A-NA	-2.06	121.68	126.40
25	2	614	ZEX	C31-C32-C33	-2.06	120.63	126.42
20	K	104	BCR	C35-C13-C14	-2.06	120.04	122.92
17	4	603	CLA	CHA-C1A-NA	-2.06	121.68	126.40
17	B	831	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
17	4	611	CLA	CHA-C4D-ND	2.06	136.80	132.50
17	O	205	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
17	5	613	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
17	A	808	CLA	C2A-C1A-CHA	2.06	127.46	123.86
17	A	828	CLA	O2D-CGD-CBD	2.06	114.92	111.27
17	A	820	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
17	3	205	CLA	CGD-CBD-CAD	-2.06	104.08	110.73
17	A	817	CLA	C1D-ND-C4D	2.06	107.80	106.33
17	A	837	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
17	1	601	CLA	O2D-CGD-CBD	2.05	114.92	111.27
17	1	610	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
17	A	848	CLA	C1-C2-C3	-2.05	122.49	126.04
17	A	829	CLA	CHA-C1A-NA	-2.05	121.70	126.40
18	B	844	PQN	O4-C4-C5	-2.05	118.24	121.56
17	5	612	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
17	5	602	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
17	2	607	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
17	A	829	CLA	CHA-C4D-ND	2.05	136.78	132.50
17	B	838	CLA	C1-C2-C3	-2.05	122.50	126.04
17	1	608	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	1	616	ZEX	C15-C35-C34	-2.05	119.28	123.47
20	K	101	BCR	C33-C5-C6	-2.05	122.23	124.53
16	A	801	CL0	CHD-C4C-NC	-2.05	120.98	124.20
17	5	606	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
25	3	218	ZEX	C17-C1-C6	-2.05	106.98	110.30
17	O	203	CLA	CHA-C1A-NA	-2.05	121.71	126.40
20	L	205	BCR	C37-C22-C21	-2.05	120.06	122.92
17	B	806	CLA	C16-C15-C13	-2.05	109.31	115.92
17	K	102	CLA	CHA-C1A-NA	-2.05	121.71	126.40
17	4	611	CLA	O2A-CGA-O1A	-2.05	118.20	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	830	CLA	CHA-C1A-NA	-2.05	121.71	126.40
17	B	843	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
17	A	817	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
17	5	613	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
17	J	101	CLA	C3A-C2A-C1A	2.04	104.40	101.34
17	3	206	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
17	5	609	CLA	C2A-C1A-CHA	2.04	127.42	123.85
17	B	815	CLA	CHA-C1A-NA	-2.04	121.72	126.40
17	A	807	CLA	C11-C12-C13	-2.04	109.32	115.92
20	B	845	BCR	C38-C26-C27	-2.04	109.69	113.62
17	A	828	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
17	B	821	CLA	O2D-CGD-CBD	2.04	114.89	111.27
17	A	823	CLA	C1-C2-C3	-2.04	122.52	126.04
17	B	802	CLA	CHD-C1D-C2D	2.04	129.76	125.48
25	3	216	ZEX	C3-C4-C5	2.04	115.92	111.85
17	3	204	CLA	C2A-C1A-CHA	2.04	127.42	123.86
17	2	608	CLA	CHA-C1A-NA	-2.03	121.74	126.40
25	4	616	ZEX	C15-C35-C34	-2.03	119.31	123.47
20	B	805	BCR	C31-C1-C6	2.03	113.60	110.30
17	O	201	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
17	2	602	CLA	O1D-CGD-CBD	2.03	128.64	124.48
17	A	808	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
17	B	820	CLA	CHA-C1A-NA	-2.03	121.75	126.40
17	B	833	CLA	CAC-C3C-C4C	2.03	127.44	124.81
17	A	807	CLA	CHA-C1A-NA	-2.03	121.75	126.40
25	4	613	ZEX	C15-C35-C34	-2.03	119.32	123.47
17	B	812	CLA	CHA-C1A-NA	-2.03	121.76	126.40
17	3	210	CLA	CBC-CAC-C3C	2.03	118.02	112.43
17	A	848	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
17	A	828	CLA	CHC-C1C-C2C	-2.03	121.12	126.72
17	B	833	CLA	C3C-C4C-NC	-2.03	108.30	110.57
20	F	304	BCR	C7-C8-C9	-2.03	123.17	126.23
17	B	802	CLA	CMC-C2C-C1C	-2.03	121.95	125.04
17	1	602	CLA	C2A-C1A-CHA	2.03	127.40	123.86
17	B	813	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
17	O	205	CLA	CHA-C1A-NA	-2.02	121.76	126.40
20	A	844	BCR	C38-C26-C27	-2.02	109.73	113.62
20	A	846	BCR	C10-C11-C12	-2.02	116.91	123.22
20	A	843	BCR	C24-C23-C22	-2.02	123.18	126.23
25	5	616	ZEX	C4-C5-C6	-2.02	116.34	120.85
17	B	825	CLA	CHA-C1A-NA	-2.02	121.77	126.40
17	A	836	CLA	C6-C7-C8	-2.02	109.39	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	608	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
17	3	209	CLA	CHD-C1D-ND	-2.02	122.60	124.45
17	B	802	CLA	CMC-C2C-C3C	2.02	131.60	126.12
25	5	616	ZEX	C3-C4-C5	2.02	115.88	111.85
16	A	801	CL0	C4-C3-C5	2.02	118.67	115.27
17	A	805	CLA	CHA-C4D-ND	2.02	136.72	132.50
17	A	809	CLA	C1-C2-C3	-2.02	122.55	126.04
17	1	611	CLA	CHD-C4C-C3C	2.02	127.81	124.84
17	B	813	CLA	C2A-C1A-CHA	2.02	127.39	123.86
17	A	825	CLA	CHA-C1A-NA	-2.02	121.78	126.40
17	4	604	CLA	CHA-C1A-NA	-2.02	121.78	126.40
17	A	812	CLA	C2A-C1A-CHA	2.02	127.38	123.86
17	1	610	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
17	4	607	CLA	O2A-CGA-O1A	-2.02	118.28	123.30
17	5	609	CLA	CHD-C1D-C2D	2.01	129.71	125.48
17	A	823	CLA	CHA-C1A-NA	-2.01	121.78	126.40
25	1	617	ZEX	C23-C24-C25	2.01	112.20	109.33
17	B	813	CLA	CHA-C1A-NA	-2.01	121.79	126.40
25	4	616	ZEX	C38-C24-C23	-2.01	109.09	112.20
17	B	811	CLA	CHC-C1C-NC	2.01	127.26	124.20
17	O	204	CLA	CHA-C1A-NA	-2.01	121.79	126.40
17	B	826	CLA	CHA-C1A-NA	-2.01	121.79	126.40
17	F	303	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	A	818	CLA	O1A-CGA-CBA	2.01	129.54	123.08
17	J	101	CLA	C1-C2-C3	-2.01	122.57	126.04
17	A	837	CLA	C1-C2-C3	-2.01	122.57	126.04
25	4	617	ZEX	C11-C12-C13	-2.01	120.77	126.42
17	A	824	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
17	1	605	CLA	C2A-C1A-CHA	2.01	127.37	123.86
17	2	608	CLA	C2A-C1A-CHA	2.01	127.37	123.86
17	B	829	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
17	B	813	CLA	CGD-CBD-CAD	-2.01	104.23	110.73
17	4	604	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
20	B	848	BCR	C33-C5-C6	-2.01	122.27	124.53
17	B	808	CLA	C2D-C1D-ND	-2.01	108.62	110.10
17	5	604	CLA	O1D-CGD-CBD	2.01	128.59	124.48
17	J	102	CLA	C2D-C1D-ND	-2.01	108.63	110.10
17	A	826	CLA	CAC-C3C-C4C	2.01	127.41	124.81
25	5	615	ZEX	C17-C1-C6	-2.00	107.05	110.30
17	5	607	CLA	CHA-C1A-NA	-2.00	121.81	126.40
17	B	824	CLA	C2A-C1A-CHA	2.00	127.36	123.86
17	A	836	CLA	CHC-C1C-NC	2.00	127.24	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	606	CLA	C2A-C1A-CHA	2.00	127.36	123.86
17	5	607	CLA	C2A-C1A-CHA	2.00	127.36	123.86
17	A	810	CLA	C2A-C1A-CHA	2.00	127.36	123.86
20	L	201	BCR	C37-C22-C21	-2.00	120.12	122.92

All (160) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	NC
16	A	801	CL0	ND
16	A	801	CL0	NA
17	A	802	CLA	ND
17	A	803	CLA	ND
17	A	804	CLA	ND
17	A	805	CLA	ND
17	A	806	CLA	ND
17	A	807	CLA	ND
17	A	808	CLA	ND
17	A	809	CLA	ND
17	A	810	CLA	ND
17	A	811	CLA	ND
17	A	812	CLA	ND
17	A	813	CLA	ND
17	A	814	CLA	ND
17	A	815	CLA	ND
17	A	816	CLA	ND
17	A	817	CLA	ND
17	A	818	CLA	ND
17	A	819	CLA	ND
17	A	820	CLA	ND
17	A	821	CLA	ND
17	A	822	CLA	ND
17	A	823	CLA	ND
17	A	824	CLA	ND
17	A	825	CLA	ND
17	A	826	CLA	ND
17	A	827	CLA	ND
17	A	828	CLA	ND
17	A	829	CLA	ND
17	A	830	CLA	ND
17	A	831	CLA	ND
17	A	832	CLA	ND

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Mol	Chain	Res	Type	Atom
17	A	833	CLA	ND
17	A	834	CLA	ND
17	A	835	CLA	ND
17	A	836	CLA	ND
17	A	837	CLA	ND
17	A	838	CLA	ND
17	A	839	CLA	ND
17	A	848	CLA	ND
17	B	801	CLA	ND
17	B	802	CLA	ND
17	B	803	CLA	ND
17	B	804	CLA	ND
17	B	806	CLA	ND
17	B	807	CLA	ND
17	B	808	CLA	ND
17	B	809	CLA	ND
17	B	810	CLA	ND
17	B	811	CLA	ND
17	B	812	CLA	ND
17	B	813	CLA	ND
17	B	814	CLA	ND
17	B	815	CLA	ND
17	B	816	CLA	ND
17	B	817	CLA	ND
17	B	818	CLA	ND
17	B	819	CLA	ND
17	B	820	CLA	ND
17	B	821	CLA	ND
17	B	822	CLA	ND
17	B	823	CLA	ND
17	B	824	CLA	ND
17	B	825	CLA	ND
17	B	826	CLA	ND
17	B	827	CLA	ND
17	B	828	CLA	ND
17	B	829	CLA	ND
17	B	830	CLA	ND
17	B	831	CLA	ND
17	B	832	CLA	ND
17	B	833	CLA	ND
17	B	834	CLA	ND
17	B	835	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B	836	CLA	ND
17	B	837	CLA	ND
17	B	838	CLA	ND
17	B	839	CLA	ND
17	B	840	CLA	ND
17	B	841	CLA	ND
17	B	842	CLA	ND
17	B	843	CLA	ND
17	F	301	CLA	ND
17	F	302	CLA	ND
17	F	303	CLA	ND
17	J	101	CLA	ND
17	J	102	CLA	ND
17	J	103	CLA	ND
17	K	102	CLA	ND
17	K	103	CLA	ND
17	L	202	CLA	ND
17	L	203	CLA	ND
17	L	204	CLA	ND
17	O	201	CLA	ND
17	O	203	CLA	ND
17	O	204	CLA	ND
17	O	205	CLA	ND
17	1	601	CLA	ND
17	1	602	CLA	ND
17	1	603	CLA	ND
17	1	604	CLA	ND
17	1	605	CLA	ND
17	1	606	CLA	ND
17	1	607	CLA	ND
17	1	608	CLA	ND
17	1	609	CLA	ND
17	1	610	CLA	ND
17	1	611	CLA	ND
17	1	612	CLA	ND
17	2	601	CLA	ND
17	2	602	CLA	ND
17	2	603	CLA	ND
17	2	604	CLA	ND
17	2	605	CLA	ND
17	2	606	CLA	ND
17	2	607	CLA	ND

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Mol	Chain	Res	Type	Atom
17	2	608	CLA	ND
17	2	609	CLA	ND
17	2	610	CLA	ND
17	2	611	CLA	ND
17	2	612	CLA	ND
17	2	613	CLA	ND
17	3	202	CLA	ND
17	3	203	CLA	ND
17	3	204	CLA	ND
17	3	205	CLA	ND
17	3	206	CLA	ND
17	3	207	CLA	ND
17	3	208	CLA	ND
17	3	209	CLA	ND
17	3	210	CLA	ND
17	3	211	CLA	ND
17	3	212	CLA	ND
17	3	213	CLA	ND
17	4	601	CLA	ND
17	4	602	CLA	ND
17	4	603	CLA	ND
17	4	604	CLA	ND
17	4	605	CLA	ND
17	4	606	CLA	ND
17	4	607	CLA	ND
17	4	608	CLA	ND
17	4	609	CLA	ND
17	4	610	CLA	ND
17	4	611	CLA	ND
17	5	601	CLA	ND
17	5	602	CLA	ND
17	5	603	CLA	ND
17	5	604	CLA	ND
17	5	605	CLA	ND
17	5	606	CLA	ND
17	5	607	CLA	ND
17	5	608	CLA	ND
17	5	609	CLA	ND
17	5	610	CLA	ND
17	5	611	CLA	ND
17	5	612	CLA	ND
17	5	613	CLA	ND

All (2345) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	802	CLA	CHA-CBD-CGD-O1D
17	A	802	CLA	CHA-CBD-CGD-O2D
17	A	804	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	CHA-CBD-CGD-O1D
17	A	805	CLA	CAD-CBD-CGD-O1D
17	A	805	CLA	CBD-CGD-O2D-CED
17	A	806	CLA	C3A-C2A-CAA-CBA
17	A	806	CLA	CHA-CBD-CGD-O2D
17	A	807	CLA	CHA-CBD-CGD-O1D
17	A	807	CLA	CAD-CBD-CGD-O1D
17	A	807	CLA	CAD-CBD-CGD-O2D
17	A	807	CLA	CBD-CGD-O2D-CED
17	A	810	CLA	C1A-C2A-CAA-CBA
17	A	810	CLA	C3A-C2A-CAA-CBA
17	A	811	CLA	CBD-CGD-O2D-CED
17	A	813	CLA	CHA-CBD-CGD-O1D
17	A	813	CLA	CHA-CBD-CGD-O2D
17	A	813	CLA	CBD-CGD-O2D-CED
17	A	814	CLA	CHA-CBD-CGD-O1D
17	A	814	CLA	CHA-CBD-CGD-O2D
17	A	816	CLA	C3A-C2A-CAA-CBA
17	A	816	CLA	CHA-CBD-CGD-O1D
17	A	816	CLA	CHA-CBD-CGD-O2D
17	A	817	CLA	C1A-C2A-CAA-CBA
17	A	817	CLA	C3A-C2A-CAA-CBA
17	A	818	CLA	C1A-C2A-CAA-CBA
17	A	818	CLA	C3A-C2A-CAA-CBA
17	A	821	CLA	CHA-CBD-CGD-O1D
17	A	821	CLA	CHA-CBD-CGD-O2D
17	A	821	CLA	CBD-CGD-O2D-CED
17	A	822	CLA	CHA-CBD-CGD-O1D
17	A	822	CLA	CHA-CBD-CGD-O2D
17	A	825	CLA	CHA-CBD-CGD-O1D
17	A	825	CLA	CHA-CBD-CGD-O2D
17	A	826	CLA	C1A-C2A-CAA-CBA
17	A	826	CLA	CHA-CBD-CGD-O1D
17	A	826	CLA	CHA-CBD-CGD-O2D
17	A	826	CLA	CBD-CGD-O2D-CED
17	A	832	CLA	CHA-CBD-CGD-O2D
17	A	833	CLA	C4-C3-C5-C6
17	A	834	CLA	C1A-C2A-CAA-CBA
17	A	834	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	A	834	CLA	CHA-CBD-CGD-O2D
17	A	835	CLA	CHA-CBD-CGD-O1D
17	A	835	CLA	CHA-CBD-CGD-O2D
17	A	835	CLA	CAD-CBD-CGD-O1D
17	A	835	CLA	C2-C3-C5-C6
17	A	836	CLA	CHA-CBD-CGD-O1D
17	A	836	CLA	CHA-CBD-CGD-O2D
17	A	836	CLA	C2-C3-C5-C6
17	A	836	CLA	C4-C3-C5-C6
17	A	848	CLA	CBD-CGD-O2D-CED
17	B	801	CLA	CHA-CBD-CGD-O1D
17	B	801	CLA	CHA-CBD-CGD-O2D
17	B	802	CLA	CBD-CGD-O2D-CED
17	B	803	CLA	CHA-CBD-CGD-O1D
17	B	803	CLA	CHA-CBD-CGD-O2D
17	B	804	CLA	CHA-CBD-CGD-O1D
17	B	804	CLA	CHA-CBD-CGD-O2D
17	B	804	CLA	CBD-CGD-O2D-CED
17	B	807	CLA	CHA-CBD-CGD-O1D
17	B	807	CLA	CHA-CBD-CGD-O2D
17	B	808	CLA	C3A-C2A-CAA-CBA
17	B	808	CLA	CHA-CBD-CGD-O1D
17	B	808	CLA	CHA-CBD-CGD-O2D
17	B	809	CLA	CBD-CGD-O2D-CED
17	B	810	CLA	CHA-CBD-CGD-O1D
17	B	810	CLA	CHA-CBD-CGD-O2D
17	B	812	CLA	C1A-C2A-CAA-CBA
17	B	812	CLA	C3A-C2A-CAA-CBA
17	B	814	CLA	CHA-CBD-CGD-O2D
17	B	815	CLA	C1A-C2A-CAA-CBA
17	B	815	CLA	C3A-C2A-CAA-CBA
17	B	815	CLA	CBD-CGD-O2D-CED
17	B	815	CLA	O1D-CGD-O2D-CED
17	B	816	CLA	C1A-C2A-CAA-CBA
17	B	816	CLA	C3A-C2A-CAA-CBA
17	B	816	CLA	CBD-CGD-O2D-CED
17	B	817	CLA	CBD-CGD-O2D-CED
17	B	819	CLA	CBD-CGD-O2D-CED
17	B	820	CLA	C1A-C2A-CAA-CBA
17	B	820	CLA	C3A-C2A-CAA-CBA
17	B	821	CLA	C1A-C2A-CAA-CBA
17	B	821	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	B	822	CLA	CHA-CBD-CGD-O1D
17	B	822	CLA	CHA-CBD-CGD-O2D
17	B	824	CLA	CBA-CGA-O2A-C1
17	B	824	CLA	CBD-CGD-O2D-CED
17	B	825	CLA	CHA-CBD-CGD-O1D
17	B	825	CLA	CHA-CBD-CGD-O2D
17	B	825	CLA	CBD-CGD-O2D-CED
17	B	829	CLA	CHA-CBD-CGD-O1D
17	B	829	CLA	CHA-CBD-CGD-O2D
17	B	829	CLA	C6-C7-C8-C9
17	B	830	CLA	CHA-CBD-CGD-O1D
17	B	830	CLA	CHA-CBD-CGD-O2D
17	B	830	CLA	C11-C10-C8-C9
17	B	831	CLA	C1A-C2A-CAA-CBA
17	B	831	CLA	CBD-CGD-O2D-CED
17	B	832	CLA	CBD-CGD-O2D-CED
17	B	835	CLA	CHA-CBD-CGD-O1D
17	B	835	CLA	CHA-CBD-CGD-O2D
17	B	836	CLA	CBD-CGD-O2D-CED
17	B	836	CLA	O1D-CGD-O2D-CED
17	B	837	CLA	C1A-C2A-CAA-CBA
17	B	837	CLA	C3A-C2A-CAA-CBA
17	B	837	CLA	CBD-CGD-O2D-CED
17	B	838	CLA	CHA-CBD-CGD-O1D
17	B	838	CLA	CHA-CBD-CGD-O2D
17	B	838	CLA	CAD-CBD-CGD-O1D
17	B	842	CLA	CHA-CBD-CGD-O1D
17	B	842	CLA	CAD-CBD-CGD-O1D
17	B	842	CLA	CAD-CBD-CGD-O2D
17	B	842	CLA	CBD-CGD-O2D-CED
17	B	842	CLA	C2-C3-C5-C6
17	B	842	CLA	C4-C3-C5-C6
17	F	301	CLA	CBD-CGD-O2D-CED
17	J	101	CLA	CHA-CBD-CGD-O1D
17	J	101	CLA	CHA-CBD-CGD-O2D
17	J	101	CLA	CAD-CBD-CGD-O1D
17	J	101	CLA	CAD-CBD-CGD-O2D
17	J	103	CLA	CHA-CBD-CGD-O1D
17	J	103	CLA	CHA-CBD-CGD-O2D
17	J	103	CLA	CAD-CBD-CGD-O1D
17	J	103	CLA	CBD-CGD-O2D-CED
17	K	103	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	K	103	CLA	CHA-CBD-CGD-O2D
17	L	202	CLA	C1A-C2A-CAA-CBA
17	L	202	CLA	CBD-CGD-O2D-CED
17	L	203	CLA	CHA-CBD-CGD-O1D
17	L	204	CLA	CBD-CGD-O2D-CED
17	O	201	CLA	CBD-CGD-O2D-CED
17	O	205	CLA	C3A-C2A-CAA-CBA
17	1	601	CLA	C1A-C2A-CAA-CBA
17	1	601	CLA	CBD-CGD-O2D-CED
17	1	604	CLA	C1A-C2A-CAA-CBA
17	1	604	CLA	CBD-CGD-O2D-CED
17	1	606	CLA	CBD-CGD-O2D-CED
17	1	611	CLA	C1A-C2A-CAA-CBA
17	1	611	CLA	C3A-C2A-CAA-CBA
17	1	611	CLA	C2C-C3C-CAC-CBC
17	1	611	CLA	C4C-C3C-CAC-CBC
17	2	604	CLA	C1A-C2A-CAA-CBA
17	2	605	CLA	CBD-CGD-O2D-CED
17	2	607	CLA	CBD-CGD-O2D-CED
17	2	607	CLA	O1D-CGD-O2D-CED
17	2	610	CLA	CHA-CBD-CGD-O1D
17	2	610	CLA	CHA-CBD-CGD-O2D
17	2	610	CLA	CBD-CGD-O2D-CED
17	2	612	CLA	CBD-CGD-O2D-CED
17	2	613	CLA	CBD-CGD-O2D-CED
17	3	202	CLA	CHA-CBD-CGD-O1D
17	3	202	CLA	CHA-CBD-CGD-O2D
17	3	202	CLA	CBD-CGD-O2D-CED
17	3	202	CLA	O1D-CGD-O2D-CED
17	3	203	CLA	CBD-CGD-O2D-CED
17	3	204	CLA	CHA-CBD-CGD-O1D
17	3	204	CLA	CHA-CBD-CGD-O2D
17	3	204	CLA	CAD-CBD-CGD-O1D
17	3	204	CLA	CAD-CBD-CGD-O2D
17	3	205	CLA	CHA-CBD-CGD-O1D
17	3	205	CLA	CHA-CBD-CGD-O2D
17	3	207	CLA	CBD-CGD-O2D-CED
17	3	208	CLA	C3A-C2A-CAA-CBA
17	3	209	CLA	CBD-CGD-O2D-CED
17	3	210	CLA	CHA-CBD-CGD-O1D
17	3	210	CLA	CHA-CBD-CGD-O2D
17	3	212	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	3	212	CLA	C3A-C2A-CAA-CBA
17	3	212	CLA	CBA-CGA-O2A-C1
17	3	212	CLA	CHA-CBD-CGD-O1D
17	3	212	CLA	CHA-CBD-CGD-O2D
17	3	212	CLA	CBD-CGD-O2D-CED
17	3	212	CLA	O1D-CGD-O2D-CED
17	4	602	CLA	C1A-C2A-CAA-CBA
17	4	602	CLA	CBD-CGD-O2D-CED
17	4	603	CLA	CBD-CGD-O2D-CED
17	4	604	CLA	C1A-C2A-CAA-CBA
17	4	604	CLA	C3A-C2A-CAA-CBA
17	4	605	CLA	C3A-C2A-CAA-CBA
17	4	606	CLA	CBD-CGD-O2D-CED
17	4	606	CLA	O1D-CGD-O2D-CED
17	4	607	CLA	C3A-C2A-CAA-CBA
17	4	607	CLA	CHA-CBD-CGD-O1D
17	4	607	CLA	CHA-CBD-CGD-O2D
17	4	611	CLA	C1A-C2A-CAA-CBA
17	4	611	CLA	C3A-C2A-CAA-CBA
17	4	611	CLA	CBD-CGD-O2D-CED
17	4	611	CLA	O1D-CGD-O2D-CED
17	5	601	CLA	CBD-CGD-O2D-CED
17	5	602	CLA	C1A-C2A-CAA-CBA
17	5	603	CLA	C4-C3-C5-C6
17	5	604	CLA	CBD-CGD-O2D-CED
17	5	605	CLA	C1A-C2A-CAA-CBA
17	5	605	CLA	C3A-C2A-CAA-CBA
17	5	607	CLA	CBD-CGD-O2D-CED
17	5	609	CLA	CBD-CGD-O2D-CED
17	5	610	CLA	C3A-C2A-CAA-CBA
17	5	610	CLA	CBD-CGD-O2D-CED
17	5	611	CLA	CHA-CBD-CGD-O1D
17	5	611	CLA	CHA-CBD-CGD-O2D
17	5	611	CLA	CBD-CGD-O2D-CED
17	5	611	CLA	O1D-CGD-O2D-CED
19	A	841	LHG	C3-O3-P-O6
19	A	842	LHG	O1-C1-C2-O2
19	A	842	LHG	O2-C2-C3-O3
20	A	843	BCR	C6-C7-C8-C9
20	A	843	BCR	C10-C11-C12-C13
20	A	843	BCR	C14-C15-C16-C17
20	A	843	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	A	844	BCR	C6-C7-C8-C9
20	A	844	BCR	C7-C8-C9-C34
20	A	844	BCR	C18-C19-C20-C21
20	A	844	BCR	C20-C21-C22-C23
20	A	844	BCR	C20-C21-C22-C37
20	A	844	BCR	C21-C22-C23-C24
20	A	845	BCR	C20-C21-C22-C37
20	A	845	BCR	C37-C22-C23-C24
20	A	845	BCR	C22-C23-C24-C25
20	A	846	BCR	C1-C6-C7-C8
20	A	846	BCR	C7-C8-C9-C10
20	A	846	BCR	C7-C8-C9-C34
20	A	846	BCR	C11-C10-C9-C8
20	A	846	BCR	C11-C10-C9-C34
20	A	846	BCR	C10-C11-C12-C13
20	A	846	BCR	C18-C19-C20-C21
20	A	846	BCR	C20-C21-C22-C23
20	A	846	BCR	C20-C21-C22-C37
20	A	846	BCR	C37-C22-C23-C24
20	A	846	BCR	C22-C23-C24-C25
20	B	805	BCR	C11-C12-C13-C35
20	B	805	BCR	C20-C21-C22-C37
20	B	805	BCR	C21-C22-C23-C24
20	B	805	BCR	C23-C24-C25-C30
20	B	845	BCR	C6-C7-C8-C9
20	B	845	BCR	C7-C8-C9-C10
20	B	845	BCR	C10-C11-C12-C13
20	B	845	BCR	C22-C23-C24-C25
20	B	846	BCR	C6-C7-C8-C9
20	B	846	BCR	C37-C22-C23-C24
20	B	847	BCR	C6-C7-C8-C9
20	B	847	BCR	C11-C10-C9-C8
20	B	847	BCR	C11-C10-C9-C34
20	B	847	BCR	C11-C12-C13-C14
20	B	847	BCR	C11-C12-C13-C35
20	B	847	BCR	C37-C22-C23-C24
20	B	847	BCR	C22-C23-C24-C25
20	B	848	BCR	C6-C7-C8-C9
20	B	848	BCR	C7-C8-C9-C34
20	B	848	BCR	C37-C22-C23-C24
20	B	849	BCR	C1-C6-C7-C8
20	B	849	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	849	BCR	C10-C11-C12-C13
20	B	849	BCR	C11-C12-C13-C14
20	B	849	BCR	C11-C12-C13-C35
20	B	849	BCR	C16-C17-C18-C19
20	B	849	BCR	C16-C17-C18-C36
20	B	849	BCR	C18-C19-C20-C21
20	B	849	BCR	C22-C23-C24-C25
20	B	849	BCR	C23-C24-C25-C26
20	B	849	BCR	C23-C24-C25-C30
20	B	850	BCR	C13-C14-C15-C16
20	B	850	BCR	C37-C22-C23-C24
20	F	304	BCR	C6-C7-C8-C9
20	F	304	BCR	C11-C12-C13-C14
20	F	304	BCR	C14-C15-C16-C17
20	F	304	BCR	C18-C19-C20-C21
20	F	304	BCR	C37-C22-C23-C24
20	F	304	BCR	C22-C23-C24-C25
20	I	101	BCR	C7-C8-C9-C34
20	I	101	BCR	C9-C10-C11-C12
20	I	101	BCR	C11-C12-C13-C14
20	I	101	BCR	C11-C12-C13-C35
20	I	101	BCR	C16-C17-C18-C36
20	I	101	BCR	C20-C21-C22-C23
20	I	101	BCR	C37-C22-C23-C24
20	I	101	BCR	C22-C23-C24-C25
20	J	104	BCR	C1-C6-C7-C8
20	J	104	BCR	C7-C8-C9-C10
20	J	104	BCR	C7-C8-C9-C34
20	J	104	BCR	C20-C21-C22-C23
20	J	104	BCR	C21-C22-C23-C24
20	J	104	BCR	C22-C23-C24-C25
20	J	104	BCR	C23-C24-C25-C30
20	J	105	BCR	C1-C6-C7-C8
20	J	105	BCR	C6-C7-C8-C9
20	J	105	BCR	C7-C8-C9-C34
20	J	105	BCR	C14-C15-C16-C17
20	J	105	BCR	C16-C17-C18-C19
20	J	105	BCR	C21-C22-C23-C24
20	J	105	BCR	C37-C22-C23-C24
20	J	105	BCR	C22-C23-C24-C25
20	K	101	BCR	C1-C6-C7-C8
20	K	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	K	101	BCR	C7-C8-C9-C34
20	K	101	BCR	C22-C23-C24-C25
20	K	104	BCR	C6-C7-C8-C9
20	K	104	BCR	C7-C8-C9-C34
20	K	104	BCR	C16-C17-C18-C19
20	K	104	BCR	C16-C17-C18-C36
20	K	104	BCR	C18-C19-C20-C21
20	K	104	BCR	C19-C20-C21-C22
20	K	104	BCR	C22-C23-C24-C25
20	L	201	BCR	C6-C7-C8-C9
20	L	201	BCR	C14-C15-C16-C17
20	L	201	BCR	C15-C16-C17-C18
20	L	201	BCR	C36-C18-C19-C20
20	L	201	BCR	C22-C23-C24-C25
20	L	205	BCR	C1-C6-C7-C8
20	L	205	BCR	C7-C8-C9-C10
20	L	205	BCR	C7-C8-C9-C34
20	L	205	BCR	C21-C22-C23-C24
20	L	205	BCR	C23-C24-C25-C26
20	L	205	BCR	C23-C24-C25-C30
20	L	206	BCR	C11-C12-C13-C14
20	L	206	BCR	C20-C21-C22-C37
20	L	206	BCR	C22-C23-C24-C25
20	O	202	BCR	C1-C6-C7-C8
20	O	202	BCR	C7-C8-C9-C10
20	O	202	BCR	C20-C21-C22-C37
20	O	202	BCR	C21-C22-C23-C24
20	O	202	BCR	C22-C23-C24-C25
20	O	202	BCR	C23-C24-C25-C30
23	B	851	DGD	C2B-C1B-O2G-C2G
23	B	851	DGD	O1B-C1B-O2G-C2G
24	J	106	3XQ	O20-C21-C22-O23
25	1	613	ZEX	C5-C6-C7-C8
25	1	613	ZEX	C25-C26-C27-C28
25	1	613	ZEX	C7-C8-C9-C19
25	1	613	ZEX	C7-C8-C9-C10
25	1	613	ZEX	C11-C10-C9-C8
25	1	613	ZEX	C11-C12-C13-C14
25	1	613	ZEX	C20-C13-C14-C15
25	1	613	ZEX	C40-C33-C34-C35
25	1	613	ZEX	C31-C32-C33-C40
25	1	613	ZEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
25	1	613	ZEX	C27-C28-C29-C30
25	1	613	ZEX	C27-C28-C29-C39
25	1	614	ZEX	C5-C6-C7-C8
25	1	614	ZEX	C25-C26-C27-C28
25	1	614	ZEX	C11-C10-C9-C19
25	1	614	ZEX	C11-C12-C13-C14
25	1	614	ZEX	C12-C13-C14-C15
25	1	614	ZEX	C40-C33-C34-C35
25	1	614	ZEX	C31-C32-C33-C40
25	1	614	ZEX	C39-C29-C30-C31
25	1	614	ZEX	C27-C28-C29-C30
25	1	614	ZEX	C27-C28-C29-C39
25	1	615	ZEX	C21-C26-C27-C28
25	1	615	ZEX	C25-C26-C27-C28
25	1	615	ZEX	C11-C10-C9-C19
25	1	615	ZEX	C11-C12-C13-C20
25	1	615	ZEX	C20-C13-C14-C15
25	1	615	ZEX	C40-C33-C34-C35
25	1	615	ZEX	C31-C32-C33-C40
25	1	615	ZEX	C29-C30-C31-C32
25	1	615	ZEX	C39-C29-C30-C31
25	1	615	ZEX	C27-C28-C29-C30
25	1	616	ZEX	C25-C26-C27-C28
25	1	616	ZEX	C11-C10-C9-C19
25	1	616	ZEX	C11-C12-C13-C20
25	1	616	ZEX	C20-C13-C14-C15
25	1	616	ZEX	C40-C33-C34-C35
25	1	616	ZEX	C32-C33-C34-C35
25	1	616	ZEX	C31-C32-C33-C40
25	1	616	ZEX	C29-C30-C31-C32
25	1	616	ZEX	C39-C29-C30-C31
25	1	616	ZEX	C27-C28-C29-C30
25	1	616	ZEX	C27-C28-C29-C39
25	1	617	ZEX	C5-C6-C7-C8
25	1	617	ZEX	C25-C26-C27-C28
25	1	617	ZEX	C7-C8-C9-C10
25	1	617	ZEX	C11-C10-C9-C19
25	1	617	ZEX	C9-C10-C11-C12
25	1	617	ZEX	C11-C12-C13-C20
25	1	617	ZEX	C11-C12-C13-C14
25	1	617	ZEX	C20-C13-C14-C15
25	1	617	ZEX	C33-C34-C35-C15

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Mol	Chain	Res	Type	Atoms
25	1	617	ZEX	C32-C33-C34-C35
25	1	617	ZEX	C39-C29-C30-C31
25	2	614	ZEX	C25-C26-C27-C28
25	2	614	ZEX	C11-C10-C9-C19
25	2	614	ZEX	C11-C12-C13-C20
25	2	614	ZEX	C11-C12-C13-C14
25	2	614	ZEX	C20-C13-C14-C15
25	2	614	ZEX	C33-C34-C35-C15
25	2	614	ZEX	C40-C33-C34-C35
25	2	614	ZEX	C31-C32-C33-C34
25	2	614	ZEX	C39-C29-C30-C31
25	2	615	ZEX	C5-C6-C7-C8
25	2	615	ZEX	C11-C10-C9-C19
25	2	615	ZEX	C11-C12-C13-C20
25	2	615	ZEX	C11-C12-C13-C14
25	2	615	ZEX	C20-C13-C14-C15
25	2	615	ZEX	C13-C14-C15-C35
25	2	615	ZEX	C40-C33-C34-C35
25	2	615	ZEX	C39-C29-C30-C31
25	2	615	ZEX	C27-C28-C29-C30
25	2	615	ZEX	C27-C28-C29-C39
25	2	616	ZEX	C25-C26-C27-C28
25	2	616	ZEX	C7-C8-C9-C19
25	2	616	ZEX	C11-C10-C9-C19
25	2	616	ZEX	C11-C12-C13-C20
25	2	616	ZEX	C11-C12-C13-C14
25	2	616	ZEX	C12-C13-C14-C15
25	2	616	ZEX	C40-C33-C34-C35
25	2	616	ZEX	C39-C29-C30-C31
25	2	617	ZEX	C25-C26-C27-C28
25	2	617	ZEX	C7-C8-C9-C19
25	2	617	ZEX	C7-C8-C9-C10
25	2	617	ZEX	C11-C10-C9-C19
25	2	617	ZEX	C11-C12-C13-C20
25	2	617	ZEX	C20-C13-C14-C15
25	2	617	ZEX	C33-C34-C35-C15
25	2	617	ZEX	C40-C33-C34-C35
25	2	617	ZEX	C39-C29-C30-C31
25	2	617	ZEX	C27-C28-C29-C30
25	2	617	ZEX	C27-C28-C29-C39
25	3	201	ZEX	C21-C26-C27-C28
25	3	201	ZEX	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	3	201	ZEX	C11-C10-C9-C8
25	3	201	ZEX	C9-C10-C11-C12
25	3	201	ZEX	C11-C12-C13-C20
25	3	201	ZEX	C20-C13-C14-C15
25	3	201	ZEX	C13-C14-C15-C35
25	3	201	ZEX	C40-C33-C34-C35
25	3	201	ZEX	C39-C29-C30-C31
25	3	201	ZEX	C27-C28-C29-C39
25	3	214	ZEX	C25-C26-C27-C28
25	3	214	ZEX	C11-C10-C9-C19
25	3	214	ZEX	C11-C12-C13-C20
25	3	214	ZEX	C20-C13-C14-C15
25	3	214	ZEX	C40-C33-C34-C35
25	3	214	ZEX	C39-C29-C30-C31
25	3	215	ZEX	C5-C6-C7-C8
25	3	215	ZEX	C25-C26-C27-C28
25	3	215	ZEX	C11-C10-C9-C19
25	3	215	ZEX	C20-C13-C14-C15
25	3	215	ZEX	C40-C33-C34-C35
25	3	215	ZEX	C31-C32-C33-C40
25	3	215	ZEX	C29-C30-C31-C32
25	3	215	ZEX	C39-C29-C30-C31
25	3	215	ZEX	C27-C28-C29-C39
25	3	216	ZEX	C21-C26-C27-C28
25	3	216	ZEX	C25-C26-C27-C28
25	3	216	ZEX	C7-C8-C9-C19
25	3	216	ZEX	C7-C8-C9-C10
25	3	216	ZEX	C11-C10-C9-C19
25	3	216	ZEX	C20-C13-C14-C15
25	3	216	ZEX	C40-C33-C34-C35
25	3	216	ZEX	C39-C29-C30-C31
25	3	216	ZEX	C27-C28-C29-C30
25	3	216	ZEX	C27-C28-C29-C39
25	3	217	ZEX	C25-C26-C27-C28
25	3	217	ZEX	C7-C8-C9-C10
25	3	217	ZEX	C11-C10-C9-C19
25	3	217	ZEX	C11-C12-C13-C20
25	3	217	ZEX	C20-C13-C14-C15
25	3	217	ZEX	C13-C14-C15-C35
25	3	217	ZEX	C40-C33-C34-C35
25	3	217	ZEX	C32-C33-C34-C35
25	3	217	ZEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
25	3	217	ZEX	C27-C28-C29-C30
25	3	217	ZEX	C27-C28-C29-C39
25	3	218	ZEX	C7-C8-C9-C19
25	3	218	ZEX	C7-C8-C9-C10
25	3	218	ZEX	C11-C10-C9-C8
25	3	218	ZEX	C11-C12-C13-C20
25	3	218	ZEX	C32-C33-C34-C35
25	3	218	ZEX	C39-C29-C30-C31
25	3	218	ZEX	C28-C29-C30-C31
25	4	612	ZEX	C5-C6-C7-C8
25	4	612	ZEX	C11-C10-C9-C8
25	4	612	ZEX	C9-C10-C11-C12
25	4	612	ZEX	C12-C13-C14-C15
25	4	612	ZEX	C20-C13-C14-C15
25	4	612	ZEX	C40-C33-C34-C35
25	4	612	ZEX	C29-C30-C31-C32
25	4	612	ZEX	C39-C29-C30-C31
25	4	612	ZEX	C28-C29-C30-C31
25	4	612	ZEX	C27-C28-C29-C39
25	4	613	ZEX	C5-C6-C7-C8
25	4	613	ZEX	C11-C10-C9-C19
25	4	613	ZEX	C20-C13-C14-C15
25	4	613	ZEX	C40-C33-C34-C35
25	4	613	ZEX	C31-C32-C33-C40
25	4	613	ZEX	C39-C29-C30-C31
25	4	613	ZEX	C28-C29-C30-C31
25	4	614	ZEX	C5-C6-C7-C8
25	4	614	ZEX	C21-C26-C27-C28
25	4	614	ZEX	C25-C26-C27-C28
25	4	614	ZEX	C7-C8-C9-C10
25	4	614	ZEX	C11-C10-C9-C19
25	4	614	ZEX	C20-C13-C14-C15
25	4	614	ZEX	C13-C14-C15-C35
25	4	614	ZEX	C40-C33-C34-C35
25	4	614	ZEX	C31-C32-C33-C34
25	4	614	ZEX	C31-C32-C33-C40
25	4	614	ZEX	C28-C29-C30-C31
25	4	615	ZEX	C25-C26-C27-C28
25	4	615	ZEX	C11-C10-C9-C19
25	4	615	ZEX	C11-C12-C13-C14
25	4	615	ZEX	C20-C13-C14-C15
25	4	615	ZEX	C33-C34-C35-C15

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Mol	Chain	Res	Type	Atoms
25	4	615	ZEX	C40-C33-C34-C35
25	4	615	ZEX	C31-C32-C33-C34
25	4	615	ZEX	C31-C32-C33-C40
25	4	615	ZEX	C28-C29-C30-C31
25	4	616	ZEX	C25-C26-C27-C28
25	4	616	ZEX	C7-C8-C9-C19
25	4	616	ZEX	C7-C8-C9-C10
25	4	616	ZEX	C11-C10-C9-C19
25	4	616	ZEX	C11-C12-C13-C20
25	4	616	ZEX	C20-C13-C14-C15
25	4	616	ZEX	C13-C14-C15-C35
25	4	616	ZEX	C40-C33-C34-C35
25	4	616	ZEX	C39-C29-C30-C31
25	4	617	ZEX	C1-C6-C7-C8
25	4	617	ZEX	C25-C26-C27-C28
25	4	617	ZEX	C11-C10-C9-C19
25	4	617	ZEX	C11-C12-C13-C20
25	4	617	ZEX	C12-C13-C14-C15
25	4	617	ZEX	C20-C13-C14-C15
25	4	617	ZEX	C33-C34-C35-C15
25	4	617	ZEX	C40-C33-C34-C35
25	4	617	ZEX	C32-C33-C34-C35
25	4	617	ZEX	C31-C32-C33-C40
25	4	617	ZEX	C28-C29-C30-C31
25	5	614	ZEX	C5-C6-C7-C8
25	5	614	ZEX	C11-C10-C9-C19
25	5	614	ZEX	C20-C13-C14-C15
25	5	614	ZEX	C40-C33-C34-C35
25	5	614	ZEX	C29-C30-C31-C32
25	5	614	ZEX	C39-C29-C30-C31
25	5	614	ZEX	C27-C28-C29-C30
25	5	614	ZEX	C27-C28-C29-C39
25	5	615	ZEX	C5-C6-C7-C8
25	5	615	ZEX	C25-C26-C27-C28
25	5	615	ZEX	C11-C10-C9-C8
25	5	615	ZEX	C11-C12-C13-C20
25	5	615	ZEX	C20-C13-C14-C15
25	5	615	ZEX	C40-C33-C34-C35
25	5	615	ZEX	C39-C29-C30-C31
25	5	616	ZEX	C25-C26-C27-C28
25	5	616	ZEX	C11-C10-C9-C19
25	5	616	ZEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	5	616	ZEX	C20-C13-C14-C15
25	5	616	ZEX	C40-C33-C34-C35
25	5	616	ZEX	C32-C33-C34-C35
25	5	616	ZEX	C31-C32-C33-C40
25	5	616	ZEX	C39-C29-C30-C31
25	5	616	ZEX	C27-C28-C29-C39
25	5	617	ZEX	C5-C6-C7-C8
25	5	617	ZEX	C25-C26-C27-C28
25	5	617	ZEX	C7-C8-C9-C10
25	5	617	ZEX	C11-C10-C9-C19
25	5	617	ZEX	C20-C13-C14-C15
25	5	617	ZEX	C40-C33-C34-C35
25	5	617	ZEX	C32-C33-C34-C35
25	5	617	ZEX	C39-C29-C30-C31
25	5	617	ZEX	C28-C29-C30-C31
17	A	813	CLA	O1D-CGD-O2D-CED
17	A	830	CLA	O1D-CGD-O2D-CED
17	B	802	CLA	O1D-CGD-O2D-CED
17	B	806	CLA	O1D-CGD-O2D-CED
17	B	809	CLA	O1D-CGD-O2D-CED
17	B	823	CLA	O1D-CGD-O2D-CED
17	B	824	CLA	O1D-CGD-O2D-CED
17	B	825	CLA	O1D-CGD-O2D-CED
17	F	301	CLA	O1D-CGD-O2D-CED
17	F	303	CLA	O1D-CGD-O2D-CED
17	L	204	CLA	O1D-CGD-O2D-CED
17	1	606	CLA	O1D-CGD-O2D-CED
17	1	610	CLA	O1D-CGD-O2D-CED
17	1	611	CLA	O1D-CGD-O2D-CED
17	2	610	CLA	O1D-CGD-O2D-CED
17	3	203	CLA	O1D-CGD-O2D-CED
17	3	207	CLA	O1D-CGD-O2D-CED
17	4	608	CLA	O1D-CGD-O2D-CED
17	5	609	CLA	O1D-CGD-O2D-CED
17	A	821	CLA	O1D-CGD-O2D-CED
17	A	827	CLA	O1D-CGD-O2D-CED
17	B	819	CLA	O1D-CGD-O2D-CED
17	B	837	CLA	O1D-CGD-O2D-CED
17	2	605	CLA	O1D-CGD-O2D-CED
17	2	611	CLA	O1D-CGD-O2D-CED
17	2	613	CLA	O1D-CGD-O2D-CED
17	3	209	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	5	610	CLA	O1D-CGD-O2D-CED
17	A	808	CLA	CBD-CGD-O2D-CED
17	A	816	CLA	CBD-CGD-O2D-CED
17	A	819	CLA	CBD-CGD-O2D-CED
17	A	827	CLA	CBD-CGD-O2D-CED
17	A	830	CLA	CBD-CGD-O2D-CED
17	A	831	CLA	CBD-CGD-O2D-CED
17	B	806	CLA	CBD-CGD-O2D-CED
17	B	808	CLA	CBD-CGD-O2D-CED
17	B	812	CLA	CBD-CGD-O2D-CED
17	B	818	CLA	CBD-CGD-O2D-CED
17	B	821	CLA	CBD-CGD-O2D-CED
17	B	823	CLA	CBD-CGD-O2D-CED
17	B	826	CLA	CBD-CGD-O2D-CED
17	B	839	CLA	CBD-CGD-O2D-CED
17	B	840	CLA	CBD-CGD-O2D-CED
17	B	843	CLA	CBD-CGD-O2D-CED
17	F	303	CLA	CBD-CGD-O2D-CED
17	J	102	CLA	CBD-CGD-O2D-CED
17	O	203	CLA	CBD-CGD-O2D-CED
17	O	204	CLA	CBD-CGD-O2D-CED
17	O	205	CLA	CBD-CGD-O2D-CED
17	1	602	CLA	CBD-CGD-O2D-CED
17	1	603	CLA	CBD-CGD-O2D-CED
17	1	608	CLA	CBD-CGD-O2D-CED
17	1	610	CLA	CBD-CGD-O2D-CED
17	1	611	CLA	CBD-CGD-O2D-CED
17	1	612	CLA	CBD-CGD-O2D-CED
17	2	602	CLA	CBD-CGD-O2D-CED
17	2	611	CLA	CBD-CGD-O2D-CED
17	3	208	CLA	CBD-CGD-O2D-CED
17	3	213	CLA	CBD-CGD-O2D-CED
17	4	604	CLA	CBD-CGD-O2D-CED
17	4	607	CLA	CBD-CGD-O2D-CED
17	4	608	CLA	CBD-CGD-O2D-CED
17	5	602	CLA	CBD-CGD-O2D-CED
17	5	603	CLA	CBD-CGD-O2D-CED
17	5	605	CLA	CBD-CGD-O2D-CED
17	5	612	CLA	CBD-CGD-O2D-CED
17	A	835	CLA	O1A-CGA-O2A-C1
17	3	212	CLA	O1A-CGA-O2A-C1
17	5	609	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
17	A	808	CLA	O1D-CGD-O2D-CED
17	A	819	CLA	O1D-CGD-O2D-CED
17	A	848	CLA	O1D-CGD-O2D-CED
17	B	808	CLA	O1D-CGD-O2D-CED
17	B	812	CLA	O1D-CGD-O2D-CED
17	B	840	CLA	O1D-CGD-O2D-CED
17	O	203	CLA	O1D-CGD-O2D-CED
17	1	608	CLA	O1D-CGD-O2D-CED
17	3	208	CLA	O1D-CGD-O2D-CED
17	5	602	CLA	O1D-CGD-O2D-CED
17	5	603	CLA	O1D-CGD-O2D-CED
17	5	609	CLA	C2C-C3C-CAC-CBC
17	A	805	CLA	O1D-CGD-O2D-CED
17	A	807	CLA	O1D-CGD-O2D-CED
17	A	811	CLA	O1D-CGD-O2D-CED
17	A	826	CLA	O1D-CGD-O2D-CED
17	B	804	CLA	O1D-CGD-O2D-CED
17	B	816	CLA	O1D-CGD-O2D-CED
17	B	817	CLA	O1D-CGD-O2D-CED
17	B	826	CLA	O1D-CGD-O2D-CED
17	B	831	CLA	O1D-CGD-O2D-CED
17	J	103	CLA	O1D-CGD-O2D-CED
17	O	201	CLA	O1D-CGD-O2D-CED
17	1	604	CLA	O1D-CGD-O2D-CED
17	2	612	CLA	O1D-CGD-O2D-CED
17	4	602	CLA	O1D-CGD-O2D-CED
17	4	603	CLA	O1D-CGD-O2D-CED
17	5	601	CLA	O1D-CGD-O2D-CED
17	5	604	CLA	O1D-CGD-O2D-CED
17	5	607	CLA	O1D-CGD-O2D-CED
17	A	803	CLA	CBD-CGD-O2D-CED
17	A	812	CLA	CBD-CGD-O2D-CED
17	A	823	CLA	CBD-CGD-O2D-CED
17	A	832	CLA	CBD-CGD-O2D-CED
17	B	841	CLA	CBD-CGD-O2D-CED
17	2	601	CLA	CBD-CGD-O2D-CED
17	2	606	CLA	CBD-CGD-O2D-CED
17	2	609	CLA	CBD-CGD-O2D-CED
17	3	206	CLA	CBD-CGD-O2D-CED
17	3	210	CLA	CBD-CGD-O2D-CED
17	5	608	CLA	CBD-CGD-O2D-CED
17	A	802	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	A	807	CLA	O1A-CGA-O2A-C1
17	A	815	CLA	O1A-CGA-O2A-C1
17	A	838	CLA	O1A-CGA-O2A-C1
17	B	814	CLA	O1A-CGA-O2A-C1
17	B	821	CLA	O1A-CGA-O2A-C1
17	L	202	CLA	O1A-CGA-O2A-C1
17	5	603	CLA	O1A-CGA-O2A-C1
24	J	106	3XQ	O19-C1-O20-C21
17	B	832	CLA	O1D-CGD-O2D-CED
17	L	202	CLA	O1D-CGD-O2D-CED
17	1	601	CLA	O1D-CGD-O2D-CED
17	B	842	CLA	O1D-CGD-O2D-CED
17	A	814	CLA	CBD-CGD-O2D-CED
17	2	608	CLA	CBD-CGD-O2D-CED
17	5	605	CLA	O1D-CGD-O2D-CED
17	B	841	CLA	O1A-CGA-O2A-C1
16	A	801	CL0	C3-C5-C6-C7
17	A	815	CLA	C3-C5-C6-C7
17	A	822	CLA	C3-C5-C6-C7
17	A	825	CLA	C3-C5-C6-C7
17	A	832	CLA	C3-C5-C6-C7
17	A	839	CLA	C3-C5-C6-C7
17	B	811	CLA	C3-C5-C6-C7
17	B	819	CLA	C3-C5-C6-C7
17	B	821	CLA	C3-C5-C6-C7
17	B	832	CLA	C3-C5-C6-C7
17	J	102	CLA	C3-C5-C6-C7
17	A	802	CLA	CBA-CGA-O2A-C1
17	A	806	CLA	CBA-CGA-O2A-C1
17	A	815	CLA	CBA-CGA-O2A-C1
17	A	829	CLA	CBA-CGA-O2A-C1
17	A	835	CLA	CBA-CGA-O2A-C1
17	B	813	CLA	CBA-CGA-O2A-C1
17	B	819	CLA	CBA-CGA-O2A-C1
17	B	820	CLA	CBA-CGA-O2A-C1
17	5	603	CLA	CBA-CGA-O2A-C1
24	J	106	3XQ	C2-C1-O20-C21
17	A	816	CLA	O1D-CGD-O2D-CED
17	B	821	CLA	O1D-CGD-O2D-CED
17	J	102	CLA	O1D-CGD-O2D-CED
17	1	602	CLA	O1D-CGD-O2D-CED
17	A	806	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	A	828	CLA	CBD-CGD-O2D-CED
17	B	814	CLA	CBD-CGD-O2D-CED
17	A	848	CLA	C2C-C3C-CAC-CBC
17	5	606	CLA	C2C-C3C-CAC-CBC
17	3	209	CLA	C3-C5-C6-C7
17	A	833	CLA	C2-C3-C5-C6
17	5	603	CLA	C2-C3-C5-C6
17	A	833	CLA	CBD-CGD-O2D-CED
17	A	835	CLA	CBD-CGD-O2D-CED
17	4	609	CLA	CBD-CGD-O2D-CED
17	B	827	CLA	C2A-CAA-CBA-CGA
17	B	835	CLA	C2A-CAA-CBA-CGA
17	2	601	CLA	C2A-CAA-CBA-CGA
17	2	606	CLA	C2A-CAA-CBA-CGA
17	4	603	CLA	C2A-CAA-CBA-CGA
17	4	607	CLA	C2A-CAA-CBA-CGA
17	5	604	CLA	C2A-CAA-CBA-CGA
17	5	606	CLA	C2A-CAA-CBA-CGA
17	5	608	CLA	C2A-CAA-CBA-CGA
17	5	610	CLA	C2A-CAA-CBA-CGA
17	2	602	CLA	O1D-CGD-O2D-CED
17	5	612	CLA	O1D-CGD-O2D-CED
17	A	837	CLA	C3-C5-C6-C7
17	B	820	CLA	C3-C5-C6-C7
17	B	831	CLA	C3-C5-C6-C7
17	A	807	CLA	CBA-CGA-O2A-C1
17	A	808	CLA	CBA-CGA-O2A-C1
17	A	817	CLA	CBA-CGA-O2A-C1
17	A	838	CLA	CBA-CGA-O2A-C1
17	B	814	CLA	CBA-CGA-O2A-C1
17	B	821	CLA	CBA-CGA-O2A-C1
17	B	841	CLA	CBA-CGA-O2A-C1
17	L	202	CLA	CBA-CGA-O2A-C1
17	4	607	CLA	O1D-CGD-O2D-CED
18	A	840	PQN	C11-C12-C13-C14
18	B	844	PQN	C11-C12-C13-C14
17	A	809	CLA	CBD-CGD-O2D-CED
17	A	837	CLA	CBD-CGD-O2D-CED
17	B	807	CLA	CBD-CGD-O2D-CED
17	B	830	CLA	CBD-CGD-O2D-CED
17	B	818	CLA	O1D-CGD-O2D-CED
17	1	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	A	808	CLA	O1A-CGA-O2A-C1
17	A	809	CLA	O1A-CGA-O2A-C1
17	A	817	CLA	O1A-CGA-O2A-C1
17	B	820	CLA	O1A-CGA-O2A-C1
17	B	826	CLA	O1A-CGA-O2A-C1
17	B	824	CLA	O1A-CGA-O2A-C1
17	O	204	CLA	O1D-CGD-O2D-CED
20	A	843	BCR	C13-C14-C15-C16
20	A	844	BCR	C19-C20-C21-C22
20	A	846	BCR	C9-C10-C11-C12
20	B	849	BCR	C13-C14-C15-C16
20	B	849	BCR	C19-C20-C21-C22
20	B	850	BCR	C15-C16-C17-C18
20	F	304	BCR	C19-C20-C21-C22
20	K	104	BCR	C15-C16-C17-C18
25	1	614	ZEX	C33-C34-C35-C15
25	1	614	ZEX	C29-C30-C31-C32
25	1	615	ZEX	C13-C14-C15-C35
25	1	616	ZEX	C33-C34-C35-C15
25	2	615	ZEX	C9-C10-C11-C12
25	2	617	ZEX	C9-C10-C11-C12
25	3	201	ZEX	C29-C30-C31-C32
25	3	216	ZEX	C33-C34-C35-C15
25	4	615	ZEX	C9-C10-C11-C12
25	4	617	ZEX	C9-C10-C11-C12
25	5	614	ZEX	C9-C10-C11-C12
25	5	614	ZEX	C33-C34-C35-C15
25	5	615	ZEX	C13-C14-C15-C35
25	5	615	ZEX	C29-C30-C31-C32
25	5	617	ZEX	C33-C34-C35-C15
25	5	617	ZEX	C29-C30-C31-C32
17	A	822	CLA	CBD-CGD-O2D-CED
17	A	834	CLA	CBD-CGD-O2D-CED
17	B	822	CLA	CBD-CGD-O2D-CED
17	B	833	CLA	CBD-CGD-O2D-CED
17	1	607	CLA	CBD-CGD-O2D-CED
17	3	205	CLA	CBD-CGD-O2D-CED
17	A	831	CLA	O1D-CGD-O2D-CED
17	B	839	CLA	O1D-CGD-O2D-CED
17	3	213	CLA	O1D-CGD-O2D-CED
17	B	838	CLA	C3-C5-C6-C7
17	A	809	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	826	CLA	CBA-CGA-O2A-C1
19	A	841	LHG	C24-C23-O8-C6
17	A	806	CLA	O1A-CGA-O2A-C1
17	A	829	CLA	O1A-CGA-O2A-C1
17	B	813	CLA	O1A-CGA-O2A-C1
17	B	819	CLA	O1A-CGA-O2A-C1
19	A	841	LHG	O10-C23-O8-C6
22	A	849	BGC	O5-C5-C6-O6
17	B	803	CLA	CBD-CGD-O2D-CED
17	K	102	CLA	CBD-CGD-O2D-CED
17	K	103	CLA	CBD-CGD-O2D-CED
17	5	606	CLA	C4C-C3C-CAC-CBC
17	O	205	CLA	O1D-CGD-O2D-CED
17	4	604	CLA	O1D-CGD-O2D-CED
19	A	841	LHG	C23-C24-C25-C26
19	A	841	LHG	O9-C7-O7-C5
17	2	611	CLA	C2C-C3C-CAC-CBC
17	5	607	CLA	C2C-C3C-CAC-CBC
17	A	815	CLA	C4-C3-C5-C6
17	B	841	CLA	C4-C3-C5-C6
17	A	815	CLA	C2-C3-C5-C6
17	B	841	CLA	C2-C3-C5-C6
17	A	839	CLA	CBD-CGD-O2D-CED
17	A	839	CLA	C2A-CAA-CBA-CGA
17	B	804	CLA	C2A-CAA-CBA-CGA
17	B	807	CLA	C2A-CAA-CBA-CGA
17	4	611	CLA	C2A-CAA-CBA-CGA
17	A	818	CLA	C2C-C3C-CAC-CBC
17	B	804	CLA	C3-C5-C6-C7
17	A	832	CLA	O1D-CGD-O2D-CED
17	1	612	CLA	O1D-CGD-O2D-CED
17	5	608	CLA	O1D-CGD-O2D-CED
17	A	803	CLA	O1D-CGD-O2D-CED
17	A	812	CLA	O1D-CGD-O2D-CED
17	B	843	CLA	O1D-CGD-O2D-CED
17	3	206	CLA	O1D-CGD-O2D-CED
19	A	842	LHG	C1-C2-C3-O3
17	2	609	CLA	O1D-CGD-O2D-CED
16	A	801	CL0	CBA-CGA-O2A-C1
17	A	819	CLA	CBA-CGA-O2A-C1
17	A	820	CLA	CBA-CGA-O2A-C1
17	A	824	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	A	826	CLA	CBA-CGA-O2A-C1
17	A	831	CLA	CBA-CGA-O2A-C1
17	A	836	CLA	CBA-CGA-O2A-C1
17	B	806	CLA	CBA-CGA-O2A-C1
17	B	831	CLA	CBA-CGA-O2A-C1
20	J	105	BCR	C19-C20-C21-C22
20	L	206	BCR	C13-C14-C15-C16
25	4	613	ZEX	C9-C10-C11-C12
25	5	615	ZEX	C33-C34-C35-C15
25	5	616	ZEX	C33-C34-C35-C15
17	A	826	CLA	C10-C11-C12-C13
24	J	106	3XQ	O20-C21-C22-C24
17	B	821	CLA	C10-C11-C12-C13
17	B	835	CLA	C15-C16-C17-C18
19	A	841	LHG	O2-C2-C3-O3
17	A	805	CLA	C3-C5-C6-C7
17	A	819	CLA	O1A-CGA-O2A-C1
17	A	820	CLA	O1A-CGA-O2A-C1
17	B	831	CLA	O1A-CGA-O2A-C1
17	A	831	CLA	C14-C13-C15-C16
17	B	804	CLA	C14-C13-C15-C16
17	B	808	CLA	C14-C13-C15-C16
17	B	811	CLA	C14-C13-C15-C16
17	B	820	CLA	C11-C10-C8-C9
17	B	829	CLA	C14-C13-C15-C16
17	F	301	CLA	C6-C7-C8-C9
17	A	823	CLA	O1D-CGD-O2D-CED
17	B	841	CLA	O1D-CGD-O2D-CED
17	J	101	CLA	CBD-CGD-O2D-CED
17	B	804	CLA	C10-C11-C12-C13
17	B	838	CLA	C5-C6-C7-C8
17	A	819	CLA	C2A-CAA-CBA-CGA
17	B	814	CLA	C2A-CAA-CBA-CGA
17	B	830	CLA	C2A-CAA-CBA-CGA
20	A	844	BCR	C36-C18-C19-C20
20	A	844	BCR	C37-C22-C23-C24
20	A	845	BCR	C7-C8-C9-C34
20	B	805	BCR	C37-C22-C23-C24
20	B	845	BCR	C7-C8-C9-C34
20	B	847	BCR	C7-C8-C9-C34
20	B	850	BCR	C7-C8-C9-C34
20	K	101	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	K	104	BCR	C36-C18-C19-C20
25	1	614	ZEX	C11-C12-C13-C20
25	1	615	ZEX	C7-C8-C9-C19
25	1	615	ZEX	C27-C28-C29-C39
25	1	617	ZEX	C7-C8-C9-C19
25	1	617	ZEX	C31-C32-C33-C40
25	1	617	ZEX	C27-C28-C29-C39
25	2	614	ZEX	C7-C8-C9-C19
25	2	614	ZEX	C27-C28-C29-C39
25	2	615	ZEX	C31-C32-C33-C40
25	3	201	ZEX	C7-C8-C9-C19
25	3	201	ZEX	C31-C32-C33-C40
25	3	214	ZEX	C7-C8-C9-C19
25	3	214	ZEX	C27-C28-C29-C39
25	3	215	ZEX	C11-C12-C13-C20
25	4	613	ZEX	C11-C12-C13-C20
25	4	614	ZEX	C27-C28-C29-C39
25	4	615	ZEX	C11-C12-C13-C20
25	4	616	ZEX	C27-C28-C29-C39
25	5	614	ZEX	C7-C8-C9-C19
25	5	614	ZEX	C31-C32-C33-C40
25	5	615	ZEX	C7-C8-C9-C19
25	5	615	ZEX	C31-C32-C33-C40
25	5	615	ZEX	C27-C28-C29-C39
25	5	616	ZEX	C11-C12-C13-C20
25	5	617	ZEX	C7-C8-C9-C19
25	5	617	ZEX	C11-C12-C13-C20
20	A	844	BCR	C17-C18-C19-C20
20	B	805	BCR	C7-C8-C9-C10
20	B	805	BCR	C11-C12-C13-C14
20	B	847	BCR	C7-C8-C9-C10
20	B	848	BCR	C11-C12-C13-C14
20	B	849	BCR	C7-C8-C9-C10
20	B	849	BCR	C21-C22-C23-C24
20	B	850	BCR	C7-C8-C9-C10
20	F	304	BCR	C21-C22-C23-C24
20	K	101	BCR	C21-C22-C23-C24
20	L	201	BCR	C17-C18-C19-C20
25	1	614	ZEX	C31-C32-C33-C34
25	1	615	ZEX	C31-C32-C33-C34
25	2	615	ZEX	C7-C8-C9-C10
25	3	201	ZEX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	3	215	ZEX	C7-C8-C9-C10
25	3	216	ZEX	C11-C12-C13-C14
25	3	217	ZEX	C31-C32-C33-C34
25	4	613	ZEX	C7-C8-C9-C10
25	4	613	ZEX	C27-C28-C29-C30
25	4	615	ZEX	C7-C8-C9-C10
25	4	615	ZEX	C27-C28-C29-C30
25	4	616	ZEX	C31-C32-C33-C34
25	4	617	ZEX	C7-C8-C9-C10
25	4	617	ZEX	C27-C28-C29-C30
25	5	617	ZEX	C31-C32-C33-C34
25	5	617	ZEX	C27-C28-C29-C30
17	A	824	CLA	O1A-CGA-O2A-C1
17	A	825	CLA	C15-C16-C17-C18
17	A	836	CLA	C13-C15-C16-C17
17	B	812	CLA	C13-C15-C16-C17
17	B	820	CLA	C5-C6-C7-C8
17	B	828	CLA	C10-C11-C12-C13
17	3	210	CLA	O1D-CGD-O2D-CED
22	A	849	BGC	C4-C5-C6-O6
17	A	848	CLA	C4C-C3C-CAC-CBC
17	F	301	CLA	C3-C5-C6-C7
17	B	834	CLA	C2A-CAA-CBA-CGA
17	A	839	CLA	CBA-CGA-O2A-C1
17	B	804	CLA	CBA-CGA-O2A-C1
17	A	833	CLA	C13-C15-C16-C17
17	A	837	CLA	C15-C16-C17-C18
17	A	839	CLA	C13-C15-C16-C17
17	B	812	CLA	C15-C16-C17-C18
17	B	815	CLA	C5-C6-C7-C8
17	B	827	CLA	C15-C16-C17-C18
17	A	807	CLA	C5-C6-C7-C8
17	A	817	CLA	C13-C15-C16-C17
17	A	827	CLA	C13-C15-C16-C17
17	A	828	CLA	C10-C11-C12-C13
17	A	839	CLA	C15-C16-C17-C18
17	B	819	CLA	C5-C6-C7-C8
17	B	820	CLA	C8-C10-C11-C12
17	B	829	CLA	C13-C15-C16-C17
17	5	603	CLA	C5-C6-C7-C8
18	B	844	PQN	C18-C20-C21-C22
16	A	801	CL0	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	842	LHG	C23-C24-C25-C26
17	A	838	CLA	C5-C6-C7-C8
17	B	806	CLA	C13-C15-C16-C17
17	B	810	CLA	C13-C15-C16-C17
17	B	816	CLA	C15-C16-C17-C18
17	B	821	CLA	C5-C6-C7-C8
17	A	832	CLA	CBA-CGA-O2A-C1
17	B	835	CLA	CBA-CGA-O2A-C1
17	A	805	CLA	C15-C16-C17-C18
17	F	301	CLA	C10-C11-C12-C13
23	B	851	DGD	C1B-C2B-C3B-C4B
24	J	106	3XQ	C1-C2-C3-C4
17	A	815	CLA	CBD-CGD-O2D-CED
17	1	605	CLA	C2A-CAA-CBA-CGA
17	A	805	CLA	C11-C12-C13-C15
17	A	806	CLA	C12-C13-C15-C16
17	B	806	CLA	C11-C12-C13-C15
17	B	820	CLA	C11-C10-C8-C7
17	B	835	CLA	C6-C7-C8-C10
17	A	807	CLA	C3-C5-C6-C7
17	J	101	CLA	C3-C5-C6-C7
17	L	202	CLA	C3-C5-C6-C7
17	A	826	CLA	O1A-CGA-O2A-C1
17	A	831	CLA	O1A-CGA-O2A-C1
17	A	836	CLA	O1A-CGA-O2A-C1
20	A	845	BCR	C9-C10-C11-C12
20	A	845	BCR	C19-C20-C21-C22
20	B	805	BCR	C9-C10-C11-C12
20	B	845	BCR	C13-C14-C15-C16
20	B	847	BCR	C9-C10-C11-C12
20	B	848	BCR	C9-C10-C11-C12
20	L	206	BCR	C9-C10-C11-C12
25	1	613	ZEX	C9-C10-C11-C12
25	1	615	ZEX	C33-C34-C35-C15
25	3	217	ZEX	C29-C30-C31-C32
25	4	616	ZEX	C9-C10-C11-C12
25	5	616	ZEX	C13-C14-C15-C35
17	2	608	CLA	CBA-CGA-O2A-C1
17	A	827	CLA	C2A-CAA-CBA-CGA
17	B	813	CLA	C2A-CAA-CBA-CGA
17	1	606	CLA	C2A-CAA-CBA-CGA
17	1	612	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	2	601	CLA	O1D-CGD-O2D-CED
17	2	606	CLA	O1D-CGD-O2D-CED
17	2	608	CLA	O1D-CGD-O2D-CED
17	A	828	CLA	C13-C15-C16-C17
17	B	841	CLA	C8-C10-C11-C12
17	J	102	CLA	C5-C6-C7-C8
17	A	818	CLA	C4C-C3C-CAC-CBC
17	B	806	CLA	O1A-CGA-O2A-C1
17	A	807	CLA	C10-C11-C12-C13
17	A	848	CLA	C10-C11-C12-C13
17	B	827	CLA	C5-C6-C7-C8
20	A	844	BCR	C10-C11-C12-C13
20	B	845	BCR	C18-C19-C20-C21
20	B	846	BCR	C18-C19-C20-C21
20	B	847	BCR	C10-C11-C12-C13
20	B	847	BCR	C18-C19-C20-C21
20	B	848	BCR	C18-C19-C20-C21
20	F	304	BCR	C10-C11-C12-C13
20	J	104	BCR	C18-C19-C20-C21
20	K	101	BCR	C10-C11-C12-C13
20	L	201	BCR	C18-C19-C20-C21
20	L	205	BCR	C10-C11-C12-C13
20	L	206	BCR	C10-C11-C12-C13
20	O	202	BCR	C10-C11-C12-C13
20	O	202	BCR	C18-C19-C20-C21
17	A	802	CLA	C3-C5-C6-C7
17	A	839	CLA	C5-C6-C7-C8
17	B	816	CLA	C10-C11-C12-C13
17	B	832	CLA	C15-C16-C17-C18
18	A	840	PQN	C18-C20-C21-C22
17	A	839	CLA	O1A-CGA-O2A-C1
17	B	835	CLA	O1A-CGA-O2A-C1
17	4	602	CLA	O1A-CGA-O2A-C1
17	A	827	CLA	C8-C10-C11-C12
17	A	831	CLA	C8-C10-C11-C12
17	B	801	CLA	C5-C6-C7-C8
17	B	812	CLA	C5-C6-C7-C8
17	B	829	CLA	C5-C6-C7-C8
17	B	835	CLA	C13-C15-C16-C17
17	B	843	CLA	C13-C15-C16-C17
17	3	203	CLA	C13-C15-C16-C17
18	B	844	PQN	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
17	B	838	CLA	C2C-C3C-CAC-CBC
17	A	814	CLA	O1D-CGD-O2D-CED
17	B	804	CLA	O1A-CGA-O2A-C1
17	2	608	CLA	O1A-CGA-O2A-C1
19	A	841	LHG	C8-C7-O7-C5
17	A	809	CLA	C8-C10-C11-C12
17	A	833	CLA	C8-C10-C11-C12
17	A	825	CLA	CBA-CGA-O2A-C1
17	A	828	CLA	CBA-CGA-O2A-C1
17	B	809	CLA	CBA-CGA-O2A-C1
17	4	602	CLA	CBA-CGA-O2A-C1
17	A	806	CLA	O1D-CGD-O2D-CED
17	B	830	CLA	O1D-CGD-O2D-CED
17	L	203	CLA	CBD-CGD-O2D-CED
17	B	822	CLA	C8-C10-C11-C12
17	B	832	CLA	C8-C10-C11-C12
17	B	836	CLA	C10-C11-C12-C13
17	B	839	CLA	C5-C6-C7-C8
17	A	823	CLA	C8-C10-C11-C12
17	B	812	CLA	C10-C11-C12-C13
17	B	830	CLA	C8-C10-C11-C12
17	4	601	CLA	CBD-CGD-O2D-CED
17	A	815	CLA	C2A-CAA-CBA-CGA
17	A	826	CLA	C2A-CAA-CBA-CGA
17	B	802	CLA	C2A-CAA-CBA-CGA
17	B	819	CLA	C2A-CAA-CBA-CGA
17	F	302	CLA	C2A-CAA-CBA-CGA
17	3	203	CLA	C2A-CAA-CBA-CGA
17	5	603	CLA	C16-C17-C18-C20
17	A	830	CLA	CBA-CGA-O2A-C1
17	B	803	CLA	C5-C6-C7-C8
20	B	847	BCR	C14-C15-C16-C17
17	4	609	CLA	O1D-CGD-O2D-CED
20	B	847	BCR	C19-C20-C21-C22
20	O	202	BCR	C9-C10-C11-C12
25	1	614	ZEX	C13-C14-C15-C35
25	2	614	ZEX	C9-C10-C11-C12
25	2	616	ZEX	C29-C30-C31-C32
25	3	214	ZEX	C33-C34-C35-C15
25	3	216	ZEX	C29-C30-C31-C32
25	4	613	ZEX	C29-C30-C31-C32
17	A	809	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	B	810	CLA	C5-C6-C7-C8
20	A	843	BCR	C20-C21-C22-C37
20	B	845	BCR	C35-C13-C14-C15
20	B	846	BCR	C20-C21-C22-C37
20	B	847	BCR	C20-C21-C22-C37
20	B	848	BCR	C16-C17-C18-C36
20	B	849	BCR	C35-C13-C14-C15
20	F	304	BCR	C35-C13-C14-C15
20	F	304	BCR	C20-C21-C22-C37
20	J	104	BCR	C16-C17-C18-C36
20	J	104	BCR	C20-C21-C22-C37
20	J	105	BCR	C16-C17-C18-C36
20	K	104	BCR	C20-C21-C22-C37
20	L	201	BCR	C11-C10-C9-C34
20	L	201	BCR	C16-C17-C18-C36
20	L	201	BCR	C20-C21-C22-C37
25	1	613	ZEX	C11-C10-C9-C19
25	1	617	ZEX	C40-C33-C34-C35
25	3	218	ZEX	C20-C13-C14-C15
25	3	218	ZEX	C40-C33-C34-C35
25	4	612	ZEX	C11-C10-C9-C19
25	4	614	ZEX	C39-C29-C30-C31
25	5	615	ZEX	C11-C10-C9-C19
19	A	841	LHG	C17-C18-C19-C20
19	A	842	LHG	C12-C13-C14-C15
23	B	851	DGD	C2A-C3A-C4A-C5A
23	B	851	DGD	C3A-C4A-C5A-C6A
17	A	828	CLA	O1D-CGD-O2D-CED
17	B	807	CLA	O1D-CGD-O2D-CED
17	A	827	CLA	C16-C17-C18-C20
17	A	833	CLA	C16-C17-C18-C19
17	B	808	CLA	C16-C17-C18-C19
17	B	838	CLA	C11-C12-C13-C14
17	J	101	CLA	C16-C17-C18-C20
17	1	608	CLA	C11-C12-C13-C14
24	J	106	3XQ	C14-C15-C16-C17
17	B	814	CLA	O1D-CGD-O2D-CED
17	F	301	CLA	C8-C10-C11-C12
17	A	837	CLA	O1D-CGD-O2D-CED
17	A	832	CLA	O1A-CGA-O2A-C1
17	5	607	CLA	C4C-C3C-CAC-CBC
23	B	851	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
24	J	106	3XQ	C12-C13-C14-C15
24	J	106	3XQ	C2-C3-C4-C5
17	B	829	CLA	C3-C5-C6-C7
17	A	833	CLA	O1D-CGD-O2D-CED
17	B	833	CLA	O1D-CGD-O2D-CED
20	A	843	BCR	C11-C10-C9-C8
20	A	843	BCR	C16-C17-C18-C19
20	A	844	BCR	C12-C13-C14-C15
20	A	845	BCR	C11-C10-C9-C8
20	A	845	BCR	C12-C13-C14-C15
20	A	845	BCR	C16-C17-C18-C19
20	B	805	BCR	C11-C10-C9-C8
20	B	847	BCR	C16-C17-C18-C19
20	B	848	BCR	C11-C10-C9-C8
20	B	848	BCR	C20-C21-C22-C23
20	B	849	BCR	C20-C21-C22-C23
20	B	850	BCR	C11-C10-C9-C8
20	I	101	BCR	C16-C17-C18-C19
20	J	104	BCR	C16-C17-C18-C19
20	K	104	BCR	C11-C10-C9-C8
20	K	104	BCR	C20-C21-C22-C23
20	L	205	BCR	C12-C13-C14-C15
20	L	205	BCR	C16-C17-C18-C19
20	L	206	BCR	C11-C10-C9-C8
20	L	206	BCR	C20-C21-C22-C23
20	O	202	BCR	C11-C10-C9-C8
20	O	202	BCR	C20-C21-C22-C23
25	1	613	ZEX	C32-C33-C34-C35
25	1	615	ZEX	C28-C29-C30-C31
25	1	616	ZEX	C11-C10-C9-C8
25	1	617	ZEX	C12-C13-C14-C15
25	2	614	ZEX	C12-C13-C14-C15
25	2	616	ZEX	C28-C29-C30-C31
25	2	617	ZEX	C11-C10-C9-C8
25	2	617	ZEX	C12-C13-C14-C15
25	2	617	ZEX	C28-C29-C30-C31
25	3	216	ZEX	C12-C13-C14-C15
25	3	216	ZEX	C28-C29-C30-C31
25	3	218	ZEX	C12-C13-C14-C15
25	4	615	ZEX	C12-C13-C14-C15
25	4	615	ZEX	C32-C33-C34-C35
25	4	616	ZEX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	5	615	ZEX	C32-C33-C34-C35
25	5	615	ZEX	C28-C29-C30-C31
17	B	810	CLA	CBA-CGA-O2A-C1
17	B	840	CLA	CBA-CGA-O2A-C1
17	3	203	CLA	CBA-CGA-O2A-C1
17	J	101	CLA	C5-C6-C7-C8
17	A	825	CLA	O1A-CGA-O2A-C1
17	A	827	CLA	C16-C17-C18-C19
17	B	814	CLA	C6-C7-C8-C10
17	B	839	CLA	C16-C17-C18-C19
17	1	607	CLA	O1D-CGD-O2D-CED
17	B	802	CLA	C4-C3-C5-C6
17	B	819	CLA	C4-C3-C5-C6
17	L	202	CLA	C4-C3-C5-C6
19	A	841	LHG	C11-C10-C9-C8
17	A	806	CLA	C11-C12-C13-C14
17	A	819	CLA	C11-C12-C13-C14
17	B	806	CLA	C11-C12-C13-C14
17	B	816	CLA	C14-C13-C15-C16
17	B	821	CLA	C6-C7-C8-C9
17	B	836	CLA	C11-C12-C13-C14
17	B	838	CLA	C6-C7-C8-C9
17	L	203	CLA	C11-C12-C13-C14
17	1	602	CLA	C11-C10-C8-C9
17	A	804	CLA	CBD-CGD-O2D-CED
19	A	841	LHG	C18-C19-C20-C21
18	A	840	PQN	C25-C26-C27-C28
17	A	822	CLA	C2A-CAA-CBA-CGA
17	O	205	CLA	C2A-CAA-CBA-CGA
17	B	809	CLA	O1A-CGA-O2A-C1
20	B	805	BCR	C7-C8-C9-C34
20	B	849	BCR	C7-C8-C9-C34
25	1	616	ZEX	C7-C8-C9-C19
25	2	616	ZEX	C31-C32-C33-C40
25	2	617	ZEX	C31-C32-C33-C40
25	3	216	ZEX	C31-C32-C33-C40
25	3	218	ZEX	C31-C32-C33-C40
25	4	612	ZEX	C11-C12-C13-C20
25	4	612	ZEX	C31-C32-C33-C40
25	4	614	ZEX	C11-C12-C13-C20
25	5	614	ZEX	C11-C12-C13-C20
25	5	616	ZEX	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
23	B	851	DGD	C4A-C5A-C6A-C7A
19	A	842	LHG	O1-C1-C2-C3
20	A	843	BCR	C7-C8-C9-C10
20	B	846	BCR	C21-C22-C23-C24
20	L	201	BCR	C21-C22-C23-C24
25	1	614	ZEX	C7-C8-C9-C10
25	1	616	ZEX	C11-C12-C13-C14
25	1	616	ZEX	C31-C32-C33-C34
25	2	614	ZEX	C27-C28-C29-C30
25	2	616	ZEX	C7-C8-C9-C10
25	2	616	ZEX	C31-C32-C33-C34
25	2	616	ZEX	C27-C28-C29-C30
25	3	214	ZEX	C31-C32-C33-C34
25	3	218	ZEX	C27-C28-C29-C30
25	4	612	ZEX	C7-C8-C9-C10
17	5	603	CLA	C3-C5-C6-C7
17	A	809	CLA	C10-C11-C12-C13
17	3	203	CLA	C8-C10-C11-C12
19	A	842	LHG	C11-C10-C9-C8
17	A	817	CLA	CBD-CGD-O2D-CED
19	A	842	LHG	C10-C11-C12-C13
23	B	851	DGD	C5B-C6B-C7B-C8B
24	J	106	3XQ	C6-C7-C8-C9
17	A	833	CLA	C16-C17-C18-C20
17	B	826	CLA	C6-C7-C8-C9
17	B	826	CLA	C6-C7-C8-C10
17	B	839	CLA	C16-C17-C18-C20
17	B	843	CLA	C16-C17-C18-C20
17	1	608	CLA	C11-C12-C13-C15
17	5	603	CLA	C16-C17-C18-C19
17	J	101	CLA	C10-C11-C12-C13
17	B	826	CLA	C5-C6-C7-C8
17	B	828	CLA	C13-C15-C16-C17
17	A	834	CLA	O1D-CGD-O2D-CED
17	B	822	CLA	O1D-CGD-O2D-CED
17	A	823	CLA	C3A-C2A-CAA-CBA
17	A	826	CLA	C3A-C2A-CAA-CBA
17	A	831	CLA	C3A-C2A-CAA-CBA
17	B	813	CLA	C3A-C2A-CAA-CBA
17	B	831	CLA	C3A-C2A-CAA-CBA
17	F	301	CLA	C3A-C2A-CAA-CBA
17	J	101	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	L	202	CLA	C3A-C2A-CAA-CBA
17	1	601	CLA	C3A-C2A-CAA-CBA
17	1	605	CLA	C3A-C2A-CAA-CBA
17	2	606	CLA	C3A-C2A-CAA-CBA
17	3	213	CLA	C3A-C2A-CAA-CBA
17	4	603	CLA	C3A-C2A-CAA-CBA
17	4	610	CLA	C3A-C2A-CAA-CBA
25	2	617	ZEX	C29-C30-C31-C32
19	A	841	LHG	C29-C30-C31-C32
19	A	842	LHG	C14-C15-C16-C17
23	B	851	DGD	C3B-C4B-C5B-C6B
17	A	835	CLA	O1D-CGD-O2D-CED
17	B	843	CLA	C16-C17-C18-C19
17	J	101	CLA	C16-C17-C18-C19
19	A	842	LHG	C25-C26-C27-C28
20	B	845	BCR	C14-C15-C16-C17
20	B	848	BCR	C14-C15-C16-C17
17	A	819	CLA	C4-C3-C5-C6
17	B	803	CLA	C4-C3-C5-C6
17	A	819	CLA	C2-C3-C5-C6
17	B	819	CLA	C2-C3-C5-C6
17	L	202	CLA	C2-C3-C5-C6
17	B	803	CLA	O1D-CGD-O2D-CED
17	A	838	CLA	C2A-CAA-CBA-CGA
17	1	603	CLA	C2A-CAA-CBA-CGA
17	B	814	CLA	C6-C7-C8-C9
17	J	101	CLA	C13-C15-C16-C17
18	A	840	PQN	C23-C25-C26-C27
23	B	851	DGD	CDA-CEA-CFA-CGA
23	B	851	DGD	CBB-CCB-CDB-CEB
23	B	851	DGD	C6A-C7A-C8A-C9A
17	A	828	CLA	O1A-CGA-O2A-C1
17	A	830	CLA	O1A-CGA-O2A-C1
17	A	833	CLA	C5-C6-C7-C8
17	A	822	CLA	O1D-CGD-O2D-CED
17	A	839	CLA	C2-C1-O2A-CGA
17	2	611	CLA	C4C-C3C-CAC-CBC
17	A	836	CLA	C15-C16-C17-C18
17	B	801	CLA	C15-C16-C17-C18
17	B	822	CLA	C15-C16-C17-C18
17	L	203	CLA	C10-C11-C12-C13
25	1	617	ZEX	C21-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	2	616	ZEX	C21-C26-C27-C28
25	5	615	ZEX	C21-C26-C27-C28
17	B	810	CLA	O1A-CGA-O2A-C1
20	A	843	BCR	C1-C6-C7-C8
20	A	843	BCR	C5-C6-C7-C8
20	A	843	BCR	C23-C24-C25-C26
20	A	843	BCR	C23-C24-C25-C30
20	A	845	BCR	C1-C6-C7-C8
20	A	845	BCR	C5-C6-C7-C8
20	A	845	BCR	C23-C24-C25-C26
20	A	845	BCR	C23-C24-C25-C30
20	A	846	BCR	C5-C6-C7-C8
20	B	805	BCR	C23-C24-C25-C26
20	B	845	BCR	C1-C6-C7-C8
20	B	845	BCR	C5-C6-C7-C8
20	B	846	BCR	C5-C6-C7-C8
20	B	847	BCR	C23-C24-C25-C26
20	B	847	BCR	C23-C24-C25-C30
20	B	848	BCR	C1-C6-C7-C8
20	B	848	BCR	C5-C6-C7-C8
20	B	849	BCR	C5-C6-C7-C8
20	B	850	BCR	C23-C24-C25-C26
20	F	304	BCR	C23-C24-C25-C26
20	F	304	BCR	C23-C24-C25-C30
20	J	104	BCR	C5-C6-C7-C8
20	J	104	BCR	C23-C24-C25-C26
20	J	105	BCR	C5-C6-C7-C8
20	J	105	BCR	C23-C24-C25-C26
20	K	101	BCR	C5-C6-C7-C8
20	K	104	BCR	C23-C24-C25-C26
20	L	201	BCR	C1-C6-C7-C8
20	L	201	BCR	C5-C6-C7-C8
20	L	201	BCR	C23-C24-C25-C26
20	L	201	BCR	C23-C24-C25-C30
20	L	205	BCR	C5-C6-C7-C8
20	L	206	BCR	C1-C6-C7-C8
20	L	206	BCR	C5-C6-C7-C8
20	O	202	BCR	C5-C6-C7-C8
20	O	202	BCR	C23-C24-C25-C26
25	1	615	ZEX	C1-C6-C7-C8
25	1	615	ZEX	C5-C6-C7-C8
25	2	614	ZEX	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	3	201	ZEX	C1-C6-C7-C8
25	3	214	ZEX	C5-C6-C7-C8
25	3	218	ZEX	C5-C6-C7-C8
25	4	614	ZEX	C1-C6-C7-C8
25	4	617	ZEX	C5-C6-C7-C8
17	3	205	CLA	O1D-CGD-O2D-CED
17	A	805	CLA	CBA-CGA-O2A-C1
17	F	301	CLA	CBA-CGA-O2A-C1
17	A	839	CLA	C8-C10-C11-C12
17	B	822	CLA	C5-C6-C7-C8
17	B	831	CLA	C8-C10-C11-C12
17	A	832	CLA	C2C-C3C-CAC-CBC
17	A	811	CLA	C5-C6-C7-C8
17	A	825	CLA	C5-C6-C7-C8
23	B	851	DGD	C5A-C6A-C7A-C8A
17	A	823	CLA	C4-C3-C5-C6
17	A	806	CLA	C11-C12-C13-C15
17	A	819	CLA	C11-C12-C13-C15
17	A	823	CLA	C2-C3-C5-C6
17	A	831	CLA	C12-C13-C15-C16
17	A	836	CLA	C6-C7-C8-C10
17	B	802	CLA	C2-C3-C5-C6
17	B	803	CLA	C2-C3-C5-C6
17	B	804	CLA	C11-C12-C13-C15
17	B	812	CLA	C6-C7-C8-C10
17	B	812	CLA	C11-C10-C8-C7
17	B	816	CLA	C11-C12-C13-C15
17	B	816	CLA	C12-C13-C15-C16
17	B	820	CLA	C6-C7-C8-C10
17	B	829	CLA	C12-C13-C15-C16
17	B	836	CLA	C11-C12-C13-C15
17	B	838	CLA	C6-C7-C8-C10
17	B	838	CLA	C11-C10-C8-C7
17	L	203	CLA	C11-C12-C13-C15
17	1	602	CLA	C11-C10-C8-C7
17	B	840	CLA	O1A-CGA-O2A-C1
17	3	203	CLA	O1A-CGA-O2A-C1
17	B	803	CLA	C10-C11-C12-C13
20	B	849	BCR	C15-C16-C17-C18
25	2	614	ZEX	C29-C30-C31-C32
25	2	616	ZEX	C13-C14-C15-C35
17	A	808	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
17	K	103	CLA	O1D-CGD-O2D-CED
17	B	802	CLA	CBA-CGA-O2A-C1
17	L	204	CLA	CBA-CGA-O2A-C1
19	A	841	LHG	C24-C25-C26-C27
26	3	219	1DO	C6-C7-C8-C9
17	A	810	CLA	C2A-CAA-CBA-CGA
17	A	811	CLA	C2A-CAA-CBA-CGA
17	A	816	CLA	C2A-CAA-CBA-CGA
17	1	602	CLA	C2A-CAA-CBA-CGA
17	1	608	CLA	C2A-CAA-CBA-CGA
17	4	604	CLA	C2A-CAA-CBA-CGA
17	5	611	CLA	C2A-CAA-CBA-CGA
17	A	817	CLA	C15-C16-C17-C18
17	A	831	CLA	C5-C6-C7-C8
17	A	823	CLA	C13-C15-C16-C17
17	B	810	CLA	C8-C10-C11-C12
17	B	842	CLA	C8-C10-C11-C12
19	A	841	LHG	C11-C12-C13-C14
20	A	844	BCR	C22-C23-C24-C25
20	L	205	BCR	C22-C23-C24-C25
17	A	837	CLA	C16-C17-C18-C19
17	B	829	CLA	C15-C16-C17-C18
17	J	101	CLA	C8-C10-C11-C12
17	B	801	CLA	C3-C5-C6-C7
17	O	201	CLA	C3-C5-C6-C7
17	B	802	CLA	C15-C16-C17-C18
17	B	813	CLA	C13-C15-C16-C17
17	B	816	CLA	C5-C6-C7-C8
17	B	830	CLA	C5-C6-C7-C8
17	A	805	CLA	C11-C12-C13-C14
17	A	806	CLA	C14-C13-C15-C16
17	A	836	CLA	C6-C7-C8-C9
17	B	803	CLA	C11-C10-C8-C9
17	B	810	CLA	C6-C7-C8-C9
17	B	812	CLA	C11-C10-C8-C9
17	B	813	CLA	C11-C10-C8-C9
17	B	816	CLA	C11-C10-C8-C9
17	B	820	CLA	C6-C7-C8-C9
17	B	835	CLA	C6-C7-C8-C9
17	B	836	CLA	C6-C7-C8-C9
17	B	838	CLA	C11-C10-C8-C9
17	B	822	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	2	602	CLA	C3-C5-C6-C7
17	A	818	CLA	C2A-CAA-CBA-CGA
17	2	608	CLA	C2A-CAA-CBA-CGA
17	3	205	CLA	C2A-CAA-CBA-CGA
17	3	206	CLA	C2A-CAA-CBA-CGA
17	5	601	CLA	C2A-CAA-CBA-CGA
20	A	843	BCR	C7-C8-C9-C34
20	B	848	BCR	C11-C12-C13-C35
20	F	304	BCR	C11-C12-C13-C35
20	L	206	BCR	C11-C12-C13-C35
25	3	215	ZEX	C7-C8-C9-C19
25	4	612	ZEX	C7-C8-C9-C19
25	4	614	ZEX	C7-C8-C9-C19
25	5	617	ZEX	C27-C28-C29-C39
17	J	101	CLA	O1D-CGD-O2D-CED
20	A	845	BCR	C7-C8-C9-C10
20	A	845	BCR	C17-C18-C19-C20
20	I	101	BCR	C21-C22-C23-C24
25	4	614	ZEX	C27-C28-C29-C30
25	4	616	ZEX	C11-C12-C13-C14
17	A	805	CLA	O1A-CGA-O2A-C1
17	F	301	CLA	O1A-CGA-O2A-C1
23	B	851	DGD	O1A-C1A-O1G-C1G
17	A	805	CLA	C1A-C2A-CAA-CBA
17	A	806	CLA	C1A-C2A-CAA-CBA
17	A	807	CLA	C1A-C2A-CAA-CBA
17	A	809	CLA	C1A-C2A-CAA-CBA
17	A	816	CLA	C1A-C2A-CAA-CBA
17	A	821	CLA	C1A-C2A-CAA-CBA
17	A	822	CLA	C1A-C2A-CAA-CBA
17	A	831	CLA	C1A-C2A-CAA-CBA
17	A	833	CLA	C1A-C2A-CAA-CBA
17	B	808	CLA	C1A-C2A-CAA-CBA
17	B	813	CLA	C1A-C2A-CAA-CBA
17	B	822	CLA	C1A-C2A-CAA-CBA
17	F	301	CLA	C1A-C2A-CAA-CBA
17	J	101	CLA	C1A-C2A-CAA-CBA
17	J	102	CLA	C1A-C2A-CAA-CBA
17	K	102	CLA	C1A-C2A-CAA-CBA
17	O	205	CLA	C1A-C2A-CAA-CBA
17	1	602	CLA	C1A-C2A-CAA-CBA
17	1	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	1	607	CLA	C1A-C2A-CAA-CBA
17	1	608	CLA	C1A-C2A-CAA-CBA
17	2	602	CLA	C1A-C2A-CAA-CBA
17	2	606	CLA	C1A-C2A-CAA-CBA
17	3	203	CLA	C1A-C2A-CAA-CBA
17	3	208	CLA	C1A-C2A-CAA-CBA
17	3	209	CLA	C1A-C2A-CAA-CBA
17	3	213	CLA	C1A-C2A-CAA-CBA
17	4	601	CLA	C1A-C2A-CAA-CBA
17	4	603	CLA	C1A-C2A-CAA-CBA
17	4	605	CLA	C1A-C2A-CAA-CBA
17	4	606	CLA	C1A-C2A-CAA-CBA
17	4	607	CLA	C1A-C2A-CAA-CBA
17	4	608	CLA	C1A-C2A-CAA-CBA
17	4	610	CLA	C1A-C2A-CAA-CBA
17	5	601	CLA	C1A-C2A-CAA-CBA
17	5	604	CLA	C1A-C2A-CAA-CBA
17	5	607	CLA	C1A-C2A-CAA-CBA
17	5	610	CLA	C1A-C2A-CAA-CBA
17	A	808	CLA	C6-C7-C8-C9
17	A	837	CLA	C16-C17-C18-C20
17	B	808	CLA	C16-C17-C18-C20
23	B	851	DGD	C8A-C9A-CAA-CBA
20	F	304	BCR	C13-C14-C15-C16
20	J	104	BCR	C19-C20-C21-C22
25	3	215	ZEX	C9-C10-C11-C12
25	4	616	ZEX	C33-C34-C35-C15
25	5	614	ZEX	C13-C14-C15-C35
25	5	617	ZEX	C13-C14-C15-C35
16	A	801	CL0	C13-C15-C16-C17
17	B	839	CLA	C13-C15-C16-C17
17	5	603	CLA	C10-C11-C12-C13
17	A	838	CLA	CBD-CGD-O2D-CED
17	B	827	CLA	C3-C5-C6-C7
19	A	841	LHG	C15-C16-C17-C18
26	3	219	1DO	O2S-C1-C2-C3
24	J	106	3XQ	C11-C12-C13-C14
17	B	838	CLA	C11-C12-C13-C15
17	A	839	CLA	O1D-CGD-O2D-CED
25	2	615	ZEX	C25-C26-C27-C28
25	3	218	ZEX	C25-C26-C27-C28
25	4	612	ZEX	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	4	613	ZEX	C25-C26-C27-C28
25	5	614	ZEX	C25-C26-C27-C28
17	B	843	CLA	C15-C16-C17-C18
17	A	804	CLA	CBA-CGA-O2A-C1
17	B	839	CLA	CBA-CGA-O2A-C1
23	B	851	DGD	O6E-C5E-C6E-O5E
17	B	816	CLA	C4-C3-C5-C6
17	4	608	CLA	C2A-CAA-CBA-CGA
23	B	851	DGD	O1G-C1G-C2G-C3G
23	B	851	DGD	C1G-C2G-C3G-O3G
17	B	802	CLA	O1A-CGA-O2A-C1
17	A	815	CLA	C10-C11-C12-C13
25	1	616	ZEX	C9-C10-C11-C12
17	4	602	CLA	C11-C12-C13-C14
18	A	840	PQN	C14-C13-C15-C16
17	L	202	CLA	C8-C10-C11-C12
17	L	204	CLA	O1A-CGA-O2A-C1
17	A	810	CLA	CBA-CGA-O2A-C1
17	A	808	CLA	C5-C6-C7-C8
17	B	841	CLA	C2A-CAA-CBA-CGA
17	A	807	CLA	C13-C15-C16-C17
16	A	801	CL0	C2-C1-O2A-CGA
17	B	830	CLA	CBA-CGA-O2A-C1
17	3	213	CLA	CBA-CGA-O2A-C1
18	A	840	PQN	C26-C27-C28-C30
17	B	806	CLA	C10-C11-C12-C13
17	K	102	CLA	O1D-CGD-O2D-CED
17	B	804	CLA	C13-C15-C16-C17
17	B	809	CLA	C8-C10-C11-C12
17	L	202	CLA	C5-C6-C7-C8
25	3	214	ZEX	C11-C10-C9-C8
17	A	809	CLA	C15-C16-C17-C18
17	A	833	CLA	C10-C11-C12-C13
17	A	815	CLA	O1D-CGD-O2D-CED
17	A	826	CLA	C4-C3-C5-C6
17	B	830	CLA	C4-C3-C5-C6
17	F	301	CLA	C4-C3-C5-C6
18	B	844	PQN	C14-C13-C15-C16
17	A	807	CLA	C11-C10-C8-C7
17	A	817	CLA	C6-C7-C8-C10
17	A	819	CLA	C6-C7-C8-C10
17	A	823	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	B	803	CLA	C11-C10-C8-C7
17	B	806	CLA	C6-C7-C8-C10
17	B	808	CLA	C12-C13-C15-C16
17	B	810	CLA	C6-C7-C8-C10
17	B	813	CLA	C11-C10-C8-C7
17	B	816	CLA	C2-C3-C5-C6
17	B	816	CLA	C11-C10-C8-C7
17	B	827	CLA	C11-C12-C13-C15
17	B	830	CLA	C2-C3-C5-C6
17	B	836	CLA	C6-C7-C8-C10
17	B	836	CLA	C11-C10-C8-C7
17	B	841	CLA	C6-C7-C8-C10
17	B	842	CLA	C11-C10-C8-C7
17	J	101	CLA	C11-C12-C13-C15
17	3	203	CLA	C6-C7-C8-C10
17	3	203	CLA	C11-C10-C8-C7
17	B	806	CLA	CAA-CBA-CGA-O2A
17	A	804	CLA	O1A-CGA-O2A-C1
17	A	807	CLA	C11-C10-C8-C9
17	A	819	CLA	C6-C7-C8-C9
17	A	823	CLA	C11-C10-C8-C9
17	A	832	CLA	C6-C7-C8-C9
17	A	833	CLA	C11-C10-C8-C9
17	A	833	CLA	C11-C12-C13-C14
17	A	839	CLA	C11-C12-C13-C14
17	B	801	CLA	C11-C10-C8-C9
17	B	812	CLA	C6-C7-C8-C9
17	B	821	CLA	C11-C10-C8-C9
17	B	827	CLA	C11-C12-C13-C14
17	B	835	CLA	C14-C13-C15-C16
17	B	836	CLA	C11-C10-C8-C9
17	B	841	CLA	C6-C7-C8-C9
17	B	842	CLA	C11-C10-C8-C9
17	J	101	CLA	C11-C12-C13-C14
17	L	202	CLA	C11-C10-C8-C9
17	3	203	CLA	C6-C7-C8-C9
17	3	203	CLA	C11-C10-C8-C9
17	5	613	CLA	CBA-CGA-O2A-C1
17	B	838	CLA	C10-C11-C12-C13
17	A	806	CLA	C2A-CAA-CBA-CGA
17	A	810	CLA	O1A-CGA-O2A-C1
20	B	849	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	L	201	BCR	C37-C22-C23-C24
20	O	202	BCR	C7-C8-C9-C34
25	3	216	ZEX	C11-C12-C13-C20
25	4	617	ZEX	C27-C28-C29-C39
17	A	832	CLA	C15-C16-C17-C18
25	1	615	ZEX	C7-C8-C9-C10
25	1	616	ZEX	C7-C8-C9-C10
25	1	617	ZEX	C27-C28-C29-C30
25	2	617	ZEX	C31-C32-C33-C34
25	3	214	ZEX	C7-C8-C9-C10
25	4	612	ZEX	C11-C12-C13-C14
25	4	612	ZEX	C27-C28-C29-C30
25	4	616	ZEX	C27-C28-C29-C30
25	5	614	ZEX	C31-C32-C33-C34
17	4	601	CLA	O1D-CGD-O2D-CED
17	B	831	CLA	C10-C11-C12-C13
17	3	203	CLA	C15-C16-C17-C18
17	A	811	CLA	CBA-CGA-O2A-C1
17	A	831	CLA	C13-C15-C16-C17
17	A	804	CLA	O1D-CGD-O2D-CED
17	A	832	CLA	C4C-C3C-CAC-CBC
23	B	851	DGD	C4B-C5B-C6B-C7B
17	L	203	CLA	CBA-CGA-O2A-C1
17	B	830	CLA	C13-C15-C16-C17
17	B	811	CLA	C4-C3-C5-C6
17	B	827	CLA	C4-C3-C5-C6
17	A	826	CLA	C2-C3-C5-C6
17	F	301	CLA	C2-C3-C5-C6
17	B	832	CLA	C13-C15-C16-C17
17	B	835	CLA	C3-C5-C6-C7
17	A	816	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	CBA-CGA-O2A-C1
17	A	812	CLA	C3A-C2A-CAA-CBA
17	A	821	CLA	C3A-C2A-CAA-CBA
17	A	834	CLA	C3A-C2A-CAA-CBA
17	1	612	CLA	C3A-C2A-CAA-CBA
17	4	601	CLA	C3A-C2A-CAA-CBA
17	4	602	CLA	C3A-C2A-CAA-CBA
20	A	843	BCR	C9-C10-C11-C12
20	I	101	BCR	C13-C14-C15-C16
20	I	101	BCR	C15-C16-C17-C18
25	2	615	ZEX	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	3	218	ZEX	C29-C30-C31-C32
17	A	811	CLA	C13-C15-C16-C17
17	B	838	CLA	CBA-CGA-O2A-C1
17	B	839	CLA	O1A-CGA-O2A-C1
23	B	851	DGD	C2B-C3B-C4B-C5B
17	B	824	CLA	CAA-CBA-CGA-O2A
17	A	836	CLA	C3-C5-C6-C7
17	B	827	CLA	C2-C3-C5-C6
17	1	602	CLA	C11-C12-C13-C14
17	2	605	CLA	C2A-CAA-CBA-CGA
17	B	832	CLA	C10-C11-C12-C13
17	1	602	CLA	CBA-CGA-O2A-C1
17	B	830	CLA	O1A-CGA-O2A-C1
17	3	213	CLA	O1A-CGA-O2A-C1
17	L	203	CLA	O1D-CGD-O2D-CED
17	A	804	CLA	C8-C10-C11-C12
17	A	838	CLA	O1D-CGD-O2D-CED
23	B	851	DGD	O2G-C2G-C3G-O3G
17	A	817	CLA	C8-C10-C11-C12
16	A	801	CL0	C16-C17-C18-C19
17	A	809	CLA	C13-C15-C16-C17
17	A	811	CLA	C15-C16-C17-C18
17	B	822	CLA	C10-C11-C12-C13
17	B	803	CLA	C3-C5-C6-C7
17	A	815	CLA	C2-C1-O2A-CGA
17	4	602	CLA	C2-C1-O2A-CGA
17	B	811	CLA	C2-C3-C5-C6
17	5	613	CLA	O1A-CGA-O2A-C1
17	A	804	CLA	C11-C10-C8-C9
17	A	805	CLA	C6-C7-C8-C9
17	A	817	CLA	C6-C7-C8-C9
17	A	817	CLA	C14-C13-C15-C16
17	A	823	CLA	C11-C12-C13-C14
17	A	827	CLA	C11-C12-C13-C14
17	B	803	CLA	C11-C12-C13-C14
17	B	809	CLA	C6-C7-C8-C9
17	B	809	CLA	C14-C13-C15-C16
17	B	822	CLA	C14-C13-C15-C16
17	B	830	CLA	C11-C12-C13-C14
17	A	827	CLA	C5-C6-C7-C8
17	B	801	CLA	C8-C10-C11-C12
17	A	835	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	1	616	ZEX	C21-C26-C27-C28
19	A	841	LHG	C9-C10-C11-C12
17	3	202	CLA	C2A-CAA-CBA-CGA
17	3	208	CLA	C2A-CAA-CBA-CGA
17	A	831	CLA	C16-C17-C18-C19
20	A	844	BCR	C23-C24-C25-C26
20	B	805	BCR	C1-C6-C7-C8
20	B	805	BCR	C5-C6-C7-C8
20	B	845	BCR	C23-C24-C25-C26
20	B	846	BCR	C1-C6-C7-C8
20	B	846	BCR	C23-C24-C25-C26
20	B	847	BCR	C1-C6-C7-C8
20	B	847	BCR	C5-C6-C7-C8
20	B	850	BCR	C5-C6-C7-C8
20	B	850	BCR	C23-C24-C25-C30
20	F	304	BCR	C5-C6-C7-C8
20	I	101	BCR	C5-C6-C7-C8
20	I	101	BCR	C23-C24-C25-C26
20	I	101	BCR	C23-C24-C25-C30
20	J	105	BCR	C23-C24-C25-C30
20	K	101	BCR	C23-C24-C25-C26
20	K	104	BCR	C1-C6-C7-C8
20	K	104	BCR	C5-C6-C7-C8
20	K	104	BCR	C23-C24-C25-C30
20	L	206	BCR	C23-C24-C25-C26
20	L	206	BCR	C23-C24-C25-C30
25	3	217	ZEX	C5-C6-C7-C8
25	5	616	ZEX	C5-C6-C7-C8
17	A	824	CLA	C2C-C3C-CAC-CBC
17	A	813	CLA	C1A-C2A-CAA-CBA
17	B	818	CLA	C1A-C2A-CAA-CBA
17	K	103	CLA	C1A-C2A-CAA-CBA
17	2	610	CLA	C1A-C2A-CAA-CBA
20	L	205	BCR	C17-C18-C19-C20
25	4	613	ZEX	C31-C32-C33-C34
25	5	616	ZEX	C27-C28-C29-C30
17	A	831	CLA	C10-C11-C12-C13
19	A	841	LHG	C28-C29-C30-C31
20	A	844	BCR	C14-C15-C16-C17
18	B	844	PQN	C26-C27-C28-C30
17	A	817	CLA	O1D-CGD-O2D-CED
17	A	804	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	A	805	CLA	C6-C7-C8-C10
17	A	809	CLA	C11-C12-C13-C15
17	A	817	CLA	C12-C13-C15-C16
17	A	827	CLA	C11-C12-C13-C15
17	A	832	CLA	C6-C7-C8-C10
17	A	833	CLA	C11-C12-C13-C15
17	A	839	CLA	C11-C12-C13-C15
17	B	801	CLA	C11-C10-C8-C7
17	B	803	CLA	C11-C12-C13-C15
17	B	808	CLA	C6-C7-C8-C10
17	B	809	CLA	C6-C7-C8-C10
17	B	809	CLA	C12-C13-C15-C16
17	B	811	CLA	C12-C13-C15-C16
17	B	821	CLA	C6-C7-C8-C10
17	B	821	CLA	C11-C10-C8-C7
17	B	822	CLA	C12-C13-C15-C16
17	B	828	CLA	C12-C13-C15-C16
17	B	829	CLA	C6-C7-C8-C10
17	B	829	CLA	C11-C12-C13-C15
17	B	830	CLA	C11-C10-C8-C7
17	B	830	CLA	C11-C12-C13-C15
17	B	830	CLA	C12-C13-C15-C16
17	B	835	CLA	C12-C13-C15-C16
17	B	839	CLA	C12-C13-C15-C16
17	F	301	CLA	C6-C7-C8-C10
17	L	202	CLA	C11-C10-C8-C7
17	5	603	CLA	C11-C12-C13-C15
20	B	845	BCR	C9-C10-C11-C12
20	B	849	BCR	C9-C10-C11-C12
20	B	850	BCR	C19-C20-C21-C22
20	L	205	BCR	C19-C20-C21-C22
20	L	206	BCR	C19-C20-C21-C22
25	3	201	ZEX	C33-C34-C35-C15
25	4	612	ZEX	C13-C14-C15-C35
18	B	844	PQN	C15-C16-C17-C18
17	B	843	CLA	CAA-CBA-CGA-O2A
17	A	811	CLA	O1A-CGA-O2A-C1
17	A	829	CLA	C2A-CAA-CBA-CGA
20	B	846	BCR	C11-C10-C9-C34
20	B	850	BCR	C20-C21-C22-C37
20	I	101	BCR	C20-C21-C22-C37
20	J	105	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
17	A	831	CLA	C16-C17-C18-C20
18	A	840	PQN	C26-C27-C28-C29
17	B	829	CLA	CBA-CGA-O2A-C1
17	4	601	CLA	O2A-C1-C2-C3
17	A	811	CLA	C8-C10-C11-C12
17	A	838	CLA	C8-C10-C11-C12
17	A	805	CLA	CAD-CBD-CGD-O2D
17	A	815	CLA	CAD-CBD-CGD-O2D
17	A	824	CLA	CAD-CBD-CGD-O2D
17	A	830	CLA	CAD-CBD-CGD-O2D
17	A	835	CLA	CAD-CBD-CGD-O2D
17	B	812	CLA	CAD-CBD-CGD-O2D
17	B	815	CLA	CAD-CBD-CGD-O2D
17	B	834	CLA	CAD-CBD-CGD-O2D
17	J	103	CLA	CAD-CBD-CGD-O2D
17	O	203	CLA	CAD-CBD-CGD-O2D
17	1	602	CLA	CAD-CBD-CGD-O2D
17	2	601	CLA	CAD-CBD-CGD-O2D
17	2	606	CLA	CAD-CBD-CGD-O2D
17	2	607	CLA	CAD-CBD-CGD-O2D
17	3	207	CLA	CAD-CBD-CGD-O2D
17	3	208	CLA	CAD-CBD-CGD-O2D
17	4	610	CLA	CAD-CBD-CGD-O2D
17	5	602	CLA	CAD-CBD-CGD-O2D
17	5	610	CLA	CAD-CBD-CGD-O2D
17	5	612	CLA	CAD-CBD-CGD-O2D
17	A	838	CLA	C3-C5-C6-C7
17	B	802	CLA	C5-C6-C7-C8
20	B	848	BCR	C22-C23-C24-C25
20	B	850	BCR	C6-C7-C8-C9
17	A	821	CLA	CBA-CGA-O2A-C1
19	A	841	LHG	C4-C5-C6-O8
17	B	829	CLA	O1A-CGA-O2A-C1
17	A	804	CLA	CAA-CBA-CGA-O2A
20	L	205	BCR	C14-C15-C16-C17
17	A	805	CLA	CHA-CBD-CGD-O2D
17	A	806	CLA	CHA-CBD-CGD-O1D
17	A	817	CLA	CHA-CBD-CGD-O1D
17	A	817	CLA	CHA-CBD-CGD-O2D
17	A	820	CLA	CHA-CBD-CGD-O1D
17	A	820	CLA	CHA-CBD-CGD-O2D
17	A	827	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	A	827	CLA	CHA-CBD-CGD-O2D
17	A	828	CLA	CHA-CBD-CGD-O1D
17	A	828	CLA	CHA-CBD-CGD-O2D
17	A	832	CLA	CHA-CBD-CGD-O1D
17	A	837	CLA	CHA-CBD-CGD-O1D
17	A	837	CLA	CHA-CBD-CGD-O2D
17	B	813	CLA	CHA-CBD-CGD-O1D
17	B	813	CLA	CHA-CBD-CGD-O2D
17	B	814	CLA	CHA-CBD-CGD-O1D
17	B	819	CLA	CHA-CBD-CGD-O1D
17	B	819	CLA	CHA-CBD-CGD-O2D
17	B	833	CLA	CHA-CBD-CGD-O1D
17	B	842	CLA	CHA-CBD-CGD-O2D
17	J	102	CLA	CHA-CBD-CGD-O1D
17	L	203	CLA	CHA-CBD-CGD-O2D
17	1	607	CLA	CHA-CBD-CGD-O1D
17	1	607	CLA	CHA-CBD-CGD-O2D
17	4	603	CLA	CHA-CBD-CGD-O1D
17	4	609	CLA	CHA-CBD-CGD-O1D
17	4	609	CLA	CHA-CBD-CGD-O2D
17	5	605	CLA	CHA-CBD-CGD-O1D
17	5	605	CLA	CHA-CBD-CGD-O2D
17	5	608	CLA	CHA-CBD-CGD-O1D
17	5	608	CLA	CHA-CBD-CGD-O2D
17	3	203	CLA	C3-C5-C6-C7
17	A	802	CLA	CBD-CGD-O2D-CED
17	A	816	CLA	O1A-CGA-O2A-C1
17	L	203	CLA	O1A-CGA-O2A-C1
20	A	845	BCR	C20-C21-C22-C23
20	B	805	BCR	C20-C21-C22-C23
25	5	614	ZEX	C11-C10-C9-C8
17	A	804	CLA	C13-C15-C16-C17
17	B	812	CLA	O1A-CGA-O2A-C1
17	B	838	CLA	O1A-CGA-O2A-C1
17	B	822	CLA	C16-C17-C18-C19
19	A	842	LHG	C8-C7-O7-C5
17	A	811	CLA	C11-C12-C13-C14
17	B	829	CLA	C11-C12-C13-C14
17	B	830	CLA	C14-C13-C15-C16
17	A	821	CLA	O1A-CGA-O2A-C1
17	B	803	CLA	C8-C10-C11-C12
24	J	106	3XQ	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
17	4	602	CLA	C2A-CAA-CBA-CGA
20	J	104	BCR	C37-C22-C23-C24
25	1	613	ZEX	C11-C12-C13-C20
25	2	615	ZEX	C7-C8-C9-C19
25	3	217	ZEX	C7-C8-C9-C19
25	4	617	ZEX	C7-C8-C9-C19
20	A	845	BCR	C21-C22-C23-C24
20	B	850	BCR	C21-C22-C23-C24
20	I	101	BCR	C7-C8-C9-C10
25	2	614	ZEX	C7-C8-C9-C10
25	3	214	ZEX	C27-C28-C29-C30
25	5	614	ZEX	C7-C8-C9-C10
17	A	823	CLA	C1A-C2A-CAA-CBA
17	B	838	CLA	C1A-C2A-CAA-CBA
17	A	839	CLA	C16-C17-C18-C20
25	5	617	ZEX	C9-C10-C11-C12
17	A	839	CLA	C10-C11-C12-C13
23	B	851	DGD	CEB-CFB-CGB-CHB
19	A	841	LHG	C3-O3-P-O5
19	A	842	LHG	C4-O6-P-O5
17	B	827	CLA	C13-C15-C16-C17
18	A	840	PQN	C20-C21-C22-C23
24	J	106	3XQ	C3-C4-C5-C6
17	3	209	CLA	C2A-CAA-CBA-CGA
17	A	823	CLA	C3-C5-C6-C7
17	A	821	CLA	C2-C3-C5-C6
17	A	836	CLA	CAD-CBD-CGD-O1D
17	B	804	CLA	CAD-CBD-CGD-O1D
17	B	829	CLA	CAD-CBD-CGD-O1D
17	4	603	CLA	CAD-CBD-CGD-O1D
23	B	851	DGD	C7B-C8B-C9B-CAB
17	1	602	CLA	O1A-CGA-O2A-C1
17	1	608	CLA	C5-C6-C7-C8
17	B	843	CLA	CBA-CGA-O2A-C1
17	B	811	CLA	C13-C15-C16-C17
17	B	806	CLA	C4-C3-C5-C6
17	B	831	CLA	C4-C3-C5-C6
17	A	811	CLA	C11-C12-C13-C15
17	A	828	CLA	C11-C12-C13-C15
17	B	804	CLA	C12-C13-C15-C16
17	B	836	CLA	C12-C13-C15-C16
17	B	841	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	3	203	CLA	C12-C13-C15-C16
17	5	603	CLA	C11-C10-C8-C7
17	5	603	CLA	C12-C13-C15-C16
18	A	840	PQN	C21-C22-C23-C25
25	4	617	ZEX	C29-C30-C31-C32
17	A	831	CLA	C2A-CAA-CBA-CGA
17	2	602	CLA	C2A-CAA-CBA-CGA
17	B	822	CLA	C16-C17-C18-C20
19	A	841	LHG	O7-C5-C6-O8
23	B	851	DGD	O1G-C1G-C2G-O2G
24	J	106	3XQ	C10-C11-C12-C13
17	B	812	CLA	CAA-CBA-CGA-O2A
17	A	836	CLA	C8-C10-C11-C12
17	A	827	CLA	C10-C11-C12-C13
17	B	810	CLA	C4-C3-C5-C6
17	B	806	CLA	C2-C3-C5-C6
17	B	843	CLA	C10-C11-C12-C13
17	A	809	CLA	C11-C12-C13-C14
17	B	806	CLA	C6-C7-C8-C9
17	B	808	CLA	C6-C7-C8-C9
17	B	839	CLA	C14-C13-C15-C16
17	3	203	CLA	C14-C13-C15-C16
17	5	603	CLA	C11-C12-C13-C14
18	A	840	PQN	C21-C22-C23-C24
17	A	827	CLA	O1A-CGA-O2A-C1
17	A	808	CLA	C3-C5-C6-C7
17	B	843	CLA	O1A-CGA-O2A-C1
17	3	213	CLA	C2A-CAA-CBA-CGA
24	J	106	3XQ	O23-C22-C24-O25
25	2	616	ZEX	C10-C11-C12-C13
25	3	216	ZEX	C13-C14-C15-C35
17	B	816	CLA	C8-C10-C11-C12
17	B	836	CLA	C8-C10-C11-C12
17	A	820	CLA	C1-C2-C3-C4
17	B	830	CLA	CAA-CBA-CGA-O2A
23	B	851	DGD	CAB-CBB-CCB-CDB
17	B	803	CLA	C2A-CAA-CBA-CGA
17	A	838	CLA	C2-C1-O2A-CGA
17	B	801	CLA	C2-C1-O2A-CGA
17	B	814	CLA	C2-C1-O2A-CGA
17	A	839	CLA	C16-C17-C18-C19
20	L	206	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	A	827	CLA	CBA-CGA-O2A-C1
20	A	844	BCR	C23-C24-C25-C30
20	B	845	BCR	C23-C24-C25-C30
20	B	846	BCR	C23-C24-C25-C30
20	I	101	BCR	C1-C6-C7-C8
25	2	617	ZEX	C5-C6-C7-C8
25	4	615	ZEX	C1-C6-C7-C8
25	5	615	ZEX	C1-C6-C7-C8
17	2	602	CLA	C16-C17-C18-C20
20	K	101	BCR	C20-C21-C22-C23
17	O	201	CLA	CBA-CGA-O2A-C1
19	A	842	LHG	C3-O3-P-O6
19	A	842	LHG	C4-O6-P-O3
17	A	833	CLA	C11-C10-C8-C7
17	B	831	CLA	C2-C3-C5-C6
17	5	603	CLA	C6-C7-C8-C10
17	O	201	CLA	O1A-CGA-O2A-C1
17	A	828	CLA	C11-C12-C13-C14
17	B	828	CLA	C14-C13-C15-C16
17	B	836	CLA	C14-C13-C15-C16
20	L	201	BCR	C13-C14-C15-C16
25	1	615	ZEX	C9-C10-C11-C12
25	5	615	ZEX	C9-C10-C11-C12
17	B	821	CLA	C11-C12-C13-C15
17	A	804	CLA	C5-C6-C7-C8
17	B	801	CLA	C16-C17-C18-C19
19	A	842	LHG	C2-C3-O3-P
17	4	603	CLA	CAA-CBA-CGA-O2A
17	A	848	CLA	C15-C16-C17-C18
17	3	203	CLA	C5-C6-C7-C8
17	B	822	CLA	CBA-CGA-O2A-C1
20	A	844	BCR	C15-C16-C17-C18
20	B	845	BCR	C15-C16-C17-C18
20	B	845	BCR	C19-C20-C21-C22
20	B	848	BCR	C19-C20-C21-C22
25	3	218	ZEX	C33-C34-C35-C15
25	4	613	ZEX	C33-C34-C35-C15
25	5	616	ZEX	C29-C30-C31-C32
17	A	819	CLA	C3-C5-C6-C7
17	4	602	CLA	C3-C5-C6-C7
17	B	801	CLA	C13-C15-C16-C17
17	B	809	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	2	601	CLA	CAA-CBA-CGA-O2A
17	B	806	CLA	C5-C6-C7-C8
17	B	838	CLA	C4C-C3C-CAC-CBC
26	3	219	1DO	C7-C8-C9-C10
17	B	803	CLA	C2-C1-O2A-CGA
17	B	808	CLA	C2-C1-O2A-CGA
17	B	820	CLA	C10-C11-C12-C13
17	B	810	CLA	C16-C17-C18-C19
18	B	844	PQN	C26-C27-C28-C29
17	B	810	CLA	C2A-CAA-CBA-CGA
17	B	816	CLA	C2A-CAA-CBA-CGA
17	A	827	CLA	C3A-C2A-CAA-CBA
17	B	803	CLA	C3A-C2A-CAA-CBA
17	1	604	CLA	CAA-CBA-CGA-O2A
17	1	607	CLA	CAA-CBA-CGA-O2A
17	B	843	CLA	C4-C3-C5-C6
17	L	203	CLA	C4-C3-C5-C6
17	B	802	CLA	C6-C7-C8-C9
17	B	843	CLA	C11-C12-C13-C14
17	4	602	CLA	C11-C10-C8-C9
17	1	610	CLA	CAA-CBA-CGA-O2A
17	4	611	CLA	CAA-CBA-CGA-O1A
20	A	846	BCR	C16-C17-C18-C36
20	B	805	BCR	C35-C13-C14-C15
20	K	104	BCR	C11-C10-C9-C34
17	A	848	CLA	C2A-CAA-CBA-CGA
17	2	602	CLA	C16-C17-C18-C19
20	B	847	BCR	C21-C22-C23-C24
17	1	604	CLA	CAA-CBA-CGA-O1A
17	1	610	CLA	CAA-CBA-CGA-O1A
17	B	801	CLA	C4-C3-C5-C6
17	A	812	CLA	C1A-C2A-CAA-CBA
17	B	830	CLA	C1A-C2A-CAA-CBA
17	B	832	CLA	C1A-C2A-CAA-CBA
17	B	843	CLA	C1A-C2A-CAA-CBA
17	1	612	CLA	C1A-C2A-CAA-CBA
17	2	605	CLA	C1A-C2A-CAA-CBA
17	2	611	CLA	C1A-C2A-CAA-CBA
17	2	613	CLA	C1A-C2A-CAA-CBA
17	A	809	CLA	C11-C10-C8-C7
17	A	838	CLA	C6-C7-C8-C10
17	B	812	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
17	B	835	CLA	C11-C10-C8-C7
17	4	602	CLA	C11-C10-C8-C7
17	B	825	CLA	C2A-CAA-CBA-CGA
17	B	807	CLA	CAA-CBA-CGA-O2A
17	3	204	CLA	CAA-CBA-CGA-O1A
25	3	218	ZEX	C9-C10-C11-C12
17	A	802	CLA	O1D-CGD-O2D-CED
17	1	601	CLA	O2A-C1-C2-C3
17	B	837	CLA	CAA-CBA-CGA-O2A
17	1	607	CLA	CAA-CBA-CGA-O1A
17	A	823	CLA	C2A-CAA-CBA-CGA
17	B	843	CLA	C2A-CAA-CBA-CGA
17	2	612	CLA	C2A-CAA-CBA-CGA
17	A	816	CLA	C15-C16-C17-C18
17	B	804	CLA	C5-C6-C7-C8
17	B	841	CLA	C15-C16-C17-C18
17	B	807	CLA	CAA-CBA-CGA-O1A
17	5	601	CLA	CAA-CBA-CGA-O1A
17	A	838	CLA	C13-C15-C16-C17
17	3	205	CLA	CAA-CBA-CGA-O2A
17	4	611	CLA	CAA-CBA-CGA-O2A
17	2	602	CLA	C15-C16-C17-C18
17	B	837	CLA	CAA-CBA-CGA-O1A
17	B	841	CLA	C13-C15-C16-C17
20	A	846	BCR	C16-C17-C18-C19
20	B	846	BCR	C11-C10-C9-C8
20	B	847	BCR	C20-C21-C22-C23
20	F	304	BCR	C12-C13-C14-C15
17	3	205	CLA	CAA-CBA-CGA-O1A
20	B	847	BCR	C13-C14-C15-C16
20	J	104	BCR	C15-C16-C17-C18
25	2	614	ZEX	C13-C14-C15-C35
17	A	834	CLA	CAA-CBA-CGA-O1A
17	5	601	CLA	CAA-CBA-CGA-O2A
23	B	851	DGD	C9B-CAB-CBB-CCB
17	A	834	CLA	CAA-CBA-CGA-O2A
17	4	603	CLA	CAA-CBA-CGA-O1A
17	J	101	CLA	C2-C1-O2A-CGA
17	L	203	CLA	C2-C3-C5-C6
17	A	832	CLA	C13-C15-C16-C17
17	2	601	CLA	CAA-CBA-CGA-O1A
17	3	204	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	A	821	CLA	C4-C3-C5-C6
25	3	215	ZEX	C21-C26-C27-C28
17	B	829	CLA	C16-C17-C18-C19
17	2	603	CLA	CAA-CBA-CGA-O2A
17	B	806	CLA	CAA-CBA-CGA-O1A
17	B	822	CLA	O1A-CGA-O2A-C1
20	A	846	BCR	C23-C24-C25-C26
20	A	846	BCR	C23-C24-C25-C30
20	B	848	BCR	C23-C24-C25-C30
20	B	850	BCR	C1-C6-C7-C8
20	F	304	BCR	C1-C6-C7-C8
20	K	101	BCR	C23-C24-C25-C30
25	1	616	ZEX	C1-C6-C7-C8
25	3	216	ZEX	C5-C6-C7-C8
19	A	841	LHG	C30-C31-C32-C33
17	5	605	CLA	CAA-CBA-CGA-O1A
20	A	845	BCR	C15-C16-C17-C18
20	K	104	BCR	C13-C14-C15-C16
17	B	809	CLA	C4-C3-C5-C6
17	B	829	CLA	C16-C17-C18-C20
17	B	810	CLA	C2-C3-C5-C6
17	B	836	CLA	C2-C3-C5-C6
17	3	207	CLA	CAA-CBA-CGA-O2A
17	4	608	CLA	CAA-CBA-CGA-O2A
17	A	848	CLA	C13-C15-C16-C17
17	4	604	CLA	CAA-CBA-CGA-O2A
19	A	841	LHG	O6-C4-C5-O7
17	K	102	CLA	CAA-CBA-CGA-O2A
17	5	604	CLA	CAA-CBA-CGA-O2A
17	5	602	CLA	CAA-CBA-CGA-O2A
16	A	801	CL0	C11-C12-C13-C15
18	A	840	PQN	C22-C23-C25-C26
17	B	836	CLA	C15-C16-C17-C18
17	A	832	CLA	C5-C6-C7-C8
17	4	608	CLA	CAA-CBA-CGA-O1A
19	A	841	LHG	O8-C23-C24-C25
17	B	803	CLA	O1A-CGA-O2A-C1
17	A	830	CLA	C2A-CAA-CBA-CGA
17	A	832	CLA	C2A-CAA-CBA-CGA
17	B	804	CLA	C15-C16-C17-C18
17	1	611	CLA	CAA-CBA-CGA-O1A
17	1	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	B	803	CLA	CBA-CGA-O2A-C1
20	B	849	BCR	C11-C10-C9-C34
17	3	203	CLA	C4-C3-C5-C6
17	5	612	CLA	CAA-CBA-CGA-O2A
17	B	809	CLA	C2-C3-C5-C6
16	A	801	CL0	C11-C12-C13-C14
17	B	816	CLA	C11-C12-C13-C14
17	B	835	CLA	C11-C10-C8-C9
17	B	841	CLA	C11-C10-C8-C9
17	5	603	CLA	C11-C10-C8-C9
17	5	603	CLA	C14-C13-C15-C16
17	1	606	CLA	CAA-CBA-CGA-O2A
17	5	610	CLA	CAA-CBA-CGA-O2A
17	B	830	CLA	C3A-C2A-CAA-CBA
17	B	838	CLA	C3A-C2A-CAA-CBA
17	O	204	CLA	C3A-C2A-CAA-CBA
17	1	604	CLA	C3A-C2A-CAA-CBA
17	2	605	CLA	C3A-C2A-CAA-CBA
17	2	613	CLA	C3A-C2A-CAA-CBA
17	K	102	CLA	CAA-CBA-CGA-O1A
17	A	810	CLA	CAD-CBD-CGD-O2D
17	A	811	CLA	CAD-CBD-CGD-O2D
17	A	819	CLA	CAD-CBD-CGD-O2D
17	A	839	CLA	CAD-CBD-CGD-O2D
17	B	817	CLA	CAD-CBD-CGD-O2D
17	B	818	CLA	CAD-CBD-CGD-O2D
17	B	820	CLA	CAD-CBD-CGD-O2D
17	B	836	CLA	CAD-CBD-CGD-O2D
17	L	202	CLA	CAD-CBD-CGD-O2D
17	O	205	CLA	CAD-CBD-CGD-O2D
17	1	601	CLA	CAD-CBD-CGD-O2D
17	1	604	CLA	CAD-CBD-CGD-O2D
17	1	606	CLA	CAD-CBD-CGD-O2D
17	2	605	CLA	CAD-CBD-CGD-O2D
17	2	608	CLA	CAD-CBD-CGD-O2D
17	2	613	CLA	CAD-CBD-CGD-O2D
17	4	602	CLA	CAD-CBD-CGD-O2D
17	4	606	CLA	CAD-CBD-CGD-O2D
17	4	611	CLA	CAD-CBD-CGD-O2D
17	5	609	CLA	CAD-CBD-CGD-O2D
17	L	203	CLA	C2-C1-O2A-CGA
17	1	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	5	612	CLA	CAA-CBA-CGA-O1A
17	A	810	CLA	CAA-CBA-CGA-O2A
17	A	823	CLA	CAA-CBA-CGA-O2A
17	2	603	CLA	CAA-CBA-CGA-O1A
17	3	207	CLA	CAA-CBA-CGA-O1A
17	5	602	CLA	CAA-CBA-CGA-O1A
17	5	604	CLA	CAA-CBA-CGA-O1A
17	5	610	CLA	CAA-CBA-CGA-O1A
17	A	831	CLA	CAA-CBA-CGA-O2A
17	1	608	CLA	CAA-CBA-CGA-O2A
17	5	613	CLA	CAA-CBA-CGA-O2A
19	A	842	LHG	C26-C27-C28-C29
20	A	846	BCR	C11-C12-C13-C14
20	B	848	BCR	C7-C8-C9-C10
25	3	215	ZEX	C31-C32-C33-C34
25	3	215	ZEX	C27-C28-C29-C30
17	3	208	CLA	CAA-CBA-CGA-O1A
17	3	208	CLA	CAA-CBA-CGA-O2A
17	B	824	CLA	CAA-CBA-CGA-O1A
17	A	806	CLA	C13-C15-C16-C17
17	1	603	CLA	CAA-CBA-CGA-O2A
17	4	604	CLA	CAA-CBA-CGA-O1A
17	5	611	CLA	CAA-CBA-CGA-O2A
17	B	804	CLA	O2A-C1-C2-C3
17	B	820	CLA	O2A-C1-C2-C3
17	L	203	CLA	O2A-C1-C2-C3
17	O	204	CLA	O2A-C1-C2-C3
17	J	102	CLA	C2A-CAA-CBA-CGA
17	B	821	CLA	C8-C10-C11-C12
17	2	602	CLA	CAA-CBA-CGA-O2A
16	A	801	CL0	C16-C17-C18-C20
24	J	106	3XQ	C13-C14-C15-C16
17	A	807	CLA	CHA-CBD-CGD-O2D
17	A	812	CLA	CHA-CBD-CGD-O1D
17	A	812	CLA	CHA-CBD-CGD-O2D
17	A	818	CLA	CHA-CBD-CGD-O1D
17	A	823	CLA	CHA-CBD-CGD-O2D
17	A	829	CLA	CHA-CBD-CGD-O2D
17	B	833	CLA	CHA-CBD-CGD-O2D
17	F	301	CLA	CHA-CBD-CGD-O2D
17	F	302	CLA	CHA-CBD-CGD-O1D
17	F	302	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	F	303	CLA	CHA-CBD-CGD-O2D
17	J	102	CLA	CHA-CBD-CGD-O2D
17	L	204	CLA	CHA-CBD-CGD-O1D
17	L	204	CLA	CHA-CBD-CGD-O2D
17	O	201	CLA	CHA-CBD-CGD-O1D
17	O	204	CLA	CHA-CBD-CGD-O1D
17	1	603	CLA	CHA-CBD-CGD-O1D
17	1	603	CLA	CHA-CBD-CGD-O2D
17	1	611	CLA	CHA-CBD-CGD-O2D
17	2	602	CLA	CHA-CBD-CGD-O2D
17	2	604	CLA	CHA-CBD-CGD-O1D
17	2	604	CLA	CHA-CBD-CGD-O2D
17	2	609	CLA	CHA-CBD-CGD-O1D
17	3	206	CLA	CHA-CBD-CGD-O2D
17	4	601	CLA	CHA-CBD-CGD-O1D
17	4	601	CLA	CHA-CBD-CGD-O2D
17	4	603	CLA	CHA-CBD-CGD-O2D
17	5	603	CLA	CHA-CBD-CGD-O1D
17	5	603	CLA	CHA-CBD-CGD-O2D
17	1	612	CLA	CAA-CBA-CGA-O1A
17	5	611	CLA	CAA-CBA-CGA-O1A
17	B	836	CLA	C4-C3-C5-C6
17	A	837	CLA	CAA-CBA-CGA-O2A
20	B	850	BCR	C16-C17-C18-C19
20	L	201	BCR	C11-C10-C9-C8
25	4	613	ZEX	C11-C10-C9-C8
17	1	603	CLA	CAA-CBA-CGA-O1A
17	1	606	CLA	CAA-CBA-CGA-O1A
19	A	841	LHG	C12-C13-C14-C15
17	A	816	CLA	C16-C17-C18-C19
17	B	808	CLA	C10-C11-C12-C13
17	B	831	CLA	CAA-CBA-CGA-O2A
17	3	203	CLA	CAA-CBA-CGA-O2A
17	A	821	CLA	CAA-CBA-CGA-O2A
17	B	803	CLA	CAA-CBA-CGA-O2A
17	B	809	CLA	CAA-CBA-CGA-O2A
17	B	810	CLA	CAA-CBA-CGA-O2A
17	B	820	CLA	CAA-CBA-CGA-O2A
17	2	608	CLA	CAA-CBA-CGA-O2A
17	A	815	CLA	C5-C6-C7-C8
17	A	805	CLA	CAA-CBA-CGA-O2A
17	B	813	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	B	835	CLA	O1D-CGD-O2D-CED
17	A	833	CLA	C6-C7-C8-C10
17	B	802	CLA	C12-C13-C15-C16
17	B	816	CLA	CAA-CBA-CGA-O2A
17	A	806	CLA	C11-C10-C8-C9
17	A	809	CLA	C11-C10-C8-C9
17	B	802	CLA	C14-C13-C15-C16
17	B	813	CLA	C14-C13-C15-C16
17	B	827	CLA	C6-C7-C8-C9
20	A	843	BCR	C15-C16-C17-C18
25	2	616	ZEX	C33-C34-C35-C15
17	A	815	CLA	C13-C15-C16-C17
19	A	842	LHG	C11-C12-C13-C14
17	B	835	CLA	CAA-CBA-CGA-O2A
17	1	608	CLA	CAA-CBA-CGA-O1A
17	5	605	CLA	CAA-CBA-CGA-O2A
17	B	821	CLA	C2A-CAA-CBA-CGA
20	L	205	BCR	C37-C22-C23-C24
17	B	810	CLA	C16-C17-C18-C20
23	B	851	DGD	CBA-CCA-CDA-CEA
17	A	807	CLA	C4-C3-C5-C6
24	J	106	3XQ	C21-C22-C24-O25
17	A	811	CLA	C1A-C2A-CAA-CBA
17	A	825	CLA	C1A-C2A-CAA-CBA
17	A	827	CLA	C1A-C2A-CAA-CBA
17	A	832	CLA	C1A-C2A-CAA-CBA
17	B	803	CLA	C1A-C2A-CAA-CBA
17	B	834	CLA	C1A-C2A-CAA-CBA
17	B	842	CLA	C1A-C2A-CAA-CBA
17	O	204	CLA	C1A-C2A-CAA-CBA
19	A	841	LHG	C1-C2-C3-O3
17	A	837	CLA	CAA-CBA-CGA-O1A
17	B	831	CLA	C2-C1-O2A-CGA
24	J	106	3XQ	C7-C8-C9-C10
17	3	209	CLA	CAA-CBA-CGA-O2A
17	B	831	CLA	CAA-CBA-CGA-O1A
19	A	841	LHG	C14-C15-C16-C17
17	B	806	CLA	C3-C5-C6-C7
17	B	809	CLA	C3-C5-C6-C7
17	B	803	CLA	CAA-CBA-CGA-O1A
17	B	835	CLA	CAA-CBA-CGA-O1A
19	A	841	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
19	A	842	LHG	C3-O3-P-O5
17	A	823	CLA	CAA-CBA-CGA-O1A
17	A	831	CLA	CAA-CBA-CGA-O1A
17	B	809	CLA	CAA-CBA-CGA-O1A
17	2	608	CLA	CAA-CBA-CGA-O1A
20	B	848	BCR	C23-C24-C25-C26
25	2	616	ZEX	C5-C6-C7-C8
25	4	616	ZEX	C1-C6-C7-C8
17	B	816	CLA	CAA-CBA-CGA-O1A
17	2	602	CLA	CAA-CBA-CGA-O1A
17	3	203	CLA	CAA-CBA-CGA-O1A
17	B	801	CLA	CAA-CBA-CGA-O2A
20	K	104	BCR	C10-C11-C12-C13
17	5	613	CLA	CAA-CBA-CGA-O1A
17	A	810	CLA	CAA-CBA-CGA-O1A
17	B	810	CLA	CAA-CBA-CGA-O1A
17	B	843	CLA	CAA-CBA-CGA-O1A
17	2	602	CLA	C4-C3-C5-C6
17	B	843	CLA	C2-C3-C5-C6
17	B	833	CLA	CAA-CBA-CGA-O2A
17	2	606	CLA	CAA-CBA-CGA-O2A
17	A	818	CLA	CAD-CBD-CGD-O1D
17	A	831	CLA	CAD-CBD-CGD-O1D
17	A	848	CLA	CAD-CBD-CGD-O1D
17	B	832	CLA	CAD-CBD-CGD-O1D
17	O	201	CLA	CAD-CBD-CGD-O1D
17	4	602	CLA	CAD-CBD-CGD-O1D
17	4	609	CLA	CAD-CBD-CGD-O1D
17	B	842	CLA	O1A-CGA-O2A-C1
17	B	813	CLA	CAA-CBA-CGA-O1A
23	B	851	DGD	O1B-C1B-C2B-C3B
17	A	827	CLA	C15-C16-C17-C18
17	L	203	CLA	C8-C10-C11-C12
17	A	837	CLA	C11-C12-C13-C14
17	B	812	CLA	C11-C12-C13-C14
23	B	851	DGD	CFB-CGB-CHB-CIB
17	A	832	CLA	CAA-CBA-CGA-O2A
19	A	842	LHG	C24-C25-C26-C27
17	1	611	CLA	C2A-CAA-CBA-CGA
17	3	210	CLA	C2C-C3C-CAC-CBC
17	B	813	CLA	C3-C5-C6-C7
17	A	804	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	B	822	CLA	C4-C3-C5-C6
16	A	801	CL0	C12-C13-C15-C16
17	A	804	CLA	C3A-C2A-CAA-CBA
17	A	806	CLA	C11-C10-C8-C7
17	A	807	CLA	C11-C12-C13-C15
17	A	837	CLA	C11-C12-C13-C15
17	B	801	CLA	C2-C3-C5-C6
17	B	808	CLA	C11-C12-C13-C15
17	B	810	CLA	C12-C13-C15-C16
17	B	813	CLA	C12-C13-C15-C16
17	B	827	CLA	C6-C7-C8-C10
17	B	832	CLA	C12-C13-C15-C16
17	B	842	CLA	C12-C13-C15-C16
17	3	211	CLA	C3A-C2A-CAA-CBA
17	5	602	CLA	C3A-C2A-CAA-CBA
17	A	807	CLA	CAA-CBA-CGA-O1A
17	A	821	CLA	CAA-CBA-CGA-O1A
17	F	302	CLA	CAA-CBA-CGA-O2A
17	4	610	CLA	CAA-CBA-CGA-O1A
17	A	807	CLA	CAA-CBA-CGA-O2A
17	A	825	CLA	CAA-CBA-CGA-O2A
20	B	848	BCR	C21-C22-C23-C24
17	B	820	CLA	CAA-CBA-CGA-O1A
17	3	209	CLA	CAA-CBA-CGA-O1A
17	2	605	CLA	CAA-CBA-CGA-O1A
17	5	607	CLA	CAA-CBA-CGA-O1A
17	B	808	CLA	CAA-CBA-CGA-O2A
23	B	851	DGD	O6E-C1E-O5D-C6D
17	A	804	CLA	CAA-CBA-CGA-O1A
17	A	832	CLA	CAA-CBA-CGA-O1A
17	B	819	CLA	CAA-CBA-CGA-O2A
17	3	213	CLA	CAA-CBA-CGA-O2A
19	A	841	LHG	C25-C26-C27-C28
17	5	607	CLA	CAA-CBA-CGA-O2A
17	A	824	CLA	C5-C6-C7-C8

There are no ring outliers.

196 monomers are involved in 583 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	3	210	CLA	1	0
17	2	606	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	810	CLA	4	0
16	A	801	CLO	59	0
17	1	612	CLA	2	0
17	2	610	CLA	2	0
17	A	813	CLA	2	0
17	B	841	CLA	9	0
17	A	822	CLA	2	0
17	2	601	CLA	4	0
17	J	102	CLA	4	0
17	2	605	CLA	2	0
17	B	828	CLA	4	0
17	2	612	CLA	1	0
17	A	838	CLA	9	0
17	A	804	CLA	5	0
25	4	613	ZEX	4	0
17	4	607	CLA	1	0
17	3	209	CLA	2	0
17	A	810	CLA	3	0
17	5	607	CLA	3	0
17	5	603	CLA	7	0
26	3	219	IDO	1	0
17	B	827	CLA	6	0
17	1	607	CLA	2	0
20	L	206	BCR	2	0
17	B	820	CLA	4	0
17	1	602	CLA	2	0
20	A	846	BCR	6	0
17	B	831	CLA	9	0
20	J	105	BCR	2	0
17	B	842	CLA	14	0
17	3	207	CLA	4	0
17	B	812	CLA	7	0
17	B	824	CLA	3	0
17	2	602	CLA	6	0
17	A	820	CLA	1	0
17	B	801	CLA	11	0
17	A	835	CLA	1	0
17	4	609	CLA	3	0
20	A	844	BCR	1	0
17	A	807	CLA	5	0
17	A	817	CLA	8	0
17	O	205	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	3	214	ZEX	3	0
17	B	808	CLA	3	0
17	1	603	CLA	2	0
17	3	212	CLA	3	0
17	B	832	CLA	5	0
17	A	836	CLA	8	0
17	B	818	CLA	3	0
17	5	612	CLA	2	0
17	A	823	CLA	5	0
17	J	103	CLA	1	0
17	A	848	CLA	9	0
17	2	613	CLA	1	0
17	3	204	CLA	3	0
17	B	811	CLA	4	0
17	F	302	CLA	3	0
17	L	204	CLA	1	0
17	B	809	CLA	6	0
25	3	217	ZEX	1	0
20	B	849	BCR	2	0
17	A	830	CLA	3	0
17	4	611	CLA	5	0
17	B	839	CLA	5	0
17	3	205	CLA	2	0
25	1	613	ZEX	3	0
25	1	615	ZEX	2	0
17	1	601	CLA	3	0
17	J	101	CLA	6	0
17	3	203	CLA	8	0
17	B	804	CLA	9	0
17	A	833	CLA	4	0
25	3	201	ZEX	4	0
17	B	816	CLA	7	0
19	A	842	LHG	3	0
17	F	301	CLA	1	0
17	L	202	CLA	1	0
17	B	834	CLA	1	0
17	A	802	CLA	1	0
20	B	845	BCR	1	0
20	B	848	BCR	4	0
17	3	206	CLA	5	0
17	4	601	CLA	3	0
20	A	845	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	803	CLA	7	0
17	5	601	CLA	2	0
25	1	617	ZEX	4	0
17	A	816	CLA	5	0
17	L	203	CLA	4	0
17	5	611	CLA	1	0
17	A	819	CLA	5	0
17	4	608	CLA	4	0
25	2	617	ZEX	2	0
20	B	846	BCR	2	0
17	A	827	CLA	5	0
17	5	608	CLA	2	0
25	5	617	ZEX	8	0
17	B	803	CLA	2	0
25	4	614	ZEX	6	0
17	A	806	CLA	8	0
18	A	840	PQN	4	0
17	K	102	CLA	1	0
17	5	605	CLA	2	0
25	4	612	ZEX	3	0
17	4	602	CLA	2	0
25	5	615	ZEX	1	0
25	5	614	ZEX	4	0
20	O	202	BCR	5	0
17	B	813	CLA	4	0
17	A	831	CLA	11	0
17	A	811	CLA	4	0
17	B	835	CLA	7	0
23	B	851	DGD	5	0
17	B	830	CLA	7	0
17	5	604	CLA	2	0
17	B	825	CLA	1	0
17	B	838	CLA	4	0
25	1	614	ZEX	8	0
17	K	103	CLA	1	0
17	B	814	CLA	2	0
17	1	604	CLA	1	0
17	4	604	CLA	3	0
17	A	825	CLA	5	0
25	2	614	ZEX	4	0
17	A	837	CLA	4	0
17	B	833	CLA	3	0

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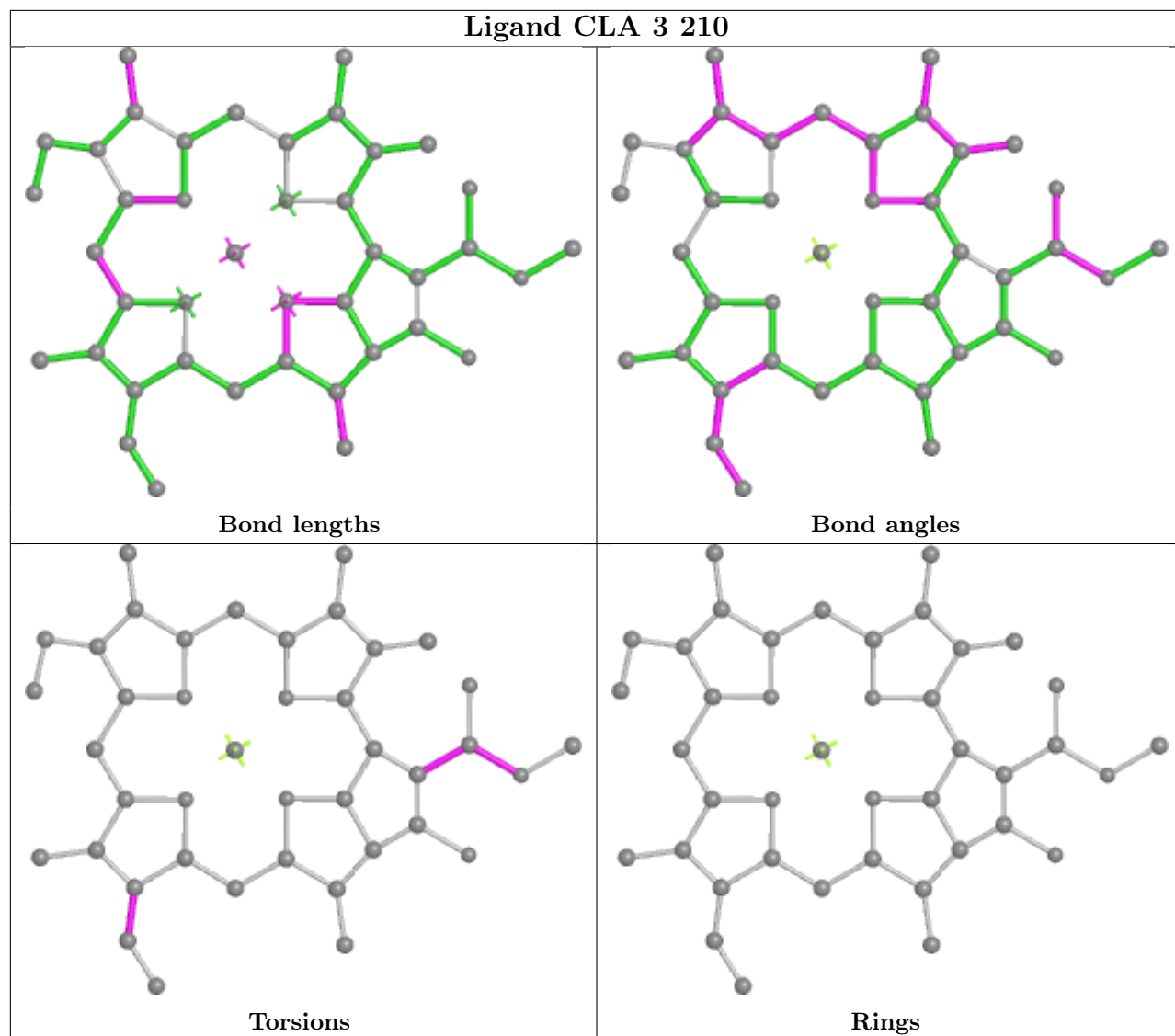
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	808	CLA	3	0
20	B	850	BCR	4	0
17	5	606	CLA	4	0
17	B	826	CLA	2	0
17	1	606	CLA	4	0
17	2	604	CLA	2	0
17	A	839	CLA	5	0
17	2	603	CLA	2	0
18	B	844	PQN	3	0
25	3	216	ZEX	1	0
17	B	821	CLA	5	0
17	1	611	CLA	1	0
20	K	104	BCR	5	0
17	1	610	CLA	1	0
20	B	847	BCR	6	0
20	L	201	BCR	3	0
17	A	821	CLA	1	0
20	L	205	BCR	6	0
17	A	826	CLA	10	0
20	I	101	BCR	4	0
25	4	615	ZEX	2	0
17	2	609	CLA	2	0
17	A	812	CLA	1	0
17	B	840	CLA	3	0
17	B	829	CLA	6	0
21	C	102	SF4	1	0
17	B	819	CLA	3	0
17	B	836	CLA	5	0
17	B	843	CLA	4	0
17	O	201	CLA	1	0
17	1	609	CLA	1	0
17	2	607	CLA	1	0
20	K	101	BCR	6	0
17	3	208	CLA	2	0
17	B	802	CLA	8	0
25	4	616	ZEX	2	0
25	1	616	ZEX	2	0
25	5	616	ZEX	3	0
17	A	805	CLA	5	0
17	B	817	CLA	2	0
17	A	824	CLA	3	0
25	2	616	ZEX	1	0

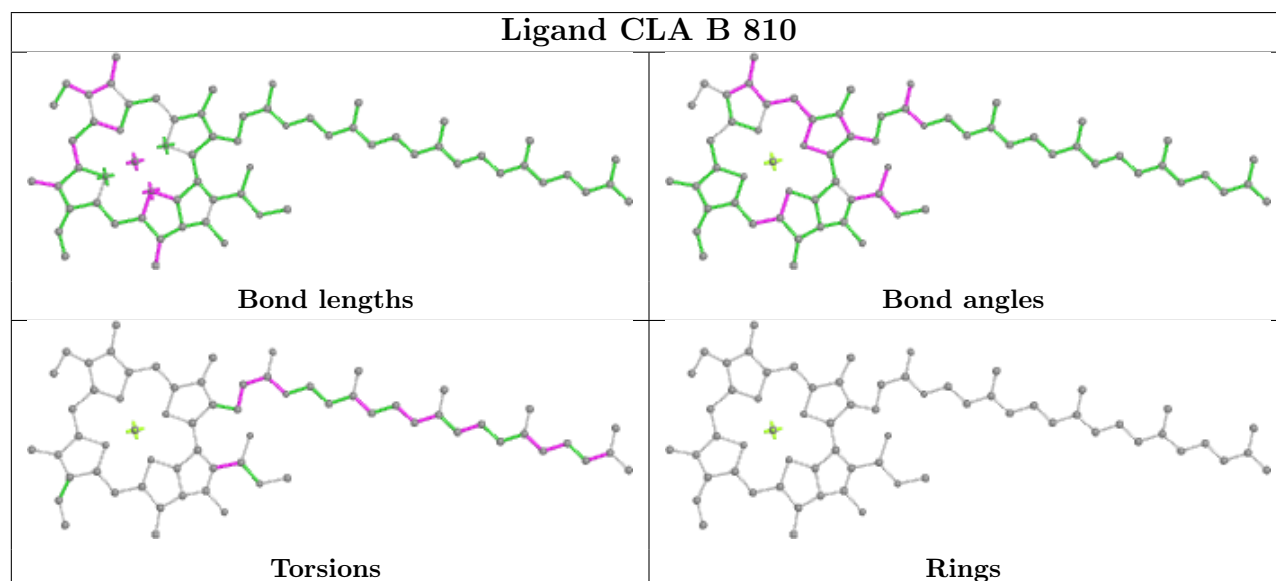
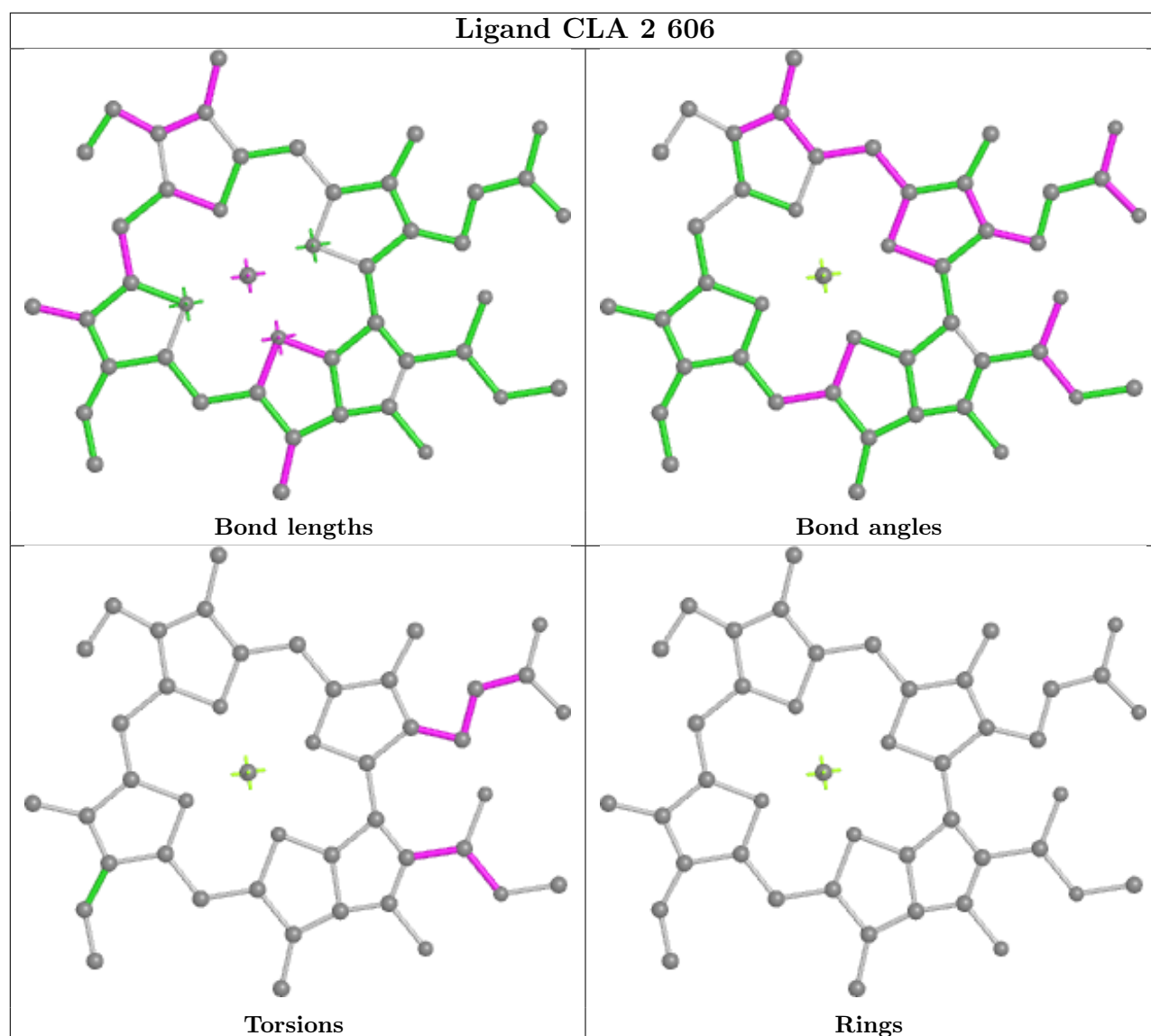
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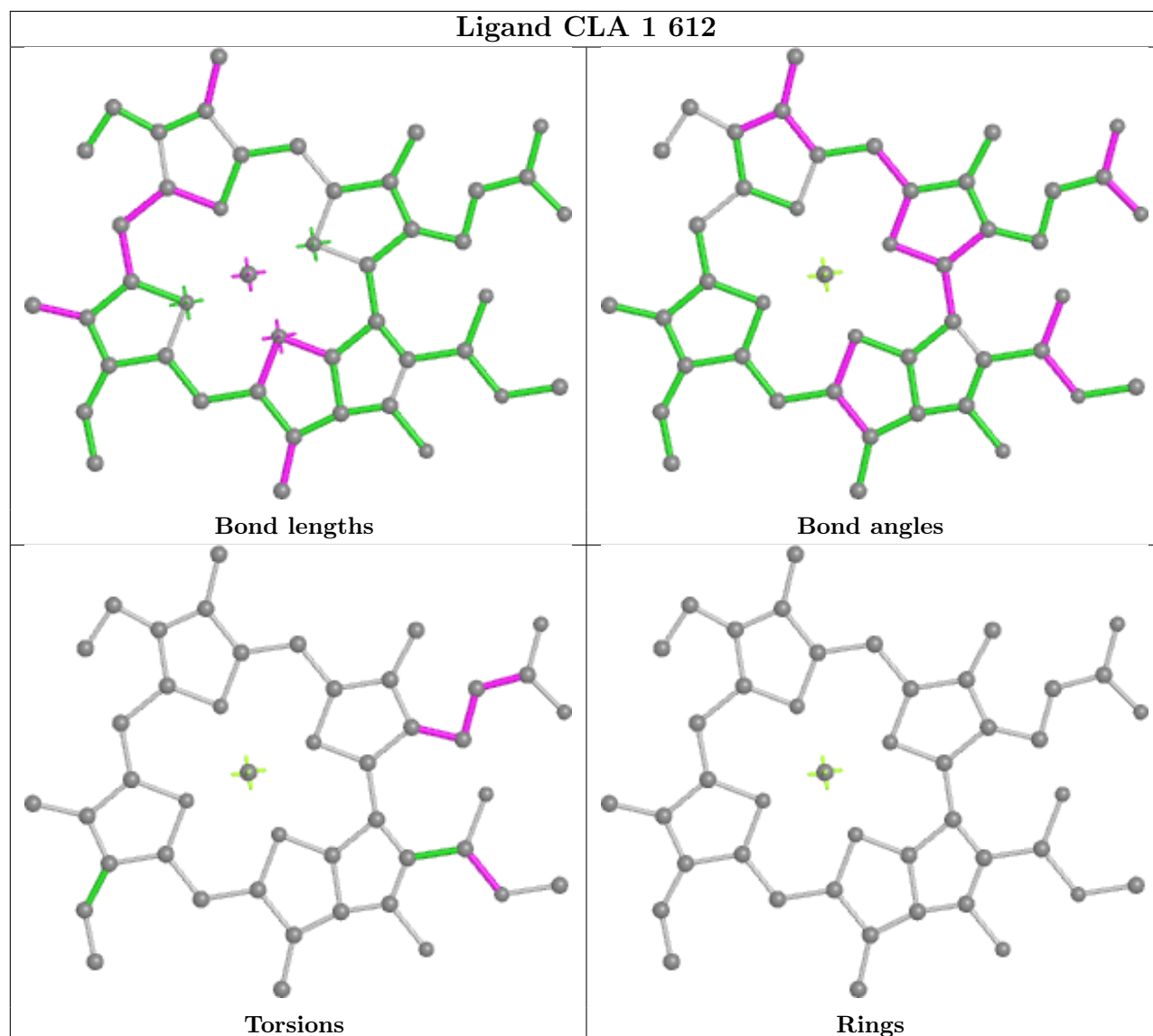
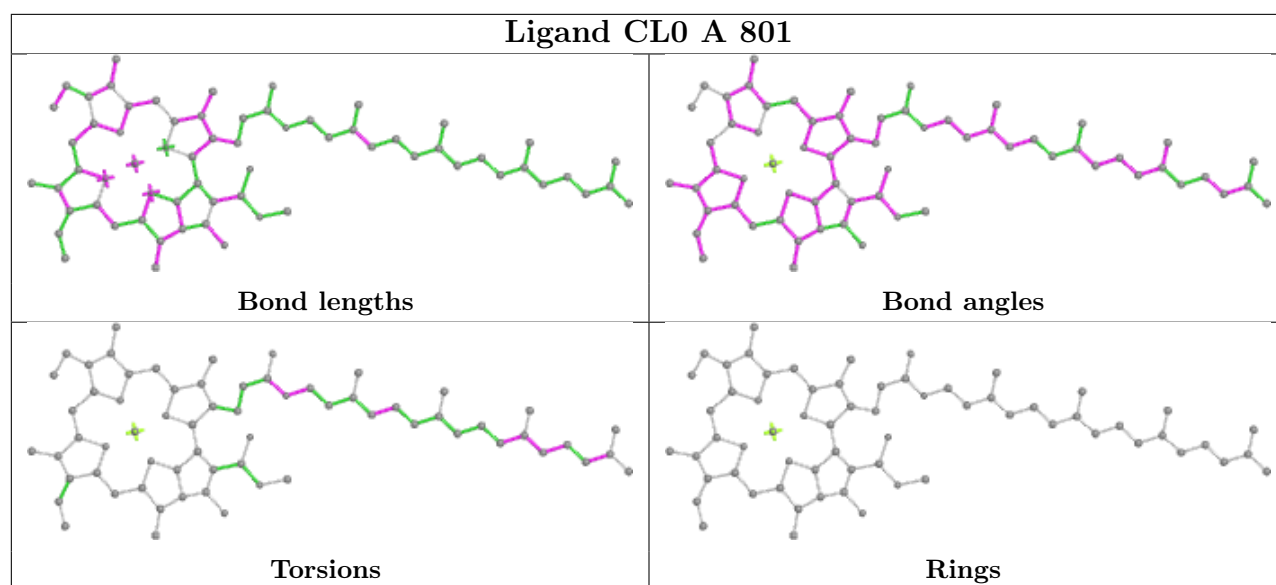
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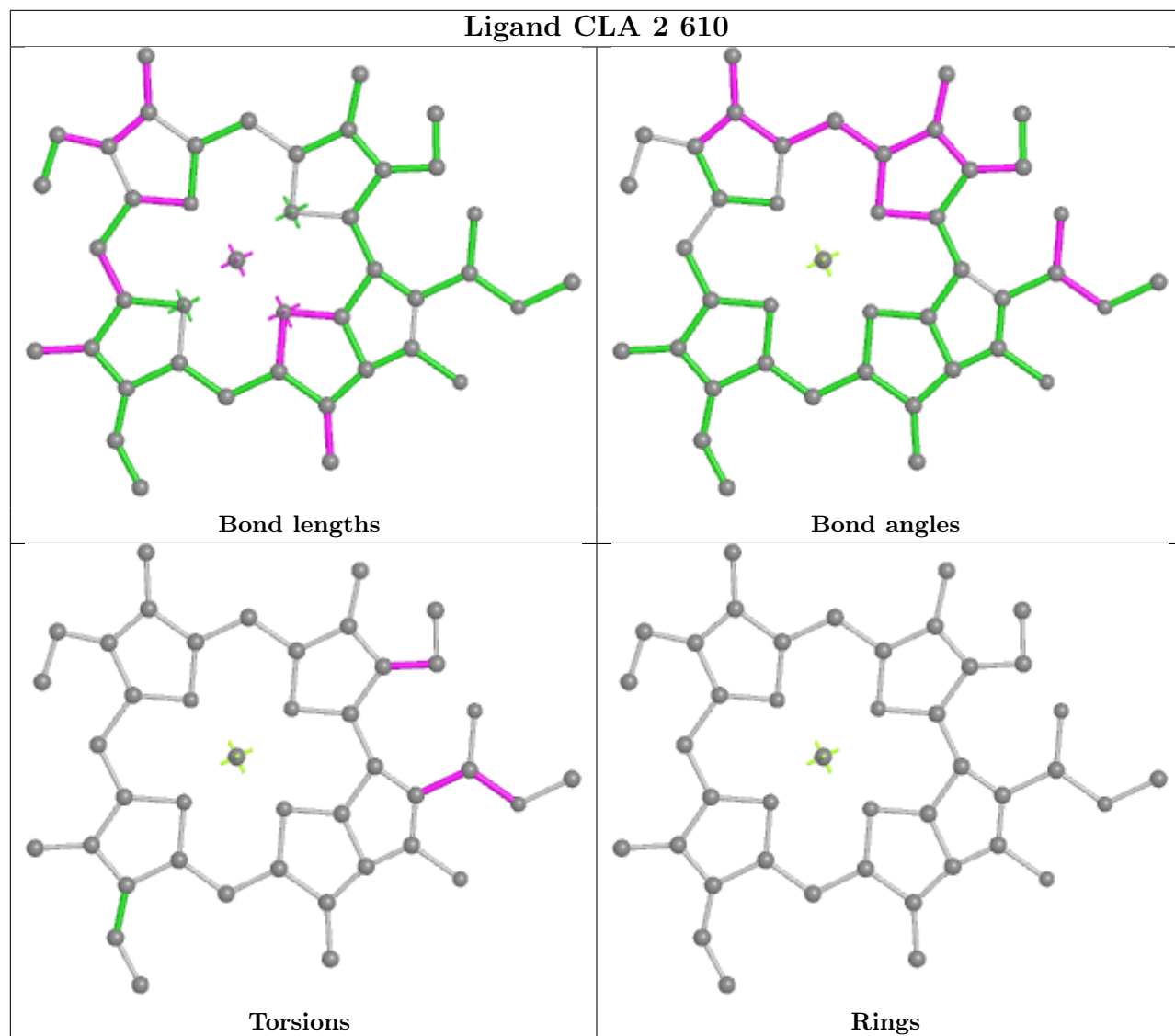
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	4	606	CLA	3	0
17	A	832	CLA	4	0
17	A	818	CLA	4	0
25	2	615	ZEX	4	0
17	A	828	CLA	5	0
17	A	815	CLA	4	0
17	O	204	CLA	2	0
20	A	843	BCR	5	0
17	B	822	CLA	4	0
17	A	814	CLA	1	0
17	B	806	CLA	11	0
17	A	829	CLA	2	0
25	3	215	ZEX	6	0
17	A	809	CLA	3	0
17	5	609	CLA	1	0
21	C	101	SF4	1	0
17	A	834	CLA	6	0
19	A	841	LHG	3	0
17	2	608	CLA	2	0
20	F	304	BCR	2	0
20	J	104	BCR	4	0
25	4	617	ZEX	1	0
17	5	602	CLA	2	0
25	3	218	ZEX	6	0
20	B	805	BCR	6	0
17	B	837	CLA	2	0

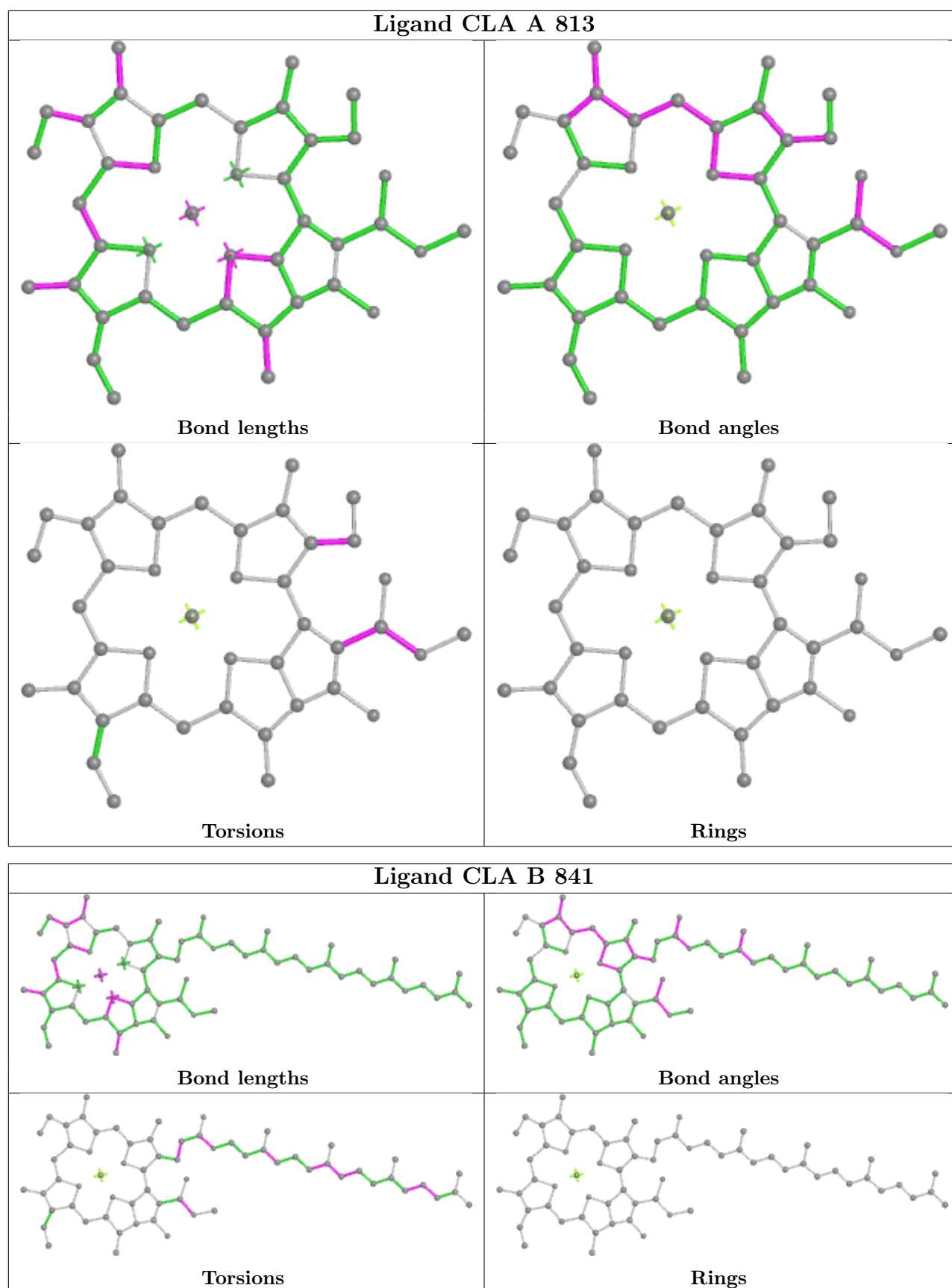
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

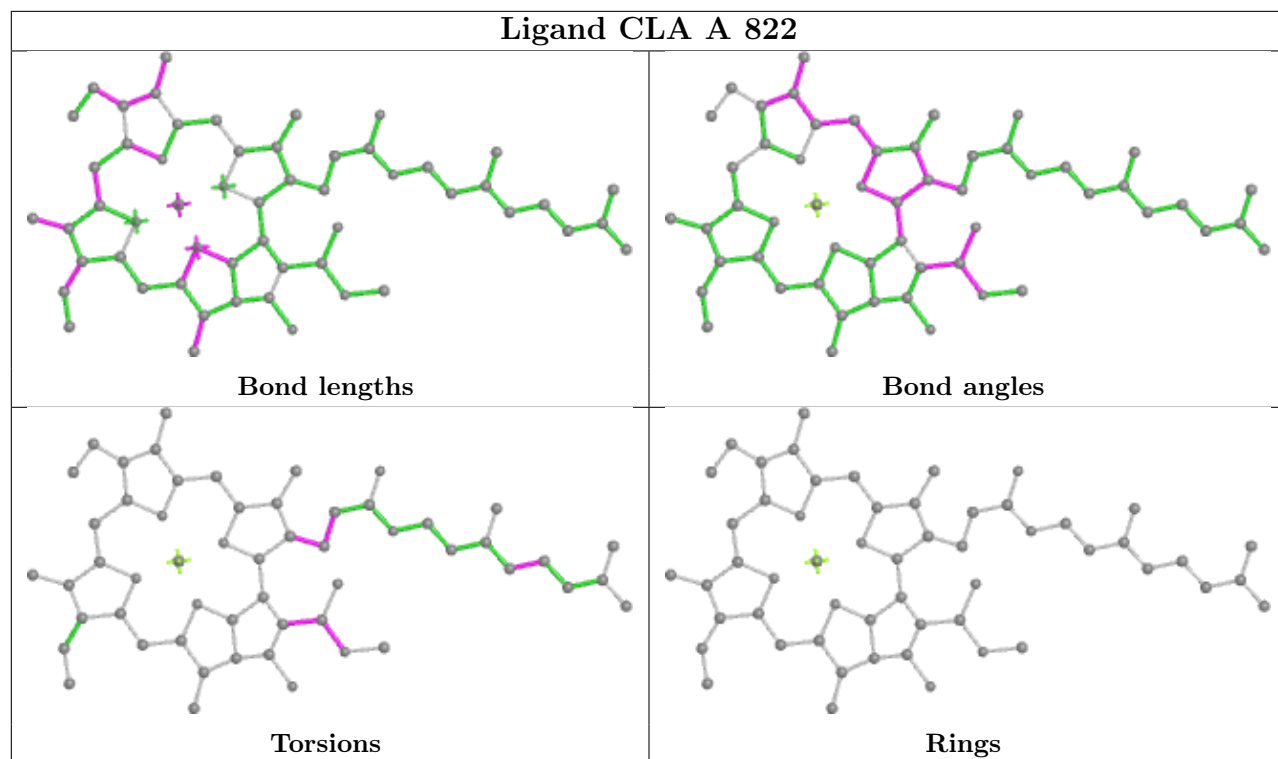


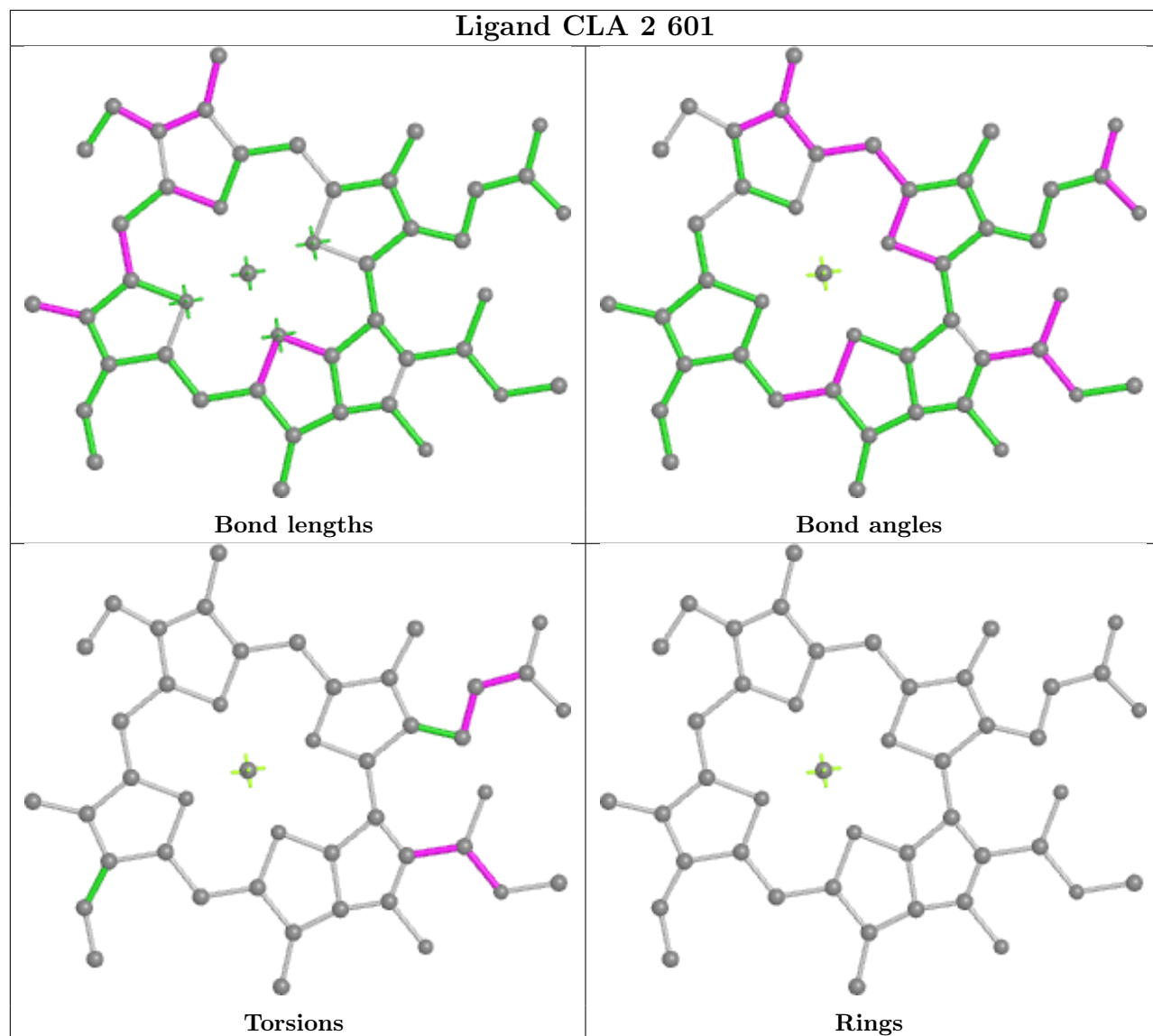


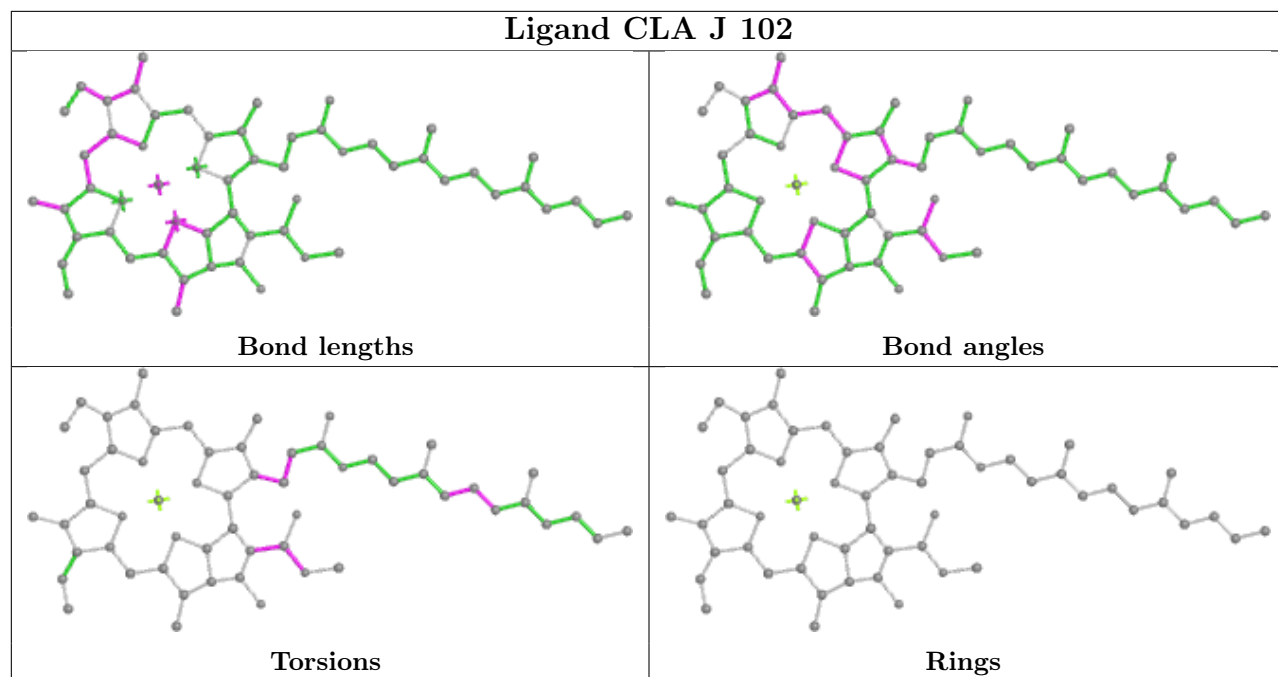


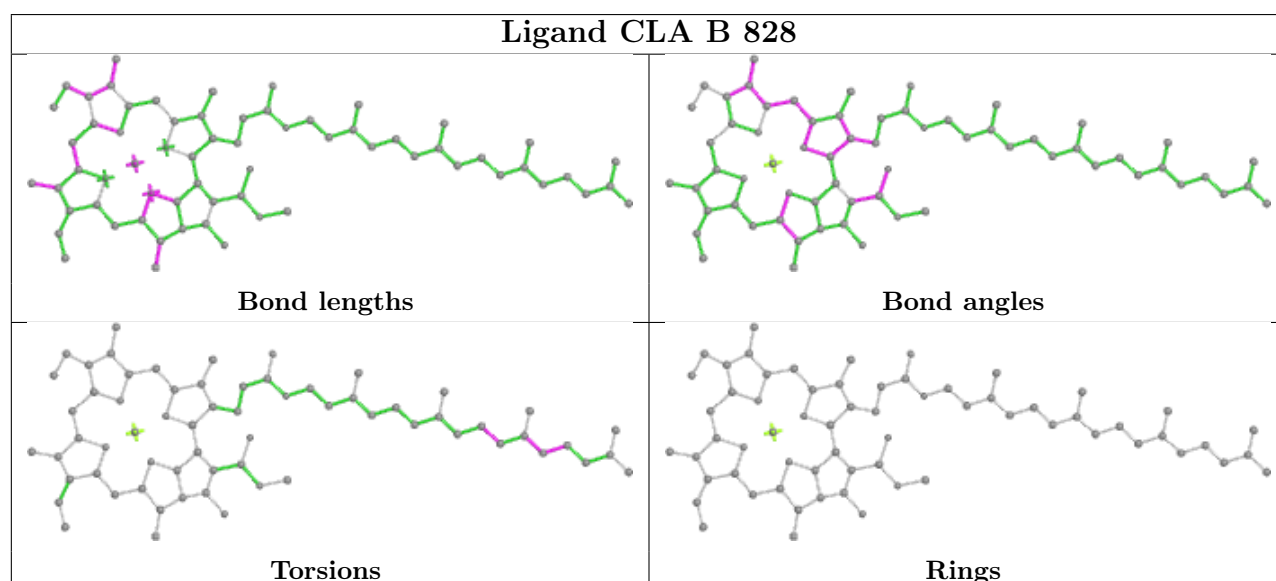
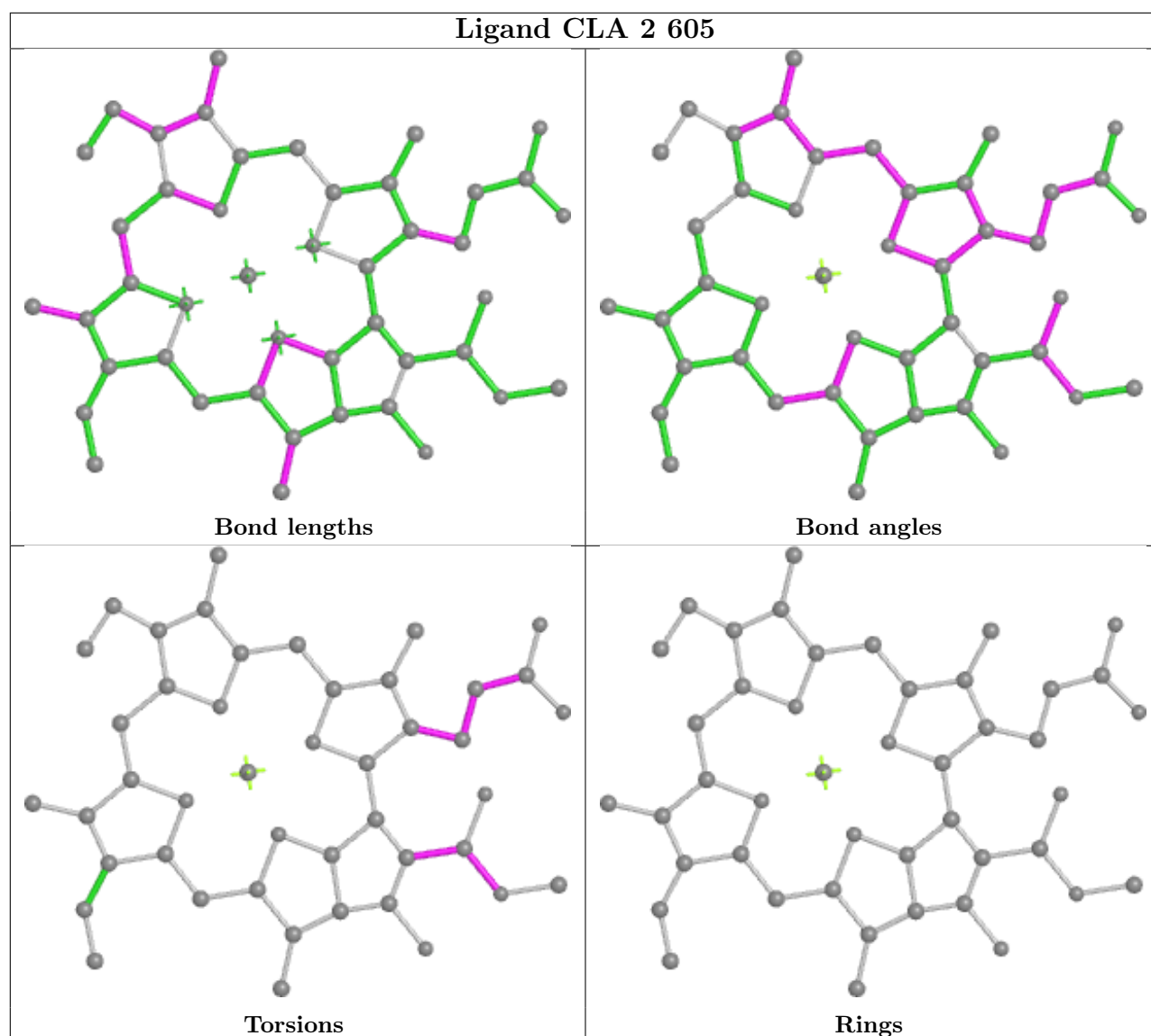


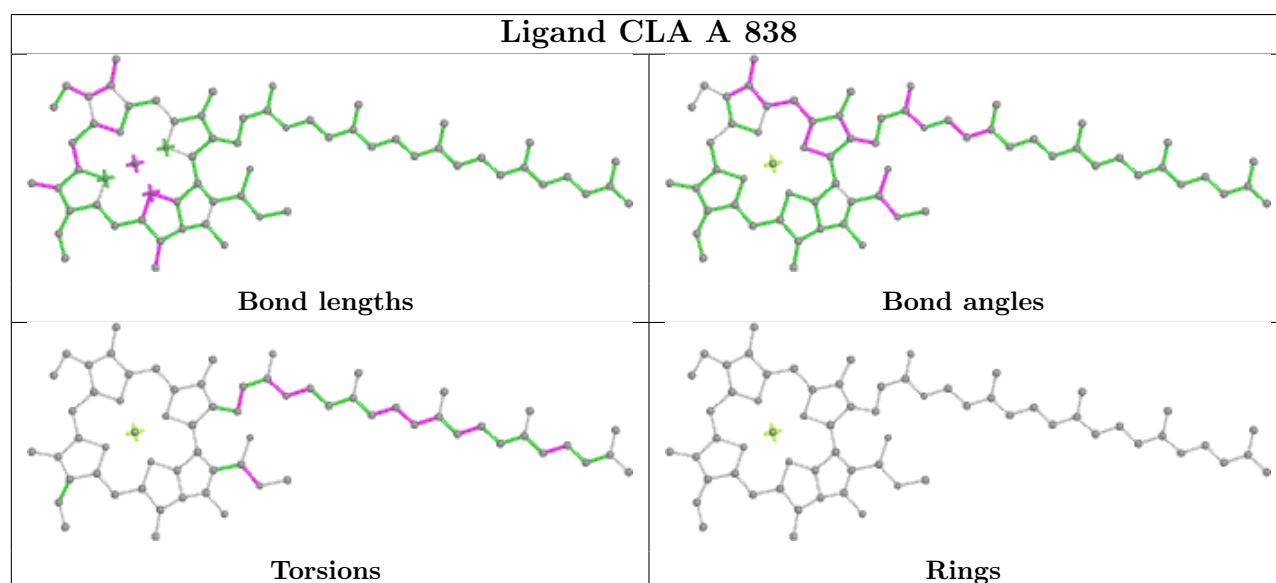
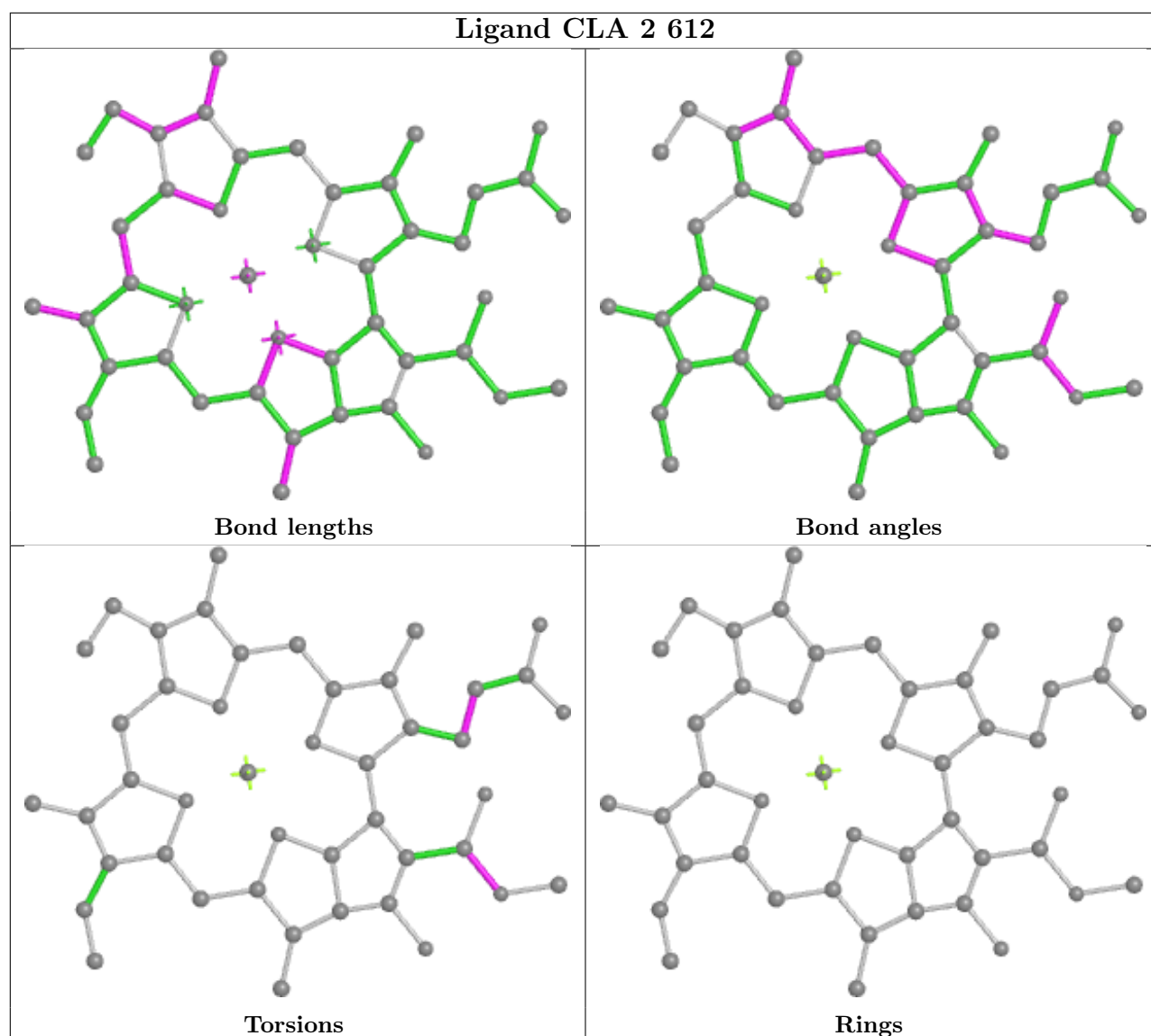


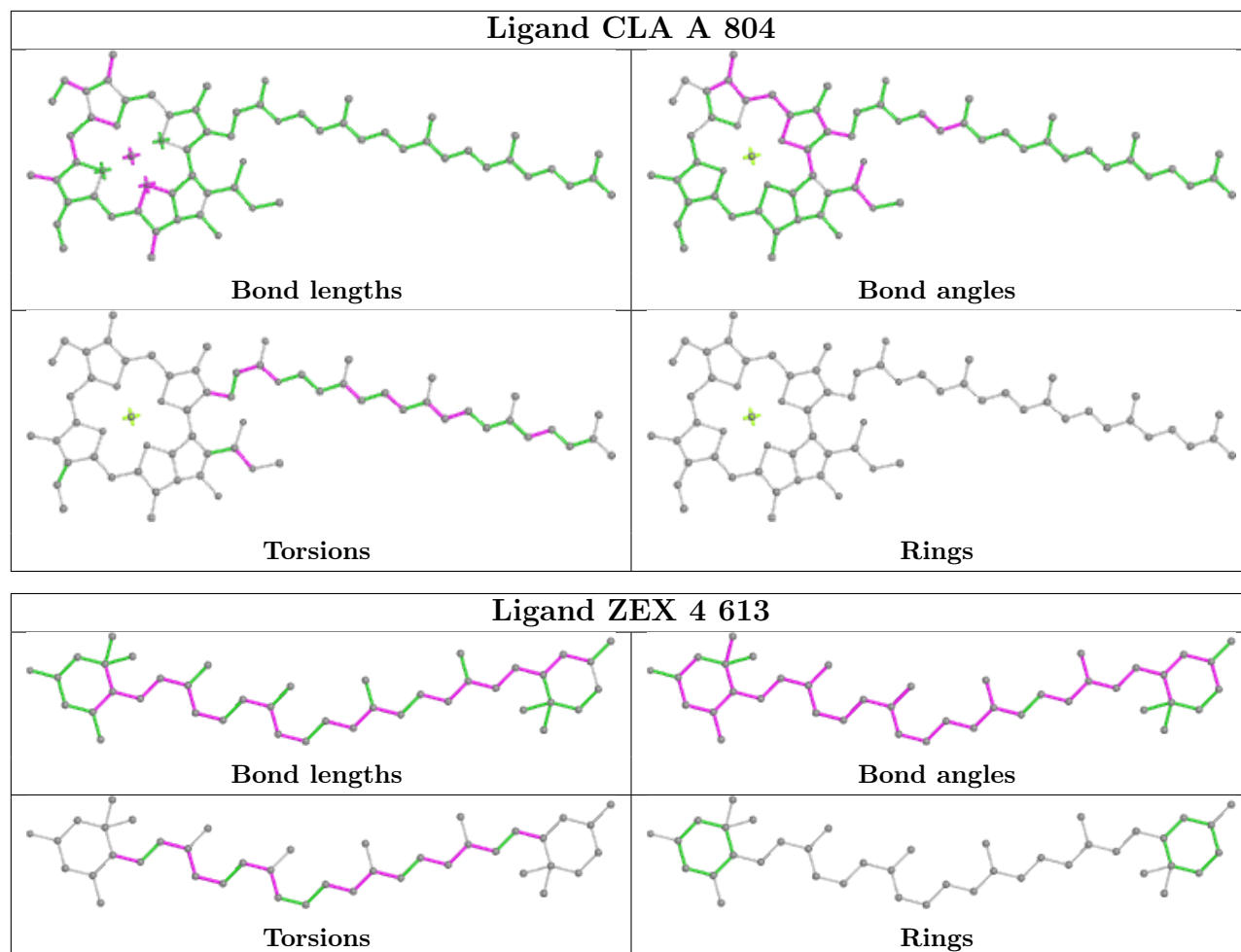


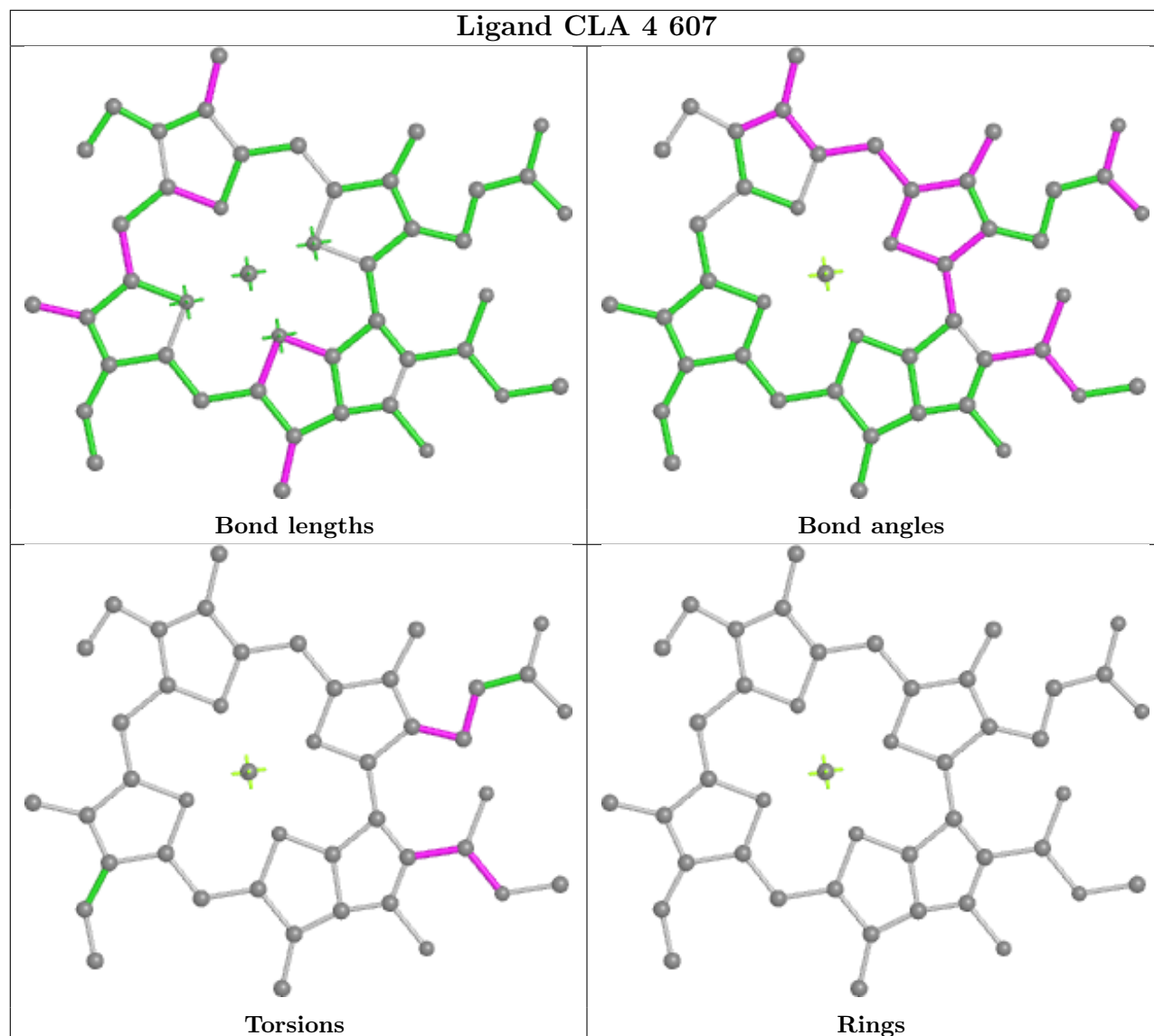


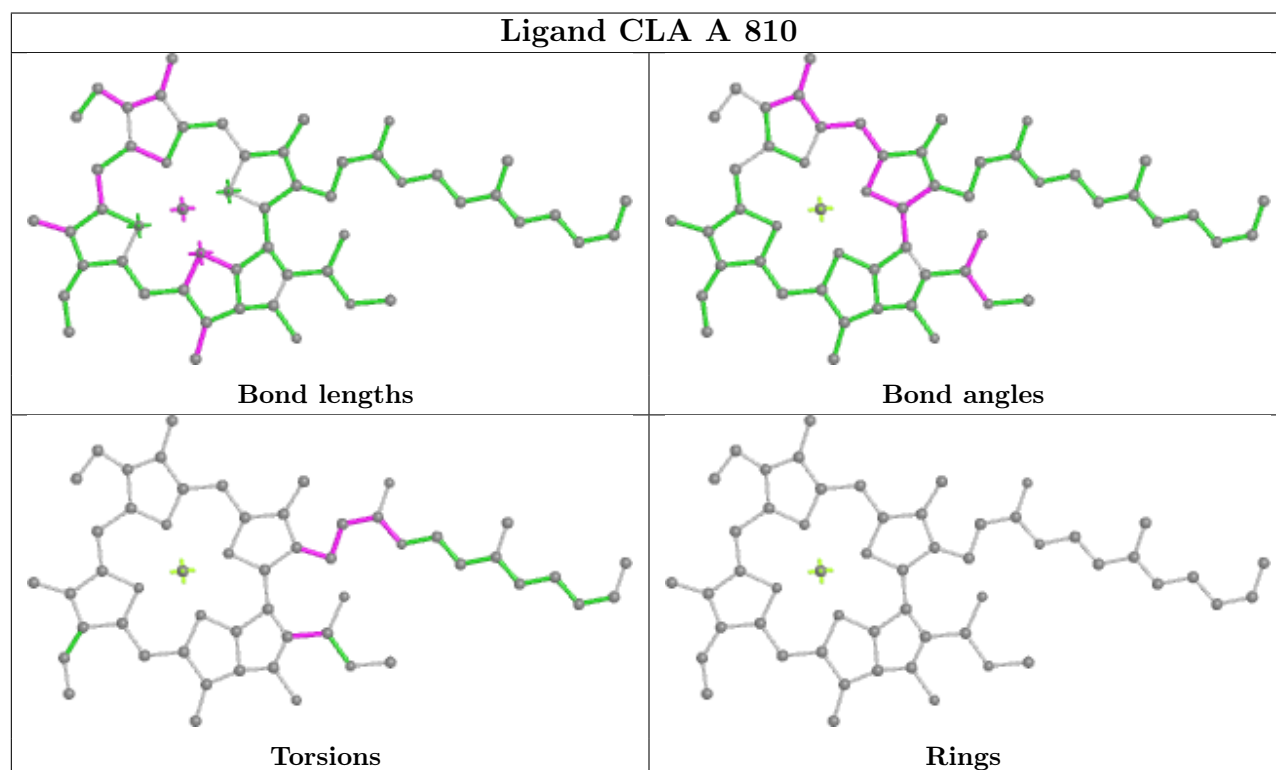
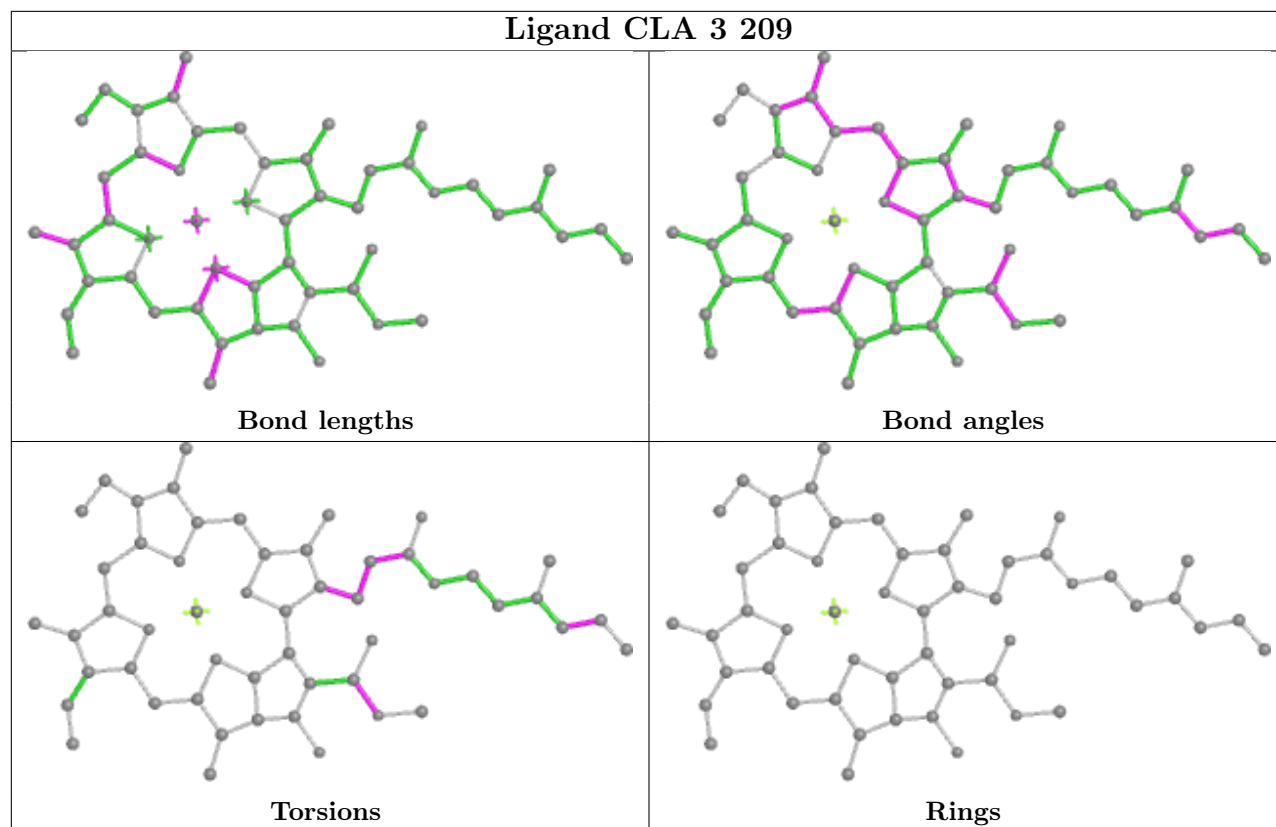




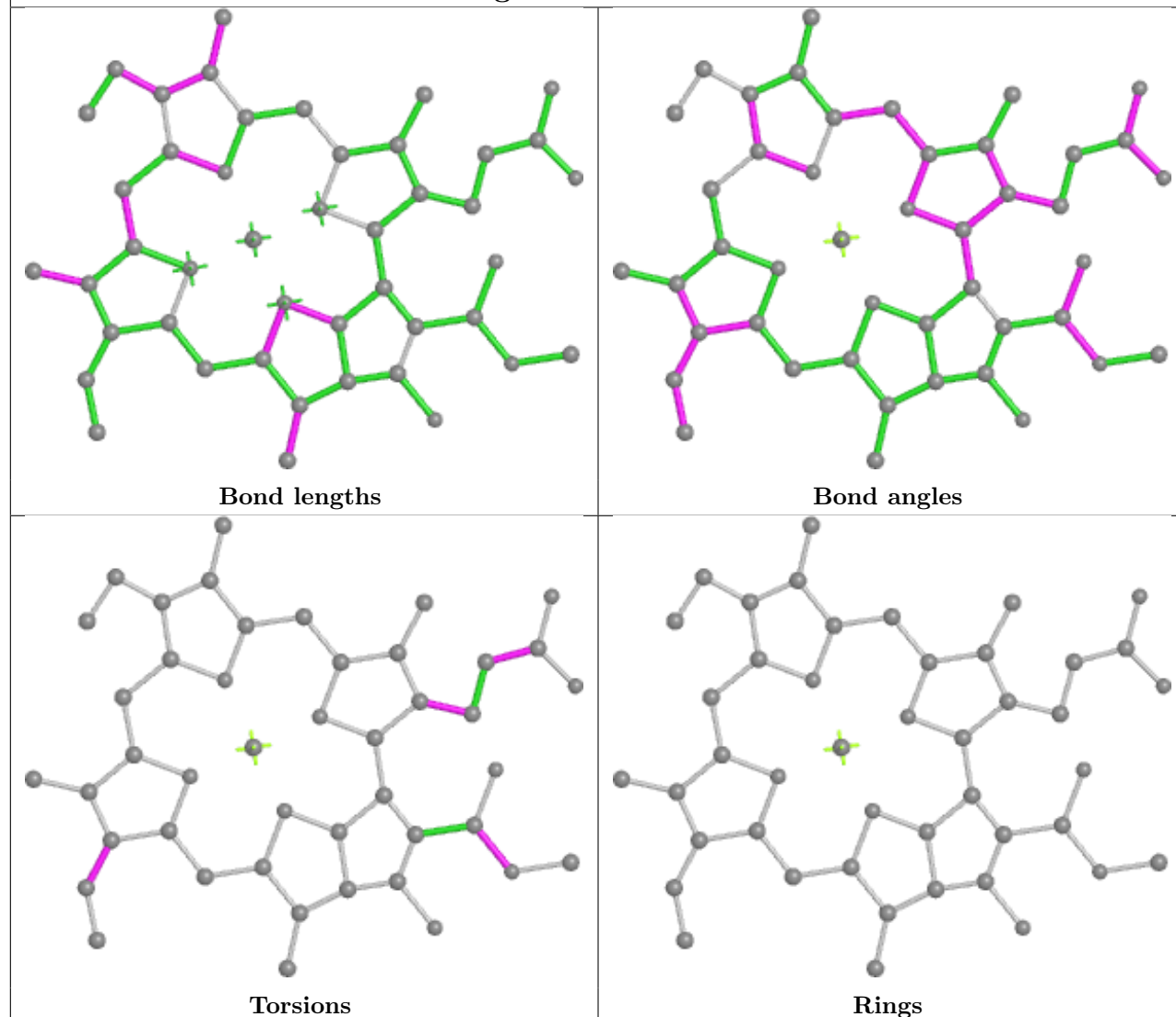




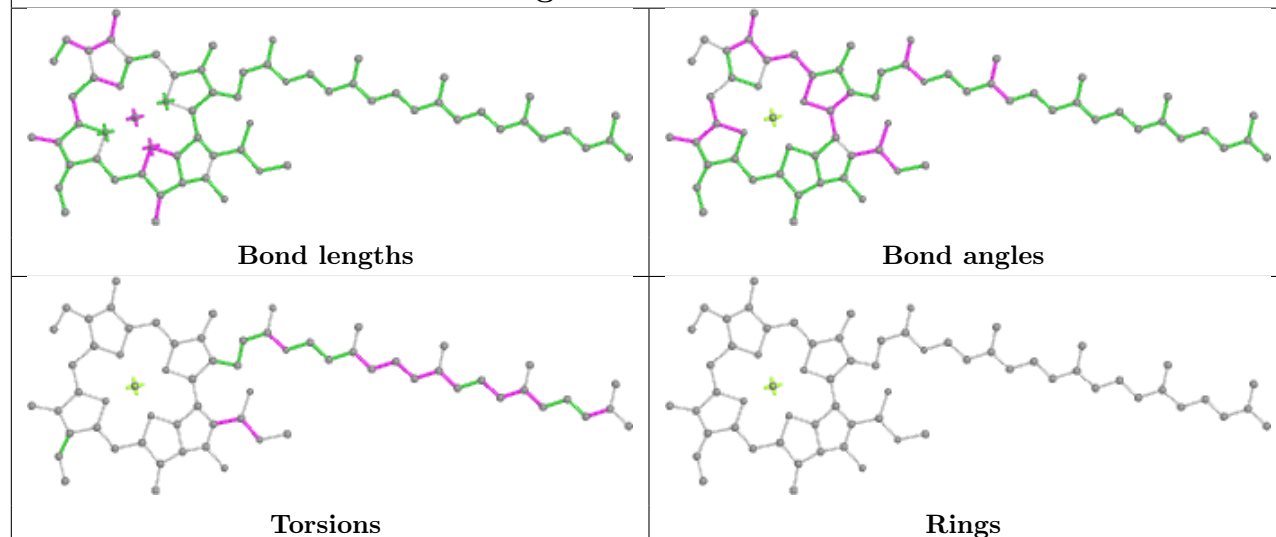


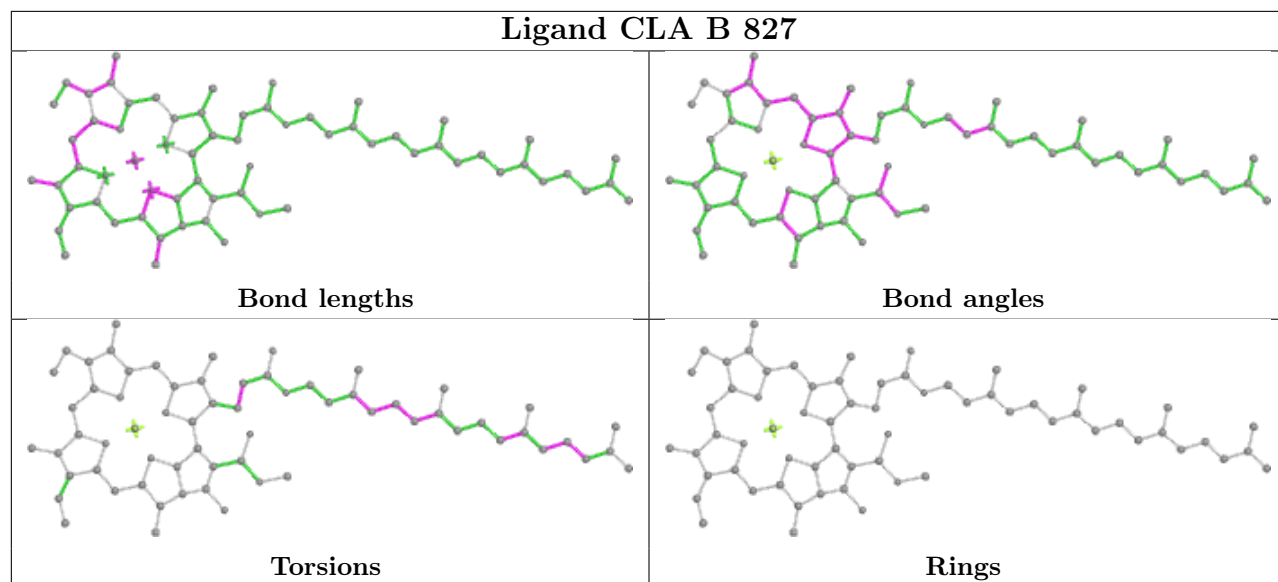


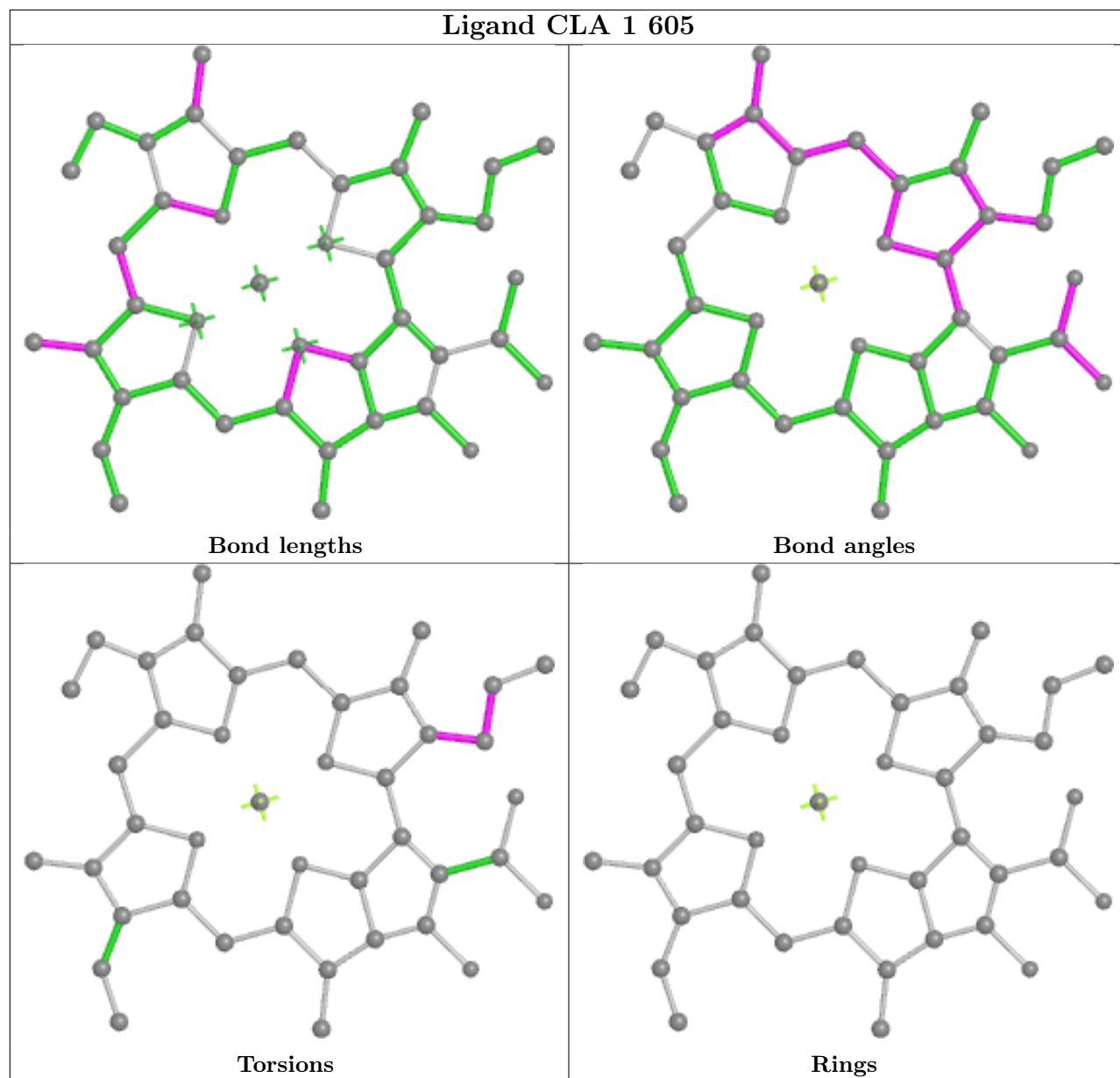
Ligand CLA 5 607

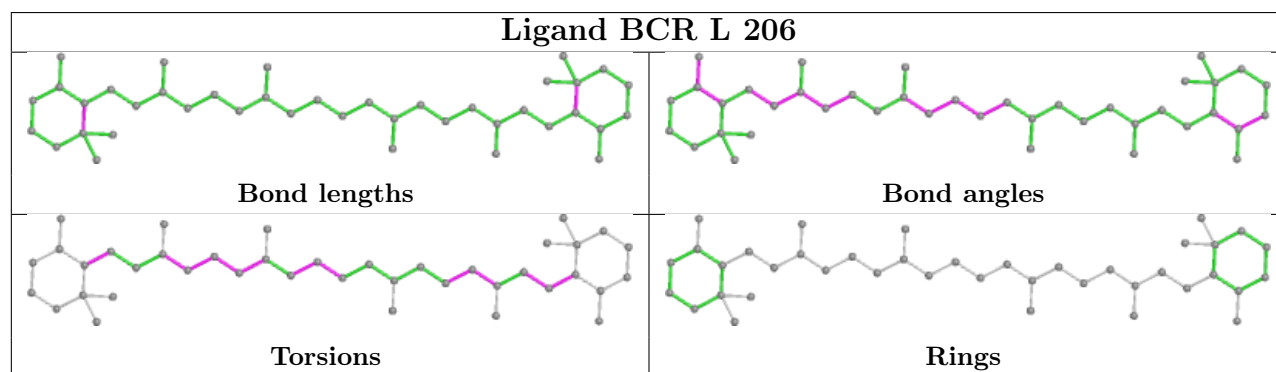
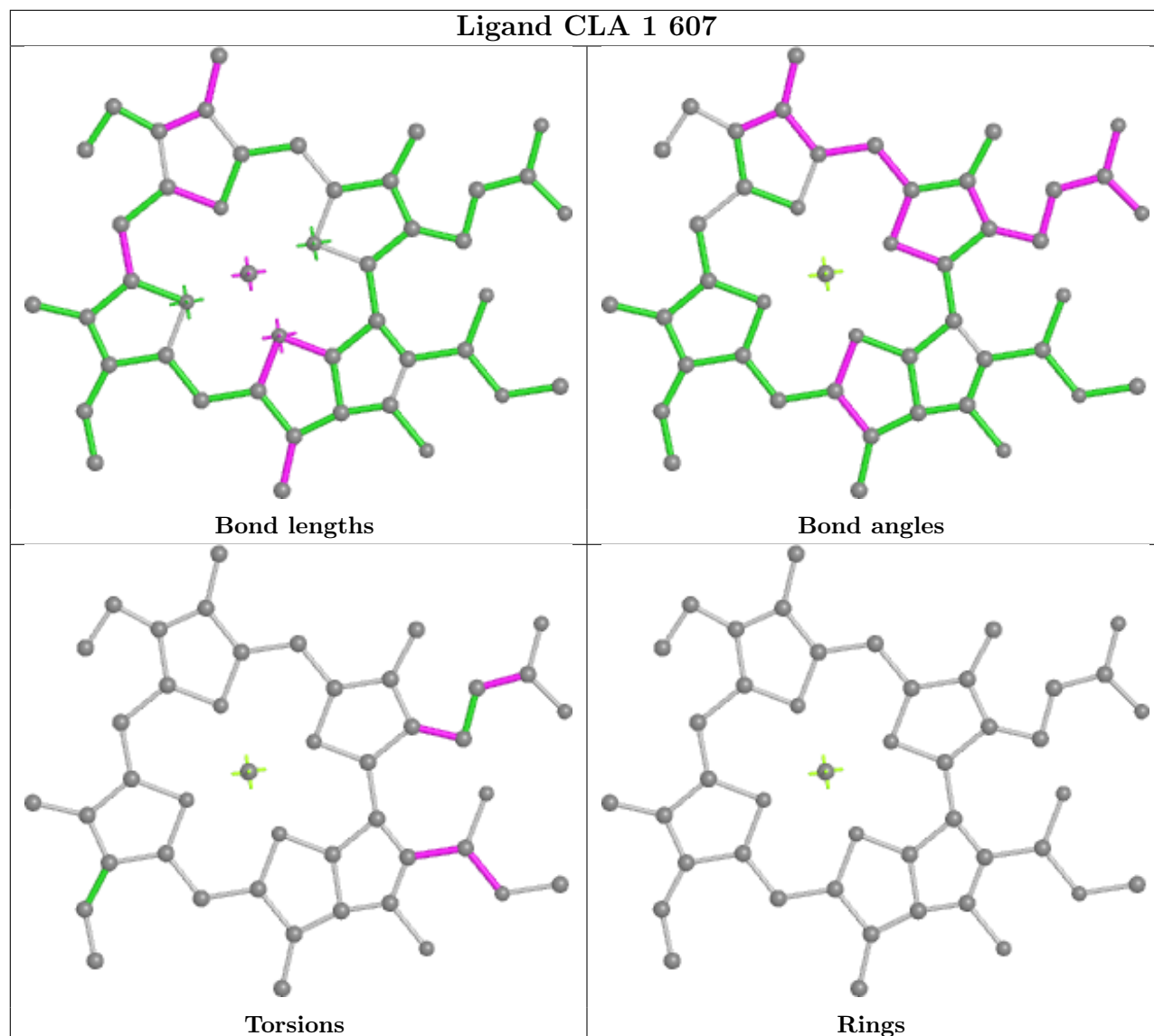


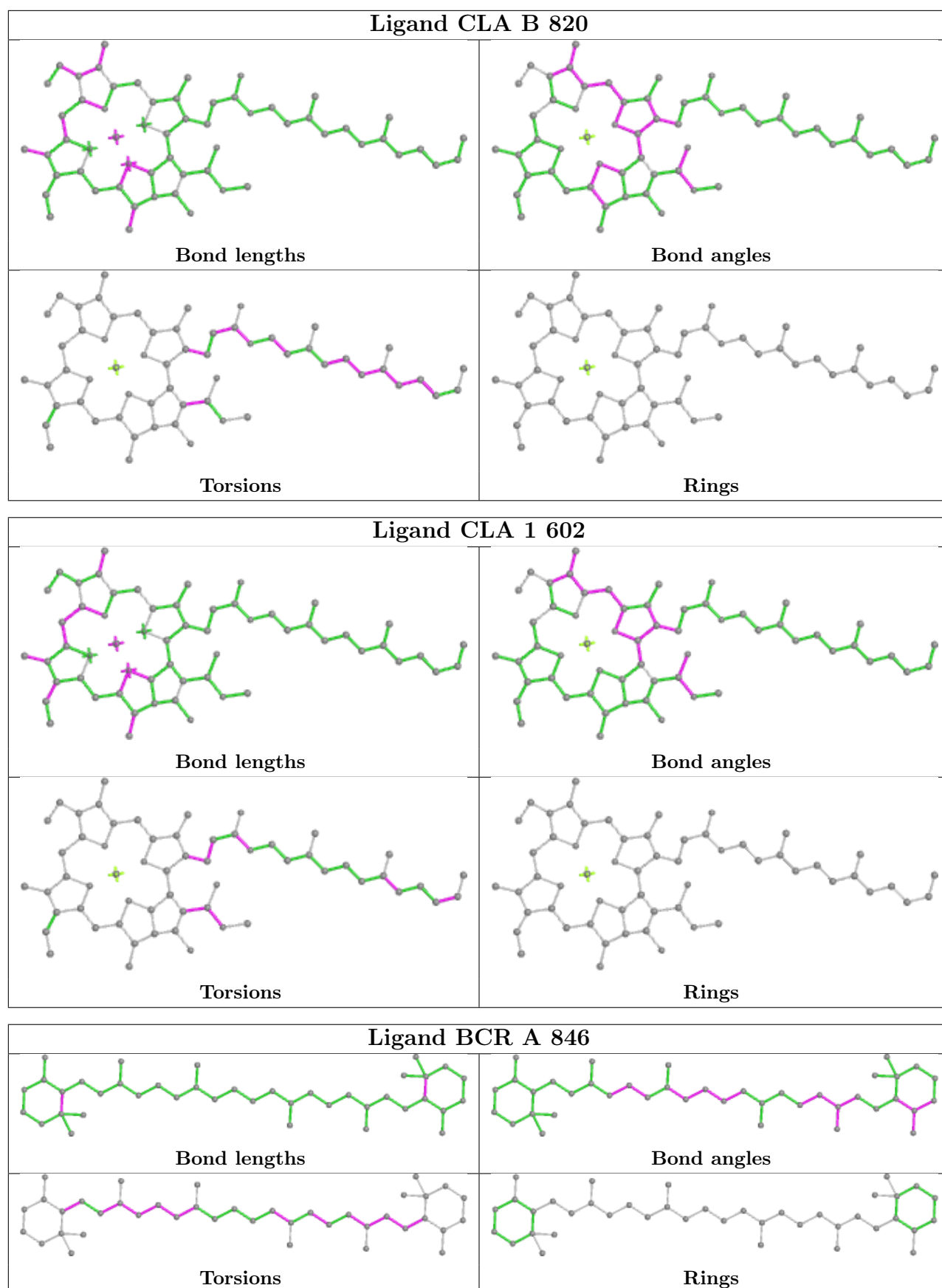
Ligand CLA 5 603

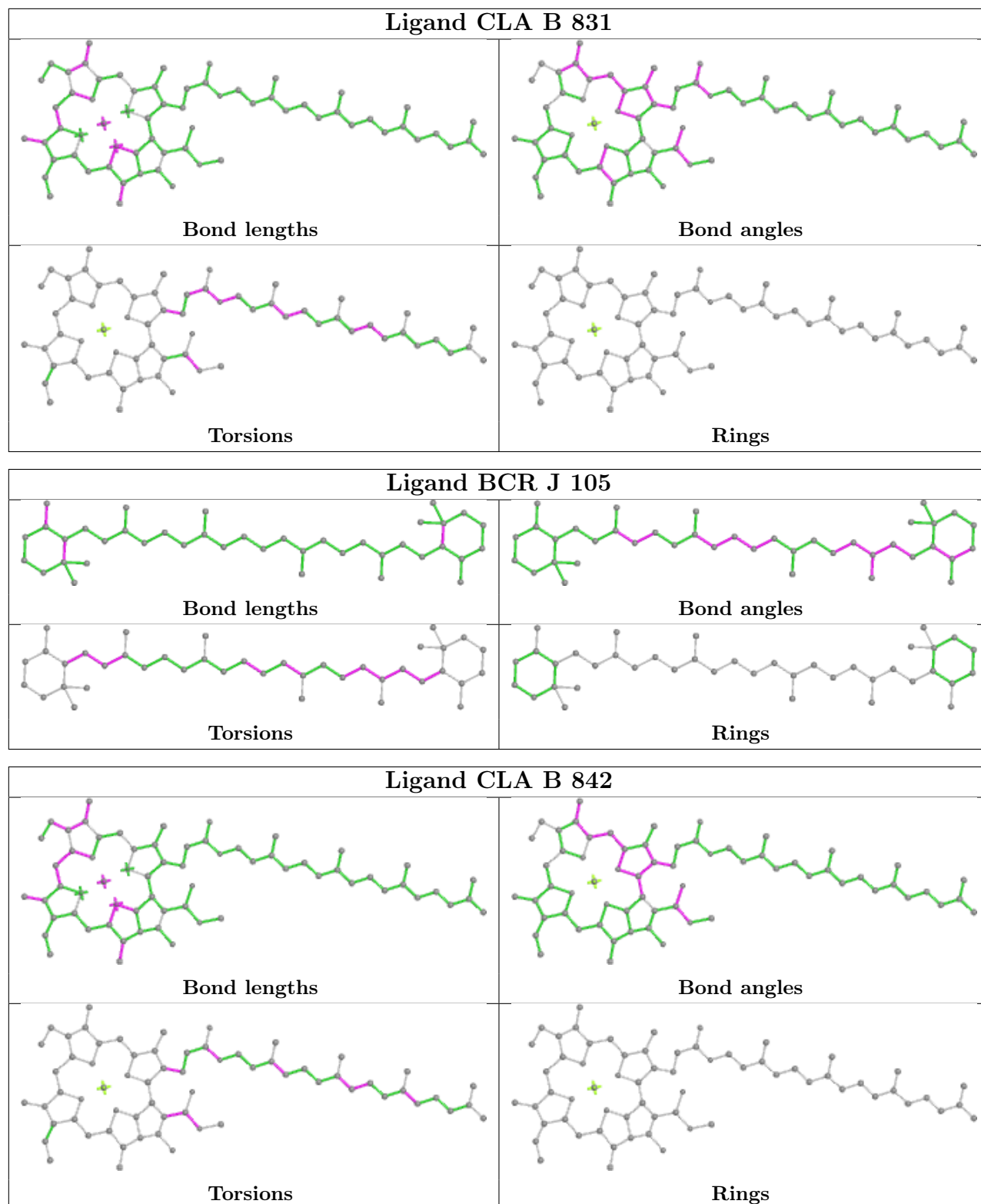


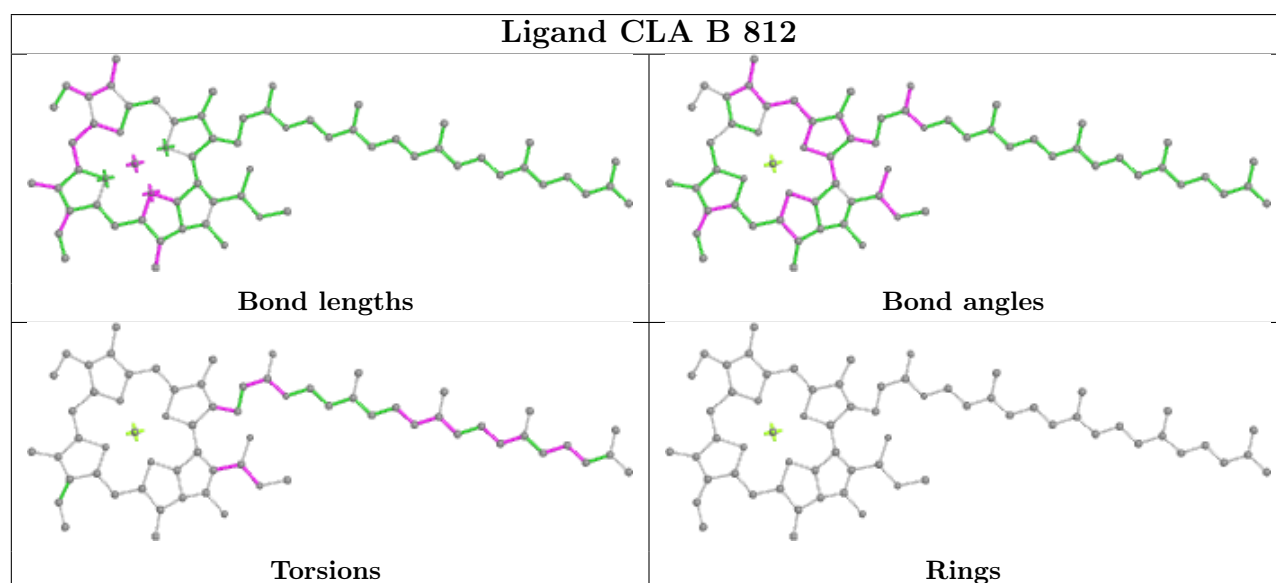
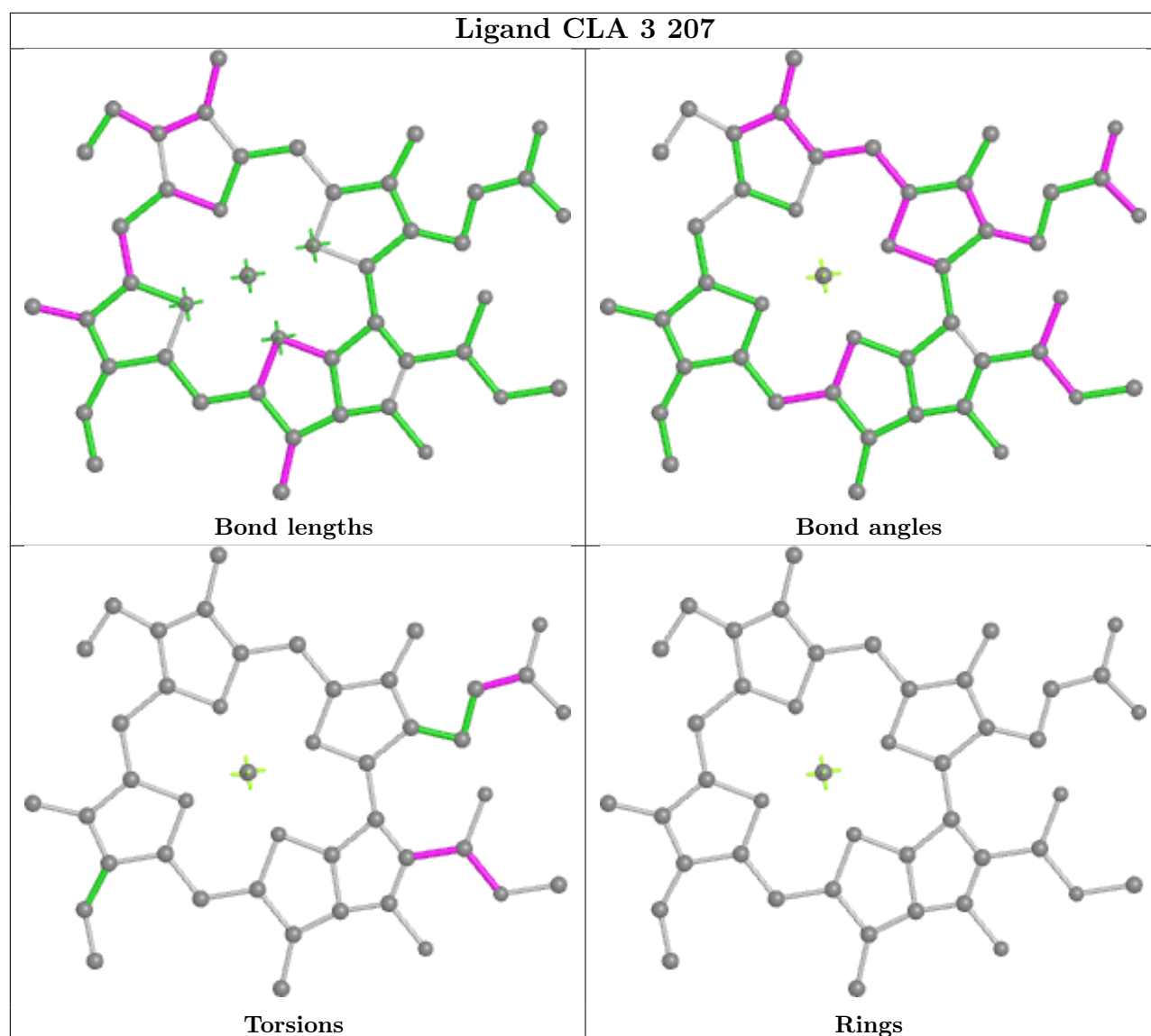


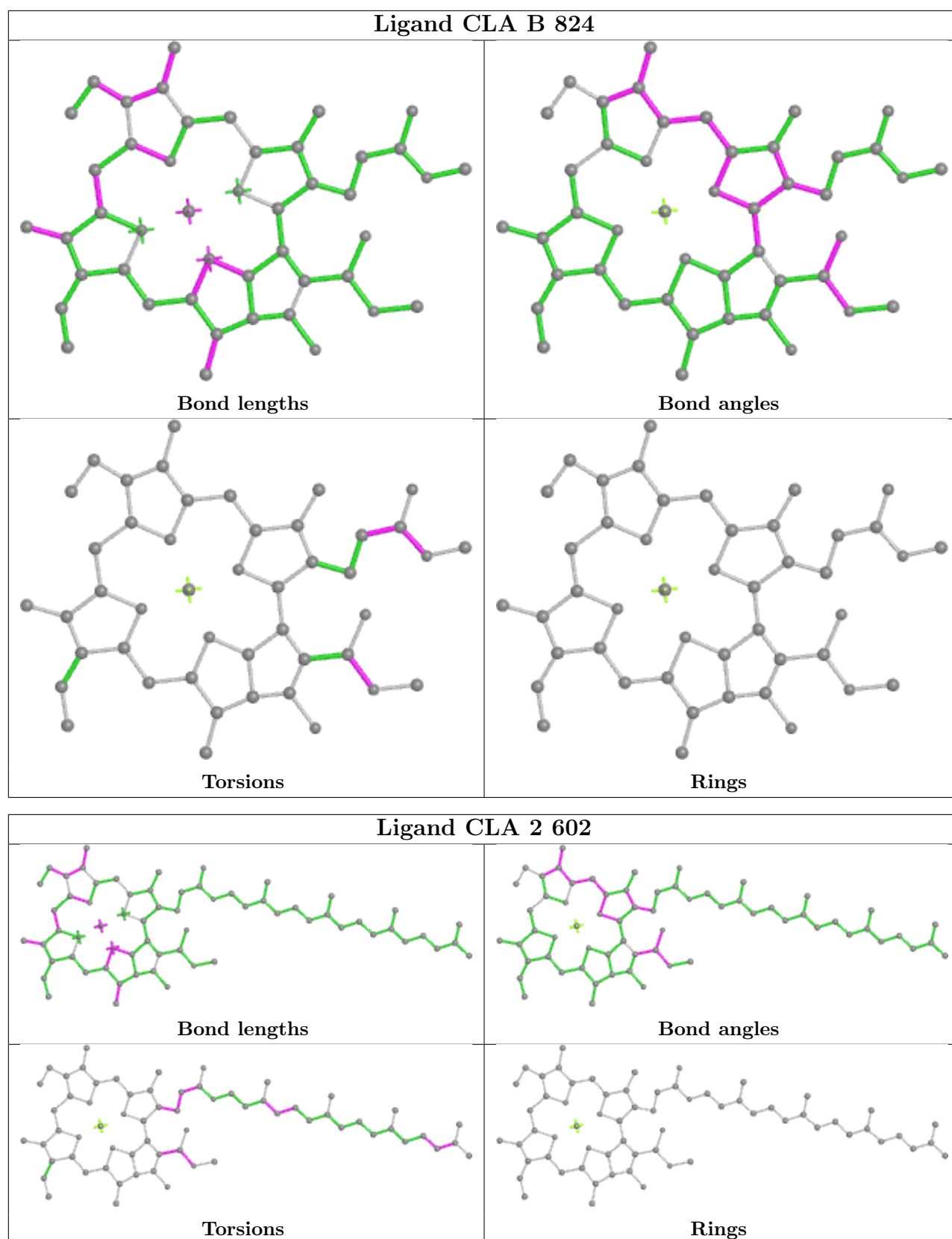


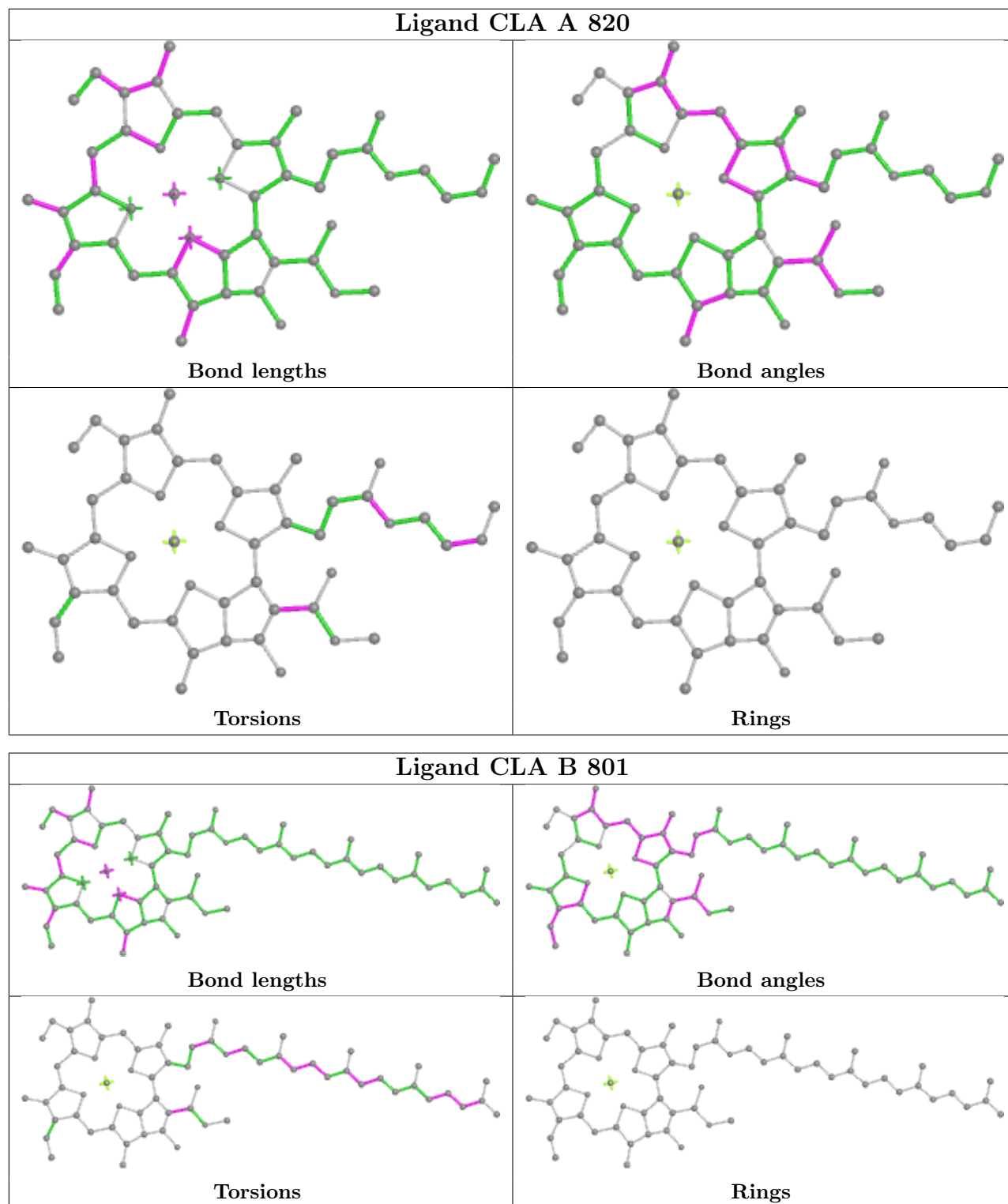


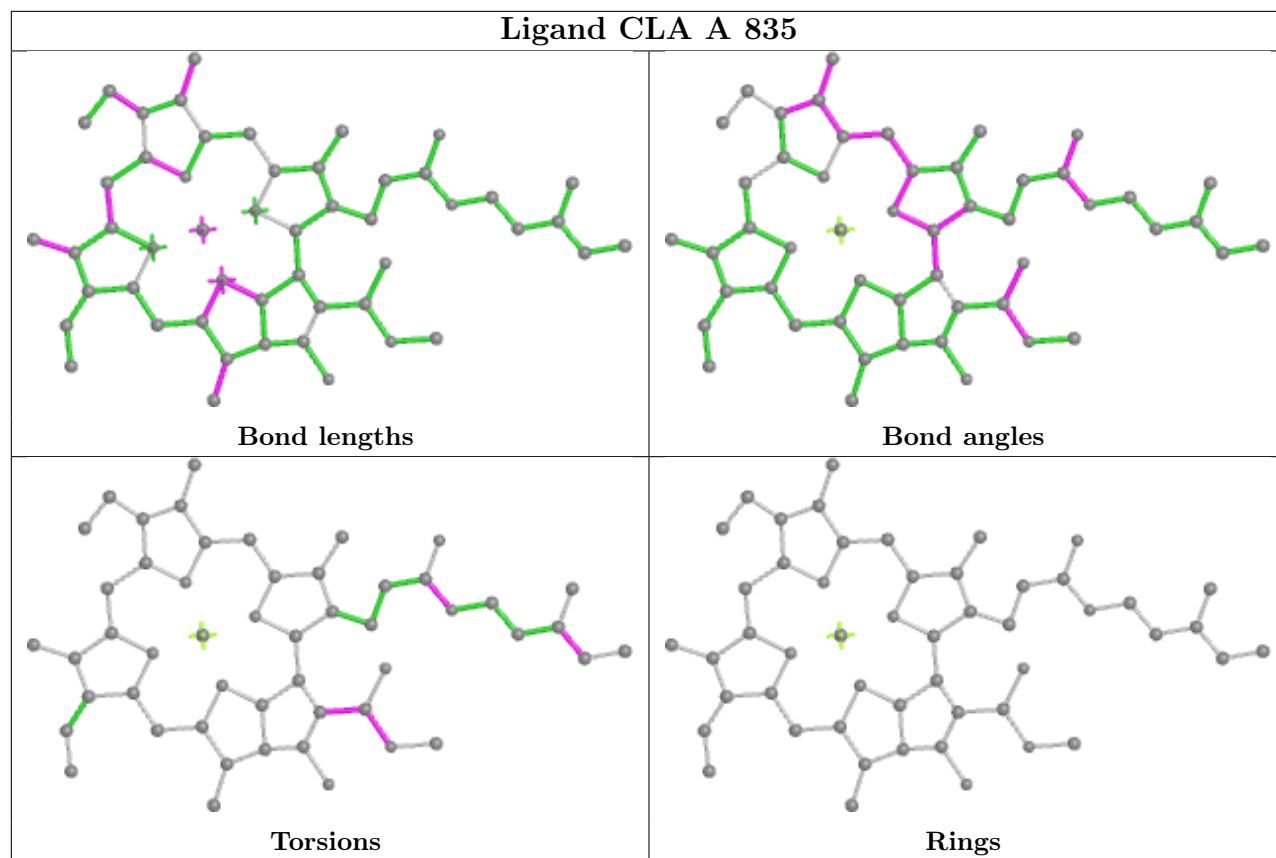


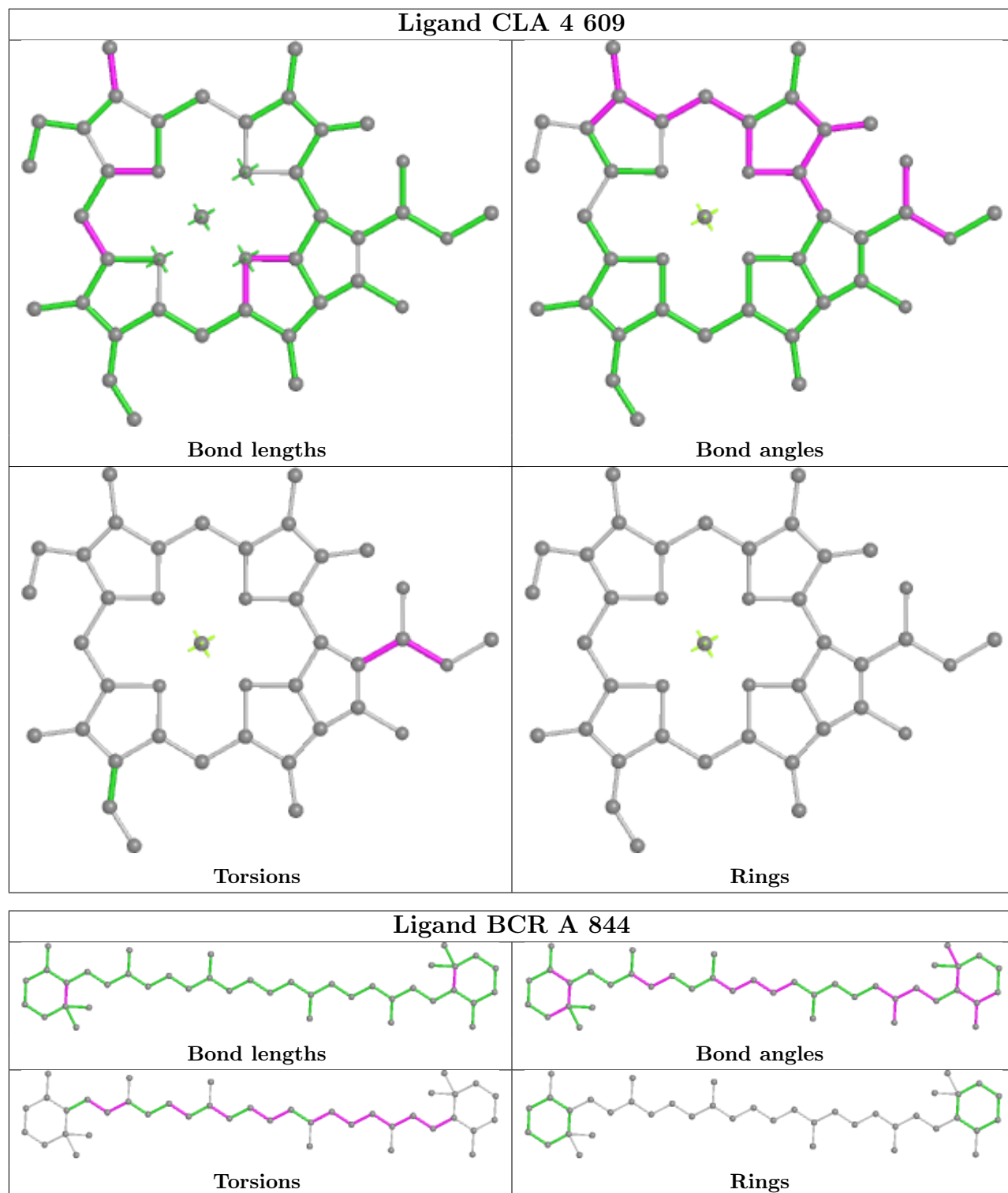


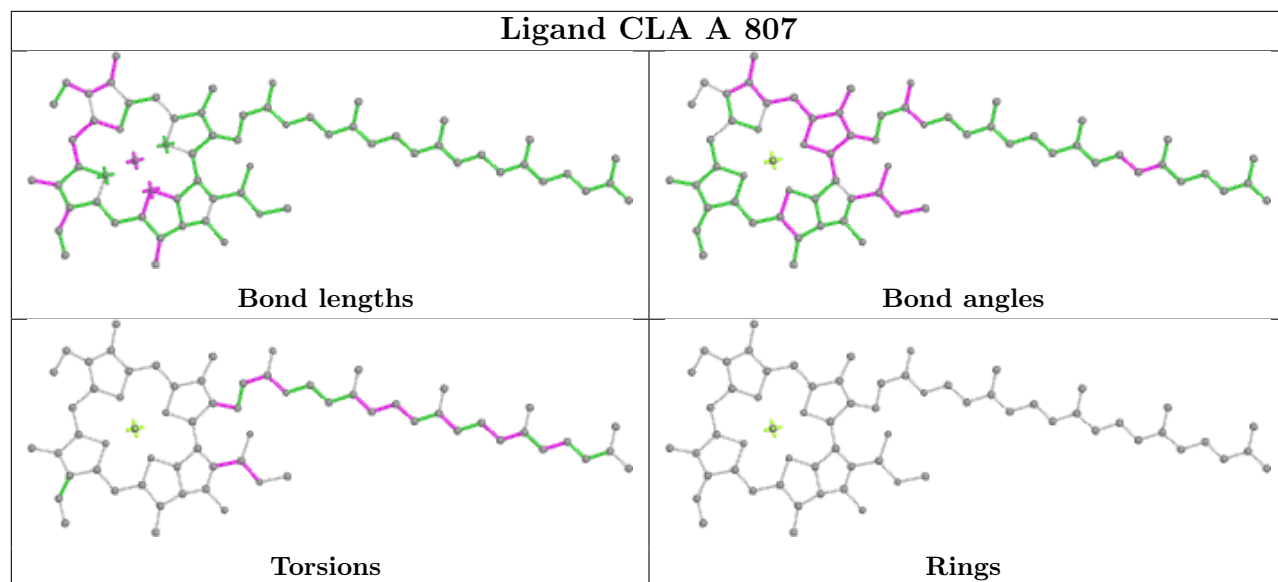


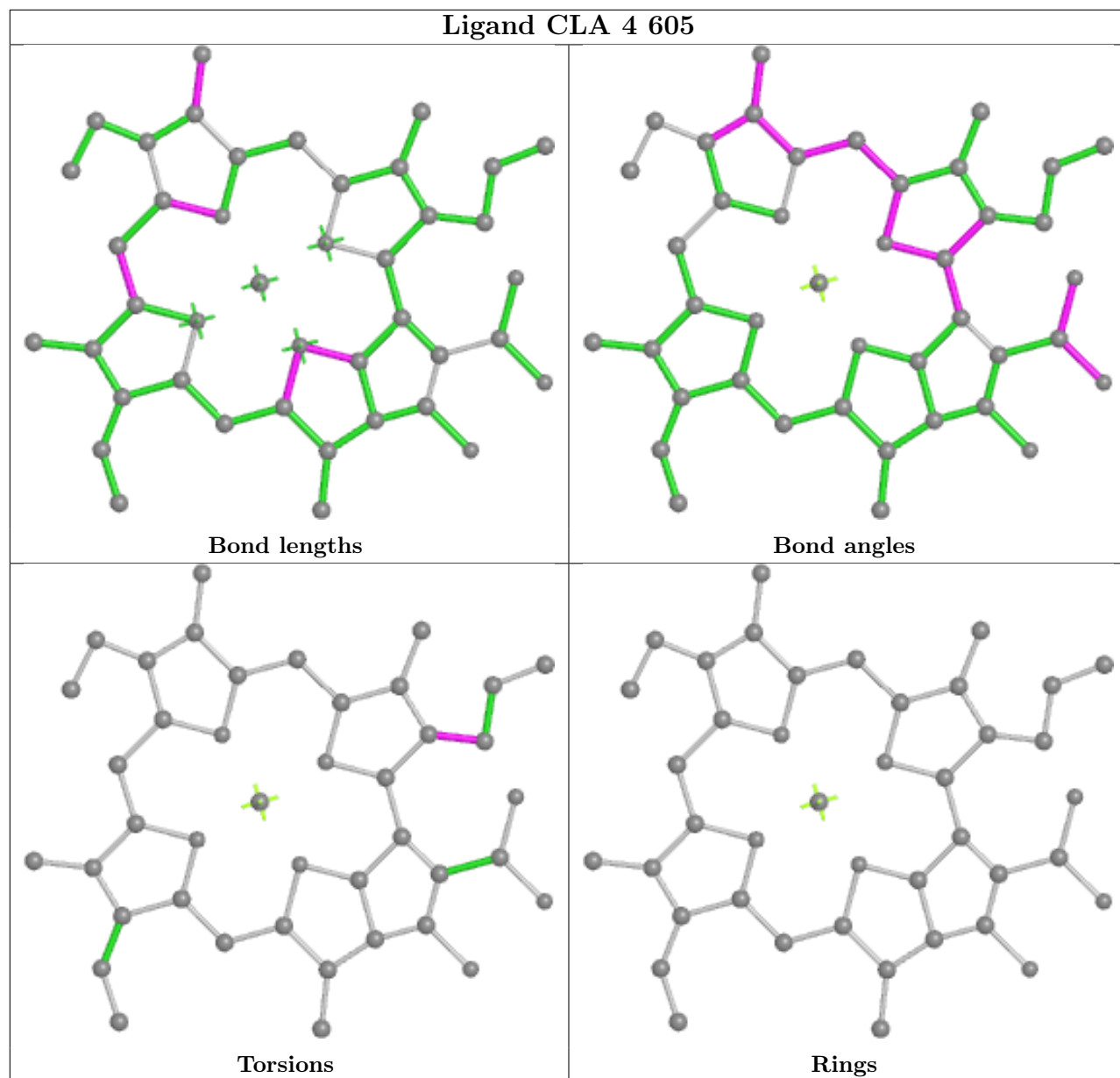


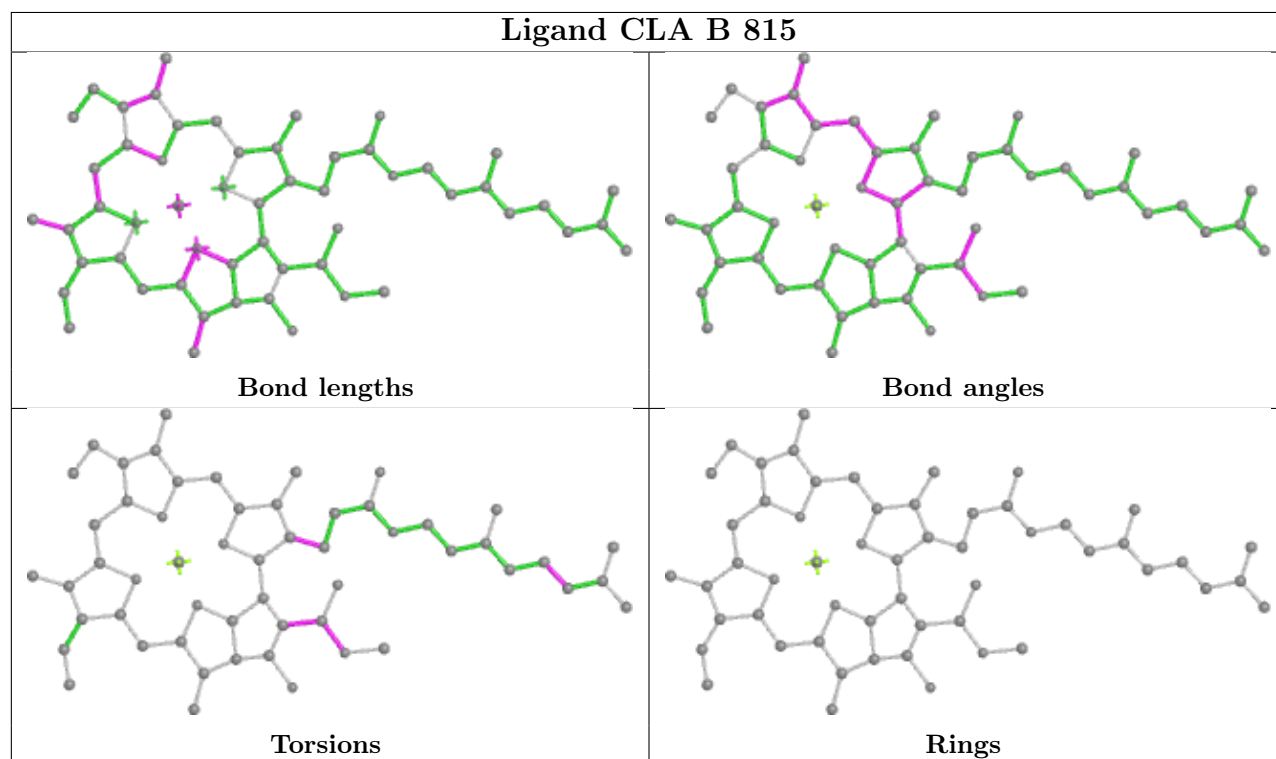
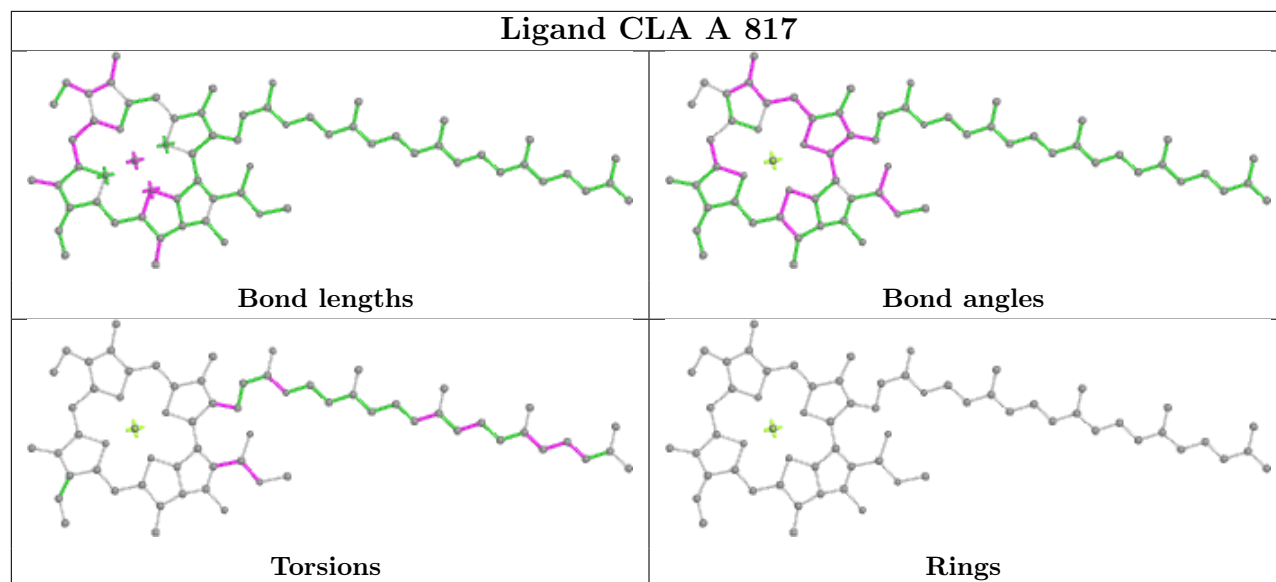


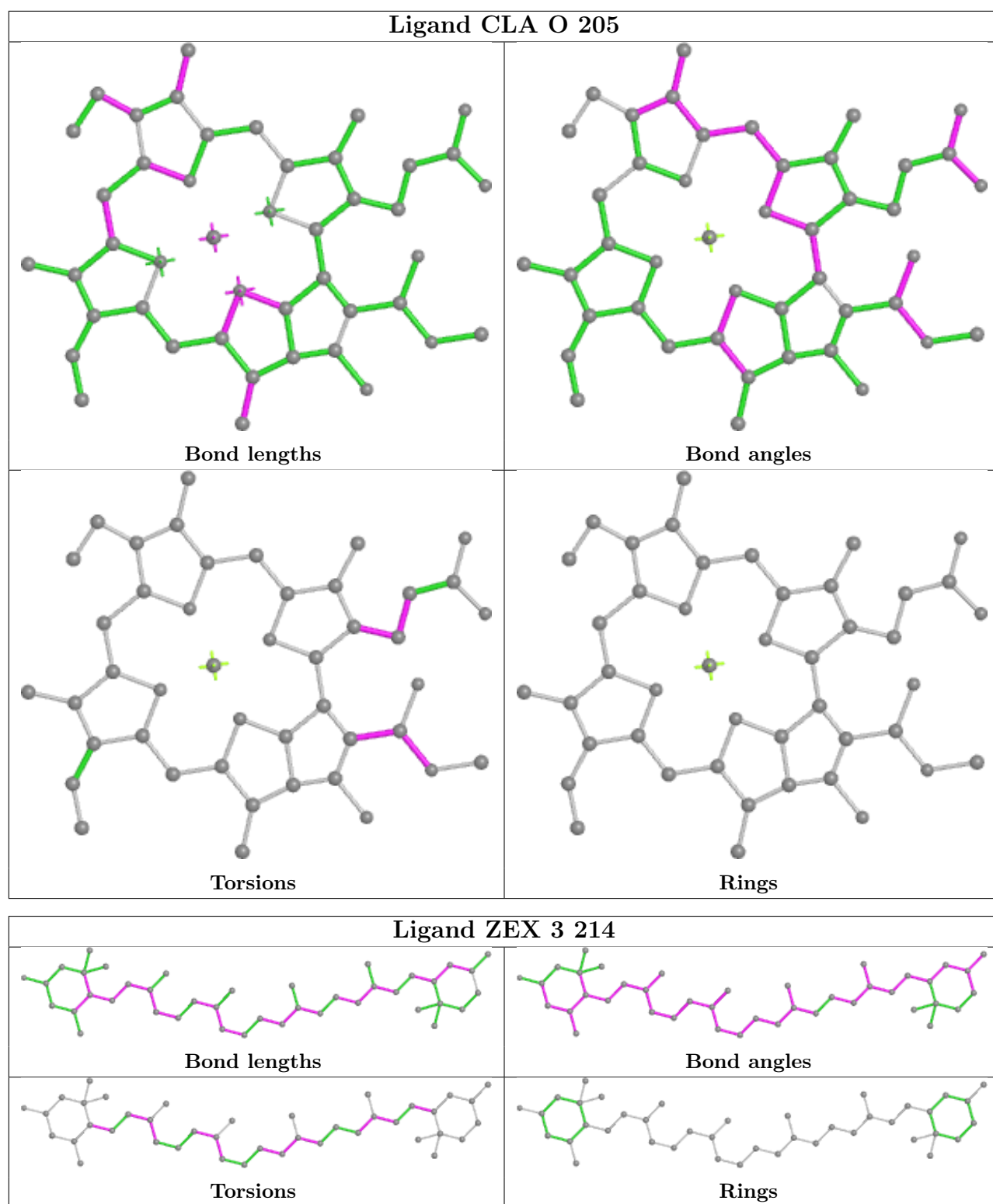


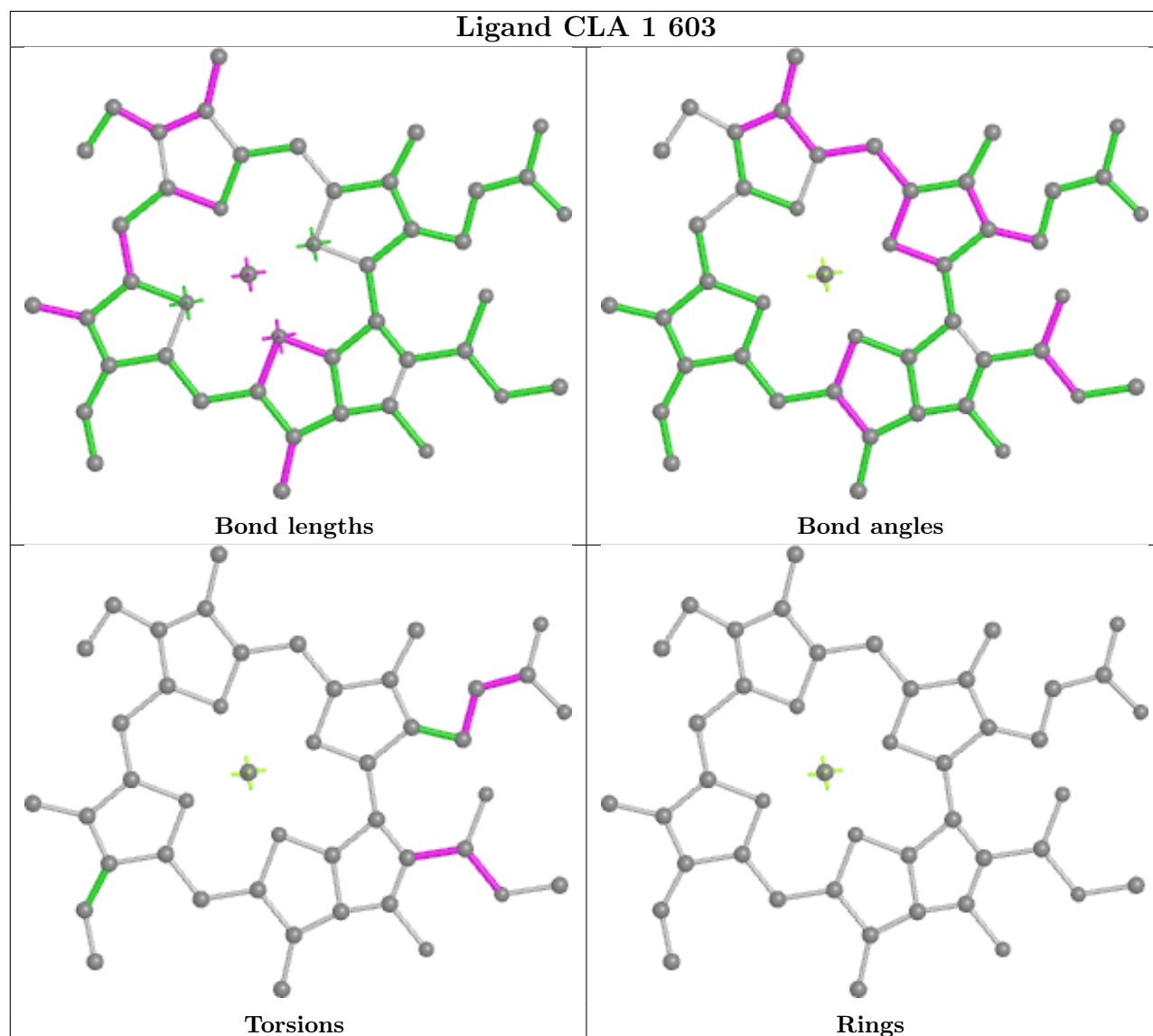
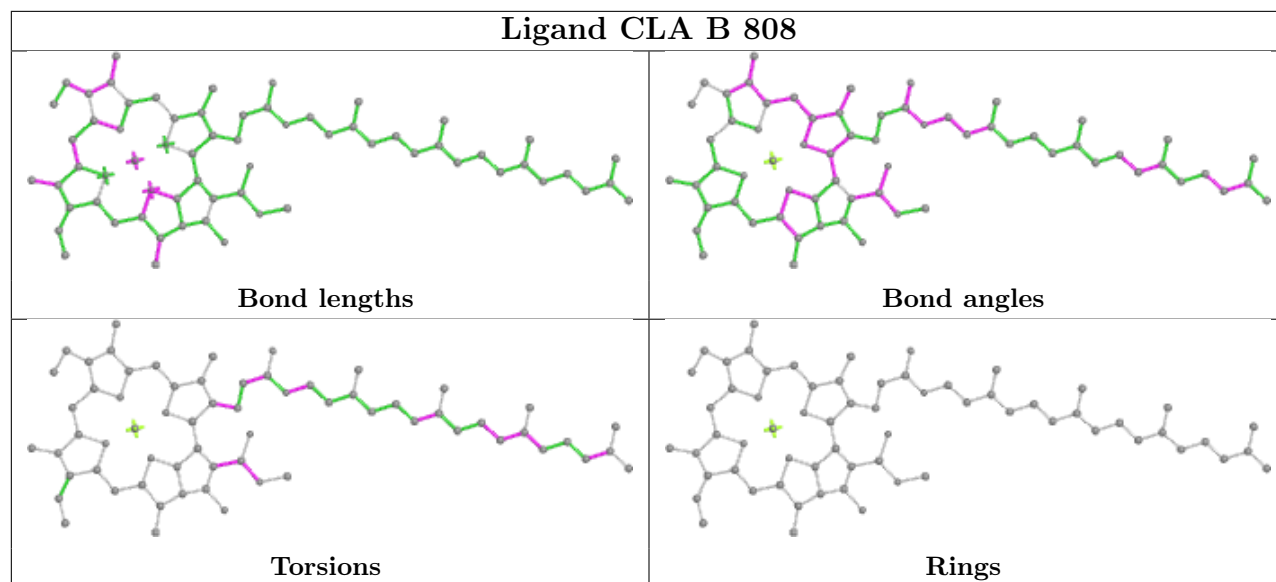


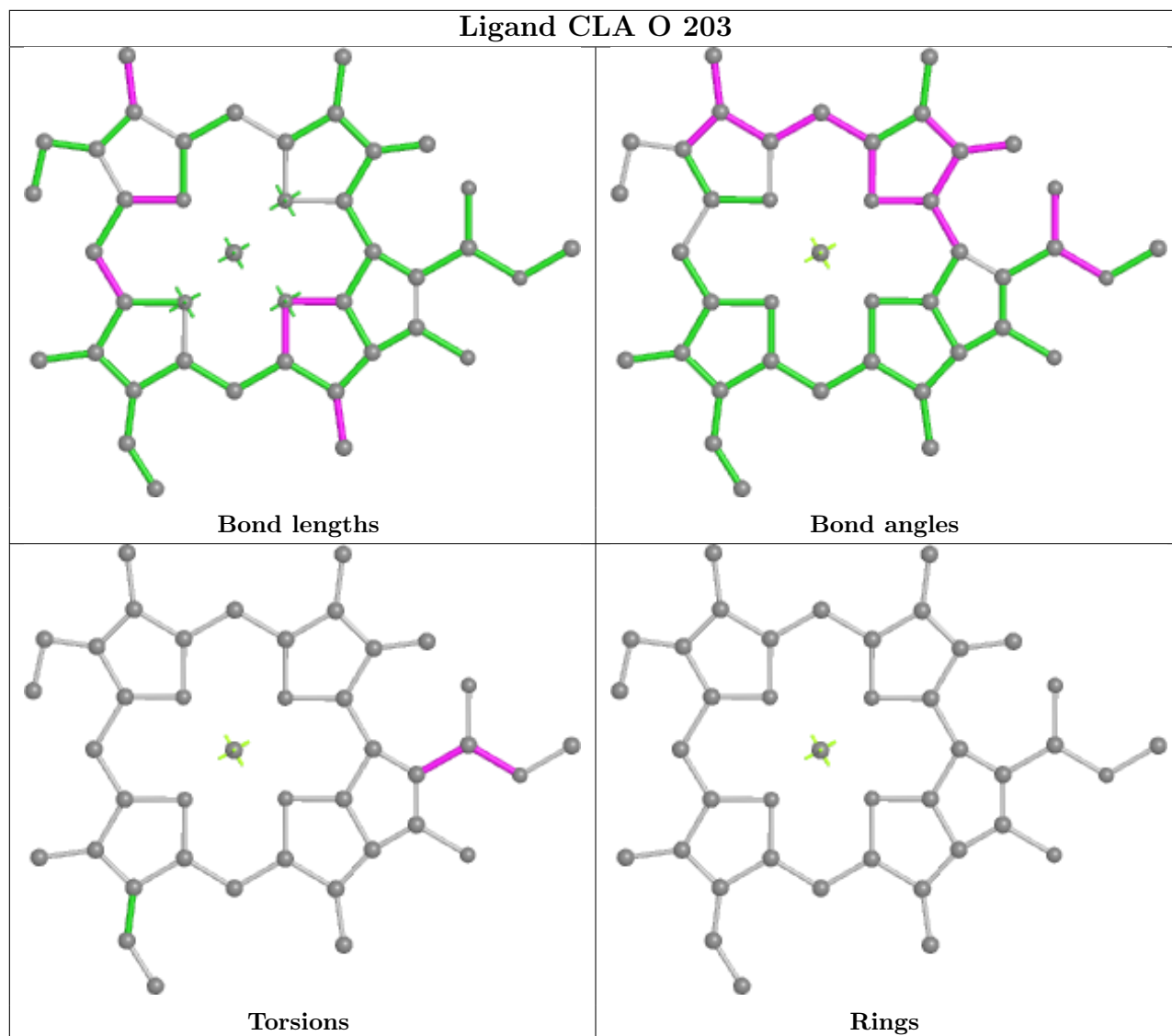


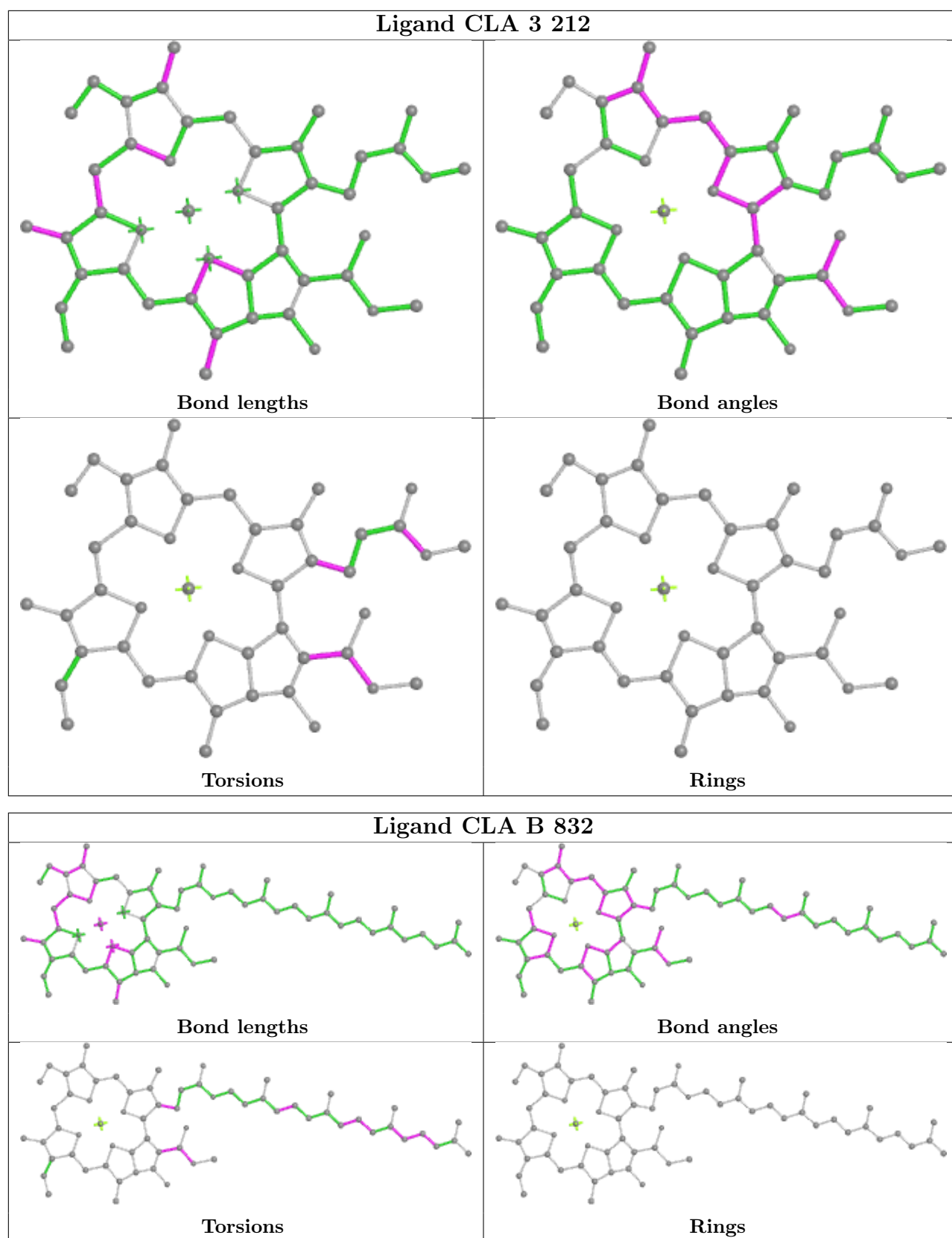


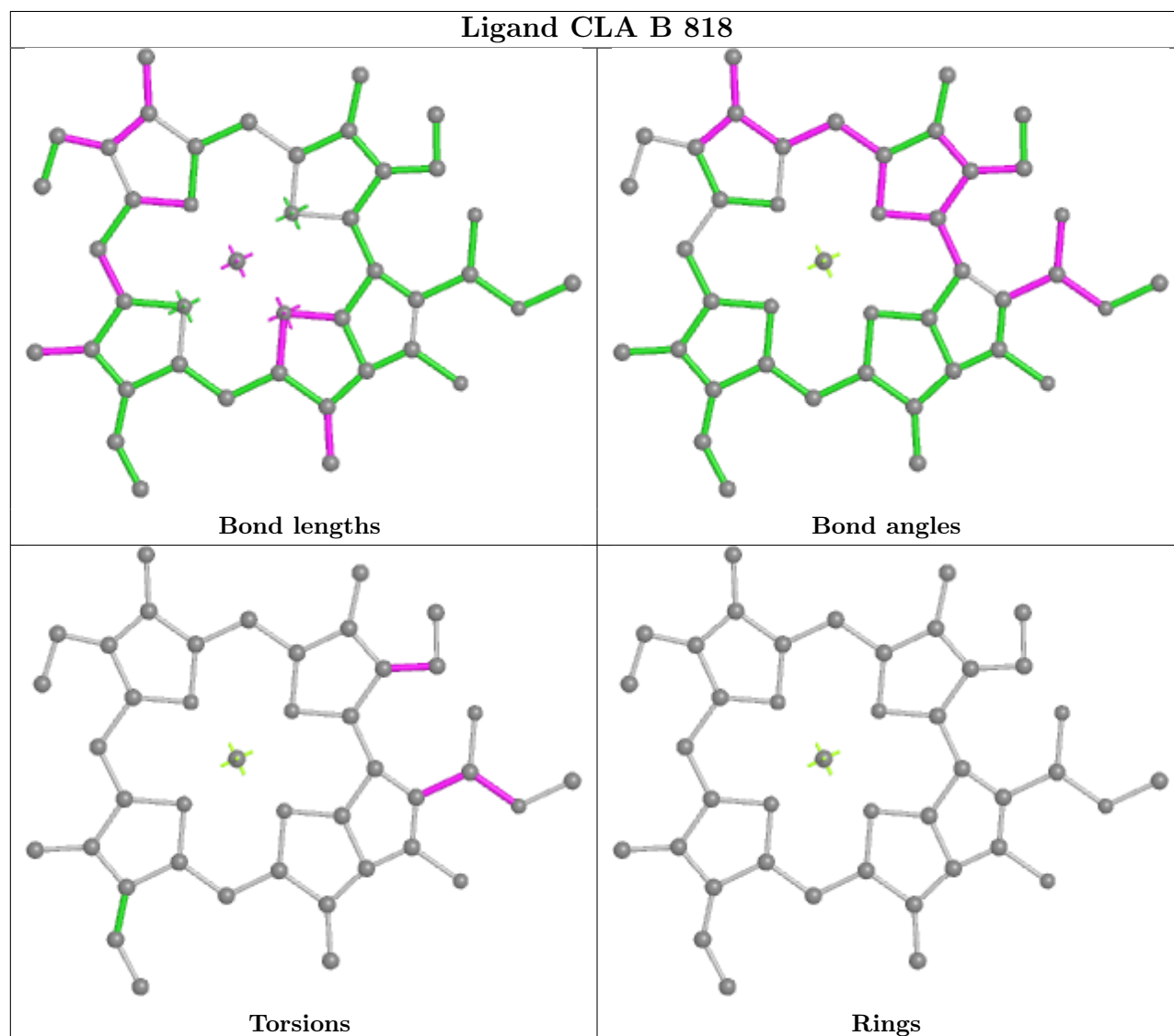
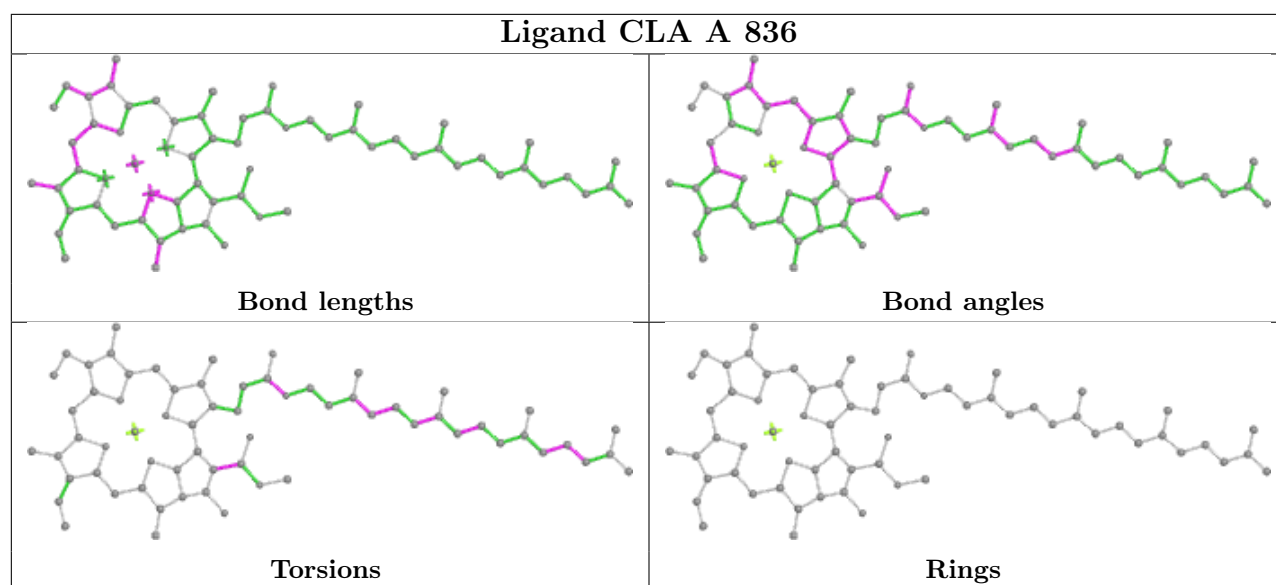




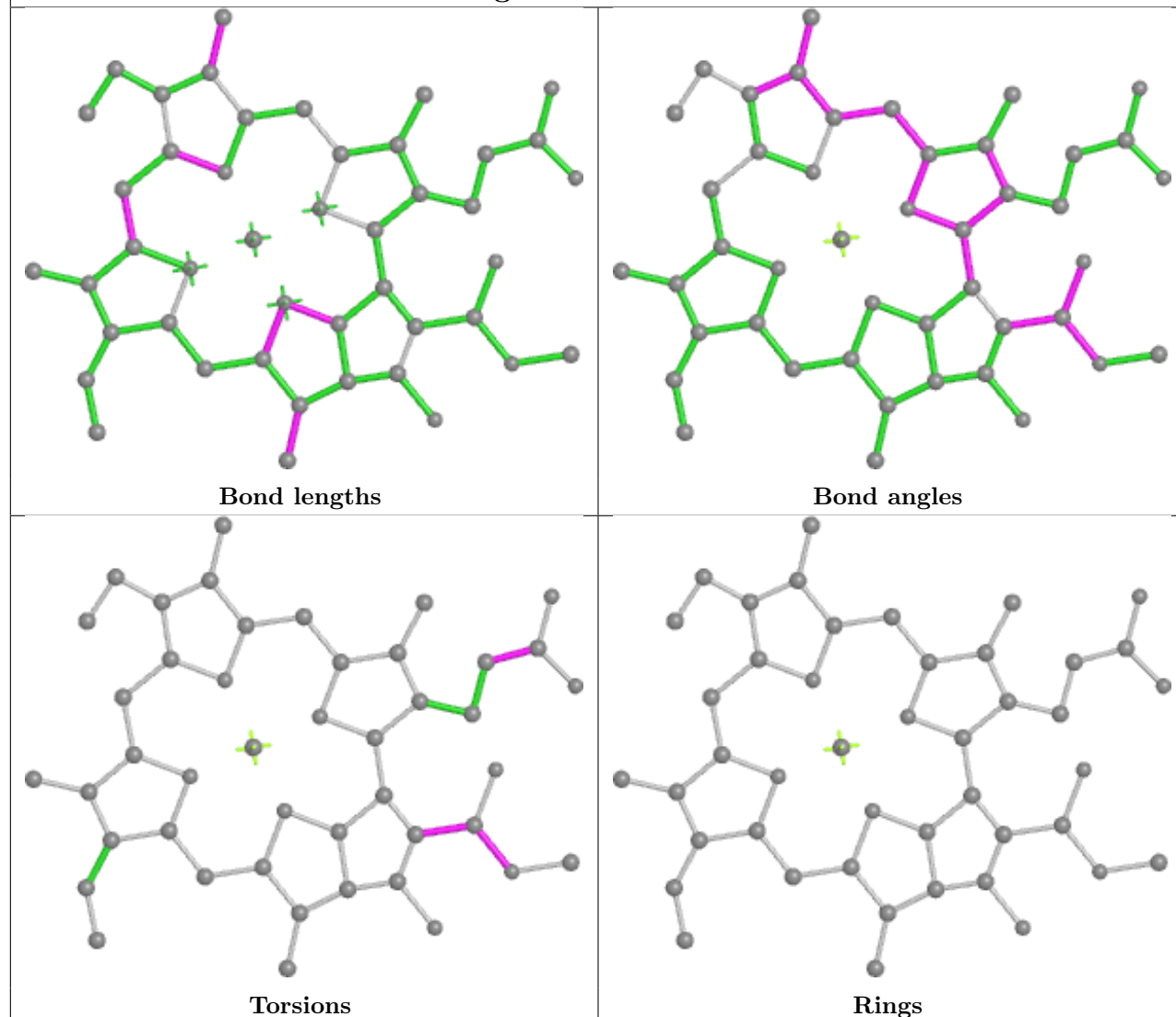




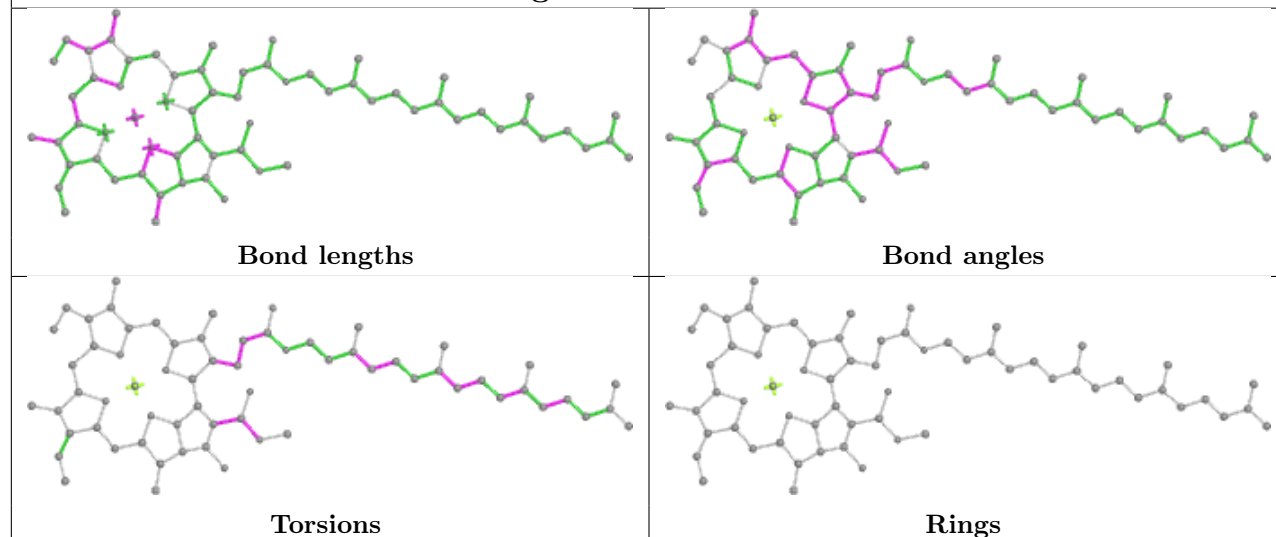


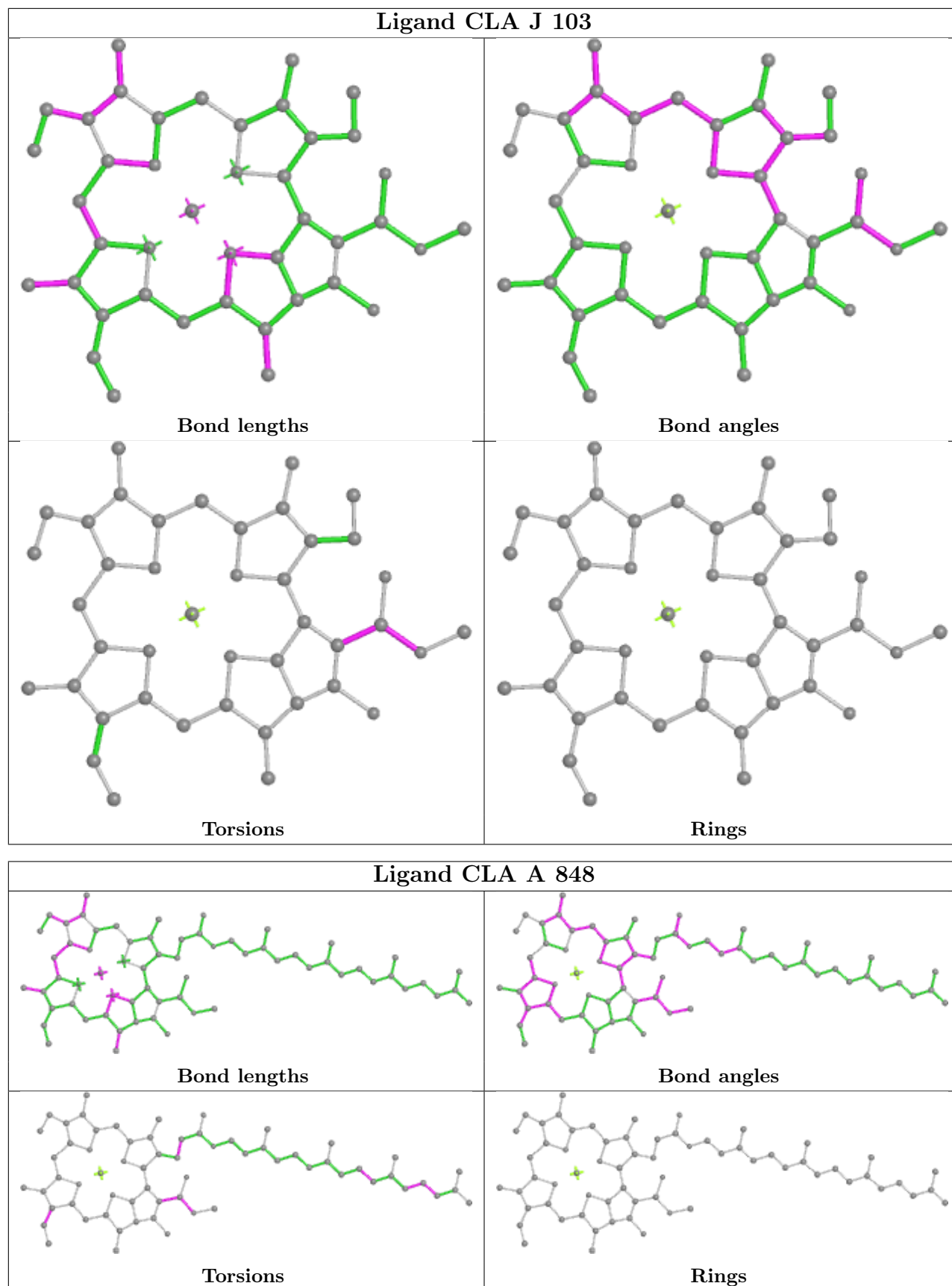


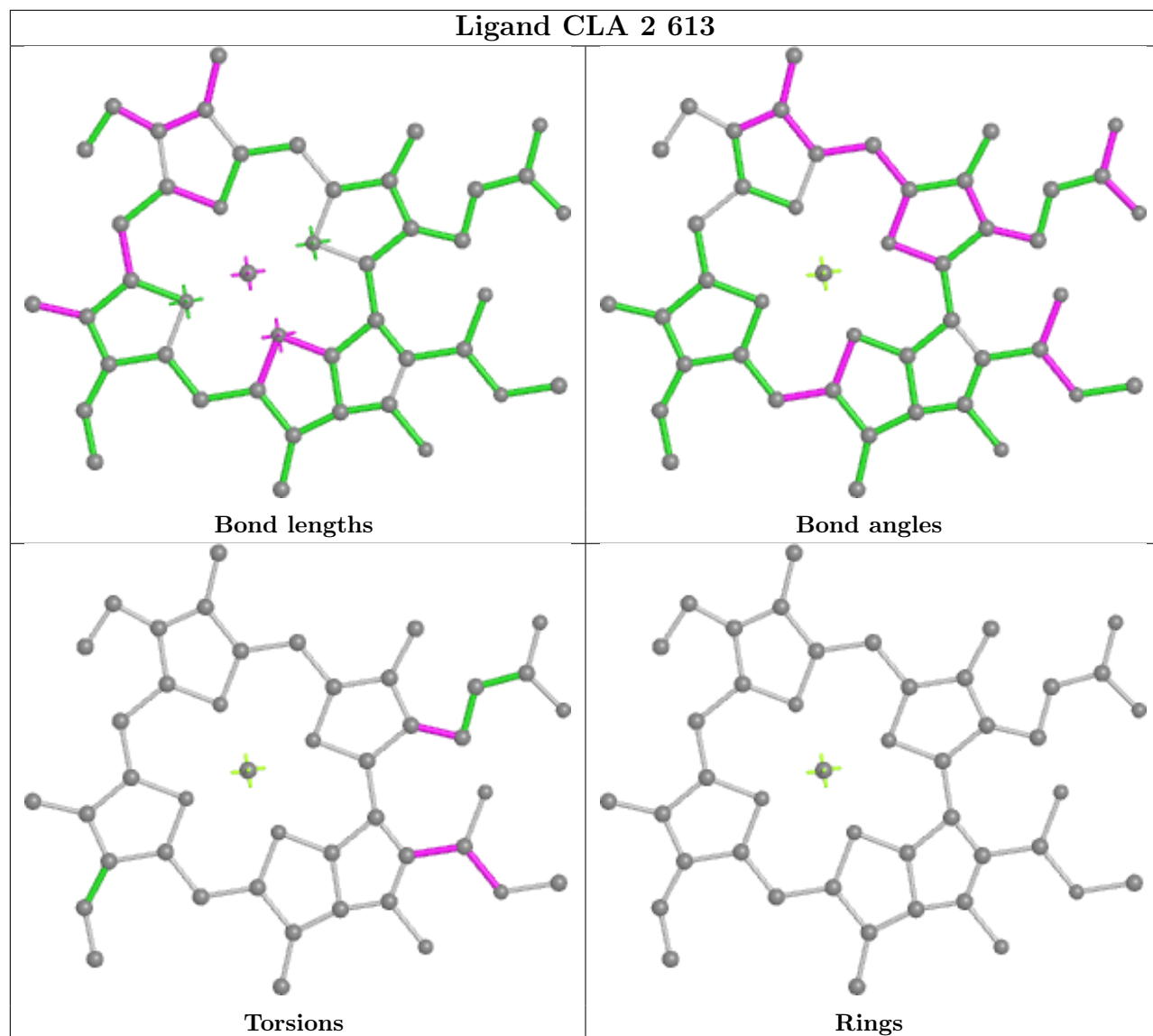
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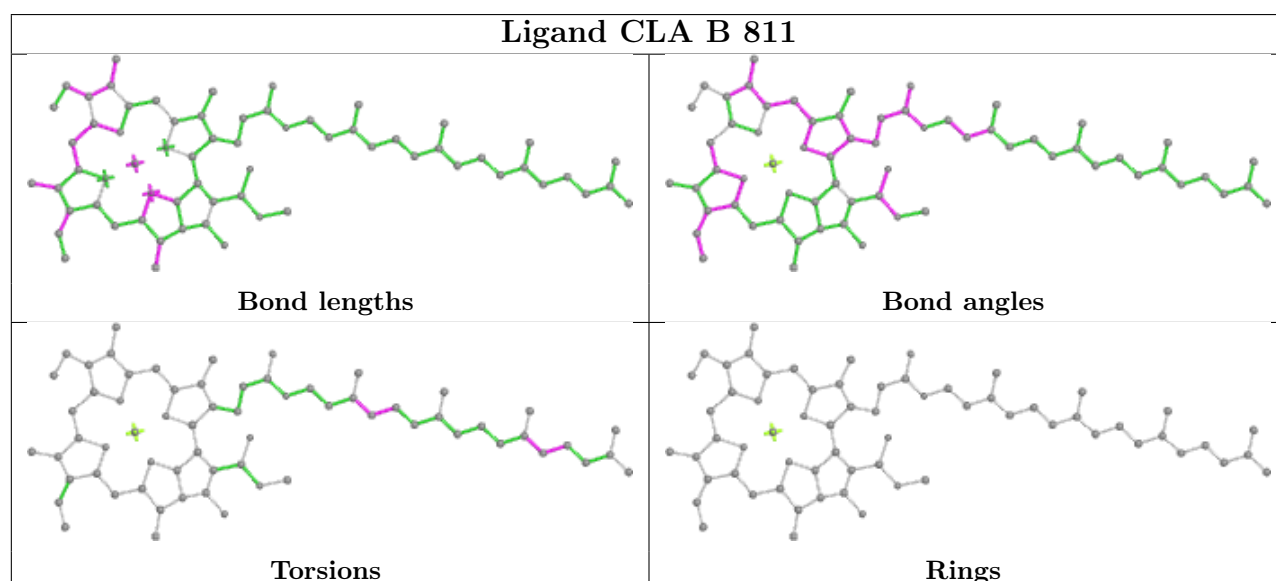
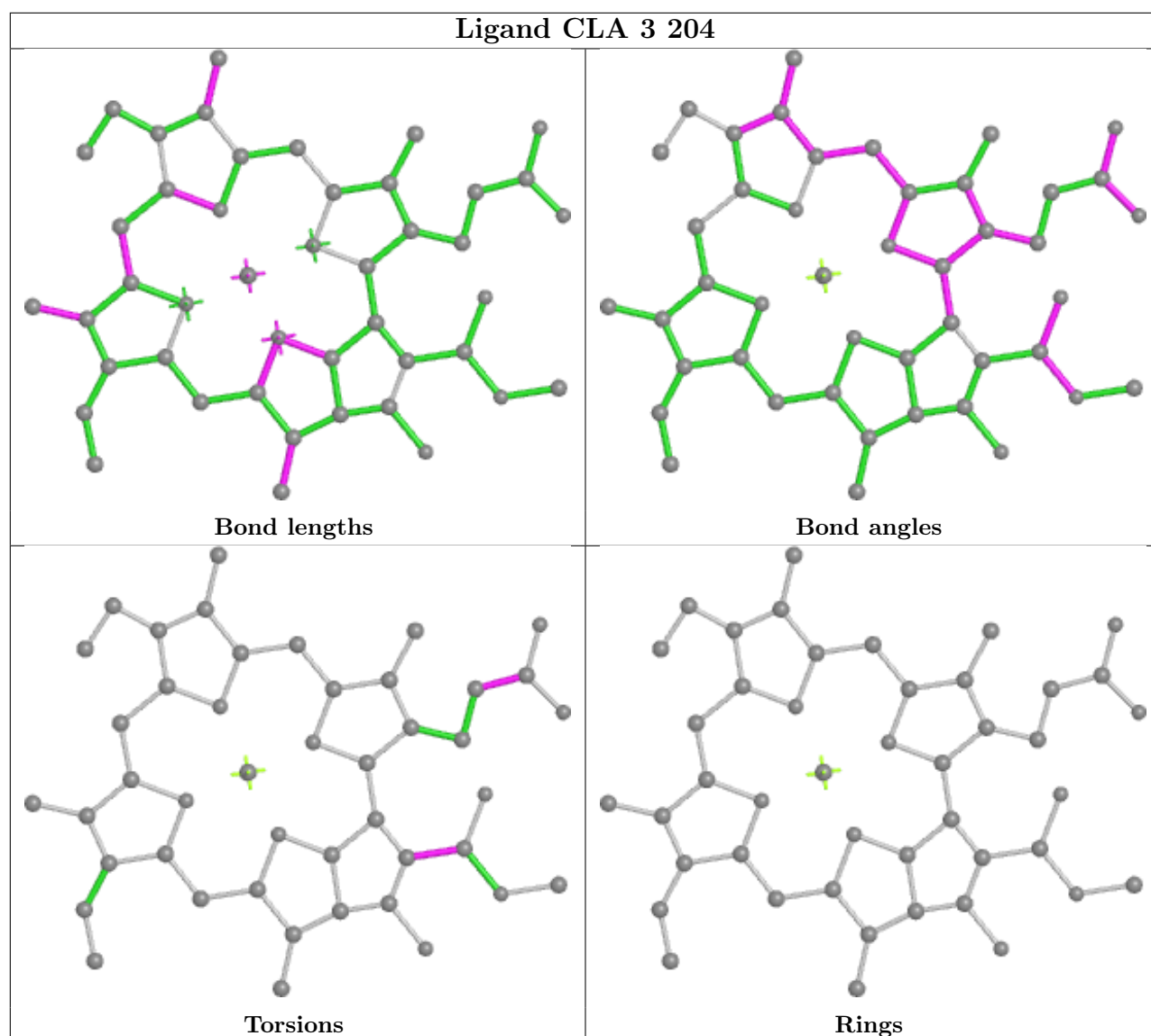


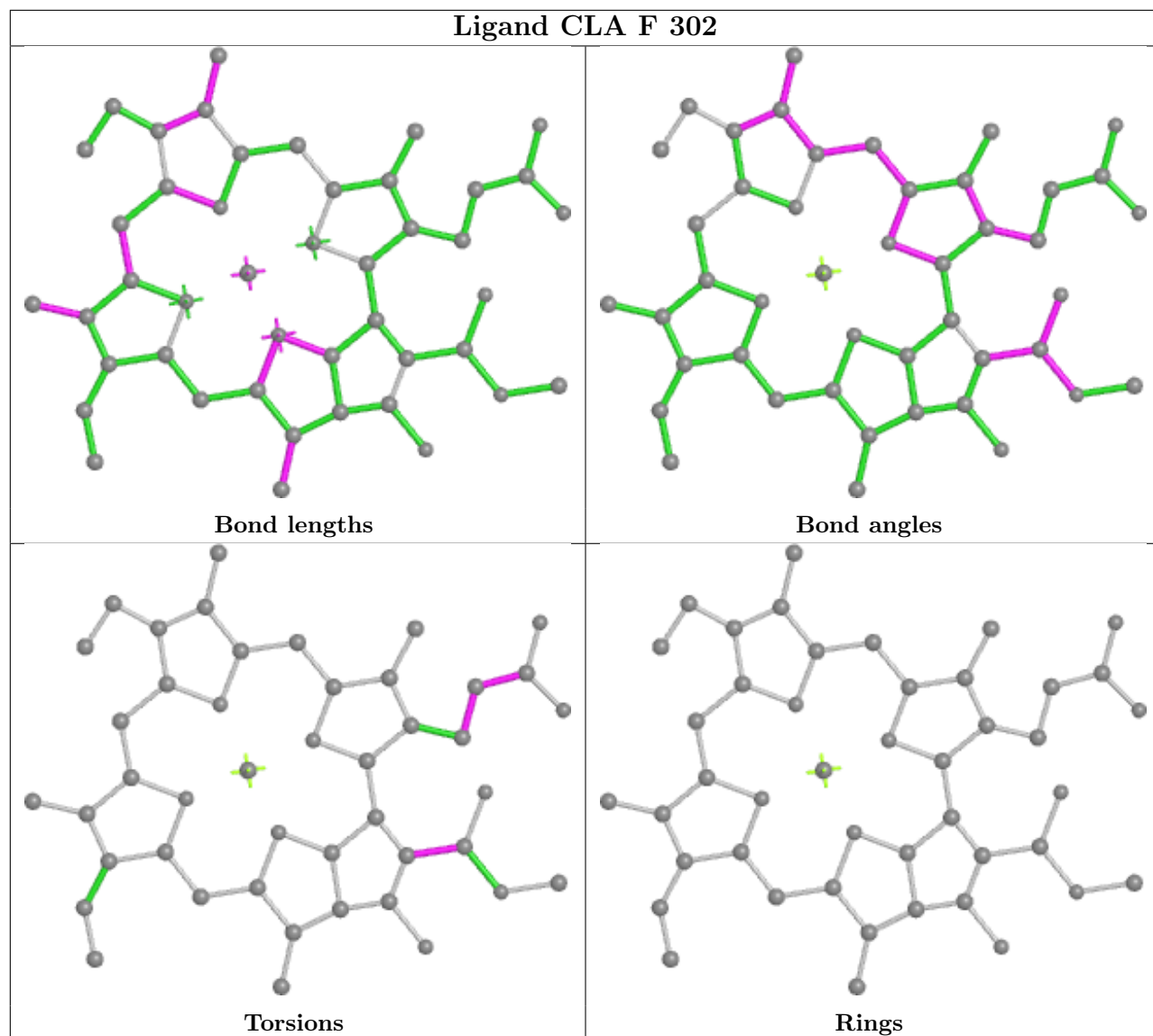
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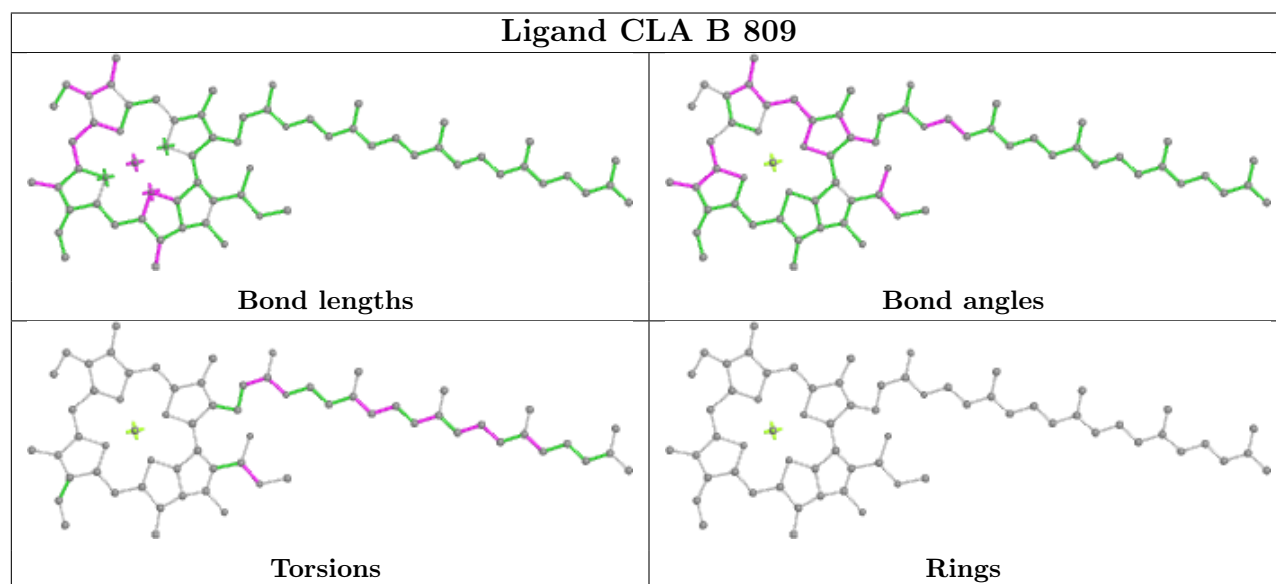
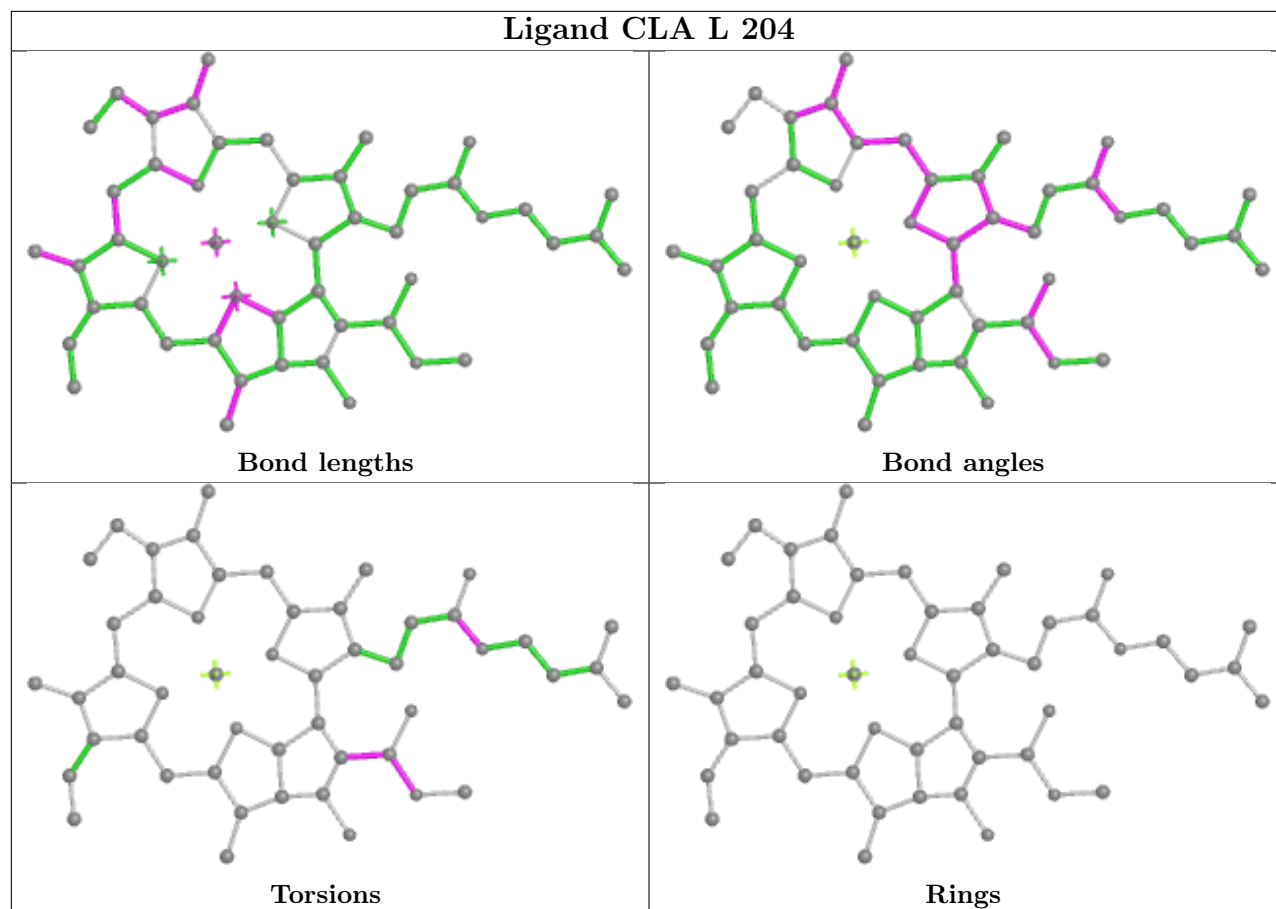


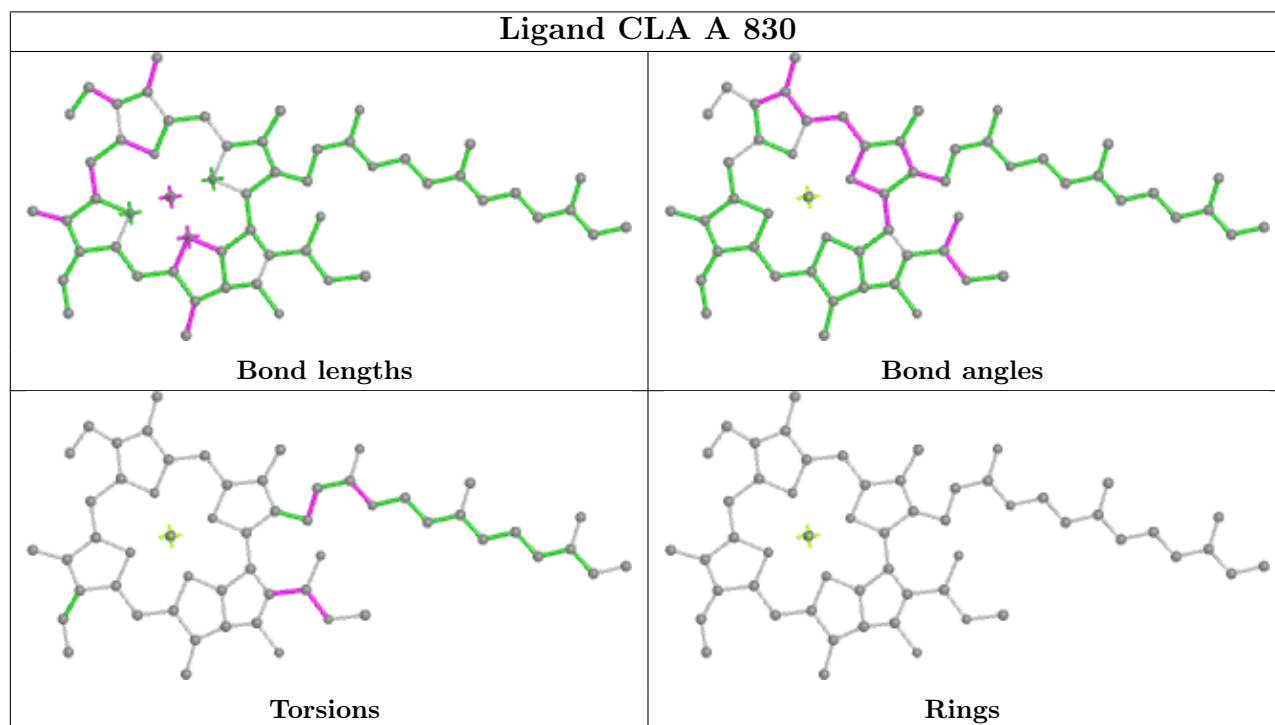
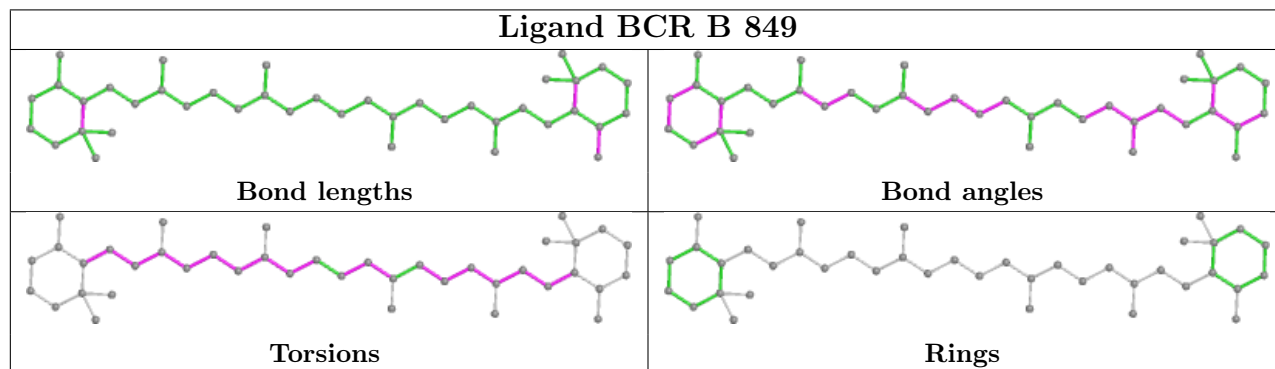
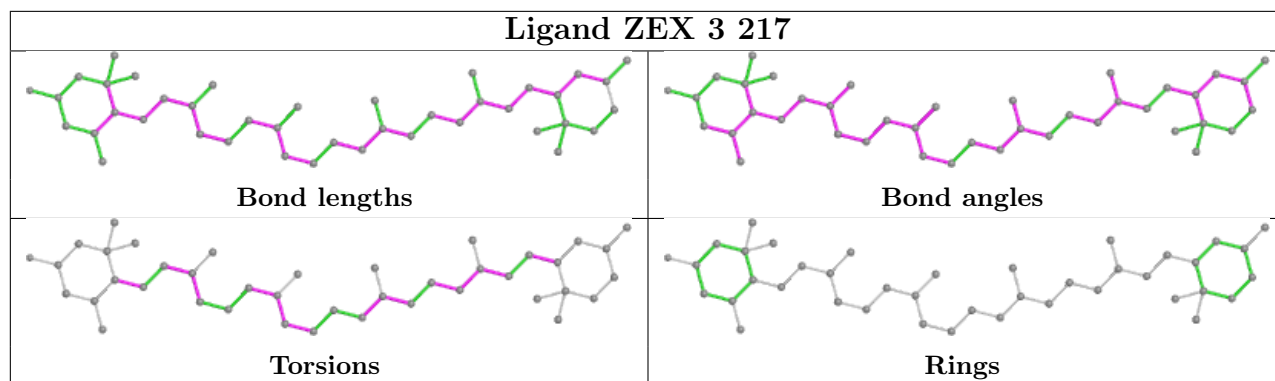


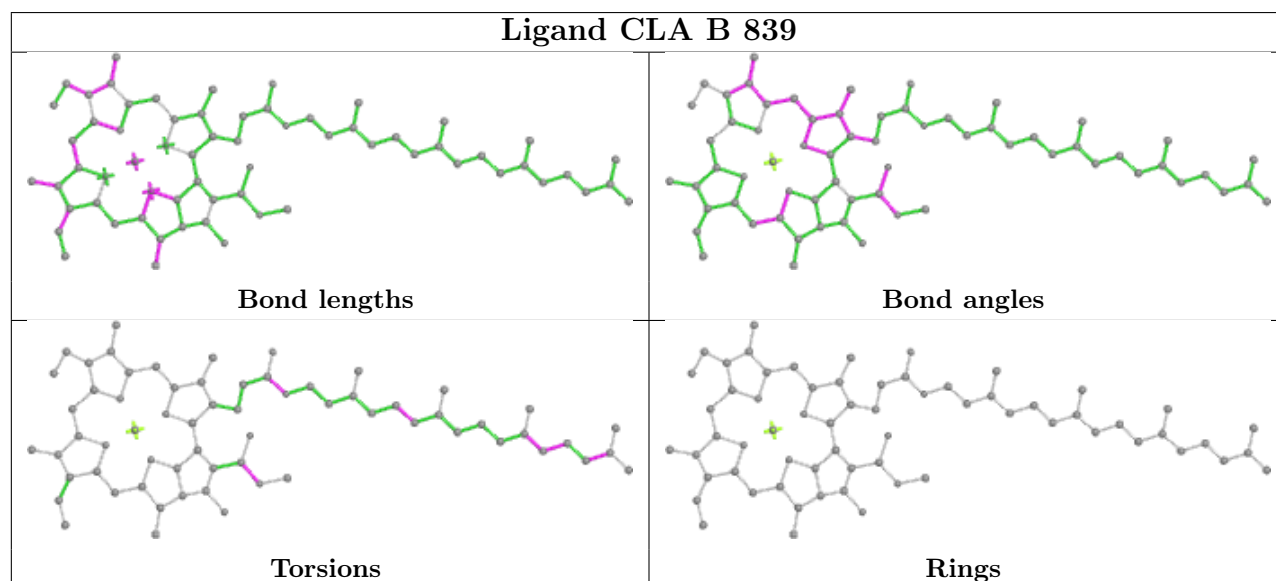
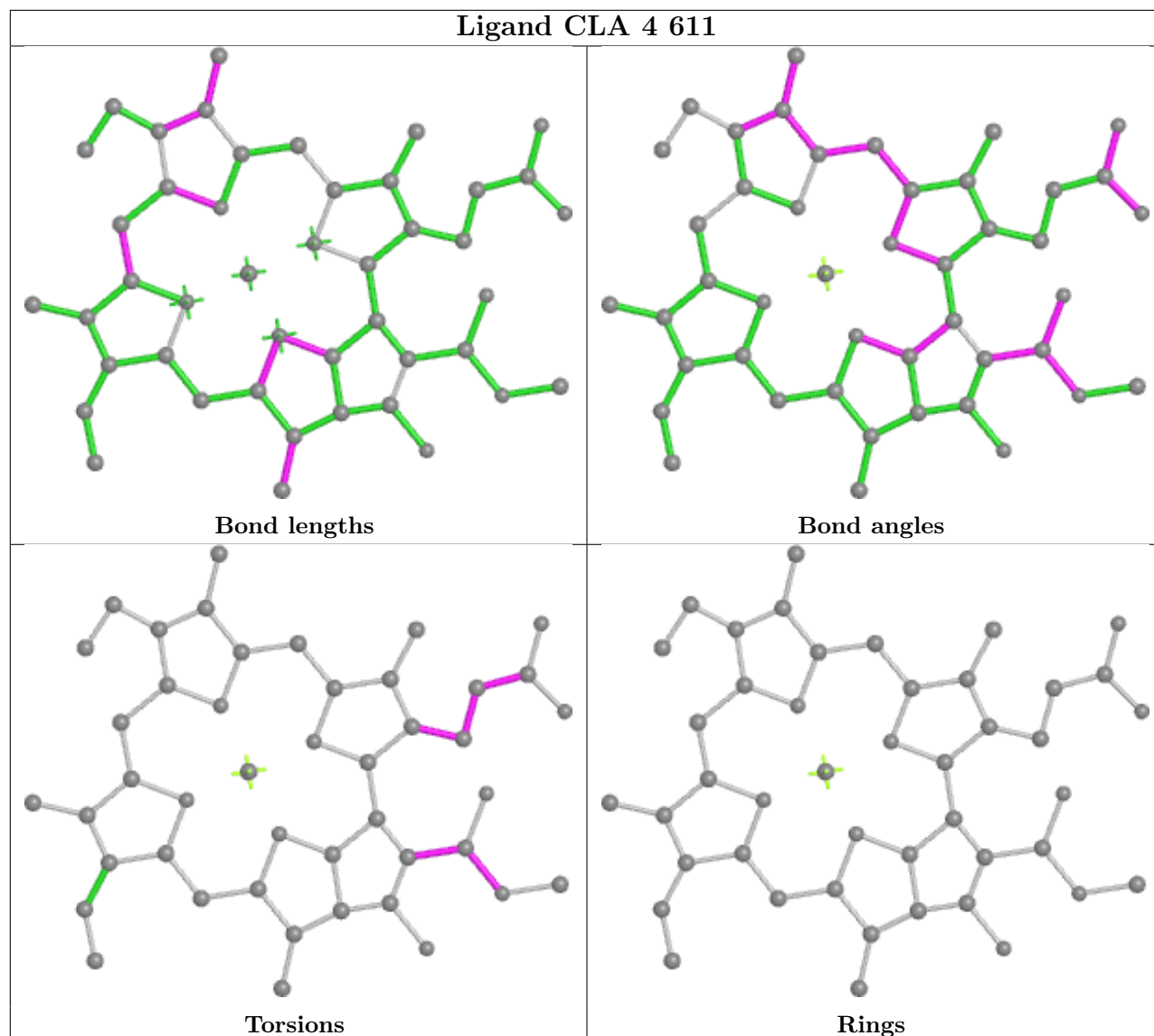


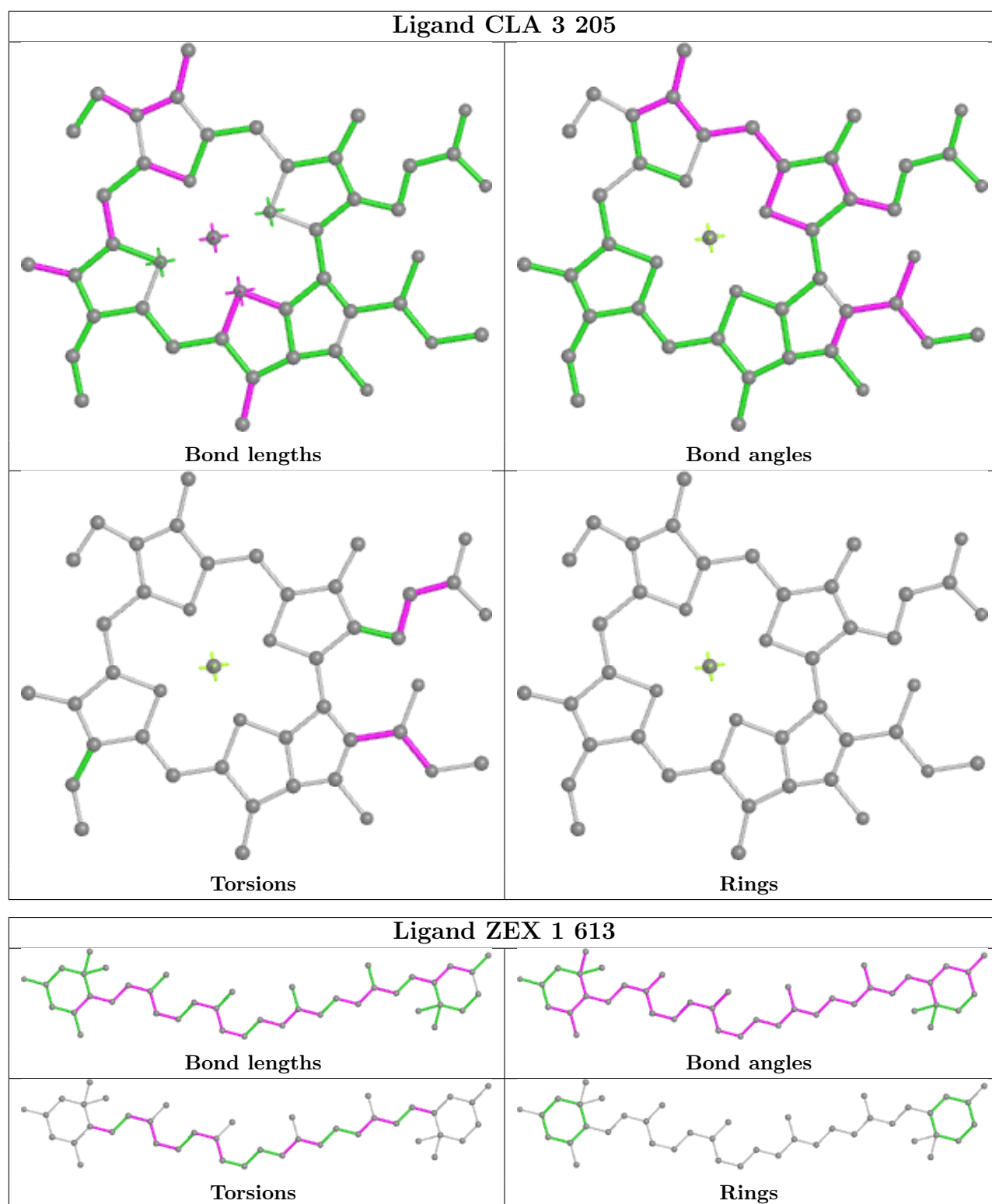


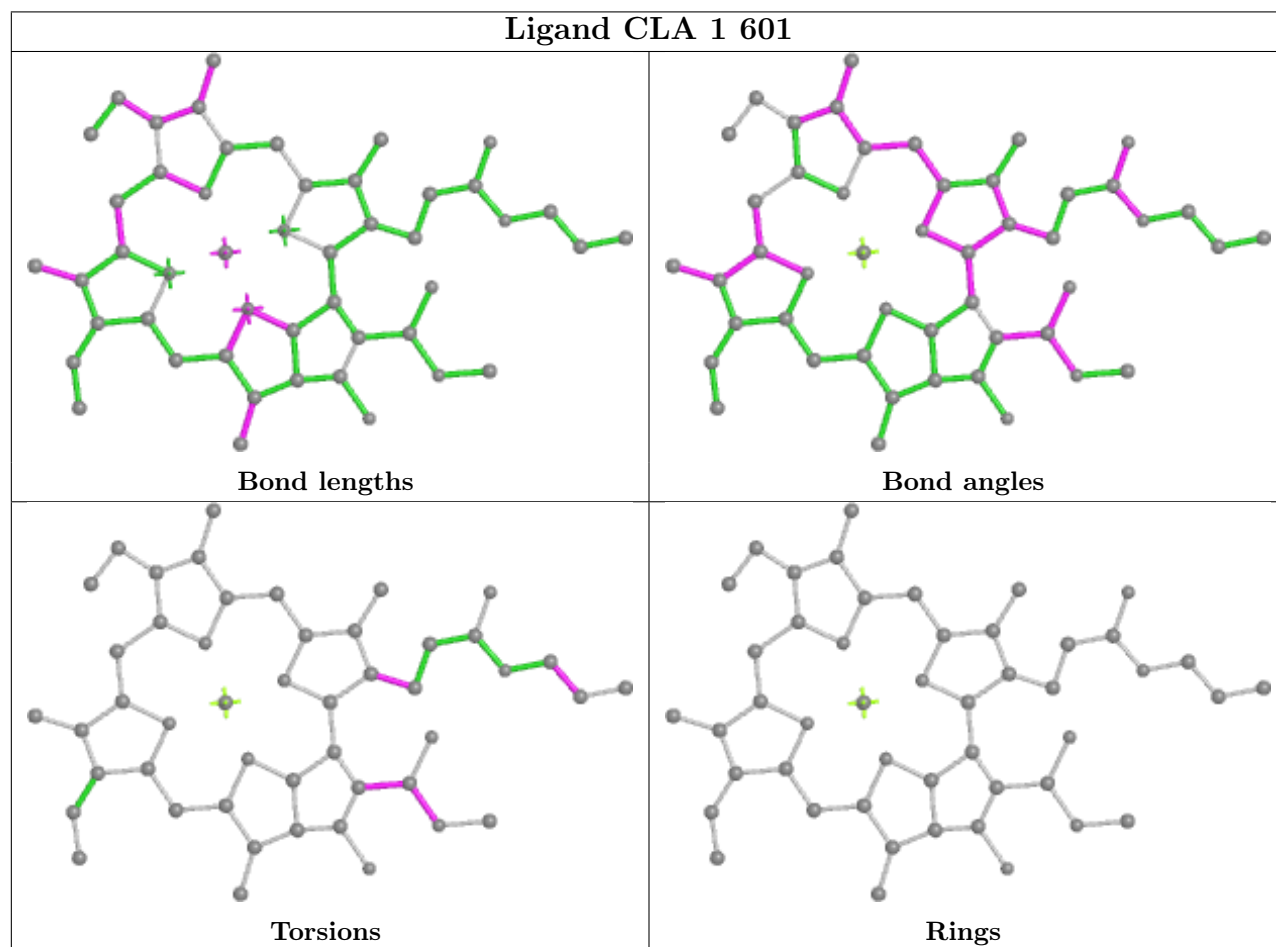
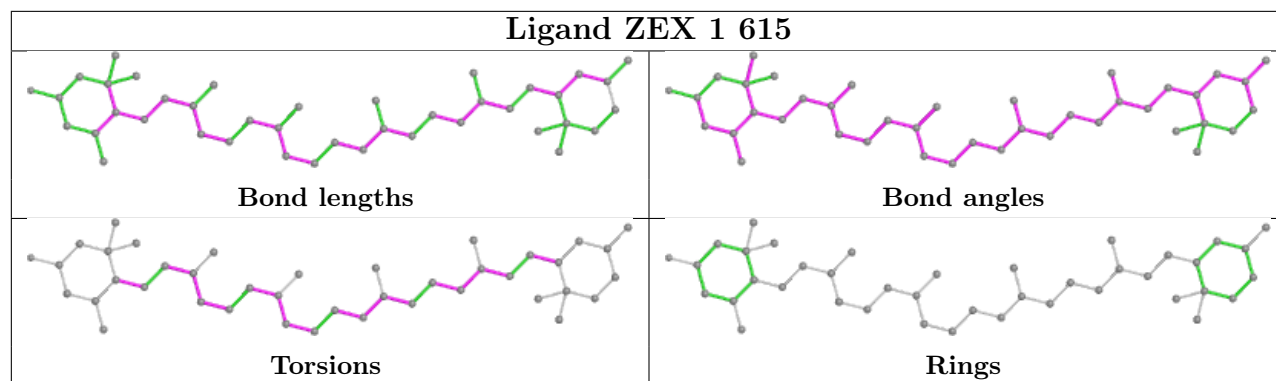


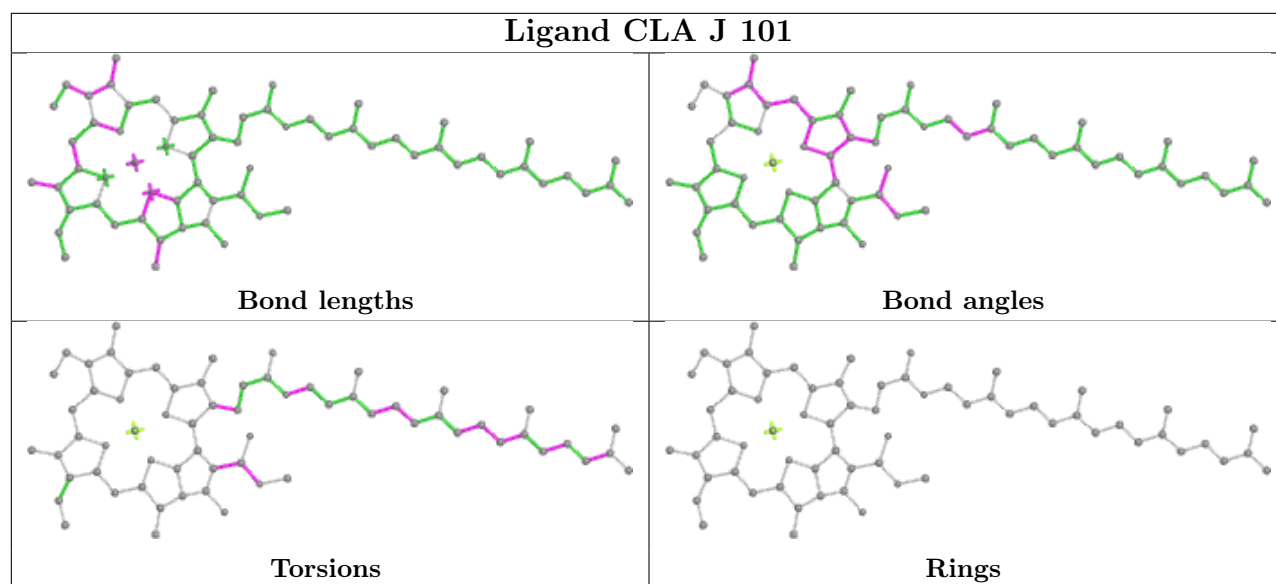
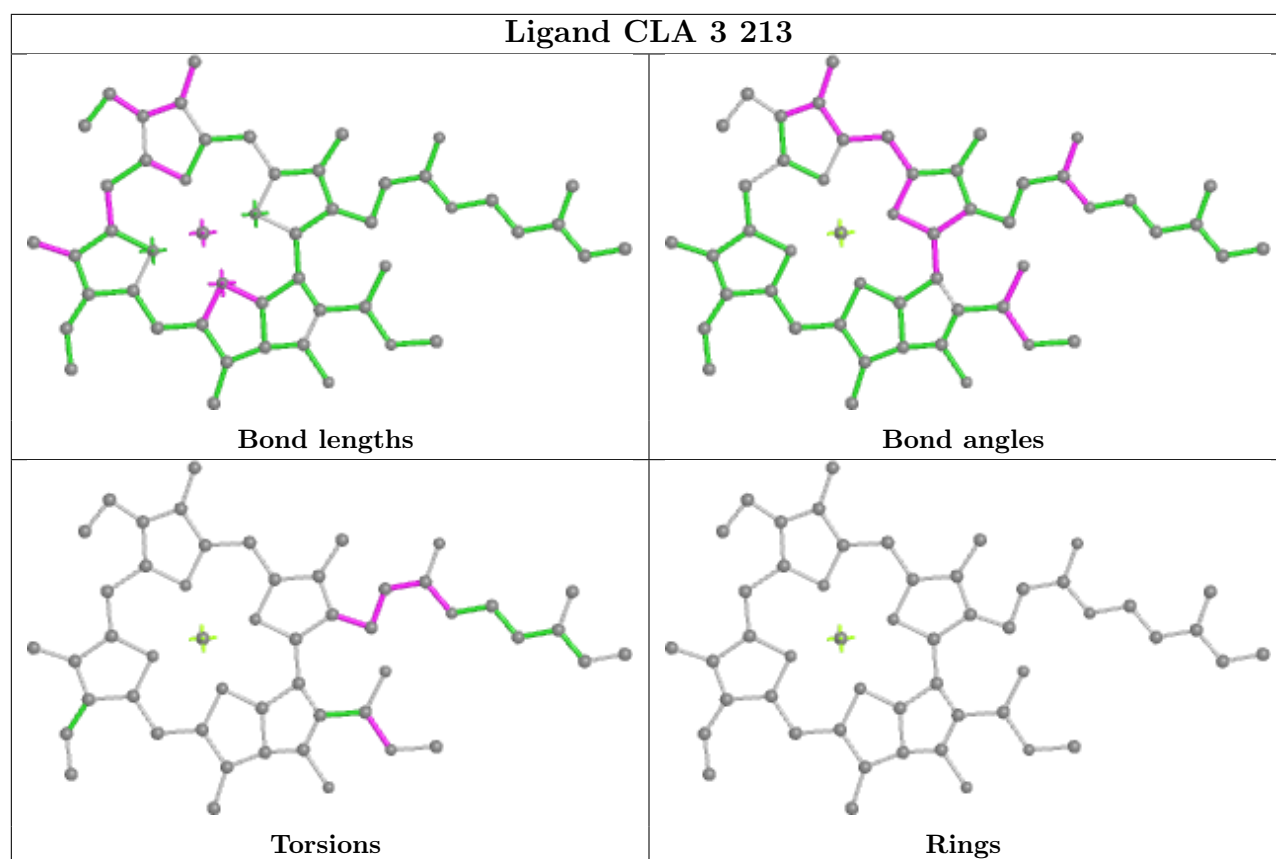


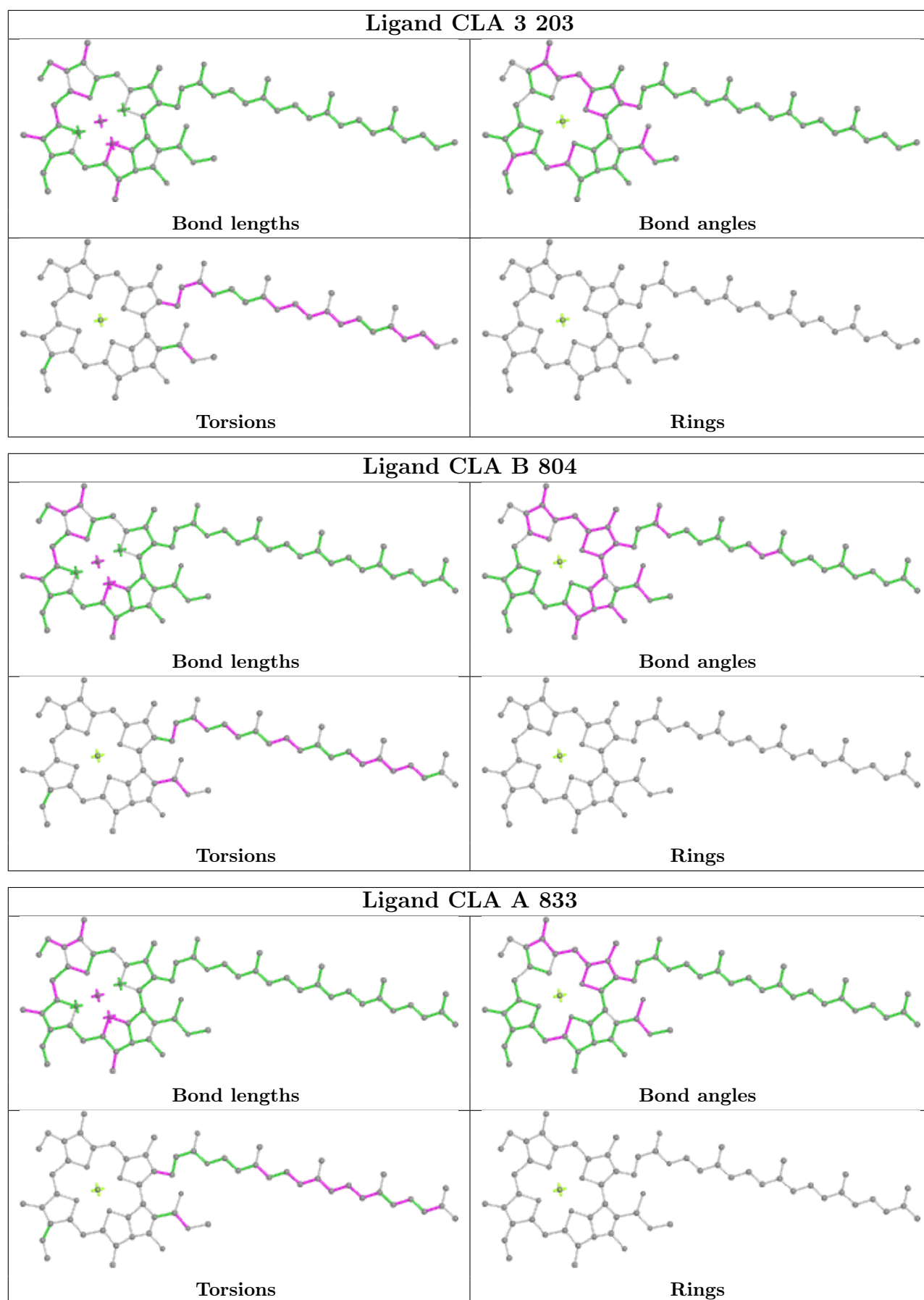


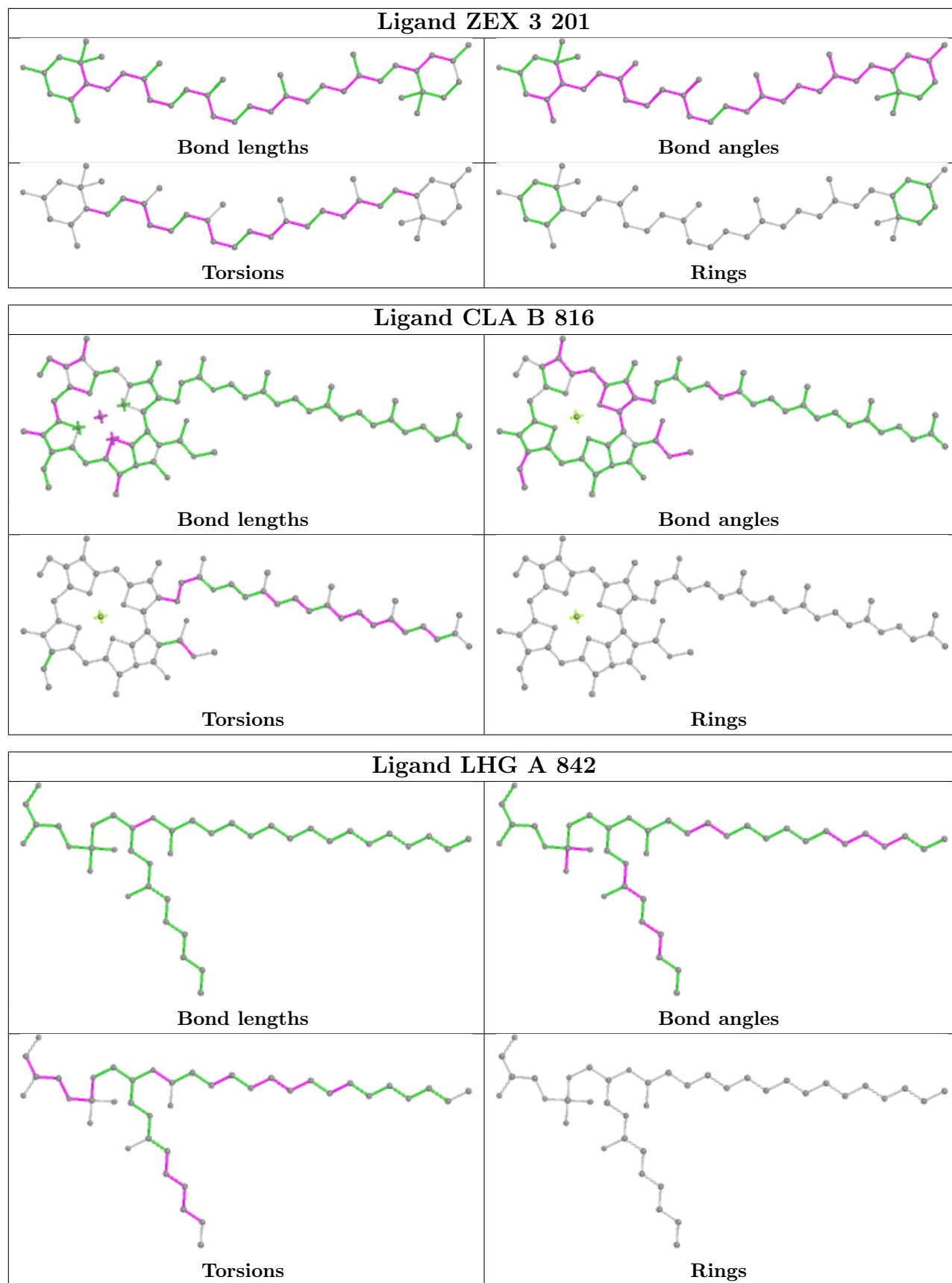


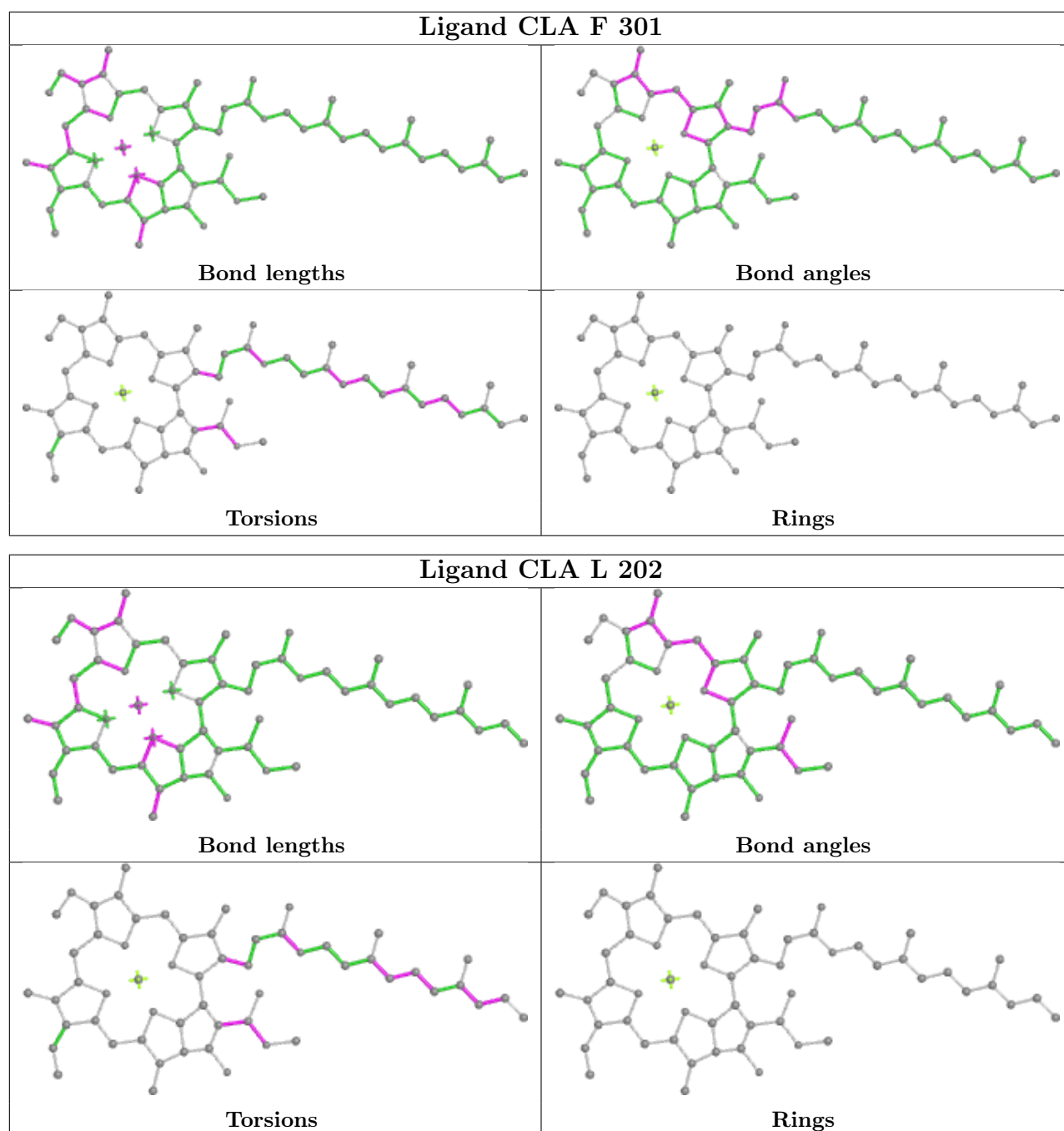


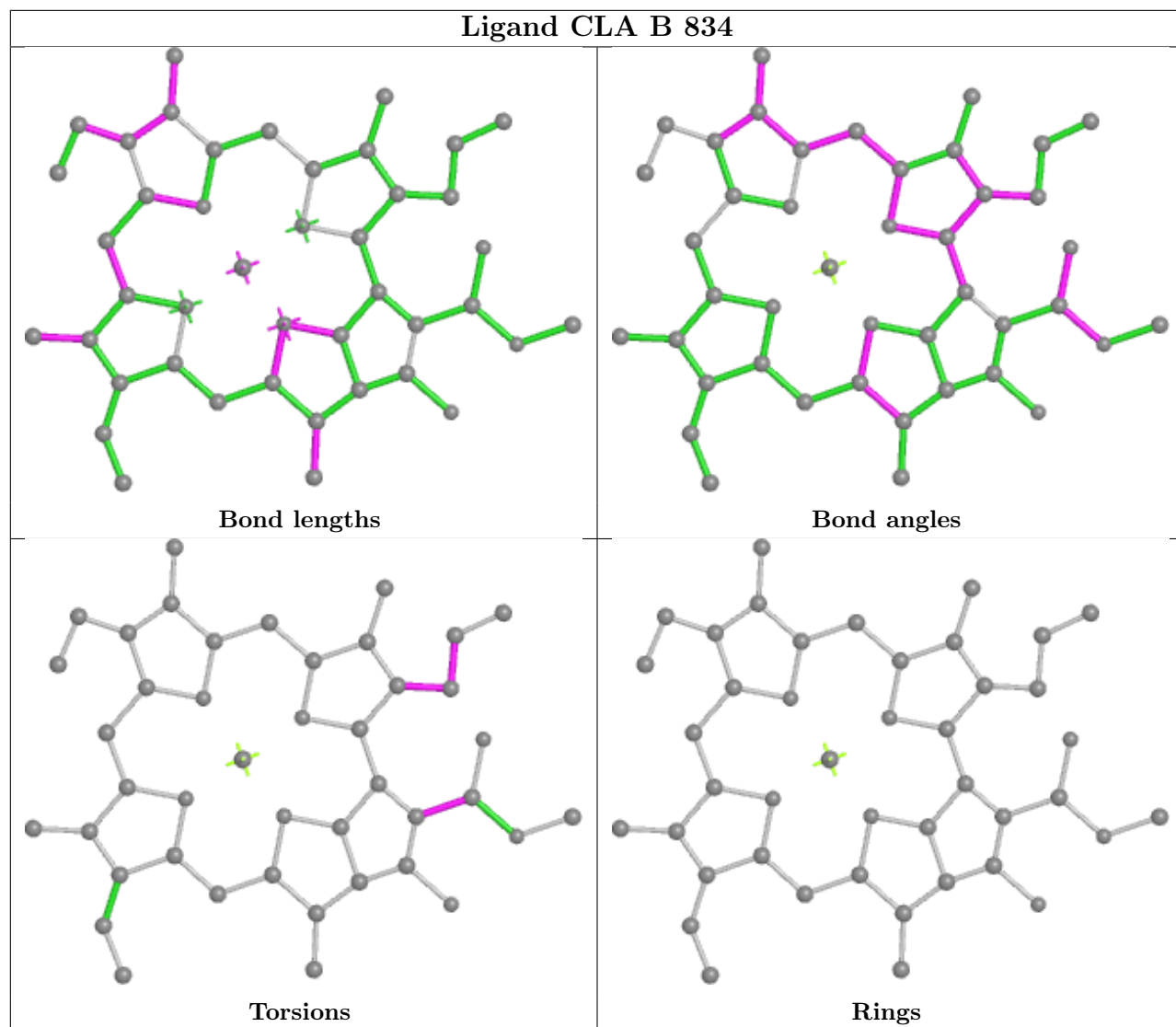


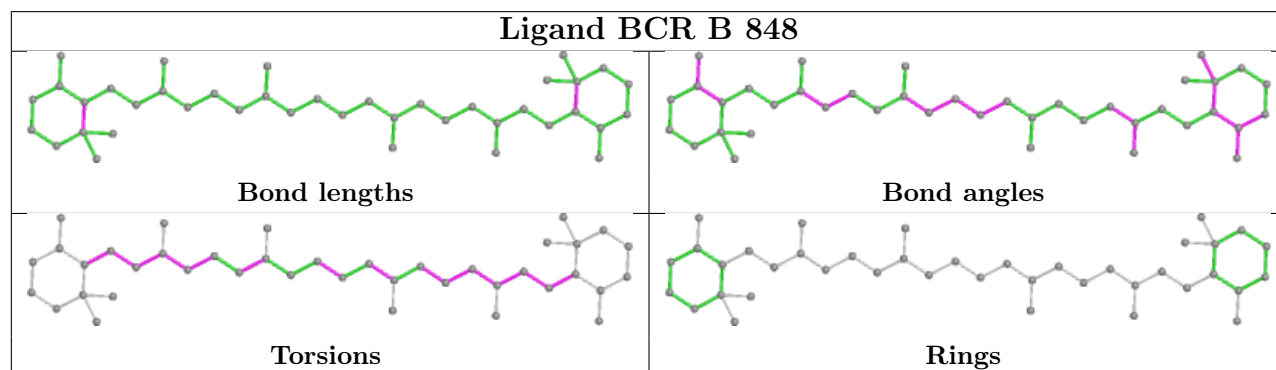
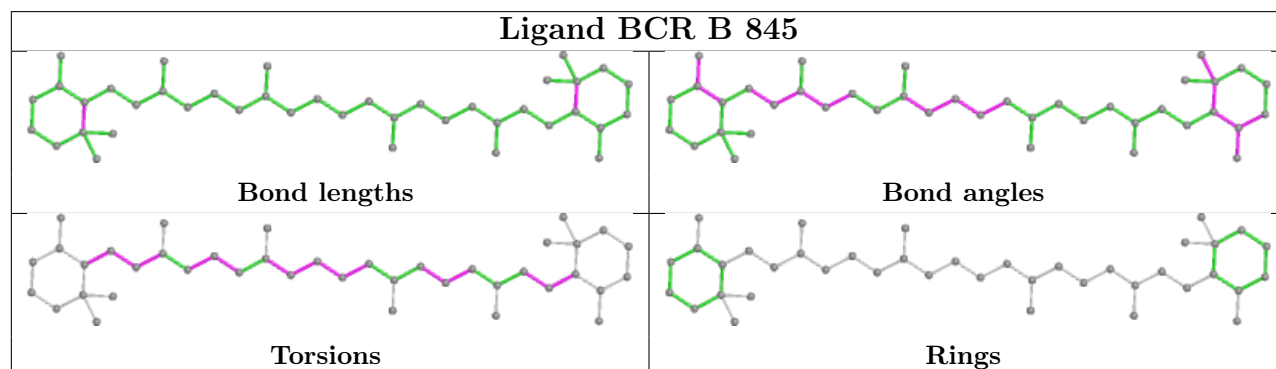
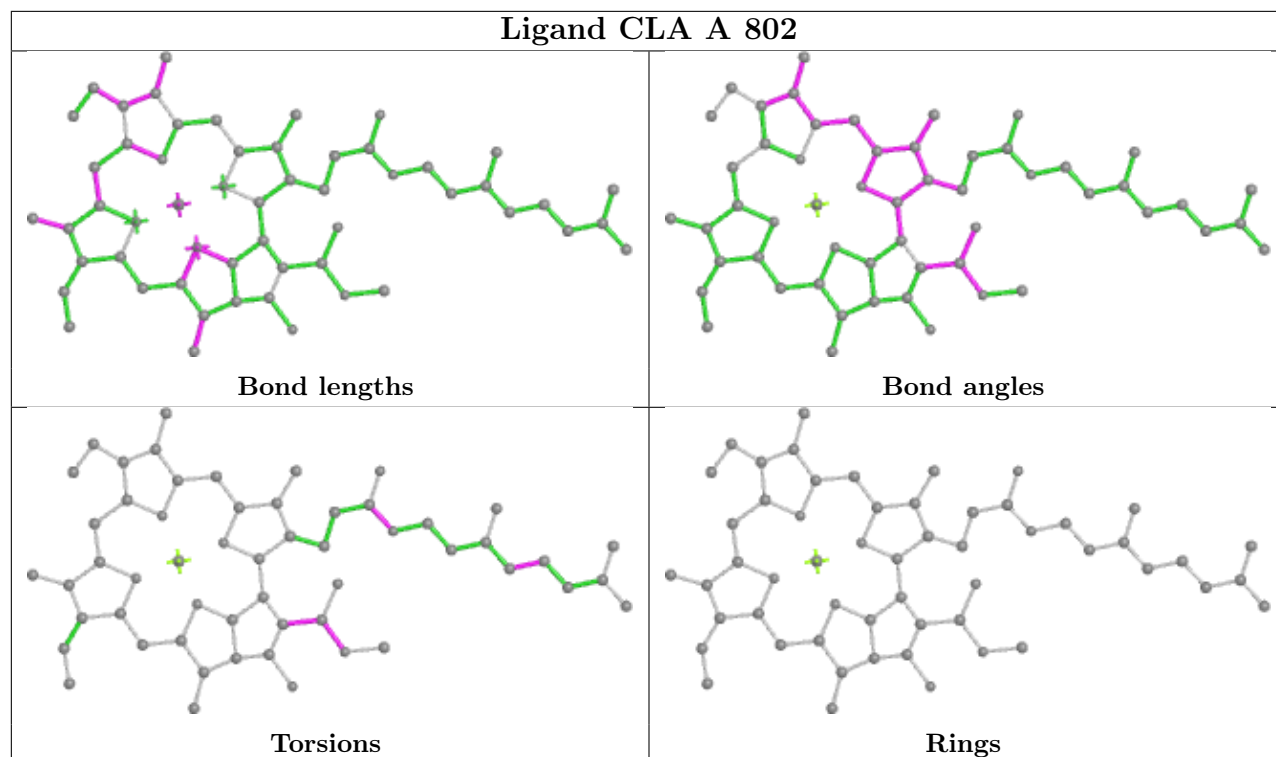


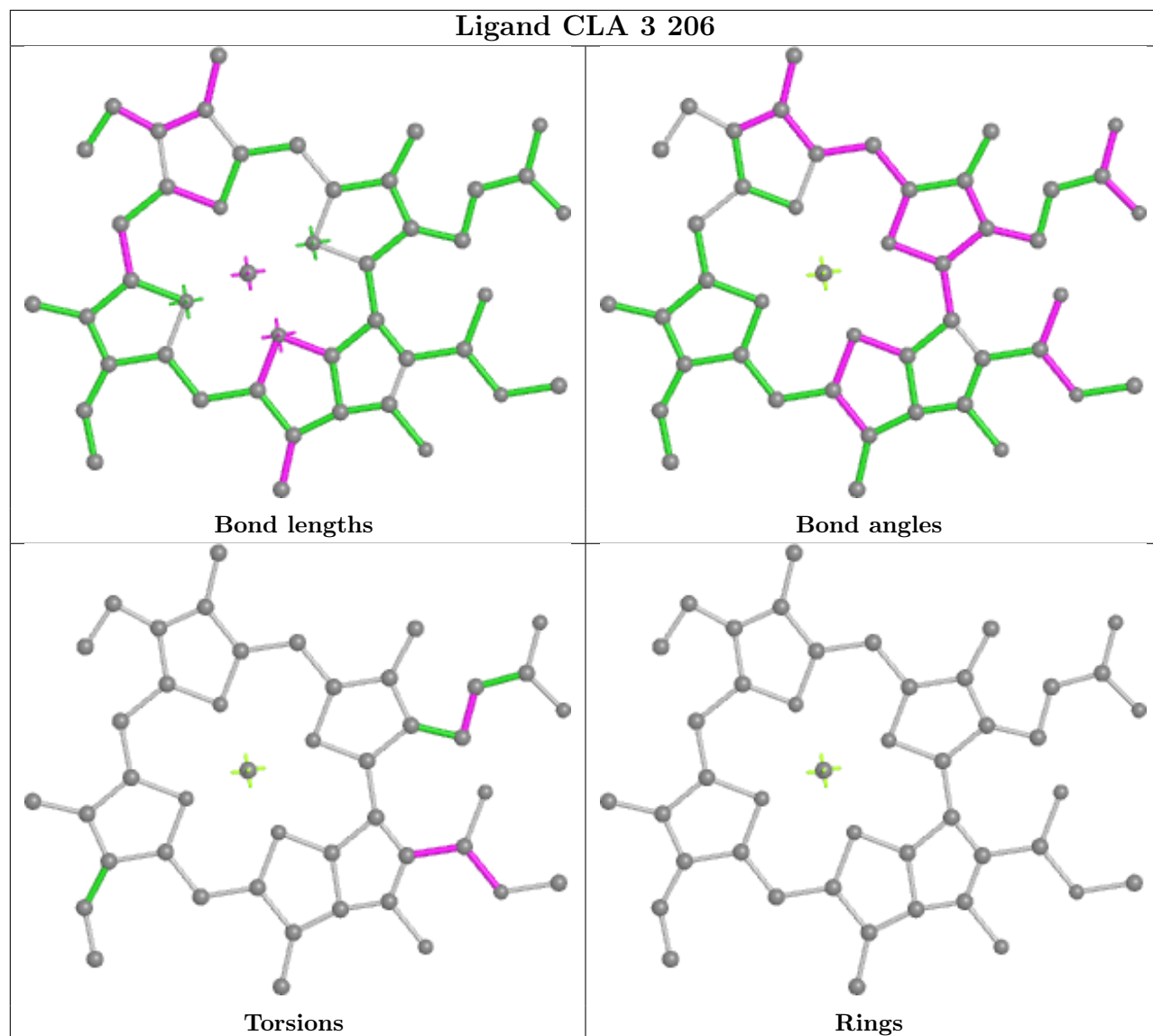


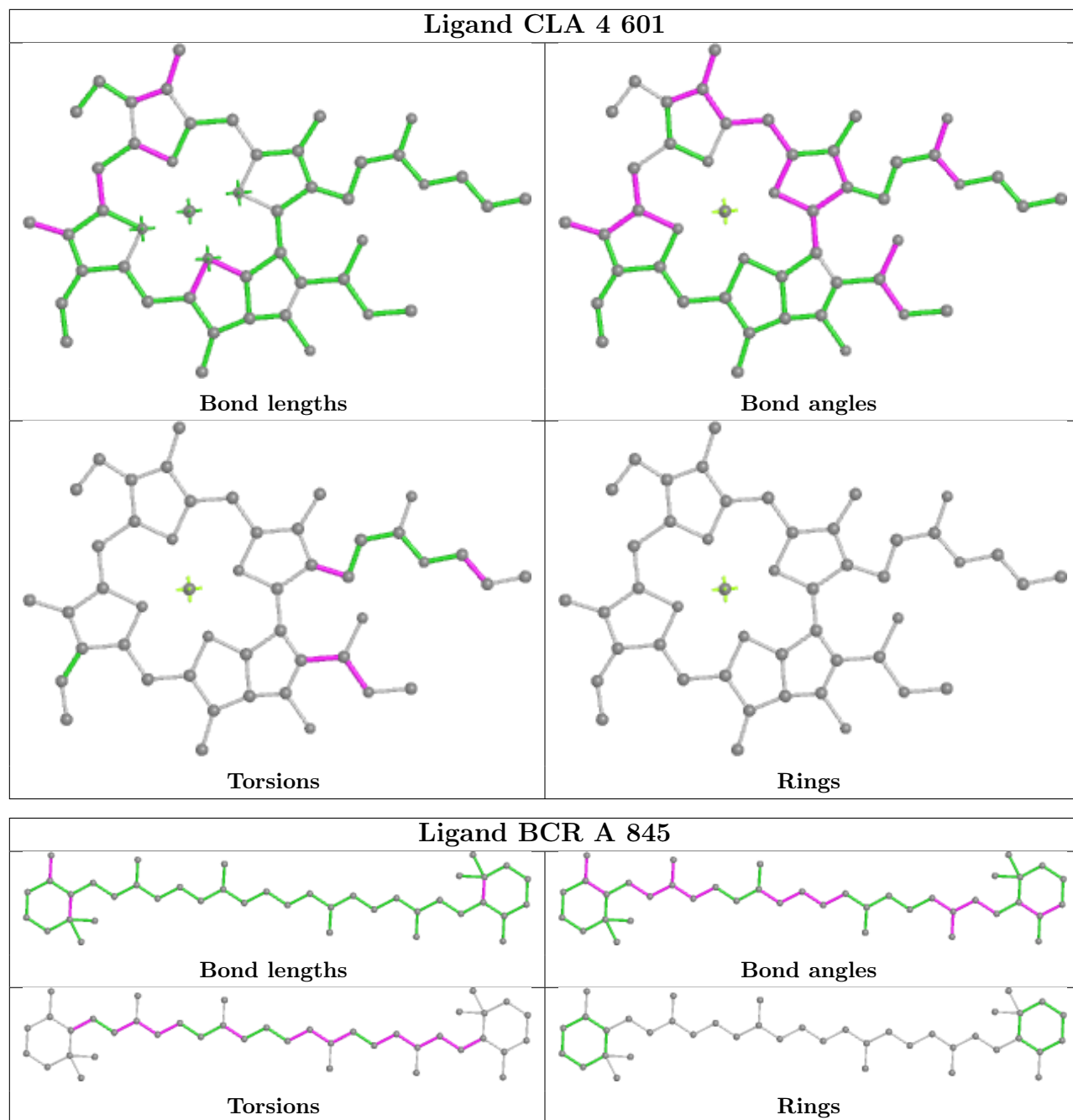


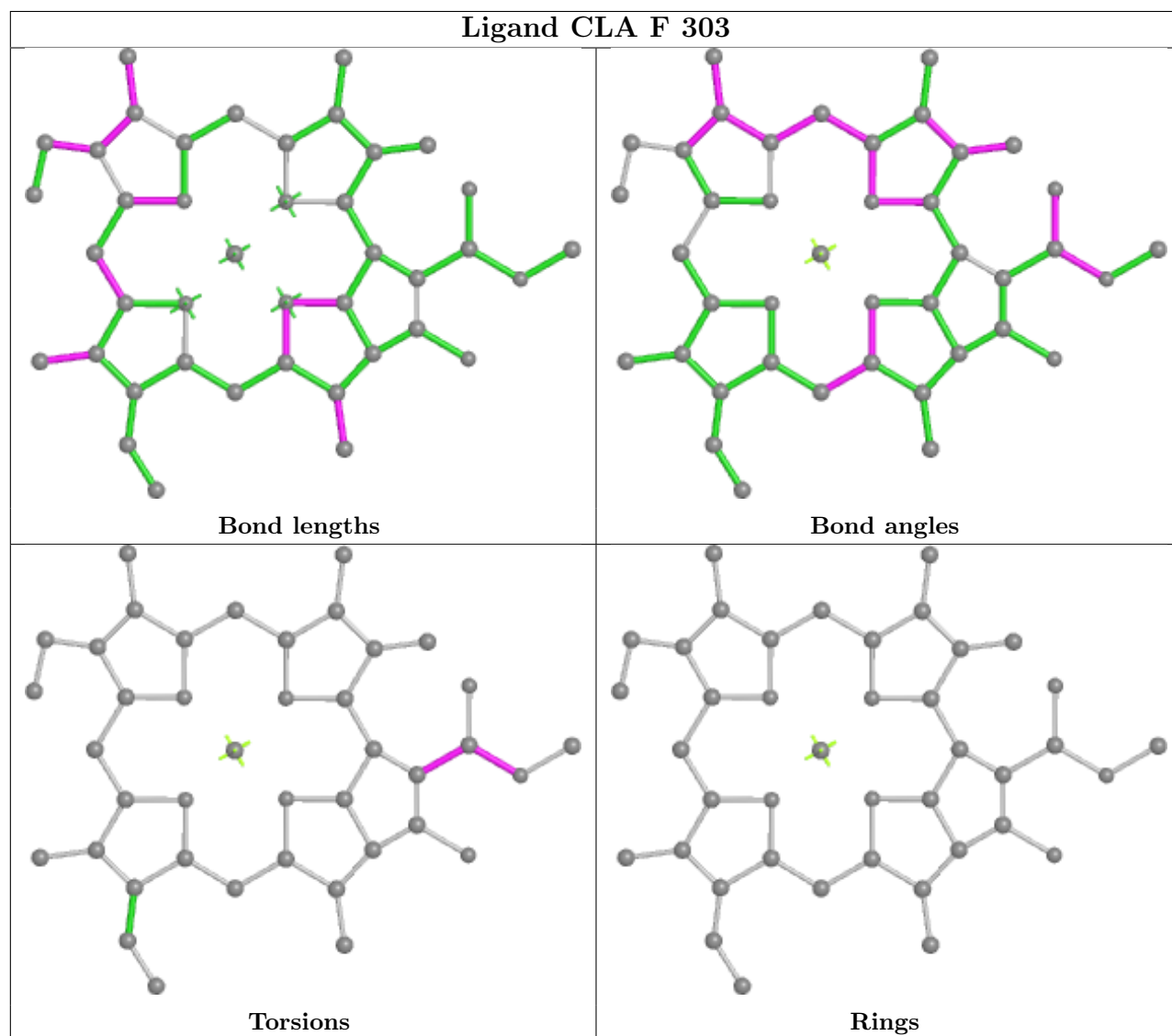
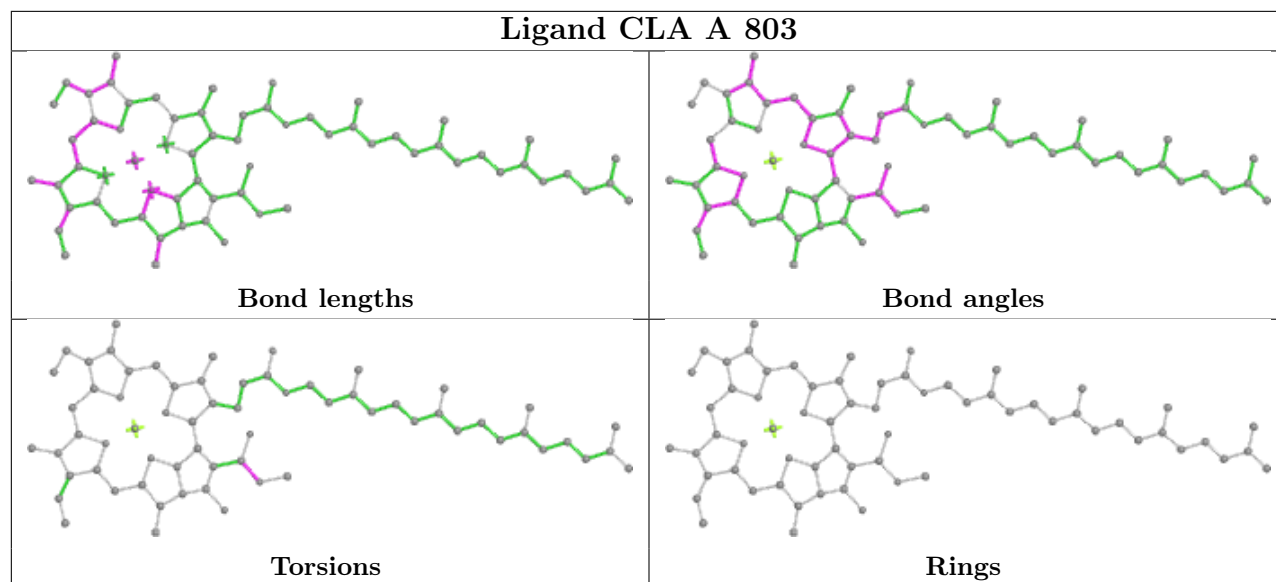


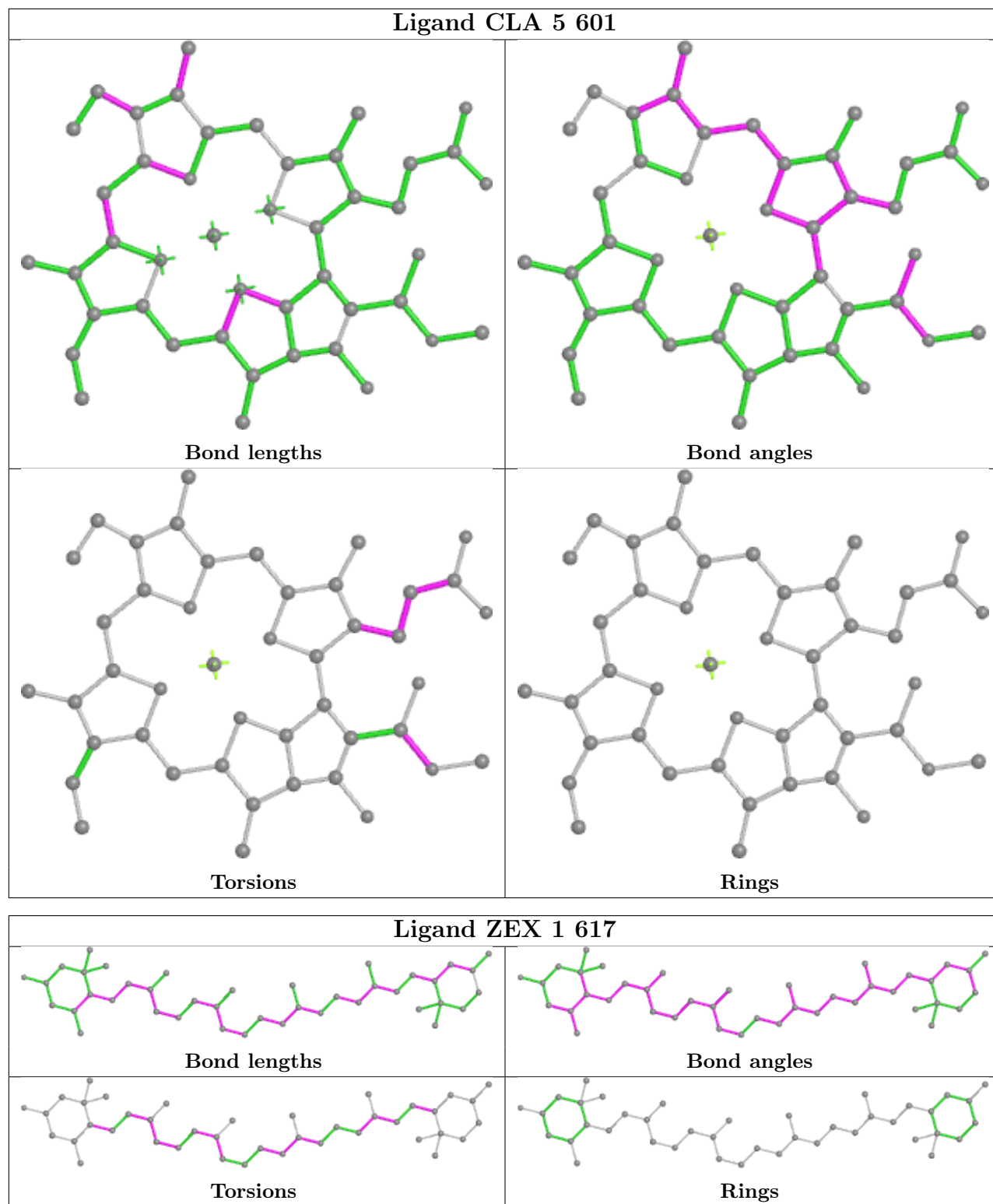


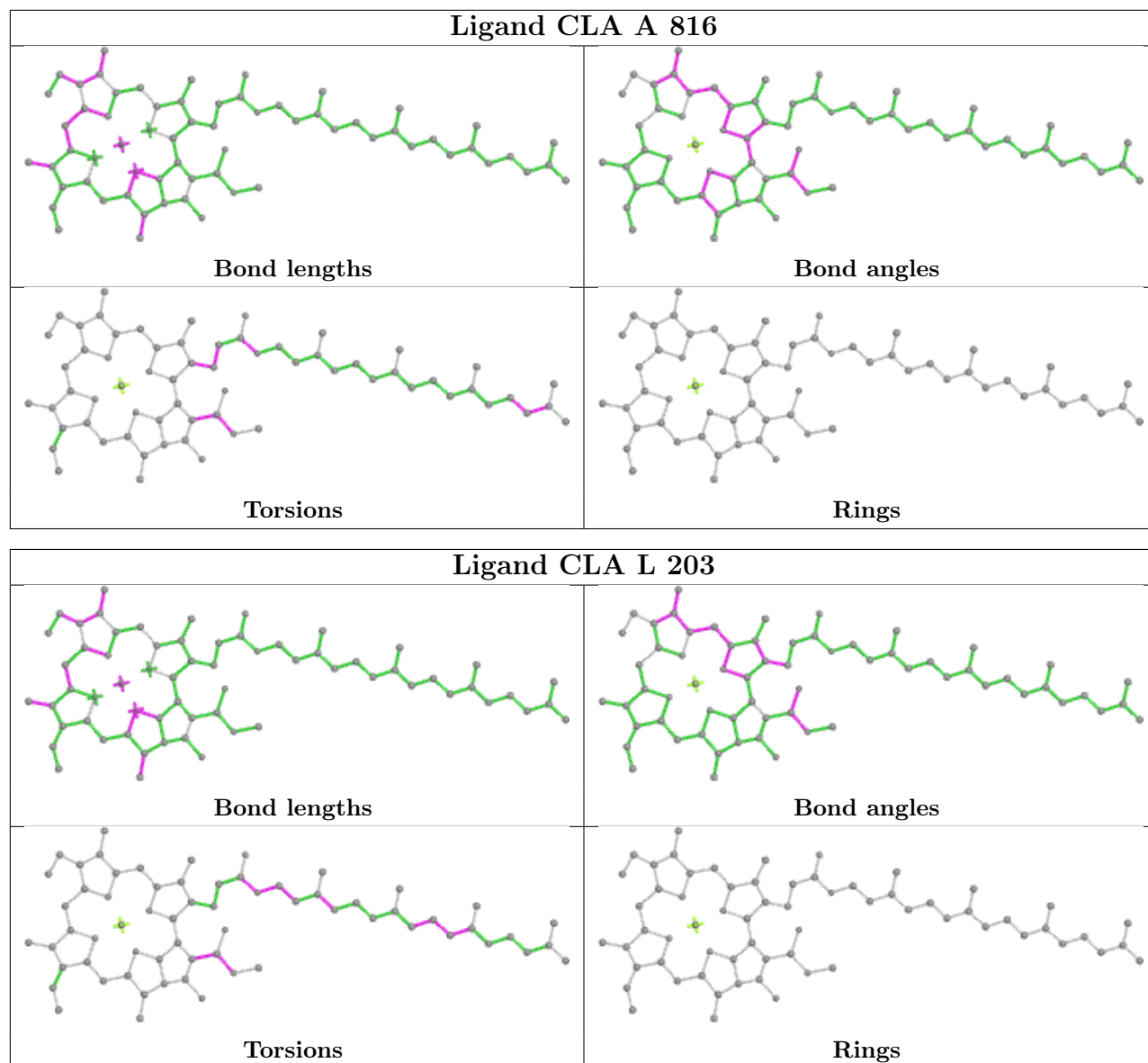


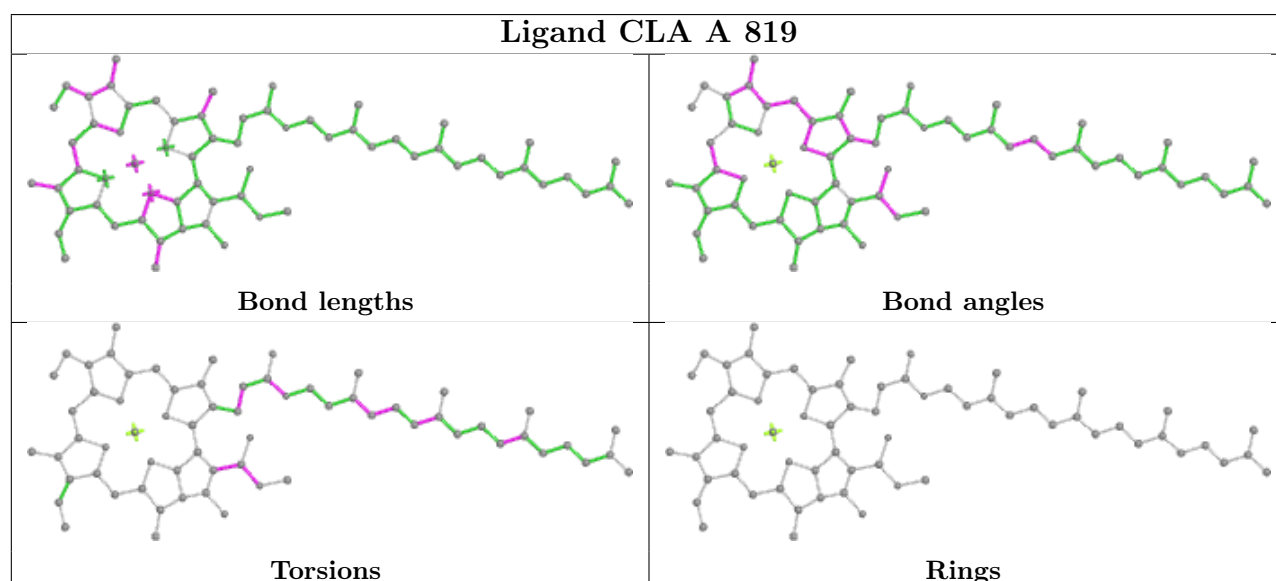
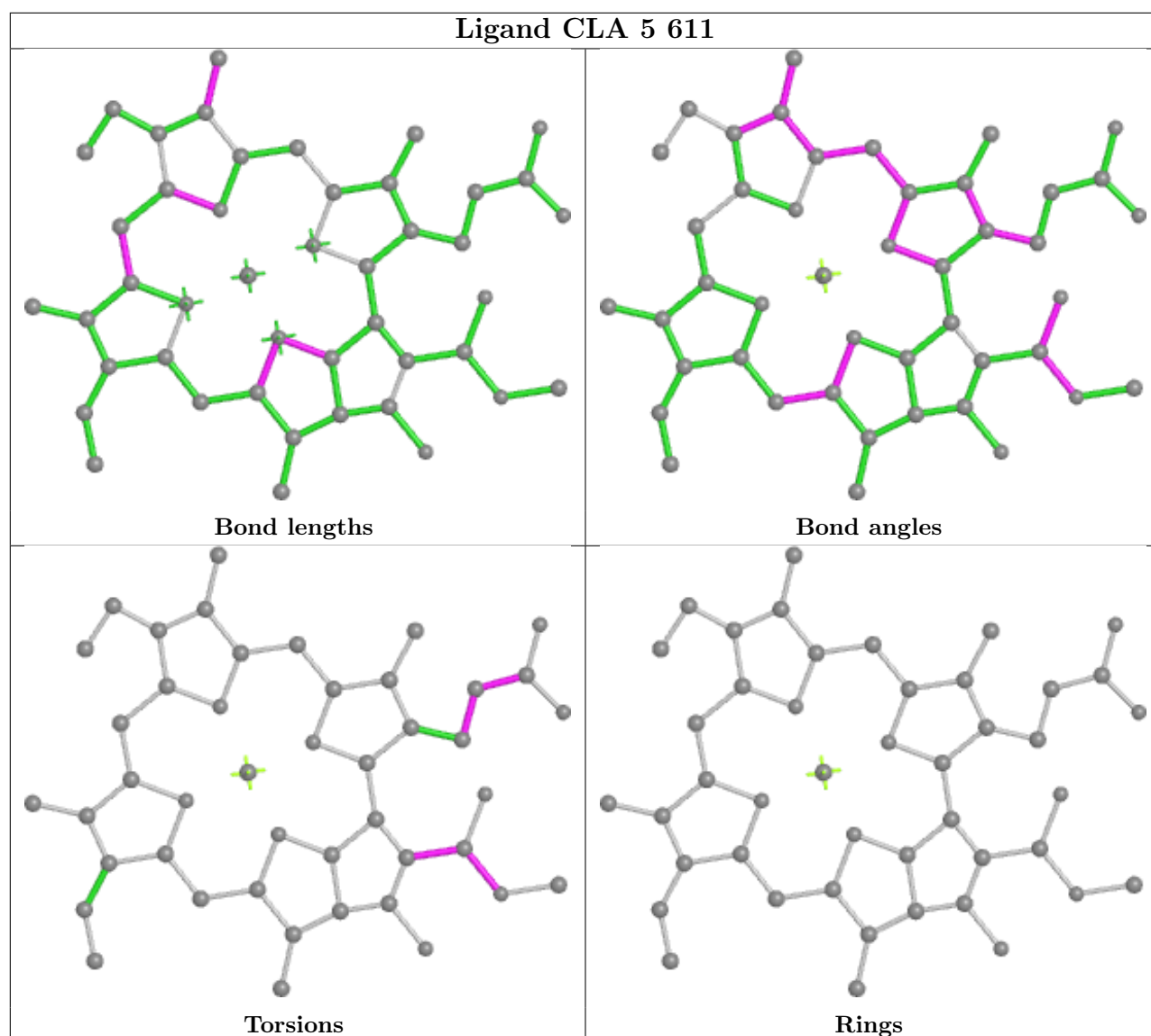


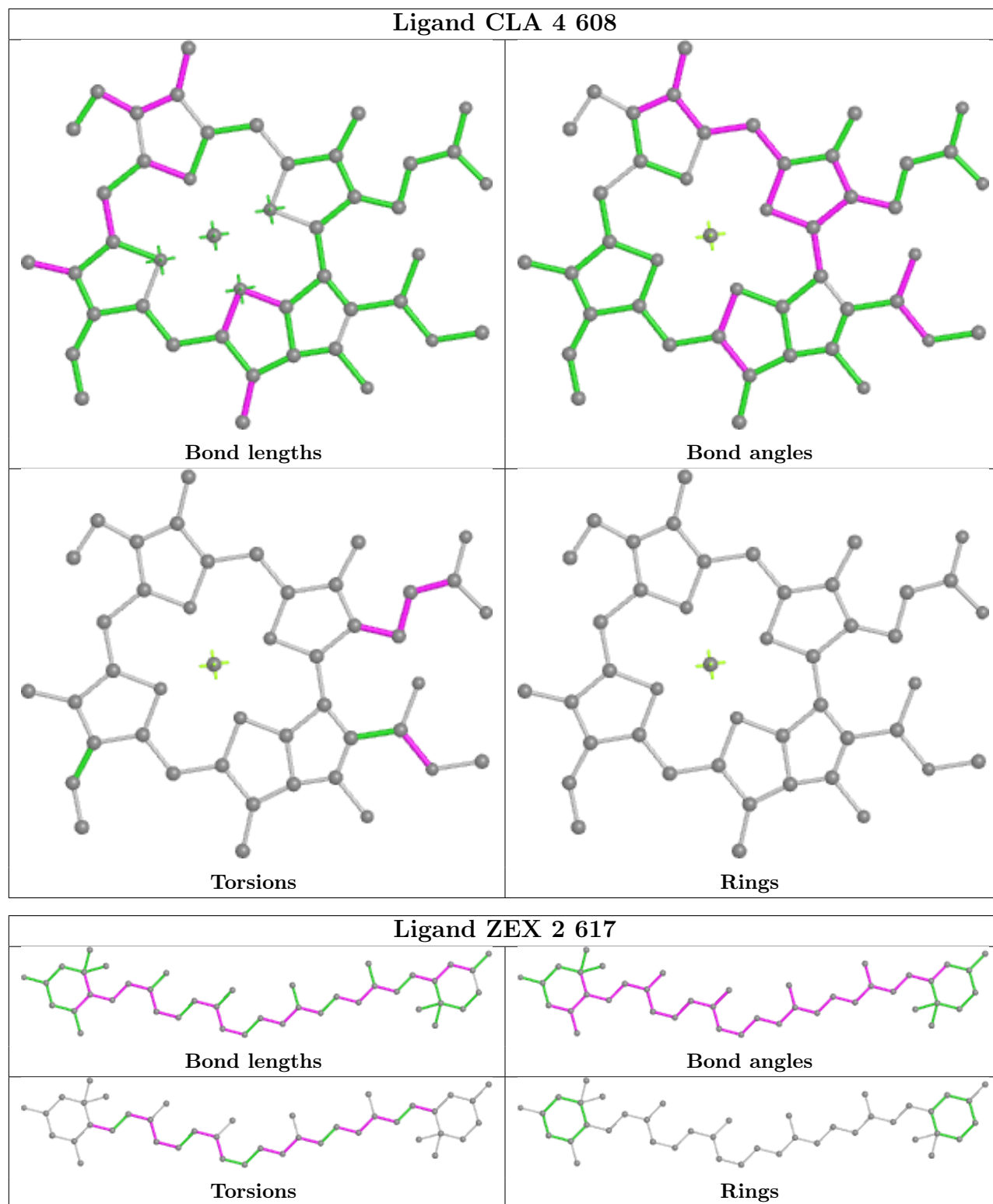


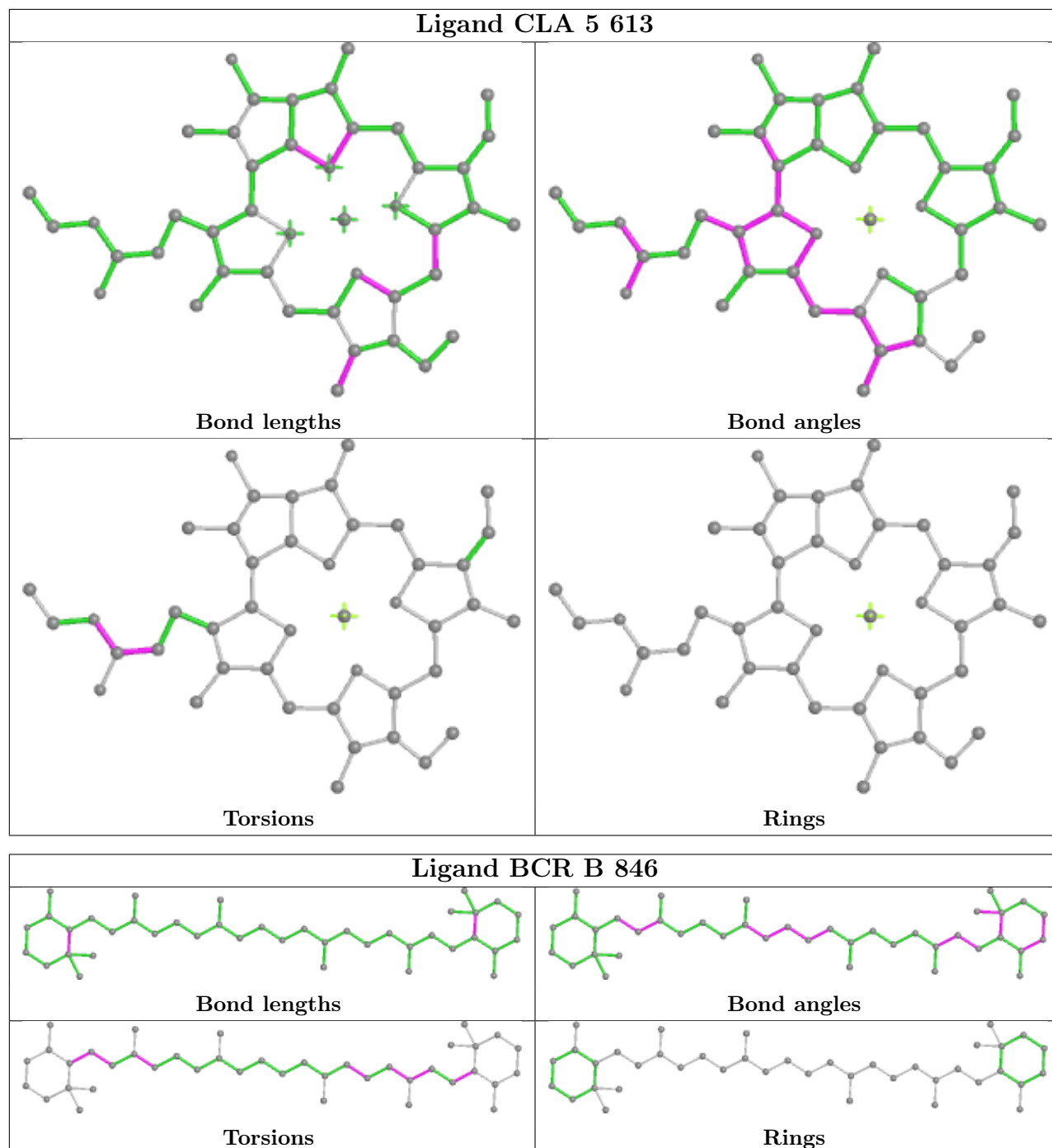


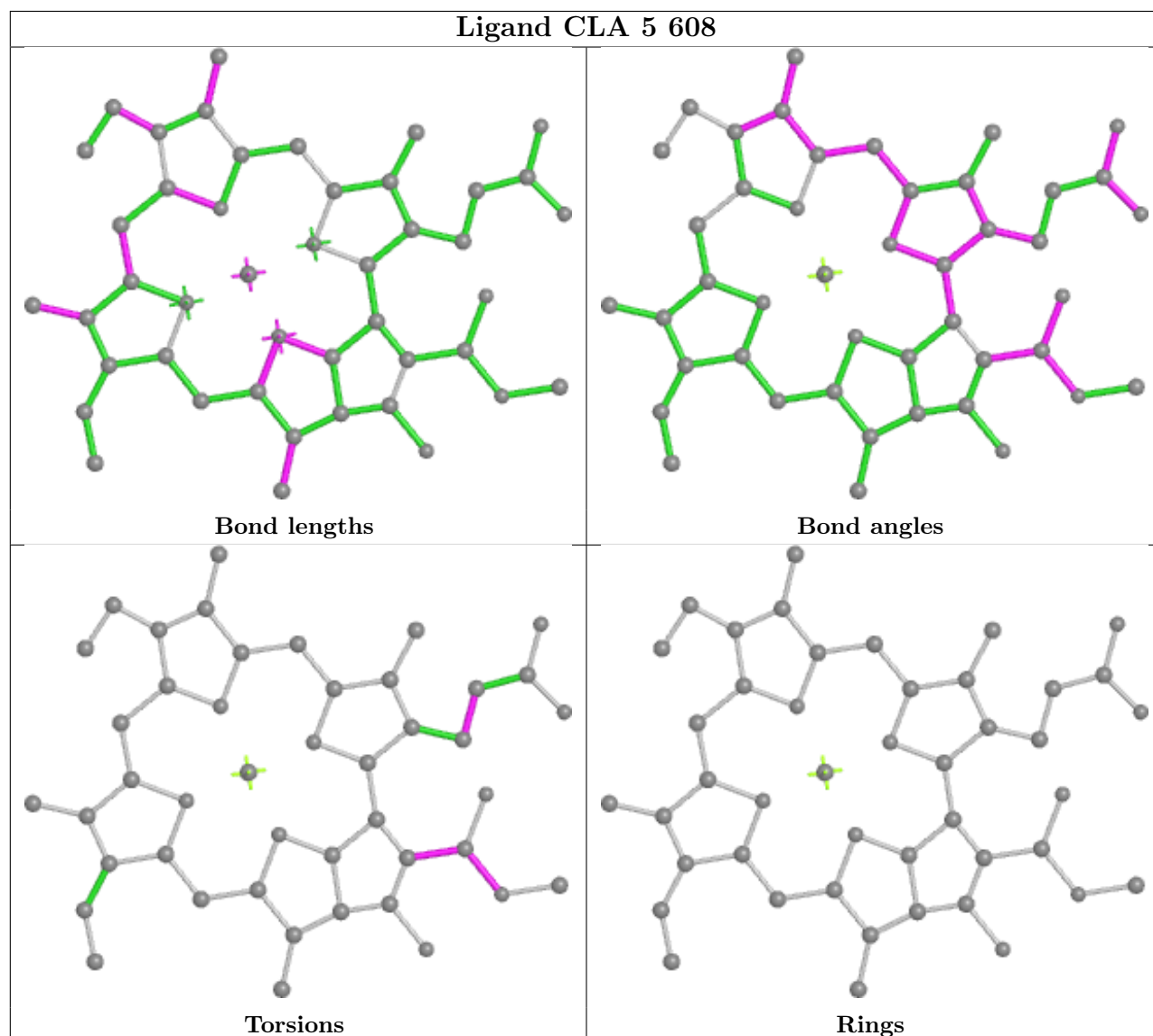
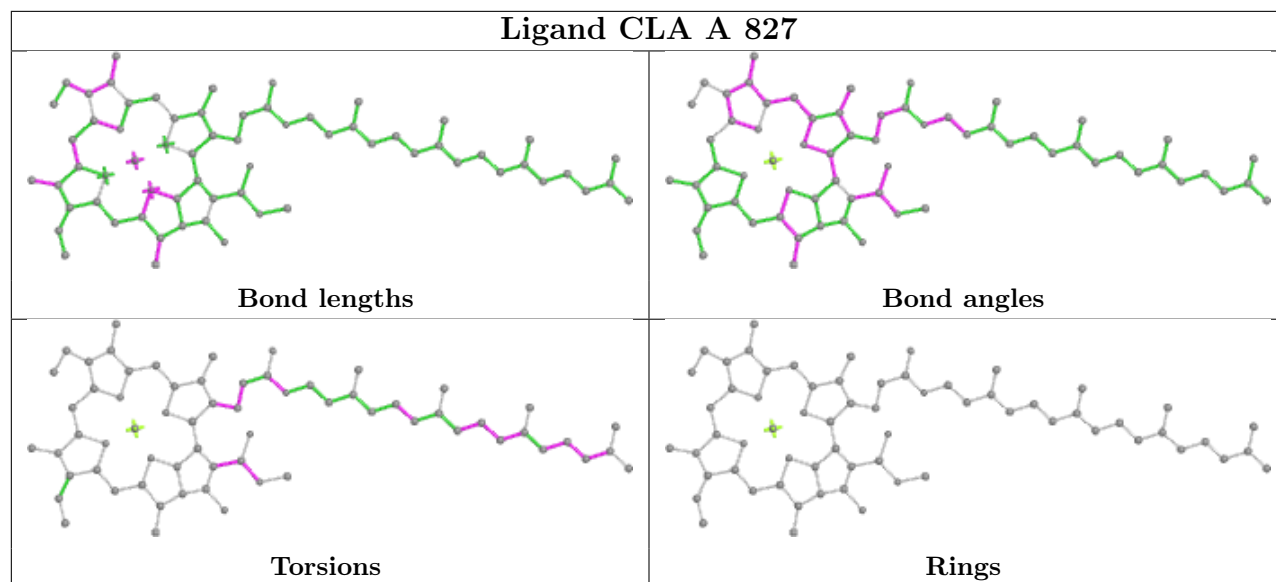


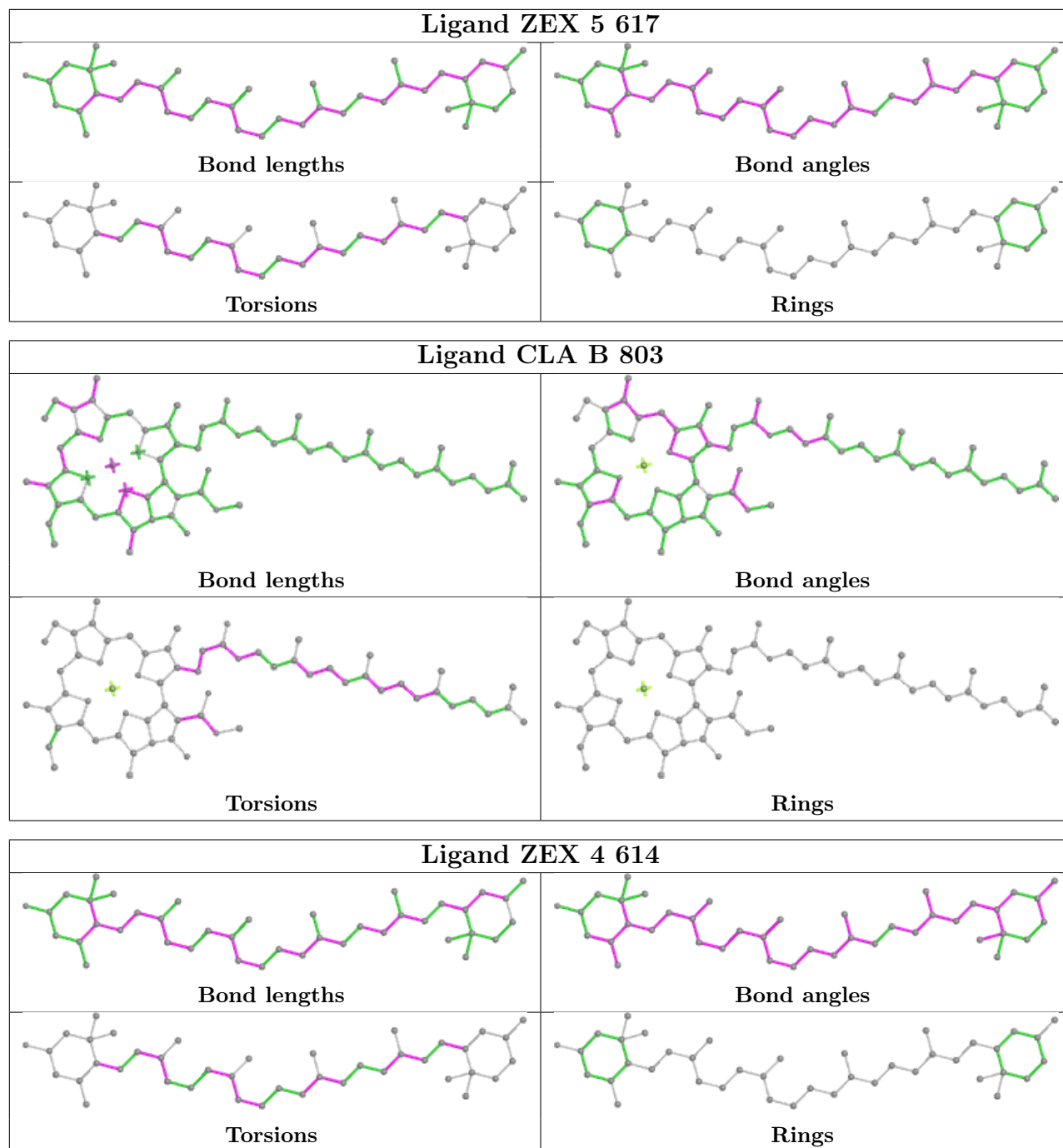


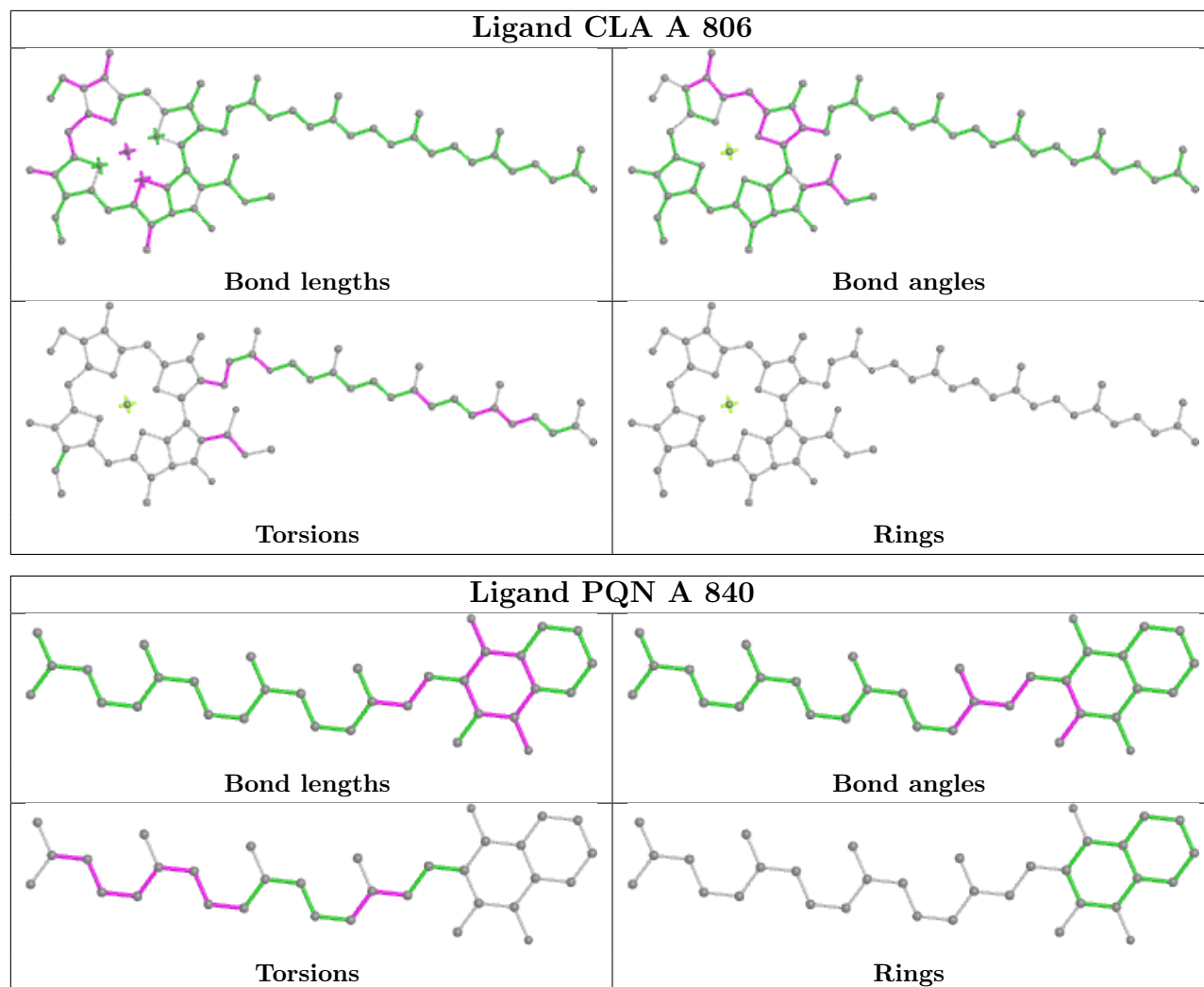


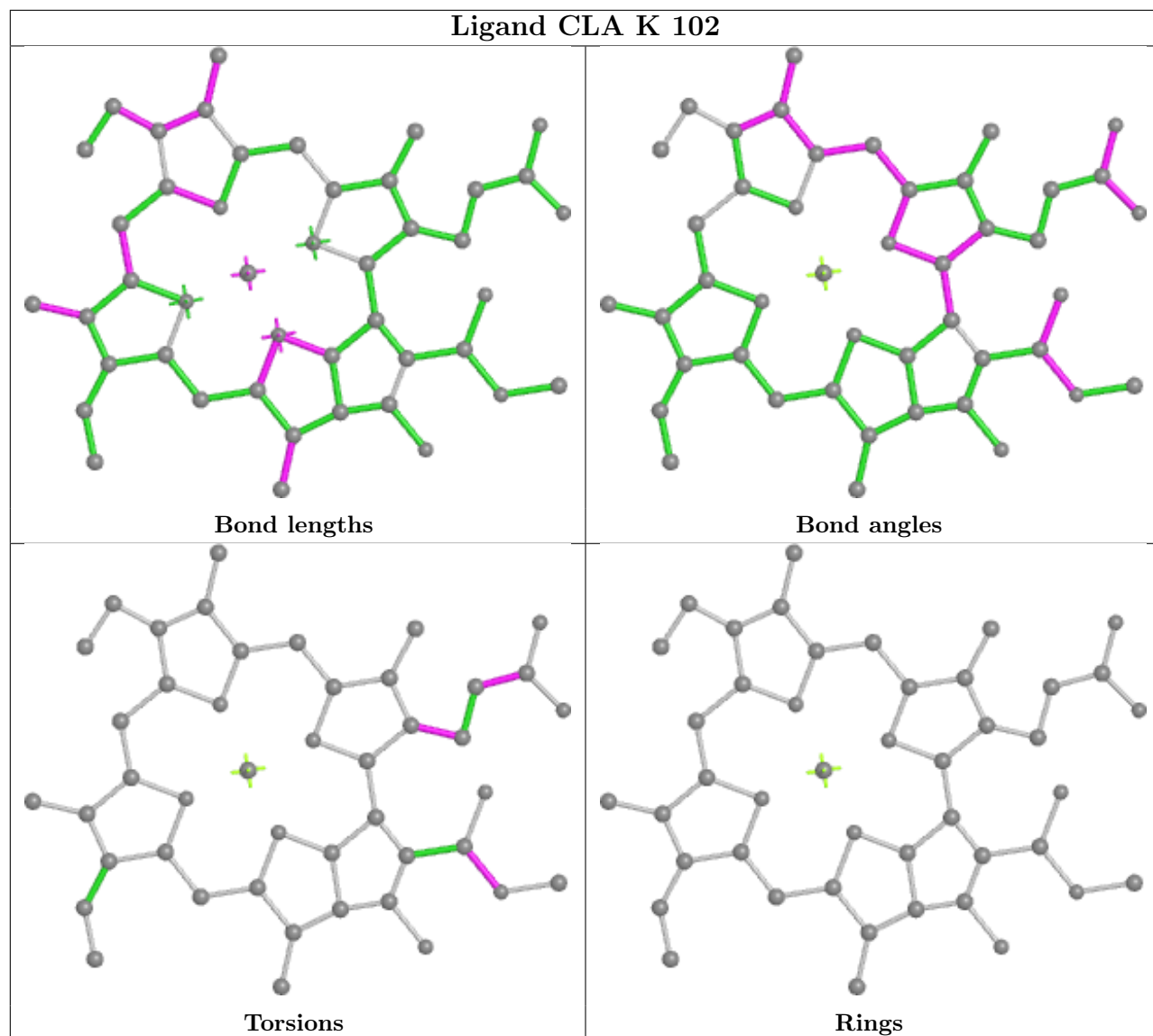


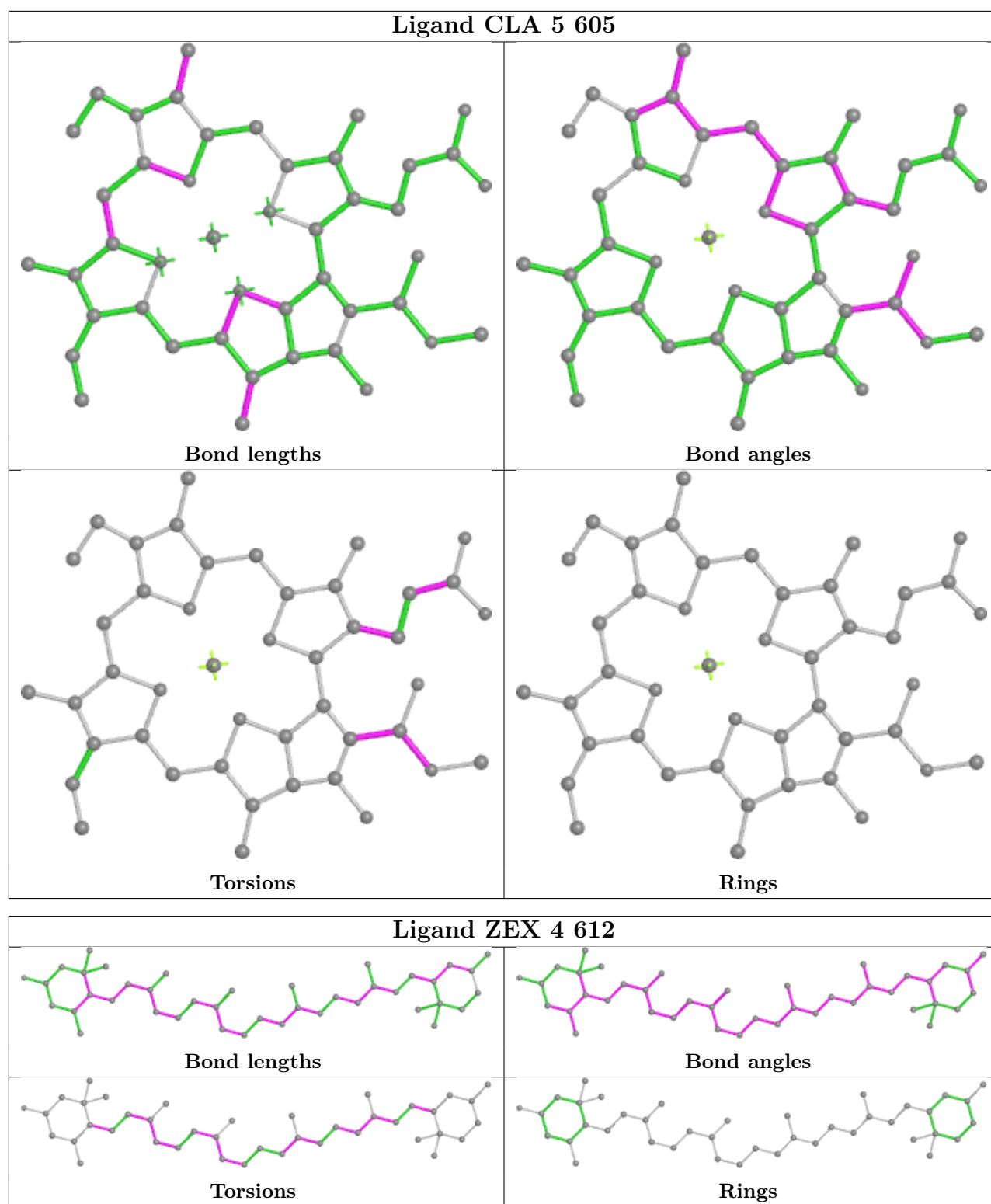


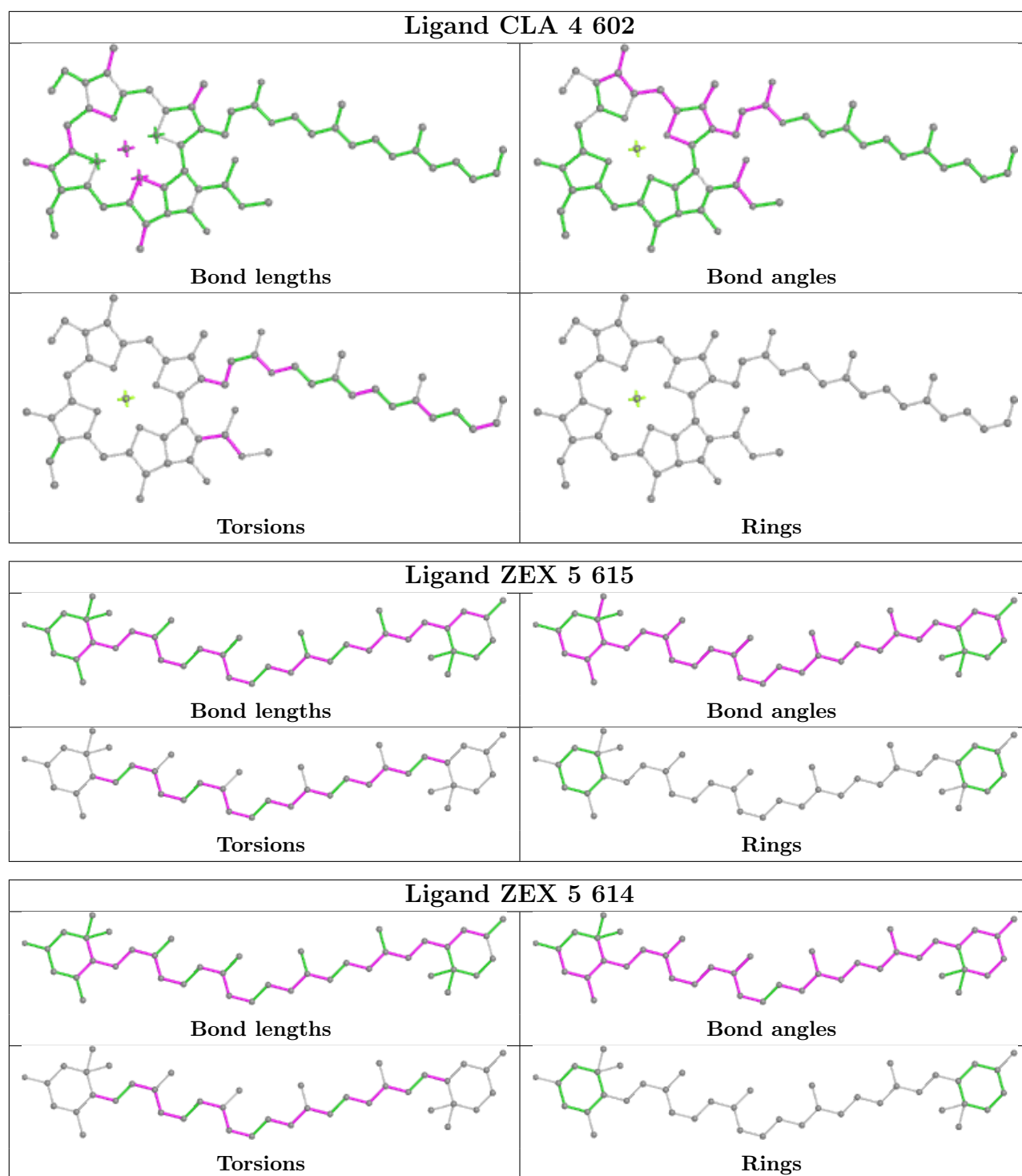


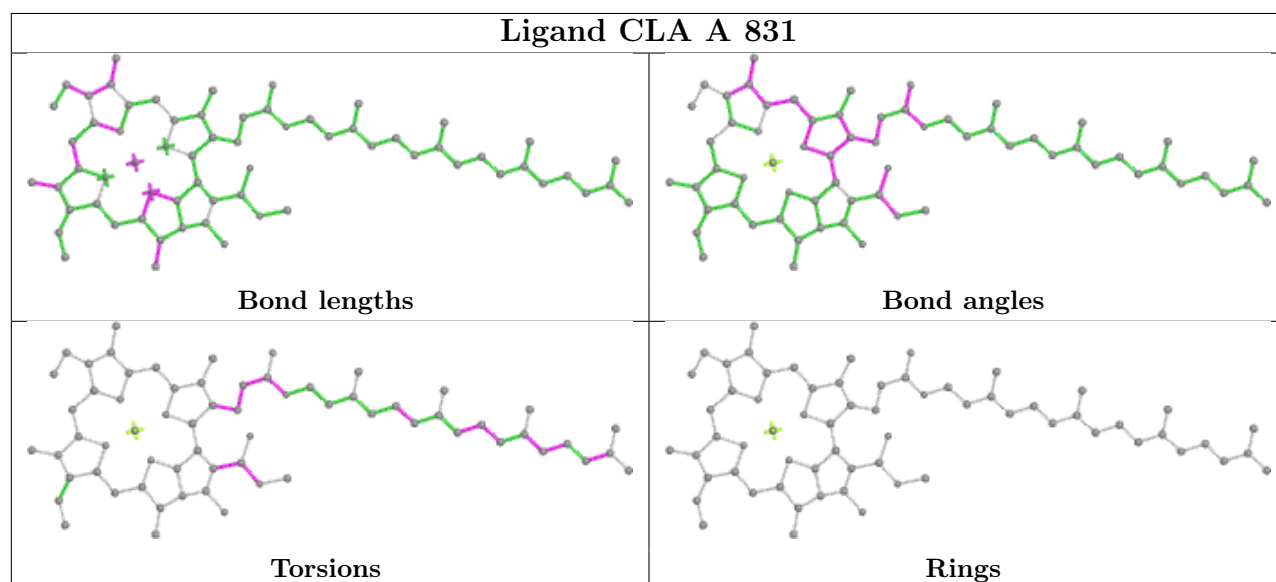
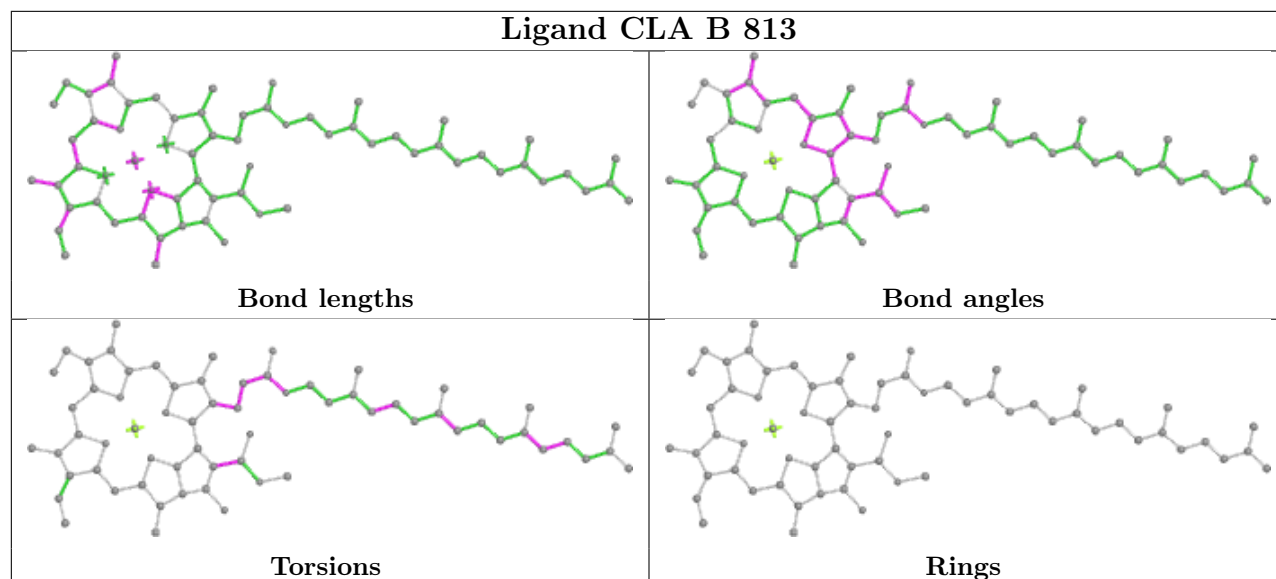
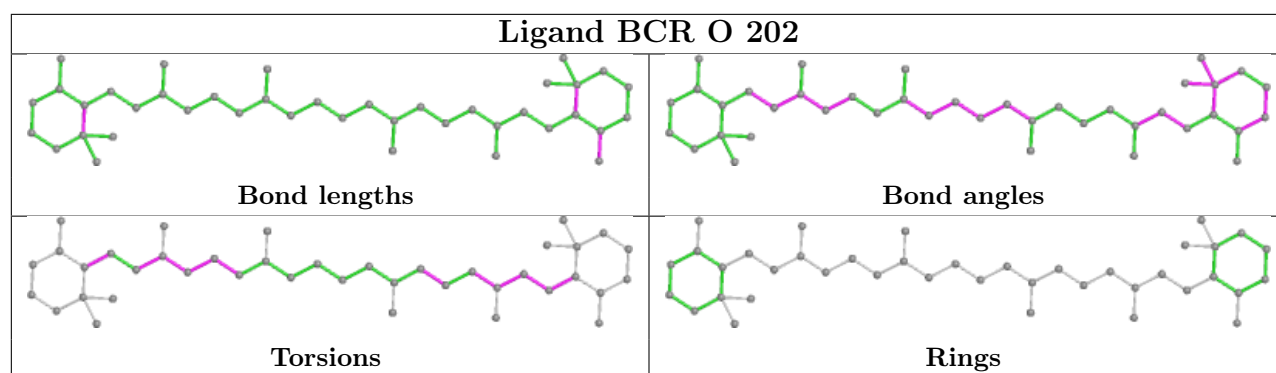


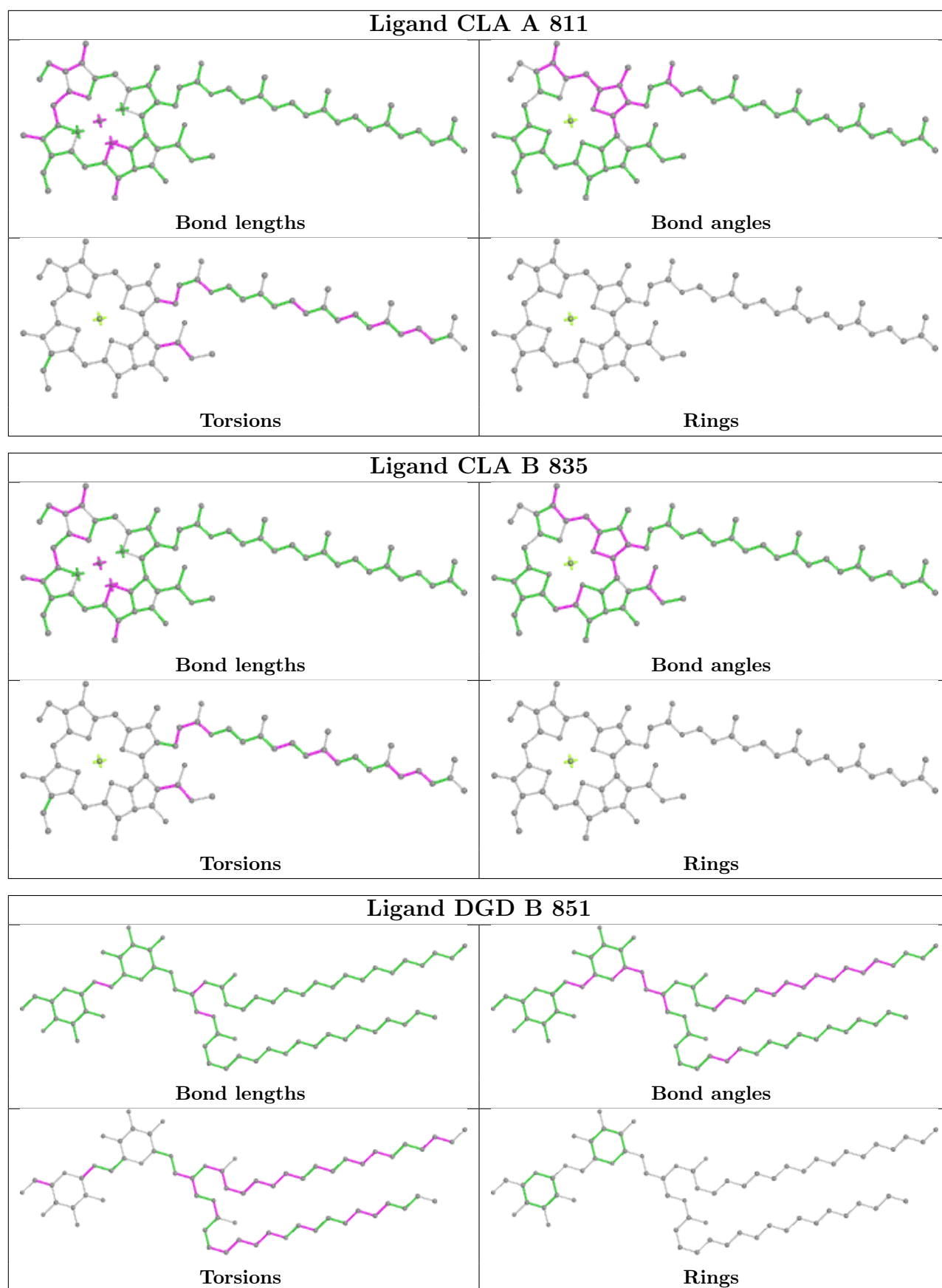


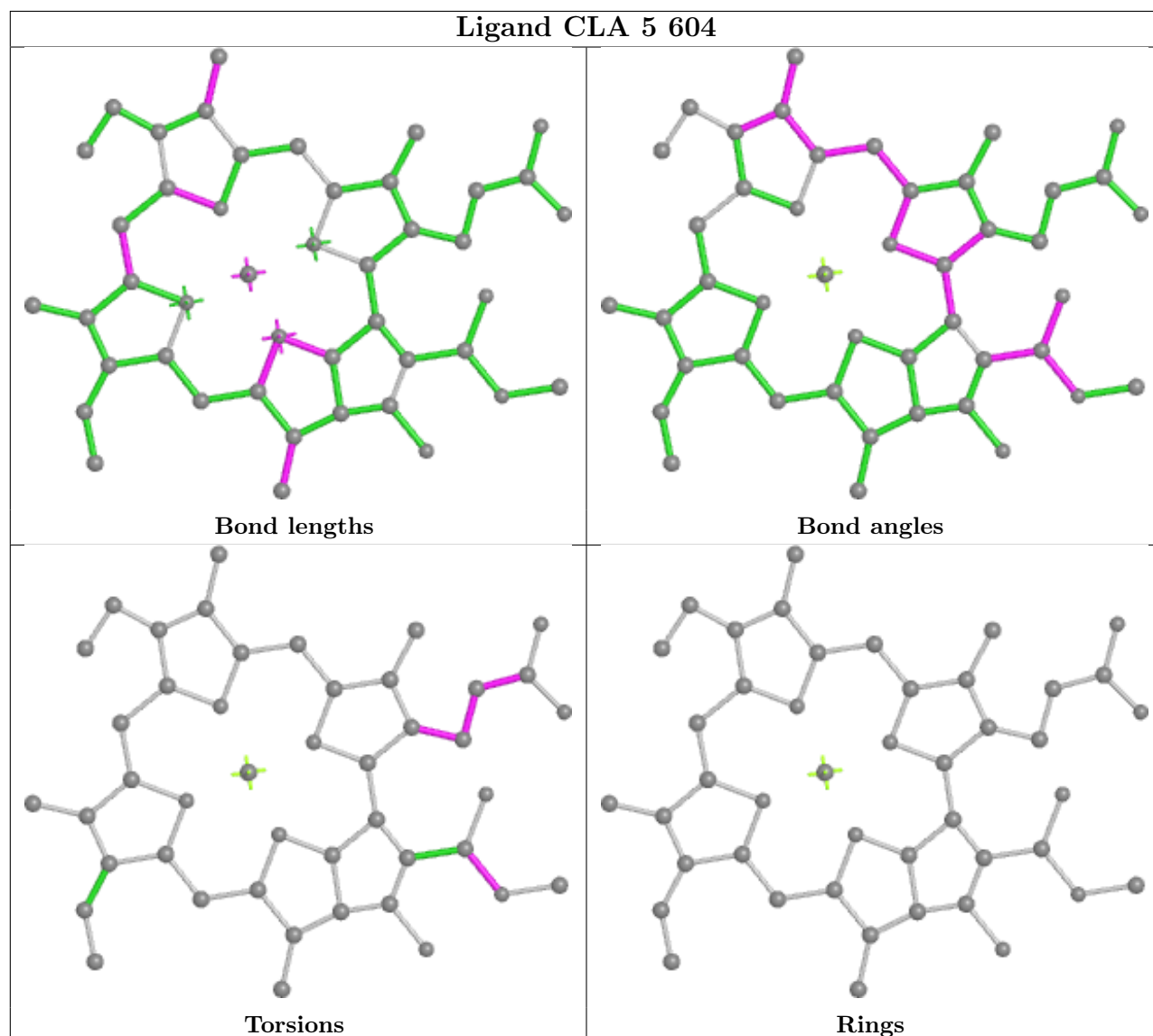
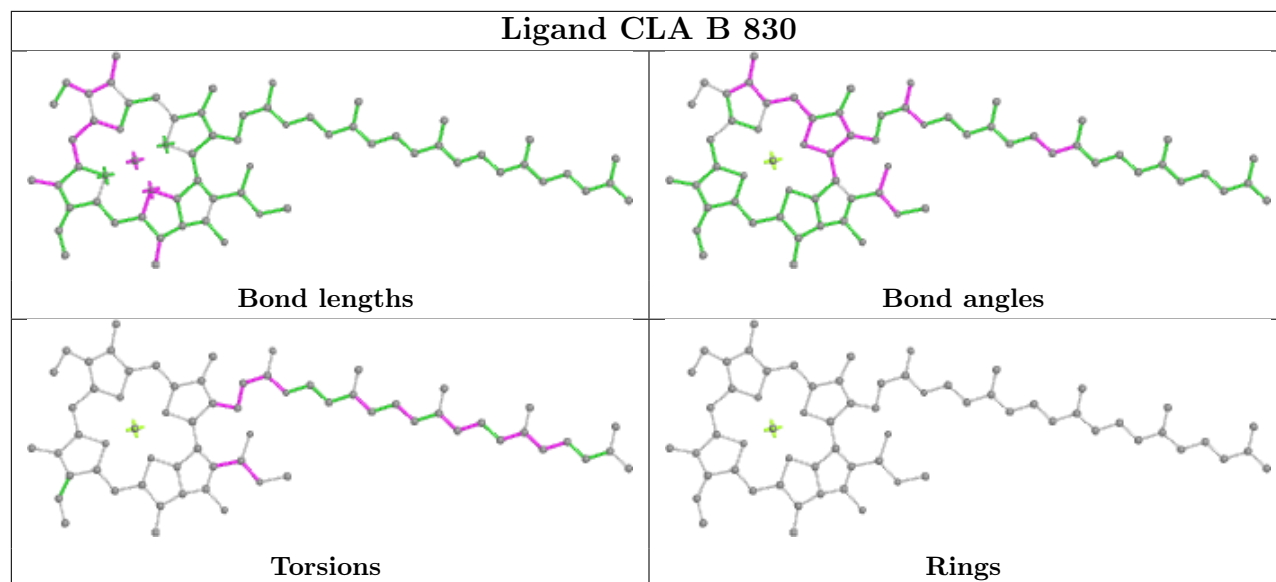


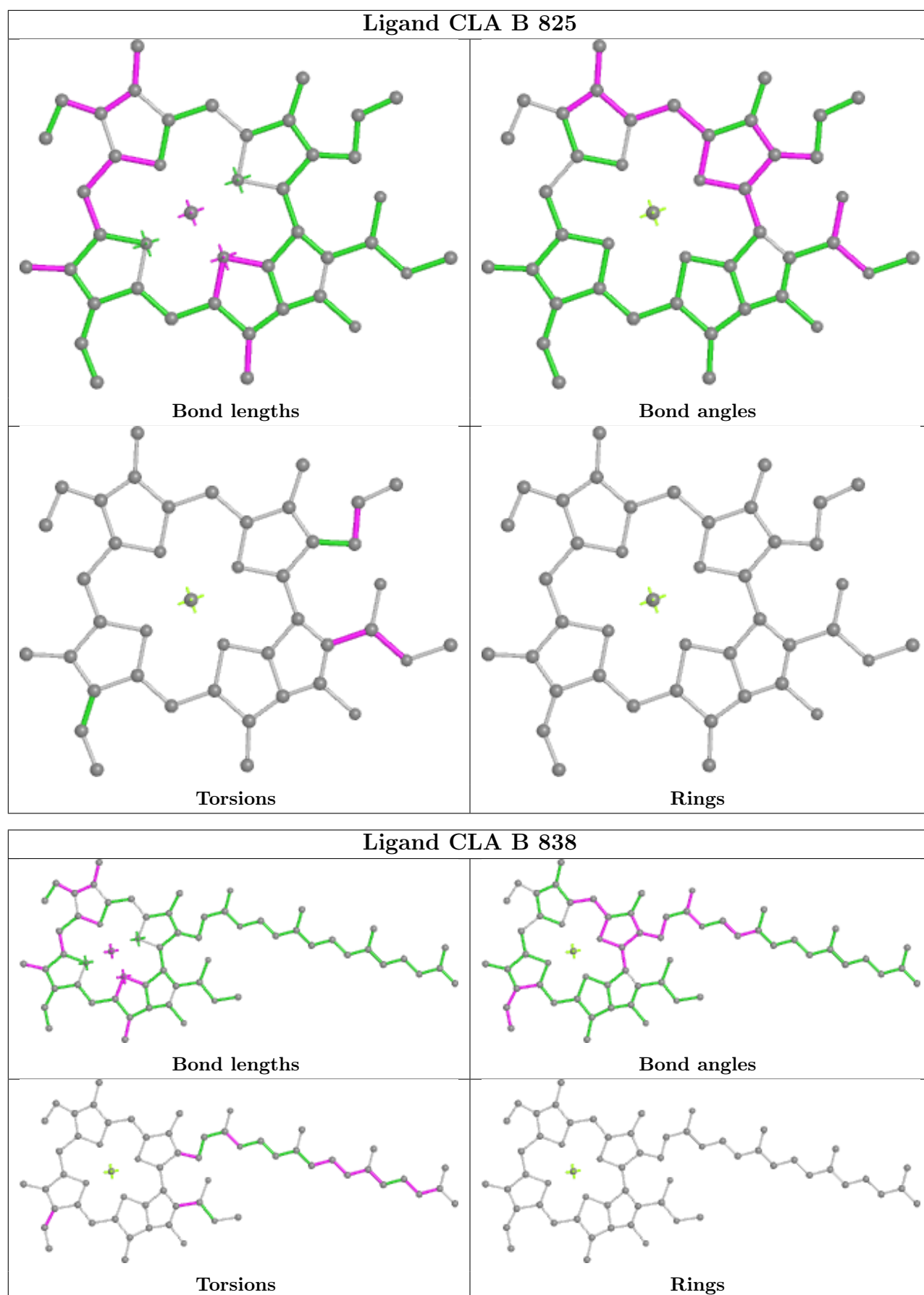


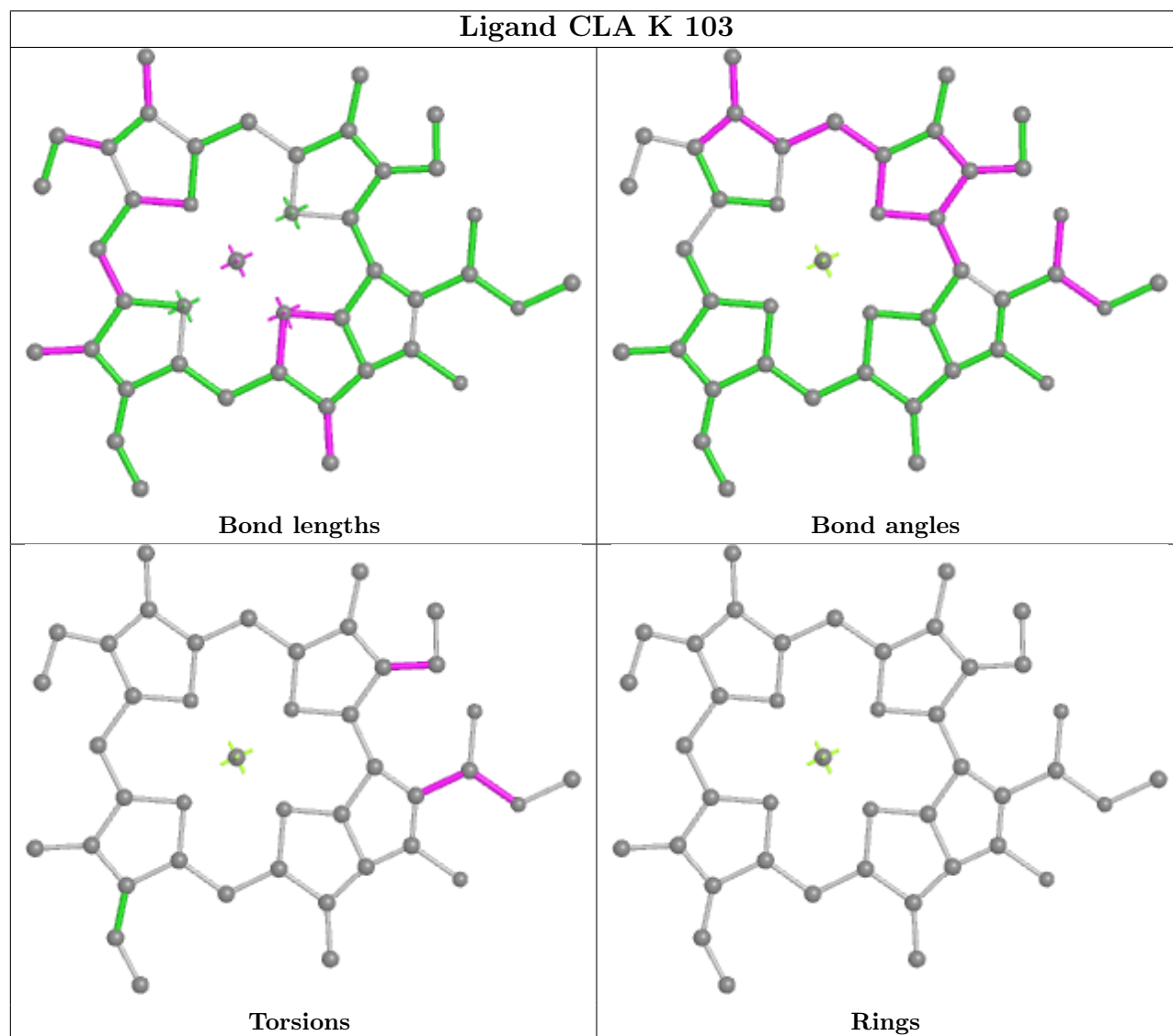
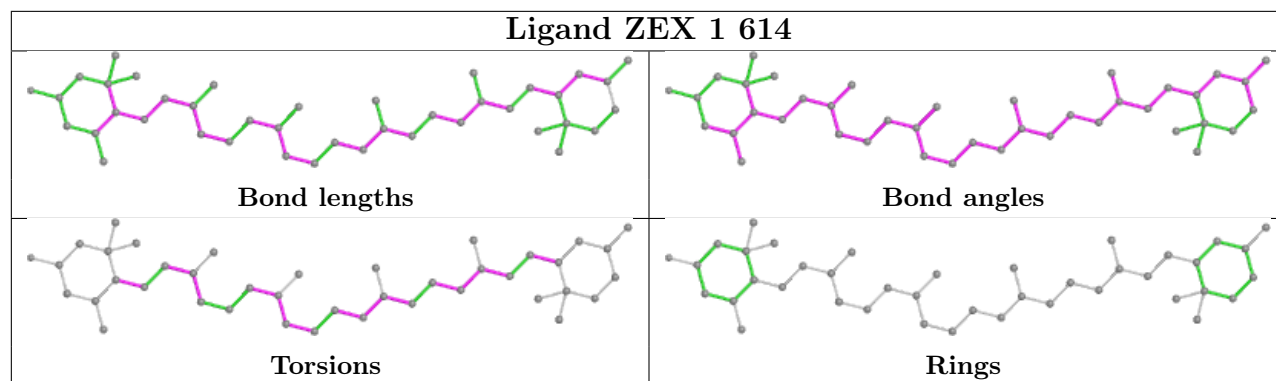


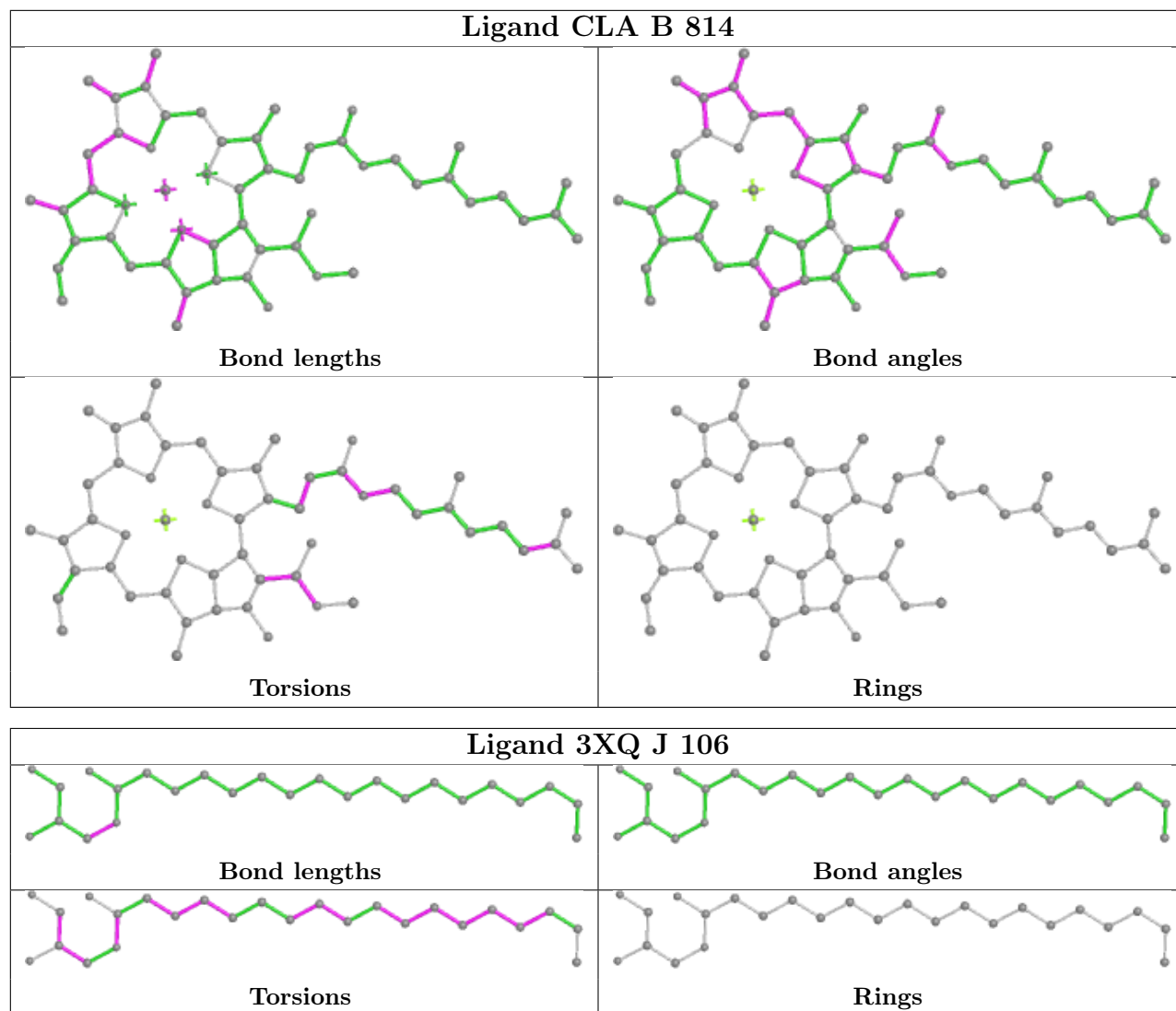


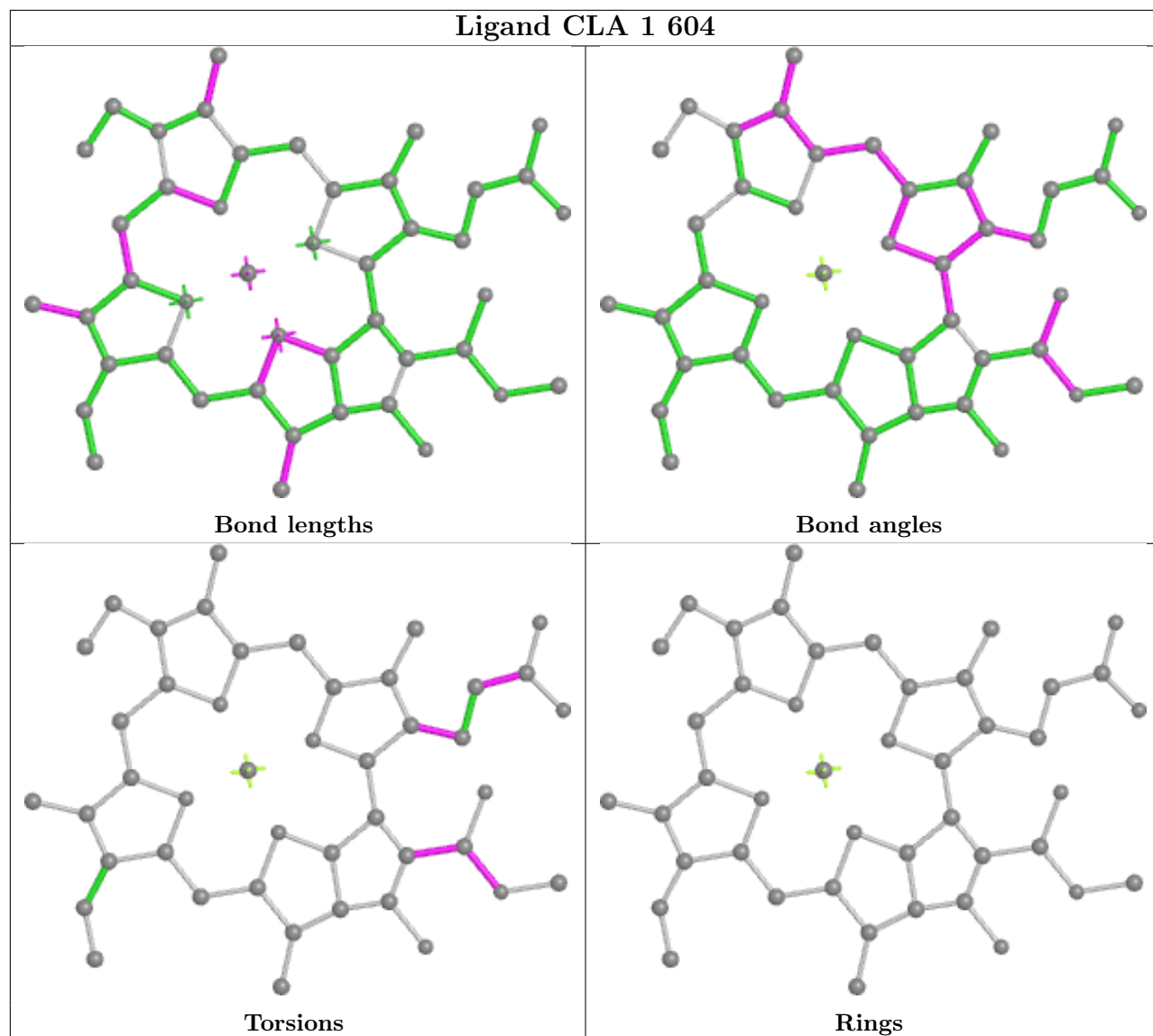


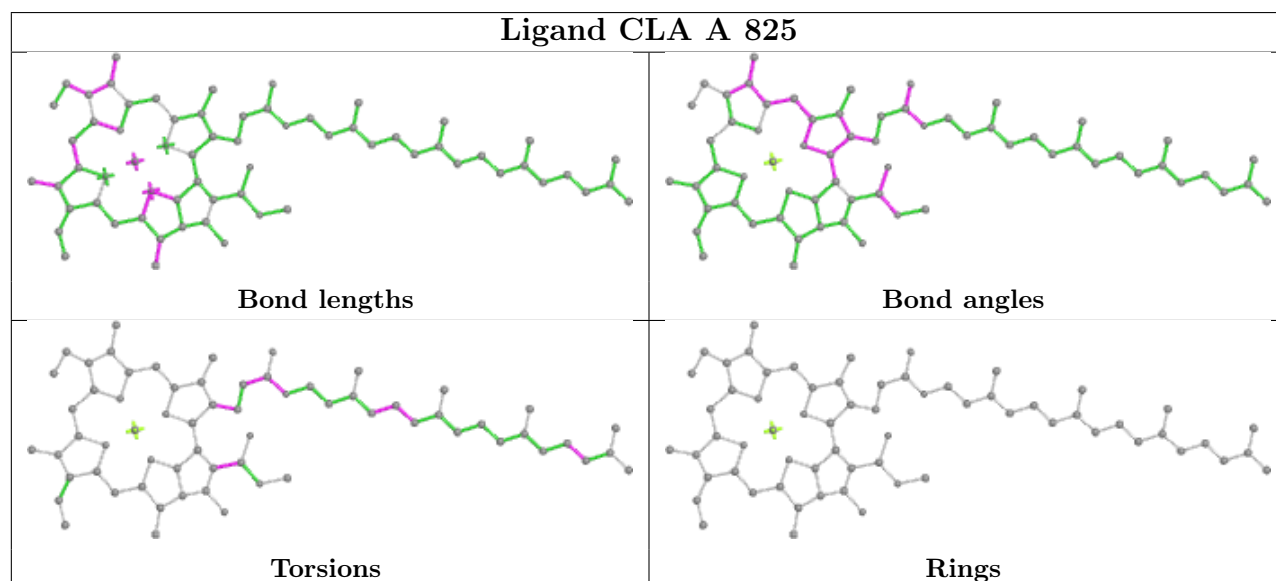
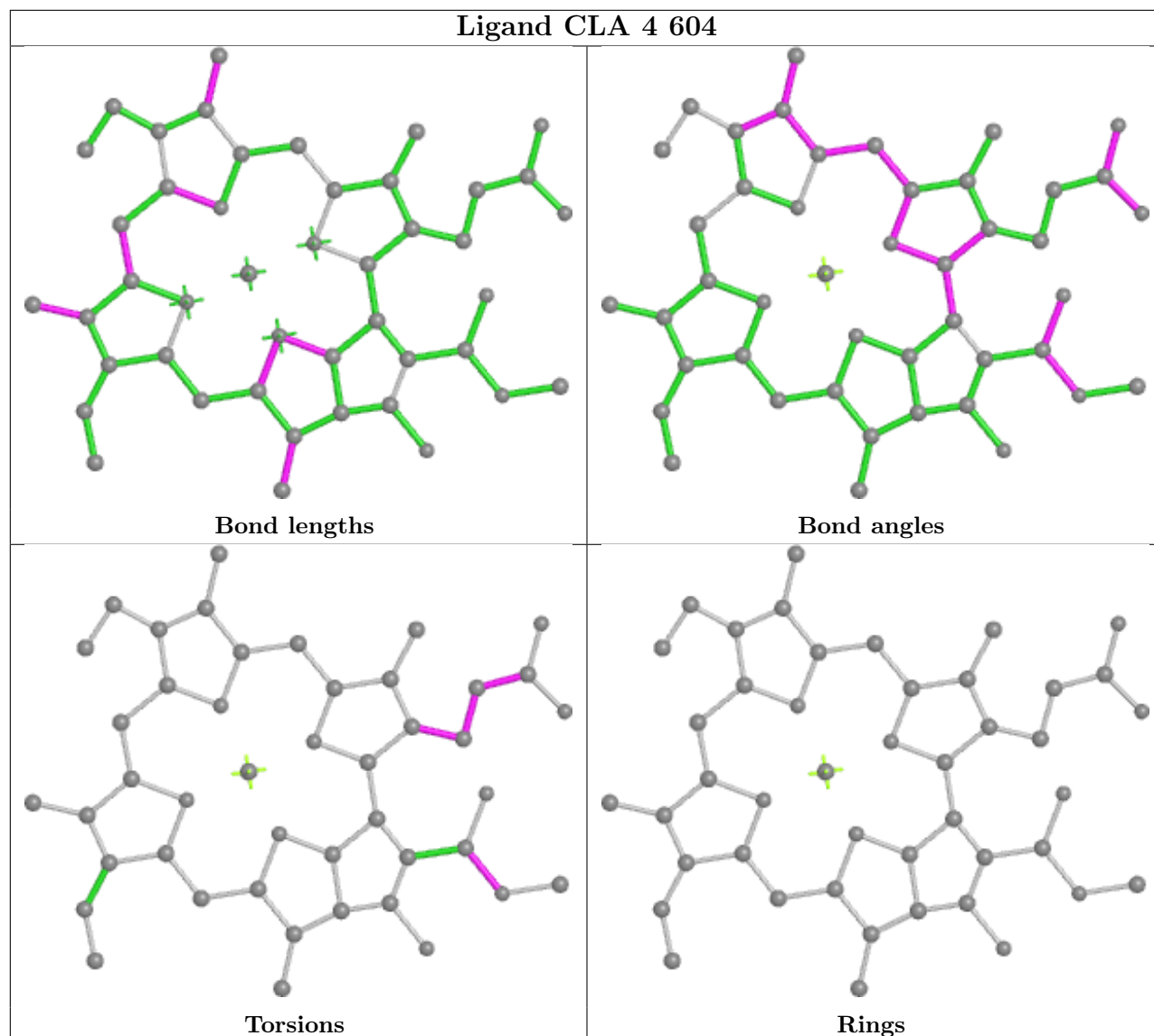


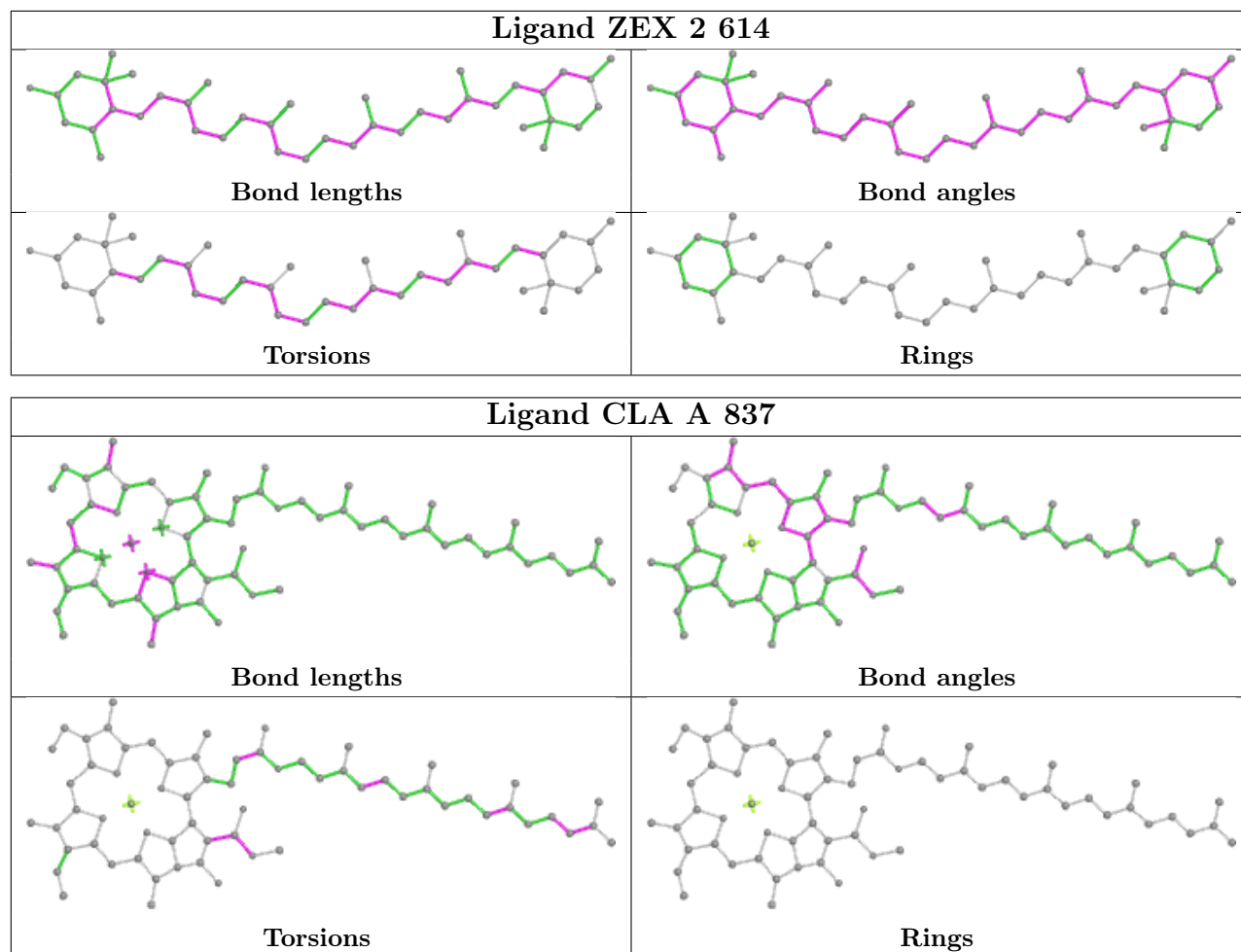


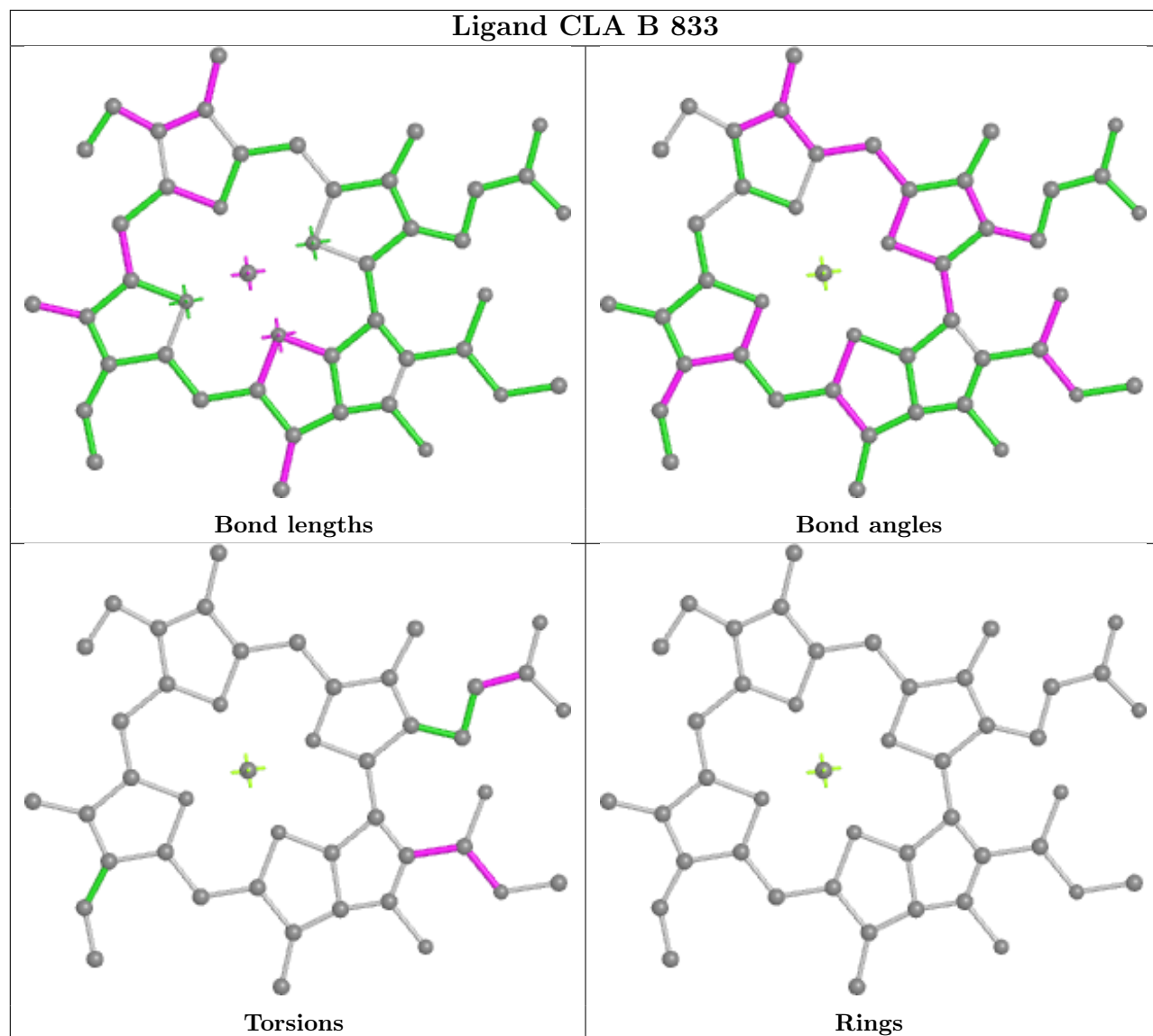


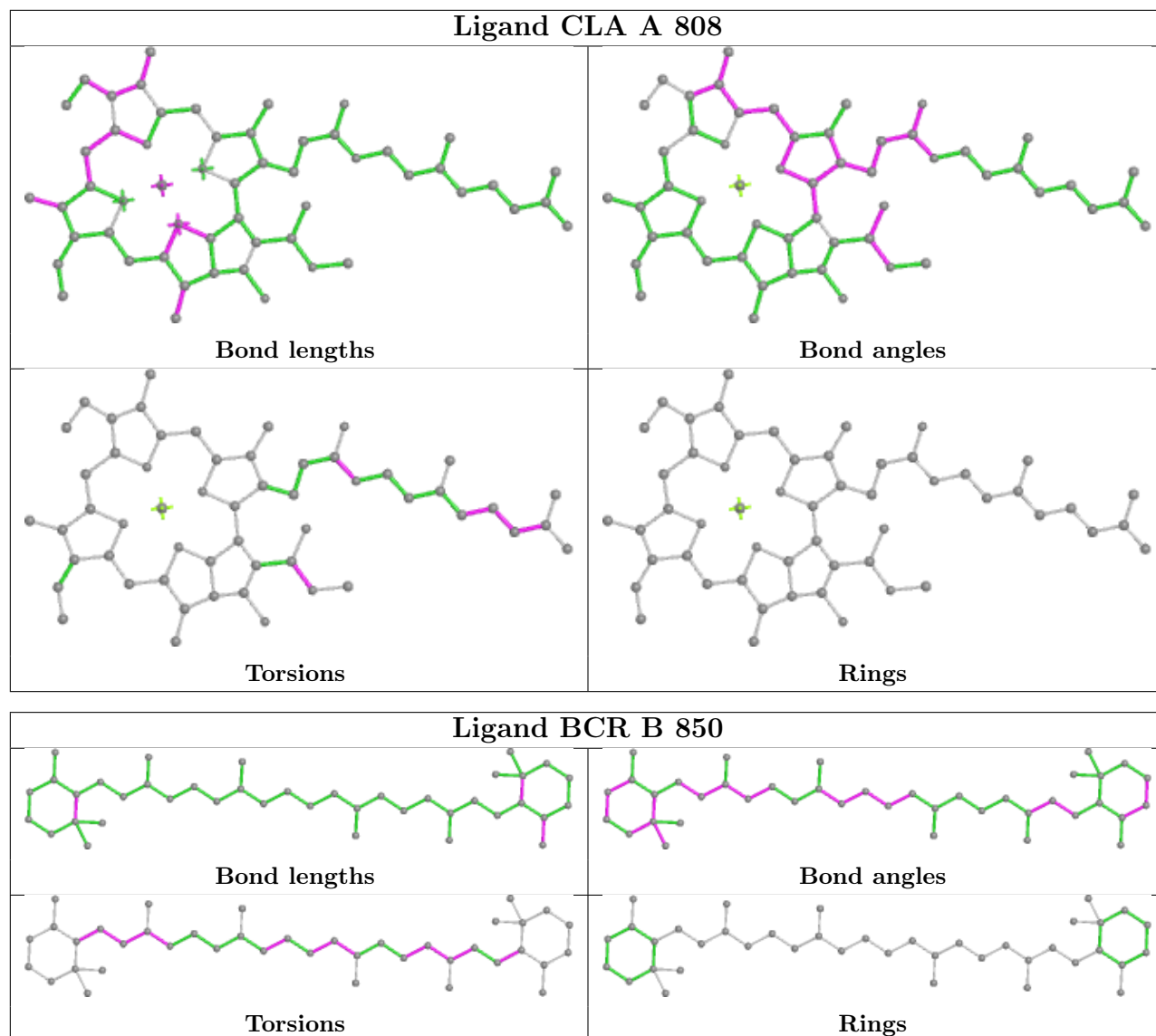


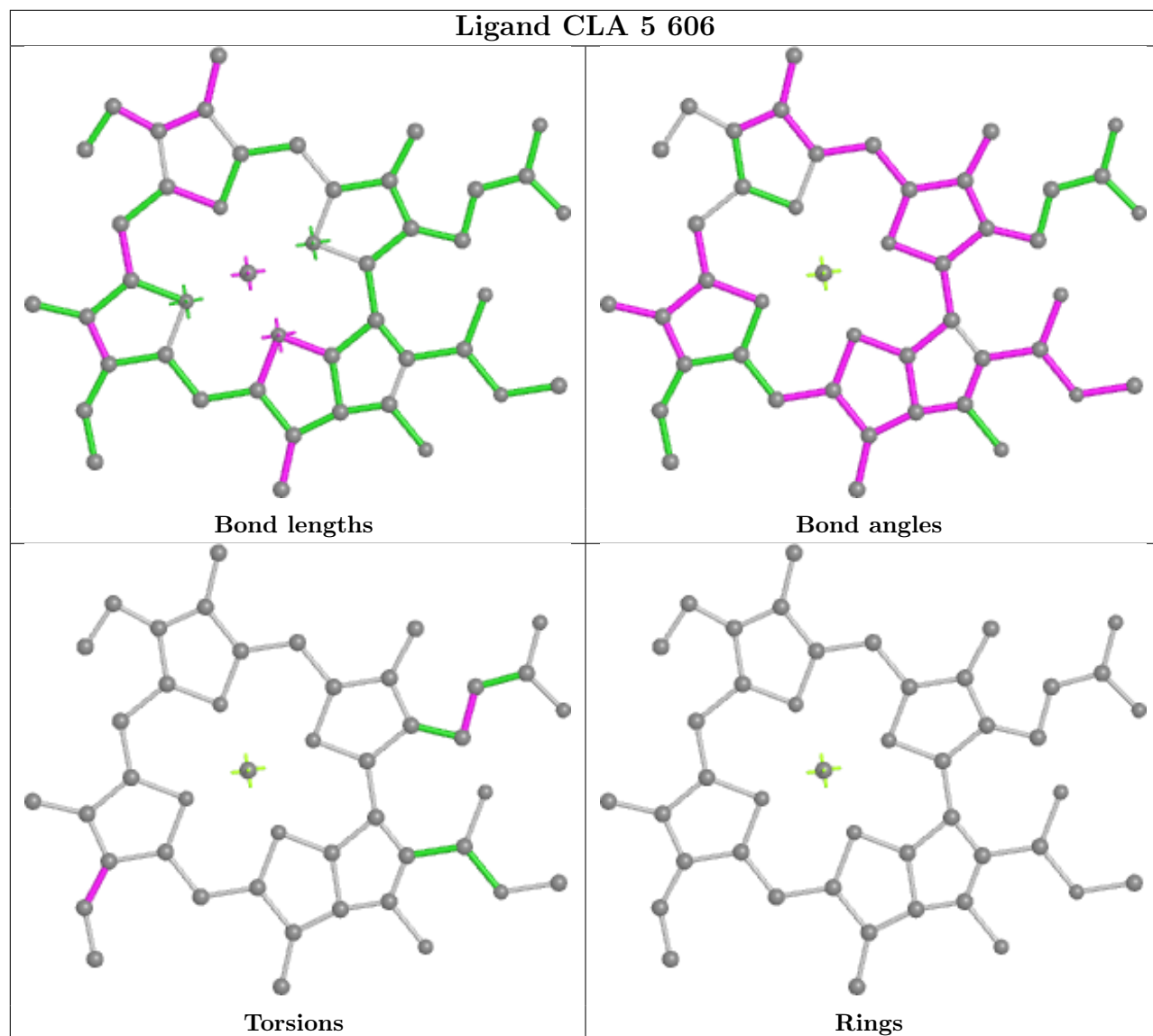


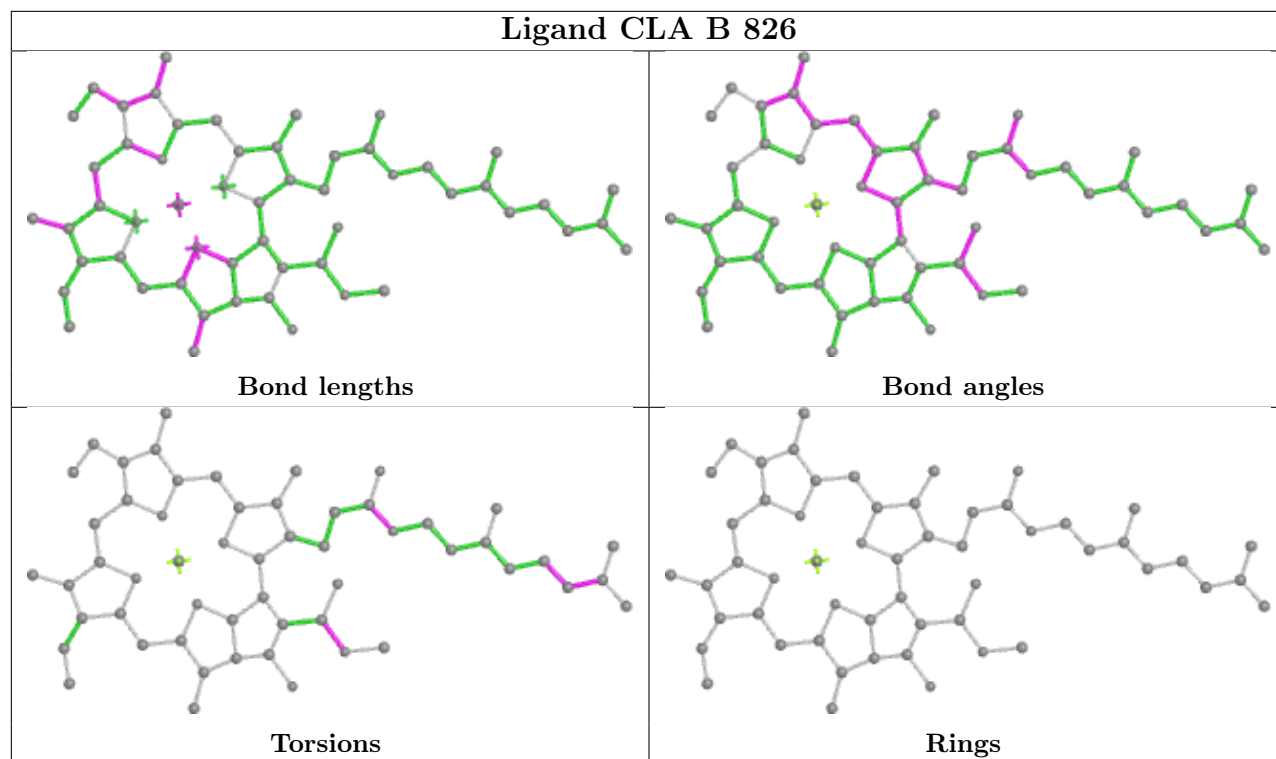


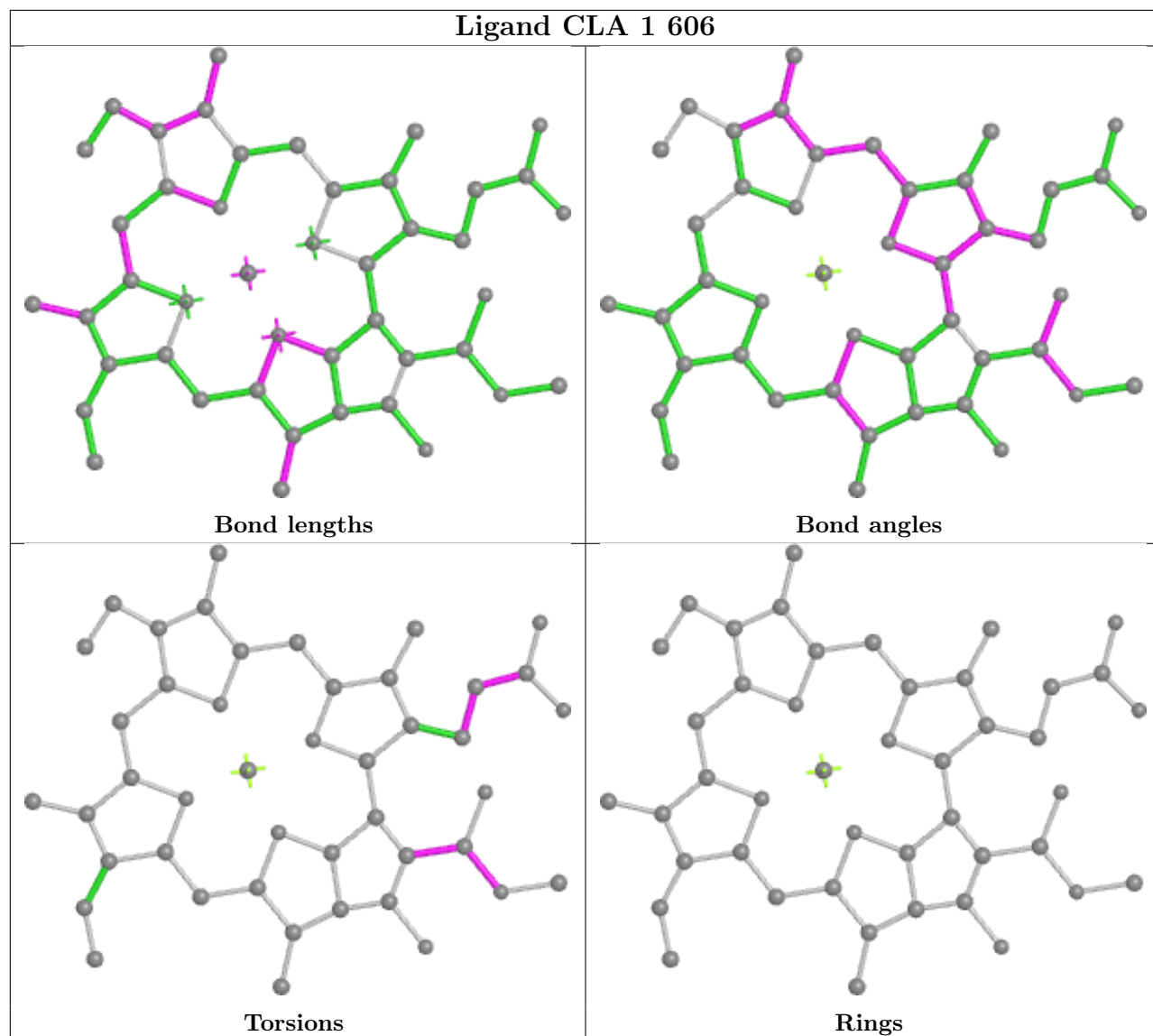


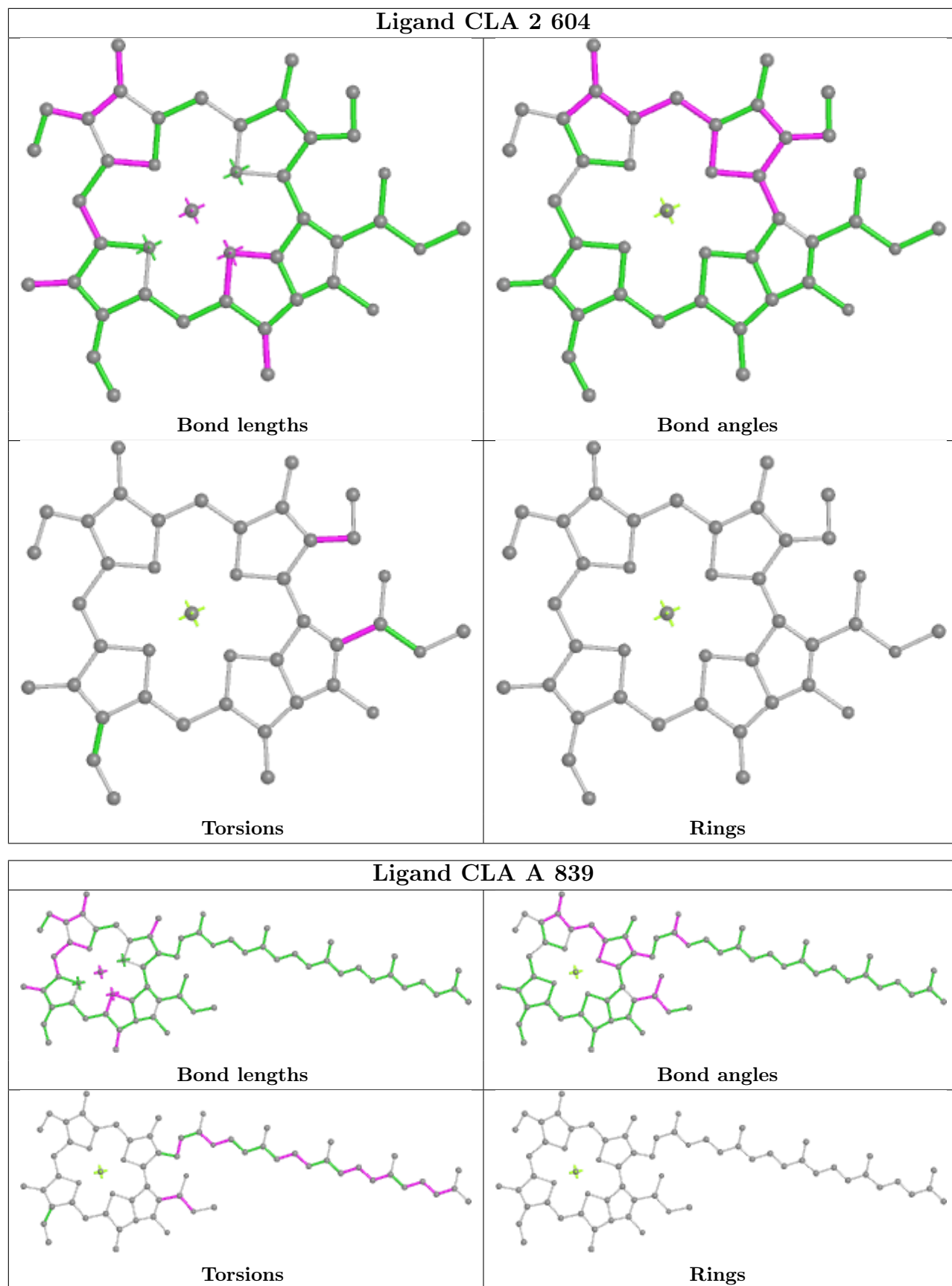


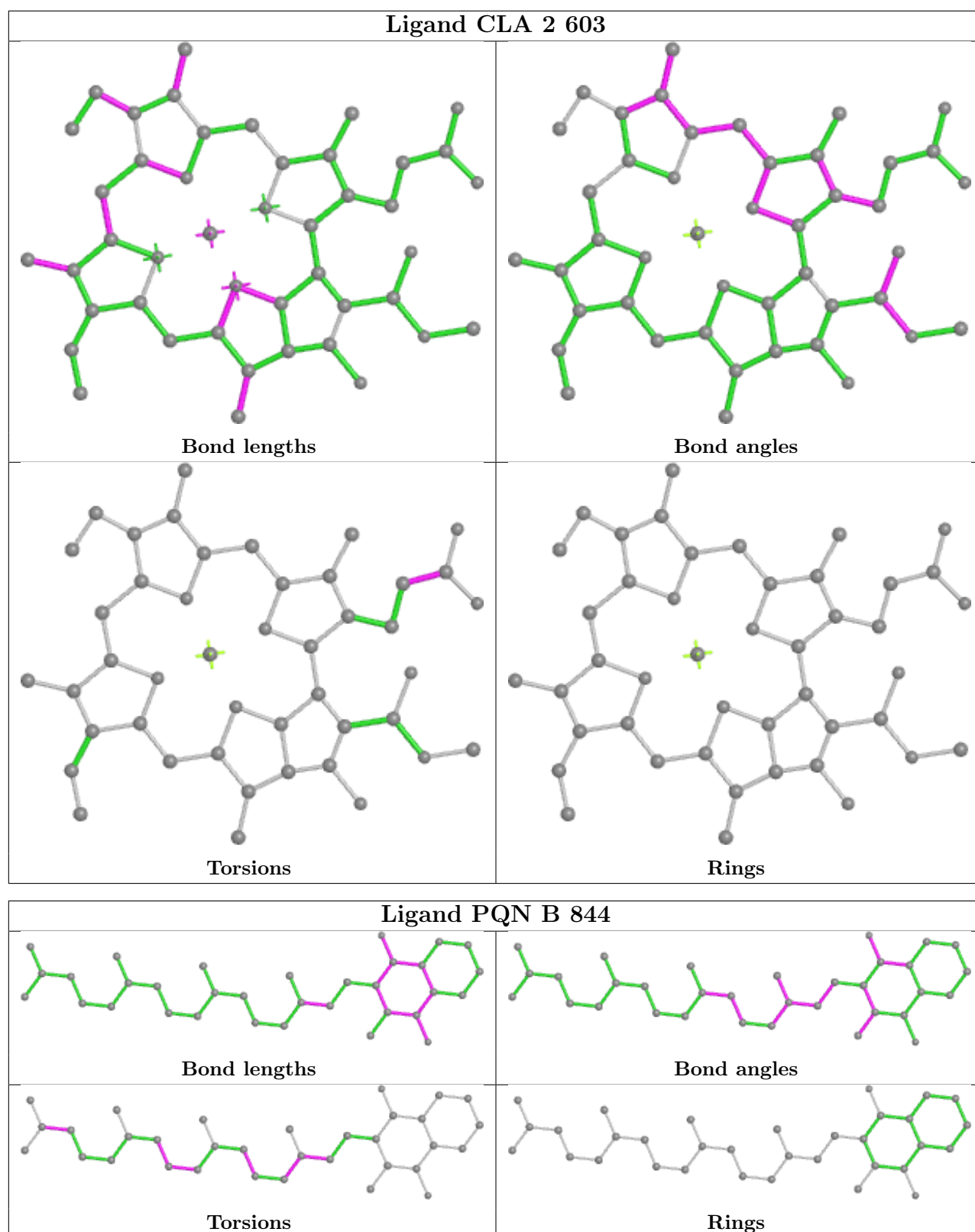


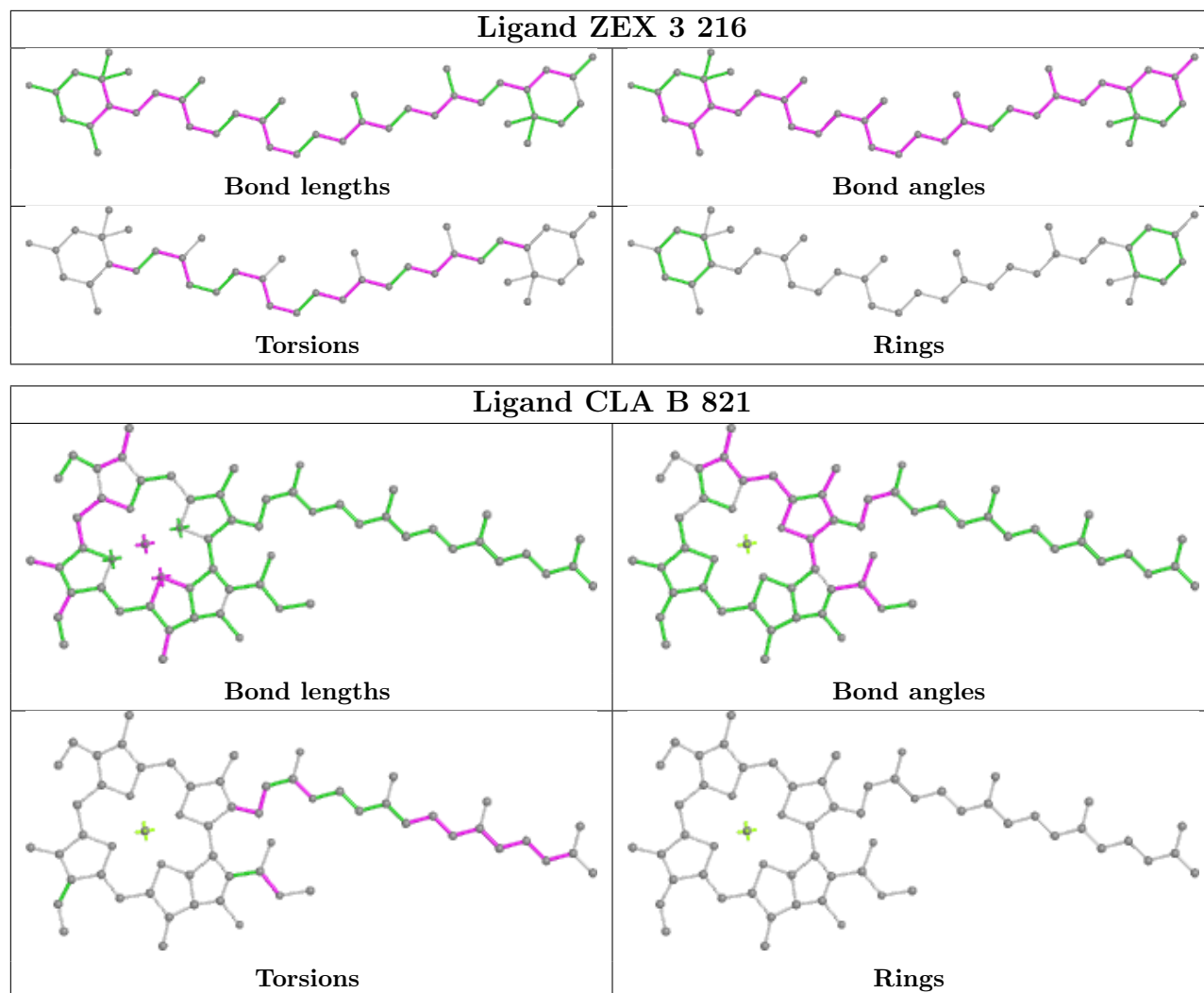


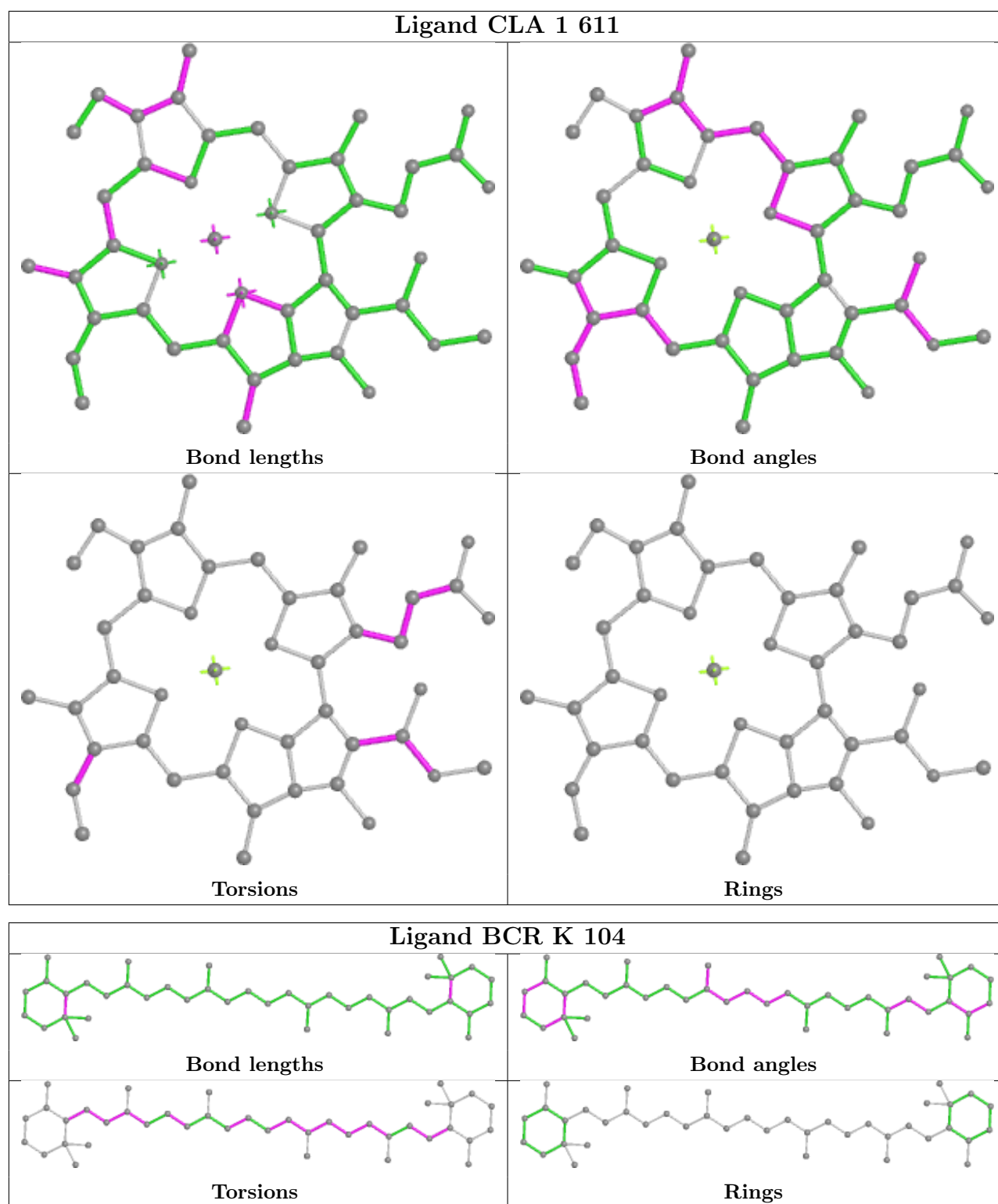


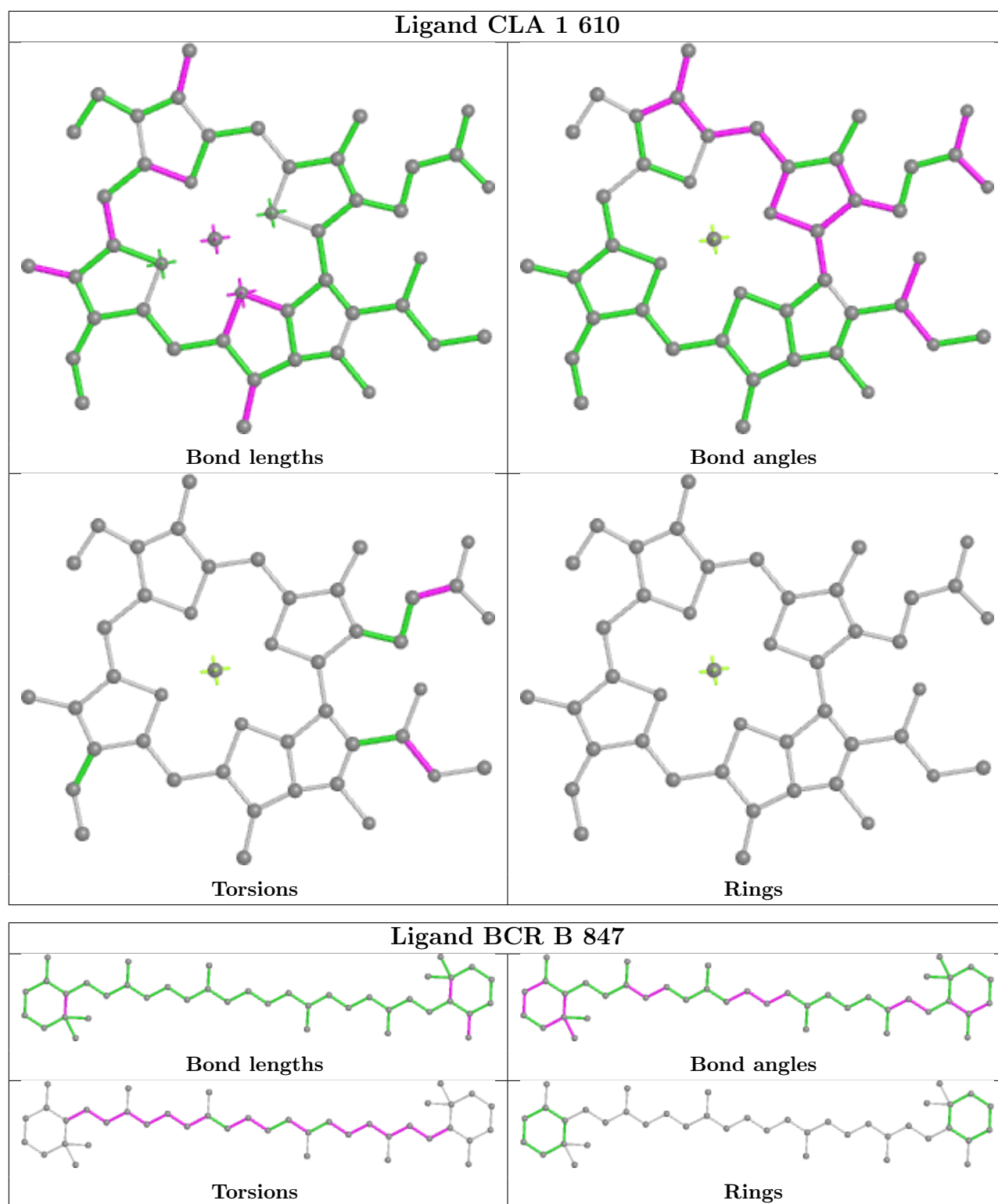


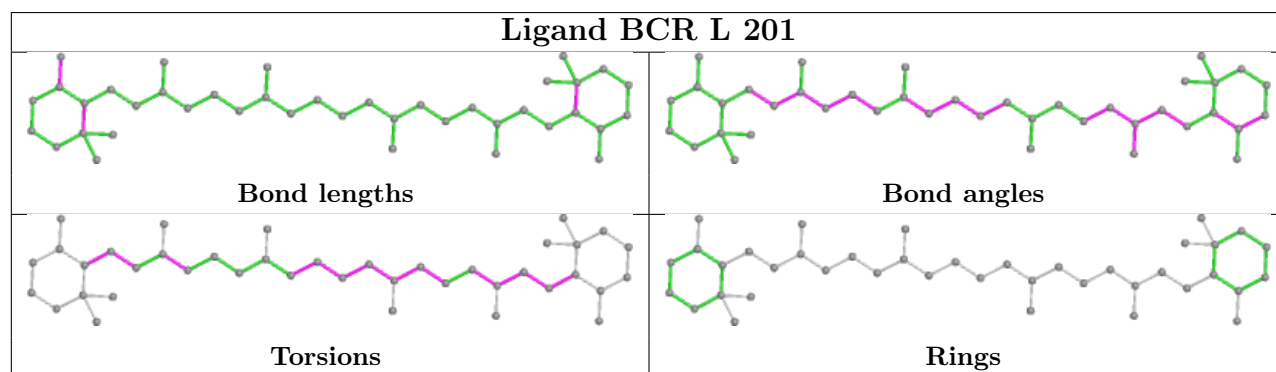
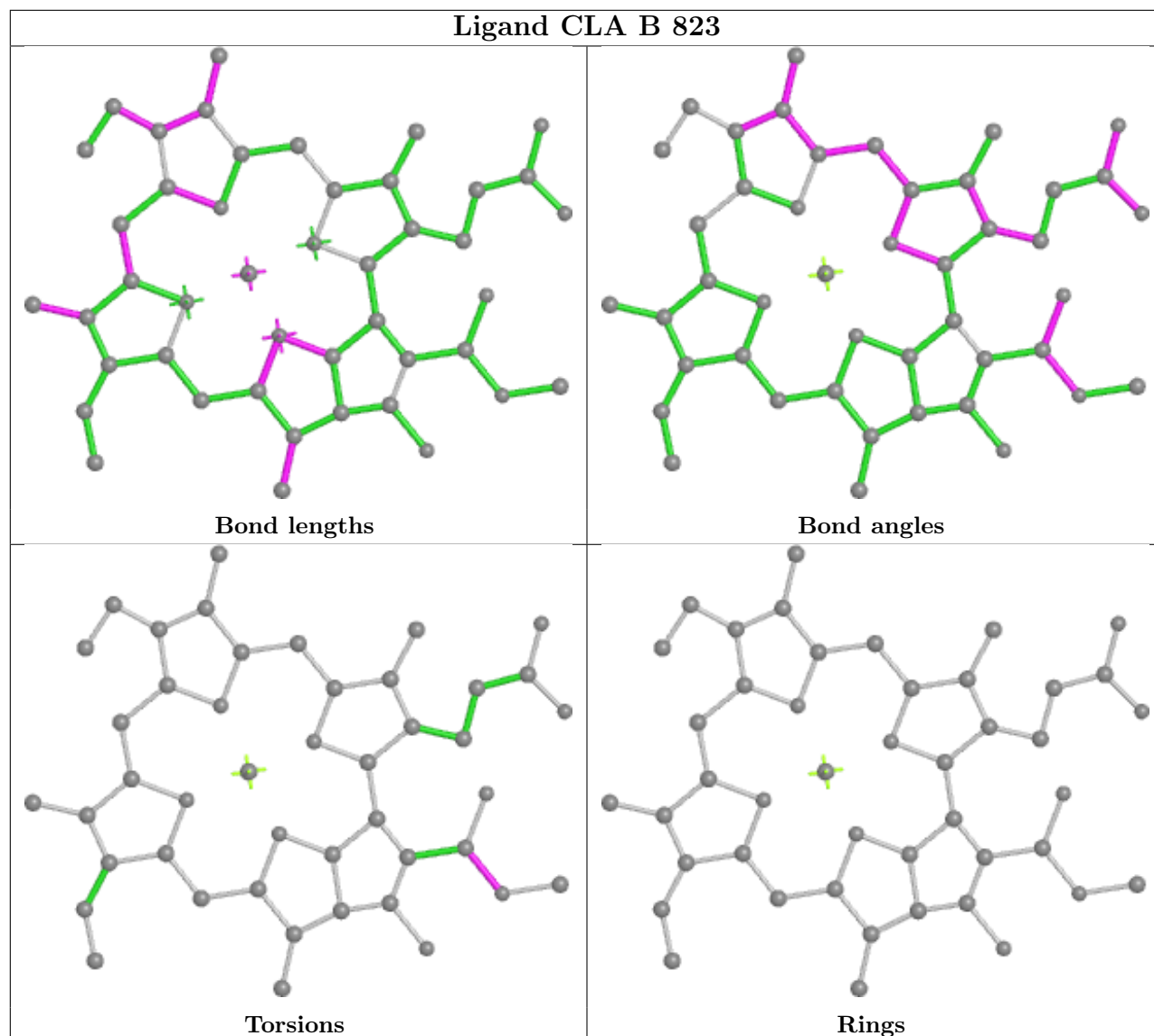


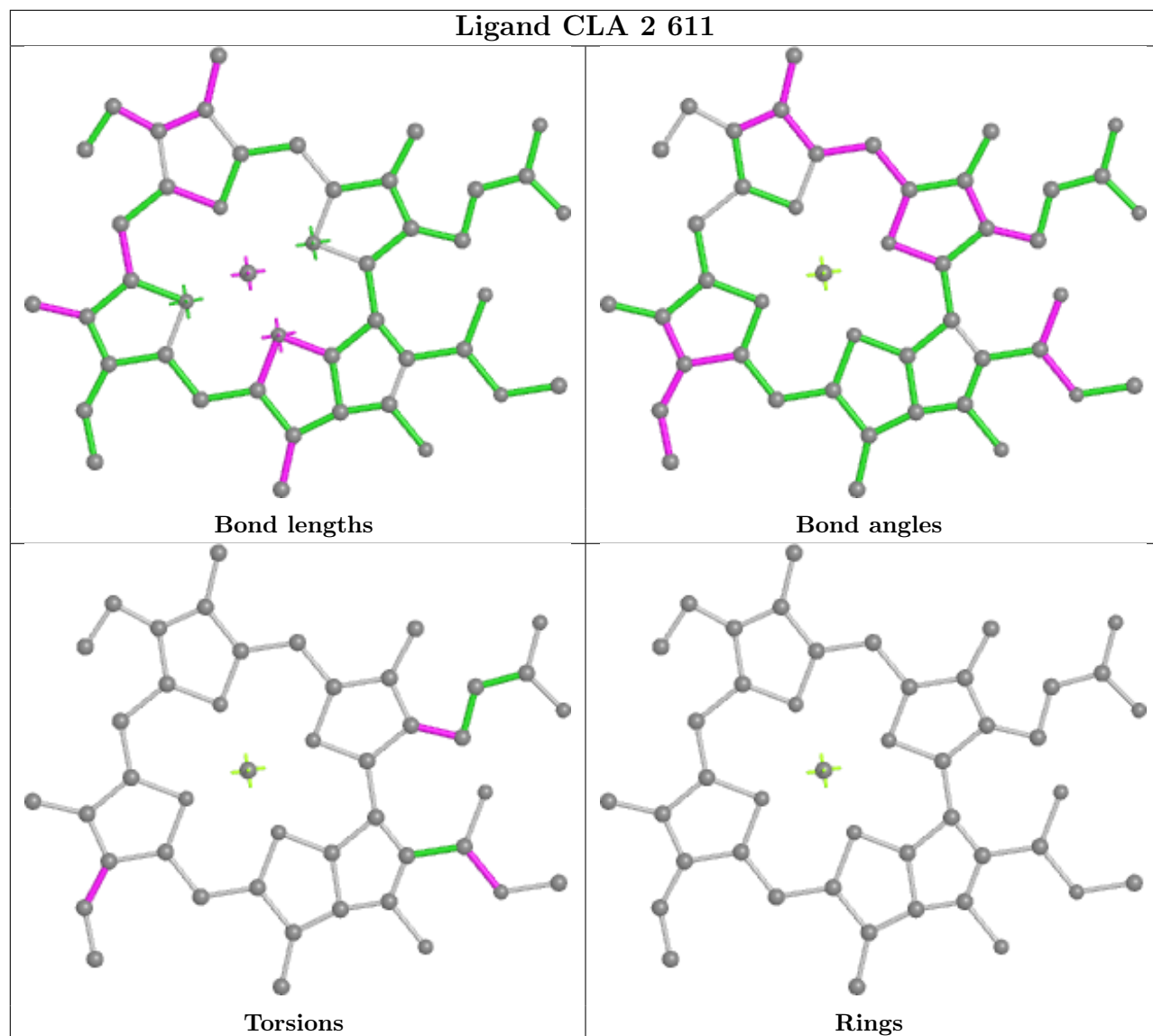


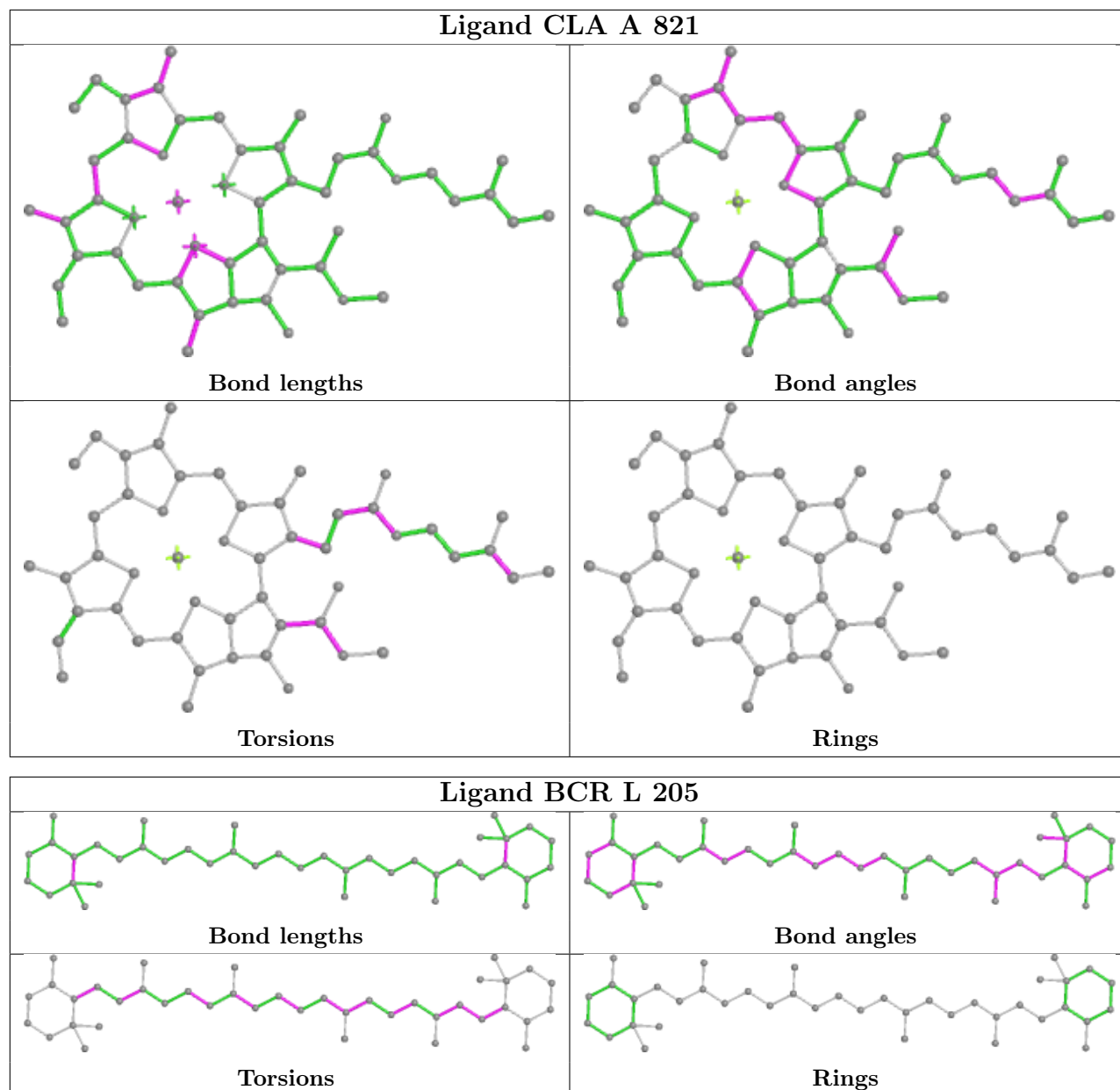


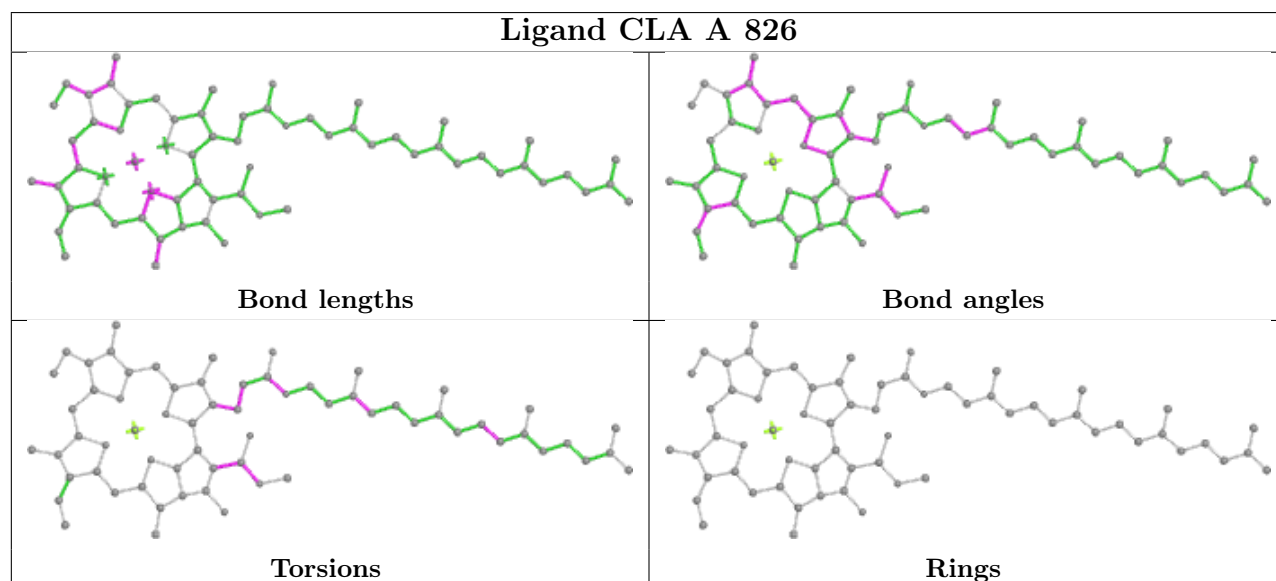
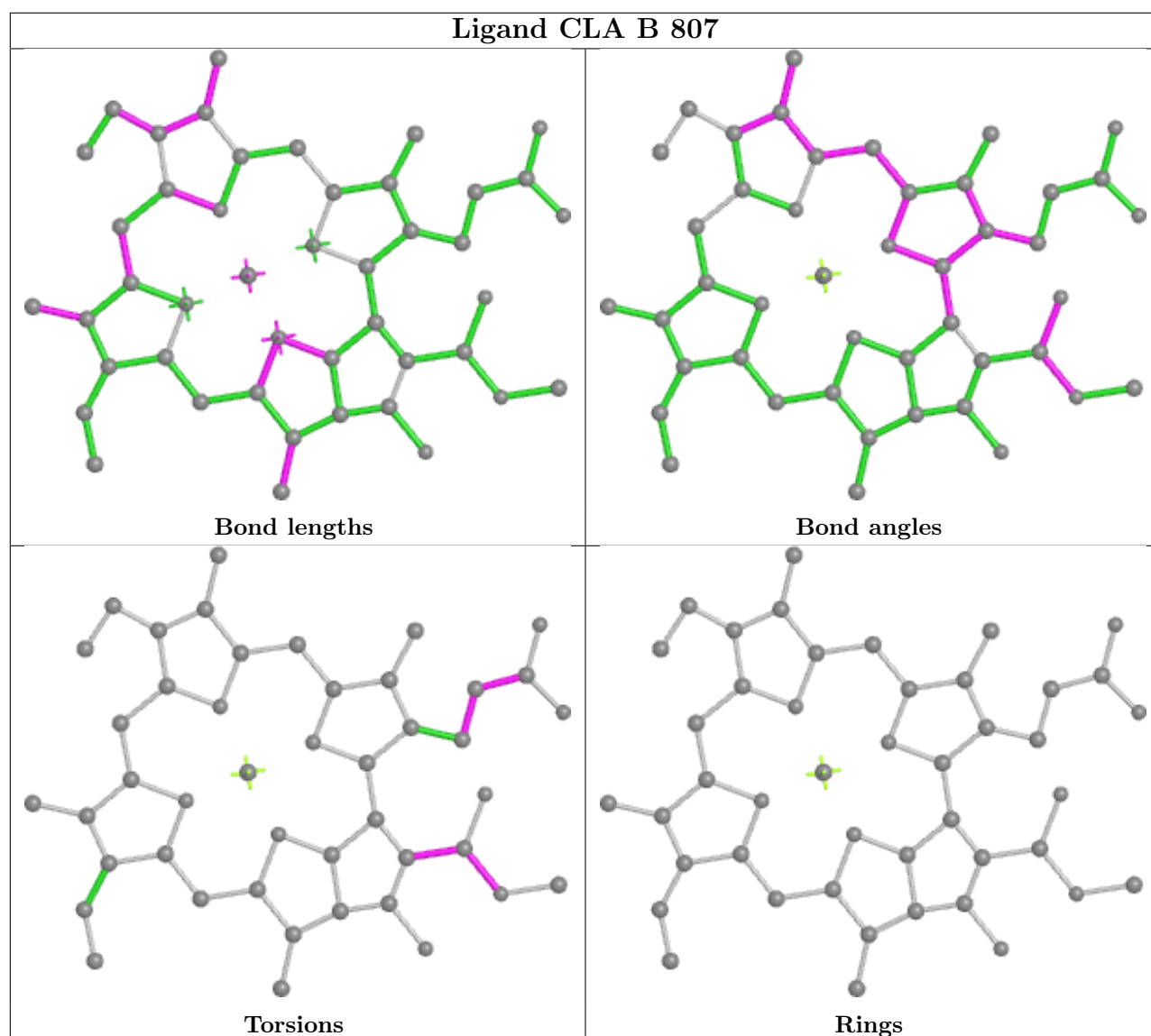


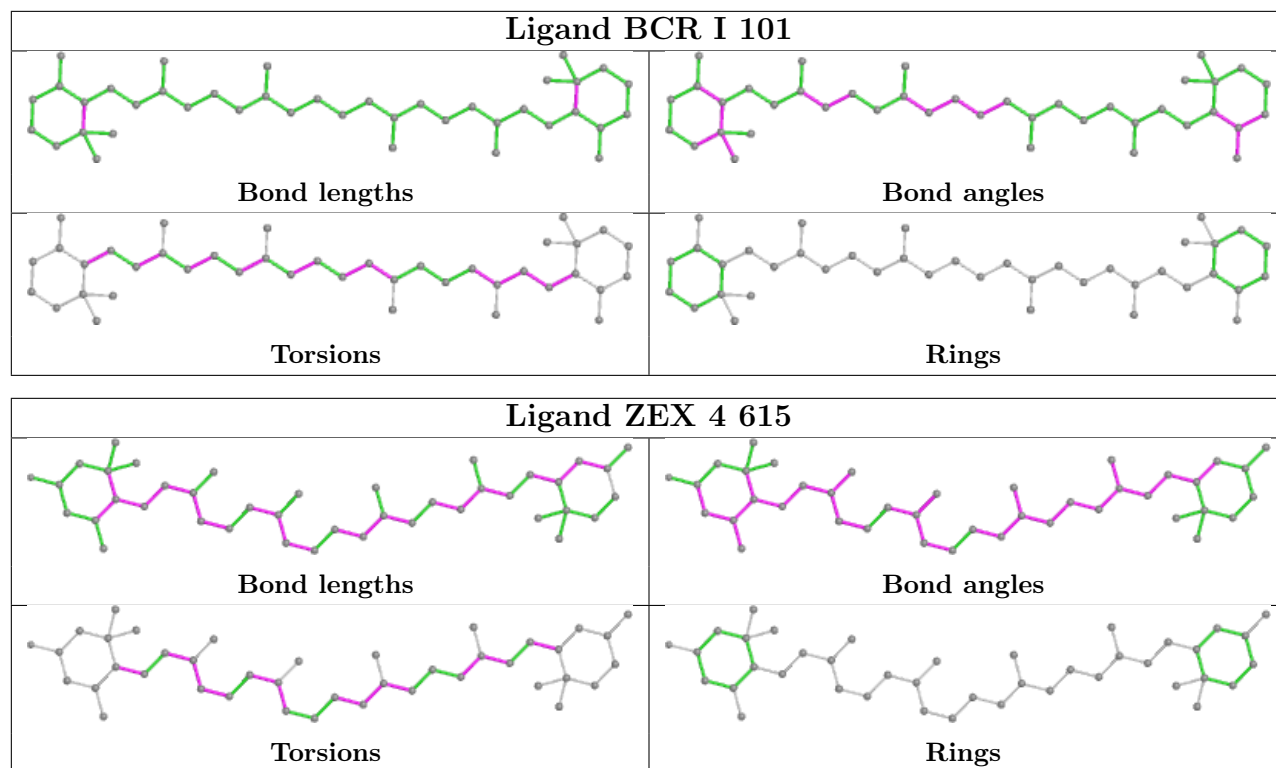


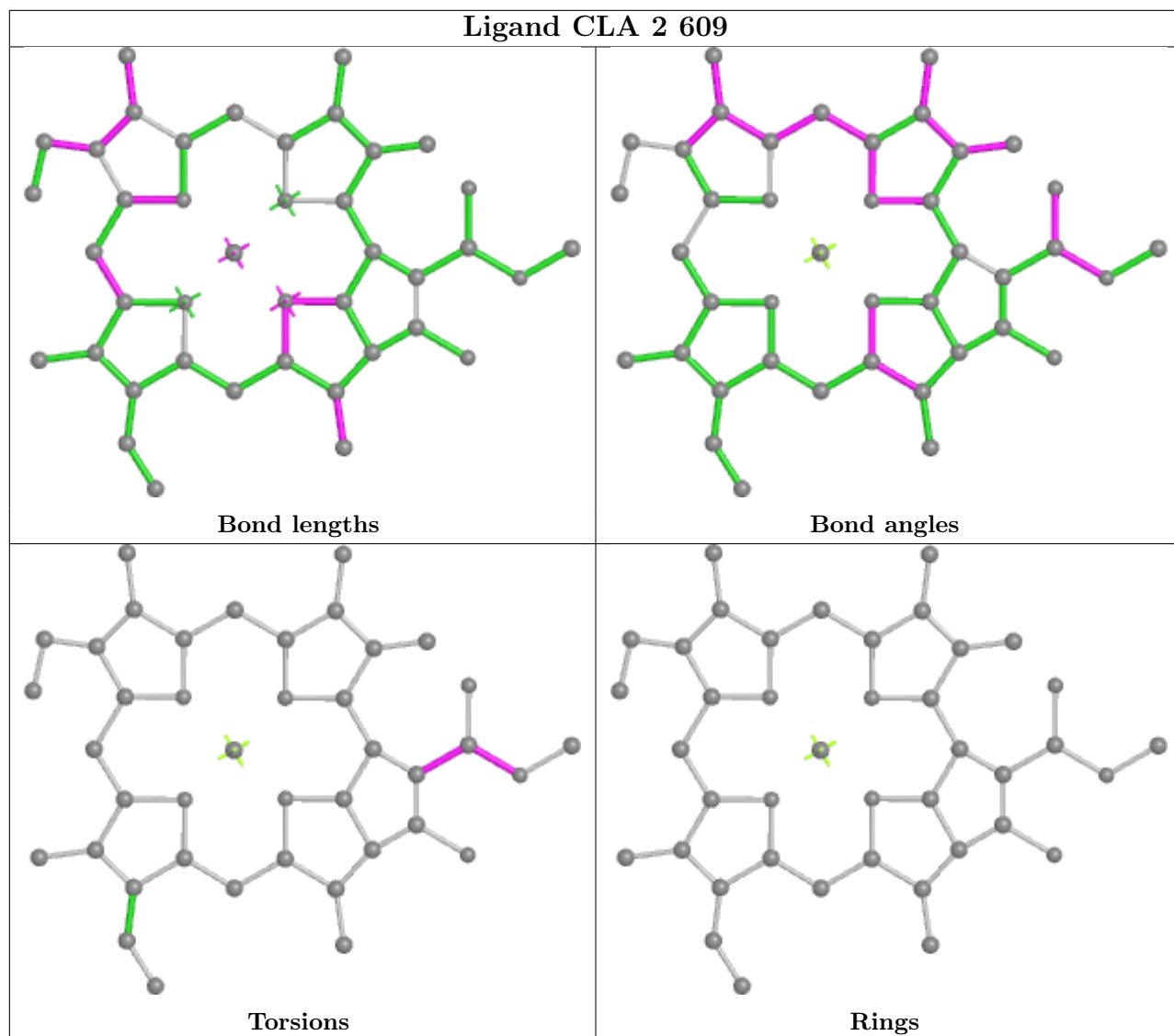


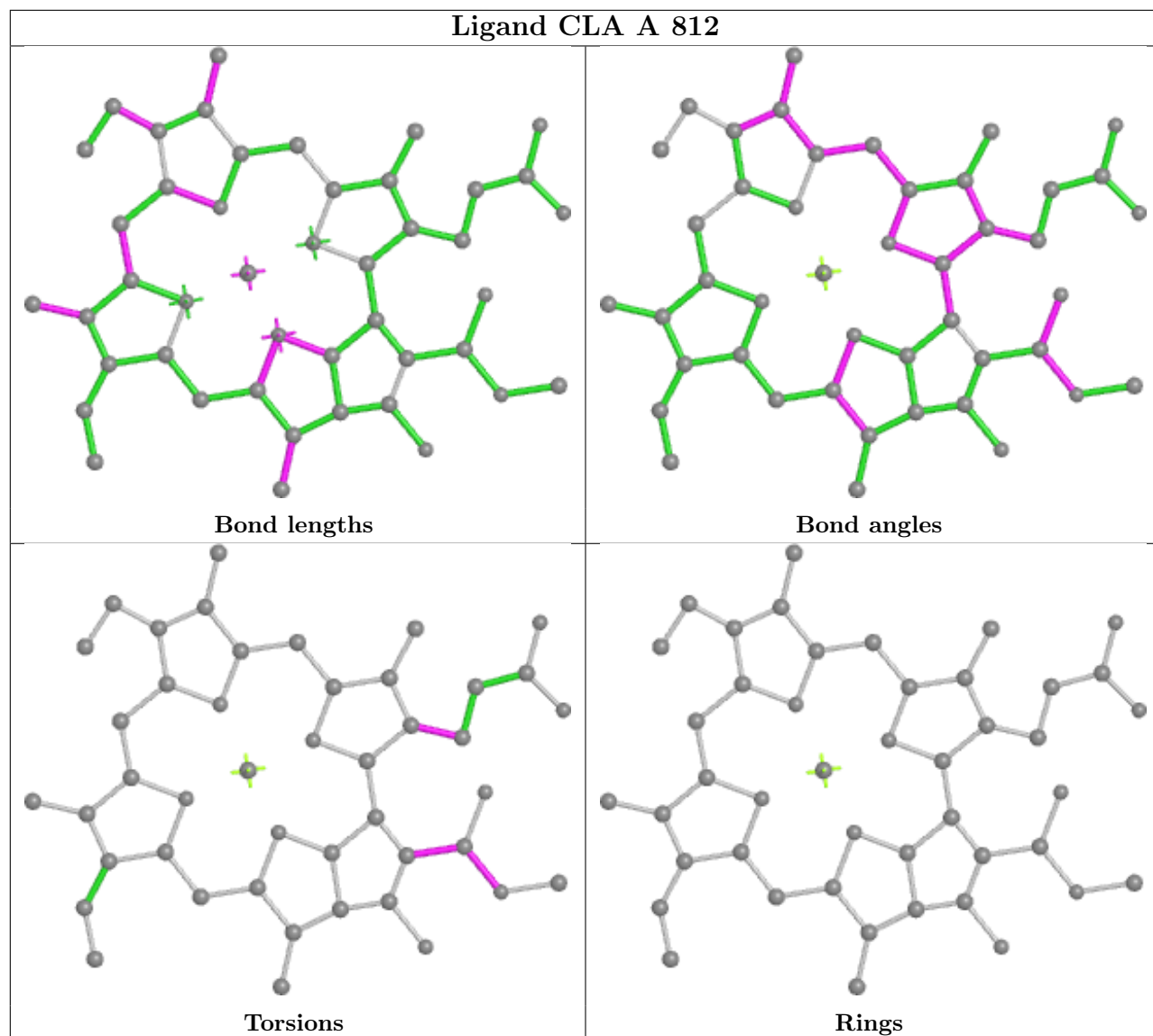


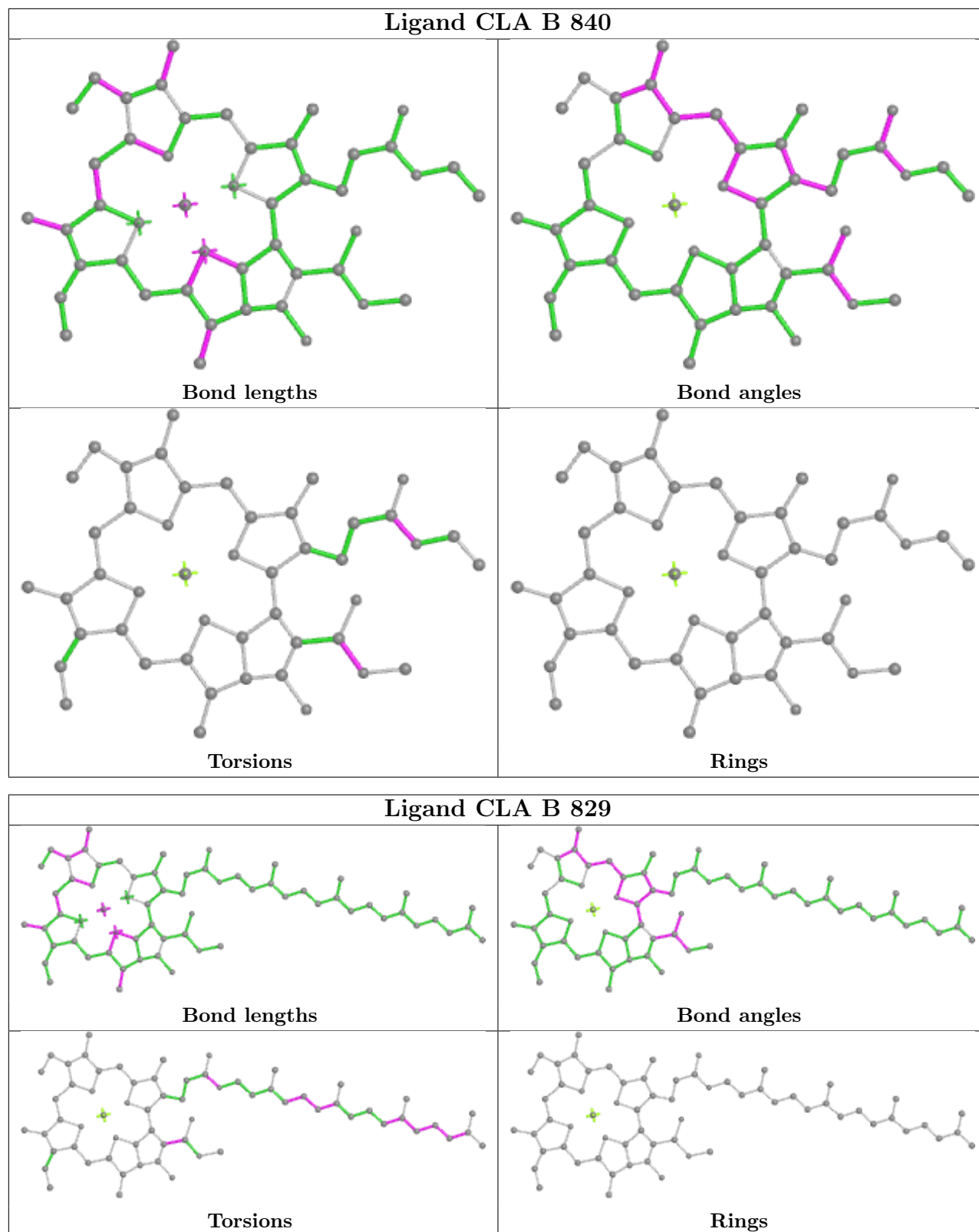


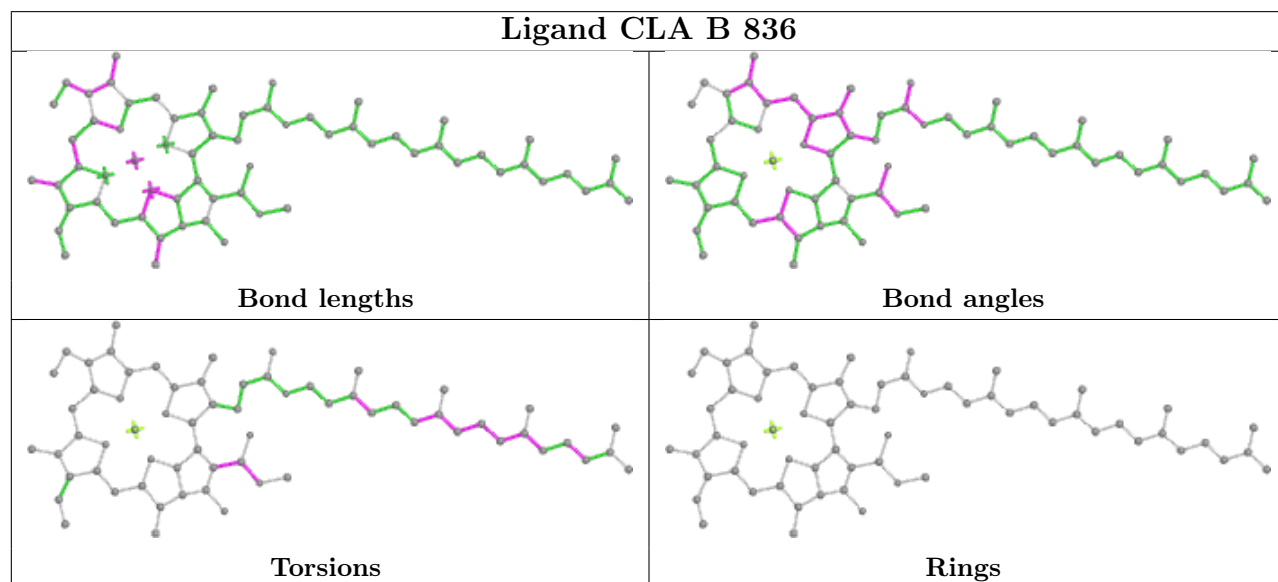
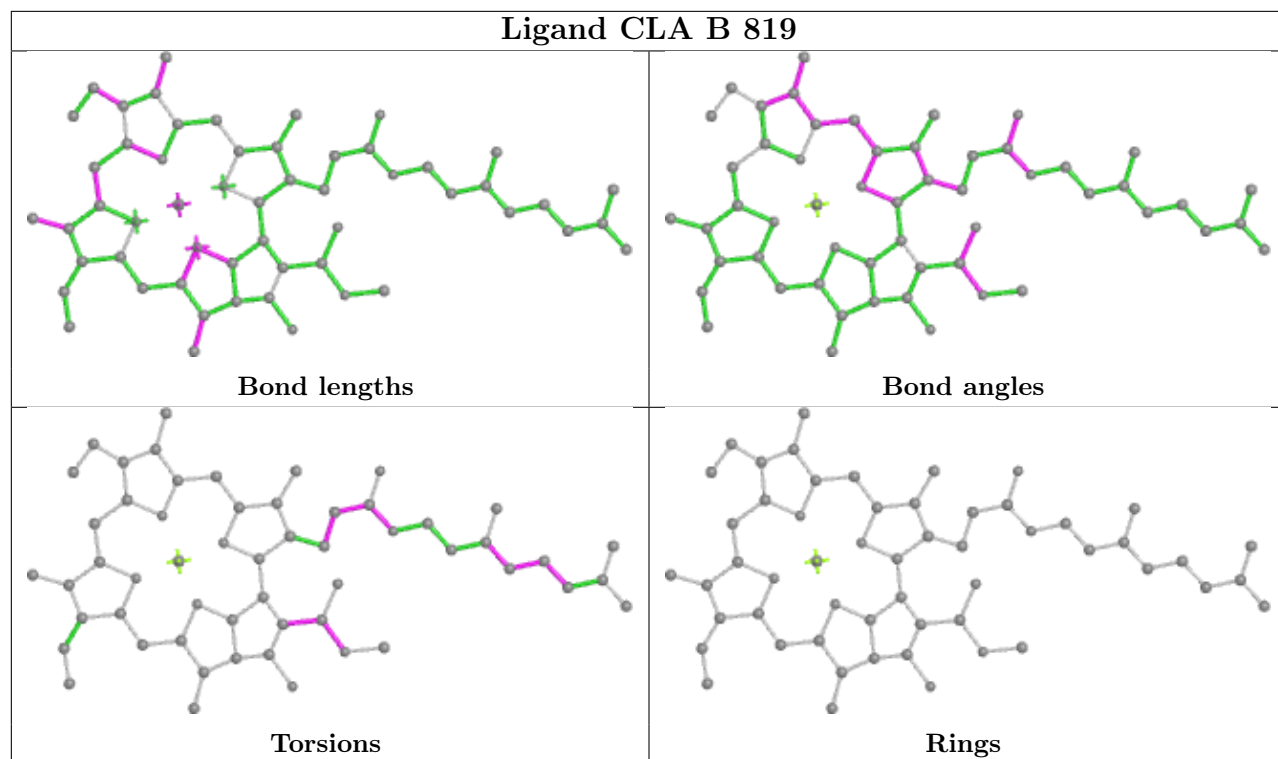


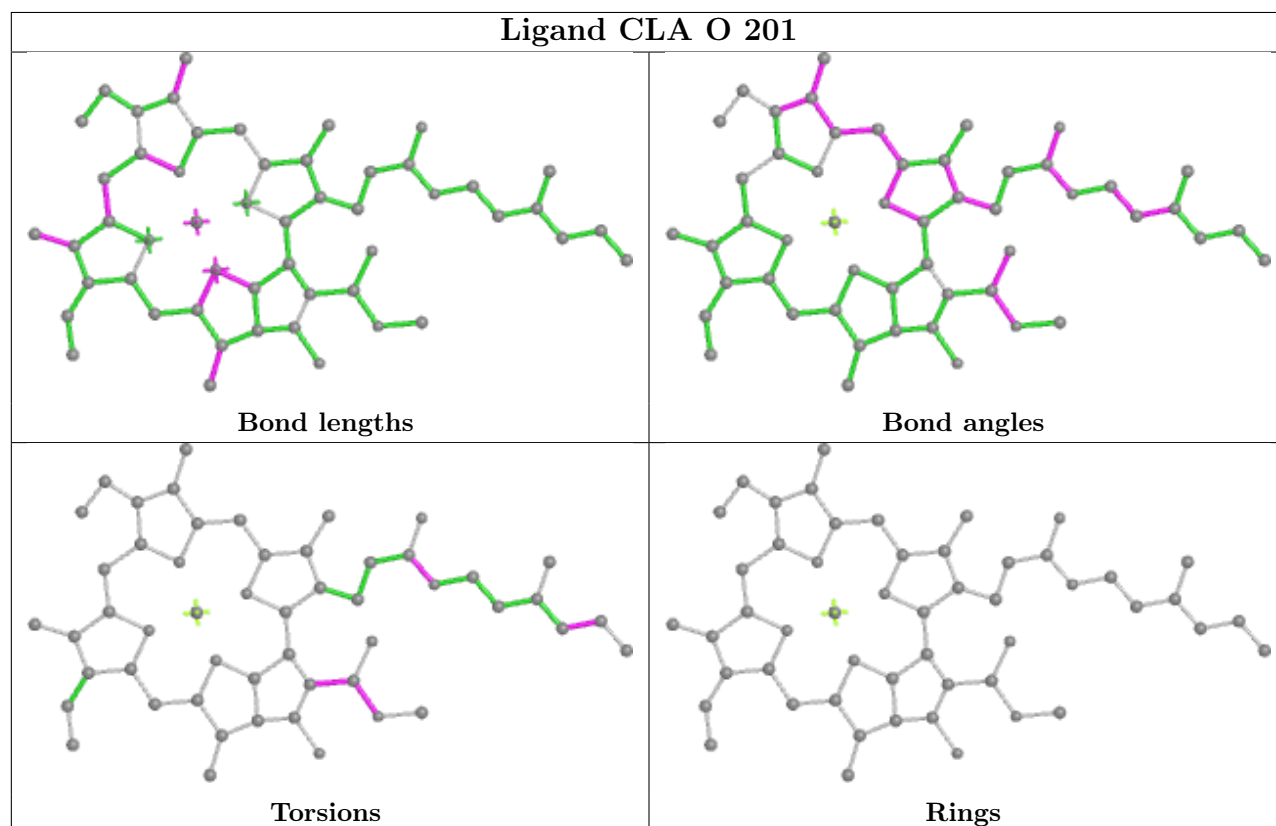
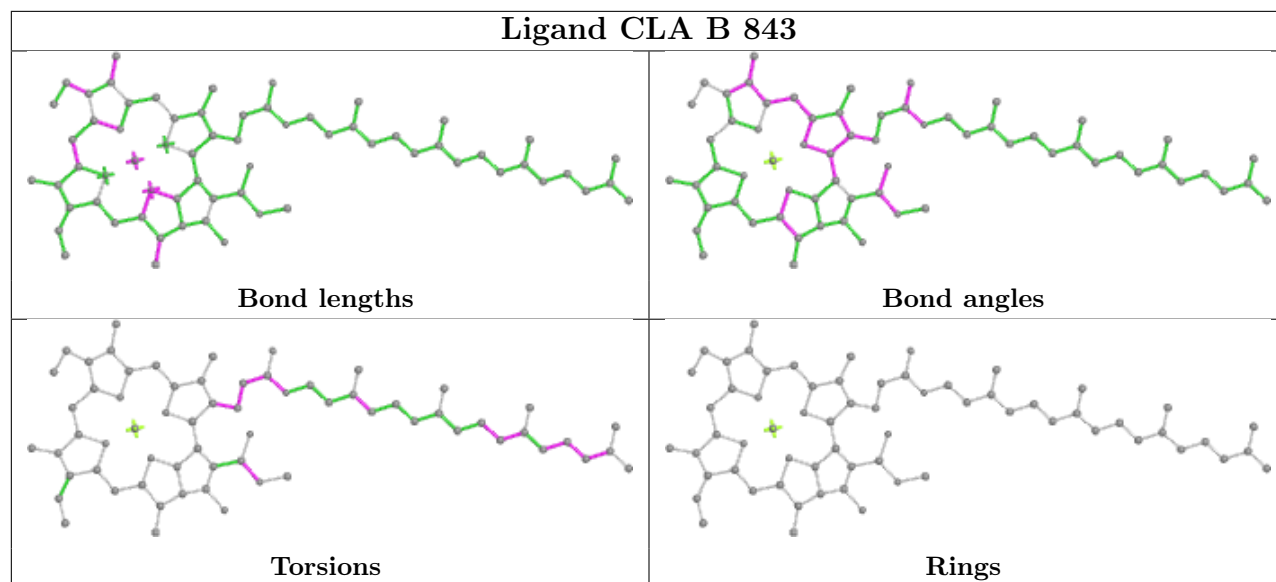


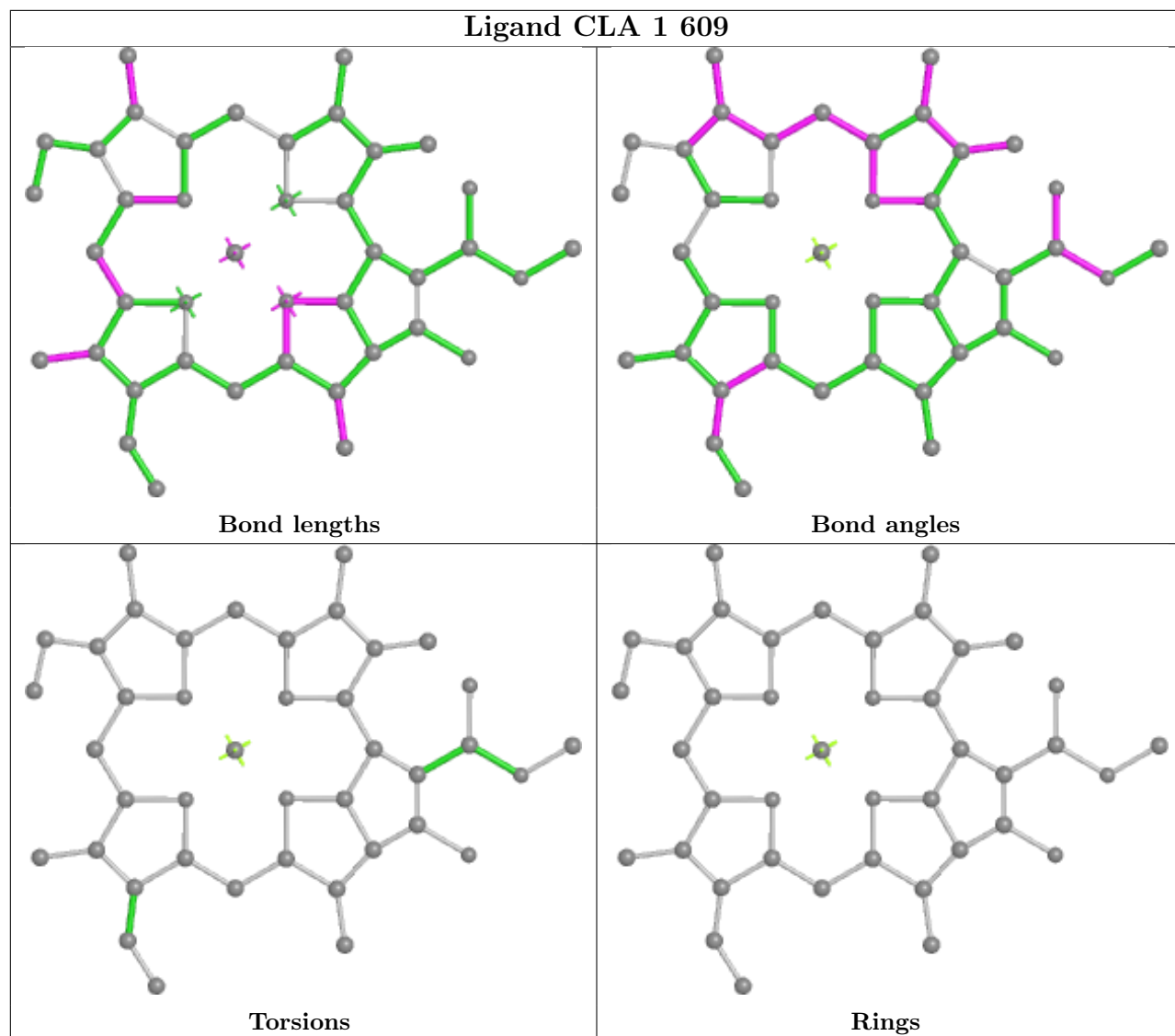


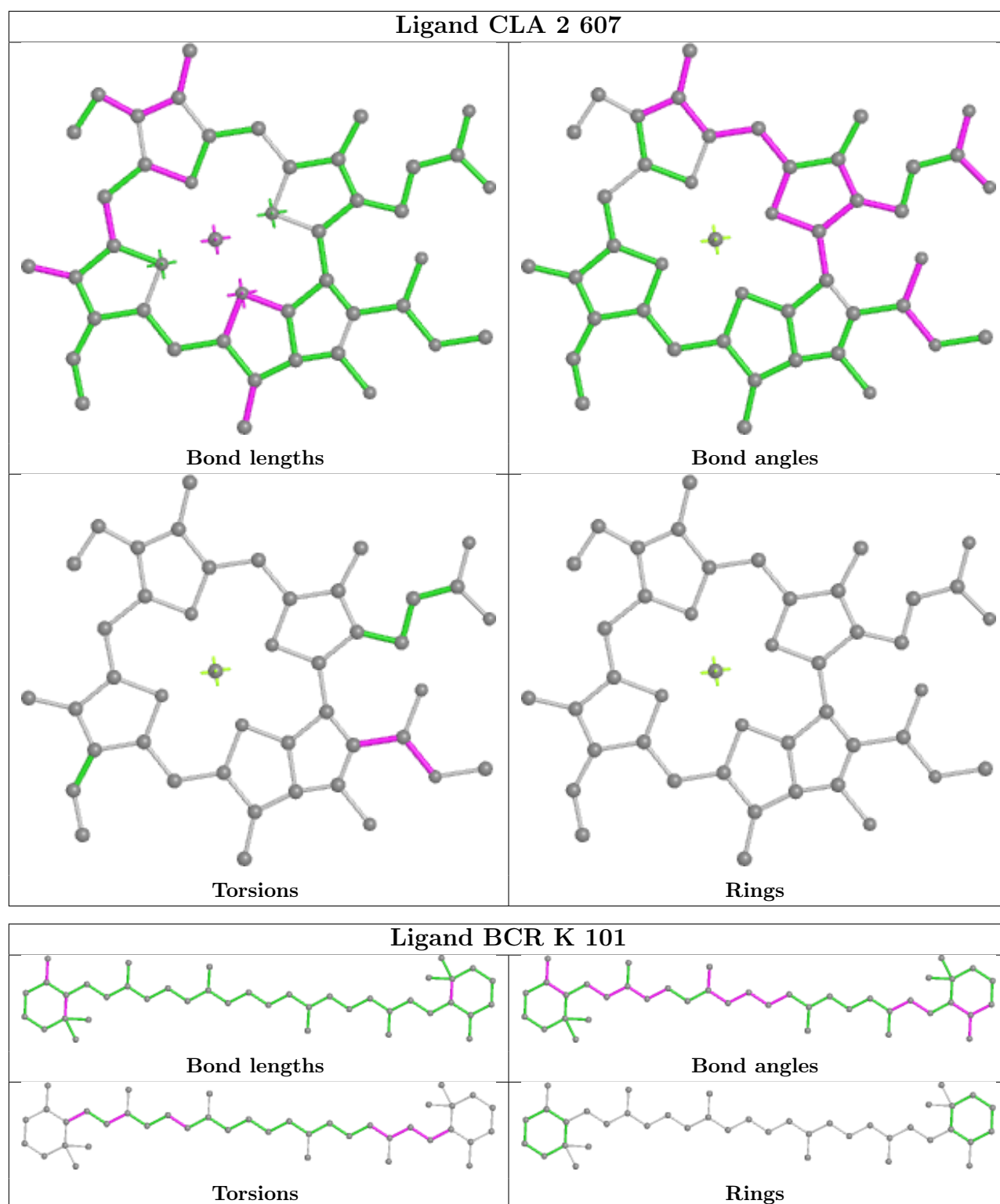


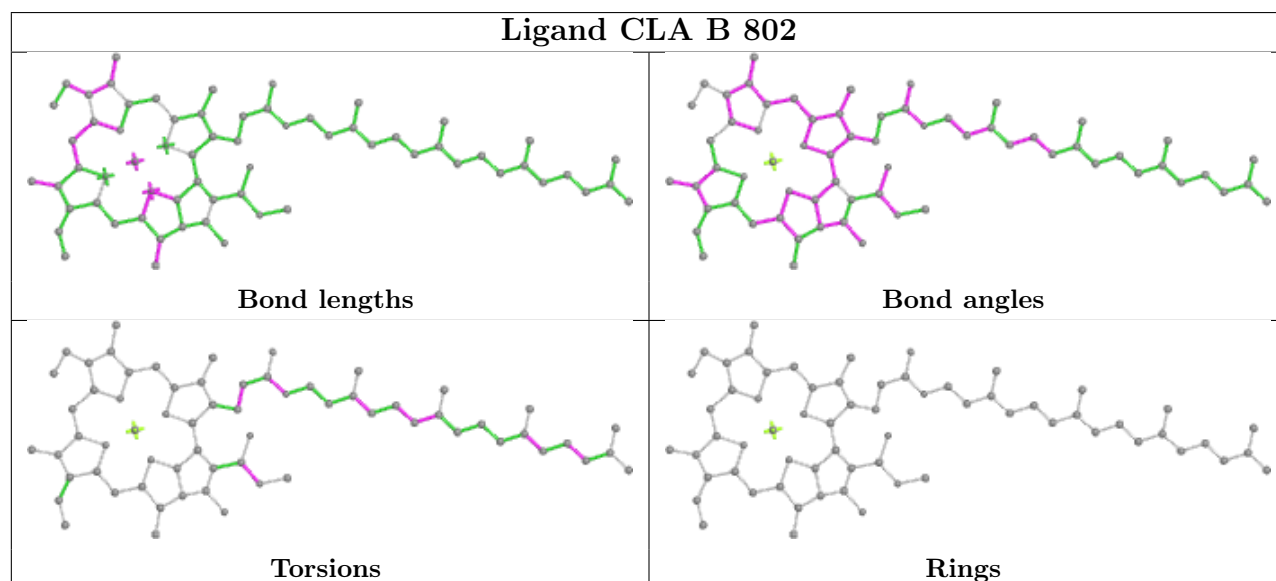
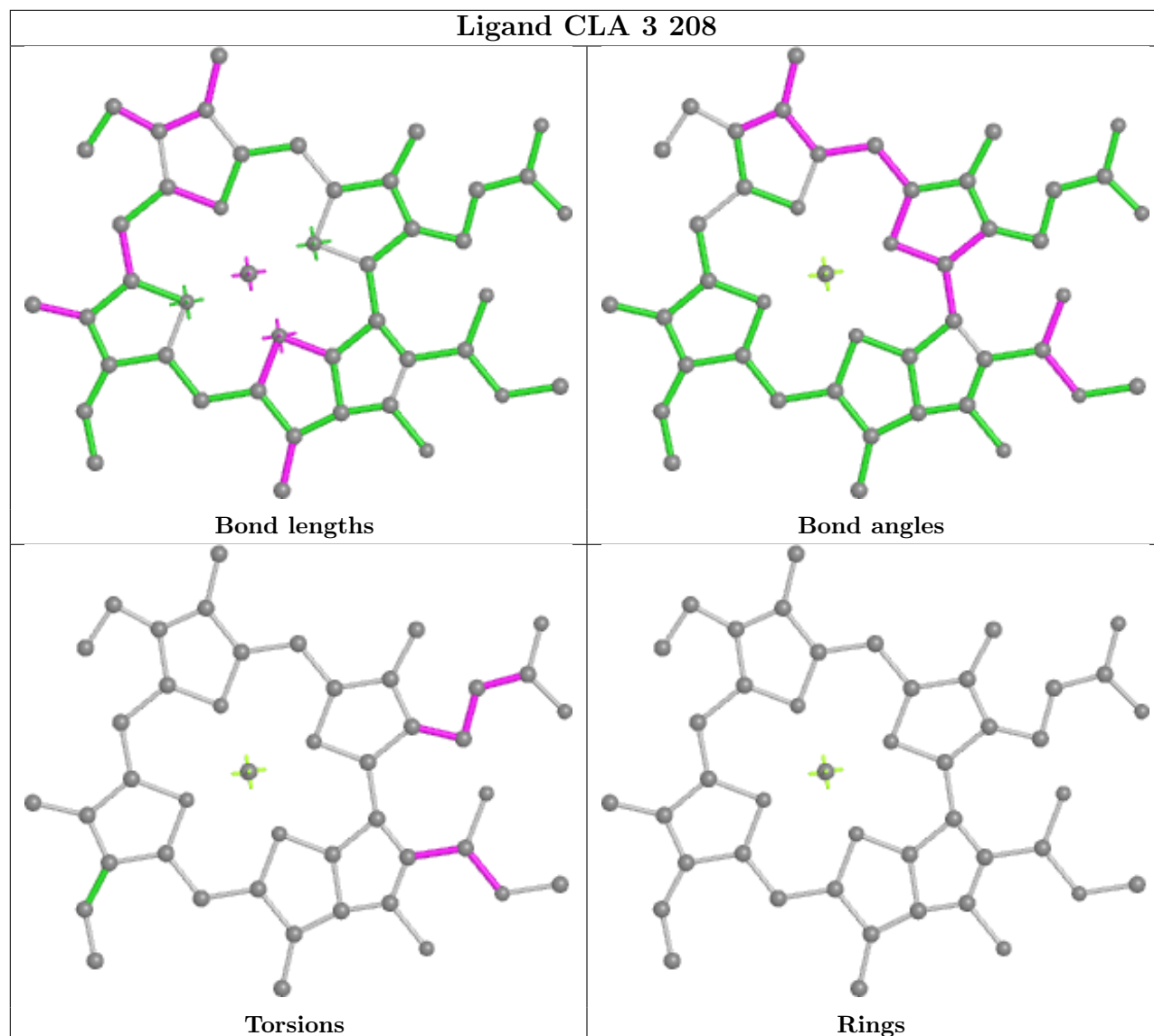


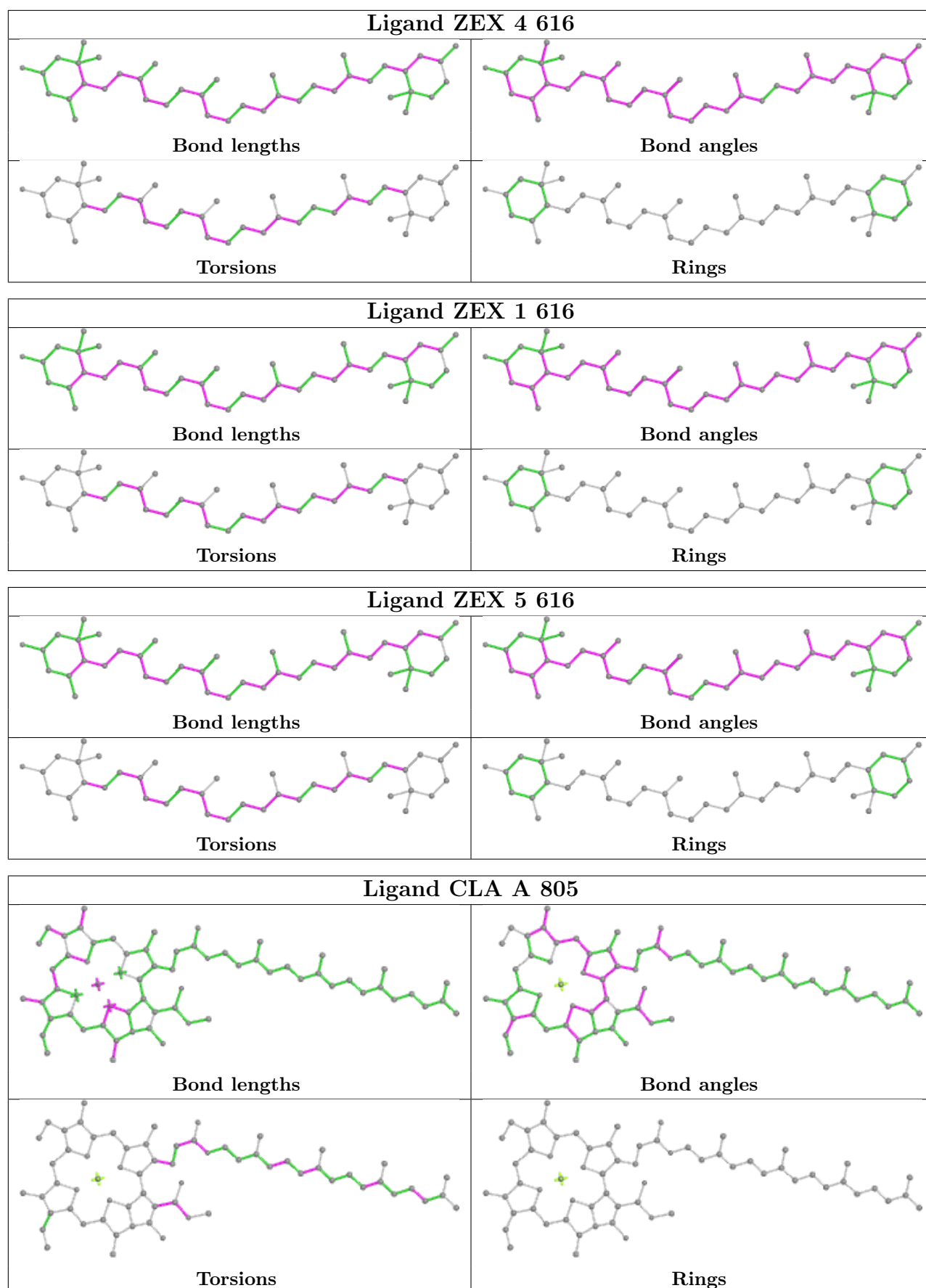


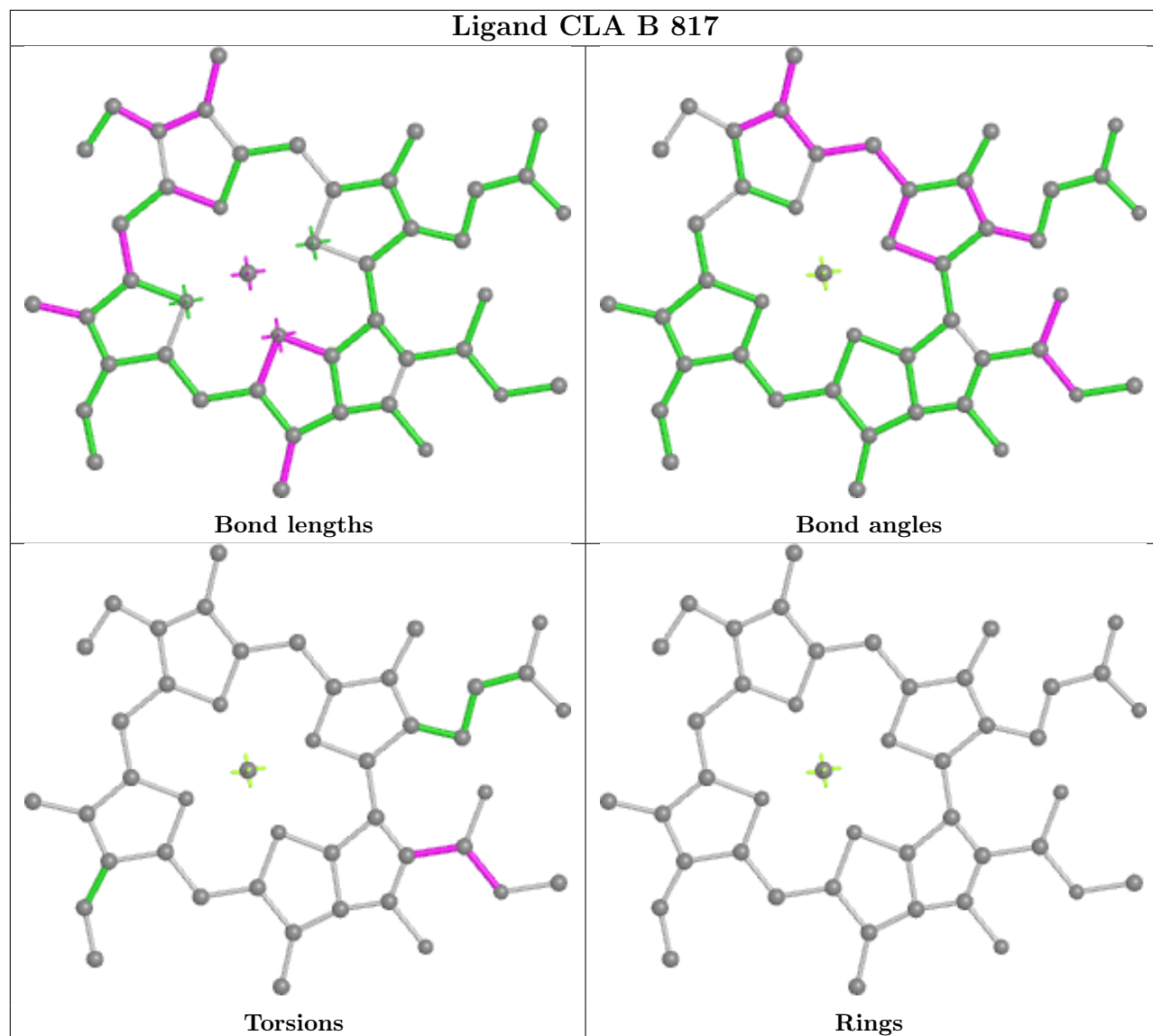


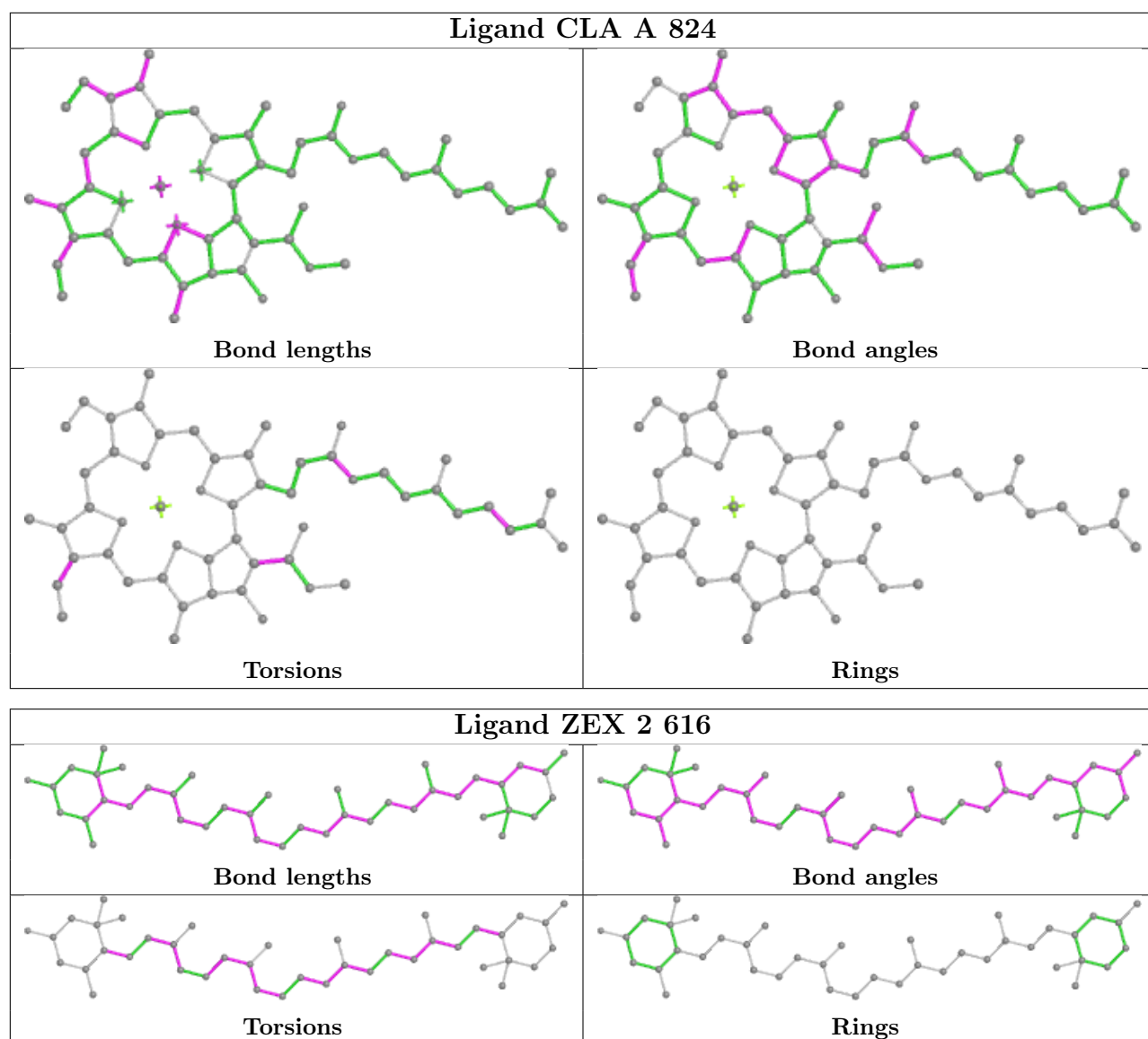


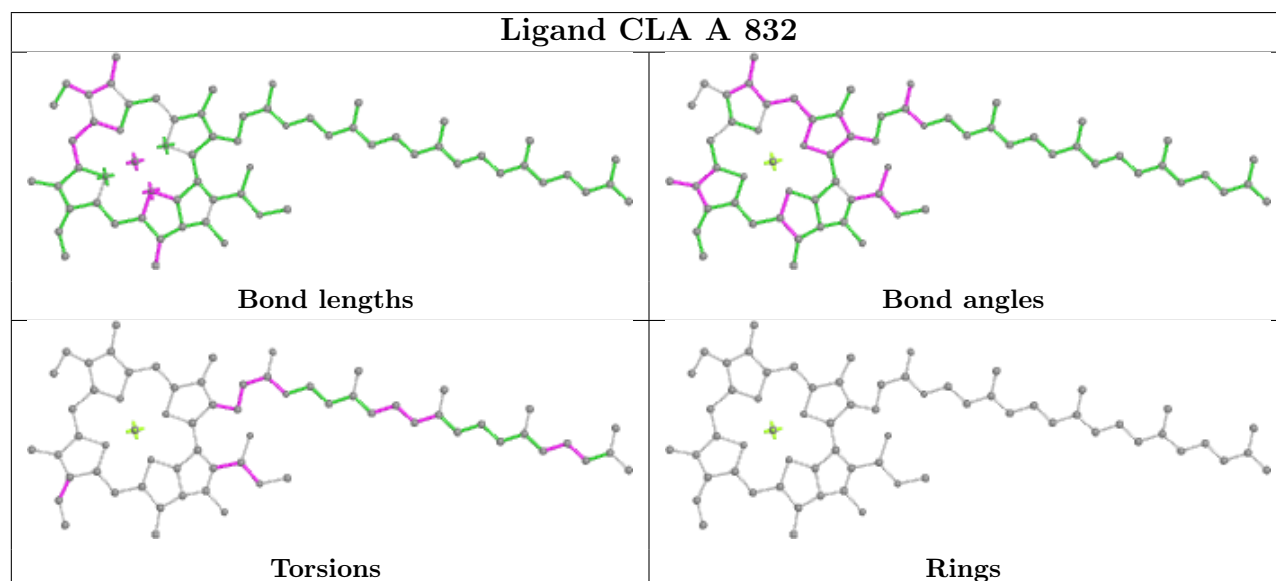
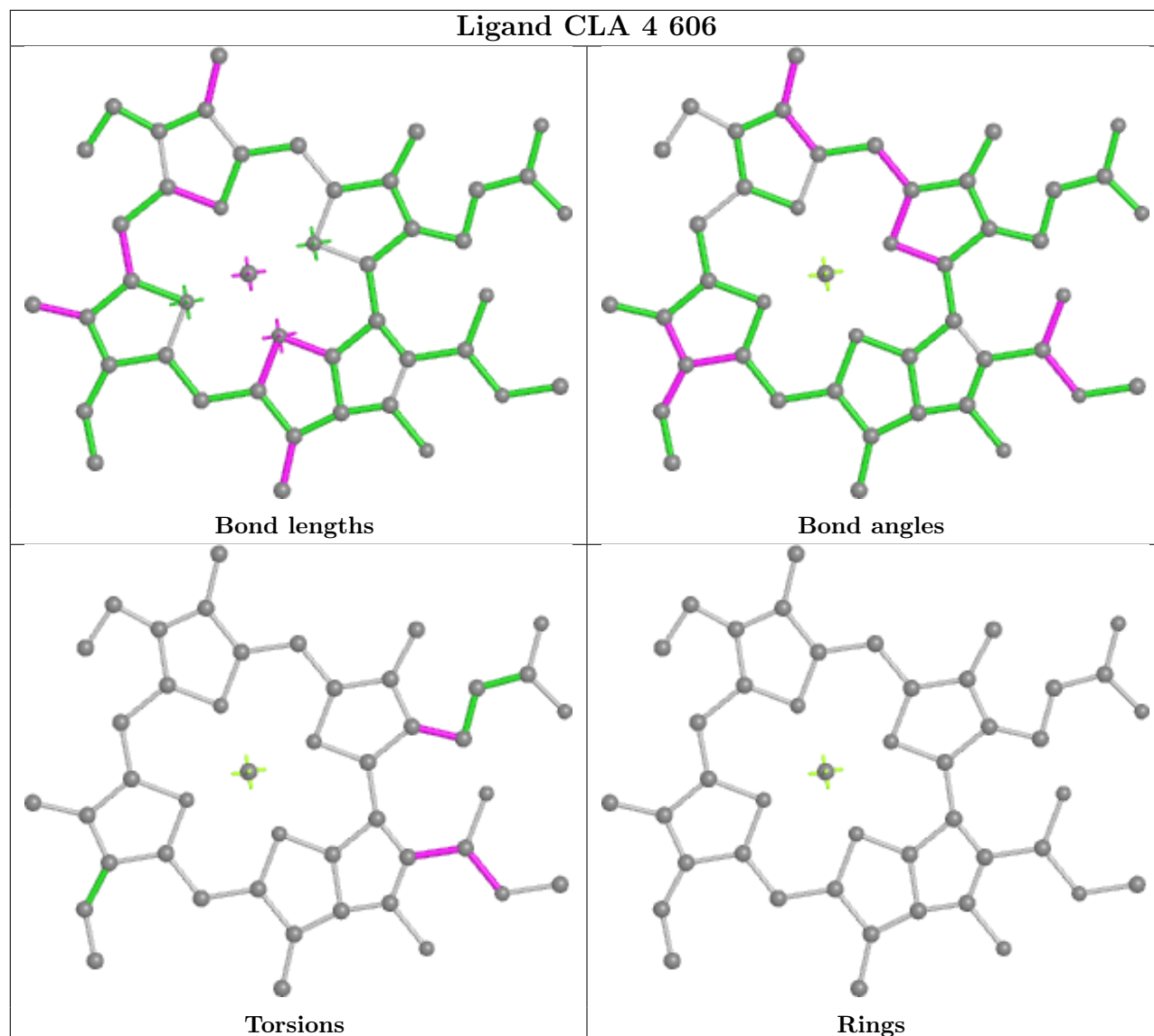


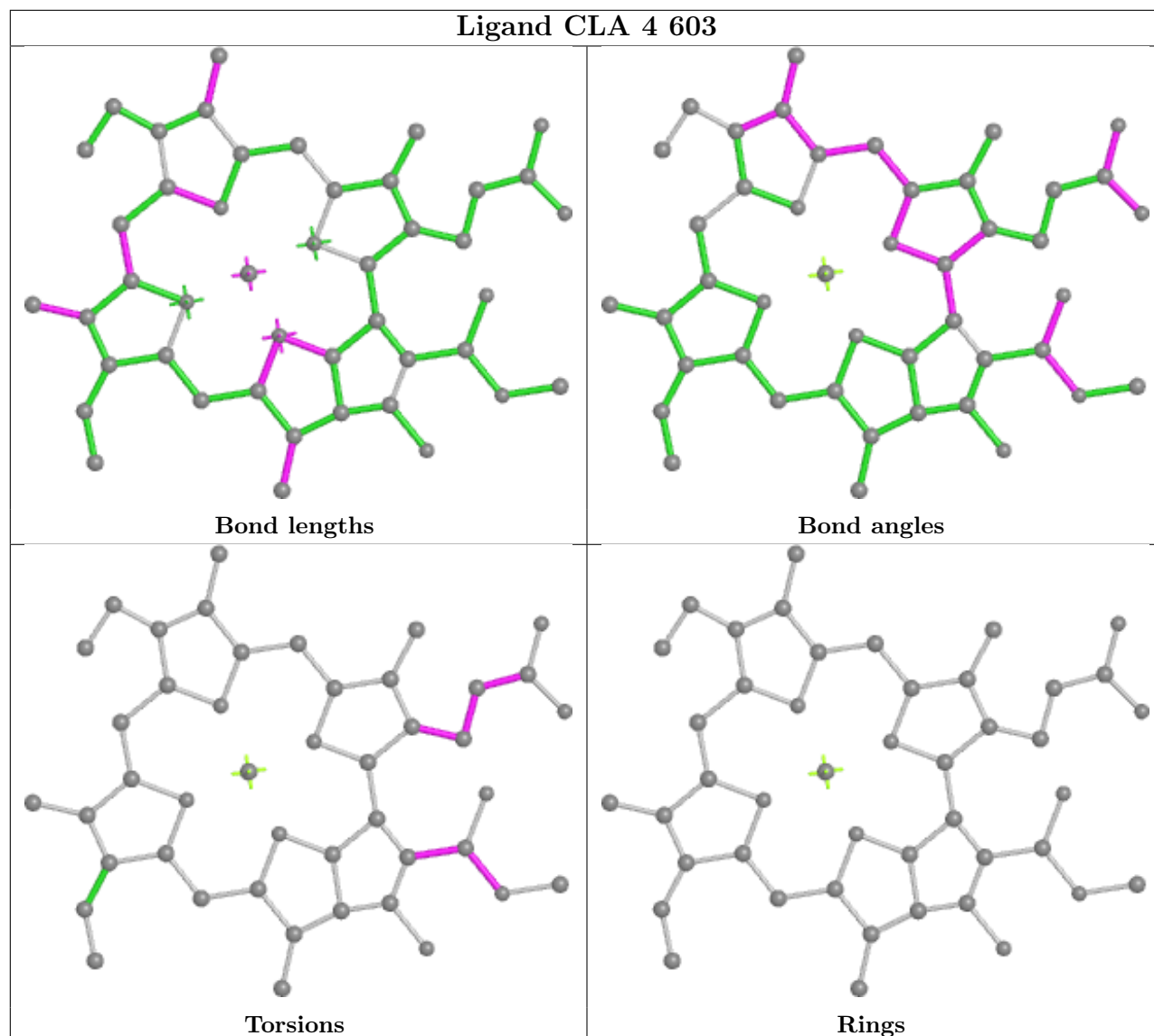


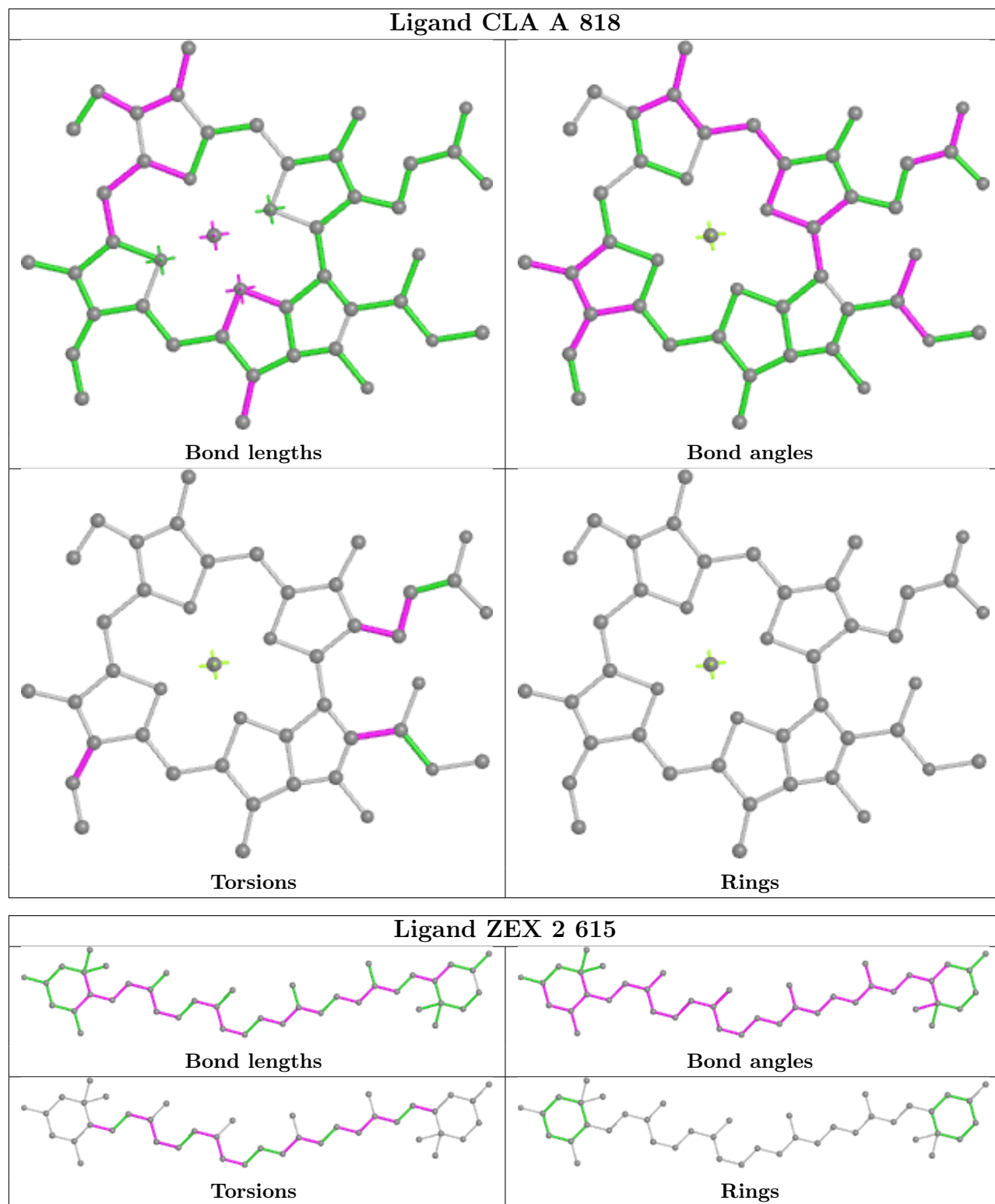


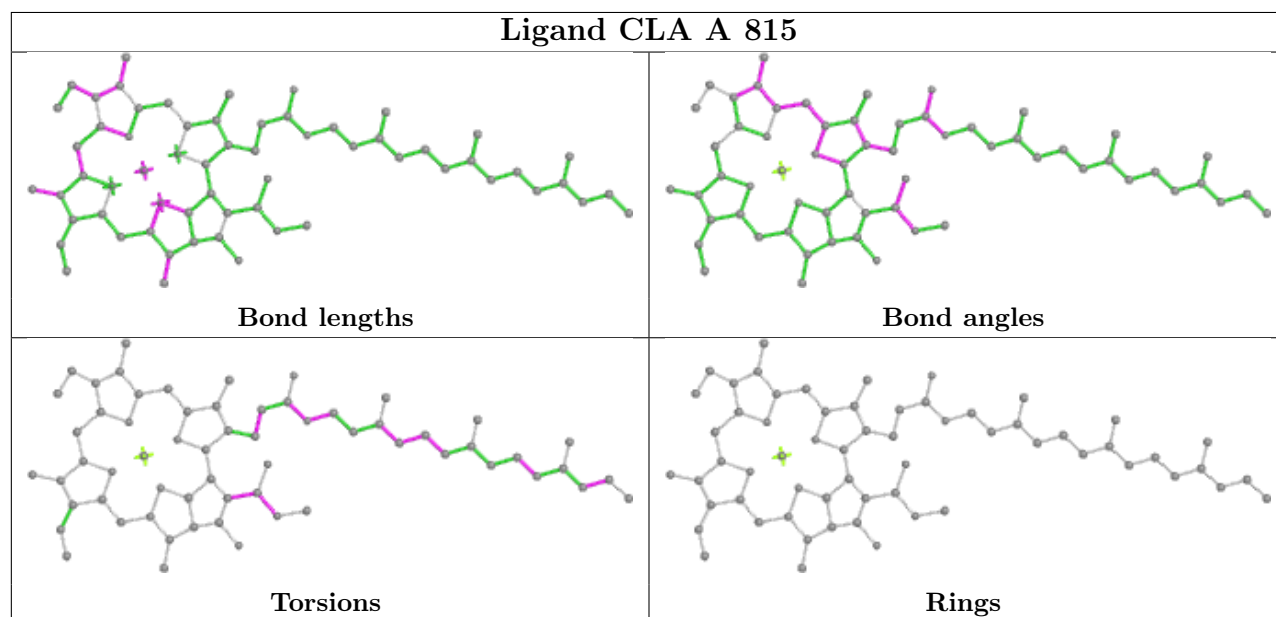
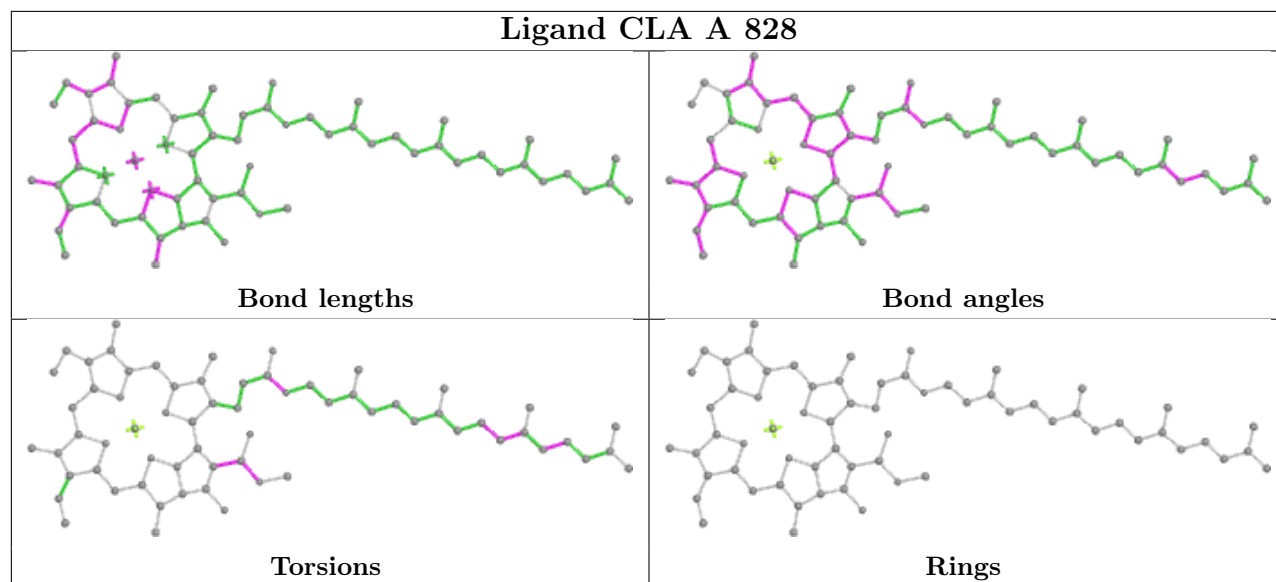


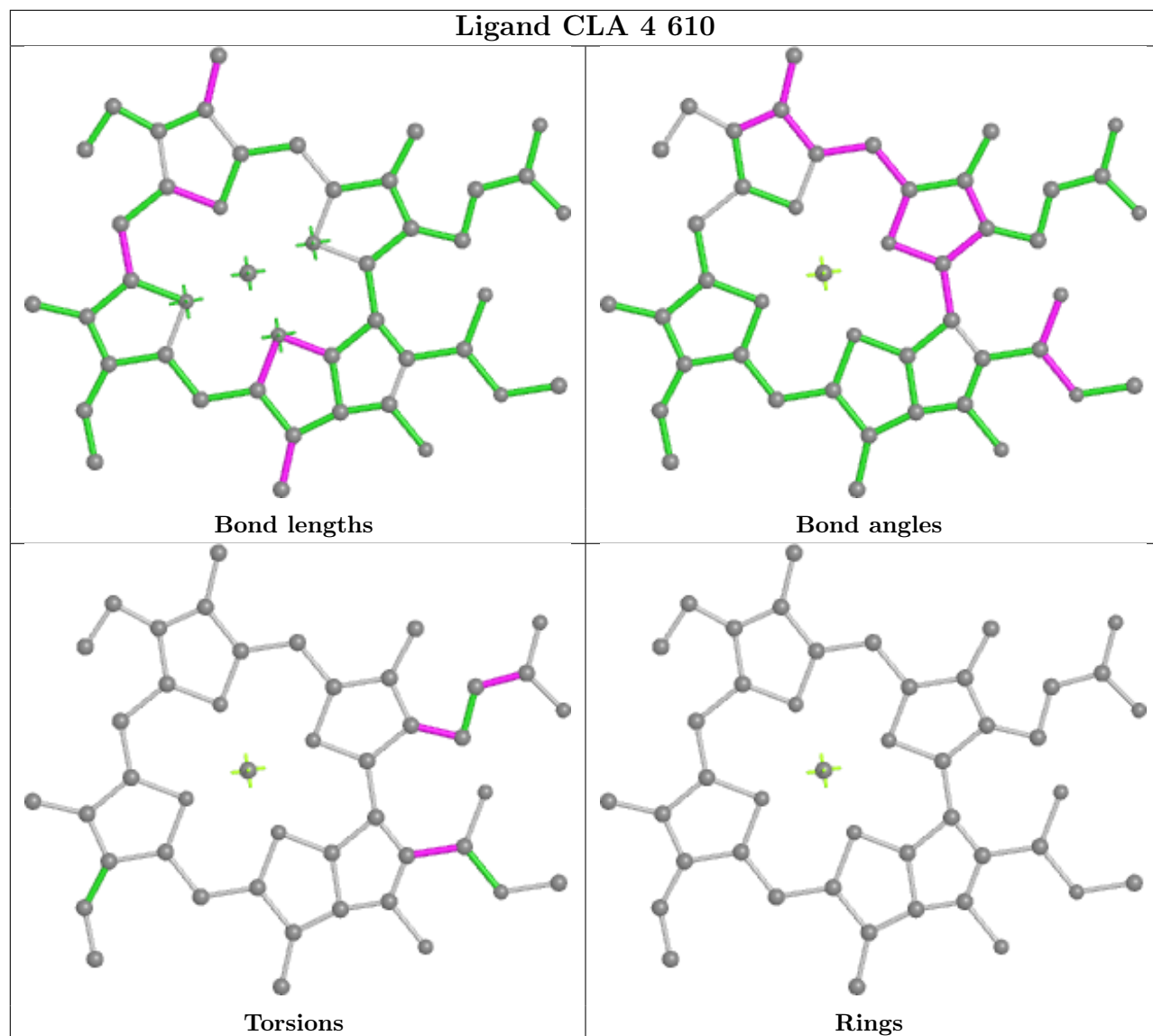


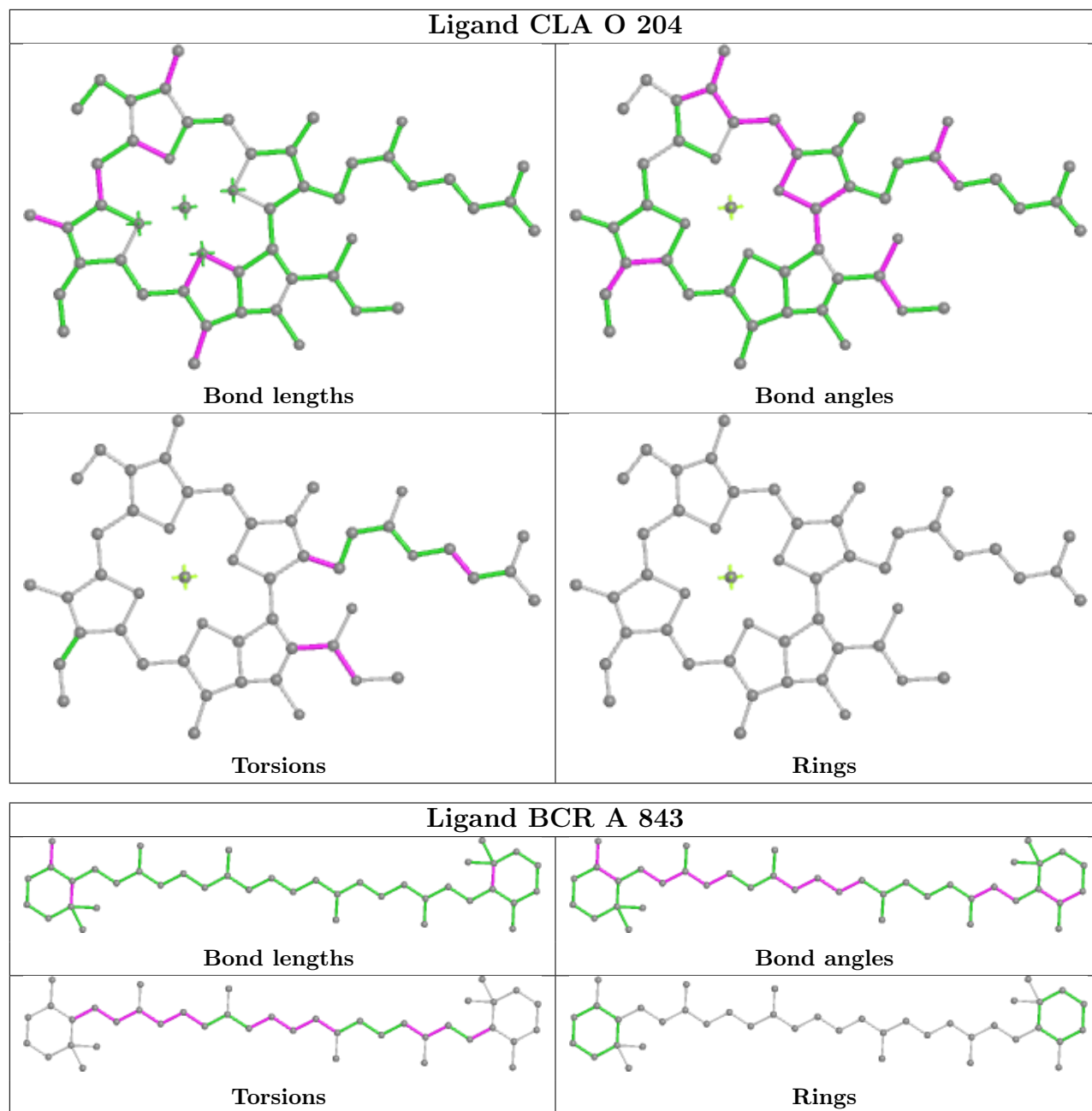


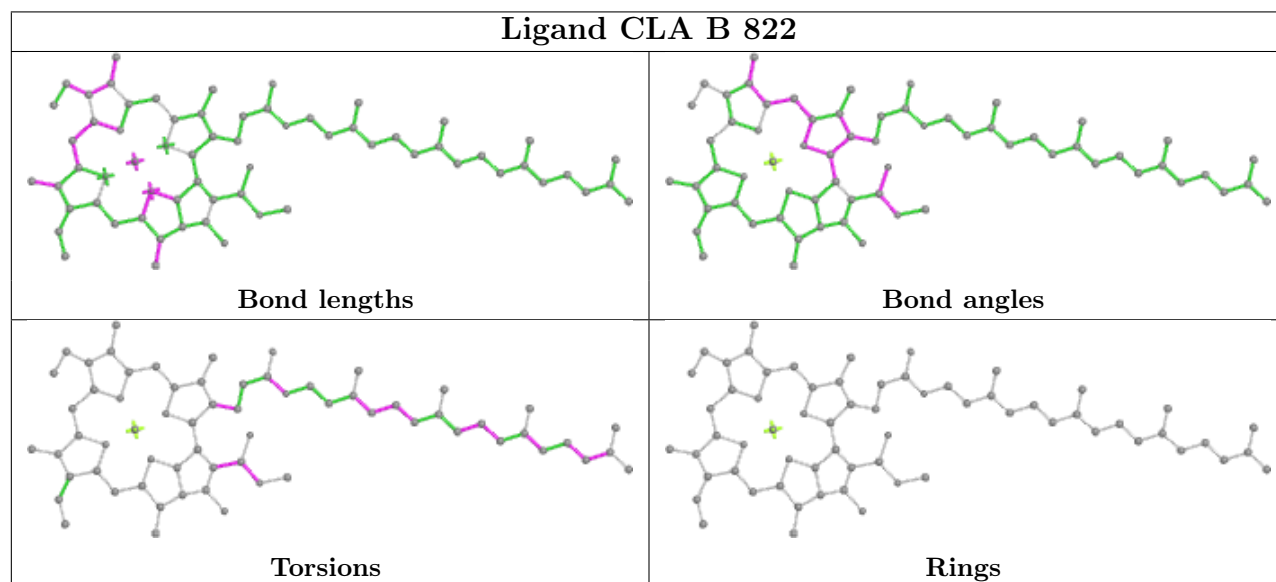
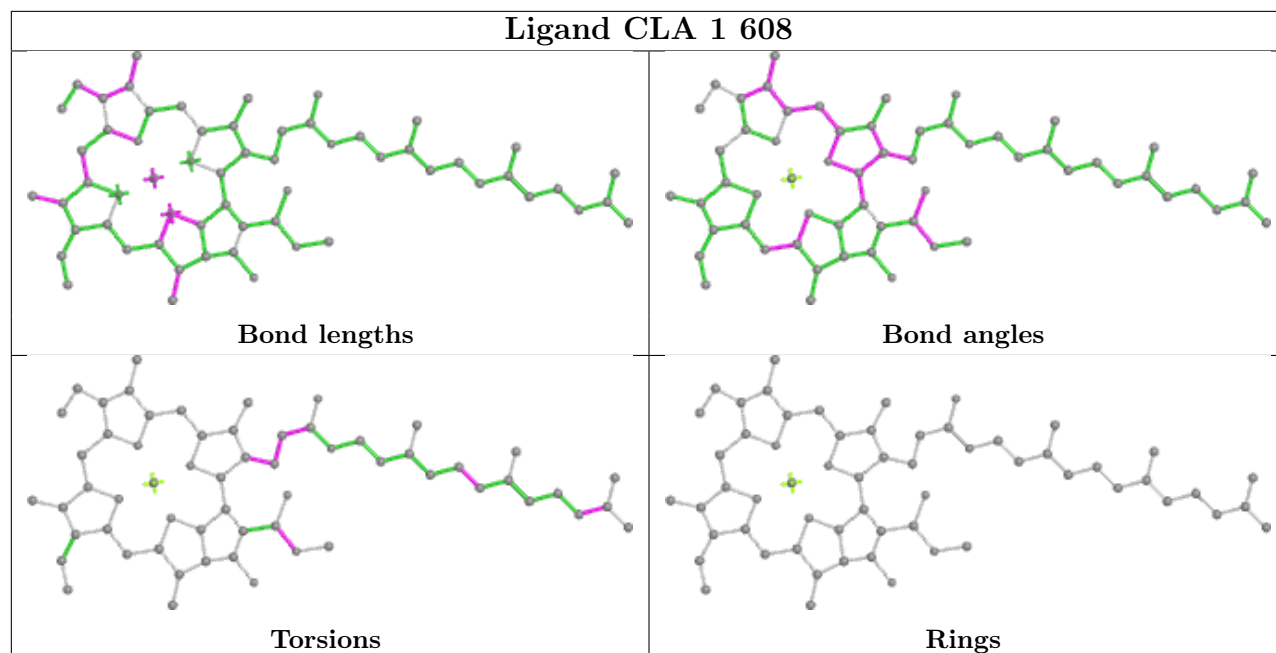


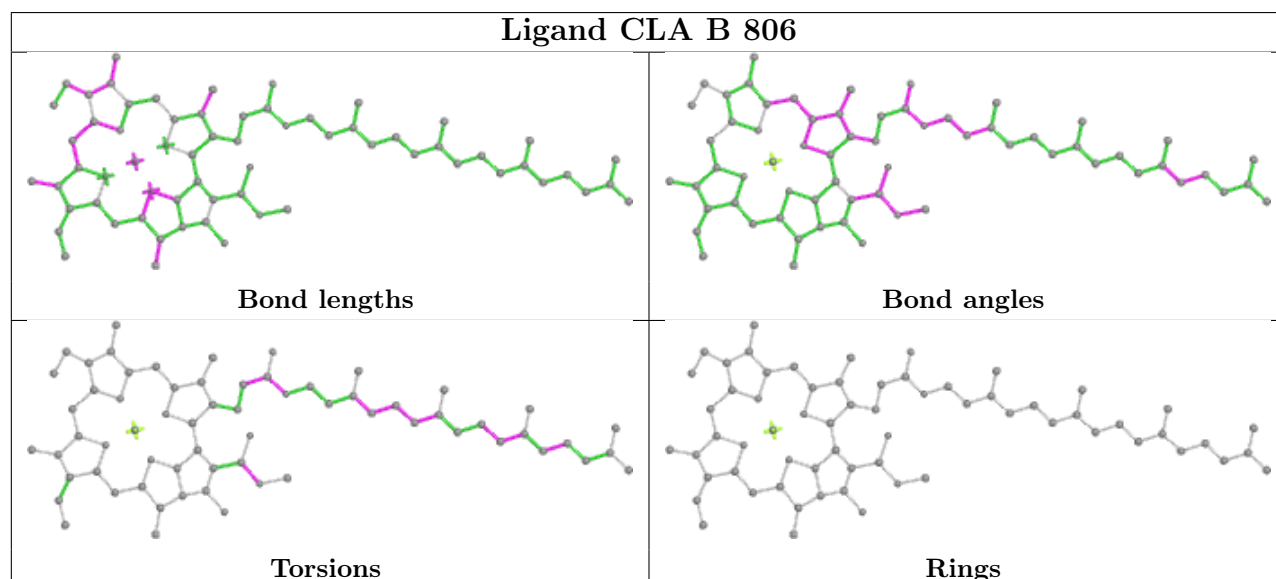
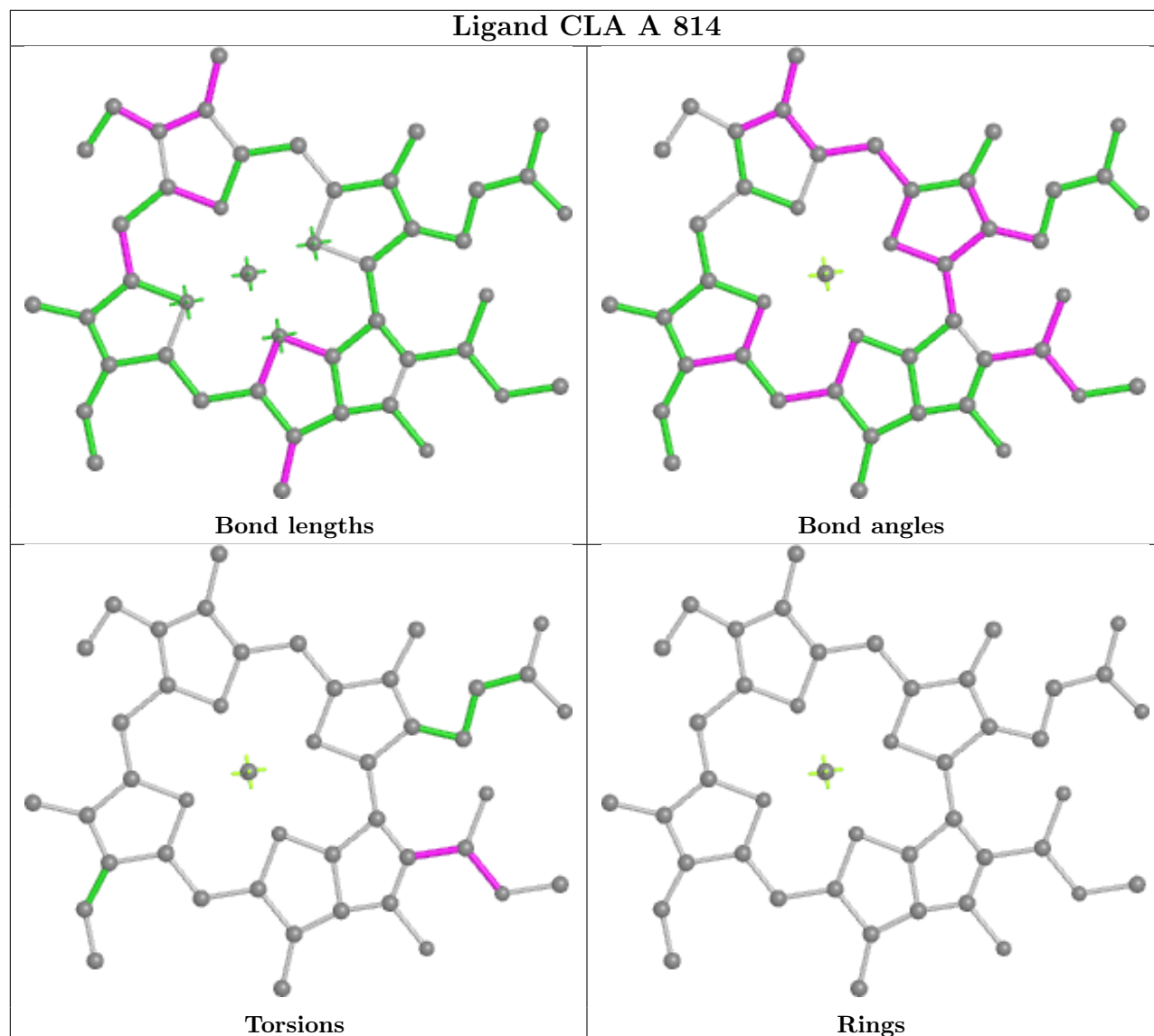


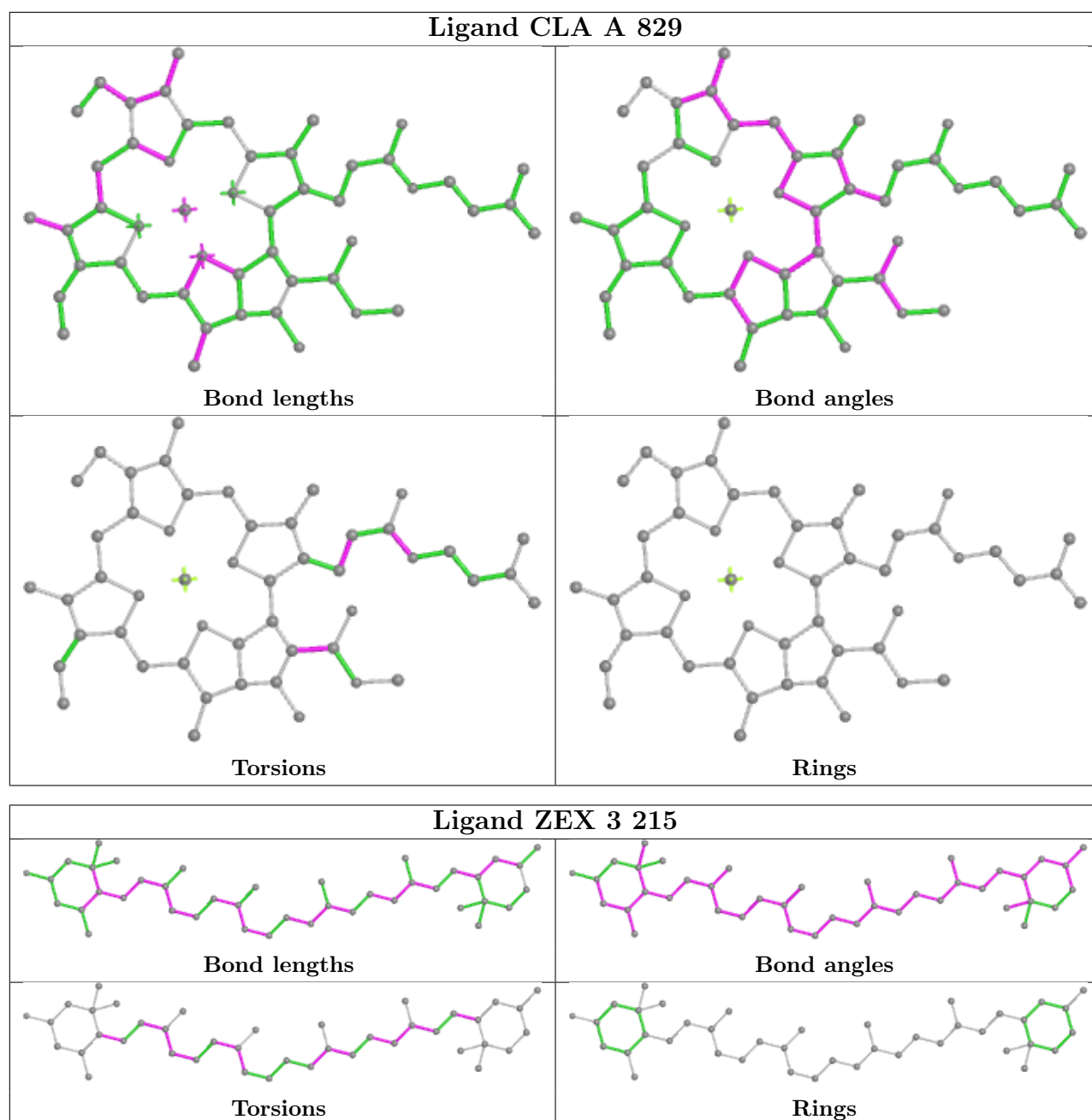


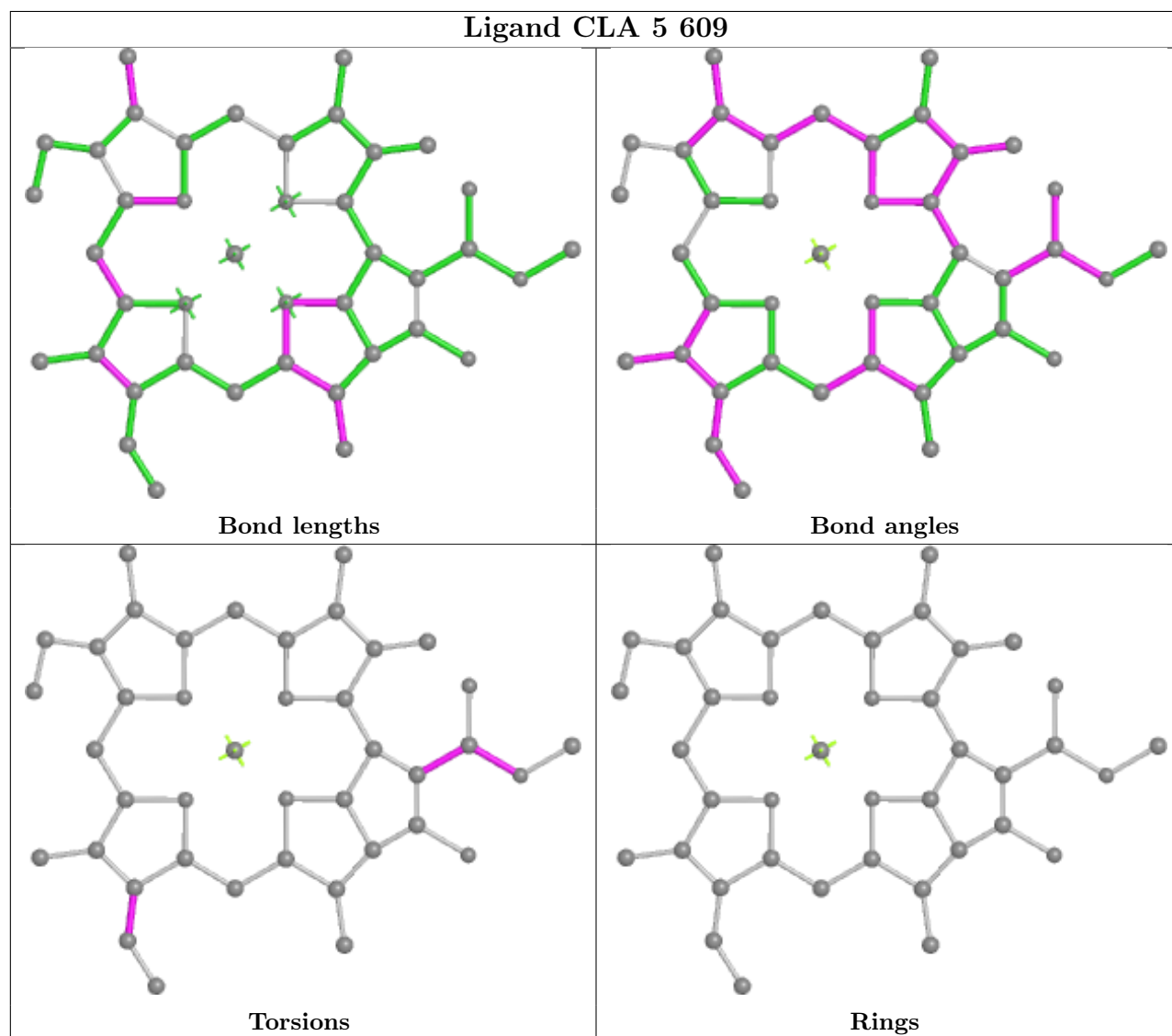
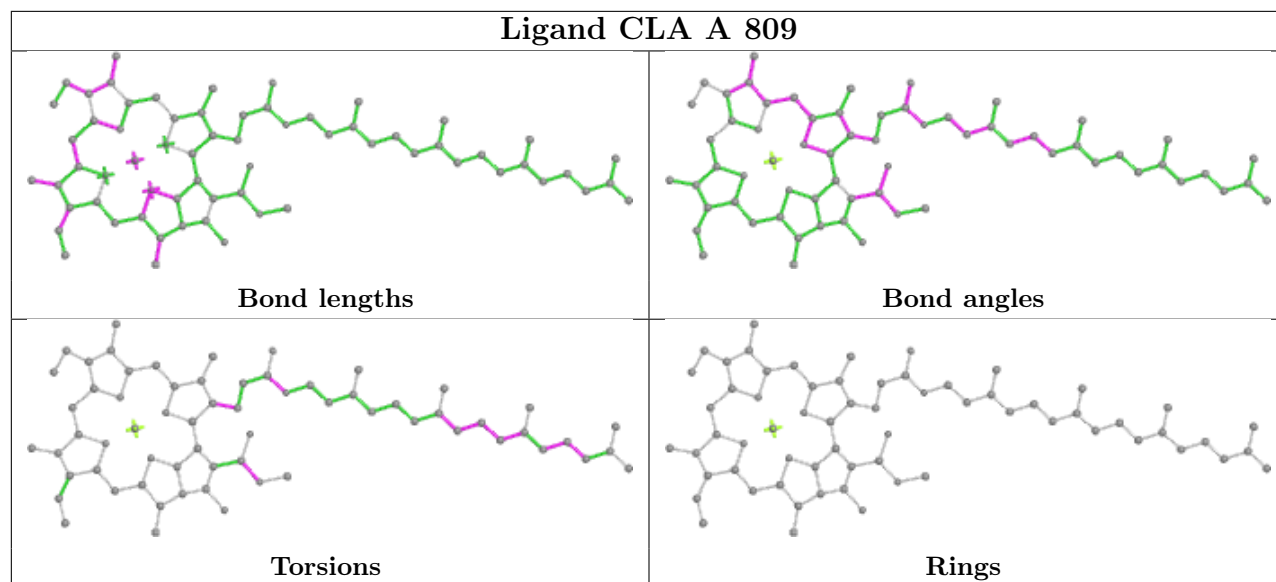




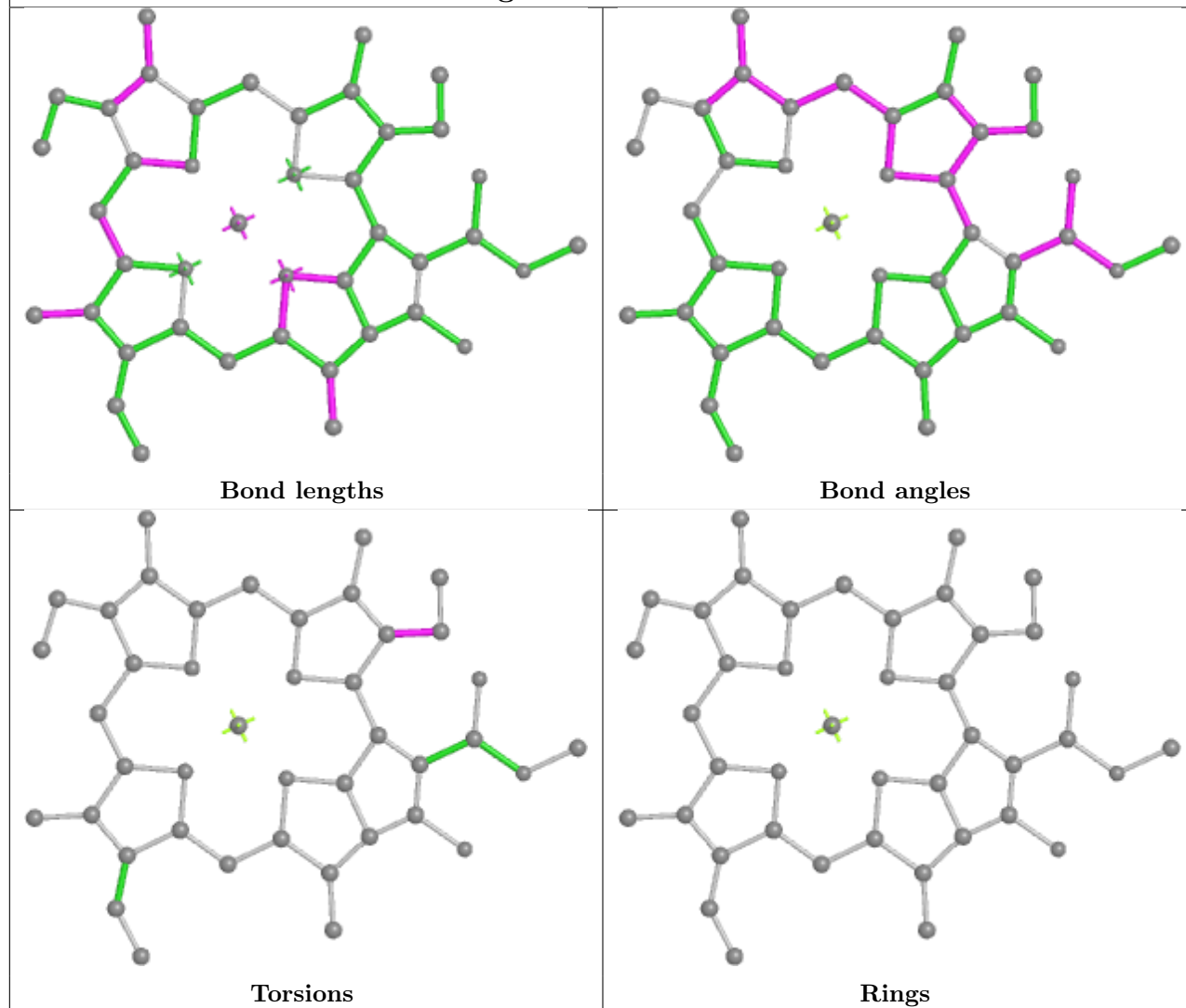


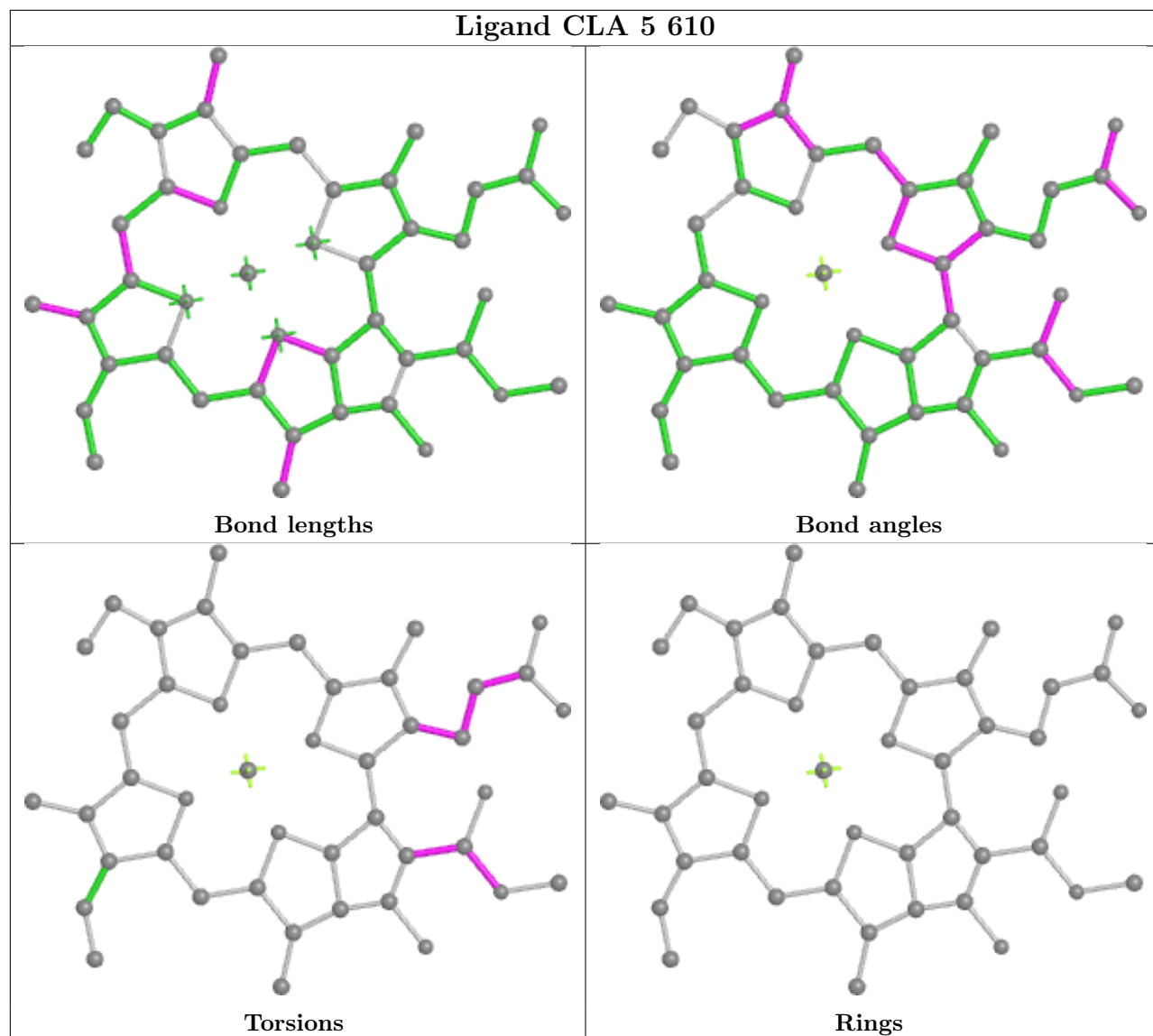


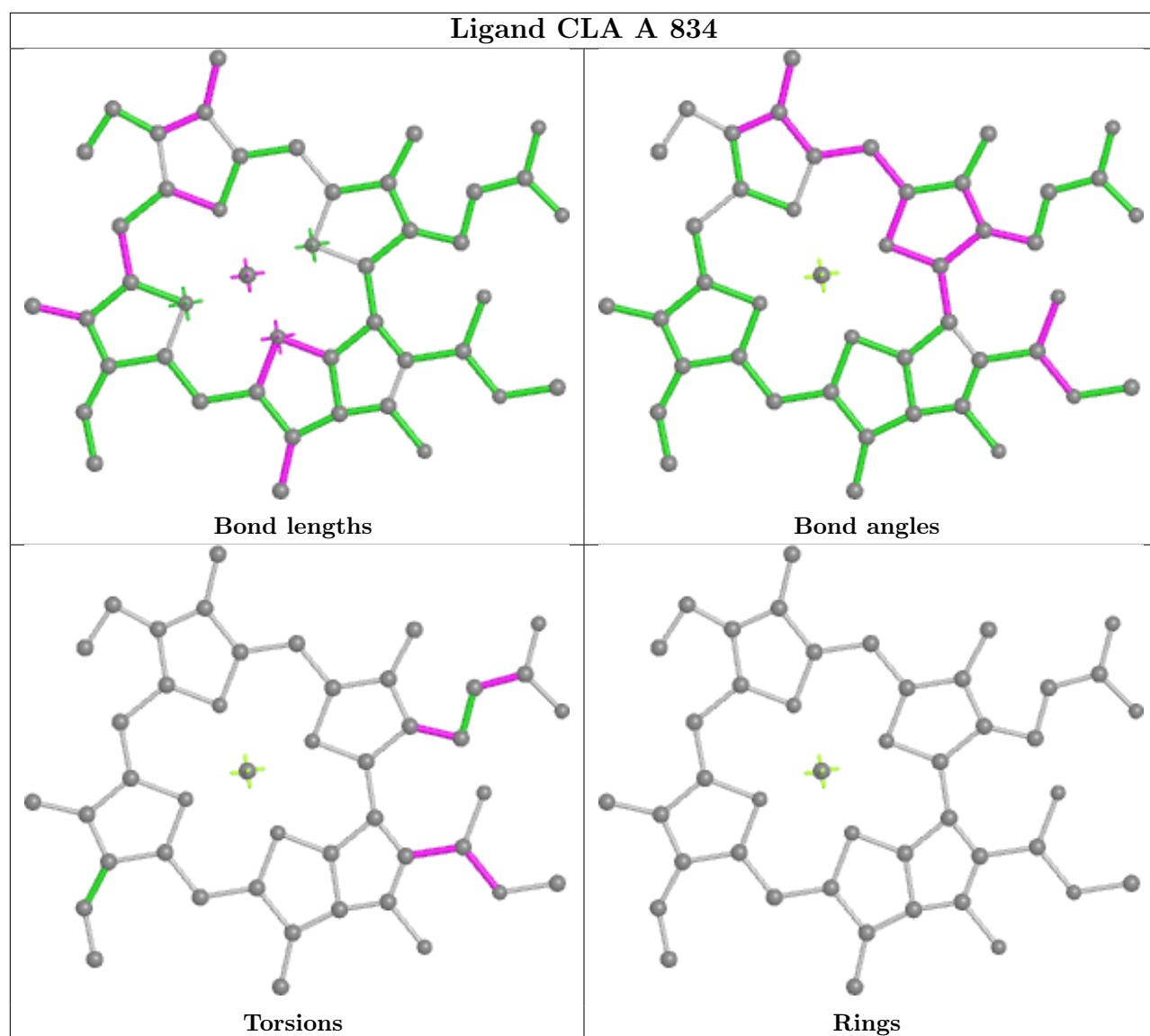


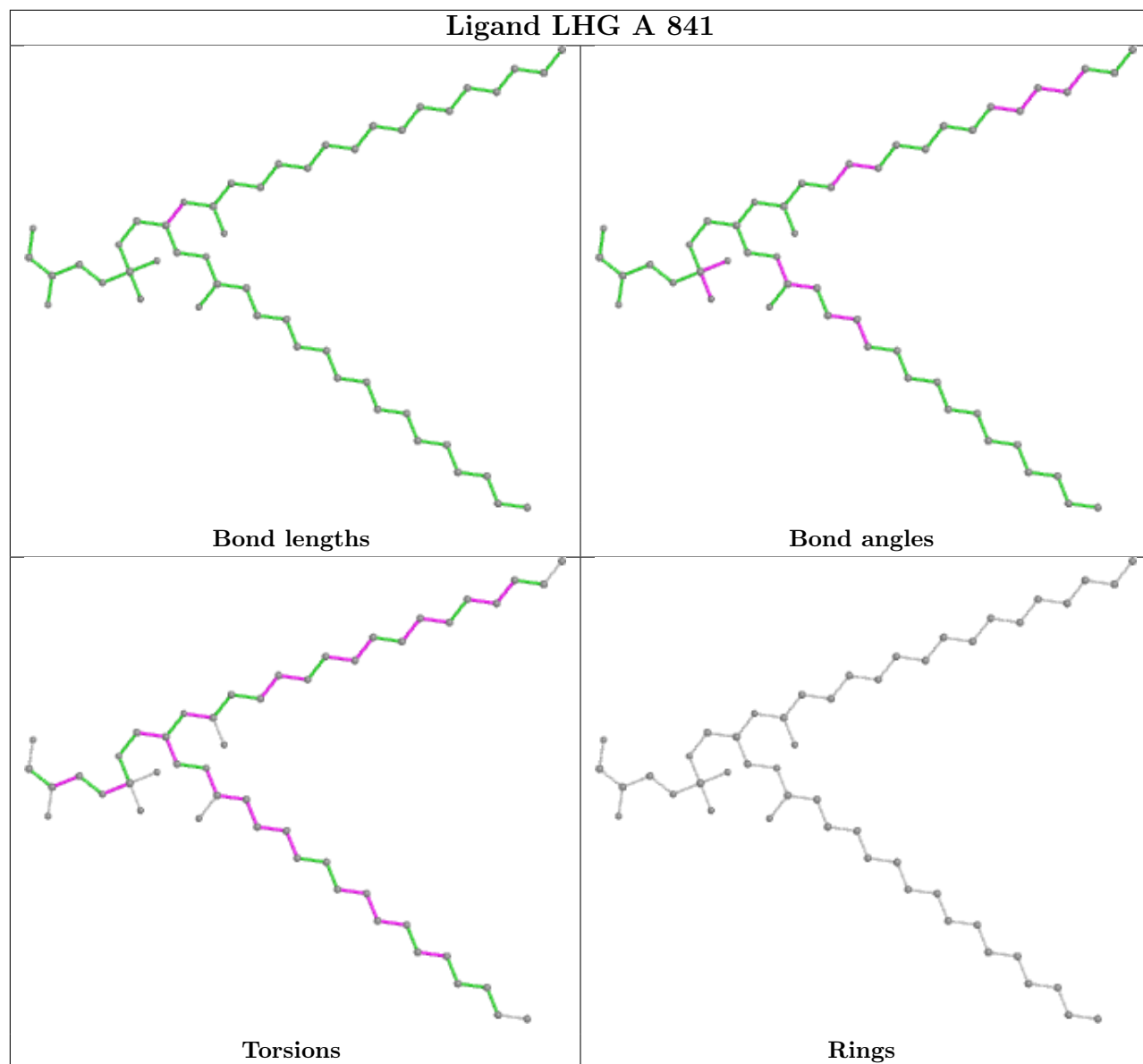


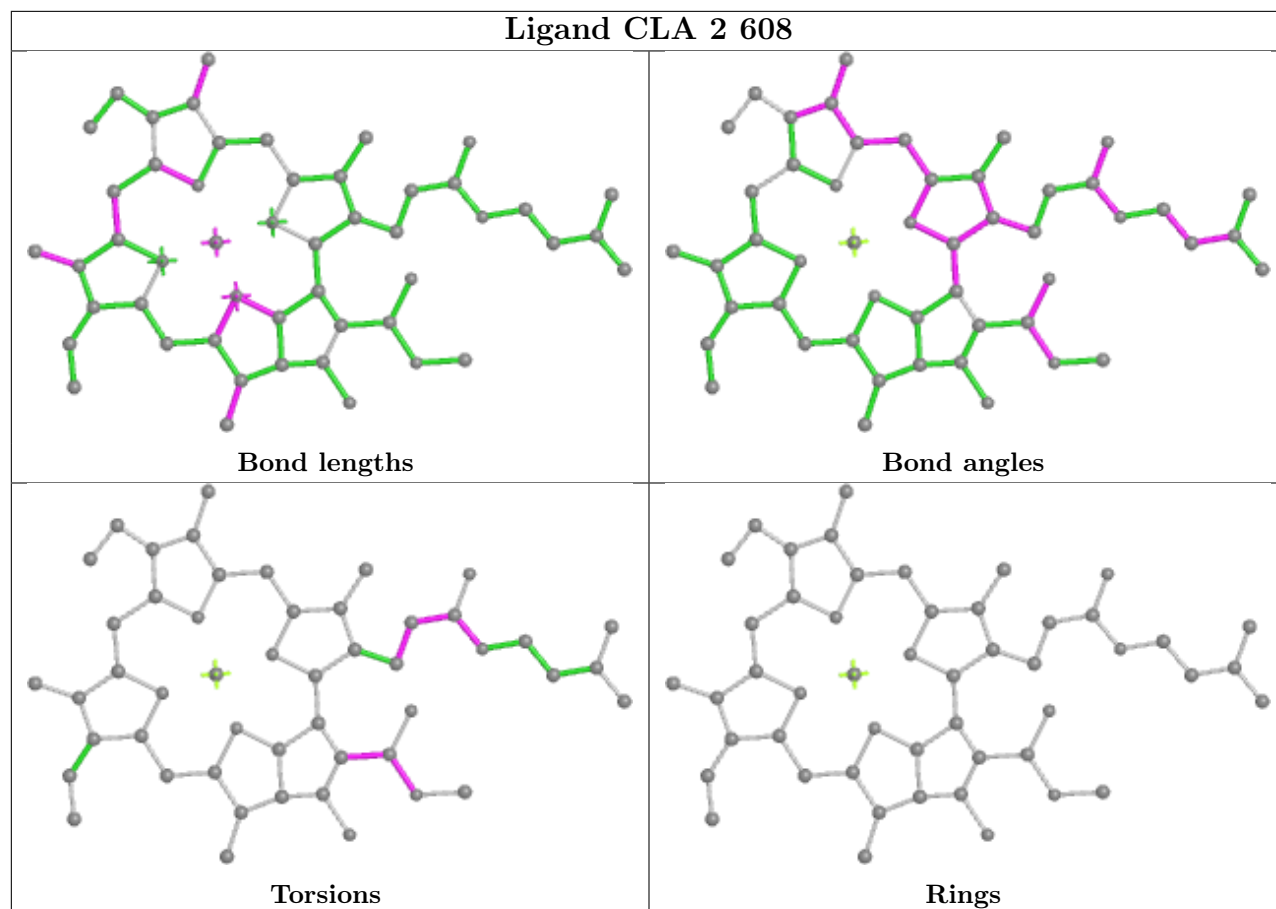
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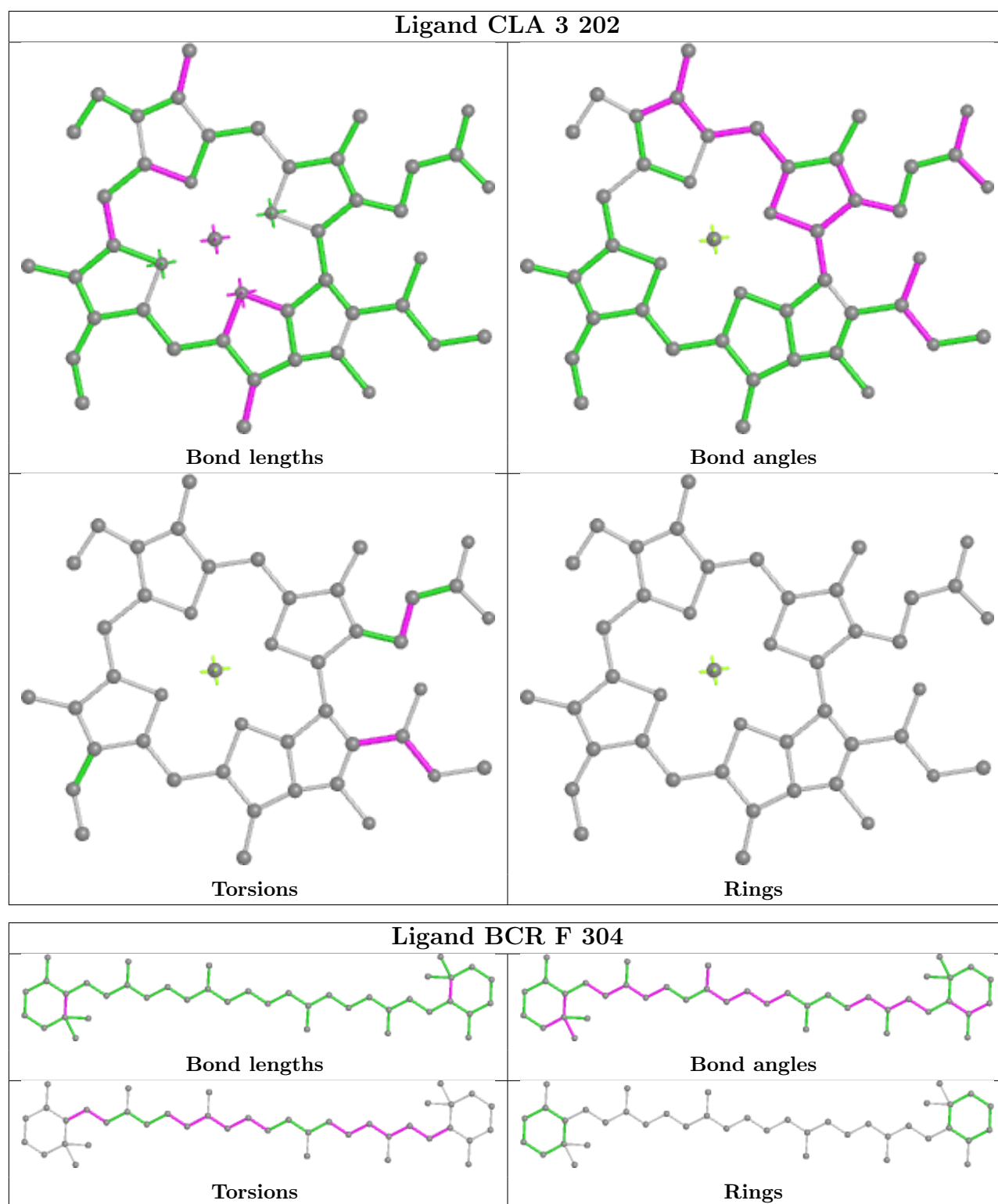


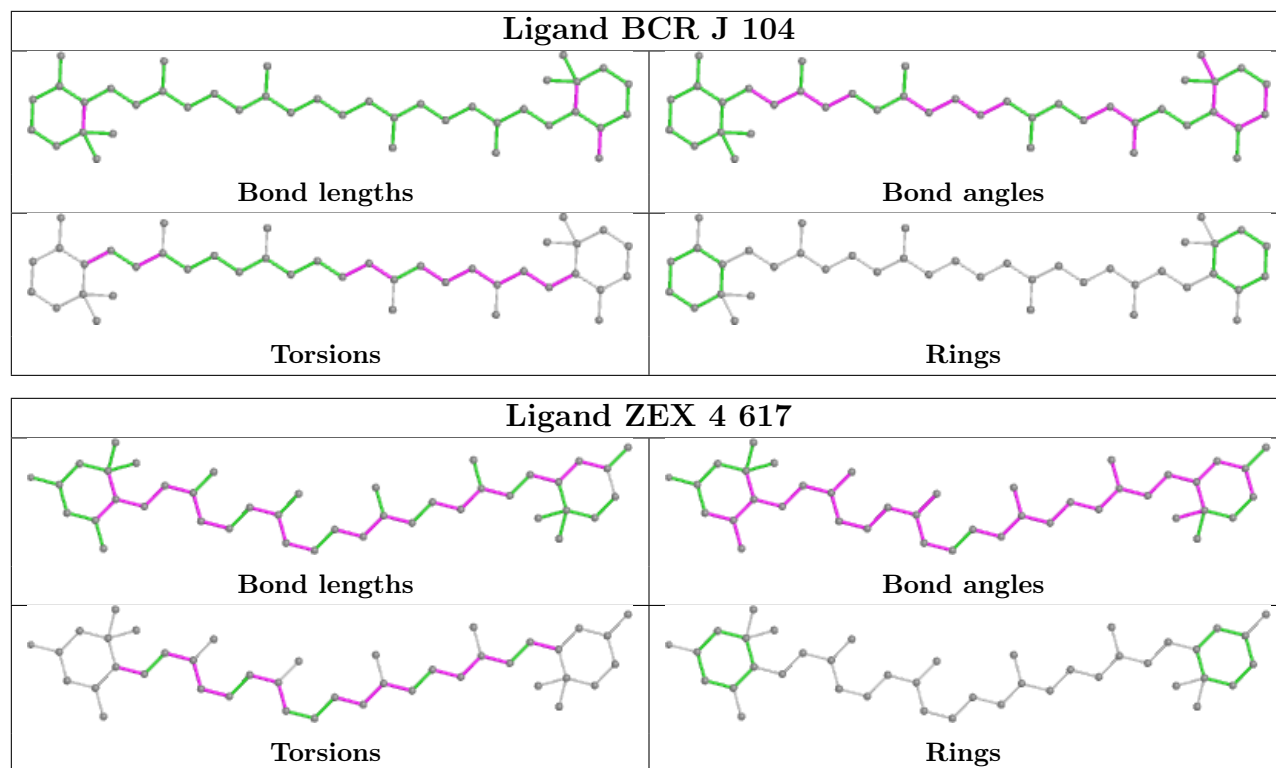


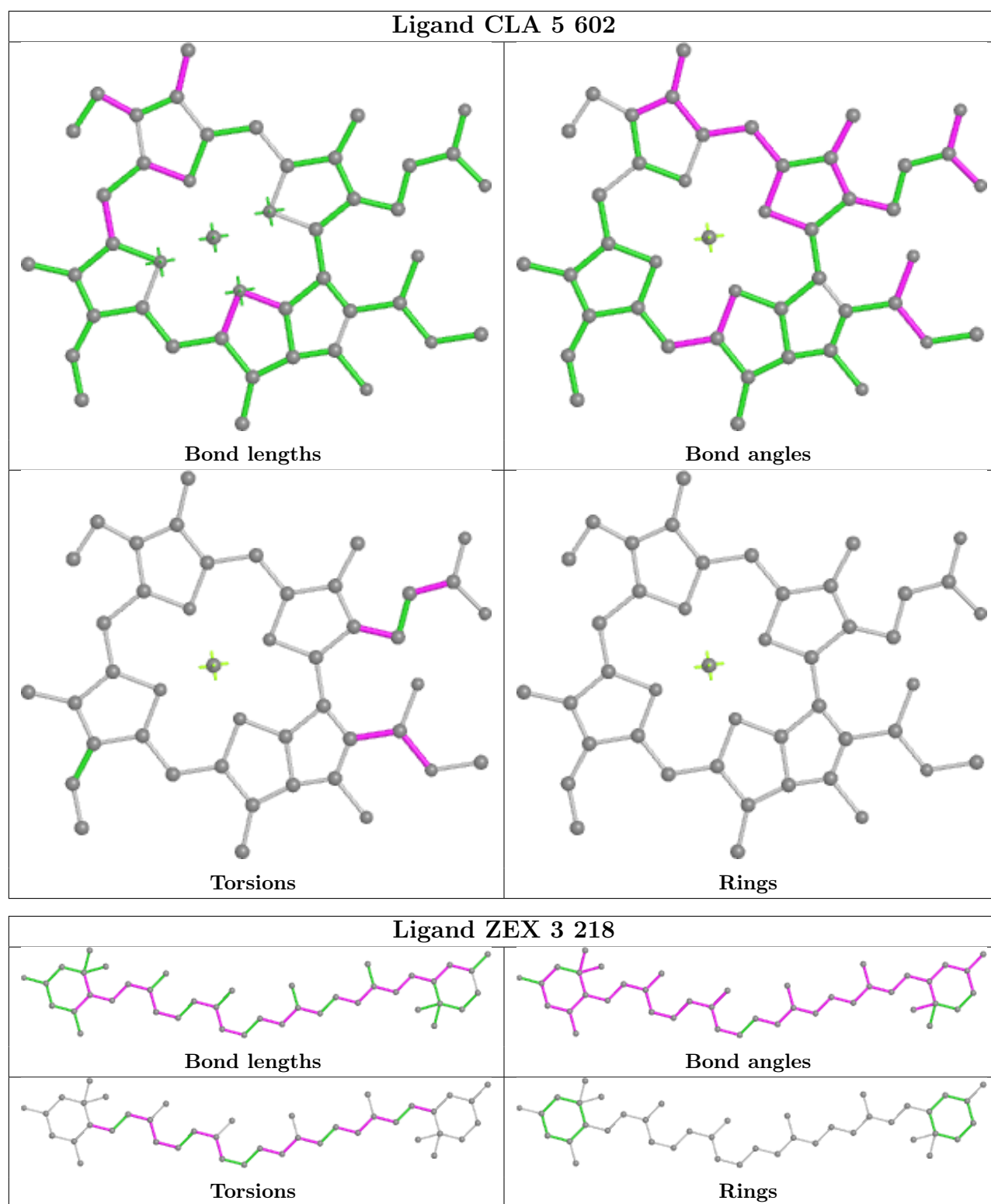


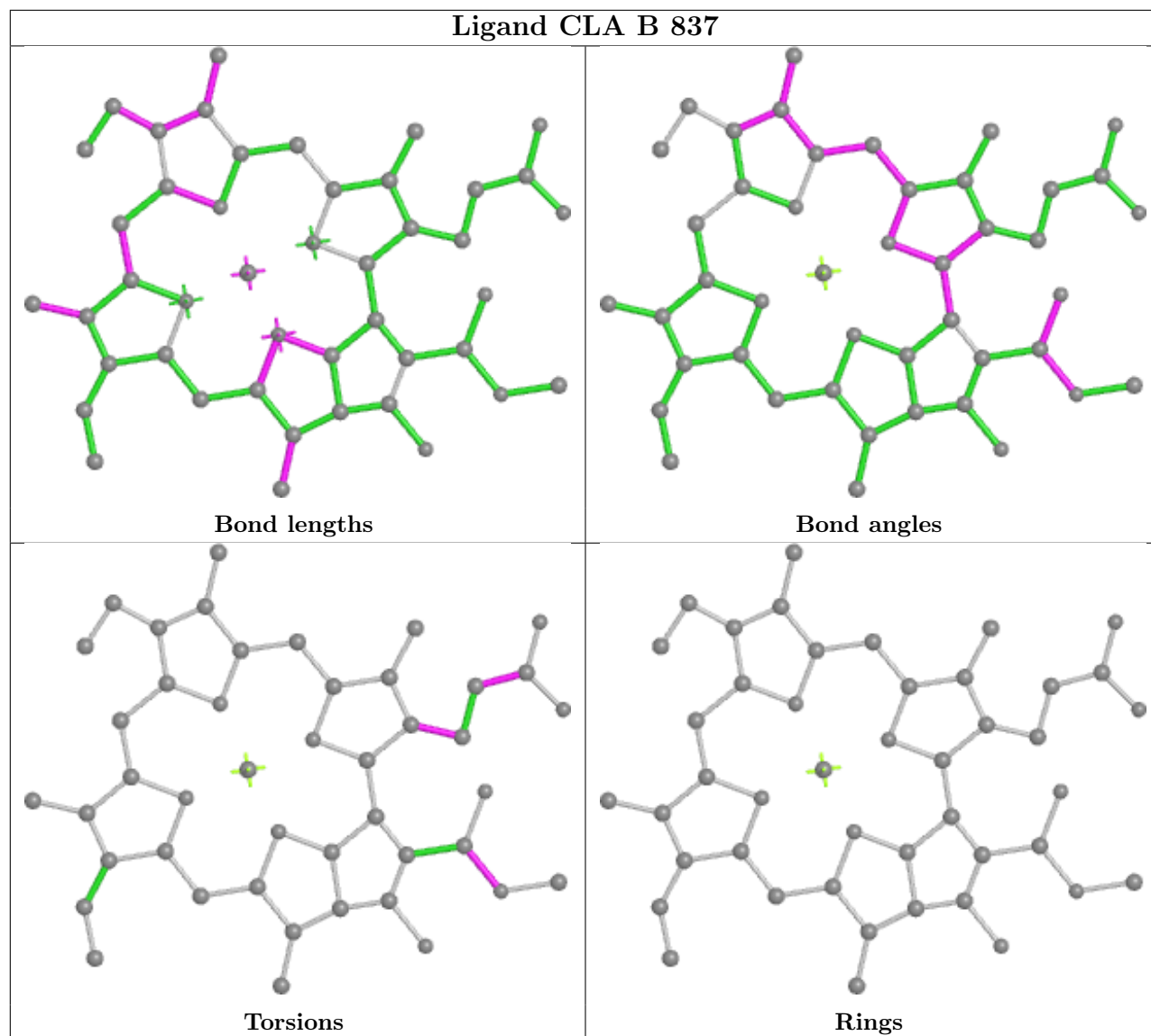
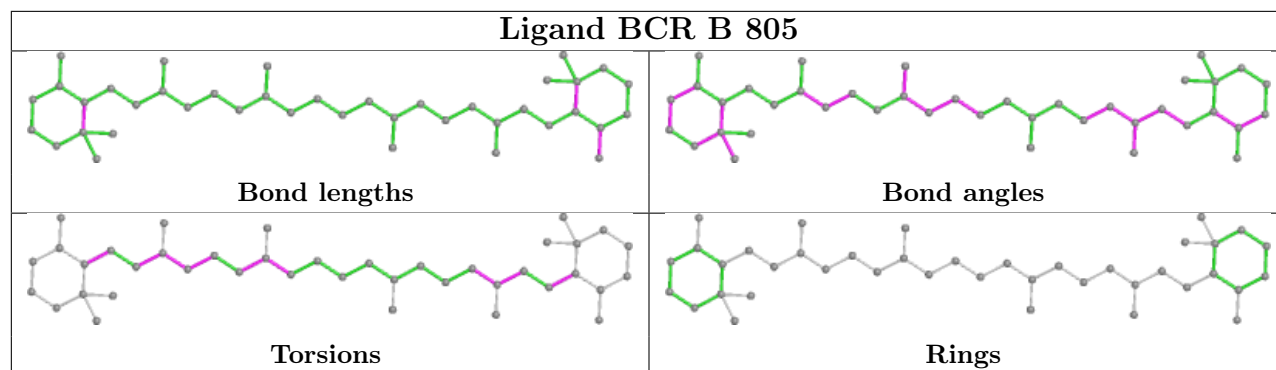












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

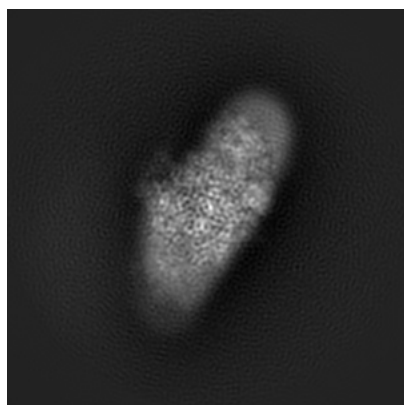
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6929. These allow visual inspection of the internal detail of the map and identification of artifacts.

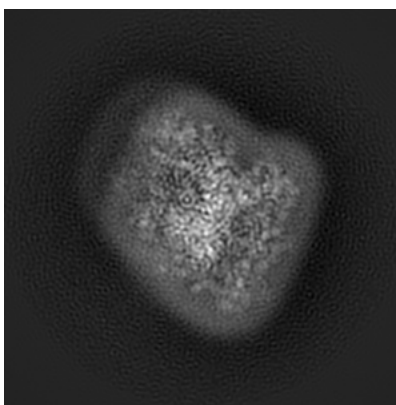
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

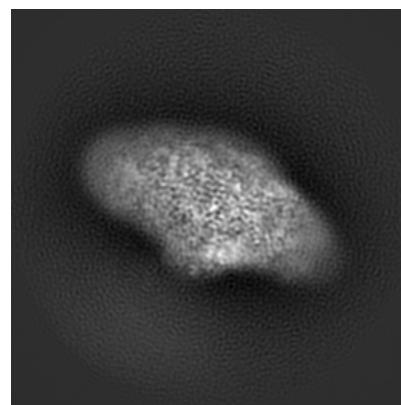
6.1.1 Primary map



X



Y

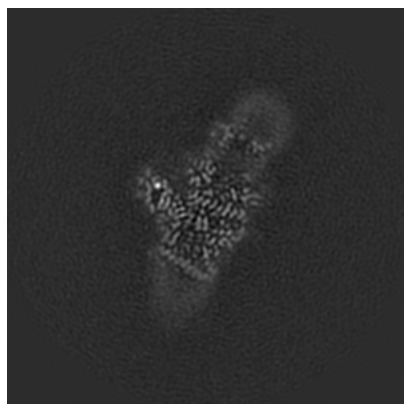


Z

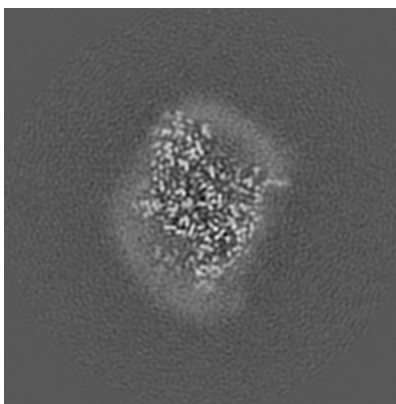
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

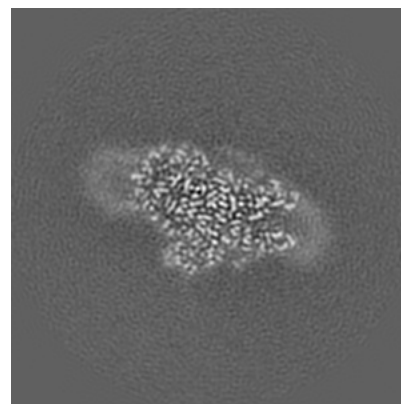
6.2.1 Primary map



X Index: 140



Y Index: 140

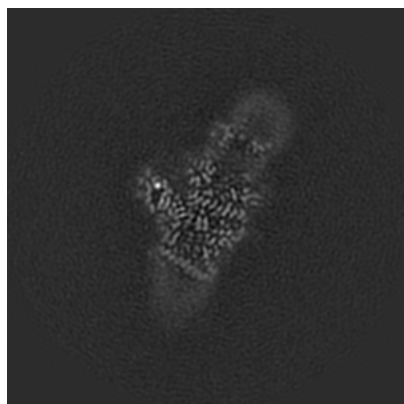


Z Index: 140

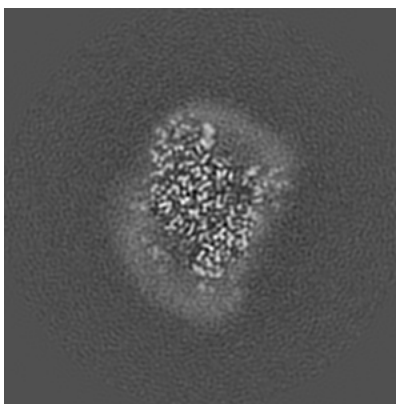
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

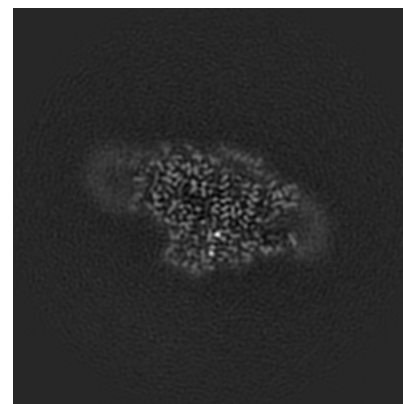
6.3.1 Primary map



X Index: 140



Y Index: 142



Z Index: 143

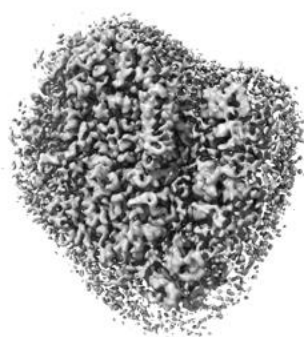
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0562. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

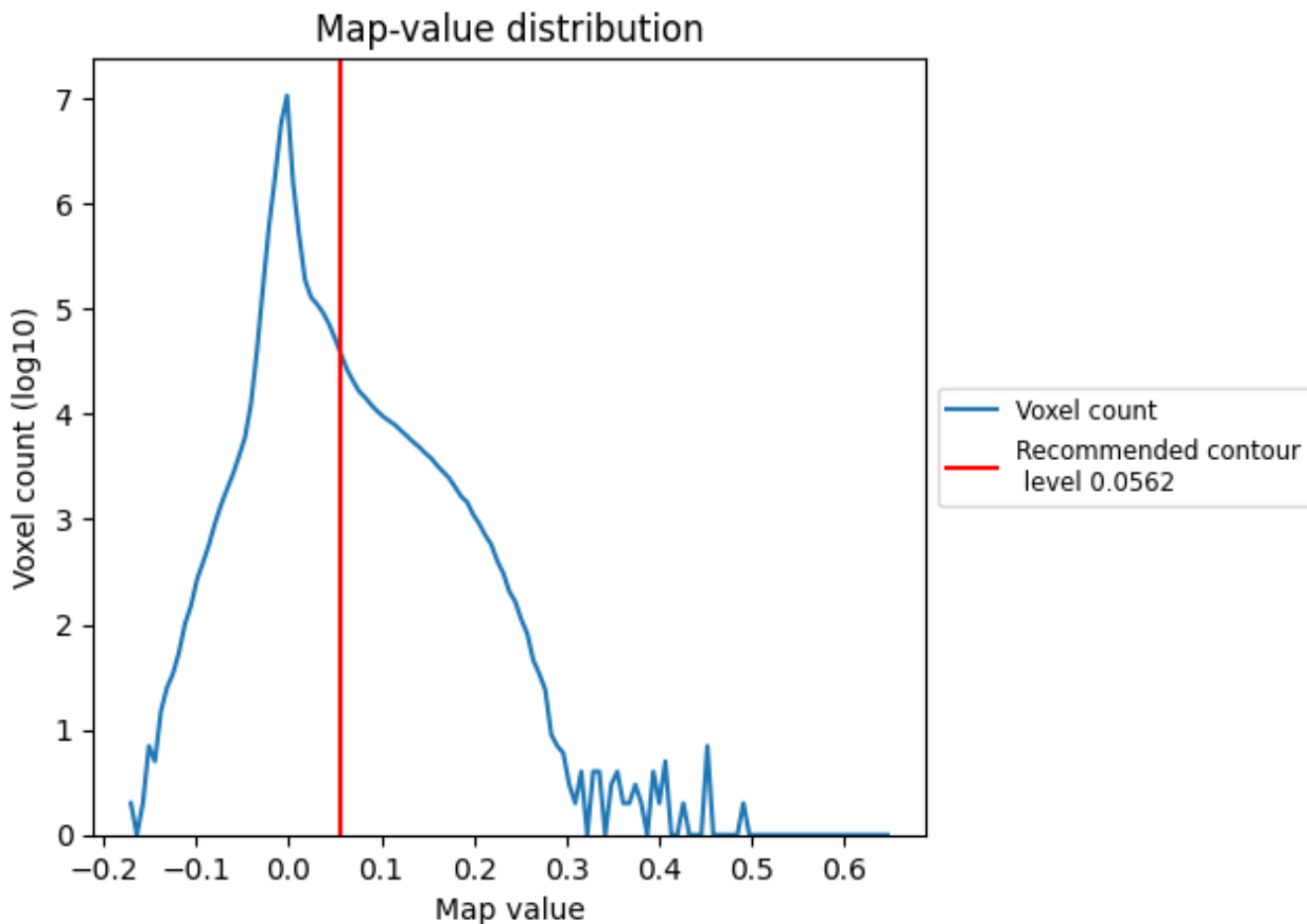
6.5 Mask visualisation

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

7 Map analysis [i](#)

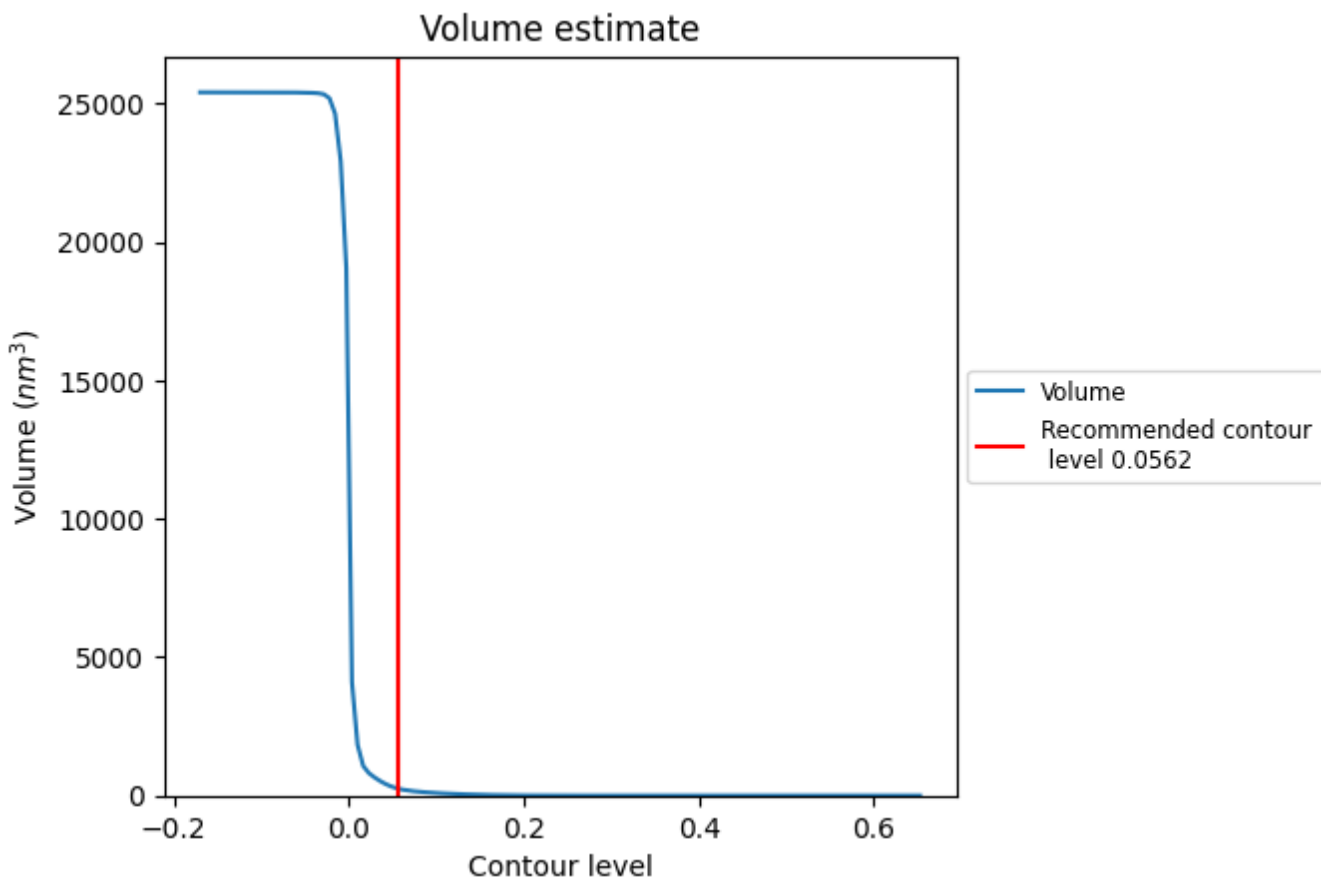
This section contains the results of statistical analysis of the map.

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.

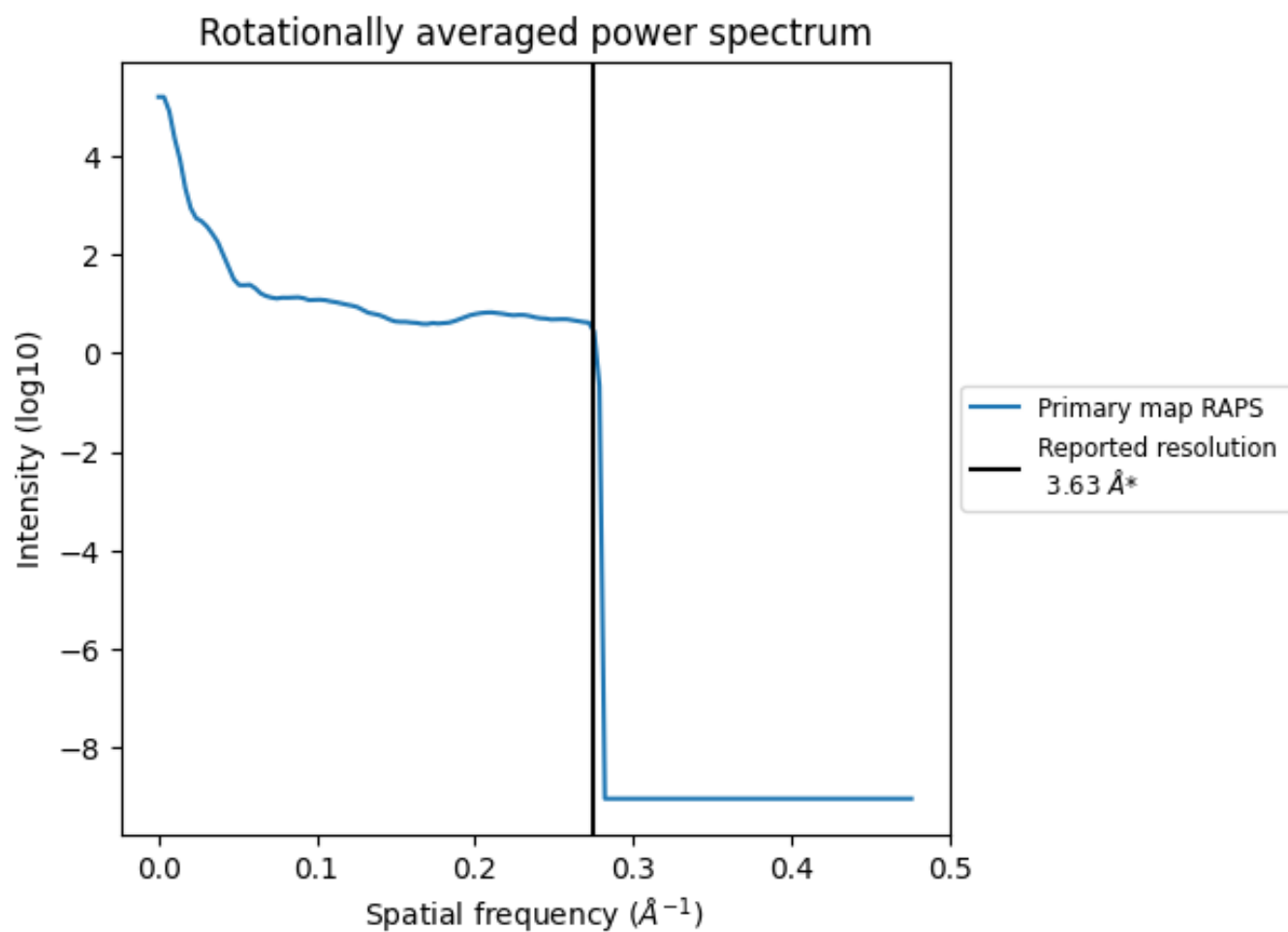
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 253 nm^3 ; this corresponds to an approximate mass of 228 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

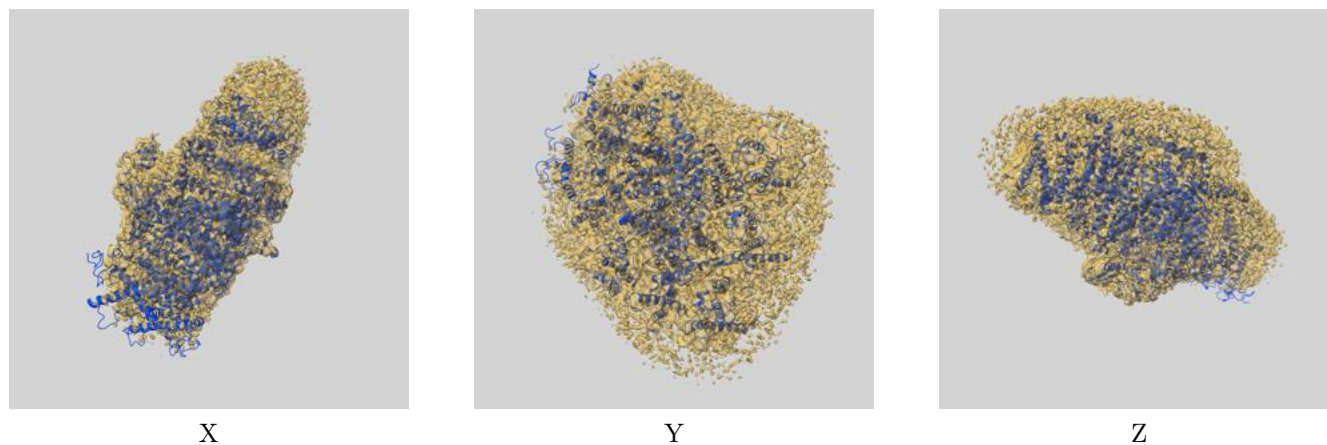
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

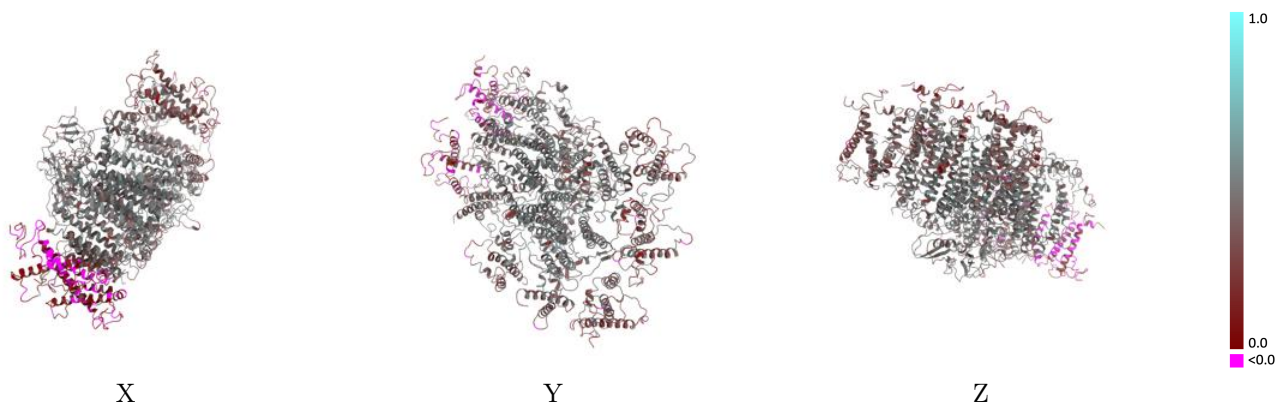
This section contains information regarding the fit between EMDB map EMD-6929 and PDB model 5ZGB. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



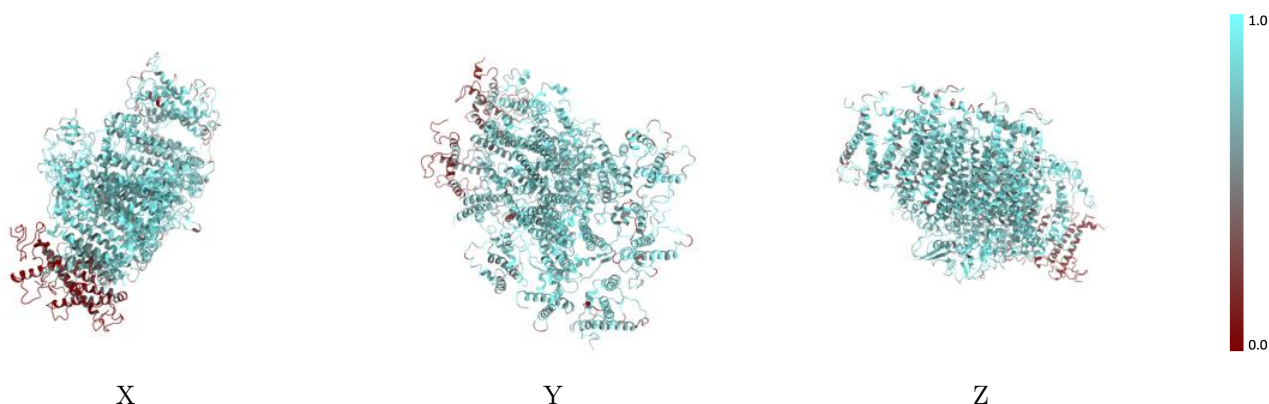
The images above show the 3D surface view of the map at the recommended contour level 0.0562 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



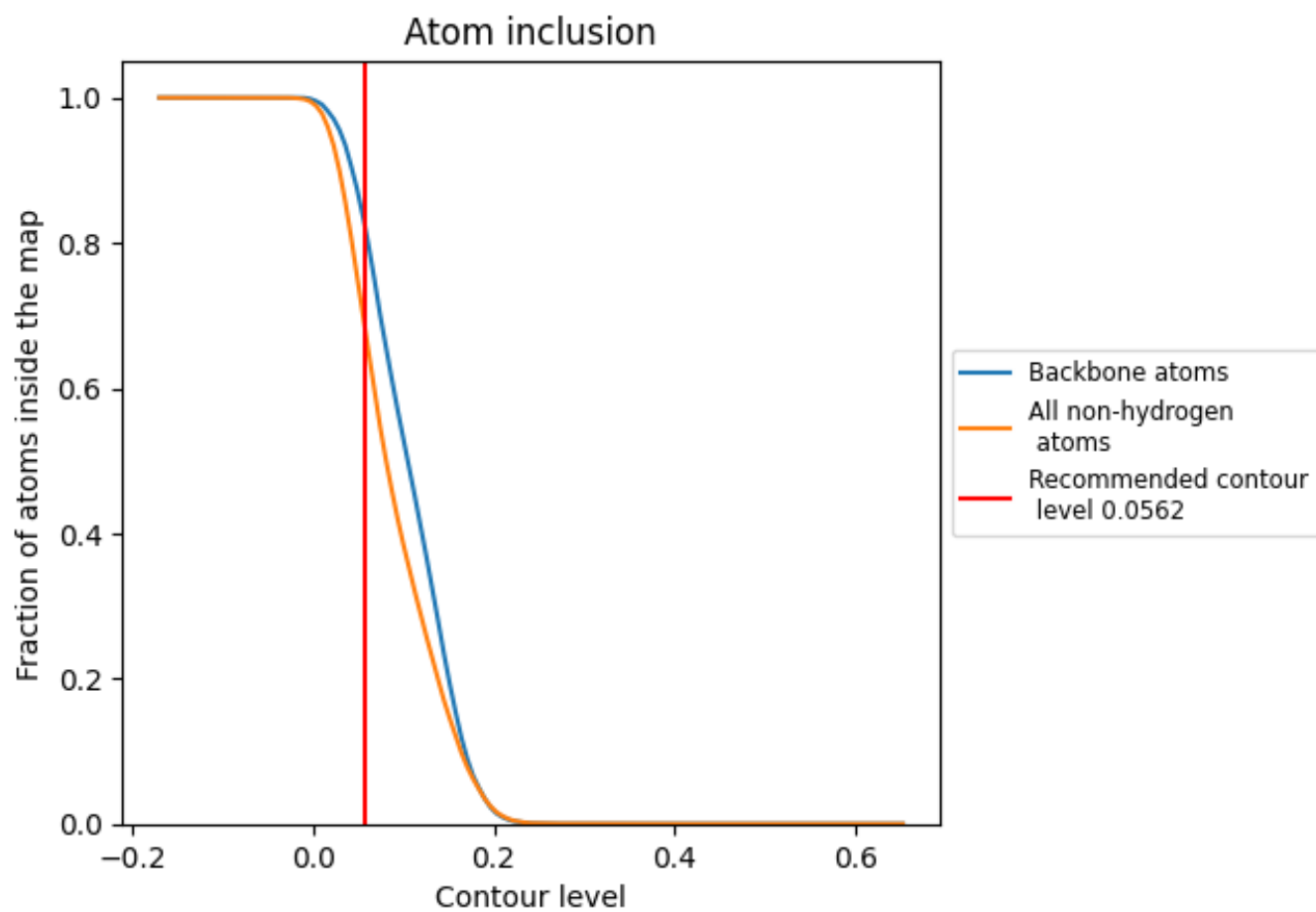
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0562).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.0562) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6923	 0.3990
1	 0.7125	 0.3420
2	 0.7002	 0.3450
3	 0.6951	 0.3520
4	 0.2513	 0.1760
5	 0.2331	 0.0920
A	 0.7893	 0.4840
B	 0.7743	 0.4690
C	 0.8664	 0.4550
D	 0.7656	 0.4340
E	 0.7588	 0.4220
F	 0.7559	 0.4220
I	 0.6877	 0.4310
J	 0.7204	 0.4820
K	 0.6954	 0.3850
L	 0.7080	 0.4100
M	 0.6453	 0.3860
O	 0.6726	 0.3670

