



Full wwPDB EM Validation Report ⓘ

Jul 2, 2026 – 01:58 pm BST

PDB ID : 9S6P / pdb_00009s6p
EMDB ID : EMD-54627
Title : Local refinement of a PSI monomer of *A. marina* NIES-2412
Authors : Consoli, G.; Leong, H.F.
Deposited on : 2025-08-01
Resolution : 2.44 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

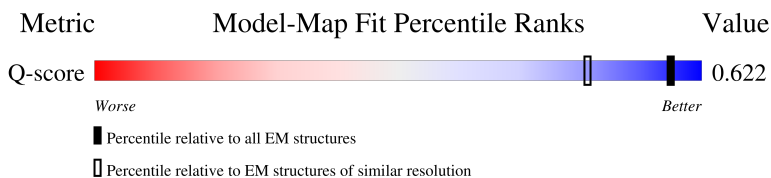
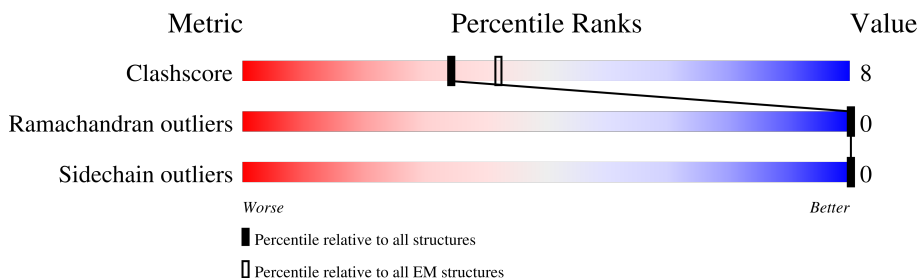
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.44 Å.

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




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5856 (1.94 - 2.94)

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	B	733	85% (green), 14% (yellow)
2	D	139	88% (green), 10% (yellow), 2% (grey)
3	E	86	6% (red), 72% (green), 7% (yellow), 15% (grey)
4	I	34	6% (red), 74% (green), 20% (yellow), 0% (grey)

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Mol	Chain	Length	Quality of chain
5	J	47	
6	K	86	
7	L	153	
8	M	31	
9	X	27	
10	A	753	
11	C	81	
12	F	167	

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
13	CL7	A	1012	X	-	-	-
13	CL7	A	1101	X	-	-	-
13	CL7	A	1102	X	-	-	-
13	CL7	A	1103	X	-	-	-
13	CL7	A	1104	X	-	-	-
13	CL7	A	1105	X	-	-	-
13	CL7	A	1106	X	-	-	-
13	CL7	A	1107	X	-	-	-
13	CL7	A	1108	X	-	-	-
13	CL7	A	1109	X	-	-	-
13	CL7	A	1110	X	-	-	-
13	CL7	A	1111	X	-	-	-
13	CL7	A	1112	X	-	-	-
13	CL7	A	1113	X	-	-	-
13	CL7	A	1114	X	-	-	-
13	CL7	A	1115	X	-	-	-
13	CL7	A	1116	X	-	-	-
13	CL7	A	1117	X	-	-	-
13	CL7	A	1118	X	-	-	-
13	CL7	A	1119	X	-	-	-
13	CL7	A	1120	X	-	-	-
13	CL7	A	1121	X	-	-	-
13	CL7	A	1122	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL7	A	1123	X	-	-	-
13	CL7	A	1124	X	-	-	-
13	CL7	A	1125	X	-	-	-
13	CL7	A	1126	X	-	-	-
13	CL7	A	1127	X	-	-	-
13	CL7	A	1128	X	-	-	-
13	CL7	A	1129	X	-	-	-
13	CL7	A	1130	X	-	-	-
13	CL7	A	1131	X	-	-	-
13	CL7	A	1132	X	-	-	-
13	CL7	A	1133	X	-	-	-
13	CL7	A	1134	X	-	-	-
13	CL7	A	1135	X	-	-	-
13	CL7	A	1136	X	-	-	-
13	CL7	A	1137	X	-	-	-
13	CL7	A	1138	X	-	-	-
13	CL7	A	1139	X	-	-	-
13	CL7	A	1140	X	-	-	-
13	CL7	A	1141	X	-	-	-
13	CL7	B	1021	X	-	-	-
13	CL7	B	1022	X	-	-	-
13	CL7	B	1201	X	-	-	-
13	CL7	B	1202	X	-	-	-
13	CL7	B	1203	X	-	-	-
13	CL7	B	1204	X	-	-	-
13	CL7	B	1205	X	-	-	-
13	CL7	B	1206	X	-	-	-
13	CL7	B	1207	X	-	-	-
13	CL7	B	1208	X	-	-	-
13	CL7	B	1209	X	-	-	-
13	CL7	B	1210	X	-	-	-
13	CL7	B	1211	X	-	-	-
13	CL7	B	1212	X	-	-	-
13	CL7	B	1213	X	-	-	-
13	CL7	B	1214	X	-	-	-
13	CL7	B	1215	X	-	-	-
13	CL7	B	1216	X	-	-	-
13	CL7	B	1217	X	-	-	-
13	CL7	B	1218	X	-	-	-
13	CL7	B	1219	X	-	-	-
13	CL7	B	1220	X	-	-	-
13	CL7	B	1221	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL7	B	1222	X	-	-	-
13	CL7	B	1223	X	-	-	-
13	CL7	B	1224	X	-	-	-
13	CL7	B	1225	X	-	-	-
13	CL7	B	1226	X	-	-	-
13	CL7	B	1227	X	-	-	-
13	CL7	B	1228	X	-	-	-
13	CL7	B	1229	X	-	-	-
13	CL7	B	1230	X	-	-	-
13	CL7	B	1231	X	-	-	-
13	CL7	B	1232	X	-	-	-
13	CL7	B	1233	X	-	-	-
13	CL7	B	1234	X	-	-	-
13	CL7	B	1235	X	-	-	-
13	CL7	B	1236	X	-	-	-
13	CL7	B	1237	X	-	-	-
13	CL7	B	1238	X	-	-	-
13	CL7	B	1239	X	-	-	-
13	CL7	B	1241	X	-	-	-
13	CL7	F	1701	X	-	-	-
13	CL7	I	1601	X	-	-	-
13	CL7	J	1301	X	-	-	-
13	CL7	J	1302	X	-	-	-
13	CL7	K	1401	X	-	-	-
13	CL7	K	1402	X	-	-	-
13	CL7	L	1501	X	-	-	-
13	CL7	L	1502	X	-	-	-
13	CL7	L	1503	X	-	-	-
20	G9R	A	1011	X	-	-	-

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 23856 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	730	5809	3819	965	1004	21	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	122	HIS	GLN	conflict	UNP A0AAT9GV97
B	240	THR	ALA	conflict	UNP A0AAT9GV97
B	247	SER	GLY	conflict	UNP A0AAT9GV97
B	258	VAL	MET	conflict	UNP A0AAT9GV97
B	318	GLU	GLN	conflict	UNP A0AAT9GV97
B	484	ALA	SER	conflict	UNP A0AAT9GV97
B	505	SER	ALA	conflict	UNP A0AAT9GV97
B	506	SER	ASN	conflict	UNP A0AAT9GV97

- Molecule 2 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	136	1039	653	180	202	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	76	ILE	THR	conflict	UNP A0AAT9GVK4
D	136	GLN	LYS	conflict	UNP A0AAT9GVK4

- Molecule 3 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	68	535	337	95	102	1	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	29	LYS	GLN	conflict	UNP A0AAT9GVJ0
E	73	ALA	GLY	conflict	UNP A0AAT9GVJ0
E	74	LYS	GLY	conflict	UNP A0AAT9GVJ0
E	75	ALA	LYS	conflict	UNP A0AAT9GVJ0
E	?	-	PRO	deletion	UNP A0AAT9GVJ0
E	?	-	ALA	deletion	UNP A0AAT9GVJ0
E	?	-	ALA	deletion	UNP A0AAT9GVJ0

- Molecule 4 is a protein called Psa27 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	33	250	167	36	44	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	J	35	291	207	40	44	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	2	PRO	LEU	conflict	UNP B0C7S6
J	3	GLN	LYS	conflict	UNP B0C7S6
J	9	GLY	ASP	conflict	UNP B0C7S6
J	22	PHE	LEU	conflict	UNP B0C7S6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	63	459	304	73	79	3	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	19	THR	ALA	conflict	UNP A0AAT9GVI7
K	30	MET	LEU	conflict	UNP A0AAT9GVI7
K	52	SER	ASN	conflict	UNP A0AAT9GVI7

- Molecule 7 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L	146	1040	665	174	194	7	0	0

- Molecule 8 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	31	223	148	34	40	1	0	0

- Molecule 9 is a protein called PsaX2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	X	27	211	146	33	32	0	0

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	A	737	5797	3785	989	991	32	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ASN	THR	conflict	UNP A0AAT9GVI9
A	367	CYS	VAL	conflict	UNP A0AAT9GVI9
A	516	MET	LEU	conflict	UNP A0AAT9GVI9
A	569	SER	ASN	conflict	UNP A0AAT9GVI9
A	622	THR	SER	conflict	UNP A0AAT9GVI9

- Molecule 11 is a protein called Photosystem I iron-sulfur center.

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

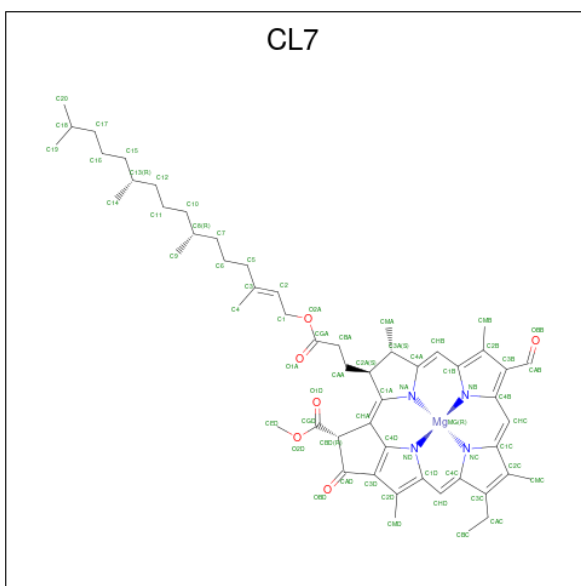
- Molecule 12 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	144	1067	672	189	202	4	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	9	VAL	LEU	conflict	UNP A0AAT9GVR1
F	11	LEU	MET	conflict	UNP A0AAT9GVR1
F	36	GLN	LYS	conflict	UNP A0AAT9GVR1
F	52	GLU	ASN	conflict	UNP A0AAT9GVR1
F	55	ARG	GLN	conflict	UNP A0AAT9GVR1
F	68	ALA	PRO	conflict	UNP A0AAT9GVR1
F	69	ASP	GLU	conflict	UNP A0AAT9GVR1
F	144	LEU	VAL	conflict	UNP A0AAT9GVR1

- Molecule 13 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	B	1	65	54	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	50	39	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	45	34	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	45	34	1	4	6	0
13	B	1	45	34	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	55	44	1	4	6	0
13	B	1	55	44	1	4	6	0
13	B	1	41	32	1	4	4	0
13	B	1	41	32	1	4	4	0
13	B	1	41	32	1	4	4	0
13	B	1	45	34	1	4	6	0
13	B	1	60	49	1	4	6	0
13	B	1	50	39	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	56	45	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	B	1	65	54	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	60	49	1	4	6	0
13	B	1	45	34	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	41	32	1	4	4	0
13	B	1	60	49	1	4	6	0
13	B	1	41	32	1	4	4	0
13	B	1	41	32	1	4	4	0
13	B	1	50	39	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	45	34	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	65	54	1	4	6	0
13	B	1	65	54	1	4	6	0
13	I	1	65	54	1	4	6	0
13	J	1	41	32	1	4	4	0
13	J	1	42	33	1	4	4	0
13	K	1	45	34	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	K	1	Total 37	C 30	Mg 1	N 4	O 2	0
13	L	1	Total 60	C 49	Mg 1	N 4	O 6	0
13	L	1	Total 65	C 54	Mg 1	N 4	O 6	0
13	L	1	Total 42	C 33	Mg 1	N 4	O 4	0
13	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
13	A	1	Total 41	C 32	Mg 1	N 4	O 4	0
13	A	1	Total 52	C 41	Mg 1	N 4	O 6	0
13	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
13	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
13	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
13	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
13	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
13	A	1	Total 51	C 40	Mg 1	N 4	O 6	0
13	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
13	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
13	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
13	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
13	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
13	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
13	A	1	Total 41	C 32	Mg 1	N 4	O 4	0
13	A	1	Total 65	C 54	Mg 1	N 4	O 6	0

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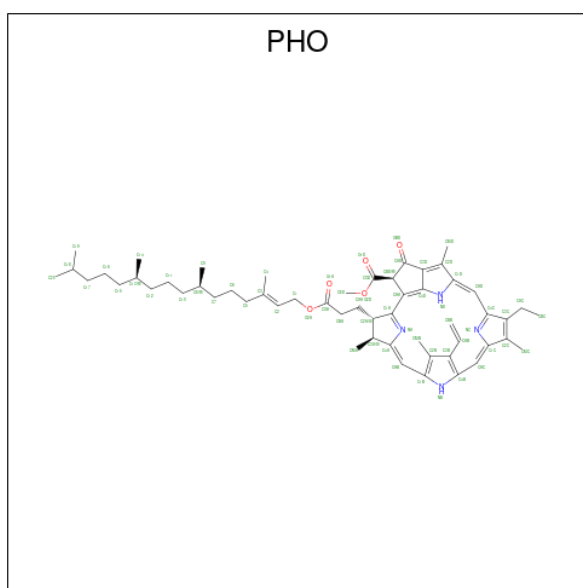
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	A	1	65	54	1	4	6	0
13	A	1	55	44	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	45	34	1	4	6	0
13	A	1	55	44	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	57	46	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	50	39	1	4	6	0
13	A	1	51	40	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	44	33	1	4	6	0
13	A	1	50	39	1	4	6	0
13	A	1	65	54	1	4	6	0
13	A	1	55	44	1	4	6	0

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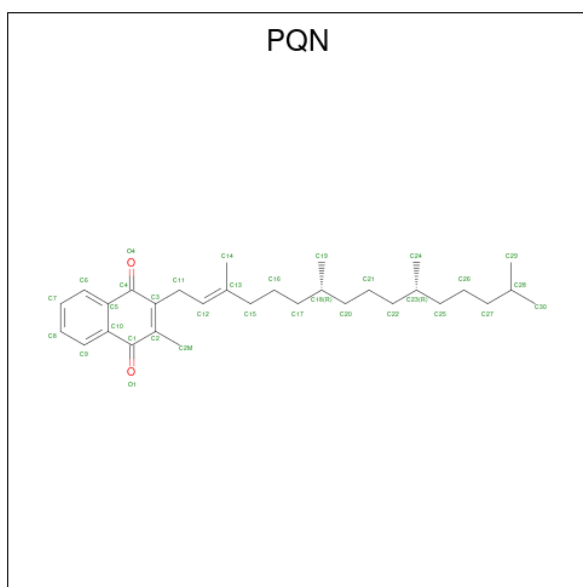
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	A	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
13	F	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

- Molecule 14 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



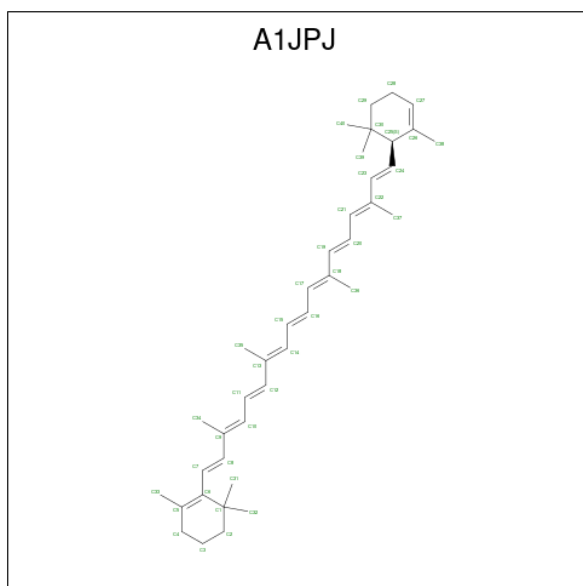
Mol	Chain	Residues	Atoms				AltConf
14	B	1	Total	C	N	O	0
			64	55	4	5	
14	A	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 16 is (6'S)-beta,epsilon-carotene (CCD ID: A1JPJ) (formula: C₄₀H₅₆).



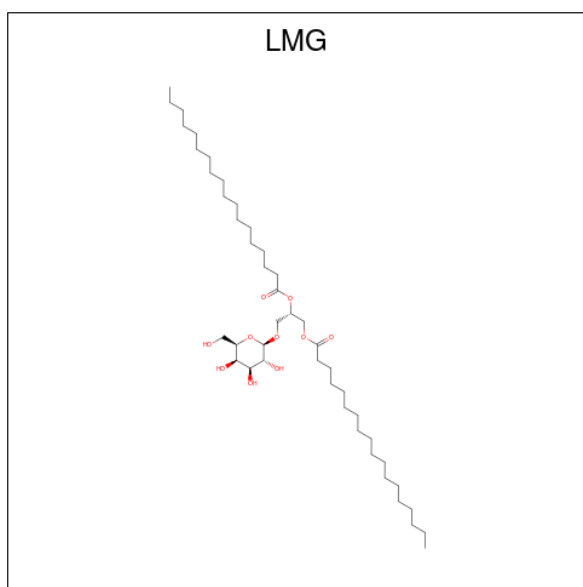
Mol	Chain	Residues	Atoms		AltConf
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	

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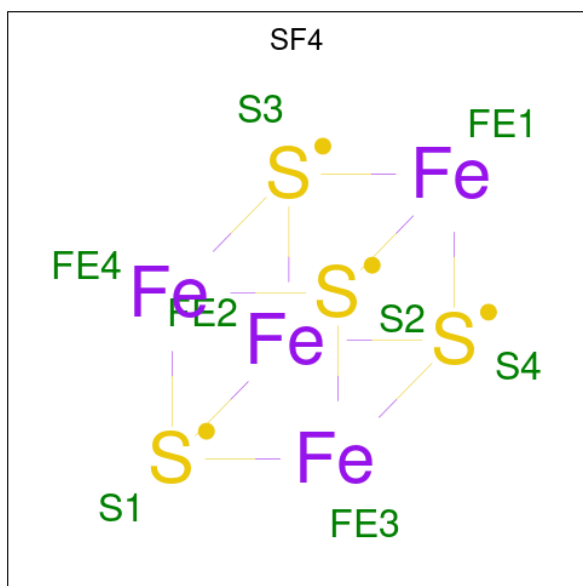
Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C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

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



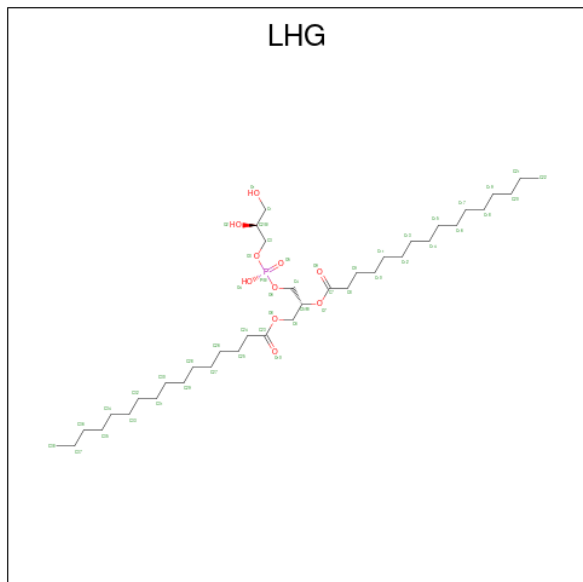
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	B	1	55	45	10	0

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



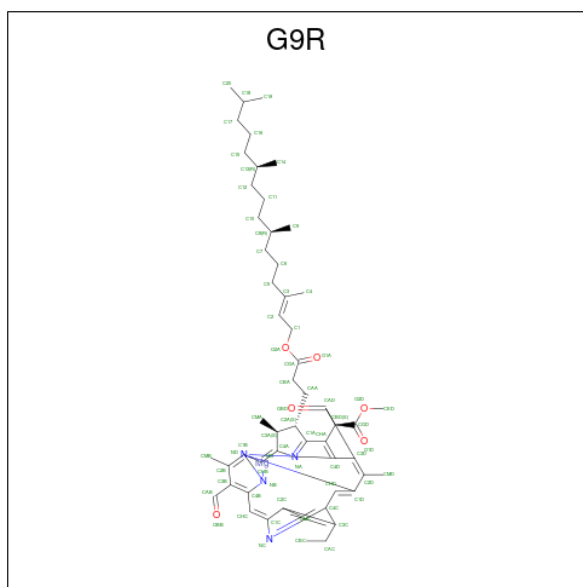
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	B	1	8	4	4	0
18	C	1	8	4	4	0
18	C	1	8	4	4	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	A	1	49	38	10	1	0
19	A	1	38	27	10	1	0

- Molecule 20 is CHLOROPHYLL D ISOMER (CCD ID: G9R) (formula: $C_{54}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
20	A	1	65	54	1	4	6	0

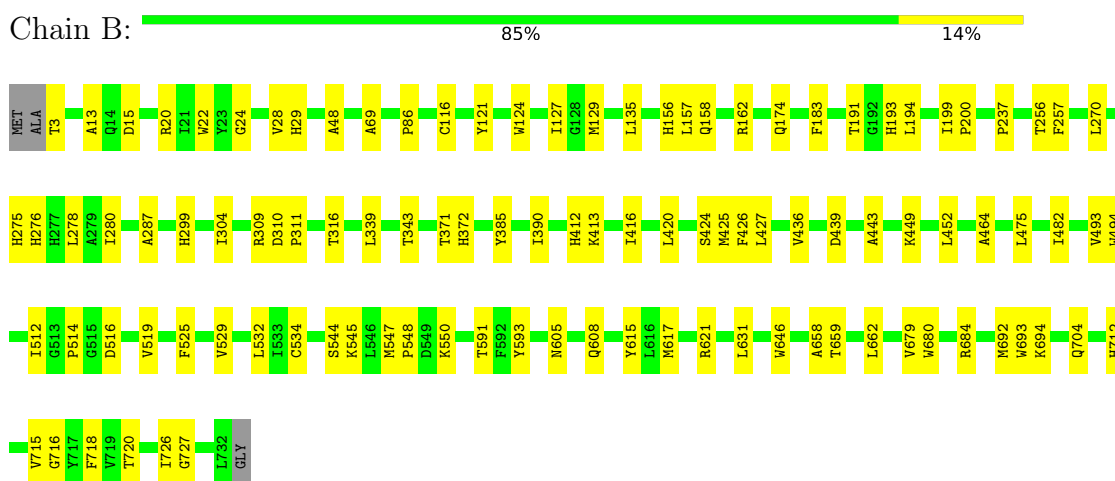
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	B	11	Total 11	O 11	0
21	B	1	Total 1	O 1	0
21	B	2	Total 2	O 2	0
21	I	2	Total 2	O 2	0
21	J	1	Total 1	O 1	0
21	L	2	Total 2	O 2	0
21	A	1	Total 1	O 1	0
21	A	18	Total 18	O 18	0
21	A	1	Total 1	O 1	0

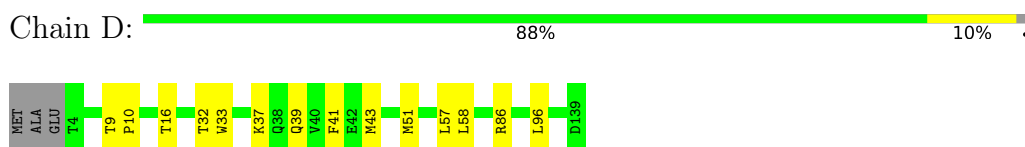
3 Residue-property plots

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

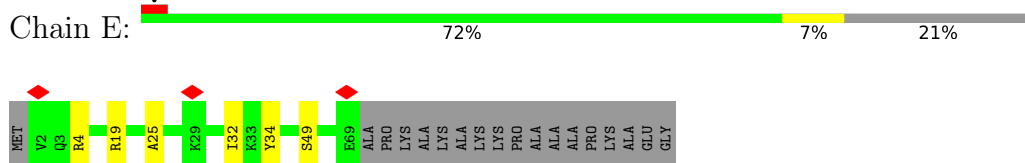
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I reaction center subunit II

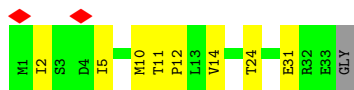


- Molecule 3: Photosystem I reaction center subunit IV

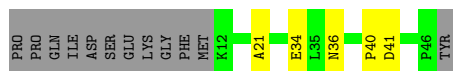


- Molecule 4: Psa27 protein





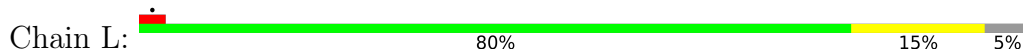
• Molecule 5: Photosystem I reaction center subunit IX



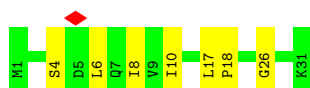
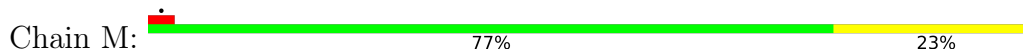
• Molecule 6: Photosystem I reaction center subunit PsaK



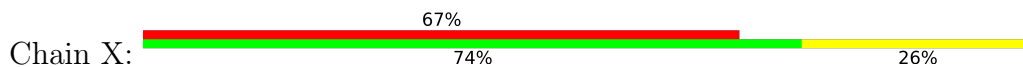
• Molecule 7: PsaL



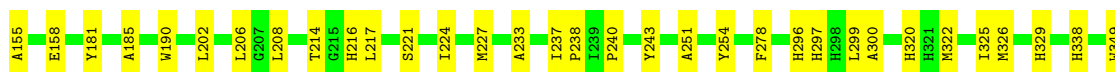
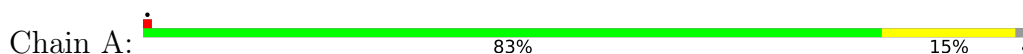
• Molecule 8: PsaM

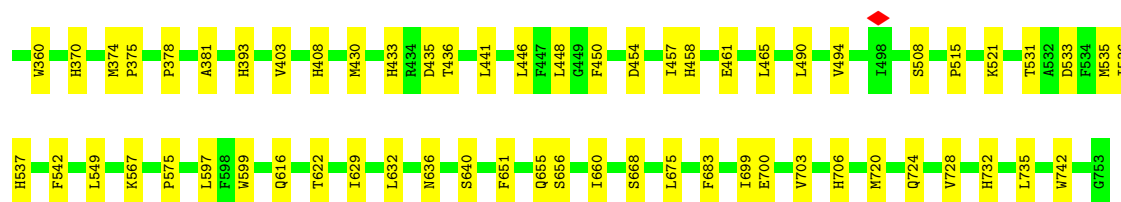


• Molecule 9: PsaX2



• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1





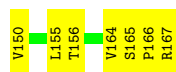
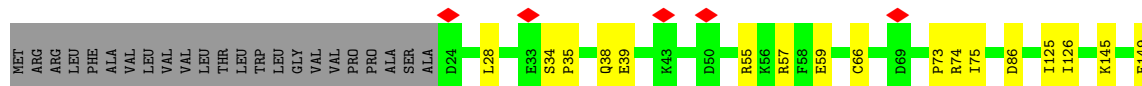
- Molecule 11: Photosystem I iron-sulfur center

Chain C: 94% 5%



- Molecule 12: Photosystem I reaction center subunit III

Chain F: 72% 14% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151833	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.634	Depositor
Minimum map value	-0.505	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	634.8, 634.8, 634.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	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: G9R, LHG, SF4, PHO, PQN, CL7, A1JPJ, LMG

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	B	0.18	0/6025	0.33	0/8244
2	D	0.18	0/1058	0.32	0/1428
3	E	0.12	0/545	0.32	0/737
4	I	0.16	0/255	0.32	0/346
5	J	0.12	0/303	0.30	0/412
6	K	0.14	0/469	0.34	0/640
7	L	0.17	0/1064	0.34	0/1448
8	M	0.16	0/223	0.29	0/304
9	X	0.17	0/219	0.34	0/303
10	A	0.18	0/5993	0.31	0/8165
11	C	0.18	0/609	0.33	0/825
12	F	0.14	0/1089	0.33	0/1478
All	All	0.17	0/17852	0.32	0/24330

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5809	0	5541	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1039	0	1043	10	0
3	E	535	0	524	4	0
4	I	250	0	260	6	0
5	J	291	0	289	4	0
6	K	459	0	470	6	0
7	L	1040	0	1047	17	0
8	M	223	0	259	4	0
9	X	211	0	225	4	0
10	A	5797	0	5623	91	0
11	C	599	0	577	2	0
12	F	1067	0	1076	19	0
13	A	2428	0	2328	106	0
13	B	2366	0	2219	95	0
13	F	41	0	27	0	0
13	I	65	0	70	2	0
13	J	83	0	55	4	0
13	K	82	0	54	0	0
13	L	167	0	156	4	0
14	A	64	0	74	3	0
14	B	64	0	74	10	0
15	A	33	0	46	0	0
15	B	33	0	46	0	0
16	A	240	0	0	0	0
16	B	320	0	0	1	0
16	F	40	0	0	0	0
16	I	40	0	0	0	0
16	J	80	0	0	1	0
16	L	120	0	0	0	0
17	B	55	0	86	3	0
18	B	8	0	0	0	0
18	C	16	0	0	0	0
19	A	87	0	123	3	0
20	A	65	0	0	0	0
21	A	20	0	0	0	0
21	B	14	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	2	0	0	0	0
All	All	23856	0	22292	371	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (371) 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:B:412:HIS:NE2	13:B:1227:CL7:ND	2.34	0.75
10:A:278:PHE:HD1	13:A:1116:CL7:HMB2	1.54	0.72
1:B:257:PHE:HE2	1:B:494:TRP:HE3	1.39	0.70
2:D:39:GLN:HG3	2:D:51:MET:HE3	1.74	0.70
14:B:1023:PHO:HED3	14:B:1023:PHO:HBA2	1.75	0.68
1:B:257:PHE:CE2	1:B:494:TRP:HE3	2.12	0.68
13:A:1138:CL7:H203	13:A:1139:CL7:H52C	1.75	0.68
1:B:427:LEU:HB3	1:B:525:PHE:HB2	1.75	0.67
1:B:15:ASP:HB3	1:B:20:ARG:HB2	1.77	0.66
10:A:374:MET:HG2	10:A:508:SER:HB2	1.76	0.66
13:J:1301:CL7:HBC1	13:A:1138:CL7:H152	1.78	0.66
10:A:75:SER:OG	10:A:181:TYR:HB2	1.96	0.66
7:L:48:LEU:HG	7:L:52:MET:HE2	1.77	0.66
4:I:24:THR:HG23	7:L:95:LEU:HD21	1.78	0.64
13:A:1102:CL7:HBD	13:A:1109:CL7:H2	1.80	0.63
9:X:9:TRP:HB2	9:X:10:PRO:HD3	1.79	0.63
3:E:49:SER:HB3	10:A:575:PRO:HG3	1.81	0.63
10:A:83:ILE:HD11	13:A:1109:CL7:H141	1.80	0.62
1:B:237:PRO:HB3	1:B:256:THR:HG21	1.80	0.62
6:K:17:THR:HG22	6:K:19:THR:H	1.63	0.62
13:A:1119:CL7:H102	13:A:1119:CL7:HBC3	1.82	0.62
12:F:55:ARG:O	12:F:59:GLU:HG3	2.00	0.62
13:B:1227:CL7:H72C	13:B:1241:CL7:H2	1.81	0.62
1:B:69:ALA:HB2	1:B:135:LEU:HB2	1.81	0.61
13:L:1502:CL7:H43C	13:A:1130:CL7:H2	1.81	0.61
1:B:299:HIS:HB3	1:B:304:ILE:HD11	1.81	0.61
10:A:720:MET:HE1	10:A:728:VAL:HG21	1.83	0.60
10:A:214:THR:HG21	10:A:299:LEU:HB2	1.83	0.59
13:B:1227:CL7:H2	13:B:1227:CL7:H92C	1.83	0.59
13:B:1241:CL7:H171	13:B:1241:CL7:H43C	1.83	0.59
12:F:75:ILE:HG23	12:F:86:ASP:HB3	1.85	0.59
13:B:1214:CL7:H93C	13:B:1231:CL7:H43C	1.82	0.59
1:B:692:MET:HB3	7:L:102:PRO:HG2	1.85	0.58
13:B:1220:CL7:HAB	13:B:1241:CL7:HBA1	1.85	0.58
10:A:217:LEU:HA	10:A:221:SER:HB3	1.85	0.58
10:A:320:HIS:NE2	13:A:1120:CL7:ND	2.51	0.58
13:A:1137:CL7:H93C	13:A:1137:CL7:H2	1.85	0.58
2:D:9:THR:HG23	7:L:13:PHE:HE2	1.68	0.58
13:B:1204:CL7:HBD	13:B:1204:CL7:HBA2	1.86	0.57
10:A:116:HIS:HD1	10:A:138:ILE:HD12	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1112:CL7:H2	13:A:1114:CL7:HMB2	1.87	0.57
10:A:227:MET:HE1	10:A:238:PRO:HD2	1.85	0.57
2:D:86:ARG:HB2	2:D:96:LEU:HD11	1.87	0.57
10:A:441:LEU:HD13	10:A:549:LEU:HA	1.87	0.57
10:A:224:ILE:HD11	10:A:240:PRO:HG3	1.87	0.57
10:A:71:ARG:HG2	10:A:185:ALA:HB1	1.87	0.56
12:F:155:LEU:HG	12:F:156:THR:HG23	1.86	0.56
13:A:1103:CL7:H62C	13:A:1111:CL7:H12C	1.88	0.56
10:A:403:VAL:HG11	10:A:597:LEU:HG	1.88	0.56
1:B:694:LYS:HG3	7:L:99:LEU:HD13	1.87	0.55
13:B:1216:CL7:H2	13:B:1221:CL7:H111	1.87	0.55
13:A:1125:CL7:HED1	13:A:1133:CL7:HAB	1.88	0.55
13:B:1227:CL7:H12C	13:B:1241:CL7:HED2	1.89	0.55
10:A:531:THR:O	10:A:535:MET:HG3	2.07	0.55
13:A:1124:CL7:HAA1	13:A:1125:CL7:OBD	2.07	0.55
13:B:1203:CL7:H202	17:B:8002:LMG:H451	1.87	0.55
14:B:1023:PHO:O1A	10:A:446:LEU:HD23	2.07	0.55
10:A:616:GLN:HB2	10:A:632:LEU:HB2	1.88	0.55
10:A:278:PHE:HZ	13:A:1116:CL7:H43C	1.72	0.54
10:A:322:MET:O	10:A:326:MET:HG3	2.06	0.54
2:D:10:PRO:HG2	2:D:58:LEU:HD23	1.89	0.54
1:B:605:ASN:HB3	1:B:608:GLN:HG2	1.88	0.54
10:A:300:ALA:HB1	13:A:1115:CL7:HBC2	1.88	0.54
12:F:145:LYS:O	12:F:149:GLU:HG3	2.07	0.54
1:B:514:PRO:HG3	12:F:74:ARG:HH12	1.71	0.54
13:J:1301:CL7:HAC2	13:A:1138:CL7:H121	1.89	0.54
10:A:208:LEU:HD11	13:A:1118:CL7:HBC1	1.90	0.54
1:B:174:GLN:HB2	13:B:1210:CL7:HBC2	1.89	0.54
1:B:482:ILE:HD13	9:X:31:ILE:HB	1.90	0.54
1:B:659:THR:HA	14:B:1023:PHO:HAB	1.90	0.54
10:A:408:HIS:CE1	13:A:1128:CL7:NA	2.76	0.53
1:B:545:LYS:HB2	10:A:700:GLU:CD	2.33	0.53
1:B:658:ALA:HB1	14:B:1023:PHO:HBB2	1.90	0.53
13:B:1206:CL7:HMC2	10:A:465:LEU:HG	1.90	0.53
1:B:621:ARG:HG3	10:A:660:ILE:HD12	1.90	0.53
11:C:15:THR:HG22	11:C:28:MET:HE2	1.91	0.53
10:A:84:VAL:HG11	13:A:1103:CL7:H72C	1.90	0.53
1:B:658:ALA:CB	14:B:1023:PHO:HBB2	2.38	0.53
7:L:93:MET:HE1	7:L:130:PHE:HB3	1.91	0.52
14:B:1023:PHO:C1D	10:A:599:TRP:HE1	2.23	0.52
10:A:190:TRP:CE2	13:A:1111:CL7:HBC3	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:448:LEU:HB3	10:A:542:PHE:HB2	1.91	0.52
1:B:439:ASP:OD1	1:B:615:TYR:HB2	2.10	0.52
10:A:430:MET:HA	10:A:433:HIS:CE1	2.45	0.52
1:B:412:HIS:HD1	1:B:416:ILE:HG13	1.75	0.52
10:A:360:TRP:HE1	13:A:1104:CL7:HAB	1.75	0.52
1:B:183:PHE:CZ	13:B:1210:CL7:H61C	2.44	0.52
13:B:1228:CL7:HMB2	13:A:1138:CL7:HAA1	1.92	0.52
7:L:19:THR:HG21	13:A:1130:CL7:OBD	2.09	0.52
1:B:29:HIS:NE2	13:B:1201:CL7:NB	2.57	0.52
1:B:385:TYR:CG	1:B:534:CYS:HB3	2.45	0.52
4:I:2:ILE:HA	4:I:5:ILE:HG22	1.93	0.51
13:B:1201:CL7:HBC3	13:B:1226:CL7:H41C	1.93	0.51
1:B:680:TRP:CE2	1:B:684:ARG:HG3	2.46	0.51
10:A:216:HIS:CE1	13:A:1112:CL7:NA	2.79	0.51
10:A:149:ARG:HD3	10:A:378:PRO:HG2	1.93	0.51
19:A:853:LHG:H251	19:A:853:LHG:H121	1.91	0.51
10:A:490:LEU:O	10:A:494:VAL:HB	2.11	0.51
12:F:125:ILE:HG13	12:F:126:ILE:HG12	1.93	0.51
7:L:19:THR:HG22	7:L:21:VAL:H	1.76	0.51
13:L:1502:CL7:H191	13:A:1136:CL7:H101	1.93	0.51
1:B:276:HIS:CE1	13:B:1214:CL7:ND	2.79	0.50
10:A:683:PHE:HA	14:A:1013:PHO:HAB	1.93	0.50
13:A:1128:CL7:O1D	13:A:1128:CL7:H2A	2.12	0.50
1:B:129:MET:HE2	13:B:1211:CL7:HMA2	1.93	0.50
13:B:1021:CL7:H122	13:A:1126:CL7:H152	1.92	0.50
10:A:370:HIS:CE1	13:A:1125:CL7:NB	2.80	0.50
10:A:706:HIS:CE1	13:A:1138:CL7:ND	2.80	0.50
1:B:275:HIS:HB3	13:B:1214:CL7:HMB2	1.93	0.50
1:B:547:MET:HE2	1:B:550:LYS:HA	1.94	0.49
1:B:194:LEU:O	1:B:199:ILE:HG12	2.12	0.49
1:B:193:HIS:CE1	13:B:1211:CL7:NA	2.81	0.49
1:B:257:PHE:HD2	1:B:493:VAL:HG23	1.77	0.49
10:A:326:MET:HE2	10:A:338:HIS:HB3	1.94	0.49
13:B:1204:CL7:H12C	4:I:14:VAL:HG21	1.93	0.49
10:A:95:ALA:HB2	10:A:144:LEU:HD21	1.95	0.49
1:B:191:THR:HG21	1:B:278:LEU:HB2	1.94	0.49
13:B:1225:CL7:H51C	16:B:4005:A1JPJ:C23	2.43	0.49
13:B:1229:CL7:O2D	13:B:1229:CL7:H2A	2.13	0.49
10:A:105:LEU:HD21	10:A:154:THR:HG22	1.93	0.49
1:B:199:ILE:HD13	1:B:270:LEU:HB3	1.95	0.49
7:L:43:ALA:HB1	7:L:126:ILE:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:LEU:HD13	1:B:727:GLY:HA3	1.94	0.49
10:A:393:HIS:CE1	13:A:1126:CL7:ND	2.80	0.49
10:A:521:LYS:HG2	10:A:622:THR:HG22	1.95	0.49
10:A:706:HIS:HE1	13:A:1138:CL7:ND	2.10	0.49
12:F:34:SER:O	12:F:38:GLN:HG2	2.13	0.49
1:B:617:MET:HB2	10:A:675:LEU:HD11	1.93	0.48
13:B:1203:CL7:H162	13:B:1203:CL7:H122	1.65	0.48
13:A:1134:CL7:H2A	13:A:1134:CL7:O2D	2.12	0.48
10:A:297:HIS:HB2	13:A:1116:CL7:CHB	2.42	0.48
1:B:424:SER:HB3	1:B:529:VAL:HG22	1.94	0.48
1:B:516:ASP:HA	1:B:519:VAL:HG12	1.96	0.48
13:B:1226:CL7:H2	17:B:8002:LMG:H312	1.94	0.48
10:A:458:HIS:CE1	13:A:1132:CL7:NA	2.82	0.48
1:B:309:ARG:HG3	1:B:316:THR:HG22	1.94	0.48
13:B:1201:CL7:H2A	13:B:1201:CL7:HED2	1.96	0.48
3:E:32:ILE:HG22	3:E:34:TYR:H	1.78	0.48
13:B:1204:CL7:HHB	13:B:1205:CL7:HMB3	1.94	0.48
10:A:240:PRO:HA	10:A:243:TYR:CE2	2.49	0.48
1:B:158:GLN:O	1:B:162:ARG:HG3	2.13	0.48
13:A:1123:CL7:H11C	13:A:1123:CL7:HBA2	1.57	0.48
10:A:329:HIS:HE2	13:A:1121:CL7:C4D	2.27	0.48
8:M:4:SER:O	8:M:8:ILE:HD12	2.14	0.47
13:A:1123:CL7:HMB3	13:A:1125:CL7:H92C	1.95	0.47
1:B:420:LEU:HD13	1:B:532:LEU:HA	1.96	0.47
1:B:716:GLY:O	1:B:720:THR:HG22	2.14	0.47
10:A:450:PHE:O	10:A:454:ASP:HB2	2.14	0.47
1:B:156:HIS:CE1	13:B:1208:CL7:NA	2.83	0.47
1:B:86:PRO:HB2	1:B:116:CYS:HB3	1.95	0.47
13:B:1021:CL7:H193	13:A:1126:CL7:H101	1.95	0.47
12:F:28:LEU:HD13	12:F:74:ARG:HD2	1.97	0.47
12:F:164:VAL:HB	12:F:167:ARG:HH22	1.79	0.47
1:B:287:ALA:HB2	13:B:1216:CL7:HBC2	1.96	0.47
13:A:1135:CL7:H2	13:A:1136:CL7:O1A	2.15	0.47
1:B:720:THR:HG23	13:B:1022:CL7:O1D	2.14	0.47
13:A:1106:CL7:HBA1	13:A:1106:CL7:H3A	1.34	0.47
12:F:66:CYS:HB3	12:F:73:PRO:HA	1.97	0.47
1:B:436:VAL:HG13	13:B:1021:CL7:H62C	1.97	0.47
13:B:1220:CL7:HED3	13:B:1220:CL7:H2A	1.97	0.47
10:A:142:SER:HA	13:A:1126:CL7:HMA2	1.95	0.47
13:B:1238:CL7:H2	13:B:1237:CL7:HMC1	1.97	0.47
13:B:1210:CL7:H3A	13:B:1210:CL7:HBA2	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:320:HIS:CE1	13:A:1120:CL7:NA	2.84	0.46
13:A:1127:CL7:H142	13:A:1127:CL7:H111	1.64	0.46
1:B:339:LEU:O	1:B:343:THR:HG22	2.15	0.46
13:B:1205:CL7:O1A	13:B:1224:CL7:HBD	2.16	0.46
10:A:320:HIS:HB3	10:A:325:ILE:HD11	1.98	0.46
13:I:1601:CL7:H91C	7:L:87:ILE:HG21	1.98	0.46
5:J:41:ASP:OD2	12:F:57:ARG:HD3	2.15	0.46
13:A:1137:CL7:H2	13:A:1137:CL7:H62C	1.57	0.46
1:B:412:HIS:NE2	13:B:1227:CL7:C4D	2.77	0.46
1:B:426:PHE:HA	13:B:1229:CL7:HED2	1.97	0.46
13:I:1601:CL7:H72C	13:I:1601:CL7:H111	1.52	0.46
13:B:1210:CL7:H2	13:B:1210:CL7:H62C	1.63	0.46
13:A:1137:CL7:H93C	13:A:1137:CL7:H62C	1.69	0.46
1:B:276:HIS:HB2	13:B:1214:CL7:C1B	2.46	0.46
14:B:1023:PHO:C1B	13:A:1012:CL7:HAB	2.46	0.46
10:A:742:TRP:HD1	13:A:1126:CL7:HMB2	1.81	0.46
13:B:1227:CL7:HMC1	13:B:1241:CL7:H42C	1.98	0.46
10:A:116:HIS:CD2	13:A:1106:CL7:NA	2.84	0.46
13:A:1106:CL7:H41C	13:A:1106:CL7:H62C	1.49	0.46
1:B:29:HIS:CE1	13:B:1201:CL7:NB	2.84	0.46
1:B:712:HIS:NE2	13:B:1239:CL7:NA	2.64	0.46
13:B:1212:CL7:H3A	13:B:1212:CL7:HBA1	1.67	0.46
6:K:32:ILE:HA	6:K:65:THR:HG21	1.98	0.46
1:B:449:LYS:HD2	13:B:1230:CL7:O1D	2.16	0.45
10:A:457:ILE:O	10:A:461:GLU:HG2	2.15	0.45
2:D:33:TRP:HZ2	2:D:51:MET:HG2	1.80	0.45
10:A:93:PHE:CG	13:A:1105:CL7:HBC3	2.52	0.45
10:A:408:HIS:HE1	13:A:1128:CL7:NA	2.14	0.45
13:B:1202:CL7:H43C	13:B:1203:CL7:HAB	1.98	0.45
10:A:699:ILE:O	10:A:703:VAL:HG13	2.16	0.45
13:A:1119:CL7:H41C	13:A:1119:CL7:H61C	1.71	0.45
13:A:1126:CL7:H172	13:A:1126:CL7:H13	1.62	0.45
1:B:452:LEU:O	12:F:74:ARG:HB2	2.16	0.45
1:B:548:PRO:HB3	12:F:166:PRO:HG3	1.98	0.45
13:L:1501:CL7:HBA1	13:L:1501:CL7:H3A	1.45	0.45
8:M:17:LEU:HB3	8:M:18:PRO:HD3	1.97	0.45
13:A:1127:CL7:H62C	13:A:1127:CL7:H102	1.34	0.45
5:J:34:GLU:HG3	13:J:1302:CL7:C1B	2.46	0.45
1:B:257:PHE:HE2	1:B:494:TRP:CE3	2.26	0.45
13:B:1227:CL7:H2	13:B:1227:CL7:H61C	1.66	0.45
13:B:1239:CL7:H101	13:B:1239:CL7:H62C	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1241:CL7:H102	13:B:1241:CL7:H13	1.66	0.45
13:B:1241:CL7:H3A	13:B:1241:CL7:HBA2	1.40	0.45
10:A:636:ASN:O	10:A:640:SER:HB2	2.17	0.45
13:A:1107:CL7:H192	13:A:1107:CL7:H162	1.75	0.45
1:B:413:LYS:HE2	12:F:167:ARG:HH21	1.82	0.44
13:B:1202:CL7:H152	13:B:1210:CL7:CAD	2.47	0.44
13:B:1021:CL7:H102	13:A:1126:CL7:H152	1.99	0.44
10:A:515:PRO:HG3	10:A:629:ILE:HD11	1.98	0.44
10:A:732:HIS:NE2	13:A:1140:CL7:NA	2.64	0.44
1:B:372:HIS:CE1	13:B:1224:CL7:ND	2.86	0.44
10:A:233:ALA:O	10:A:237:ILE:HG12	2.18	0.44
10:A:25:SER:H	13:A:1109:CL7:HMA3	1.83	0.44
13:A:1106:CL7:CHC	13:A:1107:CL7:HMD2	2.46	0.44
13:B:1213:CL7:HBA1	13:B:1213:CL7:H3A	1.44	0.44
5:J:21:ALA:HA	13:A:1139:CL7:H42C	2.00	0.44
6:K:58:SER:O	6:K:62:VAL:HG23	2.18	0.44
13:A:1119:CL7:HBA2	13:A:1123:CL7:HAB	2.00	0.44
13:A:1127:CL7:H3A	13:A:1127:CL7:HBA2	1.31	0.44
6:K:57:PHE:CE2	6:K:62:VAL:HG22	2.52	0.44
9:X:15:ILE:O	9:X:19:ILE:HG12	2.18	0.44
13:A:1138:CL7:H192	13:A:1138:CL7:H161	1.75	0.44
1:B:3:THR:HG21	1:B:20:ARG:CZ	2.48	0.44
1:B:512:ILE:HA	1:B:516:ASP:OD2	2.18	0.44
13:B:1220:CL7:HBA1	13:B:1220:CL7:H3A	1.40	0.44
13:B:1236:CL7:HBA1	13:B:1241:CL7:H143	2.00	0.44
10:A:537:HIS:CG	13:A:1136:CL7:HED3	2.53	0.44
13:A:1103:CL7:H3A	13:A:1103:CL7:HBA2	1.48	0.44
13:A:1127:CL7:H62C	13:A:1127:CL7:H41C	1.61	0.44
13:B:1211:CL7:H62C	13:B:1211:CL7:H2	1.78	0.44
13:B:1238:CL7:ND	13:B:1237:CL7:HMC2	2.33	0.44
2:D:41:PHE:CD1	2:D:51:MET:HG3	2.52	0.44
1:B:390:ILE:HG21	13:B:1226:CL7:HED1	2.00	0.44
1:B:464:ALA:HB1	1:B:475:LEU:HD12	2.00	0.44
1:B:519:VAL:HG21	1:B:593:TYR:HB2	2.00	0.44
7:L:89:LEU:O	7:L:93:MET:HG3	2.18	0.44
13:A:1116:CL7:H3A	13:A:1116:CL7:HBA1	1.31	0.44
13:B:1215:CL7:H8	13:B:1215:CL7:HAB	1.99	0.44
13:B:1229:CL7:H2	13:B:1229:CL7:H8	1.99	0.44
10:A:742:TRP:CD1	13:A:1126:CL7:HMB2	2.52	0.44
13:A:1102:CL7:HBD	13:A:1102:CL7:HED3	1.72	0.44
13:A:1103:CL7:H143	13:A:1103:CL7:H161	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:HIS:O	1:B:280:ILE:HG12	2.18	0.43
13:B:1241:CL7:H192	13:B:1241:CL7:H161	1.76	0.43
3:E:4:ARG:HD3	3:E:25:ALA:O	2.17	0.43
8:M:6:LEU:O	8:M:10:ILE:HG13	2.18	0.43
10:A:121:ILE:HG13	10:A:122:VAL:HG13	1.99	0.43
10:A:155:ALA:HB3	10:A:158:GLU:HG3	2.00	0.43
10:A:724:GLN:HG3	19:A:852:LHG:C7	2.47	0.43
1:B:199:ILE:HB	1:B:200:PRO:HD3	2.00	0.43
7:L:59:TYR:OH	7:L:75:LEU:HD13	2.18	0.43
10:A:706:HIS:HE1	13:A:1138:CL7:C4D	2.31	0.43
1:B:276:HIS:HE1	13:B:1214:CL7:ND	2.16	0.43
13:A:1107:CL7:H72C	13:A:1107:CL7:H112	1.75	0.43
13:A:1126:CL7:HBA1	13:A:1126:CL7:H3A	1.59	0.43
13:B:1212:CL7:H2A	13:B:1212:CL7:HED2	1.99	0.43
13:B:1230:CL7:CED	13:B:1230:CL7:H2A	2.49	0.43
13:B:1238:CL7:H143	13:B:1239:CL7:H203	2.00	0.43
1:B:715:VAL:HA	1:B:718:PHE:CE2	2.53	0.43
7:L:93:MET:CE	7:L:127:GLY:HA2	2.48	0.43
13:B:1205:CL7:H112	13:B:1205:CL7:H142	1.70	0.43
13:A:1102:CL7:HBA2	13:A:1102:CL7:H3A	1.66	0.43
10:A:22:VAL:HG21	13:A:1109:CL7:HED1	2.00	0.43
14:A:1013:PHO:H102	13:A:1140:CL7:HMC2	2.01	0.43
1:B:24:GLY:O	1:B:28:VAL:HG13	2.19	0.43
1:B:257:PHE:CE2	1:B:494:TRP:HB3	2.53	0.43
13:B:1226:CL7:H162	13:B:1226:CL7:H192	1.74	0.43
7:L:35:PRO:HG2	13:L:1502:CL7:HED2	2.00	0.43
1:B:443:ALA:HB1	10:A:668:SER:HB2	2.00	0.43
13:B:1239:CL7:H142	13:B:1239:CL7:H112	1.89	0.43
10:A:202:LEU:HD23	10:A:206:LEU:HD12	2.01	0.43
13:B:1201:CL7:H2	8:M:26:GLY:HA3	2.00	0.43
13:B:1207:CL7:H3A	13:B:1207:CL7:HBA2	1.82	0.43
13:B:1221:CL7:H41C	13:B:1221:CL7:H62C	1.73	0.43
1:B:425:MET:HG2	14:A:1013:PHO:O1A	2.19	0.42
13:B:1204:CL7:H11C	4:I:10:MET:HE3	2.01	0.42
13:B:1209:CL7:H3A	13:B:1209:CL7:HBA1	1.74	0.42
3:E:19:ARG:HH21	12:F:164:VAL:HG22	1.84	0.42
10:A:349:TRP:HB3	13:A:1103:CL7:HAC1	2.00	0.42
11:C:61:ASP:HA	11:C:62:PHE:HA	1.82	0.42
1:B:544:SER:HA	12:F:165:SER:HB3	2.00	0.42
10:A:251:ALA:HA	10:A:254:TYR:O	2.19	0.42
10:A:651:PHE:O	10:A:655:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1207:CL7:H51C	7:L:77:SER:HA	2.01	0.42
13:A:1110:CL7:CED	13:A:1110:CL7:H2A	2.49	0.42
13:A:1116:CL7:H11C	13:A:1116:CL7:H51C	1.84	0.42
1:B:371:THR:HG23	1:B:591:THR:HG21	2.01	0.42
13:B:1238:CL7:H62C	13:B:1238:CL7:H41C	1.58	0.42
1:B:646:TRP:CE2	1:B:726:ILE:HG21	2.54	0.42
1:B:692:MET:HE3	1:B:693:TRP:CE2	2.54	0.42
10:A:450:PHE:HB3	13:A:1131:CL7:HMA3	2.02	0.42
13:A:1108:CL7:H12C	13:A:1110:CL7:C3D	2.49	0.42
13:A:1125:CL7:HMB3	13:A:1133:CL7:H12C	2.02	0.42
13:B:1202:CL7:H111	13:B:1202:CL7:H142	1.73	0.42
13:B:1221:CL7:C2	13:B:1221:CL7:HMA2	2.50	0.42
2:D:16:THR:CG2	10:A:435:ASP:HB2	2.49	0.42
19:A:852:LHG:H342	13:A:1104:CL7:H92C	2.01	0.42
13:A:1119:CL7:HBA1	13:A:1119:CL7:C4A	2.49	0.42
13:B:1205:CL7:CGA	13:B:1205:CL7:C1A	2.98	0.42
10:A:433:HIS:O	10:A:436:THR:HG22	2.20	0.42
13:A:1104:CL7:H112	13:A:1104:CL7:H72C	1.81	0.42
1:B:662:LEU:HB2	14:B:1023:PHO:CHC	2.50	0.42
13:B:1204:CL7:H2	13:B:1204:CL7:ND	2.35	0.42
13:B:1205:CL7:H141	13:B:1205:CL7:H161	1.80	0.42
17:B:8002:LMG:H171	17:B:8002:LMG:H142	1.79	0.42
10:A:296:HIS:HE1	13:A:1115:CL7:C4D	2.32	0.42
10:A:735:LEU:HD22	13:A:1140:CL7:HMA1	2.01	0.42
1:B:694:LYS:HD2	4:I:31:GLU:OE1	2.20	0.42
13:A:1106:CL7:C1C	13:A:1107:CL7:HMD2	2.50	0.42
13:A:1133:CL7:H142	13:A:1133:CL7:H111	1.77	0.42
13:B:1235:CL7:H143	13:B:1235:CL7:H111	1.84	0.41
13:B:1241:CL7:H41C	13:B:1241:CL7:H62C	1.75	0.41
10:A:533:ASP:HA	10:A:536:ILE:HG22	2.01	0.41
13:A:1107:CL7:H162	13:A:1107:CL7:H141	1.66	0.41
1:B:48:ALA:HB2	1:B:157:LEU:HG	2.02	0.41
14:B:1023:PHO:CHB	13:A:1012:CL7:HAB	2.50	0.41
10:A:656:SER:O	10:A:660:ILE:HG12	2.20	0.41
13:B:1235:CL7:H41C	13:B:1235:CL7:H62C	1.59	0.41
13:A:1131:CL7:H62C	13:A:1131:CL7:H2	1.82	0.41
2:D:32:THR:HG22	2:D:57:LEU:HD13	2.02	0.41
10:A:83:ILE:HD12	13:A:1102:CL7:HAB	2.02	0.41
1:B:22:TRP:CG	1:B:704:GLN:HE22	2.38	0.41
1:B:276:HIS:HB2	13:B:1214:CL7:CHB	2.51	0.41
1:B:679:VAL:HG13	1:B:693:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1109:CL7:H62C	13:A:1109:CL7:H41C	1.78	0.41
1:B:494:TRP:CD1	13:B:1231:CL7:HED1	2.55	0.41
14:B:1023:PHO:H143	14:B:1023:PHO:H111	1.85	0.41
9:X:25:ILE:O	9:X:29:LEU:HG	2.20	0.41
13:A:1124:CL7:H93C	13:A:1124:CL7:H62C	1.68	0.41
13:B:1231:CL7:HAA2	13:B:1232:CL7:HMB2	2.02	0.41
5:J:36:ASN:O	5:J:40:PRO:HA	2.20	0.41
7:L:101:VAL:HG11	7:L:123:TRP:CD1	2.56	0.41
10:A:536:ILE:HD12	10:A:536:ILE:HA	1.93	0.41
1:B:3:THR:O	1:B:13:ALA:HB1	2.21	0.41
13:B:1201:CL7:HHC	13:B:1203:CL7:OBD	2.20	0.41
13:B:1239:CL7:H61C	13:B:1239:CL7:H41C	1.79	0.41
2:D:43:MET:HE3	2:D:43:MET:HB3	1.85	0.41
10:A:297:HIS:HB2	13:A:1116:CL7:C1B	2.50	0.41
13:A:1108:CL7:CHA	13:A:1108:CL7:HBA2	2.49	0.41
13:A:1109:CL7:H112	13:A:1109:CL7:H143	1.60	0.41
12:F:155:LEU:H	12:F:155:LEU:HD23	1.86	0.41
1:B:124:TRP:HA	1:B:127:ILE:HG12	2.03	0.41
13:B:1022:CL7:H142	13:B:1022:CL7:H112	1.83	0.41
2:D:37:LYS:HZ3	2:D:37:LYS:HG2	1.71	0.41
12:F:150:VAL:HA	12:F:155:LEU:HD22	2.02	0.41
10:A:128:ASN:HB3	10:A:136:HIS:HB3	2.02	0.40
10:A:375:PRO:HG3	10:A:381:ALA:HB2	2.02	0.40
13:A:1103:CL7:H142	13:A:1103:CL7:H112	1.73	0.40
13:A:1139:CL7:H202	13:A:1139:CL7:H162	1.91	0.40
12:F:35:PRO:O	12:F:39:GLU:OE1	2.39	0.40
1:B:86:PRO:HB3	1:B:121:TYR:CD2	2.56	0.40
1:B:310:ASP:HA	1:B:311:PRO:HD3	1.95	0.40
13:B:1214:CL7:H41C	13:B:1231:CL7:HAA1	2.03	0.40
13:B:1223:CL7:H91C	13:B:1223:CL7:H111	1.90	0.40
13:B:1237:CL7:H141	13:B:1237:CL7:H162	1.86	0.40
13:J:1302:CL7:H3A	13:J:1302:CL7:HBA2	1.83	0.40
10:A:91:MET:SD	13:A:1106:CL7:HAA1	2.61	0.40
13:A:1104:CL7:H111	13:A:1104:CL7:H152	1.92	0.40
13:A:1119:CL7:H93C	13:A:1125:CL7:H143	2.03	0.40
13:B:1231:CL7:HBA1	13:B:1231:CL7:H3A	1.63	0.40
6:K:32:ILE:HD13	6:K:65:THR:HG21	2.03	0.40
10:A:278:PHE:CE2	13:A:1134:CL7:HED1	2.56	0.40
10:A:567:LYS:HE3	10:A:567:LYS:HB2	1.77	0.40
4:I:11:THR:HB	4:I:12:PRO:HD3	2.04	0.40
16:J:4012:A1JPJ:C12	13:A:1107:CL7:H11C	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:20:VAL:HA	6:K:23:VAL:HG12	2.04	0.40
7:L:136:GLY:O	7:L:140:ILE:HG12	2.22	0.40
13:A:1123:CL7:H141	13:A:1123:CL7:H161	1.71	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	B	728/733 (99%)	710 (98%)	18 (2%)	0	100	100
2	D	134/139 (96%)	128 (96%)	6 (4%)	0	100	100
3	E	66/86 (77%)	63 (96%)	3 (4%)	0	100	100
4	I	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
5	J	33/47 (70%)	31 (94%)	2 (6%)	0	100	100
6	K	59/86 (69%)	57 (97%)	2 (3%)	0	100	100
7	L	144/153 (94%)	140 (97%)	4 (3%)	0	100	100
8	M	29/31 (94%)	29 (100%)	0	0	100	100
9	X	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
10	A	735/753 (98%)	719 (98%)	16 (2%)	0	100	100
11	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
12	F	142/167 (85%)	137 (96%)	5 (4%)	0	100	100
All	All	2204/2337 (94%)	2140 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	B	592/593 (100%)	592 (100%)	0	100	100
2	D	110/112 (98%)	110 (100%)	0	100	100
3	E	58/68 (85%)	58 (100%)	0	100	100
4	I	26/26 (100%)	26 (100%)	0	100	100
5	J	31/42 (74%)	31 (100%)	0	100	100
6	K	47/65 (72%)	47 (100%)	0	100	100
7	L	108/113 (96%)	108 (100%)	0	100	100
8	M	25/25 (100%)	25 (100%)	0	100	100
9	X	22/22 (100%)	22 (100%)	0	100	100
10	A	590/602 (98%)	590 (100%)	0	100	100
11	C	68/69 (99%)	68 (100%)	0	100	100
12	F	112/131 (86%)	112 (100%)	0	100	100
All	All	1789/1868 (96%)	1789 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	102	GLN
1	B	275	HIS
1	B	308	HIS
1	B	361	GLN
2	D	38	GLN
3	E	59	ASN
5	J	36	ASN
6	K	40	GLN
6	K	43	ASN
10	A	20	ASN
10	A	136	HIS

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Mol	Chain	Res	Type
10	A	259	GLN
10	A	296	HIS
10	A	442	ASN
10	A	458	HIS
10	A	493	ASN
10	A	525	GLN
10	A	616	GLN
10	A	724	GLN
12	F	46	ASN
12	F	109	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

125 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$
13	CL7	A	1103	10	71,73,73	1.32	12 (16%)	80,113,113	1.29	8 (10%)
13	CL7	B	1234	1	56,58,73	1.49	11 (19%)	62,95,113	1.41	8 (12%)
13	CL7	B	1213	1	51,53,73	1.55	10 (19%)	56,89,113	1.43	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CL7	B	1238	21	71,73,73	1.31	11 (15%)	80,113,113	1.28	8 (10%)
16	A1JPJ	A	4014	-	40,41,41	1.65	8 (20%)	50,56,56	1.54	8 (16%)
13	CL7	A	1104	10	71,73,73	1.32	12 (16%)	80,113,113	1.23	5 (6%)
13	CL7	B	1210	1	71,73,73	1.33	11 (15%)	80,113,113	1.23	6 (7%)
13	CL7	B	1216	-	61,63,73	1.44	11 (18%)	68,101,113	1.32	8 (11%)
13	CL7	A	1115	10	47,49,73	1.58	12 (25%)	51,84,113	1.49	6 (11%)
13	CL7	B	1022	1	71,73,73	1.31	10 (14%)	80,113,113	1.15	5 (6%)
13	CL7	B	1236	1	51,53,73	1.57	11 (21%)	56,89,113	1.37	6 (10%)
13	CL7	B	1223	1	71,73,73	1.33	12 (16%)	80,113,113	1.21	7 (8%)
13	CL7	L	1502	7	71,73,73	1.30	11 (15%)	80,113,113	1.30	9 (11%)
13	CL7	A	1137	10	61,63,73	1.43	11 (18%)	68,101,113	1.29	7 (10%)
13	CL7	A	1102	10,13	58,60,73	1.47	11 (18%)	64,97,113	1.39	7 (10%)
13	CL7	A	1126	10	71,73,73	1.32	11 (15%)	80,113,113	1.20	5 (6%)
16	A1JPJ	A	4001	-	40,41,41	1.70	8 (20%)	50,56,56	1.81	13 (26%)
16	A1JPJ	B	4004	-	40,41,41	1.68	8 (20%)	50,56,56	1.65	11 (22%)
15	PQN	A	2001	-	34,34,34	0.36	0	42,45,45	0.59	1 (2%)
13	CL7	B	1220	-	51,53,73	1.56	10 (19%)	56,89,113	1.39	5 (8%)
13	CL7	A	1131	10	71,73,73	1.33	11 (15%)	80,113,113	1.21	6 (7%)
19	LHG	A	852	-	48,48,48	0.51	0	51,54,54	0.52	0
13	CL7	B	1201	1	60,62,73	1.44	12 (20%)	66,99,113	1.33	6 (9%)
13	CL7	B	1206	1	56,58,73	1.48	11 (19%)	62,95,113	1.38	8 (12%)
13	CL7	B	1214	1	71,73,73	1.33	11 (15%)	80,113,113	1.28	8 (10%)
13	CL7	A	1134	10	49,52,73	1.57	11 (22%)	56,87,113	1.46	6 (10%)
16	A1JPJ	A	4008	-	40,41,41	1.68	8 (20%)	50,56,56	1.63	10 (20%)
13	CL7	I	1601	21	71,73,73	1.34	11 (15%)	80,113,113	1.25	7 (8%)
13	CL7	B	1021	21	71,73,73	1.32	11 (15%)	80,113,113	1.20	8 (10%)
20	G9R	A	1011	10	54,71,71	2.33	10 (18%)	54,104,104	1.32	9 (16%)
16	A1JPJ	J	4012	-	40,41,41	1.72	7 (17%)	50,56,56	2.23	18 (36%)
17	LMG	B	8002	-	55,55,55	0.51	0	63,63,63	0.62	0
13	CL7	A	1132	10	71,73,73	1.30	11 (15%)	80,113,113	1.29	9 (11%)
13	CL7	K	1401	-	51,53,73	1.58	11 (21%)	56,89,113	1.41	5 (8%)
16	A1JPJ	B	4006	-	40,41,41	1.69	8 (20%)	50,56,56	1.73	12 (24%)
13	CL7	A	1113	10	51,53,73	1.54	12 (23%)	56,89,113	1.42	5 (8%)
16	A1JPJ	B	4011	-	40,41,41	1.63	8 (20%)	50,56,56	1.66	8 (16%)
13	CL7	A	1119	21	71,73,73	1.31	12 (16%)	80,113,113	1.25	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CL7	B	1225	1	71,73,73	1.30	12 (16%)	80,113,113	1.20	5 (6%)
13	CL7	A	1123	21	71,73,73	1.33	11 (15%)	80,113,113	1.31	9 (11%)
13	CL7	J	1302	5	47,50,73	1.62	10 (21%)	51,85,113	1.34	4 (7%)
13	CL7	A	1122	10	71,73,73	1.32	11 (15%)	80,113,113	1.24	5 (6%)
13	CL7	A	1127	10	71,73,73	1.31	11 (15%)	80,113,113	1.19	4 (5%)
13	CL7	A	1140	10	71,73,73	1.33	12 (16%)	80,113,113	1.21	6 (7%)
13	CL7	B	1202	1	71,73,73	1.31	11 (15%)	80,113,113	1.22	5 (6%)
16	A1JPJ	I	4118	-	40,41,41	1.65	8 (20%)	50,56,56	1.46	9 (18%)
16	A1JPJ	L	4019	-	40,41,41	1.64	8 (20%)	50,56,56	2.12	13 (26%)
13	CL7	F	1701	12	47,49,73	1.59	11 (23%)	51,84,113	1.46	6 (11%)
16	A1JPJ	F	4016	-	40,41,41	1.77	8 (20%)	50,56,56	2.12	12 (24%)
13	CL7	A	1111	10	71,73,73	1.31	11 (15%)	80,113,113	1.30	8 (10%)
13	CL7	A	1112	10	71,73,73	1.33	12 (16%)	80,113,113	1.27	7 (8%)
18	SF4	C	3003	11	0,12,12	-	-	-	-	-
13	CL7	A	1106	10	71,73,73	1.30	11 (15%)	80,113,113	1.28	6 (7%)
13	CL7	A	1114	21	51,53,73	1.57	11 (21%)	56,89,113	1.40	5 (8%)
13	CL7	B	1215	1	61,63,73	1.42	11 (18%)	68,101,113	1.31	6 (8%)
13	CL7	B	1209	1	51,53,73	1.57	11 (21%)	56,89,113	1.43	7 (12%)
13	CL7	B	1230	1	47,49,73	1.58	11 (23%)	51,84,113	1.60	9 (17%)
13	CL7	A	1012	21	71,73,73	1.31	11 (15%)	80,113,113	1.21	5 (6%)
13	CL7	A	1139	21	71,73,73	1.34	11 (15%)	80,113,113	1.25	6 (7%)
18	SF4	C	3002	11	0,12,12	-	-	-	-	-
13	CL7	B	1221	1	66,68,73	1.38	13 (19%)	74,107,113	1.31	9 (12%)
13	CL7	B	1208	1	71,73,73	1.32	12 (16%)	80,113,113	1.22	6 (7%)
13	CL7	B	1203	1	71,73,73	1.32	12 (16%)	80,113,113	1.25	6 (7%)
16	A1JPJ	B	4008	-	40,41,41	1.69	8 (20%)	50,56,56	1.84	9 (18%)
13	CL7	B	1222	21	56,58,73	1.47	11 (19%)	62,95,113	1.39	7 (11%)
13	CL7	B	1229	1	71,73,73	1.33	10 (14%)	80,113,113	1.27	7 (8%)
16	A1JPJ	J	4013	-	40,41,41	1.69	8 (20%)	50,56,56	1.66	11 (22%)
13	CL7	B	1211	1	71,73,73	1.31	12 (16%)	80,113,113	1.21	5 (6%)
14	PHO	B	1023	-	58,69,69	1.96	12 (20%)	56,99,99	1.61	8 (14%)
13	CL7	A	1118	10	61,63,73	1.43	11 (18%)	68,101,113	1.32	7 (10%)
16	A1JPJ	L	4020	-	40,41,41	1.65	8 (20%)	50,56,56	1.68	10 (20%)
13	CL7	B	1226	1	71,73,73	1.32	11 (15%)	80,113,113	1.25	7 (8%)
13	CL7	B	1218	1	47,49,73	1.60	11 (23%)	51,84,113	1.48	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	A1JPJ	L	4023	-	40,41,41	1.69	8 (20%)	50,56,56	1.63	10 (20%)
13	CL7	A	1110	21	51,53,73	1.55	11 (21%)	56,89,113	1.43	7 (12%)
13	CL7	A	1121	10	61,63,73	1.43	11 (18%)	68,101,113	1.29	8 (11%)
13	CL7	A	1129	10	56,58,73	1.47	12 (21%)	62,95,113	1.40	8 (12%)
16	A1JPJ	B	4005	-	40,41,41	1.76	7 (17%)	50,56,56	2.06	14 (28%)
13	CL7	A	1130	10	57,59,73	1.48	12 (21%)	63,96,113	1.38	7 (11%)
13	CL7	A	1136	10	71,73,73	1.32	11 (15%)	80,113,113	1.26	6 (7%)
14	PHO	A	1013	-	58,69,69	1.98	12 (20%)	56,99,99	1.79	8 (14%)
13	CL7	B	1224	1	62,64,73	1.41	11 (17%)	69,102,113	1.23	5 (7%)
16	A1JPJ	B	4007	-	40,41,41	1.69	8 (20%)	50,56,56	1.69	11 (22%)
13	CL7	B	1205	1	71,73,73	1.29	12 (16%)	80,113,113	1.30	7 (8%)
13	CL7	A	1117	10	71,73,73	1.31	11 (15%)	80,113,113	1.28	7 (8%)
13	CL7	B	1241	1	71,73,73	1.33	11 (15%)	80,113,113	1.19	4 (5%)
13	CL7	A	1105	10	51,53,73	1.55	11 (21%)	56,89,113	1.43	5 (8%)
13	CL7	B	1207	1	71,73,73	1.31	11 (15%)	80,113,113	1.27	8 (10%)
13	CL7	A	1107	10	71,73,73	1.33	11 (15%)	80,113,113	1.25	7 (8%)
13	CL7	L	1501	7	66,68,73	1.39	11 (16%)	74,107,113	1.32	7 (9%)
13	CL7	L	1503	21	48,50,73	1.60	11 (22%)	51,85,113	1.43	5 (9%)
13	CL7	A	1116	10	71,73,73	1.32	12 (16%)	80,113,113	1.24	6 (7%)
13	CL7	K	1402	6	45,45,73	1.65	10 (22%)	49,78,113	1.44	5 (10%)
16	A1JPJ	A	4007	-	40,41,41	1.66	8 (20%)	50,56,56	1.67	12 (24%)
13	CL7	B	1235	1	71,73,73	1.31	11 (15%)	80,113,113	1.29	7 (8%)
16	A1JPJ	B	4021	-	40,41,41	1.77	9 (22%)	50,56,56	2.04	15 (30%)
13	CL7	B	1219	1	47,49,73	1.57	10 (21%)	51,84,113	1.47	6 (11%)
13	CL7	B	1228	1	51,53,73	1.56	11 (21%)	56,89,113	1.37	6 (10%)
13	CL7	B	1232	21	47,49,73	1.59	10 (21%)	51,84,113	1.44	6 (11%)
13	CL7	B	1237	21	71,73,73	1.31	12 (16%)	80,113,113	1.23	6 (7%)
13	CL7	B	1212	1	51,53,73	1.55	11 (21%)	56,89,113	1.40	5 (8%)
13	CL7	A	1101	10	47,49,73	1.59	11 (23%)	51,84,113	1.50	6 (11%)
18	SF4	B	3001	10,1	0,12,12	-	-	-	-	-
13	CL7	B	1217	1	47,49,73	1.59	11 (23%)	51,84,113	1.49	6 (11%)
15	PQN	B	2002	-	34,34,34	0.37	0	42,45,45	0.53	1 (2%)
13	CL7	A	1141	19	47,49,73	1.58	11 (23%)	51,84,113	1.48	6 (11%)
13	CL7	B	1204	1	71,73,73	1.33	12 (16%)	80,113,113	1.28	7 (8%)
13	CL7	A	1128	10	71,73,73	1.31	11 (15%)	80,113,113	1.29	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CL7	B	1233	-	47,49,73	1.60	9 (19%)	51,84,113	1.47	6 (11%)
19	LHG	A	853	13	37,37,48	0.57	0	40,43,54	0.57	0
13	CL7	B	1227	1	66,68,73	1.39	10 (15%)	74,107,113	1.27	6 (8%)
13	CL7	A	1125	10	71,73,73	1.31	11 (15%)	80,113,113	1.25	7 (8%)
13	CL7	A	1133	10	71,73,73	1.32	11 (15%)	80,113,113	1.27	7 (8%)
13	CL7	A	1108	10	57,59,73	1.49	11 (19%)	63,96,113	1.30	5 (7%)
16	A1JPJ	B	4009	-	40,41,41	1.71	8 (20%)	50,56,56	1.81	10 (20%)
13	CL7	A	1124	21	63,65,73	1.39	11 (17%)	70,103,113	1.34	7 (10%)
13	CL7	J	1301	21	47,49,73	1.61	11 (23%)	51,84,113	1.48	6 (11%)
13	CL7	A	1135	10	56,58,73	1.50	11 (19%)	62,95,113	1.38	7 (11%)
16	A1JPJ	A	4003	-	40,41,41	1.79	7 (17%)	50,56,56	2.02	12 (24%)
16	A1JPJ	A	4002	-	40,41,41	1.74	6 (15%)	50,56,56	1.89	12 (24%)
13	CL7	B	1231	1	66,68,73	1.38	10 (15%)	74,107,113	1.27	7 (9%)
13	CL7	A	1120	10	51,53,73	1.56	11 (21%)	56,89,113	1.42	5 (8%)
13	CL7	A	1109	10,13	71,73,73	1.32	10 (14%)	80,113,113	1.24	6 (7%)
13	CL7	B	1239	1	71,73,73	1.32	11 (15%)	80,113,113	1.25	6 (7%)
13	CL7	A	1138	10	71,73,73	1.30	11 (15%)	80,113,113	1.24	7 (8%)

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
13	CL7	A	1103	10	2/2/15/20	15/39/115/115	-
13	CL7	B	1234	1	2/2/12/20	5/21/97/115	-
13	CL7	B	1213	1	2/2/11/20	8/15/91/115	-
13	CL7	B	1238	21	2/2/15/20	8/39/115/115	-
16	A1JPJ	A	4014	-	-	4/29/63/63	0/2/2/2
13	CL7	A	1104	10	2/2/15/20	9/39/115/115	-
13	CL7	B	1210	1	2/2/15/20	17/39/115/115	-
13	CL7	B	1216	-	2/2/13/20	11/27/103/115	-
13	CL7	A	1115	10	2/2/10/20	2/10/86/115	-
13	CL7	B	1022	1	2/2/15/20	7/39/115/115	-
13	CL7	B	1236	1	2/2/11/20	6/15/91/115	-
13	CL7	B	1223	1	2/2/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL7	L	1502	7	2/2/15/20	18/39/115/115	-
13	CL7	A	1137	10	2/2/13/20	10/27/103/115	-
13	CL7	A	1102	10,13	2/2/12/20	8/24/100/115	-
13	CL7	A	1126	10	2/2/15/20	15/39/115/115	-
16	A1JPJ	A	4001	-	-	6/29/63/63	0/2/2/2
16	A1JPJ	B	4004	-	-	4/29/63/63	0/2/2/2
15	PQN	A	2001	-	-	4/23/43/43	0/2/2/2
13	CL7	B	1220	-	2/2/11/20	7/15/91/115	-
13	CL7	A	1131	10	2/2/15/20	5/39/115/115	-
19	LHG	A	852	-	-	14/53/53/53	-
13	CL7	B	1201	1	2/2/12/20	7/26/102/115	-
13	CL7	B	1206	1	2/2/12/20	6/21/97/115	-
13	CL7	B	1214	1	2/2/15/20	12/39/115/115	-
13	CL7	A	1134	10	2/2/10/20	8/15/87/115	-
16	A1JPJ	A	4008	-	-	4/29/63/63	0/2/2/2
13	CL7	I	1601	21	2/2/15/20	15/39/115/115	-
13	CL7	B	1021	21	2/2/15/20	17/39/115/115	-
20	G9R	A	1011	10	1/1/17/22	4/37/107/107	-
16	A1JPJ	J	4012	-	-	4/29/63/63	0/2/2/2
17	LMG	B	8002	-	-	15/50/70/70	0/1/1/1
13	CL7	A	1132	10	2/2/15/20	14/39/115/115	-
13	CL7	K	1401	-	2/2/11/20	2/15/91/115	-
16	A1JPJ	B	4006	-	-	5/29/63/63	0/2/2/2
13	CL7	A	1113	10	2/2/11/20	6/15/91/115	-
16	A1JPJ	B	4011	-	-	6/29/63/63	0/2/2/2
13	CL7	A	1119	21	2/2/15/20	13/39/115/115	-
13	CL7	B	1225	1	2/2/15/20	11/39/115/115	-
13	CL7	A	1123	21	2/2/15/20	15/39/115/115	-
13	CL7	J	1302	5	2/2/10/20	4/9/85/115	-
13	CL7	A	1122	10	2/2/15/20	13/39/115/115	-
13	CL7	A	1127	10	2/2/15/20	16/39/115/115	-
13	CL7	A	1140	10	2/2/15/20	10/39/115/115	-
13	CL7	B	1202	1	2/2/15/20	16/39/115/115	-
16	A1JPJ	I	4118	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	A1JPJ	L	4019	-	-	3/29/63/63	0/2/2/2
13	CL7	F	1701	12	2/2/10/20	2/10/86/115	-
16	A1JPJ	F	4016	-	-	7/29/63/63	0/2/2/2
13	CL7	A	1111	10	2/2/15/20	10/39/115/115	-
13	CL7	A	1112	10	2/2/15/20	20/39/115/115	-
18	SF4	C	3003	11	-	-	0/6/5/5
13	CL7	A	1106	10	2/2/15/20	16/39/115/115	-
13	CL7	A	1114	21	2/2/11/20	2/15/91/115	-
13	CL7	B	1215	1	2/2/13/20	7/27/103/115	-
13	CL7	B	1209	1	2/2/11/20	6/15/91/115	-
13	CL7	B	1230	1	2/2/10/20	6/10/86/115	-
13	CL7	A	1012	21	2/2/15/20	9/39/115/115	-
13	CL7	A	1139	21	2/2/15/20	13/39/115/115	-
18	SF4	C	3002	11	-	-	0/6/5/5
13	CL7	B	1221	1	2/2/14/20	14/33/109/115	-
13	CL7	B	1208	1	2/2/15/20	10/39/115/115	-
13	CL7	B	1203	1	2/2/15/20	11/39/115/115	-
16	A1JPJ	B	4008	-	-	4/29/63/63	0/2/2/2
13	CL7	B	1222	21	2/2/12/20	6/21/97/115	-
13	CL7	B	1229	1	2/2/15/20	8/39/115/115	-
16	A1JPJ	J	4013	-	-	1/29/63/63	0/2/2/2
13	CL7	B	1211	1	2/2/15/20	6/39/115/115	-
14	PHO	B	1023	-	-	14/37/103/103	0/5/6/6
13	CL7	A	1118	10	2/2/13/20	11/27/103/115	-
16	A1JPJ	L	4020	-	-	8/29/63/63	0/2/2/2
13	CL7	B	1226	1	2/2/15/20	10/39/115/115	-
13	CL7	B	1218	1	2/2/10/20	4/10/86/115	-
16	A1JPJ	L	4023	-	-	2/29/63/63	0/2/2/2
13	CL7	A	1110	21	2/2/11/20	9/15/91/115	-
13	CL7	A	1121	10	2/2/13/20	12/27/103/115	-
13	CL7	A	1129	10	2/2/12/20	5/21/97/115	-
16	A1JPJ	B	4005	-	-	6/29/63/63	0/2/2/2
13	CL7	A	1130	10	2/2/12/20	4/23/99/115	-
13	CL7	A	1136	10	2/2/15/20	15/39/115/115	-
14	PHO	A	1013	-	-	7/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL7	B	1224	1	2/2/13/20	5/29/105/115	-
16	A1JPJ	B	4007	-	-	6/29/63/63	0/2/2/2
13	CL7	B	1205	1	2/2/15/20	13/39/115/115	-
13	CL7	A	1117	10	2/2/15/20	13/39/115/115	-
13	CL7	B	1241	1	2/2/15/20	16/39/115/115	-
13	CL7	A	1105	10	2/2/11/20	3/15/91/115	-
13	CL7	B	1207	1	2/2/15/20	7/39/115/115	-
13	CL7	A	1107	10	2/2/15/20	11/39/115/115	-
13	CL7	L	1501	7	2/2/14/20	18/33/109/115	-
13	CL7	L	1503	21	2/2/10/20	3/12/88/115	-
13	CL7	A	1116	10	2/2/15/20	12/39/115/115	-
13	CL7	K	1402	6	2/2/8/20	1/4/76/115	-
16	A1JPJ	A	4007	-	-	4/29/63/63	0/2/2/2
13	CL7	B	1235	1	2/2/15/20	16/39/115/115	-
16	A1JPJ	B	4021	-	-	3/29/63/63	0/2/2/2
13	CL7	B	1219	1	2/2/10/20	2/10/86/115	-
13	CL7	B	1228	1	2/2/11/20	1/15/91/115	-
13	CL7	B	1232	21	2/2/10/20	6/10/86/115	-
13	CL7	B	1237	21	2/2/15/20	14/39/115/115	-
13	CL7	B	1212	1	2/2/11/20	11/15/91/115	-
13	CL7	A	1101	10	2/2/10/20	4/10/86/115	-
18	SF4	B	3001	10,1	-	-	0/6/5/5
13	CL7	B	1217	1	2/2/10/20	0/10/86/115	-
15	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
13	CL7	A	1141	19	2/2/10/20	5/10/86/115	-
13	CL7	B	1204	1	2/2/15/20	9/39/115/115	-
13	CL7	A	1128	10	2/2/15/20	9/39/115/115	-
13	CL7	B	1233	-	2/2/10/20	4/10/86/115	-
19	LHG	A	853	13	-	8/42/42/53	-
13	CL7	B	1227	1	2/2/14/20	17/33/109/115	-
13	CL7	A	1125	10	2/2/15/20	9/39/115/115	-
13	CL7	A	1133	10	2/2/15/20	14/39/115/115	-
13	CL7	A	1108	10	2/2/12/20	8/23/99/115	-
16	A1JPJ	B	4009	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL7	A	1124	21	2/2/13/20	13/30/106/115	-
13	CL7	J	1301	21	2/2/10/20	0/10/86/115	-
13	CL7	A	1135	10	2/2/12/20	8/21/97/115	-
16	A1JPJ	A	4003	-	-	5/29/63/63	0/2/2/2
16	A1JPJ	A	4002	-	-	5/29/63/63	0/2/2/2
13	CL7	B	1231	1	2/2/14/20	14/33/109/115	-
13	CL7	A	1120	10	2/2/11/20	4/15/91/115	-
13	CL7	A	1109	10,13	2/2/15/20	20/39/115/115	-
13	CL7	B	1239	1	2/2/15/20	11/39/115/115	-
13	CL7	A	1138	10	2/2/15/20	12/39/115/115	-

All (1229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1011	G9R	C3B-C4B	10.10	1.49	1.41
14	A	1013	PHO	C1B-C2B	8.75	1.49	1.39
14	B	1023	PHO	C1B-C2B	8.51	1.49	1.39
20	A	1011	G9R	C1B-C2B	8.01	1.49	1.39
14	A	1013	PHO	C3B-C4B	7.32	1.49	1.41
14	B	1023	PHO	C3B-C4B	7.27	1.49	1.41
20	A	1011	G9R	C1D-C2D	7.12	1.48	1.39
16	F	4016	A1JPJ	C10-C9	4.90	1.42	1.35
16	B	4021	A1JPJ	C14-C13	4.70	1.42	1.35
20	A	1011	G9R	C3D-C4D	4.64	1.47	1.41
16	B	4021	A1JPJ	C17-C18	4.41	1.41	1.35
16	A	4003	A1JPJ	C21-C22	4.41	1.41	1.35
16	A	4003	A1JPJ	C17-C18	4.39	1.41	1.35
16	B	4005	A1JPJ	C14-C13	4.32	1.41	1.35
16	A	4002	A1JPJ	C21-C22	4.32	1.41	1.35
16	A	4003	A1JPJ	C10-C9	4.31	1.41	1.35
16	A	4003	A1JPJ	C14-C13	4.28	1.41	1.35
16	B	4005	A1JPJ	C17-C18	4.28	1.41	1.35
16	A	4002	A1JPJ	C17-C18	4.21	1.41	1.35
16	F	4016	A1JPJ	C17-C18	4.17	1.41	1.35
16	J	4012	A1JPJ	C17-C18	4.17	1.41	1.35
16	B	4005	A1JPJ	C10-C9	4.15	1.41	1.35
16	J	4012	A1JPJ	C14-C13	4.14	1.41	1.35
16	B	4005	A1JPJ	C21-C22	4.13	1.41	1.35
16	A	4002	A1JPJ	C14-C13	4.11	1.41	1.35
16	J	4012	A1JPJ	C21-C22	4.10	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	4012	A1JPJ	C10-C9	4.07	1.41	1.35
16	B	4007	A1JPJ	C10-C9	4.06	1.41	1.35
16	F	4016	A1JPJ	C14-C13	4.04	1.41	1.35
16	J	4013	A1JPJ	C14-C13	4.03	1.41	1.35
16	B	4009	A1JPJ	C14-C13	4.00	1.41	1.35
16	F	4016	A1JPJ	C21-C22	4.00	1.41	1.35
16	A	4001	A1JPJ	C14-C13	3.98	1.41	1.35
16	L	4023	A1JPJ	C21-C22	3.97	1.41	1.35
16	J	4013	A1JPJ	C10-C9	3.97	1.41	1.35
13	K	1402	CL7	C1D-ND	3.96	1.42	1.37
16	A	4001	A1JPJ	C10-C9	3.95	1.41	1.35
16	L	4023	A1JPJ	C14-C13	3.95	1.41	1.35
16	B	4009	A1JPJ	C21-C22	3.95	1.41	1.35
16	J	4013	A1JPJ	C21-C22	3.94	1.41	1.35
16	A	4001	A1JPJ	C21-C22	3.92	1.41	1.35
16	J	4013	A1JPJ	C17-C18	3.91	1.41	1.35
13	B	1219	CL7	C1D-ND	3.91	1.42	1.37
16	B	4009	A1JPJ	C17-C18	3.91	1.41	1.35
16	B	4009	A1JPJ	C10-C9	3.90	1.41	1.35
16	B	4006	A1JPJ	C10-C9	3.90	1.41	1.35
13	B	1232	CL7	C1D-ND	3.90	1.42	1.37
16	B	4006	A1JPJ	C14-C13	3.89	1.40	1.35
16	A	4001	A1JPJ	C17-C18	3.89	1.40	1.35
13	B	1209	CL7	C1D-ND	3.88	1.42	1.37
16	B	4004	A1JPJ	C10-C9	3.88	1.40	1.35
16	B	4008	A1JPJ	C17-C18	3.86	1.40	1.35
16	A	4002	A1JPJ	C10-C9	3.86	1.40	1.35
16	L	4023	A1JPJ	C17-C18	3.86	1.40	1.35
16	A	4008	A1JPJ	C21-C22	3.85	1.40	1.35
16	B	4007	A1JPJ	C14-C13	3.85	1.40	1.35
16	L	4023	A1JPJ	C10-C9	3.84	1.40	1.35
13	A	1109	CL7	C1D-ND	3.84	1.42	1.37
13	B	1220	CL7	C1D-ND	3.84	1.42	1.37
13	B	1233	CL7	C1D-ND	3.84	1.42	1.37
16	B	4004	A1JPJ	C14-C13	3.83	1.40	1.35
16	B	4007	A1JPJ	C17-C18	3.83	1.40	1.35
13	B	1218	CL7	C1D-ND	3.83	1.42	1.37
13	B	1241	CL7	C1D-ND	3.82	1.42	1.37
13	A	1110	CL7	C1D-ND	3.82	1.42	1.37
16	B	4008	A1JPJ	C21-C22	3.82	1.40	1.35
16	B	4006	A1JPJ	C21-C22	3.81	1.40	1.35
13	L	1503	CL7	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1217	CL7	C1D-ND	3.80	1.42	1.37
13	A	1101	CL7	C1D-ND	3.80	1.42	1.37
13	I	1601	CL7	C1D-ND	3.80	1.42	1.37
16	B	4007	A1JPJ	C21-C22	3.80	1.40	1.35
16	A	4007	A1JPJ	C17-C18	3.79	1.40	1.35
13	J	1301	CL7	C1D-ND	3.79	1.42	1.37
16	B	4006	A1JPJ	C17-C18	3.78	1.40	1.35
13	L	1501	CL7	C1D-ND	3.78	1.42	1.37
13	A	1137	CL7	C1D-ND	3.78	1.42	1.37
16	B	4004	A1JPJ	C17-C18	3.78	1.40	1.35
13	J	1302	CL7	C1D-ND	3.77	1.42	1.37
13	A	1134	CL7	C1D-ND	3.77	1.42	1.37
13	A	1135	CL7	C1D-ND	3.77	1.42	1.37
16	A	4008	A1JPJ	C17-C18	3.76	1.40	1.35
13	F	1701	CL7	C1D-ND	3.76	1.42	1.37
16	B	4021	A1JPJ	C21-C22	3.75	1.40	1.35
13	B	1204	CL7	C1D-ND	3.75	1.42	1.37
13	B	1221	CL7	C1D-ND	3.75	1.42	1.37
16	B	4004	A1JPJ	C21-C22	3.75	1.40	1.35
13	K	1401	CL7	C1D-ND	3.74	1.42	1.37
13	A	1139	CL7	C1D-ND	3.74	1.42	1.37
16	B	4008	A1JPJ	C14-C13	3.74	1.40	1.35
13	B	1216	CL7	C1D-ND	3.73	1.42	1.37
16	L	4019	A1JPJ	C17-C18	3.72	1.40	1.35
13	A	1140	CL7	C1D-ND	3.72	1.42	1.37
14	A	1013	PHO	C1D-C2D	3.72	1.43	1.39
13	B	1231	CL7	C1D-ND	3.72	1.42	1.37
13	A	1133	CL7	C1D-ND	3.72	1.42	1.37
13	A	1115	CL7	C1D-ND	3.71	1.42	1.37
13	A	1103	CL7	C1D-ND	3.71	1.42	1.37
13	B	1236	CL7	C1D-ND	3.71	1.42	1.37
13	B	1227	CL7	C1D-ND	3.71	1.42	1.37
13	A	1114	CL7	C1D-ND	3.71	1.42	1.37
13	A	1108	CL7	C1D-ND	3.71	1.42	1.37
13	B	1223	CL7	C1D-ND	3.70	1.42	1.37
16	L	4020	A1JPJ	C14-C13	3.69	1.40	1.35
16	A	4008	A1JPJ	C14-C13	3.69	1.40	1.35
13	A	1102	CL7	C1D-ND	3.69	1.42	1.37
16	A	4007	A1JPJ	C21-C22	3.68	1.40	1.35
13	B	1230	CL7	C1D-ND	3.68	1.42	1.37
13	B	1201	CL7	C1D-ND	3.68	1.42	1.37
13	B	1022	CL7	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1213	CL7	C1D-ND	3.67	1.42	1.37
16	A	4014	A1JPJ	C21-C22	3.67	1.40	1.35
13	B	1215	CL7	C1D-ND	3.67	1.42	1.37
13	A	1116	CL7	C1D-ND	3.66	1.42	1.37
13	A	1132	CL7	C1D-ND	3.66	1.42	1.37
13	A	1136	CL7	C1D-ND	3.66	1.42	1.37
16	A	4007	A1JPJ	C14-C13	3.66	1.40	1.35
13	B	1234	CL7	C1D-ND	3.66	1.42	1.37
13	A	1012	CL7	C1D-ND	3.66	1.42	1.37
13	A	1126	CL7	C1D-ND	3.66	1.42	1.37
16	B	4008	A1JPJ	C10-C9	3.66	1.40	1.35
13	A	1111	CL7	C1D-ND	3.66	1.42	1.37
13	B	1207	CL7	C1D-ND	3.65	1.42	1.37
13	B	1222	CL7	C1D-ND	3.65	1.42	1.37
13	A	1130	CL7	C1D-ND	3.65	1.42	1.37
13	A	1104	CL7	C1D-ND	3.65	1.42	1.37
13	A	1120	CL7	C1D-ND	3.65	1.42	1.37
13	A	1113	CL7	C1D-ND	3.65	1.42	1.37
13	A	1138	CL7	C1D-ND	3.65	1.42	1.37
13	A	1122	CL7	C1D-ND	3.65	1.42	1.37
13	B	1214	CL7	C1D-ND	3.65	1.42	1.37
13	A	1105	CL7	C1D-ND	3.65	1.42	1.37
13	B	1228	CL7	C1D-ND	3.64	1.42	1.37
13	B	1021	CL7	C1D-ND	3.64	1.42	1.37
13	B	1239	CL7	C1D-ND	3.64	1.42	1.37
13	A	1118	CL7	C1D-ND	3.63	1.42	1.37
13	B	1224	CL7	C1D-ND	3.63	1.42	1.37
13	A	1106	CL7	C1D-ND	3.63	1.42	1.37
16	L	4020	A1JPJ	C10-C9	3.63	1.40	1.35
16	L	4020	A1JPJ	C17-C18	3.63	1.40	1.35
13	B	1235	CL7	C1D-ND	3.63	1.42	1.37
16	B	4011	A1JPJ	C14-C13	3.62	1.40	1.35
13	A	1112	CL7	C1D-ND	3.62	1.42	1.37
13	A	1125	CL7	C1D-ND	3.62	1.42	1.37
13	B	1205	CL7	C1D-ND	3.62	1.42	1.37
13	A	1121	CL7	C1D-ND	3.61	1.42	1.37
13	A	1131	CL7	C1D-ND	3.61	1.42	1.37
16	A	4014	A1JPJ	C17-C18	3.61	1.40	1.35
13	A	1119	CL7	C1D-ND	3.61	1.42	1.37
13	B	1229	CL7	C4B-NB	3.61	1.42	1.37
13	B	1212	CL7	C1D-ND	3.61	1.42	1.37
16	I	4118	A1JPJ	C21-C22	3.60	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	4021	A1JPJ	C10-C9	3.60	1.40	1.35
13	B	1208	CL7	C1D-ND	3.60	1.42	1.37
13	B	1229	CL7	C1D-ND	3.60	1.42	1.37
13	A	1141	CL7	C1D-ND	3.59	1.42	1.37
13	L	1502	CL7	C1D-ND	3.59	1.42	1.37
13	A	1117	CL7	C1D-ND	3.58	1.42	1.37
16	B	4011	A1JPJ	C10-C9	3.58	1.40	1.35
13	B	1203	CL7	C1D-ND	3.57	1.42	1.37
16	L	4020	A1JPJ	C21-C22	3.57	1.40	1.35
13	A	1107	CL7	C1D-ND	3.57	1.42	1.37
13	A	1124	CL7	C1D-ND	3.57	1.42	1.37
13	A	1129	CL7	C1D-ND	3.57	1.42	1.37
13	A	1127	CL7	C1D-ND	3.57	1.42	1.37
13	B	1202	CL7	C1D-ND	3.56	1.42	1.37
14	B	1023	PHO	C1D-C2D	3.54	1.43	1.39
16	A	4014	A1JPJ	C14-C13	3.54	1.40	1.35
13	B	1226	CL7	C1D-ND	3.54	1.42	1.37
13	B	1210	CL7	C1D-ND	3.54	1.42	1.37
13	A	1139	CL7	C4B-NB	3.54	1.42	1.37
13	B	1225	CL7	C1D-ND	3.54	1.42	1.37
13	B	1238	CL7	C1D-ND	3.53	1.42	1.37
16	I	4118	A1JPJ	C17-C18	3.53	1.40	1.35
13	A	1123	CL7	C1D-ND	3.52	1.42	1.37
16	L	4019	A1JPJ	C21-C22	3.52	1.40	1.35
16	A	4014	A1JPJ	C10-C9	3.52	1.40	1.35
13	B	1227	CL7	C4B-NB	3.49	1.42	1.37
13	J	1301	CL7	C4B-NB	3.49	1.42	1.37
14	B	1023	PHO	C4D-CHA	3.49	1.45	1.39
13	B	1211	CL7	C1D-ND	3.49	1.42	1.37
13	I	1601	CL7	C4B-NB	3.48	1.42	1.37
13	A	1101	CL7	C4B-NB	3.48	1.42	1.37
13	B	1233	CL7	C4B-NB	3.48	1.42	1.37
13	A	1128	CL7	C1D-ND	3.48	1.42	1.37
16	A	4008	A1JPJ	C10-C9	3.47	1.40	1.35
16	L	4019	A1JPJ	C10-C9	3.47	1.40	1.35
16	L	4019	A1JPJ	C14-C13	3.47	1.40	1.35
13	B	1206	CL7	C1D-ND	3.47	1.42	1.37
16	I	4118	A1JPJ	C14-C13	3.46	1.40	1.35
13	B	1237	CL7	C1D-ND	3.46	1.42	1.37
13	K	1402	CL7	C4B-NB	3.46	1.42	1.37
13	A	1102	CL7	C4B-NB	3.46	1.42	1.37
16	B	4011	A1JPJ	C17-C18	3.45	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1109	CL7	C4B-NB	3.45	1.42	1.37
13	A	1140	CL7	C4B-NB	3.44	1.42	1.37
13	B	1226	CL7	C4B-NB	3.44	1.42	1.37
14	A	1013	PHO	C4D-CHA	3.43	1.45	1.39
13	J	1302	CL7	C4B-NB	3.43	1.42	1.37
13	K	1401	CL7	C4B-NB	3.43	1.42	1.37
16	B	4011	A1JPJ	C21-C22	3.42	1.40	1.35
13	A	1123	CL7	C4B-NB	3.42	1.42	1.37
13	B	1224	CL7	C4B-NB	3.42	1.42	1.37
13	B	1228	CL7	C4B-NB	3.42	1.42	1.37
13	B	1231	CL7	C4B-NB	3.41	1.42	1.37
13	A	1108	CL7	C4B-NB	3.41	1.42	1.37
13	F	1701	CL7	C4B-NB	3.40	1.42	1.37
13	B	1217	CL7	C4B-NB	3.39	1.42	1.37
13	A	1121	CL7	C4B-NB	3.39	1.42	1.37
13	B	1239	CL7	C4B-NB	3.39	1.41	1.37
13	B	1213	CL7	C4B-NB	3.38	1.41	1.37
13	A	1131	CL7	C4B-NB	3.38	1.41	1.37
13	A	1141	CL7	C4B-NB	3.38	1.41	1.37
16	A	4007	A1JPJ	C10-C9	3.37	1.40	1.35
13	A	1128	CL7	C4B-NB	3.37	1.41	1.37
13	B	1236	CL7	C4B-NB	3.37	1.41	1.37
13	B	1216	CL7	C4B-NB	3.35	1.41	1.37
13	A	1105	CL7	C4B-NB	3.35	1.41	1.37
13	A	1134	CL7	C4B-NB	3.35	1.41	1.37
13	A	1117	CL7	C4B-NB	3.35	1.41	1.37
13	A	1137	CL7	C4B-NB	3.35	1.41	1.37
13	B	1208	CL7	C4B-NB	3.34	1.41	1.37
13	B	1232	CL7	C4B-NB	3.34	1.41	1.37
13	B	1219	CL7	C4B-NB	3.34	1.41	1.37
13	B	1218	CL7	C4B-NB	3.34	1.41	1.37
13	B	1221	CL7	C4B-NB	3.33	1.41	1.37
13	B	1241	CL7	C4B-NB	3.33	1.41	1.37
13	A	1120	CL7	C4B-NB	3.32	1.41	1.37
13	B	1206	CL7	C4B-NB	3.32	1.41	1.37
13	A	1118	CL7	C4B-NB	3.31	1.41	1.37
13	B	1204	CL7	C4B-NB	3.31	1.41	1.37
13	L	1503	CL7	C4B-NB	3.31	1.41	1.37
13	B	1022	CL7	C4B-NB	3.31	1.41	1.37
13	L	1501	CL7	C4B-NB	3.30	1.41	1.37
13	B	1209	CL7	C4B-NB	3.30	1.41	1.37
13	A	1115	CL7	C4B-NB	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1201	CL7	C4B-NB	3.30	1.41	1.37
13	A	1114	CL7	C4B-NB	3.30	1.41	1.37
13	A	1110	CL7	C4B-NB	3.29	1.41	1.37
13	A	1012	CL7	C4D-ND	-3.29	1.33	1.37
13	A	1106	CL7	C4B-NB	3.29	1.41	1.37
13	A	1130	CL7	C4B-NB	3.29	1.41	1.37
16	I	4118	A1JPJ	C10-C9	3.28	1.40	1.35
13	B	1222	CL7	C4B-NB	3.28	1.41	1.37
13	B	1202	CL7	C4B-NB	3.28	1.41	1.37
13	B	1237	CL7	C4B-NB	3.28	1.41	1.37
13	B	1215	CL7	C4B-NB	3.27	1.41	1.37
13	B	1021	CL7	C4B-NB	3.27	1.41	1.37
13	A	1104	CL7	C4B-NB	3.27	1.41	1.37
13	B	1223	CL7	C4B-NB	3.27	1.41	1.37
13	B	1235	CL7	C4B-NB	3.27	1.41	1.37
13	A	1136	CL7	C4B-NB	3.27	1.41	1.37
13	A	1129	CL7	C4D-ND	-3.27	1.33	1.37
13	B	1214	CL7	C4B-NB	3.26	1.41	1.37
13	A	1127	CL7	C4B-NB	3.26	1.41	1.37
13	L	1502	CL7	C4D-ND	-3.25	1.33	1.37
13	B	1212	CL7	C4B-NB	3.25	1.41	1.37
13	A	1126	CL7	C4B-NB	3.25	1.41	1.37
13	B	1211	CL7	C4B-NB	3.24	1.41	1.37
13	A	1129	CL7	C4B-NB	3.24	1.41	1.37
13	B	1205	CL7	C4B-NB	3.24	1.41	1.37
13	A	1107	CL7	C4B-NB	3.24	1.41	1.37
13	A	1113	CL7	C4B-NB	3.24	1.41	1.37
13	A	1116	CL7	C4B-NB	3.24	1.41	1.37
13	A	1133	CL7	C4B-NB	3.24	1.41	1.37
13	A	1125	CL7	C4D-ND	-3.24	1.33	1.37
13	B	1220	CL7	C4B-NB	3.24	1.41	1.37
13	A	1122	CL7	C4B-NB	3.23	1.41	1.37
13	B	1234	CL7	C4B-NB	3.22	1.41	1.37
13	B	1203	CL7	C4D-ND	-3.22	1.33	1.37
13	B	1204	CL7	C4D-ND	-3.22	1.33	1.37
13	A	1119	CL7	C4B-NB	3.22	1.41	1.37
13	B	1203	CL7	C4B-NB	3.21	1.41	1.37
13	A	1112	CL7	C4B-NB	3.20	1.41	1.37
16	B	4021	A1JPJ	C8-C9	-3.20	1.39	1.45
13	B	1230	CL7	C4B-NB	3.20	1.41	1.37
13	B	1210	CL7	C4B-NB	3.20	1.41	1.37
13	B	1207	CL7	C4D-ND	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1124	CL7	C4B-NB	3.19	1.41	1.37
16	A	4007	A1JPJ	C8-C9	-3.19	1.39	1.45
13	B	1238	CL7	C4B-NB	3.17	1.41	1.37
13	A	1124	CL7	C4D-ND	-3.17	1.33	1.37
13	J	1301	CL7	C3D-C4D	3.17	1.48	1.39
13	B	1225	CL7	C4B-NB	3.17	1.41	1.37
13	B	1202	CL7	C4D-ND	-3.17	1.33	1.37
13	B	1211	CL7	C4D-ND	-3.16	1.33	1.37
13	A	1105	CL7	C4D-ND	-3.16	1.33	1.37
13	A	1103	CL7	C4B-NB	3.16	1.41	1.37
13	A	1130	CL7	C4D-ND	-3.16	1.33	1.37
13	A	1135	CL7	C4D-ND	-3.16	1.33	1.37
13	A	1138	CL7	C4B-NB	3.16	1.41	1.37
13	B	1236	CL7	C4D-ND	-3.15	1.33	1.37
13	A	1117	CL7	C4D-ND	-3.15	1.33	1.37
13	A	1137	CL7	C4D-ND	-3.15	1.33	1.37
13	A	1136	CL7	C4D-ND	-3.15	1.33	1.37
13	A	1012	CL7	C4B-NB	3.15	1.41	1.37
13	B	1231	CL7	C3B-C4B	3.14	1.50	1.42
13	B	1222	CL7	C4D-ND	-3.14	1.33	1.37
13	B	1212	CL7	C4D-ND	-3.14	1.33	1.37
13	I	1601	CL7	C3D-C4D	3.14	1.48	1.39
13	B	1225	CL7	C4D-ND	-3.14	1.33	1.37
13	B	1233	CL7	C3B-C4B	3.14	1.50	1.42
13	A	1101	CL7	C3B-C4B	3.14	1.50	1.42
13	A	1116	CL7	C4D-ND	-3.13	1.33	1.37
13	A	1113	CL7	C4D-ND	-3.13	1.33	1.37
13	A	1133	CL7	C4D-ND	-3.13	1.33	1.37
13	B	1238	CL7	C3B-C4B	3.12	1.50	1.42
13	B	1239	CL7	C4D-ND	-3.12	1.33	1.37
13	B	1223	CL7	C4D-ND	-3.12	1.33	1.37
13	B	1208	CL7	C4D-ND	-3.12	1.33	1.37
13	A	1119	CL7	C4D-ND	-3.12	1.33	1.37
13	B	1227	CL7	C4D-ND	-3.12	1.33	1.37
13	J	1302	CL7	C3D-C4D	3.11	1.48	1.39
13	B	1221	CL7	C3D-C4D	3.11	1.48	1.39
13	B	1232	CL7	C3B-C4B	3.11	1.50	1.42
13	L	1501	CL7	C3D-C4D	3.11	1.48	1.39
13	B	1233	CL7	C3D-C4D	3.11	1.48	1.39
13	B	1217	CL7	C3D-C4D	3.11	1.48	1.39
13	A	1123	CL7	C4D-ND	-3.10	1.33	1.37
13	K	1402	CL7	C3D-C4D	3.10	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1109	CL7	C3D-C4D	3.10	1.48	1.39
13	A	1102	CL7	C3B-C4B	3.10	1.50	1.42
13	A	1132	CL7	C4B-NB	3.10	1.41	1.37
13	B	1218	CL7	C3D-C4D	3.10	1.48	1.39
13	F	1701	CL7	C3D-C4D	3.10	1.48	1.39
13	B	1215	CL7	C4D-ND	-3.10	1.33	1.37
13	J	1302	CL7	C3B-C4B	3.10	1.50	1.42
13	A	1139	CL7	C3D-C4D	3.10	1.48	1.39
13	B	1021	CL7	C4D-ND	-3.10	1.33	1.37
13	A	1103	CL7	C4D-ND	-3.10	1.33	1.37
13	B	1238	CL7	C4D-ND	-3.10	1.33	1.37
13	A	1131	CL7	C4D-ND	-3.10	1.33	1.37
13	K	1401	CL7	C3D-C4D	3.10	1.48	1.39
13	B	1219	CL7	C3D-C4D	3.10	1.48	1.39
13	A	1112	CL7	C4D-ND	-3.10	1.33	1.37
13	A	1138	CL7	C4D-ND	-3.10	1.33	1.37
13	A	1139	CL7	C3B-C4B	3.10	1.50	1.42
13	B	1232	CL7	C3D-C4D	3.10	1.48	1.39
13	A	1101	CL7	C3D-C4D	3.10	1.48	1.39
13	B	1210	CL7	C4D-ND	-3.09	1.33	1.37
13	B	1213	CL7	C3D-C4D	3.09	1.48	1.39
13	A	1122	CL7	C4D-ND	-3.09	1.33	1.37
13	B	1224	CL7	C3B-C4B	3.09	1.50	1.42
13	J	1301	CL7	C3B-C4B	3.09	1.50	1.42
13	A	1130	CL7	C3B-C4B	3.09	1.50	1.42
13	A	1135	CL7	C4B-NB	3.09	1.41	1.37
13	B	1217	CL7	C3B-C4B	3.09	1.50	1.42
16	I	4118	A1JPJ	C8-C9	-3.09	1.39	1.45
13	B	1235	CL7	C4D-ND	-3.09	1.33	1.37
13	B	1209	CL7	C3B-C4B	3.09	1.50	1.42
13	A	1113	CL7	C3B-C4B	3.09	1.50	1.42
13	A	1116	CL7	C3B-C4B	3.09	1.50	1.42
13	B	1228	CL7	C3B-C4B	3.09	1.50	1.42
13	A	1110	CL7	C3D-C4D	3.09	1.48	1.39
13	B	1229	CL7	C3D-C4D	3.08	1.48	1.39
13	A	1132	CL7	C4D-ND	-3.08	1.33	1.37
13	A	1125	CL7	C4B-NB	3.08	1.41	1.37
13	B	1214	CL7	C4D-ND	-3.08	1.33	1.37
13	B	1230	CL7	C4D-ND	-3.08	1.33	1.37
13	B	1241	CL7	C3B-C4B	3.08	1.50	1.42
13	A	1111	CL7	C4B-NB	3.08	1.41	1.37
13	B	1237	CL7	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1121	CL7	C4D-ND	-3.08	1.33	1.37
13	B	1201	CL7	C4D-ND	-3.08	1.33	1.37
13	A	1108	CL7	C4D-ND	-3.08	1.33	1.37
13	A	1140	CL7	C3B-C4B	3.08	1.50	1.42
13	A	1124	CL7	C3B-C4B	3.08	1.50	1.42
13	L	1502	CL7	C4B-NB	3.07	1.41	1.37
13	A	1114	CL7	C4D-ND	-3.07	1.33	1.37
13	A	1112	CL7	C3D-C4D	3.07	1.48	1.39
13	B	1210	CL7	C3B-C4B	3.07	1.49	1.42
13	A	1127	CL7	C4D-ND	-3.07	1.33	1.37
13	A	1106	CL7	C3B-C4B	3.07	1.49	1.42
13	B	1208	CL7	C3B-C4B	3.07	1.49	1.42
13	K	1401	CL7	C3B-C4B	3.07	1.49	1.42
13	A	1104	CL7	C4D-ND	-3.07	1.33	1.37
13	B	1227	CL7	C3D-C4D	3.06	1.48	1.39
13	A	1120	CL7	C3D-C4D	3.06	1.48	1.39
13	A	1134	CL7	C3D-C4D	3.06	1.48	1.39
13	A	1109	CL7	C3B-C4B	3.06	1.49	1.42
13	B	1220	CL7	C3D-C4D	3.06	1.48	1.39
13	A	1102	CL7	C3D-C4D	3.06	1.48	1.39
13	B	1206	CL7	C4D-ND	-3.06	1.33	1.37
13	B	1234	CL7	C4D-ND	-3.06	1.33	1.37
13	A	1107	CL7	C4D-ND	-3.06	1.33	1.37
13	A	1128	CL7	C4D-ND	-3.06	1.33	1.37
13	I	1601	CL7	C3B-C4B	3.05	1.49	1.42
13	L	1503	CL7	C3B-C4B	3.05	1.49	1.42
13	A	1105	CL7	C3B-C4B	3.05	1.49	1.42
13	B	1222	CL7	C3B-C4B	3.05	1.49	1.42
13	A	1107	CL7	C3B-C4B	3.05	1.49	1.42
13	A	1108	CL7	C3B-C4B	3.05	1.49	1.42
13	A	1121	CL7	C3B-C4B	3.05	1.49	1.42
13	A	1129	CL7	C3B-C4B	3.05	1.49	1.42
13	A	1118	CL7	C4D-ND	-3.05	1.33	1.37
13	A	1111	CL7	C4D-ND	-3.05	1.33	1.37
13	B	1218	CL7	C3B-C4B	3.05	1.49	1.42
13	A	1106	CL7	C4D-ND	-3.05	1.33	1.37
13	B	1237	CL7	C3B-C4B	3.05	1.49	1.42
13	B	1205	CL7	C4D-ND	-3.04	1.33	1.37
13	A	1108	CL7	C3D-C4D	3.04	1.47	1.39
13	A	1140	CL7	C4D-ND	-3.04	1.33	1.37
16	B	4011	A1JPJ	C8-C9	-3.04	1.39	1.45
13	B	1022	CL7	C3D-C4D	3.04	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1102	CL7	C4D-ND	-3.04	1.33	1.37
13	B	1209	CL7	C3D-C4D	3.04	1.47	1.39
13	A	1104	CL7	C3B-C4B	3.04	1.49	1.42
13	B	1231	CL7	C4D-ND	-3.04	1.33	1.37
13	A	1115	CL7	C4D-ND	-3.04	1.33	1.37
13	B	1212	CL7	C3D-C4D	3.04	1.47	1.39
13	L	1503	CL7	C3D-C4D	3.03	1.47	1.39
13	B	1201	CL7	C3D-C4D	3.03	1.47	1.39
13	B	1216	CL7	C4D-ND	-3.03	1.33	1.37
13	A	1134	CL7	C3B-C4B	3.03	1.49	1.42
13	K	1402	CL7	C3B-C4B	3.03	1.49	1.42
13	B	1209	CL7	C4D-ND	-3.03	1.33	1.37
16	A	4008	A1JPJ	C8-C9	-3.03	1.39	1.45
13	B	1221	CL7	C3B-C4B	3.03	1.49	1.42
13	A	1125	CL7	C3B-C4B	3.03	1.49	1.42
13	A	1141	CL7	C3D-C4D	3.03	1.47	1.39
13	B	1226	CL7	C3B-C4B	3.03	1.49	1.42
13	B	1202	CL7	C3B-C4B	3.03	1.49	1.42
13	B	1241	CL7	C3D-C4D	3.03	1.47	1.39
13	A	1107	CL7	C3D-C4D	3.03	1.47	1.39
13	A	1114	CL7	C3D-C4D	3.02	1.47	1.39
13	B	1227	CL7	C3B-C4B	3.02	1.49	1.42
13	F	1701	CL7	C3B-C4B	3.02	1.49	1.42
13	A	1113	CL7	C3D-C4D	3.02	1.47	1.39
13	B	1224	CL7	C4D-ND	-3.02	1.33	1.37
13	A	1133	CL7	C3D-C4D	3.02	1.47	1.39
13	B	1216	CL7	C3D-C4D	3.02	1.47	1.39
13	A	1140	CL7	C3D-C4D	3.02	1.47	1.39
13	B	1021	CL7	C3D-C4D	3.02	1.47	1.39
13	A	1115	CL7	C3D-C4D	3.02	1.47	1.39
13	B	1205	CL7	C3B-C4B	3.02	1.49	1.42
13	B	1231	CL7	C3D-C4D	3.02	1.47	1.39
13	B	1223	CL7	C3B-C4B	3.02	1.49	1.42
13	A	1117	CL7	C3B-C4B	3.02	1.49	1.42
13	B	1241	CL7	C4D-ND	-3.02	1.33	1.37
13	A	1104	CL7	C3D-C4D	3.02	1.47	1.39
16	A	4014	A1JPJ	C8-C9	-3.01	1.39	1.45
13	B	1235	CL7	C3B-C4B	3.01	1.49	1.42
13	A	1137	CL7	C3D-C4D	3.01	1.47	1.39
13	A	1105	CL7	C3D-C4D	3.01	1.47	1.39
13	F	1701	CL7	C4D-ND	-3.01	1.33	1.37
13	B	1208	CL7	C3D-C4D	3.01	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1103	CL7	C3B-C4B	3.01	1.49	1.42
16	L	4020	A1JPJ	C8-C9	-3.01	1.39	1.45
13	B	1238	CL7	C3D-C4D	3.01	1.47	1.39
13	A	1126	CL7	C3B-C4B	3.01	1.49	1.42
13	A	1118	CL7	C3D-C4D	3.01	1.47	1.39
13	B	1022	CL7	C4D-ND	-3.01	1.33	1.37
13	A	1110	CL7	C3B-C4B	3.01	1.49	1.42
13	B	1210	CL7	C3D-C4D	3.01	1.47	1.39
13	A	1128	CL7	C3D-C4D	3.01	1.47	1.39
13	B	1211	CL7	C3B-C4B	3.01	1.49	1.42
13	B	1228	CL7	C3D-C4D	3.01	1.47	1.39
13	B	1204	CL7	C3B-C4B	3.00	1.49	1.42
13	A	1132	CL7	C3D-C4D	3.00	1.47	1.39
13	A	1120	CL7	C4D-ND	-3.00	1.33	1.37
13	B	1205	CL7	C3D-C4D	3.00	1.47	1.39
13	A	1119	CL7	C3B-C4B	3.00	1.49	1.42
13	B	1206	CL7	C3D-C4D	3.00	1.47	1.39
13	A	1127	CL7	C3B-C4B	3.00	1.49	1.42
13	B	1220	CL7	C4D-ND	-3.00	1.33	1.37
13	B	1213	CL7	C3B-C4B	3.00	1.49	1.42
13	B	1216	CL7	C3B-C4B	3.00	1.49	1.42
13	A	1115	CL7	C3B-C4B	3.00	1.49	1.42
13	A	1133	CL7	C3B-C4B	3.00	1.49	1.42
13	A	1101	CL7	C4D-ND	-3.00	1.33	1.37
13	B	1225	CL7	C3B-C4B	3.00	1.49	1.42
13	B	1224	CL7	C3D-C4D	3.00	1.47	1.39
13	B	1212	CL7	C3B-C4B	3.00	1.49	1.42
13	B	1234	CL7	C3D-C4D	3.00	1.47	1.39
13	A	1106	CL7	C3D-C4D	2.99	1.47	1.39
13	A	1135	CL7	C3B-C4B	2.99	1.49	1.42
13	B	1204	CL7	C3D-C4D	2.99	1.47	1.39
13	A	1114	CL7	C3B-C4B	2.99	1.49	1.42
13	A	1120	CL7	C3B-C4B	2.99	1.49	1.42
13	A	1128	CL7	C3B-C4B	2.99	1.49	1.42
13	A	1134	CL7	C4D-ND	-2.99	1.33	1.37
13	A	1136	CL7	C3B-C4B	2.99	1.49	1.42
13	A	1112	CL7	C3B-C4B	2.99	1.49	1.42
13	B	1207	CL7	C4B-NB	2.99	1.41	1.37
13	A	1122	CL7	C3D-C4D	2.99	1.47	1.39
13	A	1117	CL7	C3D-C4D	2.99	1.47	1.39
13	B	1230	CL7	C3D-C4D	2.99	1.47	1.39
13	B	1218	CL7	C4D-ND	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1111	CL7	C3D-C4D	2.98	1.47	1.39
13	B	1228	CL7	C4D-ND	-2.98	1.33	1.37
13	A	1141	CL7	C4D-ND	-2.98	1.33	1.37
13	B	1211	CL7	C3D-C4D	2.98	1.47	1.39
13	L	1503	CL7	C4D-ND	-2.98	1.33	1.37
13	B	1239	CL7	C3D-C4D	2.98	1.47	1.39
13	B	1226	CL7	C3D-C4D	2.98	1.47	1.39
13	A	1131	CL7	C3D-C4D	2.98	1.47	1.39
13	A	1123	CL7	C3D-C4D	2.98	1.47	1.39
13	B	1220	CL7	C3B-C4B	2.98	1.49	1.42
13	L	1501	CL7	C4D-ND	-2.98	1.33	1.37
13	B	1222	CL7	C3D-C4D	2.98	1.47	1.39
13	A	1122	CL7	C3B-C4B	2.98	1.49	1.42
13	B	1236	CL7	C3D-C4D	2.97	1.47	1.39
13	B	1223	CL7	C3D-C4D	2.97	1.47	1.39
13	A	1119	CL7	C3D-C4D	2.97	1.47	1.39
13	A	1136	CL7	C3D-C4D	2.97	1.47	1.39
13	A	1126	CL7	C3D-C4D	2.97	1.47	1.39
13	B	1021	CL7	C3B-C4B	2.97	1.49	1.42
13	A	1116	CL7	C3D-C4D	2.97	1.47	1.39
13	K	1401	CL7	C4D-ND	-2.97	1.33	1.37
13	B	1229	CL7	C3B-C4B	2.97	1.49	1.42
13	B	1226	CL7	C4D-ND	-2.97	1.33	1.37
13	A	1127	CL7	C3D-C4D	2.97	1.47	1.39
13	B	1236	CL7	C3B-C4B	2.96	1.49	1.42
13	B	1237	CL7	C3D-C4D	2.96	1.47	1.39
13	B	1219	CL7	C3B-C4B	2.96	1.49	1.42
13	A	1121	CL7	C3D-C4D	2.96	1.47	1.39
13	B	1239	CL7	C3B-C4B	2.96	1.49	1.42
13	A	1141	CL7	C3B-C4B	2.95	1.49	1.42
13	B	1215	CL7	C3B-C4B	2.95	1.49	1.42
13	A	1138	CL7	C3D-C4D	2.95	1.47	1.39
13	A	1103	CL7	C3D-C4D	2.95	1.47	1.39
13	B	1214	CL7	C3B-C4B	2.95	1.49	1.42
13	A	1130	CL7	C3D-C4D	2.95	1.47	1.39
13	A	1118	CL7	C3B-C4B	2.94	1.49	1.42
13	B	1215	CL7	C3D-C4D	2.94	1.47	1.39
13	B	1207	CL7	C3D-C4D	2.94	1.47	1.39
13	B	1203	CL7	C3D-C4D	2.94	1.47	1.39
13	B	1225	CL7	C3D-C4D	2.94	1.47	1.39
13	I	1601	CL7	C4D-ND	-2.94	1.33	1.37
13	B	1214	CL7	C3D-C4D	2.94	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1012	CL7	C3D-C4D	2.94	1.47	1.39
13	B	1203	CL7	C3B-C4B	2.94	1.49	1.42
13	A	1131	CL7	C3B-C4B	2.94	1.49	1.42
13	B	1229	CL7	C4D-ND	-2.94	1.33	1.37
13	A	1129	CL7	C3D-C4D	2.93	1.47	1.39
13	B	1201	CL7	C3B-C4B	2.93	1.49	1.42
13	B	1235	CL7	C3D-C4D	2.93	1.47	1.39
13	A	1126	CL7	C4D-ND	-2.93	1.33	1.37
13	B	1234	CL7	C3B-C4B	2.93	1.49	1.42
13	B	1230	CL7	C3B-C4B	2.93	1.49	1.42
13	B	1207	CL7	C3B-C4B	2.93	1.49	1.42
13	L	1502	CL7	C3D-C4D	2.93	1.47	1.39
13	B	1202	CL7	C3D-C4D	2.92	1.47	1.39
13	B	1217	CL7	C4D-ND	-2.92	1.33	1.37
16	B	4008	A1JPJ	C8-C9	-2.92	1.39	1.45
16	L	4019	A1JPJ	C8-C9	-2.92	1.39	1.45
13	A	1137	CL7	C3B-C4B	2.91	1.49	1.42
13	A	1124	CL7	C3D-C4D	2.91	1.47	1.39
13	B	1233	CL7	C4D-ND	-2.91	1.33	1.37
13	B	1022	CL7	C3B-C4B	2.91	1.49	1.42
13	A	1139	CL7	C4D-ND	-2.91	1.33	1.37
16	B	4004	A1JPJ	C8-C9	-2.91	1.39	1.45
13	J	1301	CL7	C4D-ND	-2.91	1.33	1.37
13	A	1138	CL7	C3B-C4B	2.91	1.49	1.42
13	J	1302	CL7	C4D-ND	-2.91	1.33	1.37
13	K	1402	CL7	C4D-ND	-2.91	1.33	1.37
16	B	4009	A1JPJ	C8-C9	-2.91	1.39	1.45
13	A	1125	CL7	C3D-C4D	2.90	1.47	1.39
13	A	1111	CL7	C3B-C4B	2.90	1.49	1.42
13	B	1219	CL7	C4D-ND	-2.90	1.33	1.37
13	L	1501	CL7	C3B-C4B	2.89	1.49	1.42
13	B	1206	CL7	C3B-C4B	2.89	1.49	1.42
16	B	4006	A1JPJ	C8-C9	-2.89	1.39	1.45
13	L	1502	CL7	C3B-C4B	2.88	1.49	1.42
13	A	1135	CL7	C3D-C4D	2.88	1.47	1.39
13	A	1123	CL7	C3B-C4B	2.88	1.49	1.42
13	A	1109	CL7	C4D-ND	-2.87	1.33	1.37
13	B	1213	CL7	C4D-ND	-2.84	1.33	1.37
13	A	1110	CL7	C4D-ND	-2.84	1.33	1.37
16	A	4001	A1JPJ	C8-C9	-2.83	1.39	1.45
13	B	1232	CL7	C4D-ND	-2.82	1.33	1.37
13	A	1132	CL7	C3B-C4B	2.80	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	4007	A1JPJ	C8-C9	-2.80	1.39	1.45
13	B	1221	CL7	C4D-ND	-2.79	1.33	1.37
16	J	4013	A1JPJ	C8-C9	-2.79	1.40	1.45
14	B	1023	PHO	CMC-C2C	-2.78	1.46	1.50
16	L	4023	A1JPJ	C8-C9	-2.78	1.40	1.45
16	A	4002	A1JPJ	C8-C9	-2.75	1.40	1.45
16	F	4016	A1JPJ	C8-C9	-2.74	1.40	1.45
16	A	4003	A1JPJ	C8-C9	-2.70	1.40	1.45
16	B	4005	A1JPJ	C8-C9	-2.68	1.40	1.45
16	I	4118	A1JPJ	C12-C13	-2.68	1.40	1.45
13	J	1301	CL7	C1B-C2B	2.66	1.49	1.43
16	J	4012	A1JPJ	C8-C9	-2.64	1.40	1.45
14	A	1013	PHO	CMC-C2C	-2.64	1.46	1.50
13	F	1701	CL7	C1B-C2B	2.63	1.49	1.43
16	I	4118	A1JPJ	C19-C18	-2.63	1.40	1.45
13	A	1012	CL7	C3B-C4B	2.62	1.48	1.42
20	A	1011	G9R	CMD-C2D	-2.62	1.46	1.51
13	A	1102	CL7	CHC-C1C	2.61	1.43	1.38
13	J	1302	CL7	C1B-C2B	2.61	1.49	1.43
13	B	1201	CL7	CHC-C1C	2.61	1.43	1.38
13	B	1227	CL7	C1B-C2B	2.60	1.49	1.43
16	A	4014	A1JPJ	C12-C13	-2.59	1.40	1.45
13	K	1401	CL7	C1B-C2B	2.59	1.49	1.43
13	B	1218	CL7	C1B-C2B	2.59	1.49	1.43
13	B	1022	CL7	C1B-C2B	2.59	1.49	1.43
13	B	1241	CL7	C1B-C2B	2.58	1.49	1.43
13	A	1139	CL7	C1B-C2B	2.56	1.49	1.43
13	I	1601	CL7	C1B-C2B	2.55	1.49	1.43
13	B	1211	CL7	C1B-C2B	2.55	1.49	1.43
16	A	4008	A1JPJ	C12-C13	-2.55	1.40	1.45
20	A	1011	G9R	CMB-C2B	-2.55	1.46	1.51
16	B	4011	A1JPJ	C19-C18	-2.54	1.40	1.45
16	A	4007	A1JPJ	C12-C13	-2.54	1.40	1.45
13	K	1402	CL7	C1B-C2B	2.54	1.49	1.43
13	B	1213	CL7	C1B-C2B	2.54	1.49	1.43
13	B	1209	CL7	C1B-C2B	2.54	1.49	1.43
13	A	1110	CL7	C1B-C2B	2.54	1.49	1.43
13	B	1232	CL7	C1B-C2B	2.53	1.49	1.43
13	B	1231	CL7	C1B-C2B	2.53	1.49	1.43
16	I	4118	A1JPJ	C23-C22	-2.52	1.40	1.45
13	B	1217	CL7	C1B-C2B	2.52	1.49	1.43
13	A	1134	CL7	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1220	CL7	C1B-C2B	2.52	1.49	1.43
13	A	1121	CL7	C1B-C2B	2.52	1.49	1.43
13	A	1108	CL7	C1B-C2B	2.51	1.49	1.43
16	B	4021	A1JPJ	C12-C13	-2.51	1.40	1.45
16	B	4008	A1JPJ	C19-C18	-2.51	1.40	1.45
13	B	1230	CL7	CHC-C1C	2.51	1.43	1.38
13	A	1101	CL7	C1B-C2B	2.50	1.49	1.43
13	A	1118	CL7	C1B-C2B	2.50	1.49	1.43
13	B	1212	CL7	C1B-C2B	2.50	1.49	1.43
13	A	1131	CL7	C1B-C2B	2.49	1.49	1.43
13	B	1021	CL7	CHC-C1C	2.49	1.43	1.38
13	A	1130	CL7	CHC-C1C	2.49	1.43	1.38
13	B	1223	CL7	C1B-C2B	2.49	1.49	1.43
16	A	4014	A1JPJ	C19-C18	-2.49	1.40	1.45
14	B	1023	PHO	CMD-C2D	-2.49	1.46	1.51
13	A	1136	CL7	C1B-C2B	2.48	1.49	1.43
13	A	1105	CL7	C1B-C2B	2.48	1.49	1.43
13	A	1112	CL7	CHC-C1C	2.48	1.43	1.38
13	L	1503	CL7	C1B-C2B	2.48	1.49	1.43
13	B	1208	CL7	C1B-C2B	2.48	1.49	1.43
16	L	4019	A1JPJ	C19-C18	-2.48	1.40	1.45
14	A	1013	PHO	CMD-C2D	-2.48	1.46	1.51
13	B	1229	CL7	C1B-C2B	2.48	1.49	1.43
13	B	1239	CL7	C1B-C2B	2.48	1.49	1.43
13	B	1219	CL7	C1B-C2B	2.47	1.49	1.43
13	B	1201	CL7	C1B-C2B	2.47	1.49	1.43
14	A	1013	PHO	CAC-C3C	-2.47	1.47	1.51
13	A	1109	CL7	C1B-C2B	2.47	1.49	1.43
13	A	1114	CL7	C1B-C2B	2.47	1.49	1.43
13	B	1222	CL7	C1B-C2B	2.47	1.49	1.43
16	A	4007	A1JPJ	C19-C18	-2.47	1.40	1.45
13	B	1233	CL7	C1B-C2B	2.46	1.49	1.43
13	A	1126	CL7	CHC-C1C	2.46	1.43	1.38
16	A	4008	A1JPJ	C19-C18	-2.46	1.40	1.45
13	B	1216	CL7	CHC-C1C	2.46	1.43	1.38
13	A	1107	CL7	C1B-C2B	2.46	1.49	1.43
13	A	1140	CL7	C1B-C2B	2.46	1.49	1.43
13	B	1228	CL7	C1B-C2B	2.45	1.49	1.43
13	B	1202	CL7	C1B-C2B	2.45	1.49	1.43
13	A	1111	CL7	C1B-C2B	2.45	1.49	1.43
13	A	1138	CL7	C1B-C2B	2.45	1.49	1.43
13	L	1502	CL7	C1B-C2B	2.45	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1238	CL7	CHC-C1C	2.45	1.43	1.38
13	A	1141	CL7	C1B-C2B	2.45	1.49	1.43
14	A	1013	PHO	CMB-C2B	-2.45	1.46	1.51
14	B	1023	PHO	CMB-C2B	-2.44	1.46	1.51
13	B	1210	CL7	CHC-C1C	2.44	1.43	1.38
16	L	4020	A1JPJ	C12-C13	-2.44	1.40	1.45
13	A	1115	CL7	C1B-C2B	2.44	1.49	1.43
13	A	1122	CL7	C1B-C2B	2.44	1.49	1.43
16	L	4019	A1JPJ	C12-C13	-2.44	1.40	1.45
16	L	4019	A1JPJ	C23-C22	-2.44	1.40	1.45
13	B	1203	CL7	C1B-C2B	2.44	1.49	1.43
13	B	1216	CL7	C1B-C2B	2.44	1.49	1.43
20	A	1011	G9R	CMC-C2C	-2.44	1.46	1.50
16	B	4011	A1JPJ	C23-C22	-2.44	1.40	1.45
16	B	4011	A1JPJ	C12-C13	-2.44	1.40	1.45
13	A	1125	CL7	C1B-C2B	2.43	1.49	1.43
13	A	1112	CL7	C1B-C2B	2.43	1.49	1.43
13	B	1235	CL7	C1B-C2B	2.43	1.49	1.43
13	A	1104	CL7	C1B-C2B	2.43	1.49	1.43
13	A	1123	CL7	CHC-C1C	2.43	1.43	1.38
16	B	4004	A1JPJ	C12-C13	-2.43	1.40	1.45
13	A	1106	CL7	CHC-C1C	2.42	1.43	1.38
13	A	1103	CL7	C1B-C2B	2.42	1.49	1.43
13	B	1207	CL7	C1B-C2B	2.42	1.49	1.43
14	B	1023	PHO	C3B-C2B	-2.42	1.37	1.40
16	B	4004	A1JPJ	C19-C18	-2.42	1.40	1.45
13	B	1224	CL7	CHC-C1C	2.42	1.43	1.38
13	A	1139	CL7	CHC-C1C	2.42	1.43	1.38
13	B	1231	CL7	CHC-C1C	2.42	1.43	1.38
14	A	1013	PHO	C3D-C4D	2.42	1.44	1.41
13	A	1128	CL7	CMB-C2B	-2.42	1.45	1.50
13	B	1205	CL7	C1B-C2B	2.42	1.48	1.43
13	B	1226	CL7	CMB-C2B	-2.41	1.45	1.50
13	L	1503	CL7	CHC-C1C	2.41	1.43	1.38
13	B	1237	CL7	C1B-C2B	2.41	1.48	1.43
13	A	1133	CL7	C1B-C2B	2.41	1.48	1.43
13	L	1501	CL7	C1B-C2B	2.41	1.48	1.43
13	A	1120	CL7	C1B-C2B	2.41	1.48	1.43
13	A	1133	CL7	CHC-C1C	2.40	1.43	1.38
16	B	4006	A1JPJ	C19-C18	-2.40	1.40	1.45
13	A	1104	CL7	CHC-C1C	2.40	1.43	1.38
16	L	4020	A1JPJ	C19-C18	-2.40	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	4008	A1JPJ	C23-C22	-2.40	1.40	1.45
13	A	1137	CL7	C1B-C2B	2.40	1.48	1.43
16	B	4008	A1JPJ	C12-C13	-2.40	1.40	1.45
13	A	1012	CL7	C1B-C2B	2.40	1.48	1.43
13	B	1210	CL7	C1B-C2B	2.40	1.48	1.43
13	A	1106	CL7	C1B-C2B	2.40	1.48	1.43
16	B	4009	A1JPJ	C12-C13	-2.40	1.40	1.45
13	B	1241	CL7	CHC-C1C	2.40	1.43	1.38
13	A	1132	CL7	C1B-C2B	2.40	1.48	1.43
13	B	1219	CL7	CHC-C1C	2.40	1.43	1.38
16	B	4007	A1JPJ	C19-C18	-2.39	1.40	1.45
13	B	1236	CL7	C1B-C2B	2.39	1.48	1.43
13	A	1116	CL7	CHC-C1C	2.39	1.43	1.38
13	A	1129	CL7	CHC-C1C	2.39	1.43	1.38
13	A	1140	CL7	CHC-C1C	2.39	1.43	1.38
16	B	4021	A1JPJ	C19-C18	-2.39	1.40	1.45
13	B	1237	CL7	CHC-C1C	2.39	1.43	1.38
13	B	1225	CL7	C1B-C2B	2.39	1.48	1.43
13	A	1127	CL7	C1B-C2B	2.38	1.48	1.43
13	L	1501	CL7	CHC-C1C	2.38	1.43	1.38
13	B	1221	CL7	C1B-C2B	2.38	1.48	1.43
13	A	1135	CL7	C1B-C2B	2.38	1.48	1.43
13	A	1103	CL7	CHC-C1C	2.38	1.43	1.38
13	B	1204	CL7	C1B-C2B	2.37	1.48	1.43
13	A	1124	CL7	CHC-C1C	2.37	1.43	1.38
13	A	1124	CL7	C1B-C2B	2.37	1.48	1.43
13	A	1128	CL7	C1B-C2B	2.37	1.48	1.43
13	A	1105	CL7	CHC-C1C	2.37	1.43	1.38
13	B	1206	CL7	C1B-C2B	2.37	1.48	1.43
20	A	1011	G9R	CAC-C3C	-2.37	1.47	1.51
13	A	1101	CL7	CHC-C1C	2.36	1.43	1.38
13	F	1701	CL7	CHC-C1C	2.36	1.43	1.38
13	B	1206	CL7	CMB-C2B	-2.36	1.45	1.50
13	A	1134	CL7	CHC-C1C	2.36	1.43	1.38
16	L	4020	A1JPJ	C23-C22	-2.36	1.40	1.45
13	A	1119	CL7	CHC-C1C	2.36	1.43	1.38
13	B	1224	CL7	C1B-C2B	2.36	1.48	1.43
16	L	4023	A1JPJ	C19-C18	-2.36	1.40	1.45
13	A	1113	CL7	C1B-C2B	2.35	1.48	1.43
16	L	4023	A1JPJ	C12-C13	-2.35	1.40	1.45
16	A	4001	A1JPJ	C12-C13	-2.35	1.40	1.45
13	B	1233	CL7	CHC-C1C	2.35	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1302	CL7	CHC-C1C	2.35	1.43	1.38
13	A	1110	CL7	CHC-C1C	2.35	1.42	1.38
13	A	1120	CL7	CHC-C1C	2.35	1.42	1.38
13	B	1202	CL7	CHC-C1C	2.35	1.42	1.38
13	B	1215	CL7	C1B-C2B	2.35	1.48	1.43
13	A	1102	CL7	C1B-C2B	2.35	1.48	1.43
13	B	1208	CL7	CHC-C1C	2.34	1.42	1.38
16	B	4006	A1JPJ	C12-C13	-2.34	1.40	1.45
13	B	1231	CL7	C1D-C2D	2.34	1.48	1.43
13	B	1234	CL7	CHC-C1C	2.34	1.42	1.38
13	L	1502	CL7	CHC-C1C	2.34	1.42	1.38
13	A	1126	CL7	C1B-C2B	2.34	1.48	1.43
13	A	1119	CL7	C1B-C2B	2.34	1.48	1.43
13	A	1113	CL7	CHC-C1C	2.34	1.42	1.38
16	B	4007	A1JPJ	C23-C22	-2.34	1.40	1.45
13	B	1022	CL7	CHC-C1C	2.34	1.42	1.38
13	I	1601	CL7	CHC-C1C	2.34	1.42	1.38
13	A	1012	CL7	CHC-C1C	2.34	1.42	1.38
13	A	1135	CL7	CHC-C1C	2.34	1.42	1.38
13	A	1116	CL7	C1B-C2B	2.33	1.48	1.43
13	B	1021	CL7	C1B-C2B	2.33	1.48	1.43
13	K	1402	CL7	CHC-C1C	2.33	1.42	1.38
16	B	4008	A1JPJ	C23-C22	-2.33	1.40	1.45
13	B	1214	CL7	CMB-C2B	-2.33	1.45	1.50
13	B	1203	CL7	CHC-C1C	2.33	1.42	1.38
16	A	4014	A1JPJ	C23-C22	-2.33	1.40	1.45
13	A	1108	CL7	CHC-C1C	2.33	1.42	1.38
14	B	1023	PHO	CAC-C3C	-2.33	1.47	1.51
16	J	4013	A1JPJ	C19-C18	-2.32	1.41	1.45
13	A	1127	CL7	CHC-C1C	2.32	1.42	1.38
13	B	1235	CL7	CHC-C1C	2.32	1.42	1.38
16	A	4002	A1JPJ	C12-C13	-2.32	1.41	1.45
13	B	1228	CL7	CHC-C1C	2.32	1.42	1.38
13	B	1207	CL7	CHC-C1C	2.32	1.42	1.38
13	K	1401	CL7	CHC-C1C	2.32	1.42	1.38
13	A	1121	CL7	CHC-C1C	2.32	1.42	1.38
13	A	1115	CL7	CHC-C1C	2.32	1.42	1.38
20	A	1011	G9R	C4D-CHA	2.32	1.43	1.40
16	J	4013	A1JPJ	C12-C13	-2.32	1.41	1.45
14	B	1023	PHO	C3B-CAB	-2.32	1.43	1.47
13	B	1218	CL7	CHC-C1C	2.32	1.42	1.38
16	A	4007	A1JPJ	C23-C22	-2.32	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1213	CL7	CHC-C1C	2.32	1.42	1.38
13	A	1141	CL7	CMB-C2B	-2.31	1.45	1.50
13	A	1117	CL7	CHC-C1C	2.31	1.42	1.38
13	A	1122	CL7	CHC-C1C	2.31	1.42	1.38
13	B	1221	CL7	CHC-C1C	2.31	1.42	1.38
13	B	1223	CL7	CHC-C1C	2.31	1.42	1.38
13	A	1117	CL7	C1B-C2B	2.31	1.48	1.43
13	B	1232	CL7	CHC-C1C	2.31	1.42	1.38
13	A	1136	CL7	CHC-C1C	2.31	1.42	1.38
13	B	1230	CL7	C1B-C2B	2.31	1.48	1.43
13	B	1236	CL7	CHC-C1C	2.30	1.42	1.38
13	A	1137	CL7	CHC-C1C	2.30	1.42	1.38
13	B	1234	CL7	C1B-C2B	2.30	1.48	1.43
16	F	4016	A1JPJ	C12-C13	-2.30	1.41	1.45
13	B	1217	CL7	CHC-C1C	2.30	1.42	1.38
13	B	1227	CL7	CHC-C1C	2.30	1.42	1.38
13	B	1204	CL7	CHC-C1C	2.30	1.42	1.38
13	A	1125	CL7	CHC-C1C	2.30	1.42	1.38
16	B	4005	A1JPJ	C19-C18	-2.30	1.41	1.45
16	B	4007	A1JPJ	C12-C13	-2.29	1.41	1.45
13	B	1211	CL7	CHC-C1C	2.29	1.42	1.38
13	J	1302	CL7	C1D-C2D	2.29	1.48	1.43
14	A	1013	PHO	C3B-C2B	-2.29	1.37	1.40
16	B	4021	A1JPJ	C23-C22	-2.28	1.41	1.45
13	A	1129	CL7	C1B-C2B	2.28	1.48	1.43
13	B	1214	CL7	CHC-C1C	2.28	1.42	1.38
13	B	1238	CL7	C1B-C2B	2.28	1.48	1.43
13	B	1212	CL7	CHC-C1C	2.28	1.42	1.38
13	A	1123	CL7	CMB-C2B	-2.27	1.46	1.50
13	A	1130	CL7	C1B-C2B	2.27	1.48	1.43
16	B	4006	A1JPJ	C23-C22	-2.27	1.41	1.45
13	A	1132	CL7	CHC-C1C	2.27	1.42	1.38
13	A	1107	CL7	CHC-C1C	2.27	1.42	1.38
13	B	1230	CL7	MG-NB	-2.26	2.01	2.05
16	J	4012	A1JPJ	C19-C18	-2.26	1.41	1.45
13	B	1226	CL7	CMD-C2D	-2.26	1.46	1.50
13	B	1215	CL7	CHC-C1C	2.26	1.42	1.38
13	A	1114	CL7	CHC-C1C	2.25	1.42	1.38
13	B	1222	CL7	CHC-C1C	2.25	1.42	1.38
13	B	1225	CL7	CHC-C1C	2.25	1.42	1.38
13	A	1131	CL7	CHC-C1C	2.25	1.42	1.38
16	A	4001	A1JPJ	C23-C22	-2.25	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1226	CL7	CHC-C1C	2.25	1.42	1.38
13	A	1123	CL7	MG-NB	-2.25	2.01	2.05
16	L	4023	A1JPJ	C23-C22	-2.25	1.41	1.45
16	F	4016	A1JPJ	C23-C22	-2.24	1.41	1.45
13	A	1102	CL7	C1D-C2D	2.24	1.48	1.43
13	B	1214	CL7	MG-NB	-2.24	2.01	2.05
13	B	1229	CL7	CMB-C2B	-2.24	1.46	1.50
13	B	1234	CL7	MG-NB	-2.24	2.01	2.05
13	L	1501	CL7	CMB-C2B	-2.24	1.46	1.50
13	B	1239	CL7	CHC-C1C	2.24	1.42	1.38
13	A	1107	CL7	CMD-C2D	-2.24	1.46	1.50
13	J	1301	CL7	CHC-C1C	2.23	1.42	1.38
13	B	1226	CL7	C1B-C2B	2.23	1.48	1.43
14	B	1023	PHO	C3D-C4D	2.23	1.44	1.41
13	B	1233	CL7	C1D-C2D	2.23	1.48	1.43
13	A	1109	CL7	CHC-C1C	2.23	1.42	1.38
13	A	1117	CL7	CMB-C2B	-2.23	1.46	1.50
13	A	1103	CL7	C1D-C2D	2.23	1.48	1.43
13	B	1206	CL7	MG-NB	-2.23	2.01	2.05
16	F	4016	A1JPJ	C19-C18	-2.23	1.41	1.45
13	A	1118	CL7	CHC-C1C	2.22	1.42	1.38
13	B	1209	CL7	CHC-C1C	2.22	1.42	1.38
16	B	4004	A1JPJ	C23-C22	-2.22	1.41	1.45
13	L	1503	CL7	C1D-C2D	2.22	1.48	1.43
13	B	1206	CL7	CHC-C1C	2.22	1.42	1.38
13	B	1216	CL7	C1D-C2D	2.22	1.48	1.43
13	A	1123	CL7	CMD-C2D	-2.22	1.46	1.50
13	B	1220	CL7	CHC-C1C	2.22	1.42	1.38
13	B	1219	CL7	C1D-C2D	2.22	1.48	1.43
13	B	1205	CL7	CHC-C1C	2.20	1.42	1.38
13	A	1135	CL7	MG-NB	-2.20	2.01	2.05
13	B	1221	CL7	C2A-C1A	2.20	1.54	1.50
13	I	1601	CL7	C1D-C2D	2.20	1.48	1.43
13	A	1111	CL7	CHC-C1C	2.20	1.42	1.38
13	B	1216	CL7	CMB-C2B	-2.20	1.46	1.50
13	A	1123	CL7	C1B-C2B	2.20	1.48	1.43
13	B	1232	CL7	C1D-C2D	2.20	1.48	1.43
13	A	1138	CL7	CHC-C1C	2.20	1.42	1.38
13	A	1122	CL7	C1D-C2D	2.20	1.48	1.43
13	B	1230	CL7	C1D-C2D	2.20	1.48	1.43
13	L	1501	CL7	C1D-C2D	2.20	1.48	1.43
13	A	1128	CL7	CHC-C1C	2.19	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	1502	CL7	C1D-C2D	2.19	1.48	1.43
13	B	1211	CL7	CMD-C2D	-2.19	1.46	1.50
13	B	1210	CL7	MG-NB	-2.19	2.01	2.05
13	B	1228	CL7	C1D-C2D	2.19	1.48	1.43
13	A	1131	CL7	CMB-C2B	-2.19	1.46	1.50
13	A	1012	CL7	MG-NB	-2.19	2.01	2.05
13	B	1214	CL7	C1B-C2B	2.19	1.48	1.43
13	B	1207	CL7	MG-NB	-2.19	2.01	2.05
13	B	1238	CL7	CMD-C2D	-2.19	1.46	1.50
13	A	1141	CL7	MG-NB	-2.18	2.01	2.05
13	B	1216	CL7	MG-NB	-2.18	2.01	2.05
13	B	1241	CL7	C1D-C2D	2.18	1.48	1.43
13	F	1701	CL7	C1D-C2D	2.18	1.48	1.43
13	A	1141	CL7	CHC-C1C	2.18	1.42	1.38
13	K	1401	CL7	C1D-C2D	2.18	1.48	1.43
13	A	1111	CL7	MG-NB	-2.18	2.01	2.05
13	K	1402	CL7	C1D-C2D	2.18	1.48	1.43
13	A	1132	CL7	C1D-C2D	2.17	1.48	1.43
13	A	1108	CL7	C1D-C2D	2.17	1.48	1.43
13	B	1217	CL7	C1D-C2D	2.17	1.48	1.43
13	L	1502	CL7	MG-NB	-2.17	2.01	2.05
13	B	1215	CL7	CMB-C2B	-2.17	1.46	1.50
13	B	1215	CL7	MG-NB	-2.17	2.01	2.05
13	B	1205	CL7	CMD-C2D	-2.17	1.46	1.50
13	A	1117	CL7	C1D-C2D	2.16	1.48	1.43
14	A	1013	PHO	C4D-ND	-2.16	1.35	1.38
13	A	1125	CL7	CMC-C2C	-2.16	1.46	1.50
13	A	1130	CL7	CMB-C2B	-2.16	1.46	1.50
14	B	1023	PHO	C4D-ND	-2.16	1.35	1.38
13	B	1223	CL7	MG-NB	-2.16	2.01	2.05
16	B	4009	A1JPJ	C23-C22	-2.16	1.41	1.45
13	A	1119	CL7	MG-NB	-2.16	2.01	2.05
13	A	1137	CL7	MG-NB	-2.16	2.01	2.05
13	B	1205	CL7	CMC-C2C	-2.16	1.46	1.50
13	B	1022	CL7	CMC-C2C	-2.15	1.46	1.50
13	A	1138	CL7	MG-NB	-2.15	2.01	2.05
13	A	1132	CL7	MG-NB	-2.15	2.01	2.05
16	A	4003	A1JPJ	C12-C13	-2.15	1.41	1.45
13	A	1133	CL7	C1D-C2D	2.15	1.48	1.43
13	A	1114	CL7	C1D-C2D	2.15	1.48	1.43
13	A	1132	CL7	CMB-C2B	-2.15	1.46	1.50
13	A	1136	CL7	MG-NB	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1116	CL7	CMB-C2B	-2.15	1.46	1.50
13	B	1201	CL7	CMB-C2B	-2.15	1.46	1.50
13	B	1234	CL7	CMB-C2B	-2.15	1.46	1.50
13	A	1121	CL7	C1D-C2D	2.15	1.48	1.43
13	B	1022	CL7	CMD-C2D	-2.15	1.46	1.50
13	B	1237	CL7	C1D-C2D	2.15	1.48	1.43
13	A	1105	CL7	C1D-C2D	2.15	1.48	1.43
13	B	1209	CL7	C1D-C2D	2.15	1.48	1.43
13	B	1227	CL7	C1D-C2D	2.15	1.48	1.43
13	B	1202	CL7	MG-NB	-2.15	2.01	2.05
16	B	4021	A1JPJ	C2-C3	-2.15	1.47	1.52
13	A	1112	CL7	MG-NB	-2.15	2.01	2.05
13	B	1237	CL7	CMB-C2B	-2.15	1.46	1.50
13	A	1118	CL7	C1D-C2D	2.15	1.48	1.43
13	A	1117	CL7	MG-NB	-2.15	2.01	2.05
13	A	1119	CL7	CMB-C2B	-2.14	1.46	1.50
13	B	1212	CL7	CMB-C2B	-2.14	1.46	1.50
13	A	1112	CL7	CMB-C2B	-2.14	1.46	1.50
13	B	1226	CL7	MG-NB	-2.14	2.01	2.05
13	B	1239	CL7	MG-NB	-2.14	2.01	2.05
13	A	1105	CL7	CMD-C2D	-2.14	1.46	1.50
13	A	1112	CL7	C1D-C2D	2.14	1.48	1.43
13	B	1220	CL7	MG-NB	-2.14	2.01	2.05
13	A	1119	CL7	C1D-C2D	2.14	1.48	1.43
13	A	1012	CL7	CMB-C2B	-2.14	1.46	1.50
13	B	1203	CL7	MG-NB	-2.14	2.01	2.05
13	B	1021	CL7	MG-NB	-2.14	2.01	2.05
13	L	1502	CL7	CMD-C2D	-2.14	1.46	1.50
13	A	1140	CL7	C1D-C2D	2.14	1.48	1.43
13	B	1230	CL7	CMB-C2B	-2.14	1.46	1.50
13	A	1130	CL7	MG-NB	-2.14	2.01	2.05
13	A	1133	CL7	CMB-C2B	-2.13	1.46	1.50
13	B	1210	CL7	C1D-C2D	2.13	1.48	1.43
13	A	1101	CL7	C1D-C2D	2.13	1.48	1.43
13	L	1503	CL7	CMB-C2B	-2.13	1.46	1.50
16	J	4012	A1JPJ	C12-C13	-2.13	1.41	1.45
13	A	1114	CL7	CMB-C2B	-2.13	1.46	1.50
13	A	1115	CL7	CMC-C2C	-2.13	1.46	1.50
13	B	1229	CL7	CHC-C1C	2.13	1.42	1.38
13	B	1218	CL7	C1D-C2D	2.13	1.48	1.43
13	A	1136	CL7	C1D-C2D	2.13	1.48	1.43
13	B	1222	CL7	MG-NB	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1136	CL7	CMB-C2B	-2.13	1.46	1.50
13	A	1111	CL7	C1D-C2D	2.13	1.48	1.43
13	A	1118	CL7	CMB-C2B	-2.13	1.46	1.50
13	B	1236	CL7	CMD-C2D	-2.13	1.46	1.50
13	B	1235	CL7	C1D-C2D	2.13	1.48	1.43
13	B	1221	CL7	CMB-C2B	-2.13	1.46	1.50
13	B	1220	CL7	C1D-C2D	2.13	1.48	1.43
13	A	1127	CL7	CMD-C2D	-2.13	1.46	1.50
14	A	1013	PHO	C3B-CAB	-2.13	1.43	1.47
13	A	1135	CL7	CMD-C2D	-2.13	1.46	1.50
13	A	1107	CL7	MG-NB	-2.12	2.01	2.05
13	A	1116	CL7	MG-NB	-2.12	2.01	2.05
13	B	1225	CL7	C1D-C2D	2.12	1.48	1.43
13	A	1126	CL7	CMB-C2B	-2.12	1.46	1.50
13	A	1120	CL7	MG-NB	-2.12	2.01	2.05
13	A	1128	CL7	MG-NB	-2.12	2.01	2.05
13	B	1021	CL7	CMD-C2D	-2.12	1.46	1.50
13	A	1129	CL7	MG-NB	-2.12	2.01	2.05
13	A	1135	CL7	CMB-C2B	-2.12	1.46	1.50
13	B	1228	CL7	CMD-C2D	-2.12	1.46	1.50
13	B	1215	CL7	C1D-C2D	2.12	1.48	1.43
13	A	1106	CL7	CMB-C2B	-2.12	1.46	1.50
13	A	1126	CL7	C1D-C2D	2.12	1.48	1.43
13	L	1502	CL7	CMB-C2B	-2.12	1.46	1.50
13	B	1238	CL7	C1D-C2D	2.12	1.48	1.43
16	J	4013	A1JPJ	C23-C22	-2.11	1.41	1.45
13	A	1121	CL7	CMD-C2D	-2.11	1.46	1.50
13	B	1201	CL7	MG-NB	-2.11	2.01	2.05
13	A	1124	CL7	MG-NB	-2.11	2.01	2.05
13	A	1106	CL7	C1D-C2D	2.11	1.48	1.43
13	A	1124	CL7	CMB-C2B	-2.11	1.46	1.50
13	A	1102	CL7	MG-NB	-2.11	2.01	2.05
13	A	1113	CL7	C1D-C2D	2.11	1.48	1.43
13	A	1120	CL7	C1D-C2D	2.11	1.48	1.43
13	A	1103	CL7	CMB-C2B	-2.11	1.46	1.50
13	A	1106	CL7	MG-NB	-2.11	2.01	2.05
13	A	1012	CL7	CMD-C2D	-2.11	1.46	1.50
13	A	1130	CL7	C1D-C2D	2.11	1.48	1.43
13	A	1116	CL7	C1D-C2D	2.11	1.48	1.43
13	A	1129	CL7	CMD-C2D	-2.11	1.46	1.50
13	A	1120	CL7	CMB-C2B	-2.11	1.46	1.50
13	B	1224	CL7	C1D-C2D	2.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1134	CL7	C1D-C2D	2.11	1.48	1.43
16	A	4003	A1JPJ	C19-C18	-2.11	1.41	1.45
13	B	1207	CL7	CMB-C2B	-2.11	1.46	1.50
13	B	1204	CL7	MG-NB	-2.11	2.01	2.05
13	A	1104	CL7	C1D-C2D	2.10	1.48	1.43
13	A	1141	CL7	C1D-C2D	2.10	1.48	1.43
13	A	1138	CL7	C1D-C2D	2.10	1.48	1.43
13	A	1129	CL7	CMB-C2B	-2.10	1.46	1.50
13	L	1501	CL7	MG-NB	-2.10	2.01	2.05
13	A	1126	CL7	CMD-C2D	-2.10	1.46	1.50
13	B	1235	CL7	MG-NB	-2.10	2.01	2.05
13	B	1202	CL7	CMB-C2B	-2.10	1.46	1.50
13	B	1212	CL7	MG-NB	-2.10	2.01	2.05
13	A	1125	CL7	MG-NB	-2.10	2.01	2.05
13	B	1202	CL7	CMD-C2D	-2.10	1.46	1.50
13	A	1126	CL7	MG-NB	-2.10	2.01	2.05
13	B	1210	CL7	CMB-C2B	-2.10	1.46	1.50
13	A	1124	CL7	C1D-C2D	2.09	1.48	1.43
13	B	1230	CL7	CMD-C2D	-2.09	1.46	1.50
13	B	1235	CL7	CMB-C2B	-2.09	1.46	1.50
13	B	1236	CL7	C1D-C2D	2.09	1.48	1.43
13	B	1221	CL7	CMD-C2D	-2.09	1.46	1.50
13	B	1239	CL7	CMD-C2D	-2.09	1.46	1.50
13	B	1213	CL7	C1D-C2D	2.09	1.48	1.43
13	B	1224	CL7	CMB-C2B	-2.09	1.46	1.50
13	A	1115	CL7	CMD-C2D	-2.09	1.46	1.50
13	B	1211	CL7	C1D-C2D	2.09	1.48	1.43
13	A	1107	CL7	CMB-C2B	-2.09	1.46	1.50
13	A	1137	CL7	C1D-C2D	2.09	1.48	1.43
13	F	1701	CL7	CMD-C2D	-2.09	1.46	1.50
13	B	1234	CL7	CMD-C2D	-2.09	1.46	1.50
13	A	1114	CL7	CMD-C2D	-2.09	1.46	1.50
13	A	1125	CL7	CMB-C2B	-2.09	1.46	1.50
13	A	1127	CL7	C1D-C2D	2.09	1.48	1.43
13	A	1108	CL7	CMB-C2B	-2.09	1.46	1.50
13	B	1234	CL7	C1D-C2D	2.09	1.48	1.43
13	A	1131	CL7	C1D-C2D	2.09	1.48	1.43
20	A	1011	G9R	C3B-C2B	-2.09	1.37	1.40
13	A	1103	CL7	CMD-C2D	-2.09	1.46	1.50
13	A	1118	CL7	CMD-C2D	-2.09	1.46	1.50
13	J	1301	CL7	CMD-C2D	-2.09	1.46	1.50
13	A	1117	CL7	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1204	CL7	C1D-C2D	2.09	1.48	1.43
13	B	1205	CL7	CMB-C2B	-2.09	1.46	1.50
13	B	1239	CL7	CMB-C2B	-2.09	1.46	1.50
13	B	1222	CL7	C1D-C2D	2.09	1.48	1.43
13	B	1211	CL7	MG-NB	-2.08	2.01	2.05
13	B	1228	CL7	MG-NB	-2.08	2.01	2.05
13	B	1236	CL7	MG-NB	-2.08	2.01	2.05
13	A	1122	CL7	MG-NB	-2.08	2.01	2.05
13	B	1207	CL7	C1D-C2D	2.08	1.48	1.43
13	B	1225	CL7	CMB-C2B	-2.08	1.46	1.50
13	B	1235	CL7	CMD-C2D	-2.08	1.46	1.50
13	A	1115	CL7	CMB-C2B	-2.08	1.46	1.50
13	B	1239	CL7	C1D-C2D	2.08	1.48	1.43
13	A	1133	CL7	MG-NB	-2.08	2.01	2.05
13	B	1021	CL7	CMB-C2B	-2.08	1.46	1.50
13	B	1201	CL7	CMC-C2C	-2.08	1.46	1.50
13	A	1107	CL7	C1D-C2D	2.08	1.48	1.43
13	A	1139	CL7	C1D-C2D	2.08	1.48	1.43
13	A	1140	CL7	CMD-C2D	-2.08	1.46	1.50
13	B	1237	CL7	CMD-C2D	-2.08	1.46	1.50
13	A	1106	CL7	CMD-C2D	-2.07	1.46	1.50
13	A	1112	CL7	CMD-C2D	-2.07	1.46	1.50
13	A	1128	CL7	CMD-C2D	-2.07	1.46	1.50
13	A	1140	CL7	CMB-C2B	-2.07	1.46	1.50
13	B	1237	CL7	MG-NB	-2.07	2.01	2.05
13	K	1402	CL7	CBD-CAD	2.07	1.56	1.51
13	A	1131	CL7	MG-NB	-2.07	2.01	2.05
13	B	1225	CL7	MG-NB	-2.07	2.01	2.05
13	B	1202	CL7	C1D-C2D	2.07	1.48	1.43
13	B	1215	CL7	CMD-C2D	-2.07	1.46	1.50
13	B	1221	CL7	MG-NB	-2.07	2.01	2.05
13	A	1108	CL7	CMD-C2D	-2.07	1.46	1.50
13	J	1301	CL7	MG-NB	-2.07	2.01	2.05
13	B	1208	CL7	C1D-C2D	2.07	1.48	1.43
13	A	1012	CL7	C1D-C2D	2.07	1.48	1.43
13	L	1503	CL7	MG-NB	-2.07	2.01	2.05
13	B	1214	CL7	C1D-C2D	2.07	1.48	1.43
13	B	1208	CL7	CMD-C2D	-2.07	1.46	1.50
13	B	1225	CL7	CMD-C2D	-2.07	1.46	1.50
13	A	1109	CL7	C1D-C2D	2.07	1.48	1.43
13	B	1208	CL7	CMB-C2B	-2.07	1.46	1.50
13	A	1124	CL7	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1219	CL7	CMB-C2B	-2.07	1.46	1.50
13	B	1203	CL7	CMD-C2D	-2.07	1.46	1.50
13	B	1212	CL7	CMD-C2D	-2.07	1.46	1.50
13	B	1223	CL7	CMD-C2D	-2.07	1.46	1.50
13	B	1213	CL7	CMD-C2D	-2.07	1.46	1.50
13	B	1228	CL7	CMB-C2B	-2.07	1.46	1.50
13	A	1122	CL7	CMB-C2B	-2.07	1.46	1.50
13	A	1133	CL7	CMD-C2D	-2.07	1.46	1.50
13	A	1119	CL7	CMD-C2D	-2.06	1.46	1.50
13	B	1222	CL7	CMB-C2B	-2.06	1.46	1.50
13	A	1129	CL7	C1D-C2D	2.06	1.48	1.43
13	A	1104	CL7	MG-NB	-2.06	2.01	2.05
13	A	1137	CL7	CMB-C2B	-2.06	1.46	1.50
13	B	1206	CL7	CMC-C2C	-2.06	1.46	1.50
13	A	1104	CL7	CMB-C2B	-2.06	1.46	1.50
13	A	1131	CL7	CMD-C2D	-2.06	1.46	1.50
13	I	1601	CL7	CMC-C2C	-2.06	1.46	1.50
13	B	1208	CL7	MG-NB	-2.06	2.01	2.05
13	B	1231	CL7	CMB-C2B	-2.06	1.46	1.50
13	B	1231	CL7	CMD-C2D	-2.06	1.46	1.50
13	A	1104	CL7	CMD-C2D	-2.06	1.46	1.50
13	A	1130	CL7	CMD-C2D	-2.06	1.46	1.50
13	A	1110	CL7	MG-NB	-2.06	2.01	2.05
13	B	1217	CL7	MG-NB	-2.06	2.01	2.05
13	B	1227	CL7	CMB-C2B	-2.06	1.46	1.50
13	B	1205	CL7	MG-NB	-2.06	2.01	2.05
13	A	1127	CL7	CMB-C2B	-2.06	1.46	1.50
13	A	1139	CL7	CMD-C2D	-2.06	1.46	1.50
13	B	1021	CL7	C1D-C2D	2.06	1.48	1.43
13	B	1223	CL7	C1D-C2D	2.05	1.48	1.43
13	A	1103	CL7	MG-NB	-2.05	2.01	2.05
13	A	1114	CL7	MG-NB	-2.05	2.01	2.05
13	B	1204	CL7	CMD-C2D	-2.05	1.46	1.50
13	A	1127	CL7	MG-NB	-2.05	2.01	2.05
13	L	1503	CL7	CMD-C2D	-2.05	1.46	1.50
13	A	1116	CL7	CMD-C2D	-2.05	1.46	1.50
13	A	1116	CL7	CMC-C2C	-2.05	1.46	1.50
13	A	1136	CL7	CMD-C2D	-2.05	1.46	1.50
16	B	4009	A1JPJ	C20-C19	2.05	1.39	1.34
13	B	1207	CL7	CMD-C2D	-2.05	1.46	1.50
13	A	1139	CL7	MG-NB	-2.05	2.01	2.05
13	A	1138	CL7	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1134	CL7	CMB-C2B	-2.05	1.46	1.50
13	B	1226	CL7	C1D-C2D	2.05	1.48	1.43
13	B	1204	CL7	CMB-C2B	-2.05	1.46	1.50
13	B	1205	CL7	C1D-C2D	2.05	1.48	1.43
13	A	1111	CL7	CMB-C2B	-2.05	1.46	1.50
13	B	1238	CL7	MG-NB	-2.05	2.01	2.05
13	B	1216	CL7	CMD-C2D	-2.05	1.46	1.50
13	A	1121	CL7	CMB-C2B	-2.05	1.46	1.50
13	B	1209	CL7	CMB-C2B	-2.05	1.46	1.50
13	A	1121	CL7	MG-NB	-2.05	2.01	2.05
13	B	1218	CL7	CMD-C2D	-2.05	1.46	1.50
13	B	1236	CL7	CMB-C2B	-2.05	1.46	1.50
13	A	1134	CL7	MG-NB	-2.05	2.01	2.05
13	B	1206	CL7	CMD-C2D	-2.05	1.46	1.50
13	B	1223	CL7	CMC-C2C	-2.04	1.46	1.50
13	B	1232	CL7	CMB-C2B	-2.04	1.46	1.50
13	B	1211	CL7	CMB-C2B	-2.04	1.46	1.50
13	B	1224	CL7	MG-NB	-2.04	2.01	2.05
13	B	1022	CL7	CMB-C2B	-2.04	1.46	1.50
13	B	1203	CL7	CMB-C2B	-2.04	1.46	1.50
13	A	1118	CL7	MG-NB	-2.04	2.01	2.05
13	B	1217	CL7	CMD-C2D	-2.04	1.46	1.50
13	B	1209	CL7	CMD-C2D	-2.04	1.46	1.50
13	A	1134	CL7	CMD-C2D	-2.04	1.46	1.50
13	B	1201	CL7	CMD-C2D	-2.04	1.46	1.50
13	B	1217	CL7	CMB-C2B	-2.04	1.46	1.50
13	A	1113	CL7	CMB-C2B	-2.04	1.46	1.50
13	B	1201	CL7	C1D-C2D	2.04	1.48	1.43
13	B	1222	CL7	CMD-C2D	-2.04	1.46	1.50
13	B	1214	CL7	CMD-C2D	-2.04	1.46	1.50
13	B	1241	CL7	CMB-C2B	-2.04	1.46	1.50
13	A	1105	CL7	CMB-C2B	-2.04	1.46	1.50
16	A	4001	A1JPJ	C20-C19	2.04	1.39	1.34
16	B	4005	A1JPJ	C11-C12	2.04	1.39	1.34
13	K	1401	CL7	CMB-C2B	-2.04	1.46	1.50
13	B	1229	CL7	CMD-C2D	-2.04	1.46	1.50
13	J	1301	CL7	CMB-C2B	-2.04	1.46	1.50
13	A	1113	CL7	MG-NB	-2.03	2.01	2.05
13	A	1125	CL7	CMD-C2D	-2.03	1.46	1.50
13	B	1224	CL7	CMD-C2D	-2.03	1.46	1.50
13	A	1103	CL7	CMC-C2C	-2.03	1.46	1.50
13	A	1130	CL7	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1203	CL7	C1D-C2D	2.03	1.48	1.43
13	B	1221	CL7	C1D-C2D	2.03	1.48	1.43
13	B	1219	CL7	CMD-C2D	-2.03	1.46	1.50
13	A	1137	CL7	CMD-C2D	-2.03	1.46	1.50
13	A	1138	CL7	CMB-C2B	-2.03	1.46	1.50
13	A	1110	CL7	CMB-C2B	-2.03	1.46	1.50
13	A	1115	CL7	C1D-C2D	2.03	1.48	1.43
13	B	1221	CL7	CMC-C2C	-2.03	1.46	1.50
13	K	1402	CL7	MG-NB	-2.03	2.01	2.05
13	F	1701	CL7	MG-NB	-2.03	2.01	2.05
13	A	1101	CL7	CMB-C2B	-2.03	1.46	1.50
13	J	1301	CL7	C1D-C2D	2.03	1.48	1.43
13	B	1241	CL7	CMD-C2D	-2.03	1.46	1.50
13	A	1113	CL7	CMD-C2D	-2.03	1.46	1.50
13	B	1227	CL7	CMD-C2D	-2.03	1.46	1.50
13	A	1119	CL7	CMC-C2C	-2.03	1.46	1.50
13	A	1108	CL7	MG-NB	-2.03	2.01	2.05
13	A	1128	CL7	C1D-C2D	2.02	1.48	1.43
13	B	1213	CL7	CMB-C2B	-2.02	1.46	1.50
13	J	1302	CL7	CMD-C2D	-2.02	1.46	1.50
13	A	1132	CL7	CMD-C2D	-2.02	1.46	1.50
13	A	1105	CL7	MG-NB	-2.02	2.01	2.05
13	B	1220	CL7	CMB-C2B	-2.02	1.46	1.50
13	I	1601	CL7	CMB-C2B	-2.02	1.46	1.50
13	A	1109	CL7	CMD-C2D	-2.02	1.46	1.50
13	I	1601	CL7	MG-NB	-2.02	2.01	2.05
13	A	1129	CL7	CMC-C2C	-2.02	1.46	1.50
13	A	1109	CL7	CMB-C2B	-2.02	1.46	1.50
13	B	1232	CL7	CMD-C2D	-2.02	1.46	1.50
13	B	1238	CL7	CMB-C2B	-2.02	1.46	1.50
13	B	1218	CL7	MG-NB	-2.02	2.01	2.05
13	A	1122	CL7	CMD-C2D	-2.02	1.46	1.50
13	F	1701	CL7	CMC-C2C	-2.02	1.46	1.50
13	A	1135	CL7	C1D-C2D	2.02	1.48	1.43
13	B	1210	CL7	CMD-C2D	-2.02	1.46	1.50
13	B	1241	CL7	MG-NB	-2.02	2.01	2.05
13	A	1115	CL7	MG-NB	-2.01	2.01	2.05
13	B	1223	CL7	CMB-C2B	-2.01	1.46	1.50
13	K	1401	CL7	CMD-C2D	-2.01	1.46	1.50
13	A	1112	CL7	CMC-C2C	-2.01	1.46	1.50
13	A	1140	CL7	CMC-C2C	-2.01	1.46	1.50
13	B	1204	CL7	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1211	CL7	CMC-C2C	-2.01	1.46	1.50
13	J	1302	CL7	MG-NB	-2.01	2.01	2.05
13	B	1209	CL7	MG-NB	-2.01	2.01	2.05
13	B	1237	CL7	CMC-C2C	-2.01	1.46	1.50
13	A	1101	CL7	CMD-C2D	-2.01	1.46	1.50
13	A	1111	CL7	CMD-C2D	-2.01	1.46	1.50
13	A	1120	CL7	CMD-C2D	-2.01	1.46	1.50
13	A	1101	CL7	CMC-C2C	-2.01	1.46	1.50
13	K	1401	CL7	MG-NB	-2.01	2.01	2.05
13	A	1104	CL7	CMC-C2C	-2.01	1.46	1.50
13	A	1113	CL7	CMC-C2C	-2.01	1.46	1.50
13	B	1212	CL7	CMC-C2C	-2.01	1.46	1.50
13	B	1218	CL7	CMB-C2B	-2.01	1.46	1.50
13	B	1225	CL7	CMC-C2C	-2.01	1.46	1.50
13	A	1102	CL7	CMD-C2D	-2.01	1.46	1.50
13	B	1229	CL7	MG-NB	-2.01	2.01	2.05
13	B	1208	CL7	CMC-C2C	-2.01	1.46	1.50
13	A	1110	CL7	CMD-C2D	-2.01	1.46	1.50
13	A	1141	CL7	CMD-C2D	-2.01	1.46	1.50
13	L	1501	CL7	CMD-C2D	-2.01	1.46	1.50
13	B	1233	CL7	MG-NB	-2.00	2.01	2.05
13	A	1110	CL7	C1D-C2D	2.00	1.48	1.43
13	A	1140	CL7	MG-NB	-2.00	2.01	2.05
13	A	1102	CL7	CMC-C2C	-2.00	1.46	1.50
13	A	1139	CL7	CMB-C2B	-2.00	1.46	1.50
13	B	1203	CL7	CMC-C2C	-2.00	1.46	1.50
13	A	1123	CL7	CMC-C2C	-2.00	1.46	1.50

All (863) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1013	PHO	C4D-CHA-CBD	-9.10	104.40	108.52
14	B	1023	PHO	C4D-CHA-CBD	-7.76	105.01	108.52
16	B	4021	A1JPJ	C15-C16-C17	6.72	137.24	123.47
16	J	4012	A1JPJ	C37-C22-C23	6.41	128.18	118.08
16	L	4019	A1JPJ	C7-C8-C9	-6.17	116.91	126.23
16	L	4019	A1JPJ	C8-C9-C10	5.84	127.91	118.94
13	B	1229	CL7	C1A-NA-C4A	5.83	109.83	106.30
13	A	1134	CL7	C1A-NA-C4A	5.81	109.82	106.30
13	B	1205	CL7	C1A-NA-C4A	5.80	109.81	106.30
13	B	1213	CL7	C1A-NA-C4A	5.77	109.79	106.30
13	J	1301	CL7	C1A-NA-C4A	5.72	109.77	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1211	CL7	C1A-NA-C4A	5.69	109.75	106.30
16	B	4021	A1JPJ	C16-C15-C14	5.69	135.13	123.47
13	A	1105	CL7	C1A-NA-C4A	5.60	109.69	106.30
13	B	1235	CL7	C1A-NA-C4A	5.59	109.69	106.30
13	K	1402	CL7	C1A-NA-C4A	5.59	109.69	106.30
16	F	4016	A1JPJ	C15-C16-C17	5.58	134.90	123.47
16	B	4011	A1JPJ	C15-C16-C17	5.58	134.90	123.47
13	A	1128	CL7	C1A-NA-C4A	5.57	109.68	106.30
13	L	1502	CL7	C1A-NA-C4A	5.57	109.67	106.30
13	B	1212	CL7	C1A-NA-C4A	5.56	109.67	106.30
13	A	1101	CL7	C1A-NA-C4A	5.54	109.66	106.30
13	B	1209	CL7	C1A-NA-C4A	5.54	109.66	106.30
13	A	1139	CL7	C1A-NA-C4A	5.54	109.66	106.30
13	A	1125	CL7	C1A-NA-C4A	5.54	109.65	106.30
16	B	4005	A1JPJ	C37-C22-C23	5.53	126.80	118.08
13	K	1401	CL7	C1A-NA-C4A	5.53	109.65	106.30
13	A	1110	CL7	C1A-NA-C4A	5.53	109.65	106.30
13	I	1601	CL7	C1A-NA-C4A	5.52	109.64	106.30
13	A	1114	CL7	C1A-NA-C4A	5.49	109.63	106.30
13	A	1137	CL7	C1A-NA-C4A	5.49	109.62	106.30
13	B	1239	CL7	C1A-NA-C4A	5.47	109.61	106.30
13	L	1501	CL7	C1A-NA-C4A	5.47	109.61	106.30
16	F	4016	A1JPJ	C16-C15-C14	5.47	134.67	123.47
13	B	1201	CL7	C1A-NA-C4A	5.45	109.60	106.30
13	A	1107	CL7	C1A-NA-C4A	5.44	109.59	106.30
13	B	1222	CL7	C1A-NA-C4A	5.41	109.58	106.30
13	B	1218	CL7	C1A-NA-C4A	5.41	109.58	106.30
13	B	1227	CL7	C1A-NA-C4A	5.41	109.58	106.30
13	A	1106	CL7	C1A-NA-C4A	5.41	109.57	106.30
13	A	1118	CL7	C1A-NA-C4A	5.41	109.57	106.30
13	J	1302	CL7	C1A-NA-C4A	5.40	109.57	106.30
13	A	1140	CL7	C1A-NA-C4A	5.40	109.57	106.30
13	A	1133	CL7	C1A-NA-C4A	5.40	109.57	106.30
13	B	1217	CL7	C1A-NA-C4A	5.39	109.57	106.30
13	A	1115	CL7	C1A-NA-C4A	5.37	109.55	106.30
13	B	1206	CL7	C1A-NA-C4A	5.36	109.55	106.30
13	B	1022	CL7	C1A-NA-C4A	5.36	109.55	106.30
13	B	1238	CL7	C1A-NA-C4A	5.36	109.54	106.30
13	B	1236	CL7	C1A-NA-C4A	5.35	109.54	106.30
13	A	1136	CL7	C1A-NA-C4A	5.35	109.54	106.30
13	B	1232	CL7	C1A-NA-C4A	5.35	109.54	106.30
13	A	1131	CL7	C1A-NA-C4A	5.35	109.54	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1220	CL7	C1A-NA-C4A	5.34	109.54	106.30
13	A	1120	CL7	C1A-NA-C4A	5.33	109.53	106.30
13	B	1221	CL7	C1A-NA-C4A	5.33	109.53	106.30
13	A	1111	CL7	C1A-NA-C4A	5.33	109.53	106.30
13	A	1103	CL7	C1A-NA-C4A	5.33	109.53	106.30
13	F	1701	CL7	C1A-NA-C4A	5.32	109.52	106.30
13	A	1141	CL7	C1A-NA-C4A	5.32	109.52	106.30
13	A	1122	CL7	C1A-NA-C4A	5.30	109.51	106.30
13	A	1109	CL7	C1A-NA-C4A	5.30	109.51	106.30
13	A	1130	CL7	C1A-NA-C4A	5.30	109.51	106.30
13	B	1208	CL7	C1A-NA-C4A	5.29	109.51	106.30
13	B	1203	CL7	C1A-NA-C4A	5.28	109.50	106.30
13	A	1113	CL7	C1A-NA-C4A	5.28	109.50	106.30
13	A	1124	CL7	C1A-NA-C4A	5.26	109.48	106.30
13	A	1117	CL7	C1A-NA-C4A	5.26	109.48	106.30
13	B	1231	CL7	C1A-NA-C4A	5.25	109.48	106.30
16	B	4008	A1JPJ	C15-C16-C17	5.25	134.23	123.47
13	A	1121	CL7	C1A-NA-C4A	5.24	109.47	106.30
13	A	1108	CL7	C1A-NA-C4A	5.24	109.47	106.30
13	A	1138	CL7	C1A-NA-C4A	5.24	109.47	106.30
13	B	1241	CL7	C1A-NA-C4A	5.23	109.47	106.30
13	B	1223	CL7	C1A-NA-C4A	5.23	109.47	106.30
13	A	1126	CL7	C1A-NA-C4A	5.23	109.47	106.30
13	L	1503	CL7	C1A-NA-C4A	5.22	109.46	106.30
13	A	1119	CL7	C1A-NA-C4A	5.21	109.46	106.30
13	A	1132	CL7	C1A-NA-C4A	5.21	109.45	106.30
13	B	1219	CL7	C1A-NA-C4A	5.20	109.45	106.30
13	B	1233	CL7	C1A-NA-C4A	5.20	109.45	106.30
13	B	1224	CL7	C1A-NA-C4A	5.18	109.44	106.30
16	A	4002	A1JPJ	C21-C20-C19	5.17	139.35	123.22
13	A	1129	CL7	C1A-NA-C4A	5.15	109.42	106.30
13	B	1230	CL7	C1A-NA-C4A	5.15	109.42	106.30
13	A	1104	CL7	C1A-NA-C4A	5.15	109.42	106.30
13	B	1202	CL7	C1A-NA-C4A	5.15	109.42	106.30
13	B	1207	CL7	C1A-NA-C4A	5.14	109.42	106.30
13	B	1226	CL7	C1A-NA-C4A	5.14	109.41	106.30
13	B	1215	CL7	C1A-NA-C4A	5.13	109.41	106.30
13	A	1112	CL7	C1A-NA-C4A	5.13	109.40	106.30
13	A	1116	CL7	C1A-NA-C4A	5.12	109.40	106.30
13	B	1214	CL7	C1A-NA-C4A	5.11	109.40	106.30
16	L	4019	A1JPJ	C34-C9-C10	-5.11	115.76	122.92
16	A	4003	A1JPJ	C37-C22-C23	5.11	126.13	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1225	CL7	C1A-NA-C4A	5.11	109.39	106.30
13	A	1102	CL7	C1A-NA-C4A	5.10	109.39	106.30
13	B	1228	CL7	C1A-NA-C4A	5.09	109.38	106.30
13	B	1237	CL7	C1A-NA-C4A	5.09	109.38	106.30
13	A	1135	CL7	C1A-NA-C4A	5.04	109.35	106.30
13	B	1216	CL7	C1A-NA-C4A	5.03	109.35	106.30
13	A	1123	CL7	C1A-NA-C4A	5.03	109.34	106.30
13	A	1127	CL7	C1A-NA-C4A	5.02	109.34	106.30
13	A	1012	CL7	C1A-NA-C4A	4.97	109.31	106.30
16	A	4002	A1JPJ	C37-C22-C23	4.95	125.87	118.08
13	B	1204	CL7	C1A-NA-C4A	4.95	109.30	106.30
13	B	1234	CL7	C1A-NA-C4A	4.90	109.27	106.30
16	J	4012	A1JPJ	C25-C26-C27	-4.87	115.47	121.47
13	B	1021	CL7	C1A-NA-C4A	4.82	109.22	106.30
13	B	1210	CL7	C1A-NA-C4A	4.78	109.19	106.30
16	B	4008	A1JPJ	C25-C26-C27	-4.74	115.64	121.47
16	B	4009	A1JPJ	C16-C15-C14	4.70	133.11	123.47
16	J	4012	A1JPJ	C16-C15-C14	4.70	133.09	123.47
16	F	4016	A1JPJ	C37-C22-C21	-4.58	116.50	122.92
16	B	4009	A1JPJ	C37-C22-C21	-4.58	116.51	122.92
16	B	4005	A1JPJ	C10-C11-C12	4.58	137.51	123.22
16	J	4012	A1JPJ	C34-C9-C10	-4.51	116.61	122.92
16	B	4005	A1JPJ	C34-C9-C10	-4.47	116.67	122.92
16	B	4007	A1JPJ	C34-C9-C10	-4.46	116.68	122.92
16	A	4003	A1JPJ	C15-C16-C17	4.44	132.58	123.47
16	F	4016	A1JPJ	C23-C22-C21	4.44	125.75	118.94
16	B	4006	A1JPJ	C37-C22-C21	-4.40	116.76	122.92
16	A	4001	A1JPJ	C16-C15-C14	4.38	132.46	123.47
16	L	4019	A1JPJ	C15-C16-C17	4.38	132.45	123.47
16	A	4001	A1JPJ	C37-C22-C21	-4.36	116.81	122.92
16	A	4003	A1JPJ	C34-C9-C10	-4.34	116.84	122.92
16	A	4008	A1JPJ	C15-C16-C17	4.32	132.32	123.47
16	B	4004	A1JPJ	C16-C15-C14	4.31	132.29	123.47
16	B	4011	A1JPJ	C37-C22-C21	-4.29	116.91	122.92
16	B	4005	A1JPJ	C8-C9-C10	4.27	125.49	118.94
16	J	4012	A1JPJ	C37-C22-C21	-4.25	116.97	122.92
16	B	4006	A1JPJ	C34-C9-C10	-4.24	116.99	122.92
16	A	4008	A1JPJ	C37-C22-C21	-4.22	117.01	122.92
16	L	4020	A1JPJ	C37-C22-C21	-4.22	117.02	122.92
16	L	4019	A1JPJ	C37-C22-C21	-4.21	117.03	122.92
16	J	4013	A1JPJ	C37-C22-C21	-4.19	117.05	122.92
16	A	4002	A1JPJ	C37-C22-C21	-4.19	117.06	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	4002	A1JPJ	C34-C9-C10	-4.14	117.12	122.92
16	A	4003	A1JPJ	C12-C13-C14	4.11	125.25	118.94
16	B	4021	A1JPJ	C37-C22-C21	-4.08	117.21	122.92
16	L	4023	A1JPJ	C37-C22-C21	-4.06	117.23	122.92
16	A	4003	A1JPJ	C37-C22-C21	-4.05	117.25	122.92
16	A	4014	A1JPJ	C37-C22-C21	-4.04	117.26	122.92
16	L	4020	A1JPJ	C34-C9-C10	-4.04	117.26	122.92
16	A	4001	A1JPJ	C34-C9-C10	-4.03	117.28	122.92
16	B	4008	A1JPJ	C34-C9-C10	-4.02	117.29	122.92
16	B	4004	A1JPJ	C37-C22-C21	-4.02	117.30	122.92
16	B	4011	A1JPJ	C34-C9-C10	-4.00	117.32	122.92
16	B	4009	A1JPJ	C34-C9-C10	-3.99	117.34	122.92
16	B	4008	A1JPJ	C37-C22-C21	-3.97	117.36	122.92
16	F	4016	A1JPJ	C19-C18-C17	3.96	125.01	118.94
16	B	4007	A1JPJ	C37-C22-C21	-3.94	117.40	122.92
16	L	4023	A1JPJ	C34-C9-C10	-3.93	117.41	122.92
16	B	4005	A1JPJ	C16-C15-C14	3.93	131.53	123.47
16	A	4008	A1JPJ	C34-C9-C10	-3.93	117.42	122.92
16	A	4002	A1JPJ	C16-C15-C14	3.92	131.50	123.47
16	B	4009	A1JPJ	C23-C22-C21	3.91	124.95	118.94
16	J	4013	A1JPJ	C34-C9-C10	-3.90	117.45	122.92
16	F	4016	A1JPJ	C36-C18-C17	-3.90	117.45	122.92
16	A	4014	A1JPJ	C34-C9-C10	-3.90	117.46	122.92
16	B	4005	A1JPJ	C37-C22-C21	-3.90	117.46	122.92
16	B	4004	A1JPJ	C34-C9-C10	-3.90	117.46	122.92
16	A	4003	A1JPJ	C35-C13-C14	-3.89	117.47	122.92
16	A	4003	A1JPJ	C16-C15-C14	3.85	131.37	123.47
16	A	4007	A1JPJ	C34-C9-C10	-3.82	117.57	122.92
16	I	4118	A1JPJ	C34-C9-C10	-3.81	117.58	122.92
16	A	4001	A1JPJ	C23-C22-C21	3.81	124.79	118.94
16	L	4023	A1JPJ	C15-C16-C17	3.80	131.26	123.47
16	B	4007	A1JPJ	C8-C9-C10	3.74	124.68	118.94
16	I	4118	A1JPJ	C37-C22-C21	-3.73	117.70	122.92
16	B	4007	A1JPJ	C35-C13-C14	-3.73	117.70	122.92
16	A	4007	A1JPJ	C37-C22-C21	-3.72	117.71	122.92
16	B	4007	A1JPJ	C12-C13-C14	3.72	124.64	118.94
13	A	1128	CL7	O2D-CGD-O1D	-3.69	116.62	123.84
16	F	4016	A1JPJ	C35-C13-C14	-3.68	117.77	122.92
16	J	4013	A1JPJ	C16-C15-C14	3.65	130.95	123.47
14	A	1013	PHO	O1D-CGD-CBD	3.63	130.78	124.74
16	A	4014	A1JPJ	C16-C15-C14	3.61	130.88	123.47
16	F	4016	A1JPJ	C11-C10-C9	3.61	132.46	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	4020	A1JPJ	C16-C15-C14	3.60	130.85	123.47
16	A	4003	A1JPJ	C8-C9-C10	3.60	124.47	118.94
16	J	4012	A1JPJ	C35-C13-C14	-3.58	117.91	122.92
16	F	4016	A1JPJ	C12-C13-C14	3.58	124.43	118.94
16	B	4006	A1JPJ	C16-C15-C14	3.58	130.80	123.47
16	A	4001	A1JPJ	C21-C20-C19	3.56	134.32	123.22
16	F	4016	A1JPJ	C10-C11-C12	3.55	134.31	123.22
16	B	4005	A1JPJ	C20-C21-C22	3.55	132.38	127.31
16	B	4009	A1JPJ	C35-C13-C14	-3.55	117.96	122.92
16	B	4021	A1JPJ	C16-C17-C18	3.53	132.35	127.31
16	B	4021	A1JPJ	C34-C9-C8	3.51	123.60	118.08
16	A	4007	A1JPJ	C15-C16-C17	3.50	130.63	123.47
16	B	4008	A1JPJ	C36-C18-C17	-3.50	118.03	122.92
13	B	1230	CL7	C3B-C4B-NB	-3.48	107.29	110.52
13	B	1229	CL7	O2D-CGD-O1D	-3.47	117.05	123.84
13	A	1110	CL7	O2D-CGD-O1D	-3.46	117.07	123.84
16	A	4008	A1JPJ	C36-C18-C17	-3.46	118.07	122.92
16	A	4001	A1JPJ	C36-C18-C17	-3.46	118.08	122.92
13	A	1112	CL7	C3B-C4B-NB	-3.43	107.33	110.52
16	J	4012	A1JPJ	C28-C27-C26	-3.41	121.58	124.85
16	J	4012	A1JPJ	C12-C13-C14	3.41	124.17	118.94
16	B	4008	A1JPJ	C28-C27-C26	-3.40	121.59	124.85
13	A	1132	CL7	O2D-CGD-O1D	-3.40	117.19	123.84
16	A	4003	A1JPJ	C36-C18-C17	-3.40	118.16	122.92
16	L	4019	A1JPJ	C36-C18-C17	-3.40	118.16	122.92
16	A	4001	A1JPJ	C35-C13-C14	-3.40	118.17	122.92
13	A	1124	CL7	O2D-CGD-O1D	-3.38	117.22	123.84
14	B	1023	PHO	O1D-CGD-CBD	3.37	130.35	124.74
13	A	1102	CL7	C3B-C4B-NB	-3.36	107.39	110.52
16	J	4012	A1JPJ	C8-C9-C10	3.36	124.09	118.94
16	B	4004	A1JPJ	C35-C13-C14	-3.36	118.22	122.92
16	L	4020	A1JPJ	C35-C13-C14	-3.36	118.22	122.92
16	B	4021	A1JPJ	C34-C9-C10	-3.35	118.23	122.92
16	B	4009	A1JPJ	C36-C18-C17	-3.34	118.24	122.92
16	B	4021	A1JPJ	C7-C8-C9	3.33	131.27	126.23
16	B	4006	A1JPJ	C15-C16-C17	3.32	130.28	123.47
16	B	4009	A1JPJ	C12-C13-C14	3.31	124.02	118.94
16	B	4009	A1JPJ	C21-C20-C19	3.31	133.54	123.22
13	A	1134	CL7	O2D-CGD-O1D	-3.31	117.38	123.84
16	L	4019	A1JPJ	C35-C13-C14	-3.30	118.30	122.92
13	A	1130	CL7	C3B-C4B-NB	-3.30	107.46	110.52
13	B	1201	CL7	C3B-C4B-NB	-3.29	107.46	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	1502	CL7	O2D-CGD-O1D	-3.28	117.43	123.84
13	A	1109	CL7	O2D-CGD-O1D	-3.28	117.43	123.84
13	B	1204	CL7	O2D-CGD-O1D	-3.26	117.47	123.84
16	B	4021	A1JPJ	C15-C14-C13	3.25	131.95	127.31
16	L	4020	A1JPJ	C36-C18-C17	-3.25	118.37	122.92
13	B	1210	CL7	C3B-C4B-NB	-3.25	107.50	110.52
13	B	1205	CL7	O2D-CGD-O1D	-3.24	117.50	123.84
13	A	1124	CL7	C3B-C4B-NB	-3.24	107.51	110.52
13	A	1129	CL7	C3B-C4B-NB	-3.24	107.51	110.52
13	A	1126	CL7	C3B-C4B-NB	-3.22	107.53	110.52
16	J	4013	A1JPJ	C35-C13-C14	-3.21	118.42	122.92
16	B	4006	A1JPJ	C35-C13-C14	-3.21	118.42	122.92
13	B	1221	CL7	C3A-C4A-CHB	-3.21	118.94	123.70
16	B	4006	A1JPJ	C23-C22-C21	3.21	123.87	118.94
16	B	4006	A1JPJ	C36-C18-C17	-3.21	118.43	122.92
16	L	4023	A1JPJ	C36-C18-C17	-3.20	118.44	122.92
13	B	1209	CL7	O2D-CGD-O1D	-3.20	117.59	123.84
14	A	1013	PHO	C2B-C1B-NB	-3.19	107.32	109.53
16	B	4005	A1JPJ	C35-C13-C14	-3.19	118.46	122.92
13	B	1230	CL7	OBB-CAB-C3B	-3.18	118.49	125.69
13	A	1103	CL7	O2D-CGD-O1D	-3.18	117.62	123.84
13	A	1116	CL7	C3B-C4B-NB	-3.17	107.57	110.52
16	A	4007	A1JPJ	C28-C27-C26	-3.17	121.81	124.85
20	A	1011	G9R	O2D-CGD-O1D	-3.17	117.65	123.84
13	B	1234	CL7	C3B-C4B-NB	-3.16	107.58	110.52
16	L	4020	A1JPJ	C15-C16-C17	3.15	129.93	123.47
16	J	4013	A1JPJ	C36-C18-C17	-3.15	118.51	122.92
13	B	1207	CL7	C3B-C4B-NB	-3.14	107.60	110.52
13	B	1238	CL7	C3B-C4B-NB	-3.14	107.60	110.52
13	B	1236	CL7	O2D-CGD-O1D	-3.14	117.69	123.84
13	B	1213	CL7	O2D-CGD-O1D	-3.14	117.70	123.84
13	A	1135	CL7	C3B-C4B-NB	-3.14	107.60	110.52
13	A	1125	CL7	O2D-CGD-O1D	-3.14	117.70	123.84
13	A	1112	CL7	O2D-CGD-O1D	-3.13	117.72	123.84
13	L	1501	CL7	C3B-C4B-NB	-3.13	107.61	110.52
16	A	4014	A1JPJ	C35-C13-C14	-3.12	118.55	122.92
16	A	4002	A1JPJ	C35-C13-C14	-3.11	118.56	122.92
13	B	1203	CL7	C3B-C4B-NB	-3.11	107.63	110.52
13	B	1202	CL7	C3B-C4B-NB	-3.10	107.64	110.52
13	A	1129	CL7	O2D-CGD-O1D	-3.10	117.78	123.84
16	A	4001	A1JPJ	C12-C13-C14	3.10	123.69	118.94
13	A	1113	CL7	C3B-C4B-NB	-3.09	107.64	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1102	CL7	O2D-CGD-O1D	-3.09	117.79	123.84
13	B	1215	CL7	O2D-CGD-O1D	-3.09	117.79	123.84
16	A	4008	A1JPJ	C19-C18-C17	3.09	123.69	118.94
13	B	1216	CL7	C3B-C4B-NB	-3.08	107.66	110.52
13	A	1119	CL7	C3B-C4B-NB	-3.08	107.66	110.52
13	B	1221	CL7	O2D-CGD-O1D	-3.08	117.81	123.84
16	B	4008	A1JPJ	C19-C18-C17	3.08	123.67	118.94
13	A	1117	CL7	O2D-CGD-O1D	-3.08	117.82	123.84
13	B	1021	CL7	O2D-CGD-O1D	-3.07	117.83	123.84
13	B	1202	CL7	O2D-CGD-O1D	-3.07	117.84	123.84
13	L	1503	CL7	C3B-C4B-NB	-3.07	107.67	110.52
13	A	1137	CL7	O2D-CGD-O1D	-3.07	117.84	123.84
13	A	1123	CL7	O2D-CGD-O1D	-3.06	117.85	123.84
16	B	4006	A1JPJ	C8-C9-C10	3.06	123.63	118.94
13	B	1223	CL7	O2D-CGD-O1D	-3.06	117.86	123.84
13	A	1104	CL7	C3B-C4B-NB	-3.06	107.68	110.52
16	B	4011	A1JPJ	C35-C13-C14	-3.05	118.64	122.92
13	B	1235	CL7	O2D-CGD-O1D	-3.05	117.87	123.84
13	A	1106	CL7	O2D-CGD-O1D	-3.05	117.87	123.84
13	A	1118	CL7	O2D-CGD-O1D	-3.05	117.88	123.84
13	A	1132	CL7	C3B-C4B-NB	-3.05	107.69	110.52
13	B	1217	CL7	O2D-CGD-O1D	-3.05	117.88	123.84
16	B	4007	A1JPJ	C36-C18-C17	-3.04	118.66	122.92
13	A	1136	CL7	O2D-CGD-O1D	-3.04	117.89	123.84
13	A	1127	CL7	O2D-CGD-O1D	-3.04	117.89	123.84
13	A	1105	CL7	O2D-CGD-O1D	-3.04	117.90	123.84
13	A	1012	CL7	O2D-CGD-O1D	-3.04	117.90	123.84
13	B	1237	CL7	C3B-C4B-NB	-3.04	107.70	110.52
13	A	1103	CL7	C3B-C4B-NB	-3.03	107.70	110.52
16	F	4016	A1JPJ	C21-C20-C19	3.03	132.68	123.22
13	B	1226	CL7	O2D-CGD-O1D	-3.03	117.91	123.84
13	A	1114	CL7	O2D-CGD-O1D	-3.03	117.91	123.84
13	A	1101	CL7	C3B-C4B-NB	-3.03	107.71	110.52
13	A	1121	CL7	O2D-CGD-O1D	-3.03	117.92	123.84
16	J	4013	A1JPJ	C15-C16-C17	3.03	129.67	123.47
13	A	1138	CL7	C3B-C4B-NB	-3.02	107.71	110.52
13	B	1021	CL7	C3B-C4B-NB	-3.02	107.71	110.52
16	B	4004	A1JPJ	C12-C13-C14	3.02	123.58	118.94
13	A	1133	CL7	O2D-CGD-O1D	-3.02	117.94	123.84
16	B	4004	A1JPJ	C36-C18-C17	-3.02	118.69	122.92
16	A	4007	A1JPJ	C36-C18-C17	-3.02	118.69	122.92
13	B	1237	CL7	O2D-CGD-O1D	-3.02	117.94	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1106	CL7	C3B-C4B-NB	-3.01	107.72	110.52
13	B	1214	CL7	O2D-CGD-O1D	-3.01	117.95	123.84
13	B	1231	CL7	O2D-CGD-O1D	-3.01	117.96	123.84
16	A	4014	A1JPJ	C36-C18-C17	-3.01	118.71	122.92
13	A	1125	CL7	C3B-C4B-NB	-3.01	107.72	110.52
13	A	1139	CL7	C3B-C4B-NB	-3.00	107.73	110.52
13	B	1222	CL7	O2D-CGD-O1D	-3.00	117.97	123.84
13	B	1233	CL7	O2D-CGD-O1D	-3.00	117.97	123.84
13	A	1135	CL7	O2D-CGD-O1D	-3.00	117.98	123.84
13	A	1133	CL7	C3B-C4B-NB	-3.00	107.73	110.52
16	L	4023	A1JPJ	C35-C13-C14	-3.00	118.72	122.92
13	A	1130	CL7	O2D-CGD-O1D	-3.00	117.98	123.84
13	A	1140	CL7	O2D-CGD-O1D	-2.99	117.98	123.84
13	B	1230	CL7	O2D-CGD-O1D	-2.99	118.00	123.84
13	B	1219	CL7	C3B-C4B-NB	-2.99	107.75	110.52
13	K	1401	CL7	O2D-CGD-O1D	-2.98	118.00	123.84
13	B	1231	CL7	C3B-C4B-NB	-2.98	107.75	110.52
13	B	1226	CL7	C3B-C4B-NB	-2.98	107.75	110.52
13	B	1225	CL7	O2D-CGD-O1D	-2.98	118.02	123.84
13	A	1111	CL7	C3B-C4B-NB	-2.98	107.75	110.52
13	A	1122	CL7	C3B-C4B-NB	-2.97	107.76	110.52
13	A	1101	CL7	O2D-CGD-O1D	-2.97	118.02	123.84
13	A	1105	CL7	C3B-C4B-NB	-2.97	107.76	110.52
13	B	1207	CL7	O2D-CGD-O1D	-2.97	118.03	123.84
13	B	1212	CL7	C3B-C4B-NB	-2.97	107.76	110.52
13	A	1115	CL7	C3B-C4B-NB	-2.97	107.76	110.52
13	B	1206	CL7	C3B-C4B-NB	-2.97	107.76	110.52
13	I	1601	CL7	C3B-C4B-NB	-2.96	107.77	110.52
13	B	1208	CL7	C3B-C4B-NB	-2.96	107.77	110.52
16	A	4003	A1JPJ	C19-C18-C17	2.96	123.48	118.94
13	B	1220	CL7	C3B-C4B-NB	-2.96	107.77	110.52
13	B	1210	CL7	O2D-CGD-O1D	-2.96	118.05	123.84
13	B	1232	CL7	O2D-CGD-O1D	-2.96	118.06	123.84
16	A	4003	A1JPJ	C10-C11-C12	2.96	132.44	123.22
16	B	4005	A1JPJ	C7-C8-C9	2.95	130.69	126.23
13	L	1502	CL7	C3B-C4B-NB	-2.95	107.78	110.52
13	B	1239	CL7	O2D-CGD-O1D	-2.95	118.07	123.84
13	A	1134	CL7	C3A-C4A-CHB	-2.95	119.64	124.02
13	B	1211	CL7	C3B-C4B-NB	-2.95	107.78	110.52
13	A	1136	CL7	C3B-C4B-NB	-2.95	107.78	110.52
13	B	1212	CL7	O2D-CGD-O1D	-2.95	118.07	123.84
13	B	1208	CL7	O2D-CGD-O1D	-2.95	118.08	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1217	CL7	C3B-C4B-NB	-2.94	107.78	110.52
14	B	1023	PHO	CMB-C2B-C3B	2.94	130.18	124.68
16	I	4118	A1JPJ	C15-C16-C17	2.94	129.50	123.47
13	A	1110	CL7	C3B-C4B-NB	-2.94	107.79	110.52
16	L	4019	A1JPJ	C19-C18-C17	2.94	123.45	118.94
16	A	4008	A1JPJ	C35-C13-C14	-2.94	118.81	122.92
13	B	1216	CL7	O2D-CGD-O1D	-2.93	118.12	123.84
13	B	1234	CL7	O2D-CGD-O1D	-2.92	118.12	123.84
13	L	1503	CL7	O2D-CGD-O1D	-2.92	118.12	123.84
16	L	4023	A1JPJ	C16-C15-C14	2.92	129.46	123.47
14	A	1013	PHO	CMA-C3A-C4A	-2.92	107.98	114.38
13	B	1222	CL7	C3B-C4B-NB	-2.92	107.81	110.52
13	B	1219	CL7	O2D-CGD-O1D	-2.92	118.13	123.84
13	A	1111	CL7	O2D-CGD-O1D	-2.91	118.14	123.84
13	A	1108	CL7	C3B-C4B-NB	-2.91	107.81	110.52
13	A	1138	CL7	O2D-CGD-O1D	-2.91	118.15	123.84
16	F	4016	A1JPJ	C34-C9-C10	-2.91	118.84	122.92
13	B	1224	CL7	O2D-CGD-O1D	-2.91	118.15	123.84
16	I	4118	A1JPJ	C35-C13-C14	-2.91	118.85	122.92
13	B	1238	CL7	O2D-CGD-O1D	-2.91	118.15	123.84
13	B	1233	CL7	C3B-C4B-NB	-2.91	107.82	110.52
16	I	4118	A1JPJ	C36-C18-C17	-2.90	118.86	122.92
13	B	1235	CL7	C3B-C4B-NB	-2.90	107.82	110.52
13	A	1126	CL7	O2D-CGD-O1D	-2.90	118.16	123.84
13	B	1221	CL7	C3B-C4B-NB	-2.90	107.82	110.52
13	J	1301	CL7	O2D-CGD-O1D	-2.90	118.17	123.84
16	L	4020	A1JPJ	C12-C13-C14	2.90	123.39	118.94
13	A	1141	CL7	C3B-C4B-NB	-2.90	107.82	110.52
13	B	1211	CL7	O2D-CGD-O1D	-2.90	118.17	123.84
13	B	1238	CL7	C3A-C4A-CHB	-2.90	119.40	123.70
13	A	1128	CL7	C3B-C4B-NB	-2.90	107.83	110.52
13	A	1120	CL7	C3B-C4B-NB	-2.89	107.83	110.52
13	B	1239	CL7	C3B-C4B-NB	-2.89	107.83	110.52
13	A	1113	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
13	B	1228	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
13	A	1141	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
13	A	1120	CL7	O2D-CGD-O1D	-2.89	118.20	123.84
16	J	4012	A1JPJ	C36-C18-C17	-2.88	118.88	122.92
13	B	1232	CL7	C3B-C4B-NB	-2.88	107.84	110.52
16	B	4008	A1JPJ	C35-C13-C14	-2.88	118.89	122.92
13	L	1501	CL7	O2D-CGD-O1D	-2.88	118.20	123.84
13	K	1402	CL7	CAA-C2A-C3A	-2.88	109.38	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	1302	CL7	C3B-C4B-NB	-2.88	107.84	110.52
13	A	1123	CL7	C3B-C4B-NB	-2.88	107.85	110.52
13	I	1601	CL7	O2D-CGD-O1D	-2.88	118.22	123.84
13	K	1401	CL7	C3B-C4B-NB	-2.88	107.85	110.52
20	A	1011	G9R	O2D-CGD-CBD	2.88	114.64	111.00
13	A	1115	CL7	O2D-CGD-O1D	-2.87	118.22	123.84
16	A	4007	A1JPJ	C35-C13-C14	-2.87	118.90	122.92
13	A	1122	CL7	O2D-CGD-O1D	-2.87	118.22	123.84
13	B	1241	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
13	B	1204	CL7	CAA-C2A-C3A	-2.87	104.93	112.78
13	A	1134	CL7	C3B-C4B-NB	-2.87	107.86	110.52
13	A	1107	CL7	C3B-C4B-NB	-2.86	107.86	110.52
13	B	1206	CL7	O2D-CGD-O1D	-2.86	118.24	123.84
13	A	1139	CL7	O2D-CGD-O1D	-2.86	118.24	123.84
13	B	1215	CL7	C3B-C4B-NB	-2.86	107.86	110.52
13	B	1223	CL7	C3B-C4B-NB	-2.86	107.86	110.52
13	F	1701	CL7	O2D-CGD-O1D	-2.85	118.26	123.84
13	A	1116	CL7	O2D-CGD-O1D	-2.85	118.26	123.84
13	B	1225	CL7	C3B-C4B-NB	-2.85	107.87	110.52
14	A	1013	PHO	CMB-C2B-C3B	2.85	130.01	124.68
16	A	4007	A1JPJ	C37-C22-C23	2.85	122.56	118.08
16	I	4118	A1JPJ	C16-C15-C14	2.84	129.29	123.47
16	I	4118	A1JPJ	C37-C22-C23	2.83	122.54	118.08
16	L	4020	A1JPJ	C19-C18-C17	2.83	123.28	118.94
16	A	4001	A1JPJ	C15-C16-C17	2.83	129.26	123.47
13	L	1501	CL7	C3A-C4A-CHB	-2.82	119.51	123.70
13	B	1218	CL7	O2D-CGD-O1D	-2.82	118.33	123.84
13	A	1104	CL7	O2D-CGD-O1D	-2.82	118.33	123.84
13	A	1119	CL7	O2D-CGD-O1D	-2.82	118.33	123.84
13	B	1213	CL7	C3B-C4B-NB	-2.81	107.91	110.52
13	B	1241	CL7	C3B-C4B-NB	-2.81	107.91	110.52
13	A	1115	CL7	CAA-C2A-C3A	-2.81	109.55	116.10
13	B	1022	CL7	C3B-C4B-NB	-2.81	107.91	110.52
13	A	1135	CL7	C3A-C4A-CHB	-2.81	119.53	123.70
13	B	1234	CL7	C3A-C4A-CHB	-2.80	119.54	123.70
13	A	1114	CL7	C3B-C4B-NB	-2.80	107.92	110.52
13	B	1228	CL7	C3B-C4B-NB	-2.80	107.92	110.52
13	A	1107	CL7	O2D-CGD-O1D	-2.79	118.37	123.84
13	B	1214	CL7	C3B-C4B-NB	-2.79	107.93	110.52
13	B	1230	CL7	CAA-C2A-C3A	-2.79	109.60	116.10
13	A	1106	CL7	C1-C2-C3	-2.79	121.22	126.04
13	B	1218	CL7	CAA-C2A-C3A	-2.78	109.61	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1108	CL7	O2D-CGD-O1D	-2.78	118.40	123.84
13	B	1220	CL7	O2D-CGD-O1D	-2.78	118.41	123.84
13	B	1218	CL7	C3B-C4B-NB	-2.78	107.94	110.52
13	J	1301	CL7	C3B-C4B-NB	-2.77	107.94	110.52
13	B	1209	CL7	C3B-C4B-NB	-2.77	107.94	110.52
13	A	1131	CL7	O2D-CGD-O1D	-2.77	118.42	123.84
16	A	4007	A1JPJ	C25-C26-C27	-2.77	118.06	121.47
13	B	1214	CL7	CHB-C1B-NB	2.76	127.18	124.26
13	B	1205	CL7	C3B-C4B-NB	-2.76	107.95	110.52
16	B	4006	A1JPJ	C12-C13-C14	2.76	123.18	118.94
13	B	1022	CL7	O2D-CGD-O1D	-2.76	118.44	123.84
16	A	4002	A1JPJ	C36-C18-C17	-2.76	119.06	122.92
13	B	1201	CL7	O2D-CGD-O1D	-2.75	118.45	123.84
13	B	1205	CL7	O2A-CGA-O1A	-2.75	116.64	123.59
13	A	1134	CL7	O2D-CGD-CBD	2.74	116.14	111.27
13	F	1701	CL7	C3B-C4B-NB	-2.74	107.97	110.52
14	B	1023	PHO	C2B-C1B-NB	-2.73	107.64	109.53
16	L	4019	A1JPJ	C12-C13-C14	2.73	123.14	118.94
13	A	1117	CL7	C3B-C4B-NB	-2.73	107.98	110.52
13	B	1230	CL7	C3A-C4A-CHB	-2.73	119.65	123.70
13	A	1127	CL7	C3B-C4B-NB	-2.73	107.98	110.52
13	A	1110	CL7	O2D-CGD-CBD	2.73	116.11	111.27
13	B	1227	CL7	O2D-CGD-O1D	-2.72	118.52	123.84
13	A	1118	CL7	C3B-C4B-NB	-2.72	108.00	110.52
13	B	1213	CL7	C3A-C4A-CHB	-2.72	119.67	123.70
16	A	4003	A1JPJ	C20-C21-C22	2.72	131.19	127.31
16	B	4007	A1JPJ	C15-C16-C17	2.71	129.03	123.47
13	A	1109	CL7	C3B-C4B-NB	-2.71	108.00	110.52
13	B	1203	CL7	O2D-CGD-O1D	-2.71	118.53	123.84
16	B	4006	A1JPJ	C19-C18-C17	2.71	123.11	118.94
16	J	4013	A1JPJ	C12-C13-C14	2.71	123.10	118.94
13	B	1219	CL7	CAA-C2A-C3A	-2.71	109.78	116.10
13	B	1226	CL7	CHB-C1B-NB	2.71	127.12	124.26
16	J	4012	A1JPJ	C20-C21-C22	2.71	131.17	127.31
13	A	1112	CL7	OBB-CAB-C3B	-2.70	119.58	125.69
13	K	1402	CL7	C3B-C4B-NB	-2.70	108.01	110.52
13	A	1140	CL7	C3B-C4B-NB	-2.69	108.02	110.52
16	A	4007	A1JPJ	C16-C15-C14	2.69	128.99	123.47
14	A	1013	PHO	C1C-C2C-C3C	-2.69	106.38	108.61
13	B	1227	CL7	C3B-C4B-NB	-2.69	108.02	110.52
13	B	1210	CL7	C3A-C4A-CHB	-2.68	119.72	123.70
13	B	1235	CL7	C3A-C4A-CHB	-2.68	119.72	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1224	CL7	C3B-C4B-NB	-2.68	108.03	110.52
16	B	4007	A1JPJ	C10-C11-C12	2.68	131.57	123.22
13	A	1132	CL7	OBB-CAB-C3B	-2.68	119.64	125.69
13	A	1102	CL7	C3A-C4A-CHB	-2.67	119.73	123.70
16	J	4012	A1JPJ	C23-C22-C21	-2.67	114.84	118.94
13	B	1233	CL7	C3A-C4A-CHB	-2.67	119.73	123.70
13	A	1121	CL7	C3B-C4B-NB	-2.67	108.04	110.52
13	A	1101	CL7	CAA-C2A-C3A	-2.67	109.88	116.10
13	A	1130	CL7	CHB-C1B-NB	2.67	127.08	124.26
20	A	1011	G9R	C1C-C2C-C3C	-2.67	106.39	108.61
13	A	1129	CL7	C1-C2-C3	-2.66	122.44	126.75
13	B	1204	CL7	C3B-C4B-NB	-2.65	108.05	110.52
16	L	4020	A1JPJ	C23-C22-C21	2.65	123.01	118.94
16	B	4005	A1JPJ	C36-C18-C17	-2.65	119.21	122.92
13	B	1217	CL7	CAA-C2A-C3A	-2.65	109.92	116.10
13	A	1137	CL7	C3B-C4B-NB	-2.63	108.07	110.52
14	B	1023	PHO	CMA-C3A-C4A	-2.63	108.61	114.38
16	B	4011	A1JPJ	C36-C18-C17	-2.63	119.24	122.92
13	L	1501	CL7	OBB-CAB-C3B	-2.62	119.75	125.69
13	A	1120	CL7	C3A-C4A-CHB	-2.62	119.81	123.70
16	A	4014	A1JPJ	C12-C13-C14	2.62	122.97	118.94
13	B	1203	CL7	C3A-C4A-CHB	-2.61	119.82	123.70
16	B	4005	A1JPJ	C15-C16-C17	2.61	128.83	123.47
13	B	1210	CL7	CHB-C1B-NB	2.60	127.01	124.26
13	A	1107	CL7	C3A-C4A-CHB	-2.60	119.84	123.70
13	B	1201	CL7	OBB-CAB-C3B	-2.60	119.81	125.69
16	A	4008	A1JPJ	C16-C15-C14	2.60	128.80	123.47
20	A	1011	G9R	C3D-C4D-CHA	2.60	112.49	108.54
13	A	1101	CL7	C3A-C4A-CHB	-2.60	119.85	123.70
13	A	1112	CL7	C3A-C4A-CHB	-2.59	119.85	123.70
16	A	4002	A1JPJ	C15-C16-C17	2.59	128.77	123.47
13	B	1207	CL7	C3A-C4A-CHB	-2.59	119.86	123.70
13	A	1141	CL7	CAA-C2A-C3A	-2.58	110.07	116.10
13	K	1402	CL7	C3A-C4A-CHB	-2.58	119.87	123.70
13	B	1209	CL7	C3A-C4A-CHB	-2.58	119.87	123.70
13	A	1118	CL7	C3A-C4A-CHB	-2.58	119.88	123.70
13	B	1230	CL7	CHB-C1B-NB	2.58	126.98	124.26
16	A	4002	A1JPJ	C12-C13-C14	2.57	122.89	118.94
13	B	1229	CL7	C3A-C4A-CHB	-2.57	119.89	123.70
13	J	1301	CL7	C3A-C4A-CHB	-2.57	119.89	123.70
13	B	1218	CL7	C3A-C4A-CHB	-2.56	119.89	123.70
13	K	1401	CL7	C3A-C4A-CHB	-2.56	119.89	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1214	CL7	C3A-C4A-CHB	-2.56	119.91	123.70
13	A	1117	CL7	CHB-C1B-NB	2.55	126.96	124.26
13	B	1216	CL7	CHB-C1B-NB	2.55	126.96	124.26
13	A	1131	CL7	C3B-C4B-NB	-2.55	108.15	110.52
16	A	4008	A1JPJ	C23-C22-C21	2.54	122.84	118.94
13	A	1137	CL7	C3A-C4A-CHB	-2.54	119.93	123.70
13	A	1123	CL7	CHB-C1B-NB	2.54	126.95	124.26
16	I	4118	A1JPJ	C34-C9-C8	2.54	122.08	118.08
13	A	1109	CL7	O2D-CGD-CBD	2.54	115.78	111.27
13	B	1234	CL7	C1-C2-C3	-2.53	122.66	126.75
13	A	1139	CL7	C3A-C4A-CHB	-2.53	119.95	123.70
13	A	1012	CL7	OBB-CAB-C3B	-2.52	119.98	125.69
13	B	1215	CL7	C3A-C4A-CHB	-2.52	119.95	123.70
13	B	1021	CL7	OBB-CAB-C3B	-2.52	119.98	125.69
13	A	1110	CL7	C3A-C4A-CHB	-2.52	119.96	123.70
13	A	1122	CL7	C3A-C4A-CHB	-2.52	119.96	123.70
13	A	1138	CL7	C3A-C4A-CHB	-2.52	119.96	123.70
13	B	1227	CL7	C3A-C4A-CHB	-2.52	119.97	123.70
13	I	1601	CL7	C3A-C4A-CHB	-2.52	119.97	123.70
13	B	1217	CL7	C3A-C4A-CHB	-2.51	119.97	123.70
13	A	1128	CL7	CHB-C1B-NB	2.51	126.91	124.26
13	A	1104	CL7	C3A-C4A-CHB	-2.51	119.98	123.70
16	B	4007	A1JPJ	C16-C15-C14	2.51	128.61	123.47
20	A	1011	G9R	C4D-CHA-CBD	-2.50	106.32	108.89
13	A	1141	CL7	CHB-C1B-NB	2.50	126.90	124.26
13	A	1123	CL7	C3A-C4A-CHB	-2.49	120.00	123.70
13	A	1124	CL7	O2D-CGD-CBD	2.49	115.70	111.27
13	A	1129	CL7	CHB-C1B-NB	2.49	126.89	124.26
13	B	1204	CL7	C1-C2-C3	-2.49	121.74	126.04
13	B	1204	CL7	C3A-C4A-CHB	-2.48	120.01	123.70
13	B	1212	CL7	C3A-C4A-CHB	-2.48	120.01	123.70
13	A	1116	CL7	O2A-CGA-O1A	-2.48	117.33	123.59
16	B	4004	A1JPJ	C19-C18-C17	2.48	122.75	118.94
13	B	1221	CL7	O2A-CGA-O1A	-2.47	117.35	123.59
13	B	1234	CL7	CHB-C1B-NB	2.47	126.87	124.26
13	A	1109	CL7	C3A-C4A-CHB	-2.46	120.04	123.70
16	A	4002	A1JPJ	C20-C19-C18	2.46	133.34	126.42
14	B	1023	PHO	O2D-CGD-O1D	-2.46	119.02	123.84
13	B	1239	CL7	C3A-C4A-CHB	-2.46	120.05	123.70
13	B	1220	CL7	C3A-C4A-CHB	-2.46	120.05	123.70
16	L	4023	A1JPJ	C19-C18-C17	2.46	122.71	118.94
13	J	1301	CL7	CAA-C2A-C3A	-2.46	110.36	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1229	CL7	O2D-CGD-CBD	2.45	115.63	111.27
16	A	4014	A1JPJ	C15-C16-C17	2.45	128.50	123.47
16	L	4019	A1JPJ	C10-C11-C12	2.45	130.87	123.22
13	B	1233	CL7	CAA-C2A-C3A	-2.45	110.38	116.10
13	A	1102	CL7	CHB-C1B-NB	2.45	126.85	124.26
16	L	4019	A1JPJ	C23-C22-C21	2.45	122.70	118.94
13	A	1117	CL7	O2A-CGA-O1A	-2.45	117.42	123.59
13	A	1123	CL7	O2A-CGA-O1A	-2.45	117.42	123.59
13	A	1132	CL7	C3A-C4A-CHB	-2.45	120.07	123.70
16	L	4023	A1JPJ	C12-C13-C14	2.44	122.69	118.94
13	A	1105	CL7	C3A-C4A-CHB	-2.44	120.08	123.70
13	A	1012	CL7	C3B-C4B-NB	-2.44	108.25	110.52
16	B	4007	A1JPJ	C19-C18-C17	2.44	122.68	118.94
13	L	1502	CL7	C3A-C4A-CHB	-2.43	120.09	123.70
16	B	4011	A1JPJ	C12-C13-C14	2.43	122.67	118.94
13	B	1206	CL7	CHB-C1B-NB	2.43	126.83	124.26
13	A	1125	CL7	C3A-C4A-CHB	-2.43	120.10	123.70
13	B	1207	CL7	OBB-CAB-C3B	-2.43	120.20	125.69
20	A	1011	G9R	CMD-C2D-C3D	2.42	129.22	124.68
13	J	1302	CL7	C3A-C4A-CHB	-2.42	120.10	123.70
13	A	1124	CL7	CHB-C1B-NB	2.42	126.82	124.26
16	J	4013	A1JPJ	C19-C18-C17	2.42	122.65	118.94
13	B	1222	CL7	C3A-C4A-CHB	-2.42	120.11	123.70
16	J	4012	A1JPJ	C15-C16-C17	2.41	128.42	123.47
13	A	1119	CL7	CHB-C1B-NB	2.41	126.81	124.26
16	A	4002	A1JPJ	C8-C9-C10	2.41	122.63	118.94
16	A	4007	A1JPJ	C19-C18-C17	2.41	122.63	118.94
13	L	1503	CL7	C3A-C4A-CHB	-2.40	120.14	123.70
13	A	1114	CL7	C3A-C4A-CHB	-2.40	120.14	123.70
13	L	1502	CL7	O2D-CGD-CBD	2.40	115.53	111.27
13	A	1115	CL7	C3A-C4A-CHB	-2.40	120.14	123.70
13	F	1701	CL7	CAA-C2A-C3A	-2.39	110.51	116.10
20	A	1011	G9R	CMB-C2B-C3B	2.39	129.15	124.68
13	A	1123	CL7	OBB-CAB-C3B	-2.38	120.30	125.69
13	B	1226	CL7	C3A-C4A-CHB	-2.38	120.17	123.70
16	B	4004	A1JPJ	C2-C1-C6	2.38	114.14	110.48
16	B	4011	A1JPJ	C23-C22-C21	2.38	122.59	118.94
13	A	1111	CL7	C1-C2-C3	-2.38	121.93	126.04
13	A	1129	CL7	C3A-C4A-CHB	-2.38	120.17	123.70
13	A	1141	CL7	C3A-C4A-CHB	-2.38	120.17	123.70
13	A	1121	CL7	C3A-C4A-CHB	-2.38	120.18	123.70
16	L	4019	A1JPJ	C16-C15-C14	2.37	128.33	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1133	CL7	C3A-C4A-CHB	-2.36	120.20	123.70
16	A	4008	A1JPJ	C12-C13-C14	2.36	122.56	118.94
13	B	1206	CL7	C1-C2-C3	-2.35	122.94	126.75
13	A	1111	CL7	C3A-C4A-CHB	-2.35	120.21	123.70
16	L	4023	A1JPJ	C34-C9-C8	2.35	121.78	118.08
13	B	1239	CL7	C1-C2-C3	-2.35	121.97	126.04
13	A	1131	CL7	C1-C2-C3	-2.35	121.98	126.04
13	B	1236	CL7	C3A-C4A-CHB	-2.35	120.22	123.70
13	A	1106	CL7	CHB-C1B-NB	2.35	126.74	124.26
13	L	1502	CL7	OBB-CAB-C3B	-2.35	120.38	125.69
16	B	4009	A1JPJ	C15-C16-C17	2.35	128.28	123.47
13	A	1130	CL7	C3A-C4A-CHB	-2.34	120.23	123.70
13	B	1222	CL7	C1-C2-C3	-2.34	122.97	126.75
13	A	1124	CL7	C3A-C4A-CHB	-2.34	120.23	123.70
13	B	1201	CL7	CHB-C1B-NB	2.34	126.73	124.26
13	B	1223	CL7	C3A-C4A-CHB	-2.34	120.23	123.70
16	B	4004	A1JPJ	C37-C22-C23	2.33	121.76	118.08
13	F	1701	CL7	C3A-C4A-CHB	-2.33	120.24	123.70
13	A	1136	CL7	CHB-C1B-NB	2.33	126.73	124.26
16	B	4021	A1JPJ	C2-C1-C6	2.33	114.07	110.48
13	L	1501	CL7	CHB-C1B-NB	2.33	126.72	124.26
13	A	1112	CL7	CHB-C1B-NB	2.33	126.72	124.26
13	B	1202	CL7	C3A-C4A-CHB	-2.33	120.25	123.70
13	A	1122	CL7	CHB-C1B-NB	2.32	126.71	124.26
13	B	1226	CL7	O2A-CGA-O1A	-2.31	117.75	123.59
13	A	1116	CL7	C3A-C4A-CHB	-2.31	120.28	123.70
13	A	1132	CL7	O2D-CGD-CBD	2.31	115.37	111.27
13	B	1206	CL7	C3A-C4A-CHB	-2.31	120.28	123.70
16	A	4001	A1JPJ	C8-C9-C10	2.31	122.48	118.94
13	B	1232	CL7	CAA-C2A-C3A	-2.31	110.72	116.10
13	A	1136	CL7	C3A-C4A-CHB	-2.30	120.28	123.70
13	A	1123	CL7	C1-C2-C3	-2.30	122.06	126.04
16	J	4013	A1JPJ	C2-C1-C6	2.30	114.03	110.48
16	A	4002	A1JPJ	C16-C17-C18	2.30	130.60	127.31
13	L	1502	CL7	CHB-C1B-NB	2.30	126.69	124.26
16	B	4005	A1JPJ	C16-C17-C18	2.29	130.59	127.31
13	B	1230	CL7	O2D-CGD-CBD	2.29	115.34	111.27
13	B	1234	CL7	OBB-CAB-C3B	-2.29	120.51	125.69
13	A	1135	CL7	CHB-C1B-NB	2.29	126.68	124.26
16	B	4021	A1JPJ	C1-C6-C7	2.29	122.25	115.78
13	A	1115	CL7	CHB-C1B-NB	2.28	126.67	124.26
13	A	1121	CL7	C2D-C1D-ND	-2.28	108.70	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1215	CL7	CHB-C1B-NB	2.28	126.67	124.26
13	L	1503	CL7	CHB-C1B-NB	2.28	126.67	124.26
16	B	4004	A1JPJ	C15-C16-C17	2.28	128.15	123.47
13	B	1238	CL7	CHB-C1B-NB	2.28	126.67	124.26
13	A	1116	CL7	CHB-C1B-NB	2.28	126.67	124.26
13	A	1113	CL7	C3A-C4A-CHB	-2.28	120.32	123.70
13	B	1216	CL7	OBB-CAB-C3B	-2.28	120.54	125.69
13	A	1120	CL7	CHB-C1B-NB	2.27	126.66	124.26
13	B	1204	CL7	O2D-CGD-CBD	2.27	115.30	111.27
13	B	1223	CL7	OBB-CAB-C3B	-2.27	120.56	125.69
13	A	1109	CL7	CHB-C1B-NB	2.26	126.65	124.26
13	B	1236	CL7	C3B-C4B-NB	-2.26	108.42	110.52
16	J	4013	A1JPJ	C23-C22-C21	2.26	122.41	118.94
13	B	1203	CL7	CHB-C1B-NB	2.25	126.64	124.26
14	B	1023	PHO	O2A-CGA-O1A	-2.25	117.90	123.59
13	B	1228	CL7	C3A-C4A-CHB	-2.25	120.36	123.70
13	A	1102	CL7	OBB-CAB-C3B	-2.25	120.59	125.69
13	B	1205	CL7	C1-C2-C3	-2.25	122.15	126.04
13	A	1111	CL7	CHB-C1B-NB	2.25	126.64	124.26
13	A	1117	CL7	C3A-C4A-CHB	-2.25	120.36	123.70
16	B	4005	A1JPJ	C11-C12-C13	2.25	132.74	126.42
13	A	1103	CL7	C3A-C4A-CHB	-2.25	120.36	123.70
13	B	1212	CL7	CHB-C1B-NB	2.24	126.63	124.26
13	A	1136	CL7	O2A-CGA-O1A	-2.24	117.93	123.59
13	B	1207	CL7	CHB-C1B-NB	2.24	126.63	124.26
13	A	1119	CL7	C3A-C4A-CHB	-2.24	120.37	123.70
13	B	1203	CL7	OBB-CAB-C3B	-2.24	120.62	125.69
13	A	1101	CL7	CHB-C1B-NB	2.24	126.63	124.26
13	B	1229	CL7	C3B-C4B-NB	-2.24	108.44	110.52
13	B	1220	CL7	CHB-C1B-NB	2.24	126.62	124.26
13	B	1237	CL7	CHB-C1B-NB	2.24	126.62	124.26
16	B	4007	A1JPJ	C37-C22-C23	2.23	121.60	118.08
13	B	1225	CL7	O2A-CGA-O1A	-2.23	117.95	123.59
16	J	4012	A1JPJ	C10-C11-C12	2.23	130.19	123.22
13	B	1214	CL7	OBB-CAB-C3B	-2.22	120.66	125.69
16	J	4013	A1JPJ	C1-C6-C7	2.22	122.06	115.78
13	B	1230	CL7	C2D-C1D-ND	-2.22	108.74	110.23
13	A	1012	CL7	C2D-C1D-ND	-2.22	108.75	110.23
13	B	1235	CL7	O2A-CGA-O1A	-2.22	118.00	123.59
16	A	4014	A1JPJ	C19-C18-C17	2.22	122.34	118.94
13	B	1239	CL7	CHB-C1B-NB	2.21	126.60	124.26
13	A	1132	CL7	CHB-C1B-NB	2.21	126.60	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	2001	PQN	C11-C3-C4	-2.21	116.14	118.50
13	A	1140	CL7	C1-C2-C3	-2.21	122.22	126.04
13	A	1128	CL7	C3A-C4A-CHB	-2.21	120.42	123.70
16	B	4009	A1JPJ	C20-C19-C18	2.21	132.62	126.42
13	A	1113	CL7	CHB-C1B-NB	2.21	126.59	124.26
16	J	4012	A1JPJ	C2-C1-C6	2.20	113.87	110.48
13	B	1217	CL7	CHB-C1B-NB	2.20	126.59	124.26
16	B	4008	A1JPJ	C12-C13-C14	2.20	122.32	118.94
13	A	1133	CL7	CHB-C1B-NB	2.20	126.59	124.26
13	A	1132	CL7	C2D-C1D-ND	-2.20	108.76	110.23
16	B	4005	A1JPJ	C23-C22-C21	-2.20	115.56	118.94
13	B	1205	CL7	O2D-CGD-CBD	2.20	115.18	111.27
13	B	1221	CL7	OBB-CAB-C3B	-2.20	120.71	125.69
15	B	2002	PQN	C11-C3-C4	-2.20	116.15	118.50
13	A	1106	CL7	C3A-C4A-CHB	-2.20	120.44	123.70
13	A	1105	CL7	CHB-C1B-NB	2.20	126.58	124.26
13	A	1135	CL7	OBB-CAB-C3B	-2.20	120.72	125.69
13	A	1138	CL7	CHB-C1B-NB	2.20	126.58	124.26
16	A	4007	A1JPJ	C20-C21-C22	2.19	130.44	127.31
13	A	1107	CL7	CHB-C1B-NB	2.19	126.58	124.26
13	B	1232	CL7	C3A-C4A-CHB	-2.19	120.45	123.70
16	J	4012	A1JPJ	C1-C6-C7	2.19	121.97	115.78
16	I	4118	A1JPJ	C12-C13-C14	2.19	122.30	118.94
13	K	1401	CL7	CHB-C1B-NB	2.19	126.57	124.26
13	B	1227	CL7	C2D-C1D-ND	-2.19	108.77	110.23
13	B	1228	CL7	CHB-C1B-NB	2.19	126.57	124.26
13	A	1103	CL7	CHB-C1B-NB	2.19	126.57	124.26
13	B	1222	CL7	O2A-CGA-O1A	-2.18	118.08	123.59
13	B	1221	CL7	C2D-C1D-ND	-2.18	108.77	110.23
13	B	1209	CL7	CHC-C1C-NC	2.18	126.46	124.45
13	B	1222	CL7	CHB-C1B-NB	2.18	126.57	124.26
13	B	1208	CL7	C3A-C4A-CHB	-2.18	120.47	123.70
13	B	1219	CL7	C3A-C4A-CHB	-2.18	120.47	123.70
13	A	1118	CL7	C1-C2-C3	-2.18	122.28	126.04
13	B	1238	CL7	O2A-CGA-O1A	-2.17	118.10	123.59
13	B	1208	CL7	CHB-C1B-NB	2.17	126.56	124.26
20	A	1011	G9R	CMA-C3A-C4A	-2.17	109.62	114.38
13	B	1235	CL7	CHB-C1B-NB	2.17	126.56	124.26
13	B	1238	CL7	C2D-C1D-ND	-2.17	108.78	110.23
13	B	1205	CL7	CHB-C1B-NB	2.17	126.56	124.26
13	B	1211	CL7	C3A-C4A-CHB	-2.17	120.48	123.70
13	A	1117	CL7	C1-C2-C3	-2.17	122.29	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1233	CL7	CHB-C1B-NB	2.17	126.55	124.26
14	A	1013	PHO	C1-C2-C3	-2.17	122.29	126.04
16	A	4008	A1JPJ	C34-C9-C8	2.17	121.49	118.08
14	A	1013	PHO	O2A-CGA-O1A	-2.17	118.12	123.59
13	L	1502	CL7	O2A-CGA-O1A	-2.17	118.13	123.59
13	A	1108	CL7	C3A-C4A-CHB	-2.16	120.49	123.70
16	L	4019	A1JPJ	C1-C6-C5	-2.16	119.57	122.61
13	B	1232	CL7	CHB-C1B-NB	2.16	126.54	124.26
16	A	4007	A1JPJ	C12-C13-C14	2.16	122.25	118.94
13	B	1224	CL7	C3A-C4A-CHB	-2.16	120.50	123.70
13	B	1214	CL7	CMB-C2B-C1B	-2.16	122.08	125.37
16	A	4001	A1JPJ	C20-C19-C18	2.16	132.47	126.42
13	B	1225	CL7	CHB-C1B-NB	2.15	126.54	124.26
13	A	1139	CL7	CHB-C1B-NB	2.15	126.54	124.26
13	A	1118	CL7	O2A-CGA-O1A	-2.15	118.16	123.59
16	B	4021	A1JPJ	C23-C22-C21	2.15	122.24	118.94
13	B	1231	CL7	CHB-C1B-NB	2.15	126.53	124.26
13	B	1229	CL7	O2A-CGA-O1A	-2.15	118.18	123.59
16	B	4006	A1JPJ	C1-C6-C7	2.14	121.84	115.78
13	B	1227	CL7	C1-C2-C3	-2.14	122.34	126.04
13	B	1235	CL7	CAA-C2A-C3A	-2.14	106.91	112.78
13	B	1202	CL7	CHB-C1B-NB	2.14	126.52	124.26
13	A	1126	CL7	C3A-C4A-CHB	-2.14	120.52	123.70
13	B	1021	CL7	O2A-CGA-O1A	-2.14	118.19	123.59
13	B	1229	CL7	CHB-C1B-NB	2.14	126.52	124.26
13	A	1135	CL7	C2D-C1D-ND	-2.14	108.80	110.23
20	A	1011	G9R	O2A-CGA-O1A	-2.14	118.20	123.59
13	B	1234	CL7	O2A-CGA-O1A	-2.13	118.20	123.59
13	A	1131	CL7	O2A-CGA-O1A	-2.13	118.21	123.59
13	A	1102	CL7	O2A-CGA-O1A	-2.13	118.21	123.59
13	B	1236	CL7	CHB-C1B-NB	2.13	126.51	124.26
13	B	1223	CL7	O2A-CGA-O1A	-2.13	118.21	123.59
13	B	1231	CL7	C3A-C4A-CHB	-2.13	120.54	123.70
13	A	1138	CL7	O2A-CGA-O1A	-2.12	118.24	123.59
13	A	1114	CL7	CHB-C1B-NB	2.12	126.50	124.26
13	A	1134	CL7	CHB-C1B-NB	2.12	126.50	124.26
13	A	1111	CL7	C2D-C1D-ND	-2.12	108.81	110.23
13	B	1022	CL7	O2A-CGA-O1A	-2.12	118.25	123.59
13	A	1110	CL7	CHB-C1B-NB	2.12	126.50	124.26
13	L	1502	CL7	C3C-C4C-NC	-2.12	108.64	110.18
13	A	1104	CL7	CHB-C1B-NB	2.11	126.49	124.26
13	B	1226	CL7	C2D-C1D-ND	-2.11	108.82	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1022	CL7	C1-C2-C3	-2.11	122.39	126.04
13	A	1123	CL7	C2D-C1D-ND	-2.11	108.82	110.23
13	B	1236	CL7	O2D-CGD-CBD	2.11	115.02	111.27
13	B	1224	CL7	O2A-CGA-O1A	-2.11	118.27	123.59
13	B	1218	CL7	CHB-C1B-NB	2.11	126.49	124.26
13	B	1201	CL7	C3A-C4A-CHB	-2.11	120.57	123.70
13	B	1238	CL7	OBB-CAB-C3B	-2.11	120.92	125.69
13	A	1130	CL7	OBB-CAB-C3B	-2.11	120.92	125.69
13	B	1216	CL7	C2D-C1D-ND	-2.10	108.82	110.23
13	B	1216	CL7	O2A-CGA-O1A	-2.10	118.28	123.59
13	A	1124	CL7	O2A-CGA-O1A	-2.10	118.28	123.59
13	A	1131	CL7	C3A-C4A-CHB	-2.10	120.58	123.70
13	B	1221	CL7	CHB-C1B-NB	2.10	126.48	124.26
13	J	1301	CL7	CHB-C1B-NB	2.10	126.48	124.26
13	B	1214	CL7	O2A-CGA-O1A	-2.10	118.30	123.59
13	A	1121	CL7	O2A-CGA-O1A	-2.10	118.30	123.59
16	B	4004	A1JPJ	C34-C9-C8	2.10	121.38	118.08
13	B	1216	CL7	C3A-C4A-CHB	-2.09	120.59	123.70
13	A	1107	CL7	C2D-C1D-ND	-2.09	108.83	110.23
13	A	1103	CL7	C1-C2-C3	-2.09	122.43	126.04
13	A	1127	CL7	C3A-C4A-CHB	-2.09	120.60	123.70
13	A	1107	CL7	O2A-CGA-O1A	-2.08	118.33	123.59
13	A	1128	CL7	O2A-CGA-O1A	-2.08	118.33	123.59
13	B	1219	CL7	CHB-C1B-NB	2.08	126.46	124.26
16	B	4021	A1JPJ	C11-C10-C9	2.08	130.28	127.31
13	A	1119	CL7	OBB-CAB-C3B	-2.08	120.98	125.69
13	L	1501	CL7	O2A-CGA-O1A	-2.08	118.34	123.59
13	A	1132	CL7	O2A-CGA-O1A	-2.08	118.35	123.59
13	K	1402	CL7	CHB-C1B-NB	2.08	126.45	124.26
13	A	1103	CL7	CHC-C1C-NC	2.07	126.36	124.45
13	A	1137	CL7	CHB-C1B-NB	2.07	126.45	124.26
13	B	1208	CL7	O2A-CGA-O1A	-2.07	118.37	123.59
13	B	1228	CL7	C2D-C1D-ND	-2.07	108.84	110.23
13	B	1241	CL7	C3A-C4A-CHB	-2.07	120.63	123.70
13	B	1206	CL7	OBB-CAB-C3B	-2.07	121.01	125.69
13	A	1137	CL7	O2A-CGA-O1A	-2.07	118.38	123.59
16	J	4012	A1JPJ	C1-C6-C5	-2.06	119.71	122.61
16	L	4020	A1JPJ	C1-C6-C7	2.06	121.61	115.78
13	B	1209	CL7	CHB-C1B-NB	2.06	126.44	124.26
14	B	1023	PHO	C1C-C2C-C3C	-2.06	106.90	108.61
13	B	1231	CL7	O2A-CGA-O1A	-2.06	118.39	123.59
13	A	1128	CL7	O1D-CGD-CBD	2.06	128.70	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1103	CL7	C2D-C1D-ND	-2.05	108.86	110.23
13	A	1125	CL7	C1-C2-C3	-2.05	122.49	126.04
16	B	4021	A1JPJ	C35-C13-C14	-2.05	120.05	122.92
13	B	1021	CL7	C1-C2-C3	-2.05	122.50	126.04
13	A	1118	CL7	CHB-C1B-NB	2.05	126.43	124.26
13	A	1139	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
13	J	1302	CL7	CHB-C1B-NB	2.05	126.42	124.26
13	A	1108	CL7	CHB-C1B-NB	2.05	126.42	124.26
13	A	1137	CL7	OBB-CAB-C3B	-2.05	121.06	125.69
13	A	1129	CL7	O2A-CGA-O1A	-2.04	118.44	123.59
13	B	1211	CL7	O2A-CGA-O1A	-2.04	118.44	123.59
13	B	1207	CL7	O2A-CGA-O1A	-2.04	118.44	123.59
16	A	4001	A1JPJ	C33-C5-C6	2.04	126.82	124.53
16	L	4023	A1JPJ	C23-C22-C21	2.04	122.07	118.94
13	B	1209	CL7	O2D-CGD-CBD	2.04	114.89	111.27
13	B	1237	CL7	C1-C2-C3	-2.04	122.52	126.04
13	A	1140	CL7	CHB-C1B-NB	2.04	126.41	124.26
13	B	1223	CL7	CHB-C1B-NB	2.04	126.41	124.26
13	A	1125	CL7	CHB-C1B-NB	2.03	126.41	124.26
13	A	1140	CL7	C3A-C4A-CHB	-2.03	120.68	123.70
13	B	1231	CL7	C2D-C1D-ND	-2.03	108.87	110.23
16	J	4012	A1JPJ	C19-C18-C17	2.03	122.06	118.94
13	A	1111	CL7	O2A-CGA-O1A	-2.03	118.46	123.59
13	I	1601	CL7	O2A-CGA-O1A	-2.03	118.47	123.59
13	B	1213	CL7	O2D-CGD-CBD	2.03	114.88	111.27
13	I	1601	CL7	CHC-C1C-NC	2.03	126.32	124.45
13	A	1121	CL7	O2D-CGD-CBD	2.03	114.87	111.27
13	B	1213	CL7	CHB-C1B-NB	2.03	126.40	124.26
13	A	1130	CL7	O2A-CGA-O1A	-2.02	118.48	123.59
16	B	4021	A1JPJ	C36-C18-C17	-2.02	120.09	122.92
13	A	1119	CL7	O2A-CGA-O1A	-2.02	118.49	123.59
13	B	1210	CL7	C2D-C1D-ND	-2.02	108.88	110.23
13	B	1215	CL7	O2A-CGA-O1A	-2.02	118.49	123.59
13	F	1701	CL7	CHC-C1C-NC	2.02	126.31	124.45
13	B	1207	CL7	C2D-C1D-ND	-2.02	108.88	110.23
13	A	1133	CL7	O2A-CGA-O1A	-2.02	118.50	123.59
13	A	1138	CL7	C2D-C1D-ND	-2.02	108.88	110.23
13	A	1121	CL7	CHB-C1B-NB	2.02	126.39	124.26
13	A	1112	CL7	O2D-CGD-CBD	2.02	114.85	111.27
13	A	1110	CL7	OBB-CAB-C3B	-2.02	121.13	125.69
13	B	1206	CL7	O2A-CGA-O1A	-2.02	118.50	123.59
16	B	4011	A1JPJ	C8-C9-C10	2.01	122.03	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I	1601	CL7	CHB-C1B-NB	2.01	126.39	124.26
16	A	4001	A1JPJ	C19-C18-C17	2.01	122.03	118.94
13	A	1133	CL7	C2D-C1D-ND	-2.01	108.88	110.23
13	B	1021	CL7	C2D-C1D-ND	-2.01	108.88	110.23
13	A	1125	CL7	O2A-CGA-O1A	-2.01	118.52	123.59
16	B	4006	A1JPJ	C1-C6-C5	-2.01	119.79	122.61
13	A	1129	CL7	OBB-CAB-C3B	-2.01	121.15	125.69
13	A	1126	CL7	C2D-C1D-ND	-2.00	108.89	110.23
16	B	4021	A1JPJ	C1-C6-C5	-2.00	119.79	122.61
13	B	1021	CL7	C3A-C4A-CHB	-2.00	120.73	123.70
13	B	1237	CL7	O2A-CGA-O1A	-2.00	118.54	123.59
13	B	1221	CL7	O2D-CGD-CBD	2.00	114.82	111.27

All (187) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	1022	CL7	NC
13	B	1022	CL7	NA
13	B	1201	CL7	NC
13	B	1201	CL7	NA
13	B	1202	CL7	NC
13	B	1202	CL7	NA
13	B	1203	CL7	NC
13	B	1203	CL7	NA
13	B	1204	CL7	NC
13	B	1204	CL7	NA
13	B	1205	CL7	NC
13	B	1205	CL7	NA
13	B	1206	CL7	NC
13	B	1206	CL7	NA
13	B	1207	CL7	NC
13	B	1207	CL7	NA
13	B	1208	CL7	NC
13	B	1208	CL7	NA
13	B	1209	CL7	NC
13	B	1209	CL7	NA
13	B	1210	CL7	NC
13	B	1210	CL7	NA
13	B	1211	CL7	NC
13	B	1211	CL7	NA
13	B	1212	CL7	NC
13	B	1212	CL7	NA

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Mol	Chain	Res	Type	Atom
13	B	1213	CL7	NC
13	B	1213	CL7	NA
13	B	1214	CL7	NC
13	B	1214	CL7	NA
13	B	1215	CL7	NC
13	B	1215	CL7	NA
13	B	1216	CL7	NC
13	B	1216	CL7	NA
13	B	1217	CL7	NC
13	B	1217	CL7	NA
13	B	1218	CL7	NC
13	B	1218	CL7	NA
13	B	1219	CL7	NC
13	B	1219	CL7	NA
13	B	1220	CL7	NC
13	B	1220	CL7	NA
13	B	1221	CL7	NC
13	B	1221	CL7	NA
13	B	1222	CL7	NC
13	B	1222	CL7	NA
13	B	1223	CL7	NC
13	B	1223	CL7	NA
13	B	1224	CL7	NC
13	B	1224	CL7	NA
13	B	1225	CL7	NC
13	B	1225	CL7	NA
13	B	1226	CL7	NC
13	B	1226	CL7	NA
13	B	1227	CL7	NC
13	B	1227	CL7	NA
13	B	1228	CL7	NC
13	B	1228	CL7	NA
13	B	1229	CL7	NC
13	B	1229	CL7	NA
13	B	1230	CL7	NC
13	B	1230	CL7	NA
13	B	1231	CL7	NC
13	B	1231	CL7	NA
13	B	1232	CL7	NC
13	B	1232	CL7	NA
13	B	1233	CL7	NC
13	B	1233	CL7	NA

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Mol	Chain	Res	Type	Atom
13	B	1234	CL7	NC
13	B	1234	CL7	NA
13	B	1235	CL7	NC
13	B	1235	CL7	NA
13	B	1236	CL7	NC
13	B	1236	CL7	NA
13	B	1238	CL7	NC
13	B	1238	CL7	NA
13	B	1239	CL7	NC
13	B	1239	CL7	NA
13	B	1241	CL7	NC
13	B	1241	CL7	NA
13	B	1021	CL7	NC
13	B	1021	CL7	NA
13	B	1237	CL7	NC
13	B	1237	CL7	NA
13	I	1601	CL7	NC
13	I	1601	CL7	NA
13	J	1301	CL7	NC
13	J	1301	CL7	NA
13	J	1302	CL7	NC
13	J	1302	CL7	NA
13	K	1401	CL7	NC
13	K	1401	CL7	NA
13	K	1402	CL7	NC
13	K	1402	CL7	NA
13	L	1501	CL7	NC
13	L	1501	CL7	NA
13	L	1502	CL7	NC
13	L	1502	CL7	NA
13	L	1503	CL7	NC
13	L	1503	CL7	NA
13	A	1012	CL7	NC
13	A	1012	CL7	NA
13	A	1101	CL7	NC
13	A	1101	CL7	NA
13	A	1102	CL7	NC
13	A	1102	CL7	NA
13	A	1103	CL7	NC
13	A	1103	CL7	NA
13	A	1104	CL7	NC
13	A	1104	CL7	NA

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Mol	Chain	Res	Type	Atom
13	A	1105	CL7	NC
13	A	1105	CL7	NA
13	A	1106	CL7	NC
13	A	1106	CL7	NA
13	A	1107	CL7	NC
13	A	1107	CL7	NA
13	A	1108	CL7	NC
13	A	1108	CL7	NA
13	A	1109	CL7	NC
13	A	1109	CL7	NA
13	A	1110	CL7	NC
13	A	1110	CL7	NA
13	A	1111	CL7	NC
13	A	1111	CL7	NA
13	A	1112	CL7	NC
13	A	1112	CL7	NA
13	A	1113	CL7	NC
13	A	1113	CL7	NA
13	A	1114	CL7	NC
13	A	1114	CL7	NA
13	A	1115	CL7	NC
13	A	1115	CL7	NA
13	A	1116	CL7	NC
13	A	1116	CL7	NA
13	A	1117	CL7	NC
13	A	1117	CL7	NA
13	A	1118	CL7	NC
13	A	1118	CL7	NA
13	A	1119	CL7	NC
13	A	1119	CL7	NA
13	A	1120	CL7	NC
13	A	1120	CL7	NA
13	A	1121	CL7	NC
13	A	1121	CL7	NA
13	A	1122	CL7	NC
13	A	1122	CL7	NA
13	A	1123	CL7	NC
13	A	1123	CL7	NA
13	A	1124	CL7	NC
13	A	1124	CL7	NA
13	A	1125	CL7	NC
13	A	1125	CL7	NA

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Mol	Chain	Res	Type	Atom
13	A	1126	CL7	NC
13	A	1126	CL7	NA
13	A	1127	CL7	NC
13	A	1127	CL7	NA
13	A	1128	CL7	NC
13	A	1128	CL7	NA
13	A	1129	CL7	NC
13	A	1129	CL7	NA
13	A	1130	CL7	NC
13	A	1130	CL7	NA
13	A	1131	CL7	NC
13	A	1131	CL7	NA
13	A	1132	CL7	NC
13	A	1132	CL7	NA
13	A	1133	CL7	NC
13	A	1133	CL7	NA
13	A	1134	CL7	NC
13	A	1134	CL7	NA
13	A	1135	CL7	NC
13	A	1135	CL7	NA
13	A	1136	CL7	NC
13	A	1136	CL7	NA
13	A	1137	CL7	NC
13	A	1137	CL7	NA
13	A	1138	CL7	NC
13	A	1138	CL7	NA
13	A	1140	CL7	NC
13	A	1140	CL7	NA
13	A	1141	CL7	NC
13	A	1141	CL7	NA
13	A	1139	CL7	NC
13	A	1139	CL7	NA
13	F	1701	CL7	NC
13	F	1701	CL7	NA
20	A	1011	G9R	ND

All (1052) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	1022	CL7	CHA-CBD-CGD-O2D
13	B	1022	CL7	CHA-CBD-CGD-O1D
13	B	1201	CL7	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	B	1201	CL7	C4-C3-C5-C6
13	B	1201	CL7	C2B-C3B-CAB-OBB
13	B	1201	CL7	C4B-C3B-CAB-OBB
13	B	1203	CL7	C4B-C3B-CAB-OBB
13	B	1207	CL7	C4B-C3B-CAB-OBB
13	B	1209	CL7	C1A-C2A-CAA-CBA
13	B	1210	CL7	C1A-C2A-CAA-CBA
13	B	1210	CL7	C3A-C2A-CAA-CBA
13	B	1212	CL7	C1A-C2A-CAA-CBA
13	B	1212	CL7	C3A-C2A-CAA-CBA
13	B	1213	CL7	C1A-C2A-CAA-CBA
13	B	1213	CL7	C3A-C2A-CAA-CBA
13	B	1214	CL7	C4B-C3B-CAB-OBB
13	B	1216	CL7	C2B-C3B-CAB-OBB
13	B	1216	CL7	C4B-C3B-CAB-OBB
13	B	1219	CL7	CHA-CBD-CGD-O2D
13	B	1219	CL7	CHA-CBD-CGD-O1D
13	B	1220	CL7	C1A-C2A-CAA-CBA
13	B	1220	CL7	C3A-C2A-CAA-CBA
13	B	1220	CL7	CHA-CBD-CGD-O2D
13	B	1220	CL7	CHA-CBD-CGD-O1D
13	B	1221	CL7	C4B-C3B-CAB-OBB
13	B	1223	CL7	C1A-C2A-CAA-CBA
13	B	1223	CL7	C4B-C3B-CAB-OBB
13	B	1230	CL7	CHA-CBD-CGD-O2D
13	B	1230	CL7	CHA-CBD-CGD-O1D
13	B	1230	CL7	C2B-C3B-CAB-OBB
13	B	1230	CL7	C4B-C3B-CAB-OBB
13	B	1231	CL7	O1A-CGA-O2A-C1
13	B	1231	CL7	C3A-C2A-CAA-CBA
13	B	1234	CL7	C4B-C3B-CAB-OBB
13	B	1235	CL7	C2-C3-C5-C6
13	B	1235	CL7	C4-C3-C5-C6
13	B	1235	CL7	C1A-C2A-CAA-CBA
13	B	1235	CL7	C3A-C2A-CAA-CBA
13	B	1235	CL7	CHA-CBD-CGD-O2D
13	B	1235	CL7	CHA-CBD-CGD-O1D
13	B	1238	CL7	C2-C3-C5-C6
13	B	1238	CL7	C4-C3-C5-C6
13	B	1241	CL7	C3A-C2A-CAA-CBA
13	B	1021	CL7	CHA-CBD-CGD-O2D
13	B	1021	CL7	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	B	1021	CL7	CAD-CBD-CGD-O1D
13	J	1302	CL7	C1A-C2A-CAA-CBA
13	L	1501	CL7	C1A-C2A-CAA-CBA
13	L	1501	CL7	C3A-C2A-CAA-CBA
13	L	1501	CL7	C2B-C3B-CAB-OBB
13	L	1501	CL7	C4B-C3B-CAB-OBB
13	L	1502	CL7	C6-C7-C8-C9
13	L	1502	CL7	C2B-C3B-CAB-OBB
13	L	1502	CL7	C4B-C3B-CAB-OBB
13	A	1012	CL7	C2B-C3B-CAB-OBB
13	A	1012	CL7	C4B-C3B-CAB-OBB
13	A	1102	CL7	C1A-C2A-CAA-CBA
13	A	1102	CL7	C3A-C2A-CAA-CBA
13	A	1102	CL7	CBD-CGD-O2D-CED
13	A	1102	CL7	C4B-C3B-CAB-OBB
13	A	1103	CL7	C1A-C2A-CAA-CBA
13	A	1103	CL7	C3A-C2A-CAA-CBA
13	A	1106	CL7	C2A-CAA-CBA-CGA
13	A	1106	CL7	C1A-C2A-CAA-CBA
13	A	1106	CL7	C3A-C2A-CAA-CBA
13	A	1108	CL7	C1A-C2A-CAA-CBA
13	A	1108	CL7	C3A-C2A-CAA-CBA
13	A	1108	CL7	CBD-CGD-O2D-CED
13	A	1109	CL7	C1A-C2A-CAA-CBA
13	A	1109	CL7	C3A-C2A-CAA-CBA
13	A	1112	CL7	C1A-C2A-CAA-CBA
13	A	1112	CL7	C2B-C3B-CAB-OBB
13	A	1112	CL7	C4B-C3B-CAB-OBB
13	A	1113	CL7	C1A-C2A-CAA-CBA
13	A	1116	CL7	C3A-C2A-CAA-CBA
13	A	1118	CL7	C2-C3-C5-C6
13	A	1118	CL7	C4-C3-C5-C6
13	A	1121	CL7	C2A-CAA-CBA-CGA
13	A	1121	CL7	C1A-C2A-CAA-CBA
13	A	1122	CL7	CHA-CBD-CGD-O2D
13	A	1122	CL7	CHA-CBD-CGD-O1D
13	A	1123	CL7	O1A-CGA-O2A-C1
13	A	1123	CL7	CBA-CGA-O2A-C1
13	A	1123	CL7	C2B-C3B-CAB-OBB
13	A	1123	CL7	C4B-C3B-CAB-OBB
13	A	1124	CL7	C6-C7-C8-C9
13	A	1124	CL7	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	A	1126	CL7	C1A-C2A-CAA-CBA
13	A	1126	CL7	C3A-C2A-CAA-CBA
13	A	1127	CL7	C2A-CAA-CBA-CGA
13	A	1127	CL7	C3A-C2A-CAA-CBA
13	A	1128	CL7	CAD-CBD-CGD-O2D
13	A	1128	CL7	CAD-CBD-CGD-O1D
13	A	1129	CL7	C1A-C2A-CAA-CBA
13	A	1129	CL7	C3A-C2A-CAA-CBA
13	A	1132	CL7	CHA-CBD-CGD-O2D
13	A	1132	CL7	CHA-CBD-CGD-O1D
13	A	1132	CL7	C2B-C3B-CAB-OBB
13	A	1132	CL7	C4B-C3B-CAB-OBB
13	A	1135	CL7	C1A-C2A-CAA-CBA
13	A	1135	CL7	C3A-C2A-CAA-CBA
13	A	1135	CL7	CBD-CGD-O2D-CED
13	A	1136	CL7	C2-C3-C5-C6
13	A	1136	CL7	C4-C3-C5-C6
13	A	1138	CL7	CHA-CBD-CGD-O2D
13	A	1138	CL7	CHA-CBD-CGD-O1D
13	A	1140	CL7	C2-C3-C5-C6
13	A	1140	CL7	C4-C3-C5-C6
13	A	1140	CL7	C1A-C2A-CAA-CBA
13	A	1141	CL7	CBD-CGD-O2D-CED
13	A	1139	CL7	CHA-CBD-CGD-O2D
13	A	1139	CL7	CHA-CBD-CGD-O1D
13	A	1139	CL7	CBD-CGD-O2D-CED
14	B	1023	PHO	CBD-CGD-O2D-CED
14	A	1013	PHO	C1A-C2A-CAA-CBA
14	A	1013	PHO	C3A-C2A-CAA-CBA
16	B	4004	A1JPJ	C23-C24-C25-C26
16	B	4004	A1JPJ	C23-C24-C25-C30
16	B	4007	A1JPJ	C23-C24-C25-C26
16	B	4007	A1JPJ	C23-C24-C25-C30
16	B	4008	A1JPJ	C1-C6-C7-C8
16	B	4008	A1JPJ	C5-C6-C7-C8
16	B	4008	A1JPJ	C23-C24-C25-C26
16	B	4008	A1JPJ	C23-C24-C25-C30
16	B	4009	A1JPJ	C23-C24-C25-C26
16	B	4009	A1JPJ	C23-C24-C25-C30
16	B	4021	A1JPJ	C23-C24-C25-C26
16	J	4012	A1JPJ	C7-C8-C9-C10
16	J	4012	A1JPJ	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	J	4012	A1JPJ	C23-C24-C25-C30
16	L	4020	A1JPJ	C7-C8-C9-C34
16	L	4020	A1JPJ	C23-C24-C25-C26
16	L	4020	A1JPJ	C23-C24-C25-C30
16	A	4003	A1JPJ	C23-C24-C25-C26
16	A	4007	A1JPJ	C23-C24-C25-C26
16	A	4007	A1JPJ	C23-C24-C25-C30
16	A	4008	A1JPJ	C21-C22-C23-C24
16	A	4008	A1JPJ	C37-C22-C23-C24
16	A	4014	A1JPJ	C23-C24-C25-C30
16	F	4016	A1JPJ	C37-C22-C23-C24
13	B	1022	CL7	O1D-CGD-O2D-CED
13	A	1102	CL7	O1D-CGD-O2D-CED
13	B	1229	CL7	O1D-CGD-O2D-CED
13	B	1233	CL7	O1D-CGD-O2D-CED
13	B	1022	CL7	CBD-CGD-O2D-CED
13	B	1229	CL7	CBD-CGD-O2D-CED
13	B	1232	CL7	CBD-CGD-O2D-CED
13	B	1233	CL7	CBD-CGD-O2D-CED
13	A	1126	CL7	CBD-CGD-O2D-CED
13	B	1227	CL7	O1A-CGA-O2A-C1
13	L	1501	CL7	O1A-CGA-O2A-C1
13	A	1118	CL7	O1A-CGA-O2A-C1
13	A	1121	CL7	O1A-CGA-O2A-C1
13	A	1108	CL7	O1D-CGD-O2D-CED
14	B	1023	PHO	O1D-CGD-O2D-CED
13	B	1227	CL7	CBA-CGA-O2A-C1
13	B	1201	CL7	CBD-CGD-O2D-CED
13	B	1208	CL7	CBD-CGD-O2D-CED
13	B	1218	CL7	CBD-CGD-O2D-CED
13	B	1222	CL7	CBD-CGD-O2D-CED
13	L	1501	CL7	CBD-CGD-O2D-CED
13	A	1107	CL7	CBD-CGD-O2D-CED
13	A	1112	CL7	CBD-CGD-O2D-CED
13	A	1113	CL7	CBD-CGD-O2D-CED
13	A	1128	CL7	CBD-CGD-O2D-CED
13	B	1237	CL7	O1A-CGA-O2A-C1
13	A	1133	CL7	O1A-CGA-O2A-C1
14	A	1013	PHO	O1A-CGA-O2A-C1
13	A	1141	CL7	O1D-CGD-O2D-CED
13	A	1139	CL7	O1D-CGD-O2D-CED
13	B	1220	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	B	1230	CL7	CBD-CGD-O2D-CED
13	A	1135	CL7	O1D-CGD-O2D-CED
13	A	1102	CL7	O1A-CGA-O2A-C1
13	B	1227	CL7	C3-C5-C6-C7
13	B	1229	CL7	C3-C5-C6-C7
13	B	1231	CL7	C3-C5-C6-C7
13	B	1241	CL7	C3-C5-C6-C7
13	B	1237	CL7	C3-C5-C6-C7
13	L	1501	CL7	C3-C5-C6-C7
13	L	1502	CL7	C3-C5-C6-C7
13	A	1103	CL7	C3-C5-C6-C7
13	A	1112	CL7	C3-C5-C6-C7
13	A	1118	CL7	C3-C5-C6-C7
13	A	1122	CL7	C3-C5-C6-C7
13	A	1137	CL7	C3-C5-C6-C7
14	A	1013	PHO	C3-C5-C6-C7
13	B	1231	CL7	CBA-CGA-O2A-C1
13	B	1237	CL7	CBA-CGA-O2A-C1
13	L	1501	CL7	CBA-CGA-O2A-C1
13	A	1118	CL7	CBA-CGA-O2A-C1
13	A	1121	CL7	CBA-CGA-O2A-C1
14	A	1013	PHO	CBA-CGA-O2A-C1
13	A	1111	CL7	C2C-C3C-CAC-CBC
13	A	1109	CL7	C4-C3-C5-C6
13	A	1133	CL7	C4-C3-C5-C6
13	A	1109	CL7	C2-C3-C5-C6
13	B	1212	CL7	CBD-CGD-O2D-CED
13	I	1601	CL7	CBD-CGD-O2D-CED
13	A	1134	CL7	CBD-CGD-O2D-CED
13	B	1209	CL7	C2A-CAA-CBA-CGA
13	B	1212	CL7	C2A-CAA-CBA-CGA
13	B	1214	CL7	C2A-CAA-CBA-CGA
13	B	1228	CL7	C2A-CAA-CBA-CGA
13	B	1238	CL7	C2A-CAA-CBA-CGA
13	A	1118	CL7	C2A-CAA-CBA-CGA
13	A	1107	CL7	C3-C5-C6-C7
13	A	1102	CL7	CBA-CGA-O2A-C1
13	A	1119	CL7	CBA-CGA-O2A-C1
13	A	1127	CL7	CBA-CGA-O2A-C1
13	A	1133	CL7	CBA-CGA-O2A-C1
13	B	1224	CL7	CBD-CGD-O2D-CED
13	A	1012	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	1110	CL7	CBD-CGD-O2D-CED
13	B	1232	CL7	O1D-CGD-O2D-CED
13	B	1225	CL7	O1A-CGA-O2A-C1
13	A	1119	CL7	O1A-CGA-O2A-C1
16	B	4021	A1JPJ	C13-C14-C15-C16
16	B	4021	A1JPJ	C15-C16-C17-C18
16	F	4016	A1JPJ	C9-C10-C11-C12
13	B	1236	CL7	CBD-CGD-O2D-CED
13	B	1021	CL7	CBD-CGD-O2D-CED
13	A	1132	CL7	CBD-CGD-O2D-CED
13	B	1205	CL7	C3-C5-C6-C7
13	A	1116	CL7	C3-C5-C6-C7
13	A	1127	CL7	O1A-CGA-O2A-C1
13	B	1227	CL7	CBD-CGD-O2D-CED
13	A	1119	CL7	CBD-CGD-O2D-CED
13	A	1111	CL7	C4C-C3C-CAC-CBC
13	A	1140	CL7	C3-C5-C6-C7
13	B	1225	CL7	CBA-CGA-O2A-C1
13	A	1126	CL7	O1D-CGD-O2D-CED
13	A	1106	CL7	C4-C3-C5-C6
13	A	1127	CL7	C4-C3-C5-C6
13	A	1106	CL7	C2-C3-C5-C6
13	A	1127	CL7	C2-C3-C5-C6
13	B	1237	CL7	C2A-CAA-CBA-CGA
13	A	1111	CL7	C2A-CAA-CBA-CGA
13	A	1116	CL7	O1A-CGA-O2A-C1
13	B	1214	CL7	CBA-CGA-O2A-C1
13	A	1116	CL7	CBA-CGA-O2A-C1
13	A	1128	CL7	O1D-CGD-O2D-CED
13	B	1222	CL7	O1D-CGD-O2D-CED
13	B	1202	CL7	CBA-CGA-O2A-C1
13	B	1207	CL7	CBA-CGA-O2A-C1
13	B	1208	CL7	CBA-CGA-O2A-C1
13	A	1135	CL7	CBA-CGA-O2A-C1
13	B	1229	CL7	C15-C16-C17-C18
13	B	1241	CL7	C13-C15-C16-C17
13	L	1502	CL7	C13-C15-C16-C17
13	A	1124	CL7	C5-C6-C7-C8
13	B	1202	CL7	O1A-CGA-O2A-C1
13	B	1208	CL7	O1A-CGA-O2A-C1
13	A	1133	CL7	C2-C3-C5-C6
13	B	1202	CL7	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	B	1208	CL7	C14-C13-C15-C16
13	B	1214	CL7	C11-C10-C8-C9
13	B	1223	CL7	C11-C10-C8-C9
13	B	1225	CL7	C6-C7-C8-C9
13	B	1226	CL7	C14-C13-C15-C16
13	B	1239	CL7	C14-C13-C15-C16
13	B	1021	CL7	C11-C12-C13-C14
13	A	1106	CL7	C11-C10-C8-C9
13	A	1109	CL7	C11-C12-C13-C14
13	A	1109	CL7	C14-C13-C15-C16
13	A	1112	CL7	C11-C12-C13-C14
13	A	1117	CL7	C11-C10-C8-C9
13	A	1127	CL7	C11-C12-C13-C14
13	A	1107	CL7	O1D-CGD-O2D-CED
13	A	1131	CL7	C15-C16-C17-C18
13	I	1601	CL7	C2A-CAA-CBA-CGA
16	B	4005	A1JPJ	C7-C8-C9-C34
16	J	4012	A1JPJ	C7-C8-C9-C34
16	F	4016	A1JPJ	C11-C12-C13-C35
16	B	4005	A1JPJ	C7-C8-C9-C10
16	F	4016	A1JPJ	C11-C12-C13-C14
16	F	4016	A1JPJ	C21-C22-C23-C24
13	B	1207	CL7	O1A-CGA-O2A-C1
13	B	1221	CL7	C8-C10-C11-C12
13	B	1231	CL7	C5-C6-C7-C8
13	A	1112	CL7	O1D-CGD-O2D-CED
13	A	1136	CL7	CBA-CGA-O2A-C1
13	B	1203	CL7	C8-C10-C11-C12
13	B	1210	CL7	C8-C10-C11-C12
13	B	1226	CL7	C13-C15-C16-C17
13	A	1109	CL7	C5-C6-C7-C8
13	A	1109	CL7	C10-C11-C12-C13
13	A	1127	CL7	C10-C11-C12-C13
13	A	1139	CL7	C8-C10-C11-C12
13	A	1139	CL7	C15-C16-C17-C18
13	A	1113	CL7	O1D-CGD-O2D-CED
13	B	1201	CL7	O1D-CGD-O2D-CED
13	B	1229	CL7	C13-C15-C16-C17
13	B	1235	CL7	C13-C15-C16-C17
13	B	1239	CL7	C13-C15-C16-C17
13	B	1241	CL7	C15-C16-C17-C18
13	A	1104	CL7	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	A	1104	CL7	C15-C16-C17-C18
13	A	1106	CL7	C13-C15-C16-C17
13	A	1109	CL7	C13-C15-C16-C17
13	A	1117	CL7	C10-C11-C12-C13
13	A	1127	CL7	C5-C6-C7-C8
13	A	1128	CL7	C5-C6-C7-C8
13	A	1138	CL7	C8-C10-C11-C12
15	A	2001	PQN	C23-C25-C26-C27
13	B	1208	CL7	O1D-CGD-O2D-CED
13	B	1218	CL7	O1D-CGD-O2D-CED
13	B	1021	CL7	C5-C6-C7-C8
13	A	1106	CL7	C3-C5-C6-C7
13	B	1216	CL7	CBA-CGA-O2A-C1
13	B	1225	CL7	C10-C11-C12-C13
13	B	1241	CL7	CBD-CGD-O2D-CED
13	A	1122	CL7	CBD-CGD-O2D-CED
13	B	1223	CL7	C12-C13-C15-C16
13	B	1237	CL7	C11-C10-C8-C7
13	A	1109	CL7	C11-C12-C13-C15
13	A	1126	CL7	C11-C10-C8-C7
13	A	1127	CL7	C6-C7-C8-C10
13	A	1136	CL7	C12-C13-C15-C16
13	B	1225	CL7	C3-C5-C6-C7
13	A	1135	CL7	O1A-CGA-O2A-C1
13	A	1108	CL7	C2A-CAA-CBA-CGA
13	A	1110	CL7	C2A-CAA-CBA-CGA
13	A	1125	CL7	C2A-CAA-CBA-CGA
13	L	1501	CL7	O1D-CGD-O2D-CED
13	B	1214	CL7	C5-C6-C7-C8
13	L	1501	CL7	C5-C6-C7-C8
13	A	1116	CL7	C15-C16-C17-C18
13	A	1138	CL7	C15-C16-C17-C18
15	B	2002	PQN	C25-C26-C27-C28
13	B	1220	CL7	O1D-CGD-O2D-CED
13	A	1137	CL7	C5-C6-C7-C8
13	A	1137	CL7	CBA-CGA-O2A-C1
13	B	1214	CL7	O1A-CGA-O2A-C1
13	B	1225	CL7	C5-C6-C7-C8
13	B	1239	CL7	C15-C16-C17-C18
13	L	1502	CL7	C8-C10-C11-C12
13	B	1226	CL7	C15-C16-C17-C18
13	A	1106	CL7	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	A	1121	CL7	C5-C6-C7-C8
13	A	1133	CL7	C15-C16-C17-C18
13	A	1104	CL7	C3-C5-C6-C7
13	B	1210	CL7	CBA-CGA-O2A-C1
13	B	1231	CL7	C10-C11-C12-C13
15	B	2002	PQN	C18-C20-C21-C22
13	B	1230	CL7	O1D-CGD-O2D-CED
13	A	1140	CL7	C2A-CAA-CBA-CGA
13	B	1212	CL7	O1D-CGD-O2D-CED
13	I	1601	CL7	CBA-CGA-O2A-C1
13	A	1109	CL7	CBA-CGA-O2A-C1
13	I	1601	CL7	O1D-CGD-O2D-CED
13	B	1206	CL7	CBD-CGD-O2D-CED
13	B	1202	CL7	C15-C16-C17-C18
13	A	1134	CL7	O1D-CGD-O2D-CED
13	B	1202	CL7	C16-C17-C18-C19
13	B	1215	CL7	C6-C7-C8-C10
13	B	1225	CL7	C16-C17-C18-C19
13	A	1109	CL7	C16-C17-C18-C20
13	A	1125	CL7	C16-C17-C18-C20
17	B	8002	LMG	C36-C37-C38-C39
19	A	852	LHG	C10-C11-C12-C13
13	A	1110	CL7	O1D-CGD-O2D-CED
13	B	1216	CL7	O1A-CGA-O2A-C1
13	A	1136	CL7	O1A-CGA-O2A-C1
19	A	852	LHG	C26-C27-C28-C29
13	B	1208	CL7	C3-C5-C6-C7
13	A	1012	CL7	O1D-CGD-O2D-CED
17	B	8002	LMG	C33-C34-C35-C36
13	B	1221	CL7	C11-C12-C13-C14
13	A	1132	CL7	O1D-CGD-O2D-CED
13	A	1112	CL7	C11-C10-C8-C9
13	A	1116	CL7	C11-C10-C8-C9
17	B	8002	LMG	C19-C20-C21-C22
19	A	853	LHG	C14-C15-C16-C17
13	A	1107	CL7	C10-C11-C12-C13
13	B	1210	CL7	C2A-CAA-CBA-CGA
13	A	1113	CL7	C2A-CAA-CBA-CGA
13	A	1116	CL7	C2A-CAA-CBA-CGA
13	A	1117	CL7	C8-C10-C11-C12
13	B	1224	CL7	O1D-CGD-O2D-CED
13	B	1221	CL7	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
13	B	1237	CL7	C16-C17-C18-C19
13	A	1109	CL7	C16-C17-C18-C19
13	A	1125	CL7	C16-C17-C18-C19
13	A	1138	CL7	C13-C15-C16-C17
15	B	2002	PQN	C23-C25-C26-C27
13	A	1112	CL7	C5-C6-C7-C8
13	B	1210	CL7	O1A-CGA-O2A-C1
13	A	1137	CL7	O1A-CGA-O2A-C1
13	B	1202	CL7	C3A-C2A-CAA-CBA
13	B	1204	CL7	C3A-C2A-CAA-CBA
13	B	1223	CL7	C3A-C2A-CAA-CBA
13	A	1104	CL7	C3A-C2A-CAA-CBA
13	A	1111	CL7	C3A-C2A-CAA-CBA
13	A	1113	CL7	C3A-C2A-CAA-CBA
13	A	1120	CL7	C3A-C2A-CAA-CBA
13	A	1121	CL7	C3A-C2A-CAA-CBA
13	A	1116	CL7	C13-C15-C16-C17
13	B	1202	CL7	C16-C17-C18-C20
13	B	1237	CL7	C16-C17-C18-C20
13	B	1210	CL7	C2-C3-C5-C6
13	A	1107	CL7	C2A-CAA-CBA-CGA
14	A	1013	PHO	C13-C15-C16-C17
13	B	1221	CL7	C3-C5-C6-C7
13	I	1601	CL7	O1A-CGA-O2A-C1
13	A	1109	CL7	O1A-CGA-O2A-C1
13	B	1214	CL7	C2-C1-O2A-CGA
13	A	1127	CL7	C15-C16-C17-C18
16	B	4004	A1JPJ	C1-C6-C7-C8
16	B	4004	A1JPJ	C5-C6-C7-C8
16	B	4005	A1JPJ	C1-C6-C7-C8
16	B	4005	A1JPJ	C5-C6-C7-C8
16	B	4007	A1JPJ	C1-C6-C7-C8
16	B	4007	A1JPJ	C5-C6-C7-C8
16	B	4009	A1JPJ	C1-C6-C7-C8
16	B	4009	A1JPJ	C5-C6-C7-C8
16	B	4011	A1JPJ	C1-C6-C7-C8
16	B	4011	A1JPJ	C5-C6-C7-C8
16	I	4118	A1JPJ	C1-C6-C7-C8
16	I	4118	A1JPJ	C5-C6-C7-C8
16	L	4019	A1JPJ	C1-C6-C7-C8
16	L	4019	A1JPJ	C5-C6-C7-C8
16	L	4023	A1JPJ	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	L	4023	A1JPJ	C5-C6-C7-C8
16	A	4001	A1JPJ	C1-C6-C7-C8
16	A	4001	A1JPJ	C5-C6-C7-C8
16	A	4003	A1JPJ	C1-C6-C7-C8
16	A	4003	A1JPJ	C5-C6-C7-C8
16	A	4007	A1JPJ	C1-C6-C7-C8
16	A	4014	A1JPJ	C1-C6-C7-C8
16	A	4014	A1JPJ	C5-C6-C7-C8
16	F	4016	A1JPJ	C1-C6-C7-C8
16	F	4016	A1JPJ	C5-C6-C7-C8
13	B	1226	CL7	CBA-CGA-O2A-C1
13	B	1205	CL7	C10-C11-C12-C13
13	A	1107	CL7	C13-C15-C16-C17
13	A	1139	CL7	C10-C11-C12-C13
13	B	1236	CL7	O1D-CGD-O2D-CED
13	B	1210	CL7	C4-C3-C5-C6
13	B	1237	CL7	C4-C3-C5-C6
13	B	1021	CL7	O1D-CGD-O2D-CED
13	B	1205	CL7	C2-C3-C5-C6
13	B	1205	CL7	C6-C7-C8-C10
13	B	1226	CL7	C12-C13-C15-C16
13	B	1238	CL7	C12-C13-C15-C16
13	B	1239	CL7	C12-C13-C15-C16
13	B	1241	CL7	C12-C13-C15-C16
13	L	1501	CL7	C6-C7-C8-C10
13	A	1112	CL7	C6-C7-C8-C10
13	A	1112	CL7	C11-C10-C8-C7
13	A	1116	CL7	C11-C10-C8-C7
13	A	1117	CL7	C11-C10-C8-C7
13	A	1124	CL7	C2-C3-C5-C6
13	A	1124	CL7	C6-C7-C8-C10
13	A	1124	CL7	C11-C10-C8-C7
15	A	2001	PQN	C21-C22-C23-C25
13	B	1225	CL7	C16-C17-C18-C20
13	B	1215	CL7	CBA-CGA-O2A-C1
13	B	1224	CL7	CBA-CGA-O2A-C1
13	B	1207	CL7	C2A-CAA-CBA-CGA
13	A	1109	CL7	C2A-CAA-CBA-CGA
13	A	1119	CL7	C2A-CAA-CBA-CGA
13	A	1134	CL7	C2A-CAA-CBA-CGA
13	A	1119	CL7	O1D-CGD-O2D-CED
17	B	8002	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
13	B	1203	CL7	C3-C5-C6-C7
13	B	1202	CL7	C10-C11-C12-C13
13	B	1211	CL7	C5-C6-C7-C8
13	B	1227	CL7	O1D-CGD-O2D-CED
19	A	852	LHG	C8-C7-O7-C5
13	B	1210	CL7	C3-C5-C6-C7
13	B	1235	CL7	C16-C17-C18-C20
13	B	1221	CL7	C4-C3-C5-C6
13	A	1124	CL7	C4-C3-C5-C6
13	B	1223	CL7	C14-C13-C15-C16
13	B	1238	CL7	C14-C13-C15-C16
13	B	1237	CL7	C11-C10-C8-C9
13	L	1501	CL7	C6-C7-C8-C9
13	A	1112	CL7	C6-C7-C8-C9
13	A	1126	CL7	C11-C10-C8-C9
13	A	1127	CL7	C11-C10-C8-C9
13	A	1136	CL7	C14-C13-C15-C16
13	A	1138	CL7	C6-C7-C8-C9
14	B	1023	PHO	C11-C10-C8-C9
13	A	1119	CL7	C3-C5-C6-C7
13	B	1227	CL7	C2A-CAA-CBA-CGA
13	B	1021	CL7	C2A-CAA-CBA-CGA
13	A	1012	CL7	C2A-CAA-CBA-CGA
13	B	1204	CL7	C1A-C2A-CAA-CBA
13	B	1227	CL7	C1A-C2A-CAA-CBA
13	B	1231	CL7	C1A-C2A-CAA-CBA
13	B	1241	CL7	C1A-C2A-CAA-CBA
13	A	1104	CL7	C1A-C2A-CAA-CBA
13	A	1111	CL7	C1A-C2A-CAA-CBA
13	A	1116	CL7	C1A-C2A-CAA-CBA
13	A	1120	CL7	C1A-C2A-CAA-CBA
13	A	1124	CL7	C1A-C2A-CAA-CBA
13	A	1127	CL7	C1A-C2A-CAA-CBA
13	B	1208	CL7	C13-C15-C16-C17
17	B	8002	LMG	C34-C35-C36-C37
13	B	1226	CL7	O1A-CGA-O2A-C1
13	B	1205	CL7	C8-C10-C11-C12
13	A	1121	CL7	CBD-CGD-O2D-CED
13	B	1215	CL7	C6-C7-C8-C9
13	A	1106	CL7	CBA-CGA-O2A-C1
13	B	1205	CL7	C4-C3-C5-C6
13	B	1241	CL7	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	1123	CL7	C4-C3-C5-C6
13	B	1237	CL7	C2-C3-C5-C6
19	A	852	LHG	C25-C26-C27-C28
13	B	1239	CL7	C16-C17-C18-C19
13	A	1112	CL7	C10-C11-C12-C13
13	B	1224	CL7	O1A-CGA-O2A-C1
13	B	1215	CL7	O1A-CGA-O2A-C1
13	A	1136	CL7	C5-C6-C7-C8
13	A	1111	CL7	CBD-CGD-O2D-CED
13	B	1203	CL7	C2B-C3B-CAB-OBB
13	B	1206	CL7	C2B-C3B-CAB-OBB
13	B	1207	CL7	C2B-C3B-CAB-OBB
13	B	1214	CL7	C2B-C3B-CAB-OBB
13	B	1221	CL7	C2B-C3B-CAB-OBB
13	B	1223	CL7	C2B-C3B-CAB-OBB
13	B	1234	CL7	C2B-C3B-CAB-OBB
13	B	1236	CL7	C2B-C3B-CAB-OBB
13	B	1021	CL7	C2B-C3B-CAB-OBB
13	L	1503	CL7	C2B-C3B-CAB-OBB
13	A	1102	CL7	C2B-C3B-CAB-OBB
13	A	1110	CL7	C2B-C3B-CAB-OBB
13	A	1118	CL7	C2B-C3B-CAB-OBB
13	A	1119	CL7	C2B-C3B-CAB-OBB
13	A	1130	CL7	C2B-C3B-CAB-OBB
13	A	1133	CL7	C2B-C3B-CAB-OBB
13	A	1134	CL7	C2B-C3B-CAB-OBB
13	A	1135	CL7	C2B-C3B-CAB-OBB
13	A	1137	CL7	C2B-C3B-CAB-OBB
13	B	1235	CL7	C16-C17-C18-C19
13	B	1021	CL7	C4B-C3B-CAB-OBB
13	A	1130	CL7	C4B-C3B-CAB-OBB
13	A	1137	CL7	C4B-C3B-CAB-OBB
13	B	1203	CL7	C5-C6-C7-C8
13	B	1202	CL7	C3-C5-C6-C7
17	B	8002	LMG	C15-C16-C17-C18
13	B	1241	CL7	O1D-CGD-O2D-CED
13	A	1125	CL7	C15-C16-C17-C18
13	B	1237	CL7	C5-C6-C7-C8
19	A	852	LHG	O9-C7-O7-C5
13	B	1223	CL7	C11-C10-C8-C7
13	B	1225	CL7	C6-C7-C8-C10
13	B	1226	CL7	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	B	1235	CL7	C6-C7-C8-C10
13	B	1235	CL7	C11-C10-C8-C7
13	B	1237	CL7	C6-C7-C8-C10
13	L	1502	CL7	C12-C13-C15-C16
13	A	1106	CL7	C12-C13-C15-C16
13	A	1112	CL7	C11-C12-C13-C15
13	A	1119	CL7	C6-C7-C8-C10
13	A	1123	CL7	C11-C12-C13-C15
13	A	1127	CL7	C11-C10-C8-C7
14	B	1023	PHO	C11-C10-C8-C7
13	A	1106	CL7	O1A-CGA-O2A-C1
13	B	1226	CL7	C11-C10-C8-C9
13	B	1235	CL7	C6-C7-C8-C9
13	B	1235	CL7	C11-C10-C8-C9
13	B	1021	CL7	C14-C13-C15-C16
13	A	1103	CL7	C11-C10-C8-C9
13	A	1104	CL7	C6-C7-C8-C9
13	A	1106	CL7	C11-C12-C13-C14
13	A	1123	CL7	C11-C12-C13-C14
13	A	1124	CL7	C11-C10-C8-C9
13	A	1126	CL7	C11-C12-C13-C14
13	A	1127	CL7	C6-C7-C8-C9
15	B	2002	PQN	C16-C17-C18-C19
13	B	1239	CL7	C16-C17-C18-C20
13	A	1122	CL7	O1D-CGD-O2D-CED
14	B	1023	PHO	C2C-C3C-CAC-CBC
13	A	1117	CL7	CBD-CGD-O2D-CED
13	B	1206	CL7	O1D-CGD-O2D-CED
13	B	1209	CL7	C3A-C2A-CAA-CBA
13	B	1221	CL7	C3A-C2A-CAA-CBA
13	J	1302	CL7	C3A-C2A-CAA-CBA
13	A	1112	CL7	C3A-C2A-CAA-CBA
13	A	1140	CL7	C3A-C2A-CAA-CBA
13	B	1211	CL7	CBA-CGA-O2A-C1
13	B	1235	CL7	C5-C6-C7-C8
13	A	1132	CL7	C13-C15-C16-C17
13	A	1111	CL7	CBA-CGA-O2A-C1
13	A	1123	CL7	C2-C3-C5-C6
13	B	1201	CL7	C6-C7-C8-C9
13	B	1021	CL7	C3-C5-C6-C7
13	A	1136	CL7	C3-C5-C6-C7
19	A	852	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
19	A	852	LHG	C13-C14-C15-C16
13	B	1223	CL7	C2-C1-O2A-CGA
13	B	1235	CL7	C2-C1-O2A-CGA
13	A	1103	CL7	C13-C15-C16-C17
13	B	1202	CL7	C6-C7-C8-C9
13	B	1205	CL7	C11-C10-C8-C9
13	B	1223	CL7	C11-C12-C13-C14
13	B	1227	CL7	C11-C10-C8-C9
13	B	1231	CL7	C11-C10-C8-C9
13	B	1237	CL7	C6-C7-C8-C9
13	A	1109	CL7	C11-C10-C8-C9
13	A	1140	CL7	C6-C7-C8-C9
13	B	1227	CL7	C8-C10-C11-C12
13	A	1130	CL7	C4-C3-C5-C6
13	A	1128	CL7	C16-C17-C18-C19
16	L	4020	A1JPJ	C5-C6-C7-C8
16	A	4002	A1JPJ	C1-C6-C7-C8
13	B	1227	CL7	C5-C6-C7-C8
16	L	4020	A1JPJ	C7-C8-C9-C10
13	L	1502	CL7	C16-C17-C18-C20
13	A	1116	CL7	C8-C10-C11-C12
13	B	1227	CL7	C4-C3-C5-C6
13	B	1203	CL7	C6-C7-C8-C10
13	B	1205	CL7	C11-C10-C8-C7
13	B	1208	CL7	C12-C13-C15-C16
13	B	1223	CL7	C11-C12-C13-C15
13	B	1227	CL7	C11-C10-C8-C7
13	B	1231	CL7	C11-C10-C8-C7
13	B	1021	CL7	C11-C12-C13-C15
13	B	1021	CL7	C12-C13-C15-C16
13	I	1601	CL7	C6-C7-C8-C10
13	L	1502	CL7	C6-C7-C8-C10
13	L	1502	CL7	C11-C10-C8-C7
13	A	1103	CL7	C11-C10-C8-C7
13	A	1104	CL7	C6-C7-C8-C10
13	A	1106	CL7	C11-C12-C13-C15
13	A	1109	CL7	C11-C10-C8-C7
13	A	1109	CL7	C12-C13-C15-C16
13	A	1117	CL7	C6-C7-C8-C10
13	A	1133	CL7	C2A-CAA-CBA-CGA
13	A	1101	CL7	CBD-CGD-O2D-CED
20	A	1011	G9R	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	A	1104	CL7	CBA-CGA-O2A-C1
13	A	1118	CL7	CBD-CGD-O2D-CED
13	B	1209	CL7	CAD-CBD-CGD-O2D
13	B	1210	CL7	CAD-CBD-CGD-O2D
13	B	1211	CL7	CAD-CBD-CGD-O2D
13	B	1234	CL7	CAD-CBD-CGD-O2D
13	L	1501	CL7	CAD-CBD-CGD-O2D
13	L	1503	CL7	CAD-CBD-CGD-O2D
13	A	1111	CL7	CAD-CBD-CGD-O2D
13	A	1116	CL7	CAD-CBD-CGD-O2D
13	A	1125	CL7	CAD-CBD-CGD-O2D
13	A	1129	CL7	CAD-CBD-CGD-O2D
13	A	1131	CL7	CAD-CBD-CGD-O2D
13	A	1140	CL7	CAD-CBD-CGD-O2D
13	A	1132	CL7	C5-C6-C7-C8
19	A	853	LHG	C4-C5-C6-O8
14	A	1013	PHO	C15-C16-C17-C18
13	A	1138	CL7	C16-C17-C18-C19
14	B	1023	PHO	C16-C17-C18-C19
13	B	1221	CL7	CHA-CBD-CGD-O2D
13	B	1221	CL7	CHA-CBD-CGD-O1D
13	B	1222	CL7	CHA-CBD-CGD-O2D
13	B	1222	CL7	CHA-CBD-CGD-O1D
13	B	1232	CL7	CHA-CBD-CGD-O2D
13	B	1232	CL7	CHA-CBD-CGD-O1D
13	B	1233	CL7	CHA-CBD-CGD-O1D
13	A	1103	CL7	CHA-CBD-CGD-O2D
13	A	1103	CL7	CHA-CBD-CGD-O1D
13	A	1110	CL7	CHA-CBD-CGD-O2D
13	A	1110	CL7	CHA-CBD-CGD-O1D
13	A	1112	CL7	CHA-CBD-CGD-O1D
13	A	1137	CL7	CHA-CBD-CGD-O2D
13	A	1137	CL7	CHA-CBD-CGD-O1D
13	A	1141	CL7	CHA-CBD-CGD-O2D
13	A	1141	CL7	CHA-CBD-CGD-O1D
13	A	1104	CL7	O1A-CGA-O2A-C1
13	B	1203	CL7	C13-C15-C16-C17
19	A	853	LHG	O7-C5-C6-O8
13	B	1211	CL7	O1A-CGA-O2A-C1
13	A	1111	CL7	O1A-CGA-O2A-C1
13	A	1122	CL7	C6-C7-C8-C9
13	A	1122	CL7	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	A	1122	CL7	C5-C6-C7-C8
14	B	1023	PHO	C8-C10-C11-C12
13	B	1223	CL7	C3-C5-C6-C7
19	A	852	LHG	C27-C28-C29-C30
13	B	1216	CL7	C5-C6-C7-C8
13	A	1133	CL7	C10-C11-C12-C13
13	B	1202	CL7	C1A-C2A-CAA-CBA
13	B	1225	CL7	C1A-C2A-CAA-CBA
13	B	1234	CL7	C1A-C2A-CAA-CBA
13	A	1121	CL7	O1D-CGD-O2D-CED
13	B	1221	CL7	C2-C3-C5-C6
19	A	853	LHG	C7-C8-C9-C10
13	A	1103	CL7	CBA-CGA-O2A-C1
13	B	1210	CL7	C2C-C3C-CAC-CBC
13	A	1111	CL7	O1D-CGD-O2D-CED
13	B	1208	CL7	C5-C6-C7-C8
13	L	1502	CL7	C16-C17-C18-C19
13	A	1128	CL7	C16-C17-C18-C20
13	B	1232	CL7	CAD-CBD-CGD-O1D
13	A	1103	CL7	CAD-CBD-CGD-O1D
13	A	1112	CL7	CAD-CBD-CGD-O1D
13	A	1130	CL7	C2-C3-C5-C6
13	A	1141	CL7	CAD-CBD-CGD-O1D
13	A	1117	CL7	O1D-CGD-O2D-CED
19	A	853	LHG	C13-C14-C15-C16
13	A	1119	CL7	C4-C3-C5-C6
13	B	1202	CL7	C6-C7-C8-C10
13	B	1204	CL7	C12-C13-C15-C16
13	B	1229	CL7	C6-C7-C8-C10
13	B	1241	CL7	C11-C12-C13-C15
13	L	1501	CL7	C11-C10-C8-C7
13	A	1117	CL7	C11-C12-C13-C15
13	A	1122	CL7	C6-C7-C8-C10
13	A	1131	CL7	C11-C12-C13-C15
13	A	1139	CL7	C12-C13-C15-C16
16	J	4013	A1JPJ	C23-C24-C25-C26
16	A	4002	A1JPJ	C23-C24-C25-C26
16	A	4008	A1JPJ	C23-C24-C25-C26
16	A	4014	A1JPJ	C23-C24-C25-C26
13	B	1214	CL7	C3-C5-C6-C7
13	B	1231	CL7	C8-C10-C11-C12
13	B	1229	CL7	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	A	1134	CL7	C3A-C2A-CAA-CBA
13	A	1138	CL7	C16-C17-C18-C20
13	B	1223	CL7	C10-C11-C12-C13
13	B	1227	CL7	C2-C3-C5-C6
13	B	1203	CL7	C6-C7-C8-C9
13	B	1021	CL7	C11-C10-C8-C9
13	I	1601	CL7	C6-C7-C8-C9
13	A	1117	CL7	C6-C7-C8-C9
13	A	1103	CL7	O1A-CGA-O2A-C1
13	B	1237	CL7	C8-C10-C11-C12
20	A	1011	G9R	CAA-CBA-CGA-O2A
16	B	4005	A1JPJ	C10-C11-C12-C13
16	B	4009	A1JPJ	C18-C19-C20-C21
16	A	4001	A1JPJ	C18-C19-C20-C21
16	A	4002	A1JPJ	C18-C19-C20-C21
13	A	1101	CL7	O1D-CGD-O2D-CED
13	A	1140	CL7	C5-C6-C7-C8
15	B	2002	PQN	C20-C21-C22-C23
13	A	1126	CL7	C2B-C3B-CAB-OBB
13	A	1121	CL7	C6-C7-C8-C10
14	B	1023	PHO	C16-C17-C18-C20
13	A	1118	CL7	O1D-CGD-O2D-CED
13	B	1241	CL7	C2-C3-C5-C6
13	A	1137	CL7	C6-C7-C8-C9
13	A	1126	CL7	C13-C15-C16-C17
13	B	1206	CL7	C4B-C3B-CAB-OBB
13	B	1212	CL7	C4B-C3B-CAB-OBB
13	B	1213	CL7	C4B-C3B-CAB-OBB
13	B	1215	CL7	C4B-C3B-CAB-OBB
13	B	1218	CL7	C4B-C3B-CAB-OBB
13	B	1227	CL7	C4B-C3B-CAB-OBB
13	B	1232	CL7	C4B-C3B-CAB-OBB
13	B	1235	CL7	C4B-C3B-CAB-OBB
13	B	1236	CL7	C4B-C3B-CAB-OBB
13	B	1238	CL7	C4B-C3B-CAB-OBB
13	J	1302	CL7	C4B-C3B-CAB-OBB
13	K	1402	CL7	C4B-C3B-CAB-OBB
13	L	1503	CL7	C4B-C3B-CAB-OBB
13	A	1103	CL7	C4B-C3B-CAB-OBB
13	A	1105	CL7	C4B-C3B-CAB-OBB
13	A	1110	CL7	C4B-C3B-CAB-OBB
13	A	1115	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
13	A	1117	CL7	C4B-C3B-CAB-OBB
13	A	1118	CL7	C4B-C3B-CAB-OBB
13	A	1119	CL7	C4B-C3B-CAB-OBB
13	A	1124	CL7	C4B-C3B-CAB-OBB
13	A	1126	CL7	C4B-C3B-CAB-OBB
13	A	1129	CL7	C4B-C3B-CAB-OBB
13	A	1133	CL7	C4B-C3B-CAB-OBB
13	A	1134	CL7	C4B-C3B-CAB-OBB
13	A	1135	CL7	C4B-C3B-CAB-OBB
13	A	1139	CL7	C4B-C3B-CAB-OBB
13	F	1701	CL7	C4B-C3B-CAB-OBB
13	B	1224	CL7	C2A-CAA-CBA-CGA
13	A	1117	CL7	C2A-CAA-CBA-CGA
13	A	1119	CL7	C10-C11-C12-C13
13	B	1210	CL7	C2-C1-O2A-CGA
13	A	1122	CL7	C16-C17-C18-C20
13	B	1210	CL7	C4C-C3C-CAC-CBC
13	B	1225	CL7	C8-C10-C11-C12
13	B	1223	CL7	C2A-CAA-CBA-CGA
19	A	852	LHG	C3-O3-P-O6
19	A	853	LHG	C3-O3-P-O6
13	B	1241	CL7	C10-C11-C12-C13
13	A	1136	CL7	C10-C11-C12-C13
14	B	1023	PHO	CHA-CBD-CGD-O1D
14	B	1023	PHO	CHA-CBD-CGD-O2D
20	A	1011	G9R	CHA-CBD-CGD-O1D
20	A	1011	G9R	CHA-CBD-CGD-O2D
13	B	1210	CL7	C11-C10-C8-C7
13	A	1128	CL7	C11-C10-C8-C7
13	A	1136	CL7	C11-C10-C8-C7
17	B	8002	LMG	C20-C21-C22-C23
13	A	1140	CL7	CAA-CBA-CGA-O2A
13	L	1502	CL7	C11-C10-C8-C9
13	L	1502	CL7	C14-C13-C15-C16
13	A	1117	CL7	C11-C12-C13-C14
13	A	1119	CL7	C6-C7-C8-C9
13	A	1128	CL7	C11-C10-C8-C9
13	A	1136	CL7	C11-C10-C8-C9
13	L	1502	CL7	C2A-CAA-CBA-CGA
13	A	1139	CL7	C13-C15-C16-C17
13	B	1205	CL7	C16-C17-C18-C20
13	A	1132	CL7	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	A	1126	CL7	CBA-CGA-O2A-C1
17	B	8002	LMG	C17-C18-C19-C20
13	B	1215	CL7	C2A-CAA-CBA-CGA
14	B	1023	PHO	C2A-CAA-CBA-CGA
13	A	1126	CL7	O1A-CGA-O2A-C1
15	B	2002	PQN	C26-C27-C28-C29
13	A	1118	CL7	C2-C1-O2A-CGA
13	B	1211	CL7	C10-C11-C12-C13
13	B	1213	CL7	C2A-CAA-CBA-CGA
13	B	1231	CL7	C2A-CAA-CBA-CGA
13	B	1216	CL7	C3A-C2A-CAA-CBA
13	B	1222	CL7	C3A-C2A-CAA-CBA
13	B	1234	CL7	C3A-C2A-CAA-CBA
13	I	1601	CL7	C3A-C2A-CAA-CBA
13	L	1502	CL7	C3A-C2A-CAA-CBA
13	A	1012	CL7	C3A-C2A-CAA-CBA
13	A	1123	CL7	C3A-C2A-CAA-CBA
13	A	1125	CL7	C3A-C2A-CAA-CBA
13	A	1133	CL7	C3A-C2A-CAA-CBA
13	B	1226	CL7	C16-C17-C18-C19
13	B	1204	CL7	C14-C13-C15-C16
13	A	1103	CL7	C11-C12-C13-C14
13	A	1139	CL7	C14-C13-C15-C16
14	B	1023	PHO	C11-C12-C13-C14
15	A	2001	PQN	C24-C23-C25-C26
16	B	4006	A1JPJ	C11-C10-C9-C34
16	B	4006	A1JPJ	C20-C21-C22-C37
16	B	4007	A1JPJ	C35-C13-C14-C15
16	B	4009	A1JPJ	C20-C21-C22-C37
16	B	4011	A1JPJ	C11-C10-C9-C34
16	B	4011	A1JPJ	C16-C17-C18-C36
16	L	4020	A1JPJ	C11-C10-C9-C34
16	A	4001	A1JPJ	C20-C21-C22-C37
16	A	4003	A1JPJ	C35-C13-C14-C15
13	B	1204	CL7	C16-C17-C18-C20
13	A	1126	CL7	O2A-C1-C2-C3
13	B	1209	CL7	CAA-CBA-CGA-O1A
13	B	1222	CL7	C1A-C2A-CAA-CBA
13	I	1601	CL7	C1A-C2A-CAA-CBA
13	A	1012	CL7	C1A-C2A-CAA-CBA
13	A	1123	CL7	C1A-C2A-CAA-CBA
13	A	1125	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	B	1210	CL7	C6-C7-C8-C10
13	B	1223	CL7	C6-C7-C8-C10
13	I	1601	CL7	C11-C10-C8-C7
13	A	1127	CL7	C11-C12-C13-C15
13	A	1133	CL7	C6-C7-C8-C10
13	A	1138	CL7	C6-C7-C8-C10
13	A	1123	CL7	C13-C15-C16-C17
13	A	1136	CL7	C2A-CAA-CBA-CGA
13	A	1126	CL7	C10-C11-C12-C13
13	A	1124	CL7	C8-C10-C11-C12
16	B	4006	A1JPJ	C20-C21-C22-C23
16	B	4007	A1JPJ	C12-C13-C14-C15
16	B	4009	A1JPJ	C20-C21-C22-C23
16	B	4011	A1JPJ	C16-C17-C18-C19
16	A	4001	A1JPJ	C20-C21-C22-C23
16	A	4002	A1JPJ	C20-C21-C22-C23
16	A	4003	A1JPJ	C12-C13-C14-C15
13	A	1133	CL7	C5-C6-C7-C8
17	B	8002	LMG	C13-C14-C15-C16
13	B	1238	CL7	C3-C5-C6-C7
13	A	1108	CL7	C2-C1-O2A-CGA
13	A	1136	CL7	C2-C1-O2A-CGA
13	B	1212	CL7	CAA-CBA-CGA-O2A
13	A	1138	CL7	C11-C10-C8-C9
13	B	1209	CL7	CAA-CBA-CGA-O2A
13	B	1212	CL7	CAA-CBA-CGA-O1A
16	A	4007	A1JPJ	C5-C6-C7-C8
16	A	4008	A1JPJ	C1-C6-C7-C8
13	A	1103	CL7	CAA-CBA-CGA-O2A
13	A	1132	CL7	C2-C3-C5-C6
13	A	1134	CL7	CAA-CBA-CGA-O2A
13	A	1110	CL7	CAA-CBA-CGA-O2A
13	A	1114	CL7	CAA-CBA-CGA-O2A
13	B	1241	CL7	C2A-CAA-CBA-CGA
13	B	1213	CL7	CAA-CBA-CGA-O2A
13	A	1137	CL7	C6-C7-C8-C10
13	B	1216	CL7	C4-C3-C5-C6
13	B	1239	CL7	C4-C3-C5-C6
13	A	1132	CL7	C4-C3-C5-C6
13	B	1214	CL7	C11-C12-C13-C15
13	B	1239	CL7	C6-C7-C8-C10
15	B	2002	PQN	C17-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
13	A	1112	CL7	O1A-CGA-O2A-C1
13	A	1121	CL7	CAA-CBA-CGA-O2A
13	B	1212	CL7	C2B-C3B-CAB-OBB
13	B	1213	CL7	C2B-C3B-CAB-OBB
13	B	1215	CL7	C2B-C3B-CAB-OBB
13	B	1218	CL7	C2B-C3B-CAB-OBB
13	B	1227	CL7	C2B-C3B-CAB-OBB
13	B	1238	CL7	C2B-C3B-CAB-OBB
13	J	1302	CL7	C2B-C3B-CAB-OBB
13	A	1103	CL7	C2B-C3B-CAB-OBB
13	A	1105	CL7	C2B-C3B-CAB-OBB
13	A	1115	CL7	C2B-C3B-CAB-OBB
13	A	1117	CL7	C2B-C3B-CAB-OBB
13	A	1124	CL7	C2B-C3B-CAB-OBB
13	A	1129	CL7	C2B-C3B-CAB-OBB
13	A	1139	CL7	C2B-C3B-CAB-OBB
13	F	1701	CL7	C2B-C3B-CAB-OBB
13	A	1112	CL7	CBA-CGA-O2A-C1
13	A	1110	CL7	CAA-CBA-CGA-O1A
13	B	1214	CL7	C8-C10-C11-C12
13	B	1236	CL7	CAA-CBA-CGA-O2A
16	A	4002	A1JPJ	C20-C21-C22-C37
15	B	2002	PQN	C26-C27-C28-C30
13	B	1231	CL7	CAA-CBA-CGA-O2A
13	B	1205	CL7	C6-C7-C8-C9
13	B	1210	CL7	C6-C7-C8-C9
13	B	1229	CL7	C6-C7-C8-C9
13	B	1241	CL7	C11-C12-C13-C14
13	L	1501	CL7	C11-C10-C8-C9
13	A	1126	CL7	C6-C7-C8-C9
13	A	1131	CL7	C11-C12-C13-C14
13	A	1133	CL7	C6-C7-C8-C9
13	B	1213	CL7	CAA-CBA-CGA-O1A
13	A	1114	CL7	CAA-CBA-CGA-O1A
13	B	1204	CL7	C4B-C3B-CAB-OBB
13	A	1120	CL7	C4B-C3B-CAB-OBB
13	A	1122	CL7	C4B-C3B-CAB-OBB
13	A	1131	CL7	C4B-C3B-CAB-OBB
19	A	852	LHG	O8-C23-C24-C25
13	B	1208	CL7	CAD-CBD-CGD-O2D
13	B	1227	CL7	CAD-CBD-CGD-O2D
13	I	1601	CL7	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	A	1105	CL7	CAD-CBD-CGD-O2D
13	A	1113	CL7	CAD-CBD-CGD-O2D
13	A	1124	CL7	CAD-CBD-CGD-O2D
13	B	1204	CL7	C16-C17-C18-C19
13	A	1107	CL7	C8-C10-C11-C12
15	B	2002	PQN	C15-C16-C17-C18
13	B	1203	CL7	CAA-CBA-CGA-O2A
17	B	8002	LMG	O7-C10-C11-C12
13	K	1401	CL7	CAA-CBA-CGA-O2A
13	A	1107	CL7	CAA-CBA-CGA-O2A
13	A	1134	CL7	CAA-CBA-CGA-O1A
13	B	1221	CL7	CAA-CBA-CGA-O2A
13	B	1236	CL7	CAA-CBA-CGA-O1A
13	B	1202	CL7	O2A-C1-C2-C3
13	B	1231	CL7	O2A-C1-C2-C3
13	A	1138	CL7	C2A-CAA-CBA-CGA
19	A	852	LHG	C29-C30-C31-C32
13	B	1226	CL7	C16-C17-C18-C20
13	B	1202	CL7	CHA-CBD-CGD-O1D
13	B	1204	CL7	CHA-CBD-CGD-O2D
13	B	1204	CL7	CHA-CBD-CGD-O1D
13	B	1205	CL7	CHA-CBD-CGD-O2D
13	B	1205	CL7	CHA-CBD-CGD-O1D
13	B	1211	CL7	CHA-CBD-CGD-O2D
13	B	1212	CL7	CHA-CBD-CGD-O2D
13	B	1212	CL7	CHA-CBD-CGD-O1D
13	B	1213	CL7	CHA-CBD-CGD-O2D
13	B	1216	CL7	CHA-CBD-CGD-O2D
13	B	1216	CL7	CHA-CBD-CGD-O1D
13	B	1233	CL7	CHA-CBD-CGD-O2D
13	B	1241	CL7	CHA-CBD-CGD-O1D
13	L	1501	CL7	CHA-CBD-CGD-O2D
13	L	1502	CL7	CHA-CBD-CGD-O2D
13	L	1502	CL7	CHA-CBD-CGD-O1D
13	A	1012	CL7	CHA-CBD-CGD-O2D
13	A	1012	CL7	CHA-CBD-CGD-O1D
13	A	1101	CL7	CHA-CBD-CGD-O2D
13	A	1101	CL7	CHA-CBD-CGD-O1D
13	A	1106	CL7	CHA-CBD-CGD-O1D
13	A	1108	CL7	CHA-CBD-CGD-O2D
13	A	1108	CL7	CHA-CBD-CGD-O1D
13	A	1112	CL7	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	A	1120	CL7	CHA-CBD-CGD-O1D
13	A	1123	CL7	CHA-CBD-CGD-O1D
13	K	1401	CL7	CAA-CBA-CGA-O1A
13	B	1207	CL7	CAA-CBA-CGA-O2A
16	B	4006	A1JPJ	C11-C10-C9-C8
16	B	4011	A1JPJ	C11-C10-C9-C8
16	L	4020	A1JPJ	C11-C10-C9-C8
13	A	1109	CL7	CAA-CBA-CGA-O2A
13	A	1123	CL7	CAA-CBA-CGA-O2A
13	A	1125	CL7	CAA-CBA-CGA-O2A
13	A	1121	CL7	C3-C5-C6-C7
13	A	1122	CL7	CAA-CBA-CGA-O2A
13	B	1214	CL7	C11-C10-C8-C7
13	B	1216	CL7	C2-C3-C5-C6
13	B	1021	CL7	C6-C7-C8-C10
13	A	1107	CL7	C11-C12-C13-C15
13	A	1119	CL7	C2-C3-C5-C6
13	A	1132	CL7	C16-C17-C18-C19
13	I	1601	CL7	C11-C12-C13-C14
13	B	1022	CL7	CAA-CBA-CGA-O2A
16	L	4019	A1JPJ	C11-C12-C13-C35
19	A	852	LHG	C23-C24-C25-C26
13	B	1022	CL7	C1A-C2A-CAA-CBA
13	B	1216	CL7	C1A-C2A-CAA-CBA
13	B	1221	CL7	C1A-C2A-CAA-CBA
13	B	1239	CL7	C1A-C2A-CAA-CBA
13	L	1502	CL7	C1A-C2A-CAA-CBA
13	A	1133	CL7	C1A-C2A-CAA-CBA
13	B	1231	CL7	CAA-CBA-CGA-O1A
17	B	8002	LMG	O9-C10-C11-C12
19	A	852	LHG	O10-C23-C24-C25
19	A	852	LHG	C4-C5-C6-O8
13	B	1227	CL7	C11-C12-C13-C14
13	A	1107	CL7	C16-C17-C18-C19
13	A	1121	CL7	CAA-CBA-CGA-O1A
14	B	1023	PHO	CAA-CBA-CGA-O2A
19	A	853	LHG	C3-O3-P-O5
13	B	1022	CL7	CAA-CBA-CGA-O1A
13	B	1207	CL7	CAA-CBA-CGA-O1A
13	A	1123	CL7	CAA-CBA-CGA-O1A
16	L	4020	A1JPJ	C1-C6-C7-C8
13	B	1203	CL7	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	B	1221	CL7	CBA-CGA-O2A-C1
17	B	8002	LMG	C18-C19-C20-C21
13	B	1202	CL7	CAA-CBA-CGA-O2A
19	A	853	LHG	O7-C7-C8-C9
13	A	1107	CL7	CAA-CBA-CGA-O1A
13	A	1123	CL7	CAD-CBD-CGD-O1D
13	A	1132	CL7	O1A-CGA-O2A-C1
13	A	1109	CL7	CAA-CBA-CGA-O1A
13	B	1223	CL7	C6-C7-C8-C9
13	B	1021	CL7	C6-C7-C8-C9
15	A	2001	PQN	C21-C22-C23-C24
13	A	1122	CL7	CAA-CBA-CGA-O1A
17	B	8002	LMG	C38-C39-C40-C41
13	A	1132	CL7	CBA-CGA-O2A-C1
13	A	1136	CL7	CAA-CBA-CGA-O2A
13	A	1125	CL7	CAA-CBA-CGA-O1A
13	B	1206	CL7	CAA-CBA-CGA-O2A
13	I	1601	CL7	CAA-CBA-CGA-O2A
13	L	1501	CL7	CAA-CBA-CGA-O2A
13	A	1139	CL7	CAA-CBA-CGA-O2A
13	B	1220	CL7	CAA-CBA-CGA-O2A
13	B	1203	CL7	C12-C13-C15-C16
13	B	1210	CL7	C11-C12-C13-C15
13	I	1601	CL7	C11-C12-C13-C15
13	A	1106	CL7	C11-C10-C8-C7
13	A	1138	CL7	C11-C10-C8-C7
16	B	4005	A1JPJ	C23-C24-C25-C26
16	B	4006	A1JPJ	C23-C24-C25-C26
16	A	4001	A1JPJ	C23-C24-C25-C26
13	B	1239	CL7	CAA-CBA-CGA-O2A
17	B	8002	LMG	C28-C29-C30-C31
13	B	1206	CL7	CAA-CBA-CGA-O1A
13	B	1239	CL7	CAA-CBA-CGA-O1A
13	I	1601	CL7	CAA-CBA-CGA-O1A
14	B	1023	PHO	CAA-CBA-CGA-O1A
13	L	1501	CL7	CAA-CBA-CGA-O1A
13	B	1241	CL7	C16-C17-C18-C19
13	B	1205	CL7	C13-C15-C16-C17
17	B	8002	LMG	C31-C32-C33-C34
13	B	1202	CL7	CAA-CBA-CGA-O1A
13	A	1136	CL7	CAA-CBA-CGA-O1A

There are no ring outliers.

84 monomers are involved in 216 short contacts:

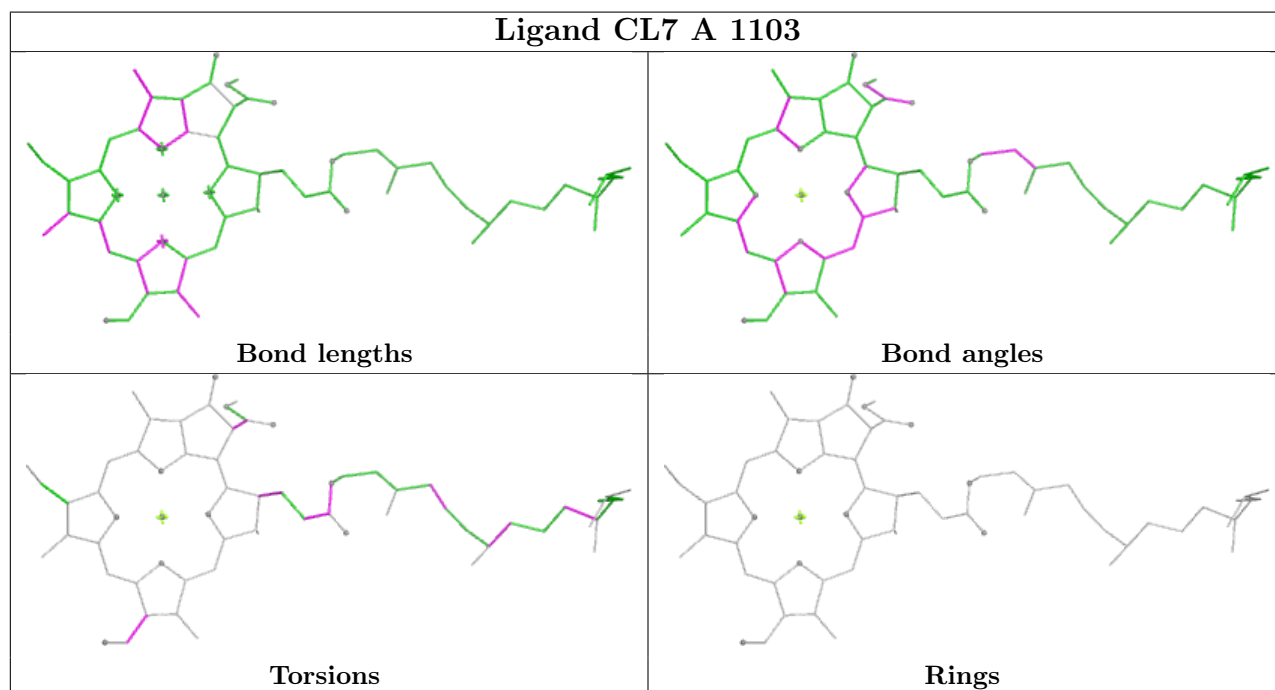
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1103	CL7	6	0
13	B	1213	CL7	1	0
13	B	1238	CL7	4	0
13	A	1104	CL7	4	0
13	B	1210	CL7	5	0
13	B	1216	CL7	2	0
13	A	1115	CL7	2	0
13	B	1022	CL7	2	0
13	B	1236	CL7	1	0
13	B	1223	CL7	1	0
13	L	1502	CL7	3	0
13	A	1137	CL7	3	0
13	A	1102	CL7	4	0
13	A	1126	CL7	9	0
13	B	1220	CL7	3	0
13	A	1131	CL7	2	0
19	A	852	LHG	2	0
13	B	1201	CL7	6	0
13	B	1206	CL7	1	0
13	B	1214	CL7	7	0
13	A	1134	CL7	2	0
13	I	1601	CL7	2	0
13	B	1021	CL7	4	0
16	J	4012	A1JPJ	1	0
17	B	8002	LMG	3	0
13	A	1132	CL7	1	0
13	A	1119	CL7	5	0
13	B	1225	CL7	1	0
13	A	1123	CL7	4	0
13	J	1302	CL7	2	0
13	A	1127	CL7	4	0
13	A	1140	CL7	3	0
13	B	1202	CL7	3	0
13	A	1111	CL7	2	0
13	A	1112	CL7	2	0
13	A	1106	CL7	6	0
13	A	1114	CL7	1	0
13	B	1215	CL7	1	0
13	B	1209	CL7	1	0
13	B	1230	CL7	2	0
13	A	1012	CL7	2	0
13	A	1139	CL7	3	0

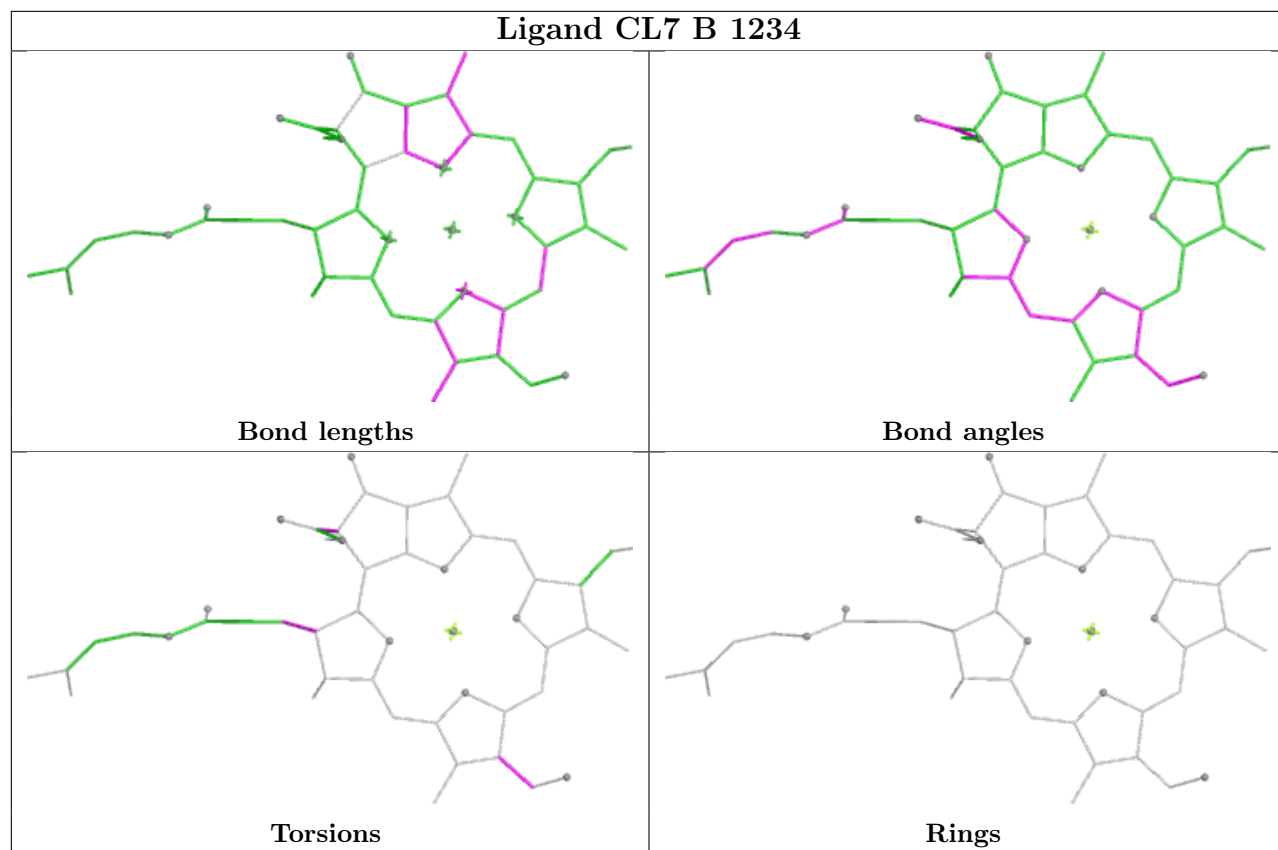
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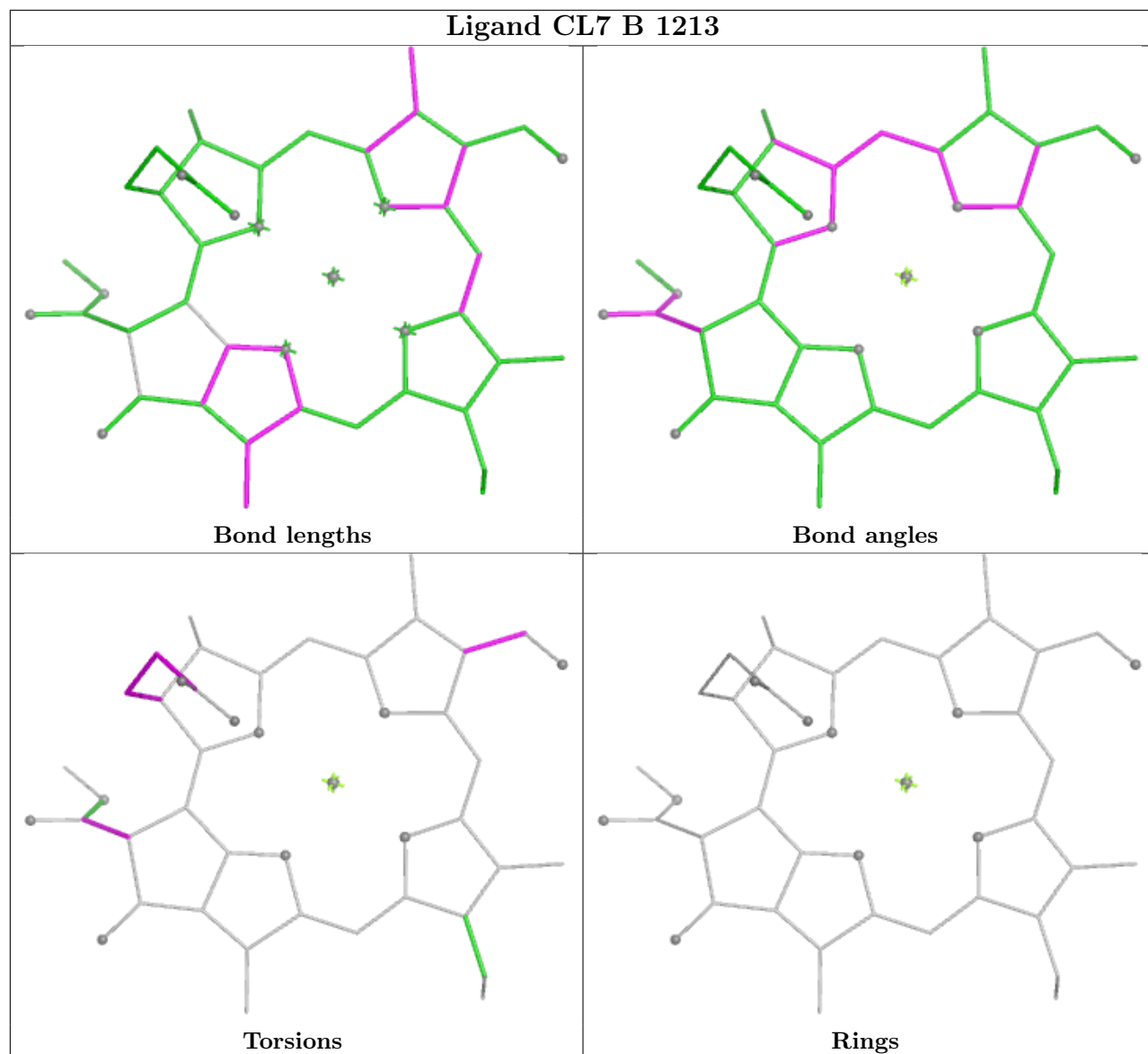
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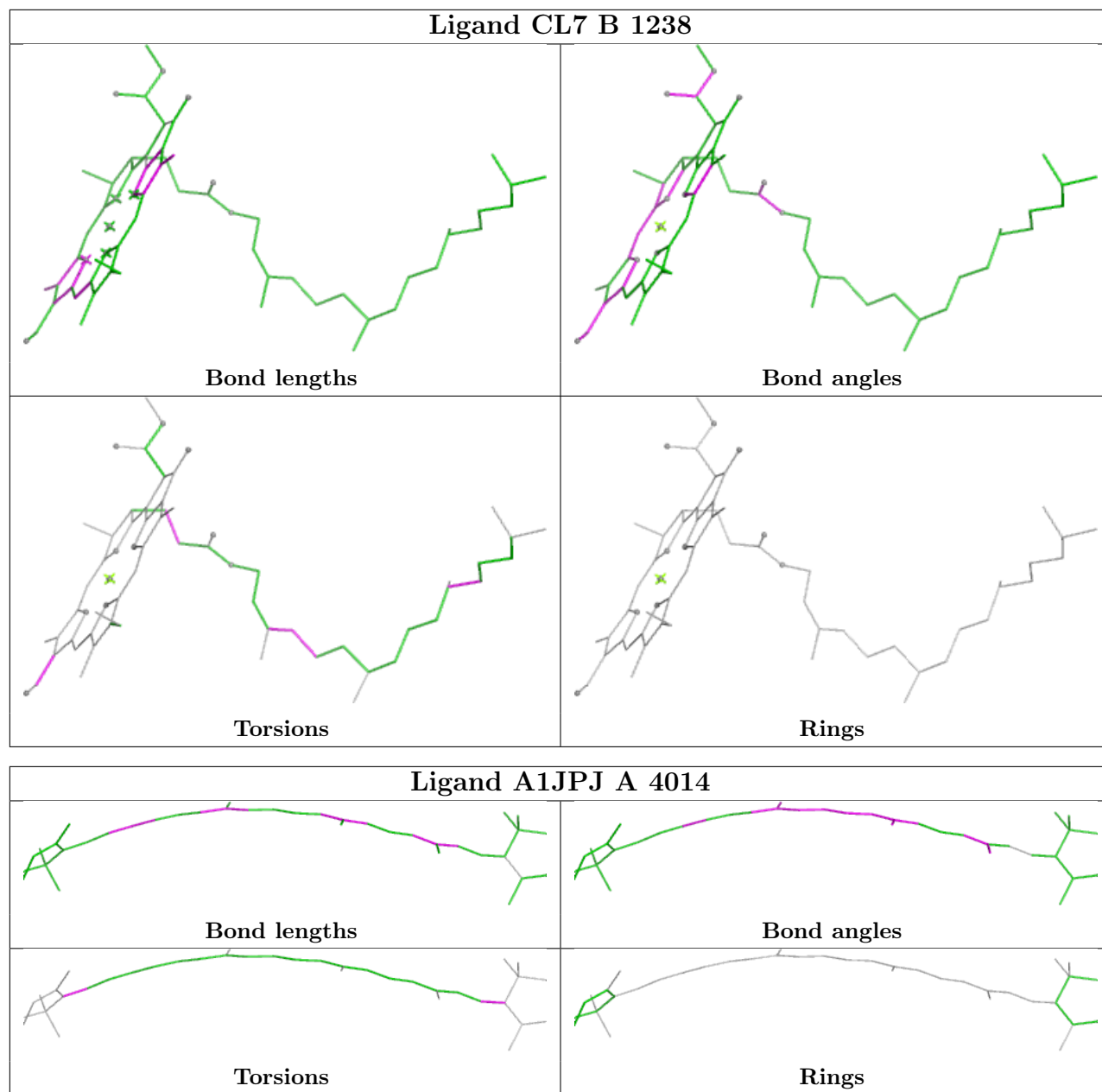
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1221	CL7	3	0
13	B	1208	CL7	1	0
13	B	1203	CL7	4	0
13	B	1229	CL7	3	0
13	B	1211	CL7	3	0
14	B	1023	PHO	10	0
13	A	1118	CL7	1	0
13	B	1226	CL7	4	0
13	A	1110	CL7	2	0
13	A	1121	CL7	1	0
16	B	4005	A1JPJ	1	0
13	A	1130	CL7	2	0
13	A	1136	CL7	3	0
14	A	1013	PHO	3	0
13	B	1224	CL7	2	0
13	B	1205	CL7	5	0
13	B	1241	CL7	10	0
13	A	1105	CL7	1	0
13	B	1207	CL7	2	0
13	A	1107	CL7	6	0
13	L	1501	CL7	1	0
13	A	1116	CL7	6	0
13	B	1235	CL7	2	0
13	B	1228	CL7	1	0
13	B	1232	CL7	1	0
13	B	1237	CL7	3	0
13	B	1212	CL7	2	0
13	B	1204	CL7	5	0
13	A	1128	CL7	3	0
19	A	853	LHG	1	0
13	B	1227	CL7	7	0
13	A	1125	CL7	6	0
13	A	1133	CL7	3	0
13	A	1108	CL7	2	0
13	A	1124	CL7	2	0
13	J	1301	CL7	2	0
13	A	1135	CL7	1	0
13	B	1231	CL7	5	0
13	A	1120	CL7	2	0
13	A	1109	CL7	6	0
13	B	1239	CL7	5	0
13	A	1138	CL7	8	0

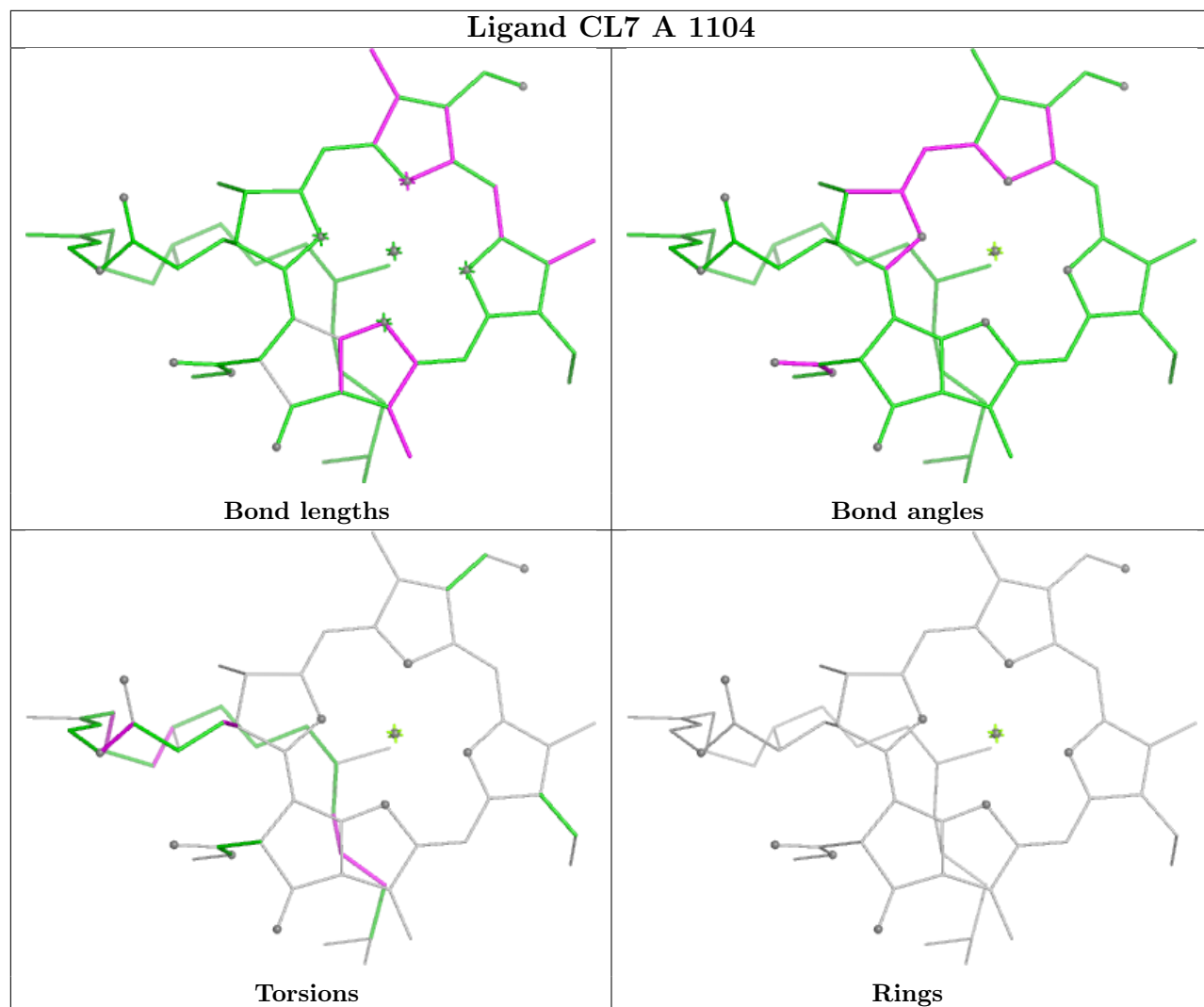
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

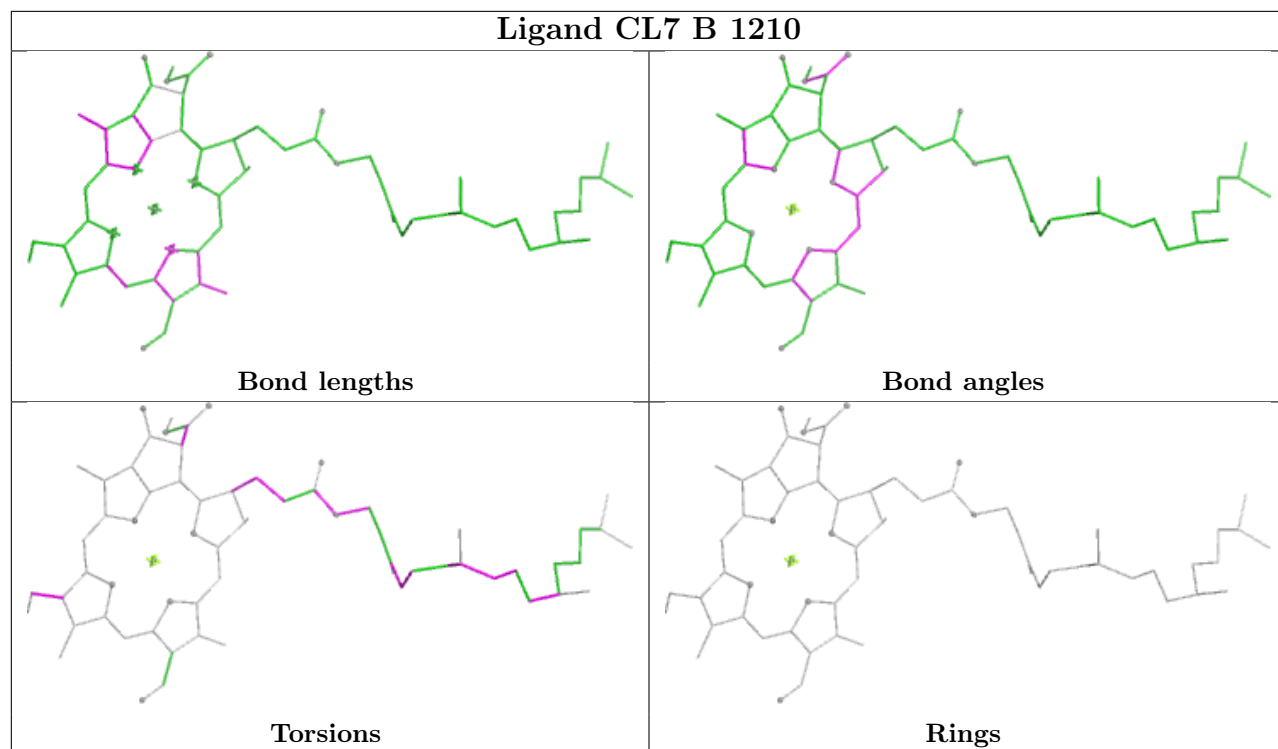


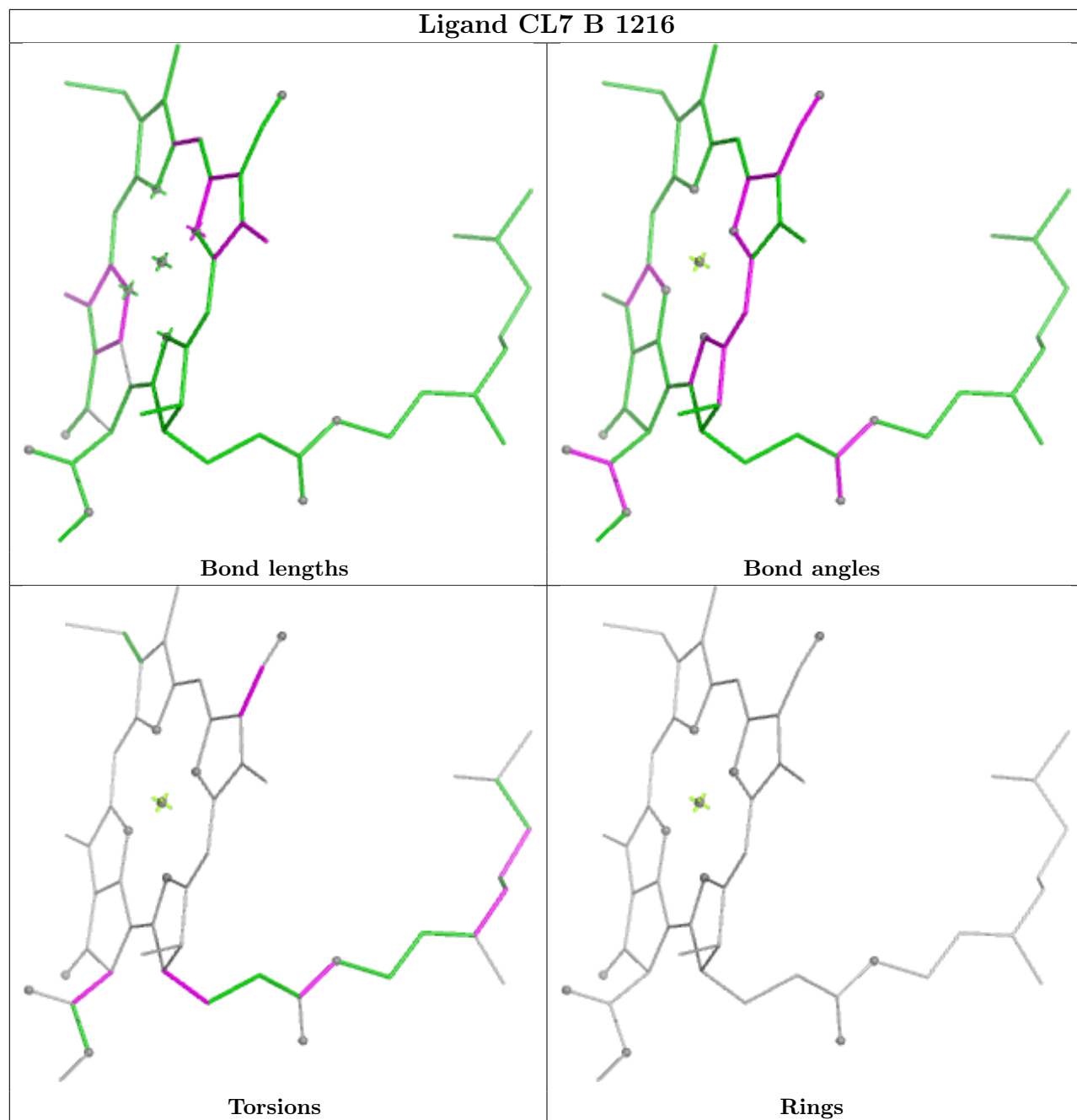


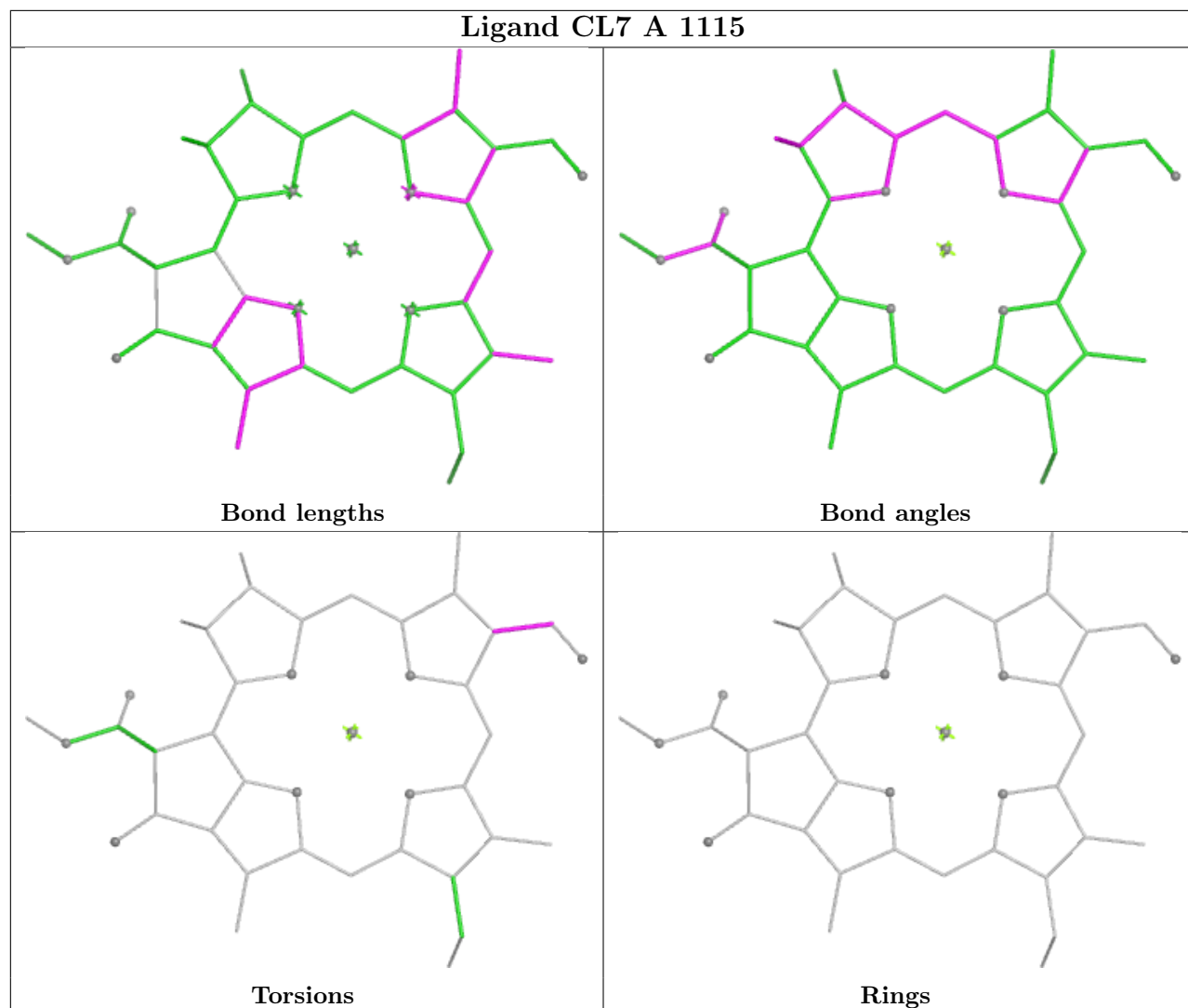


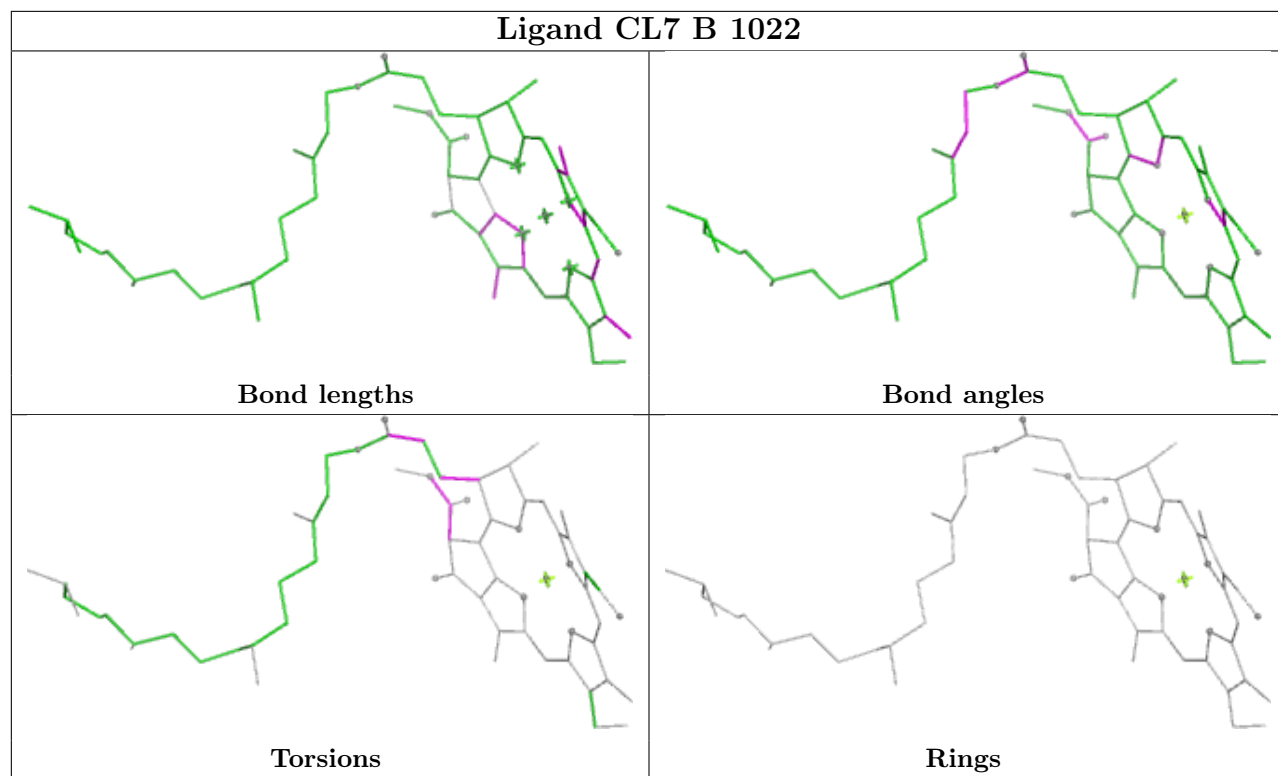


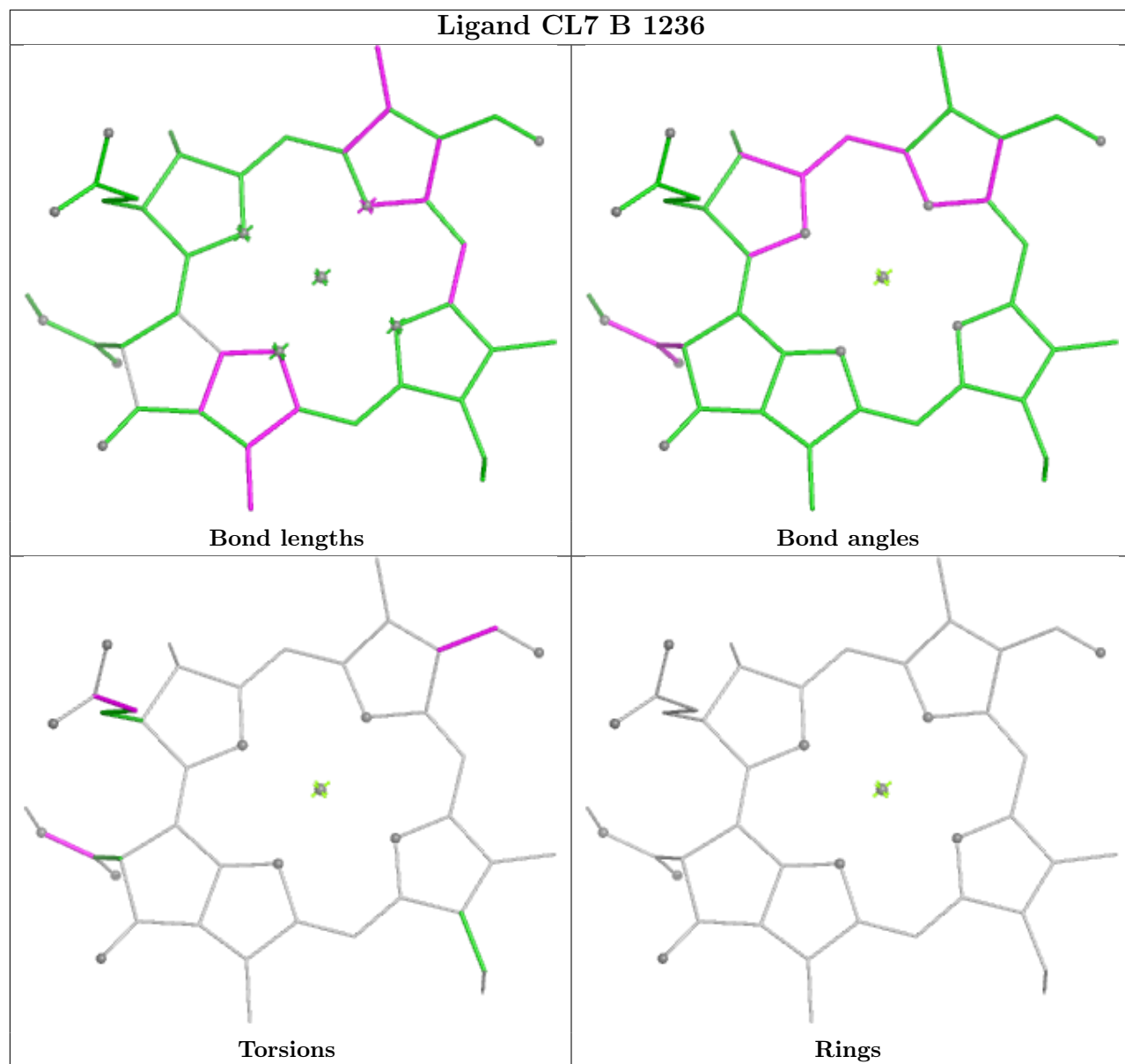


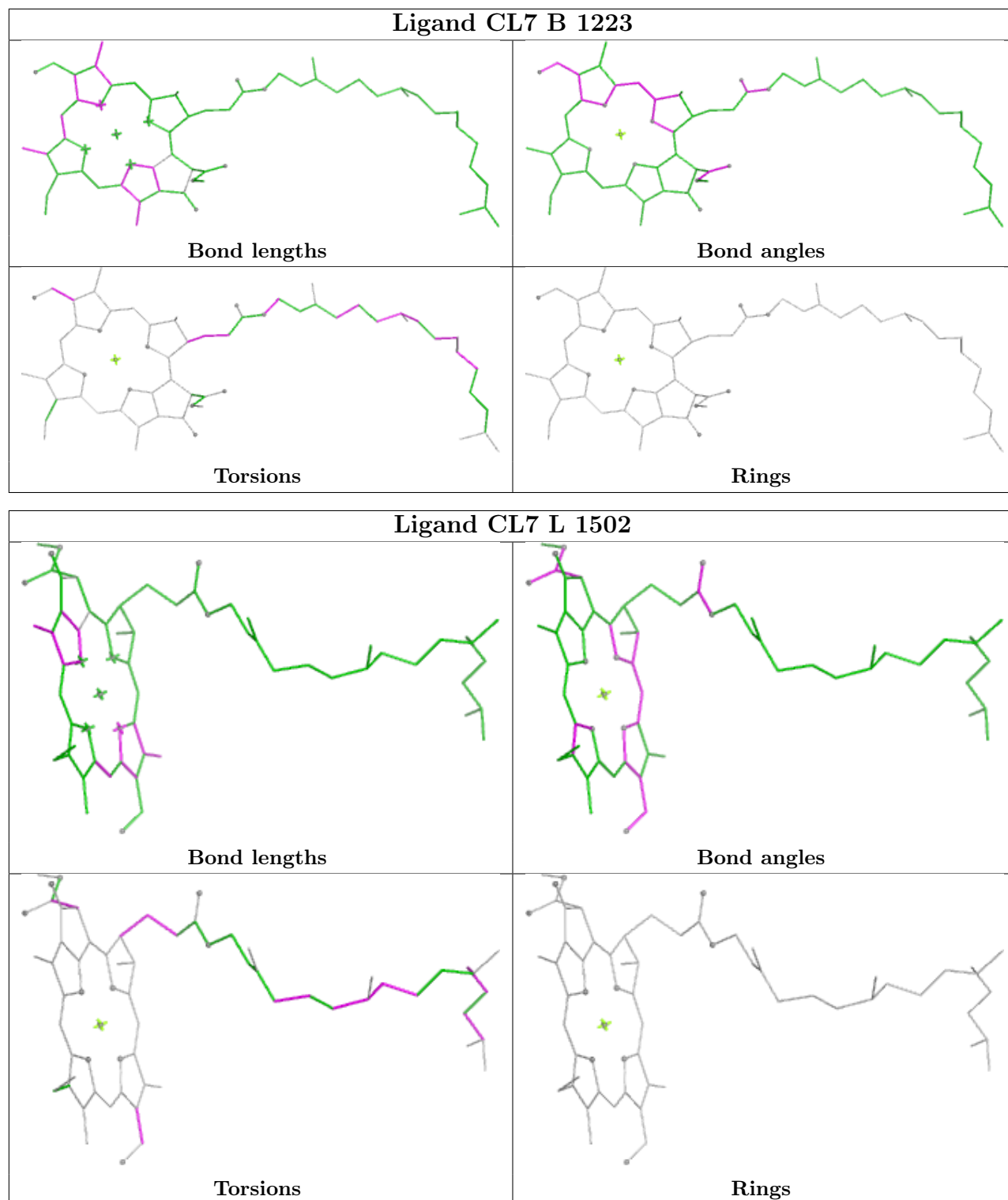


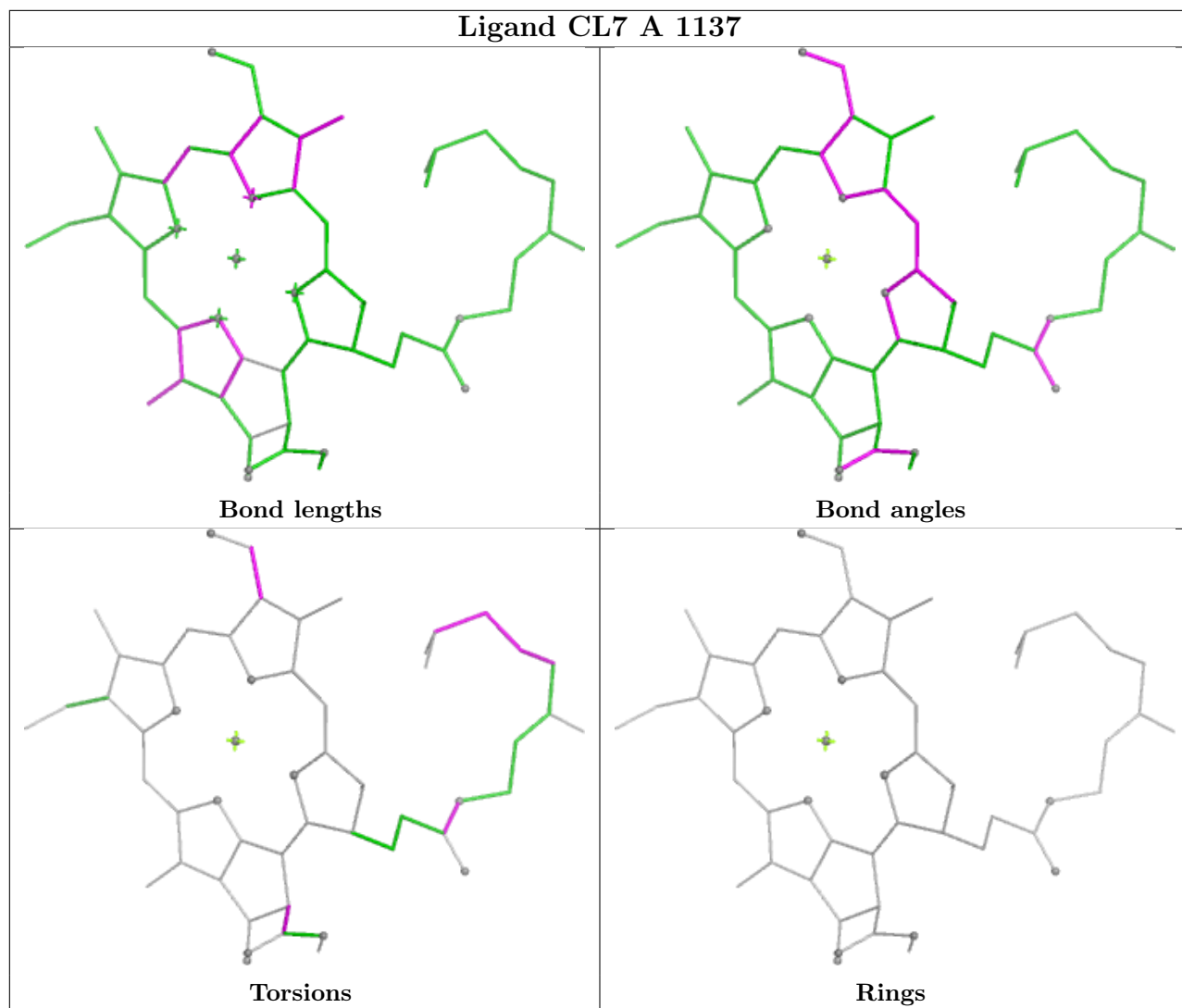


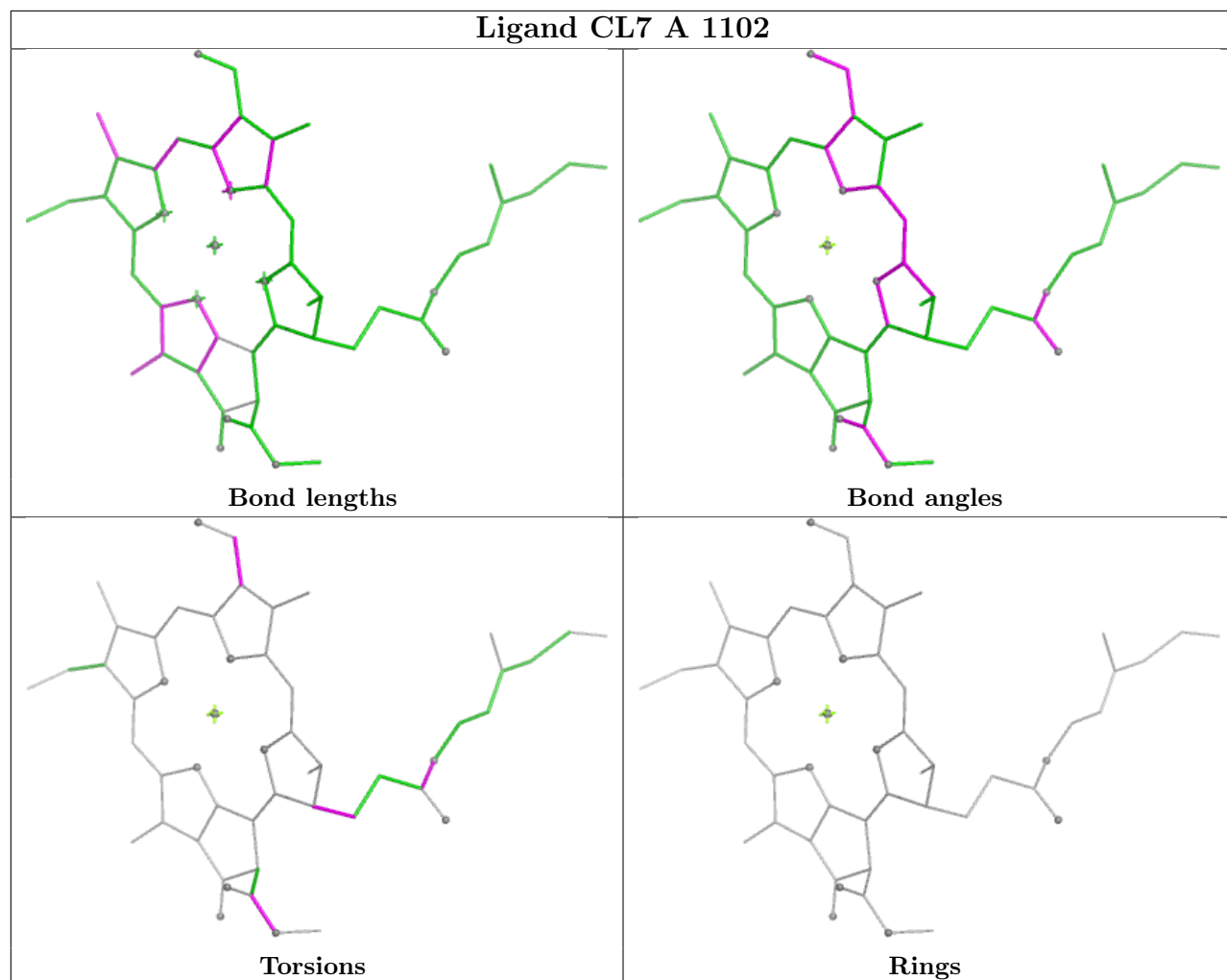


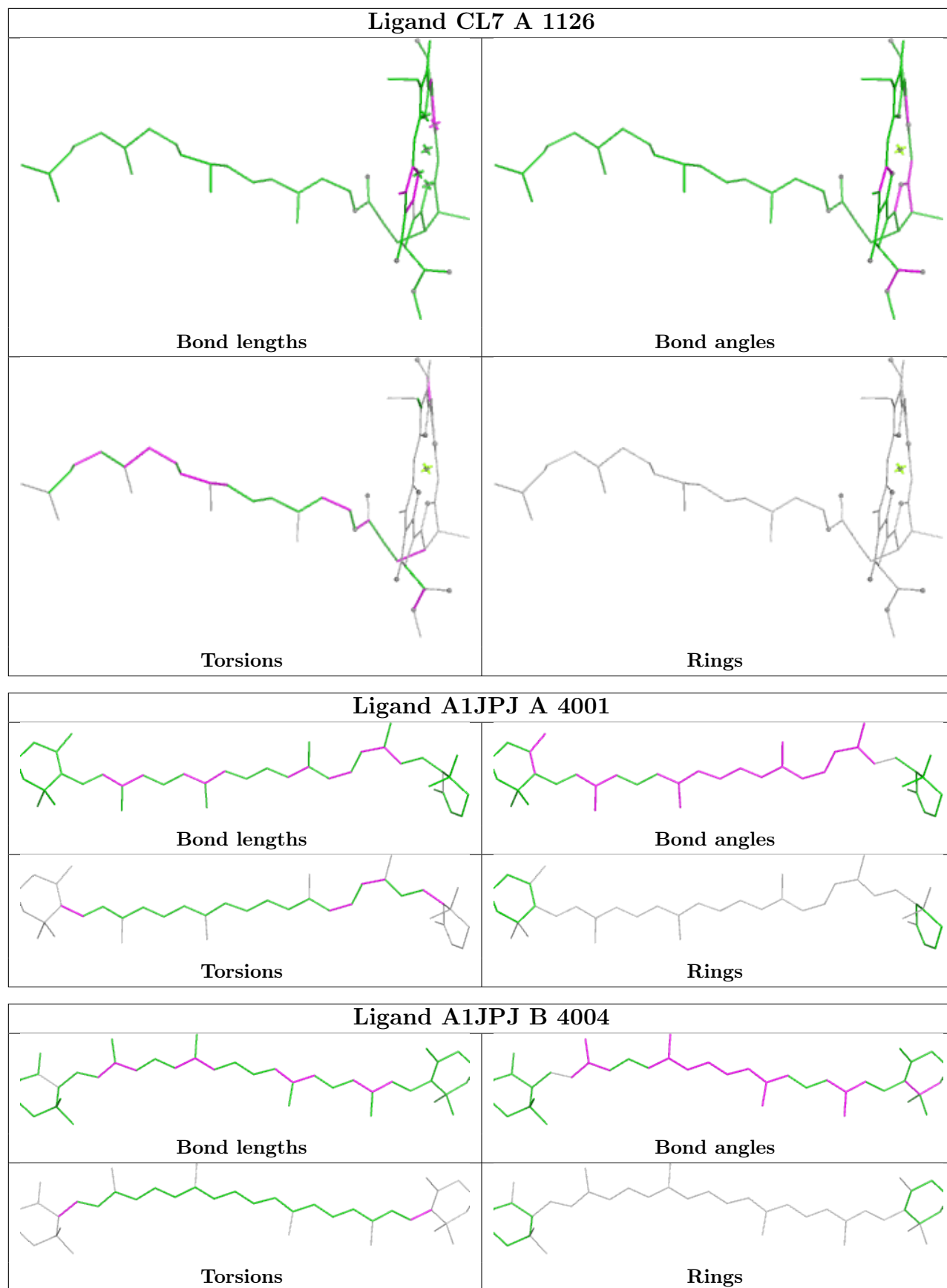


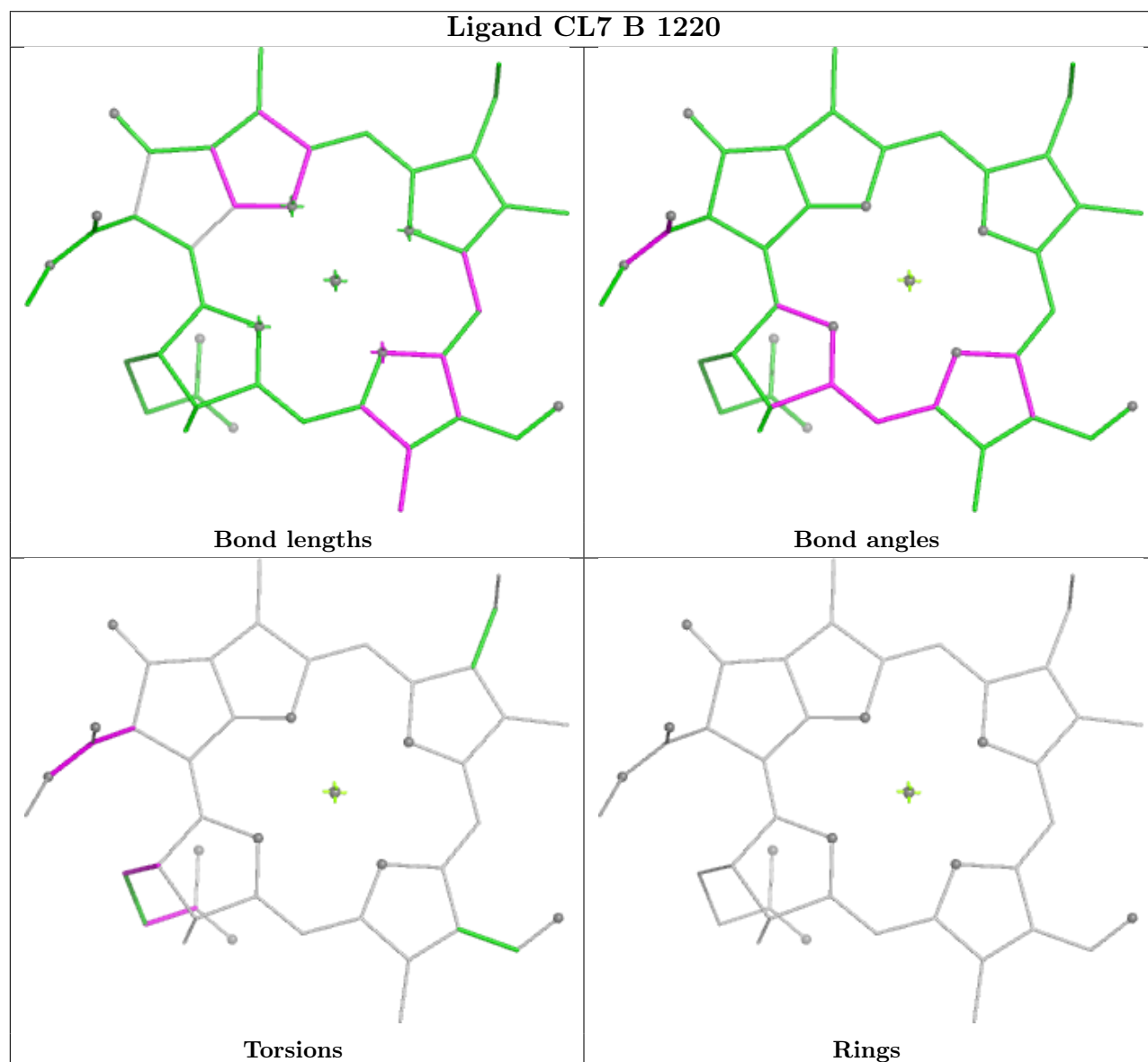
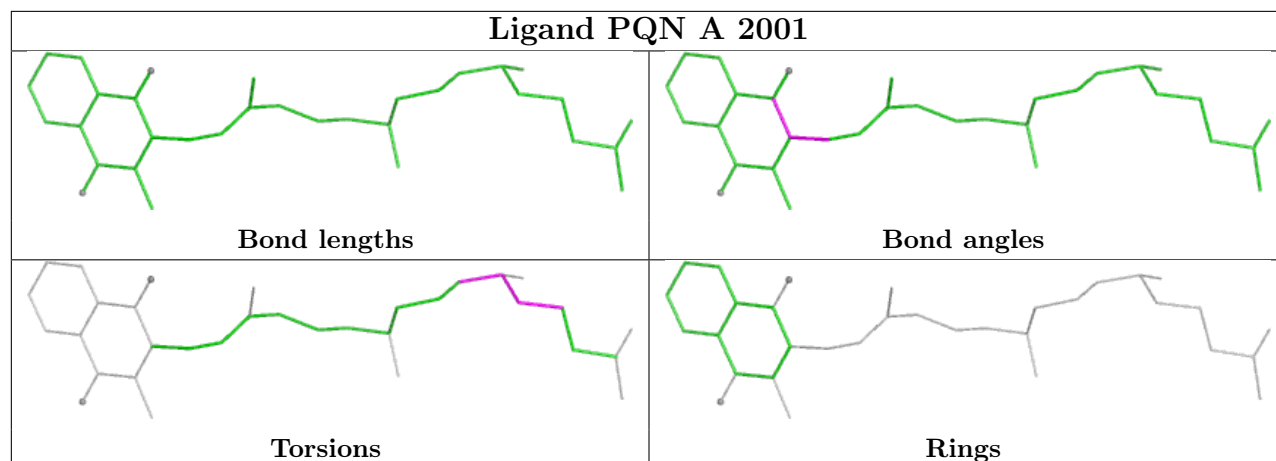


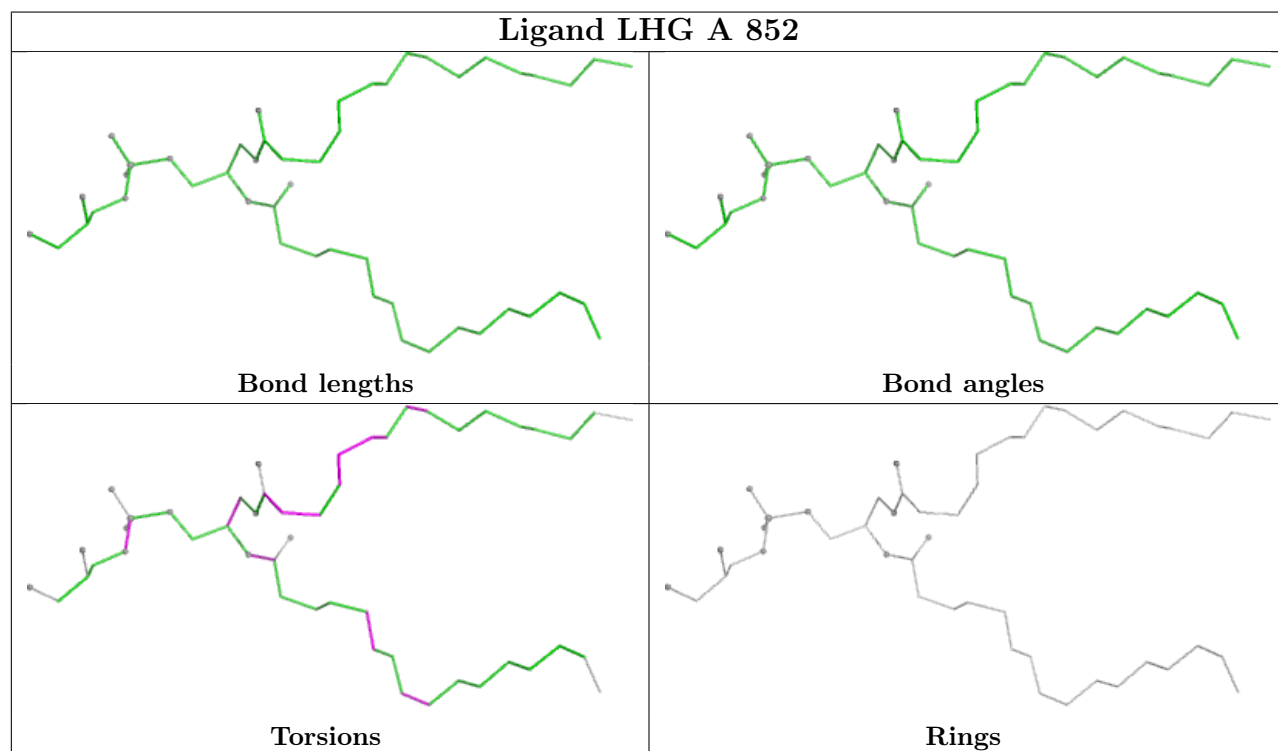
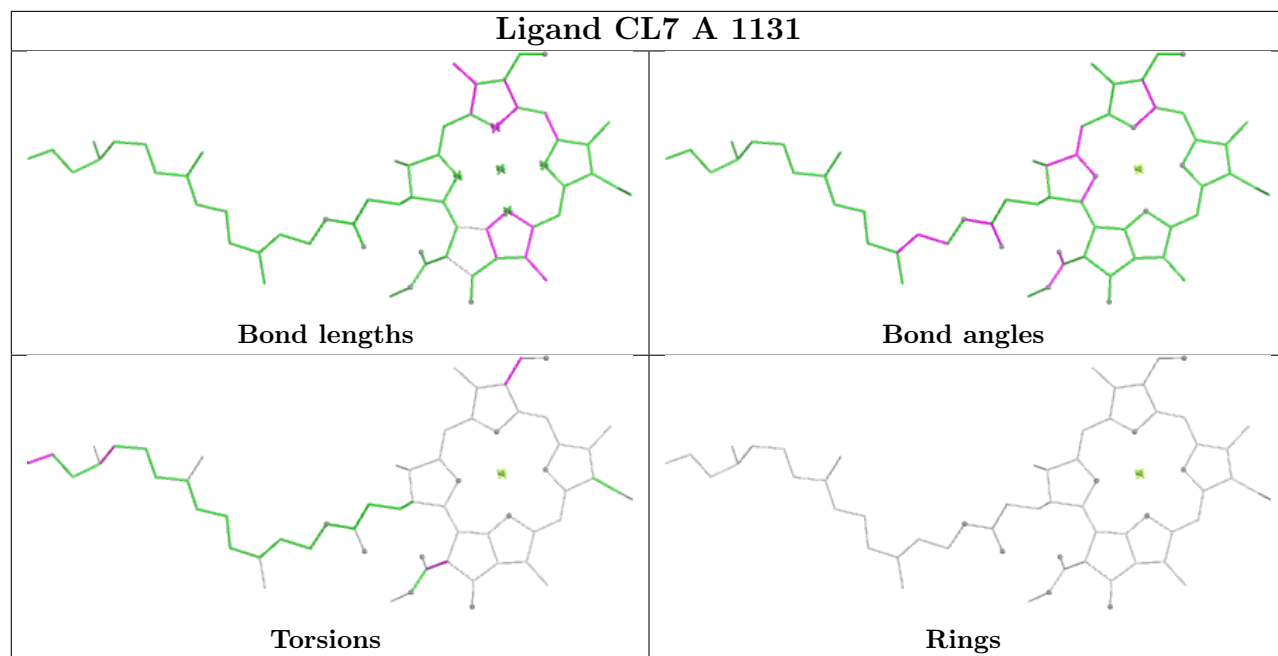


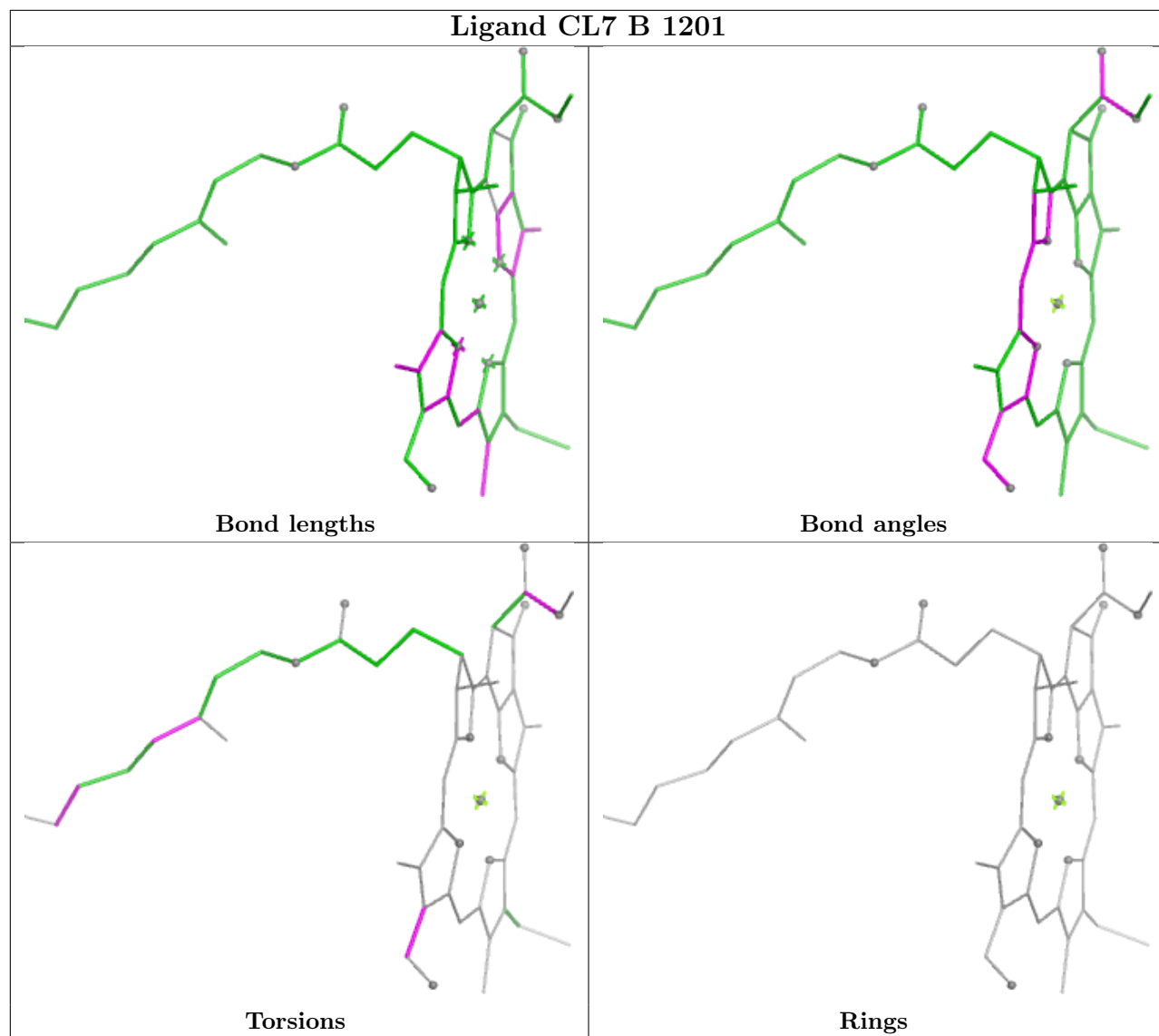


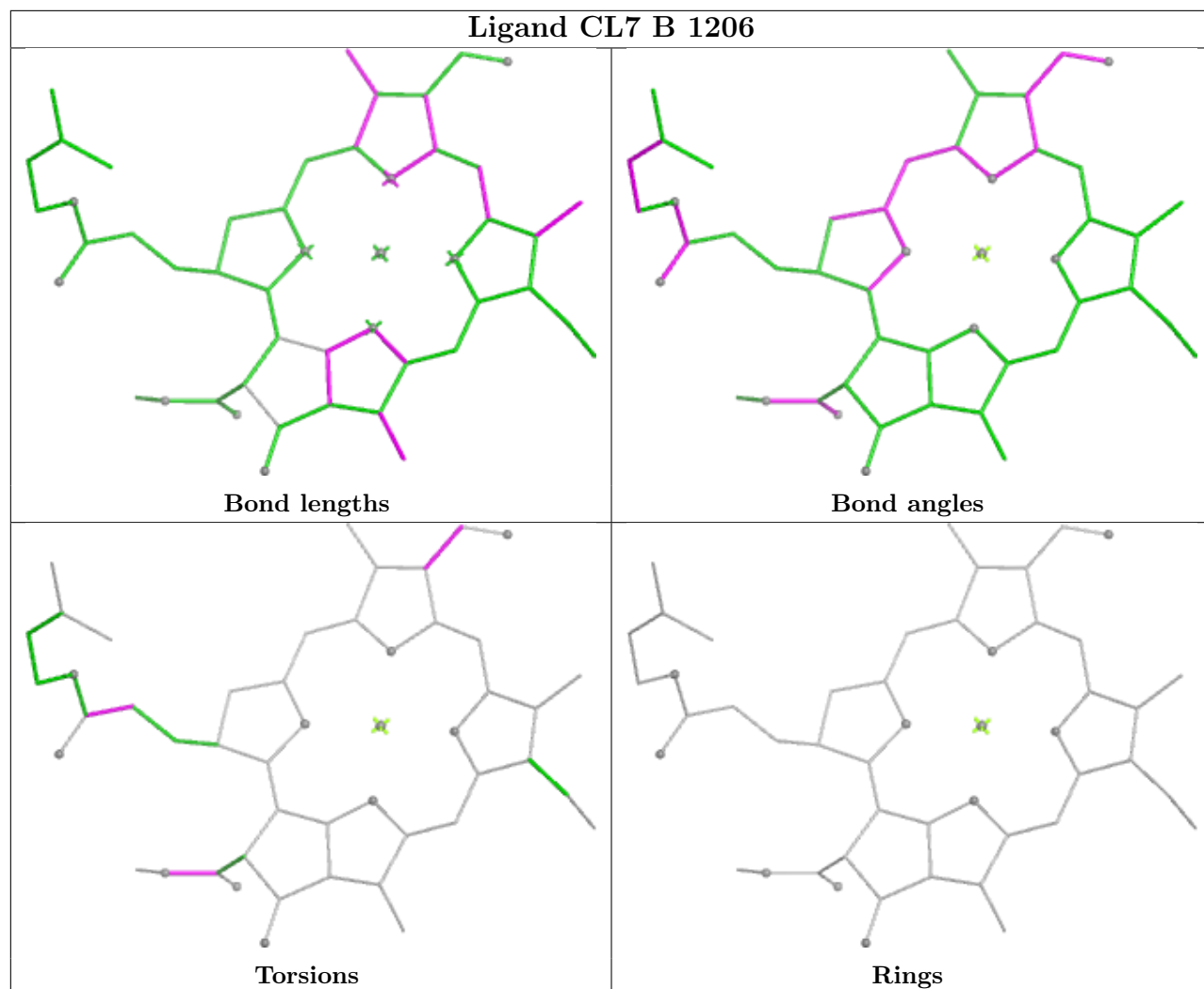


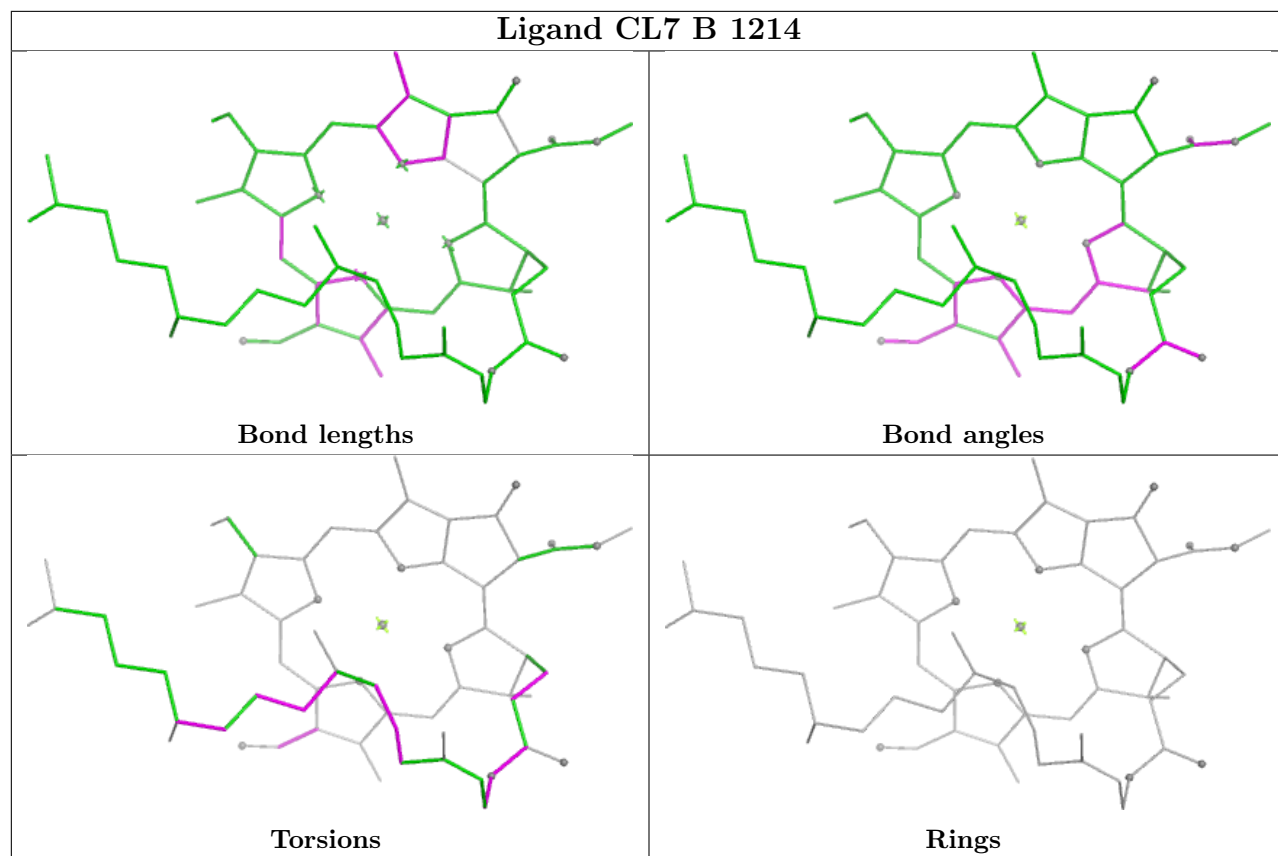


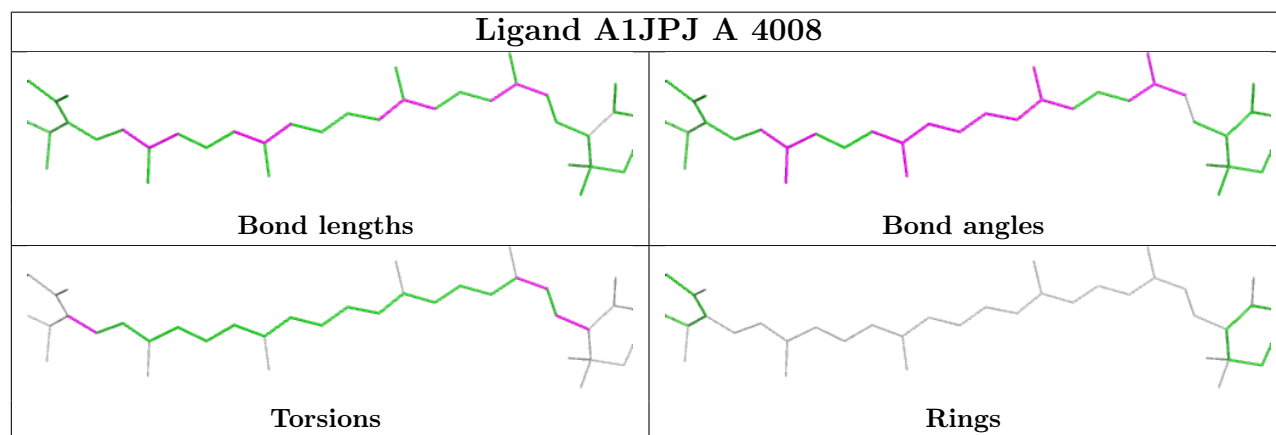
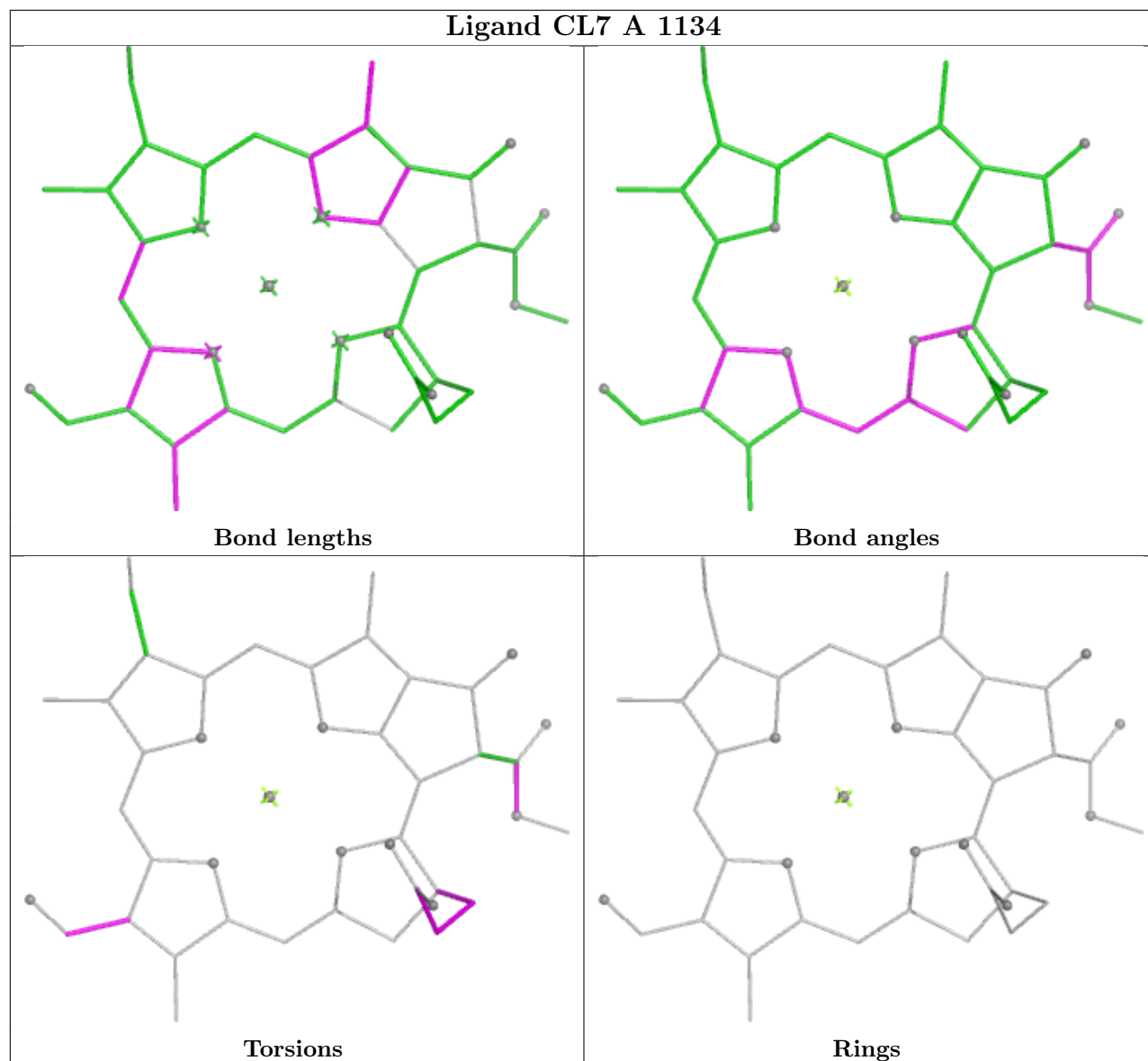


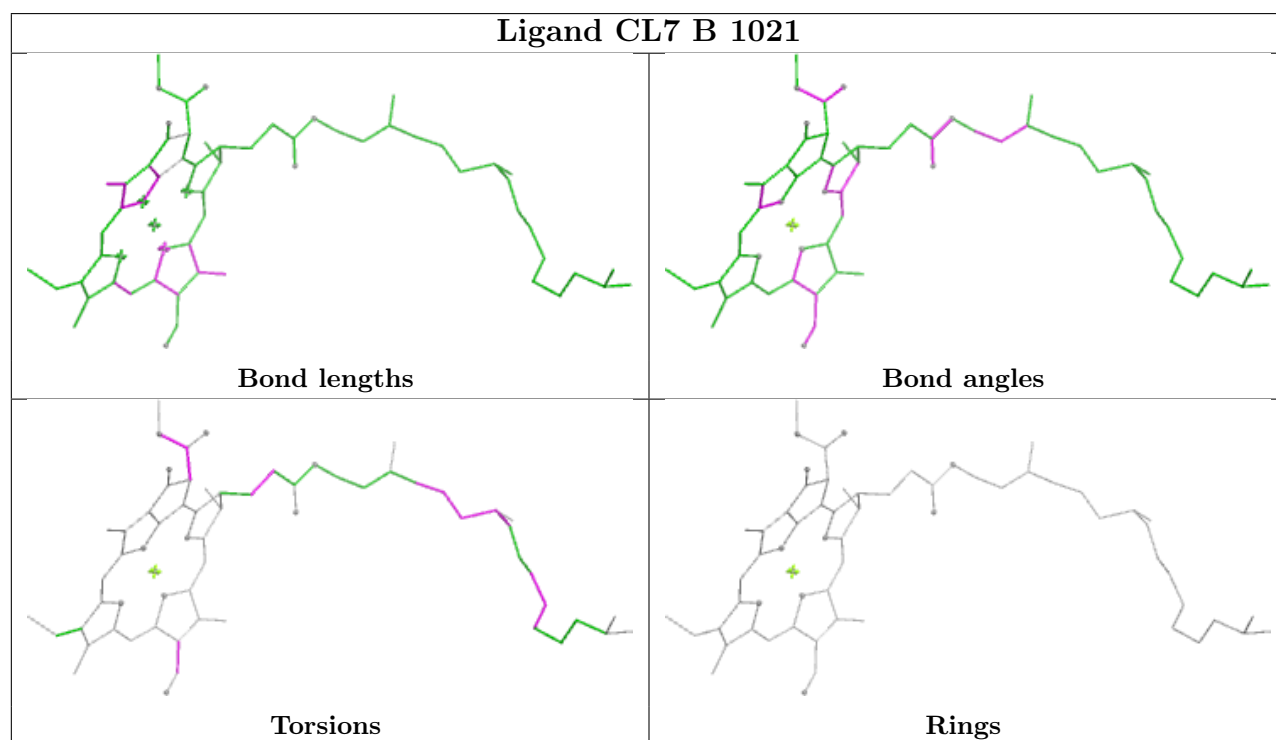
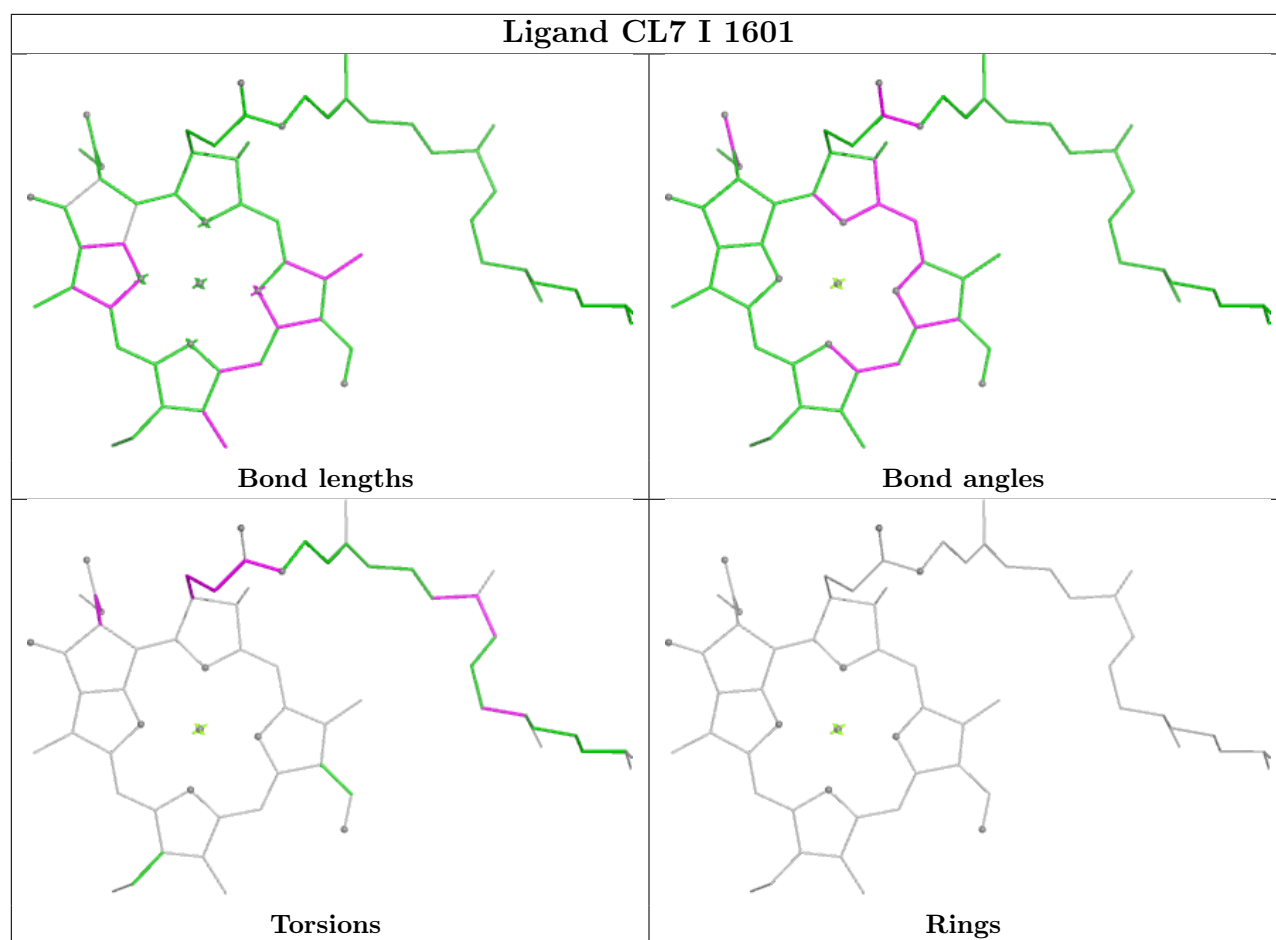


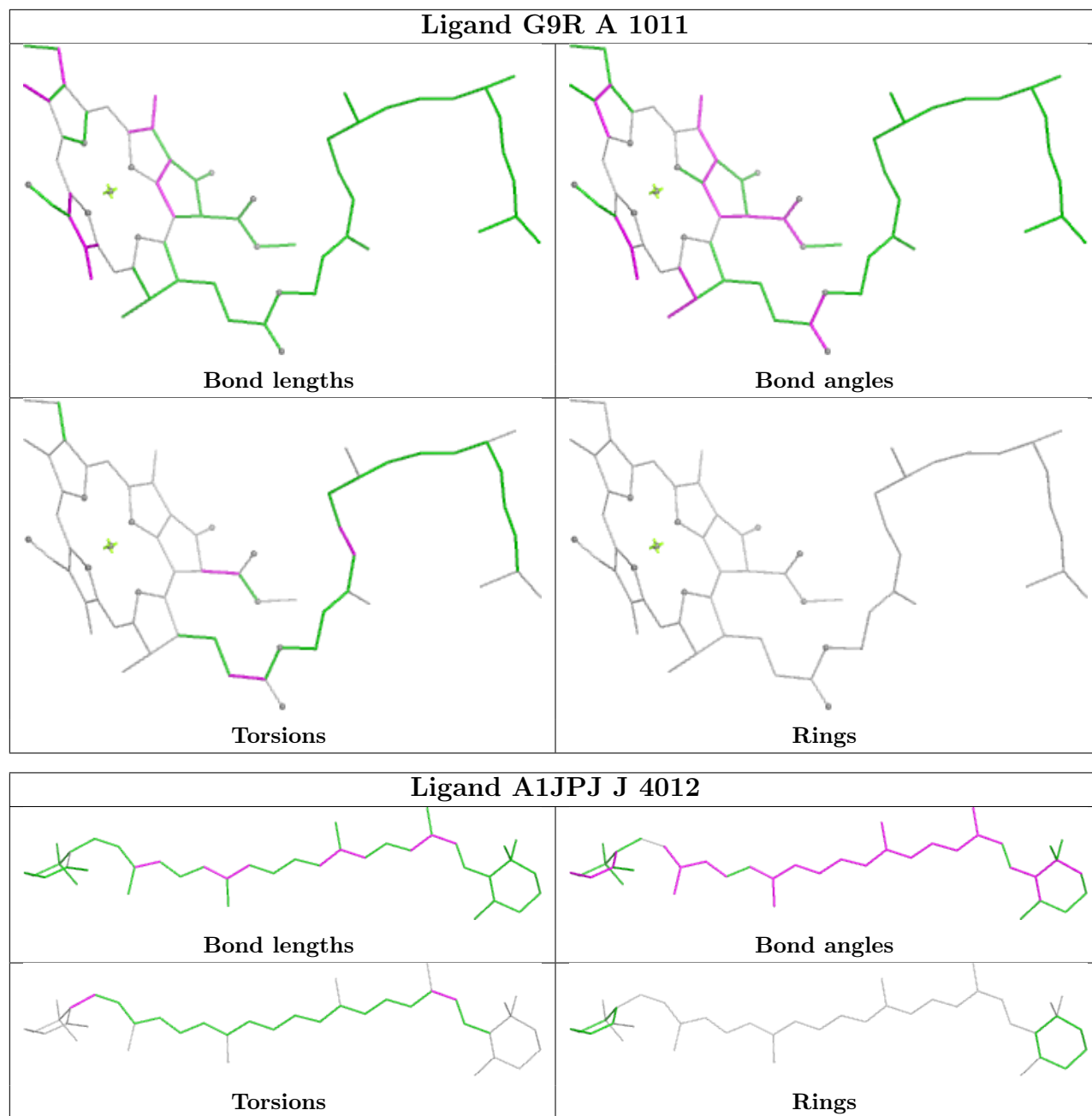


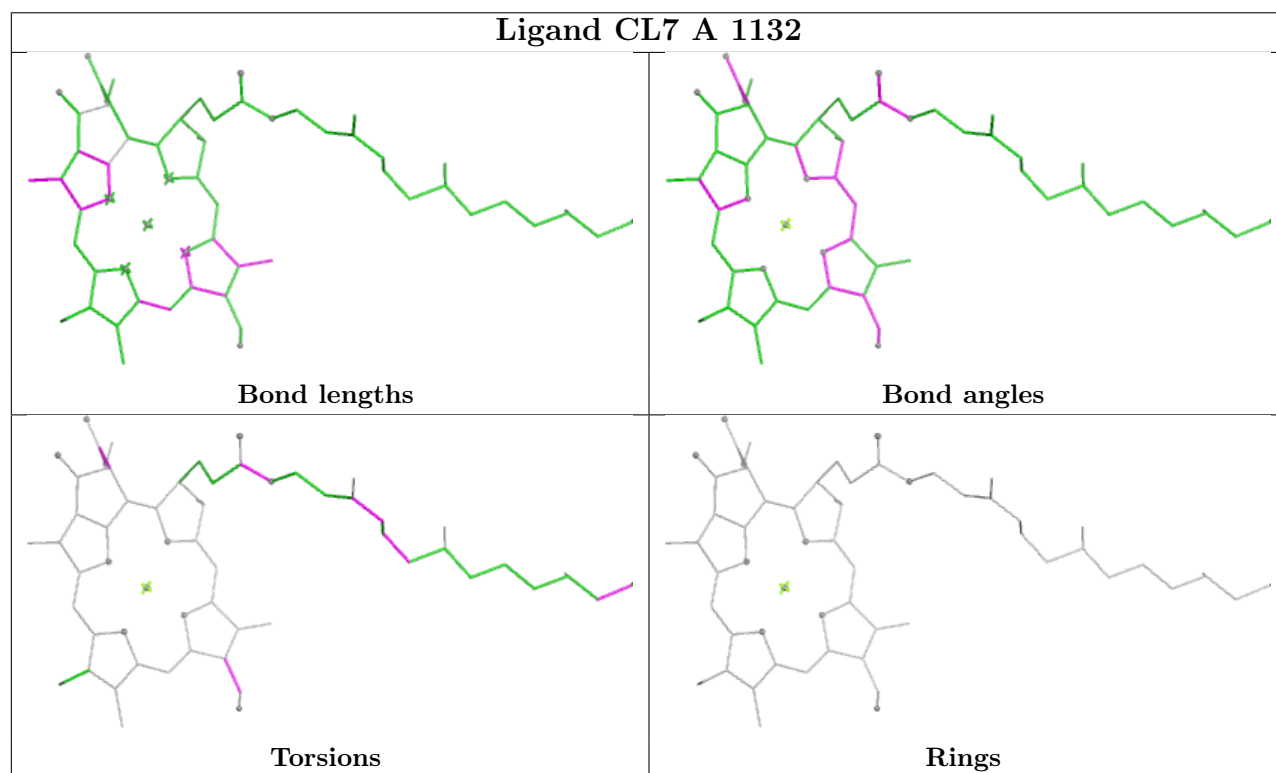
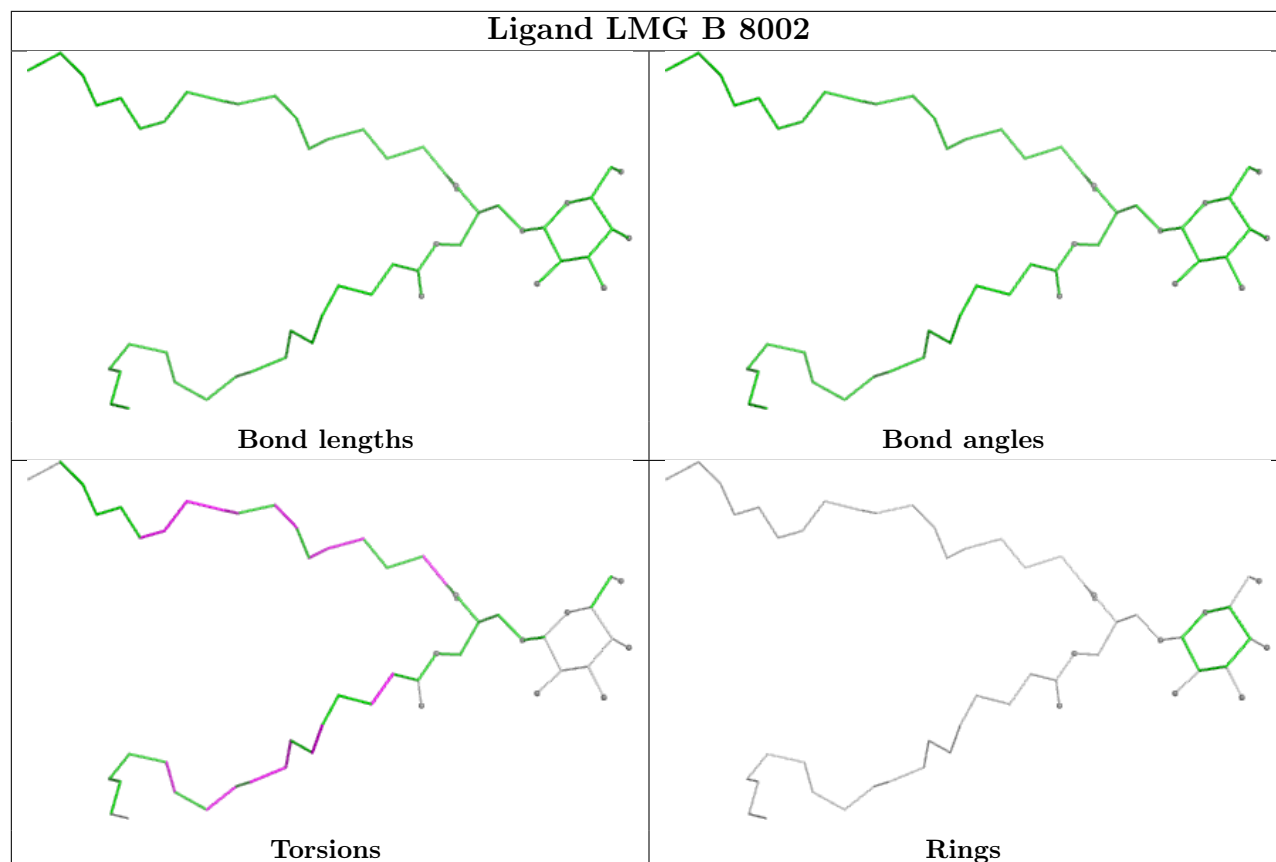


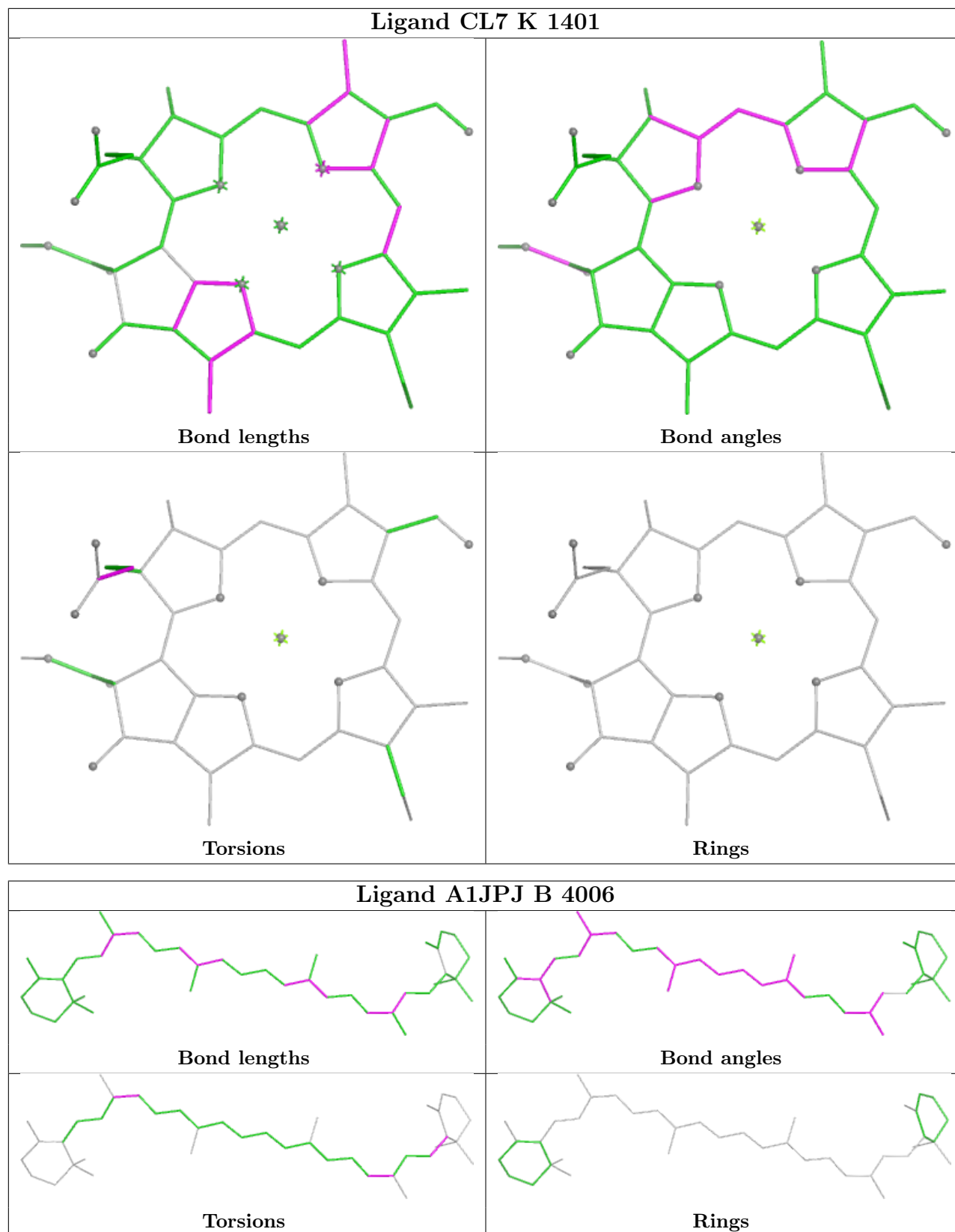


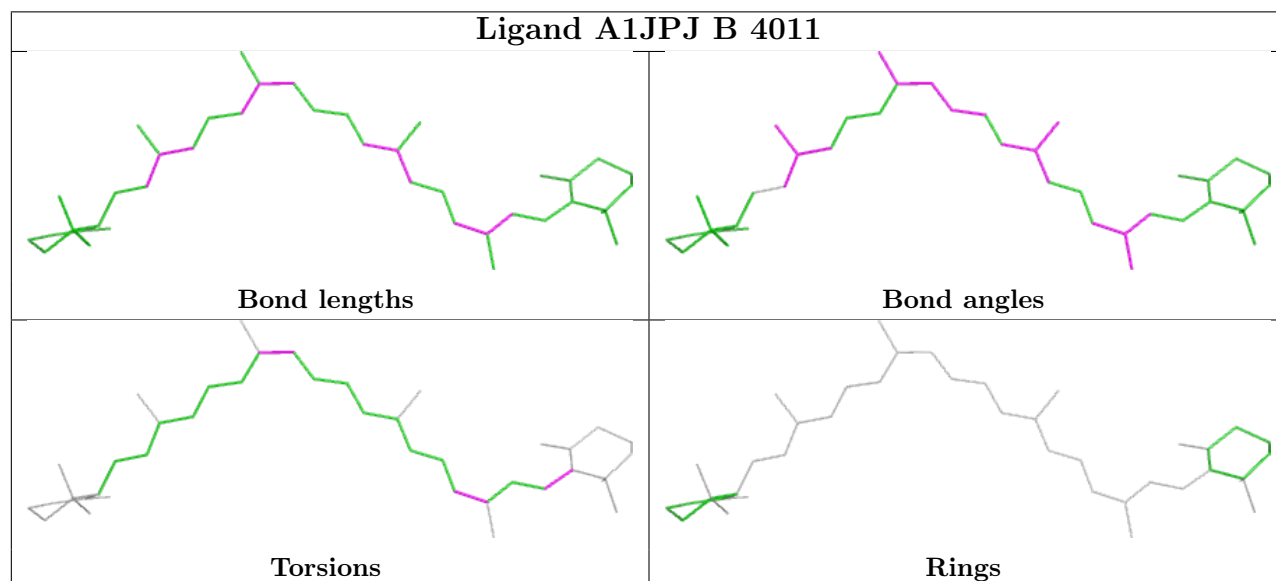
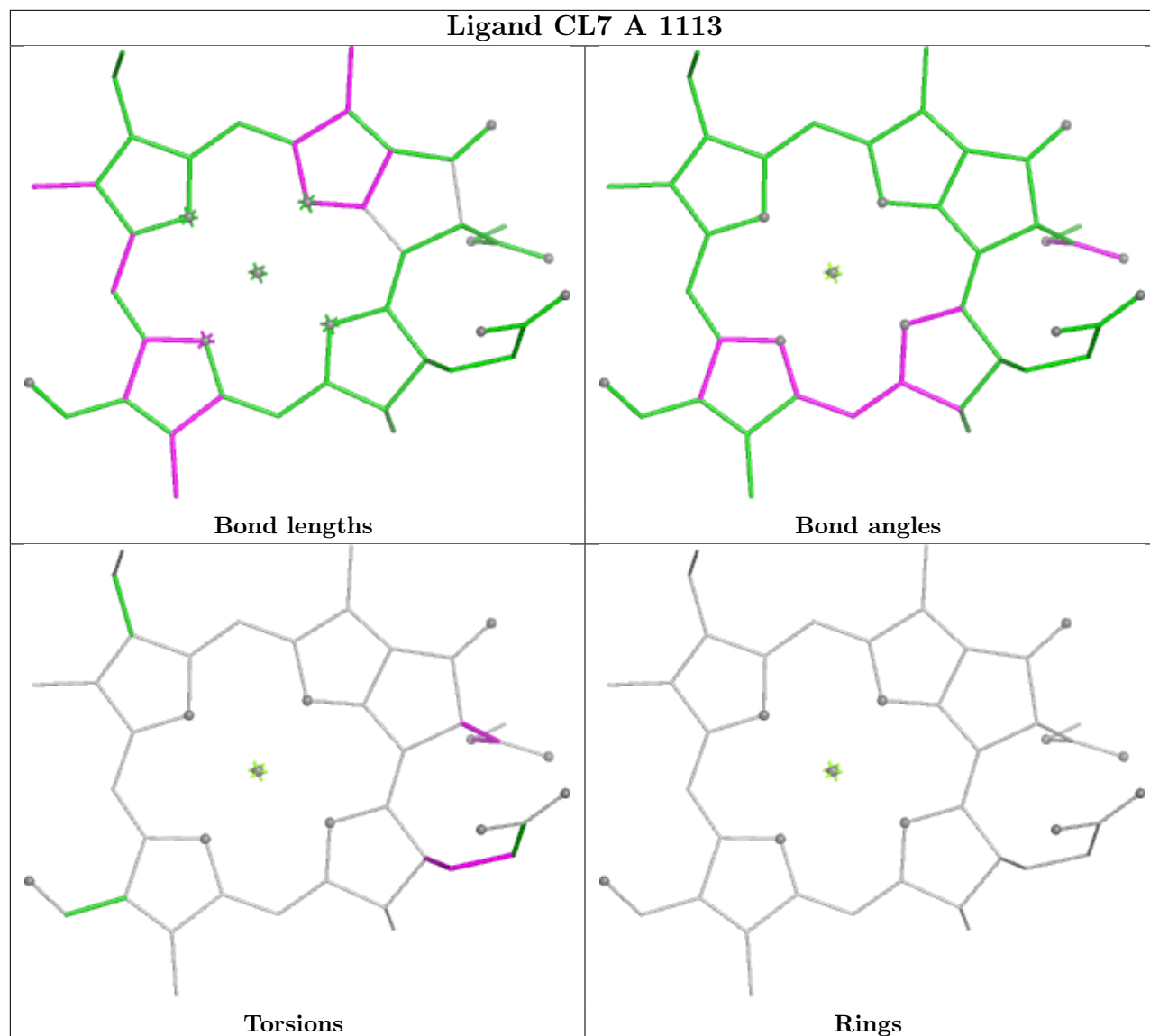


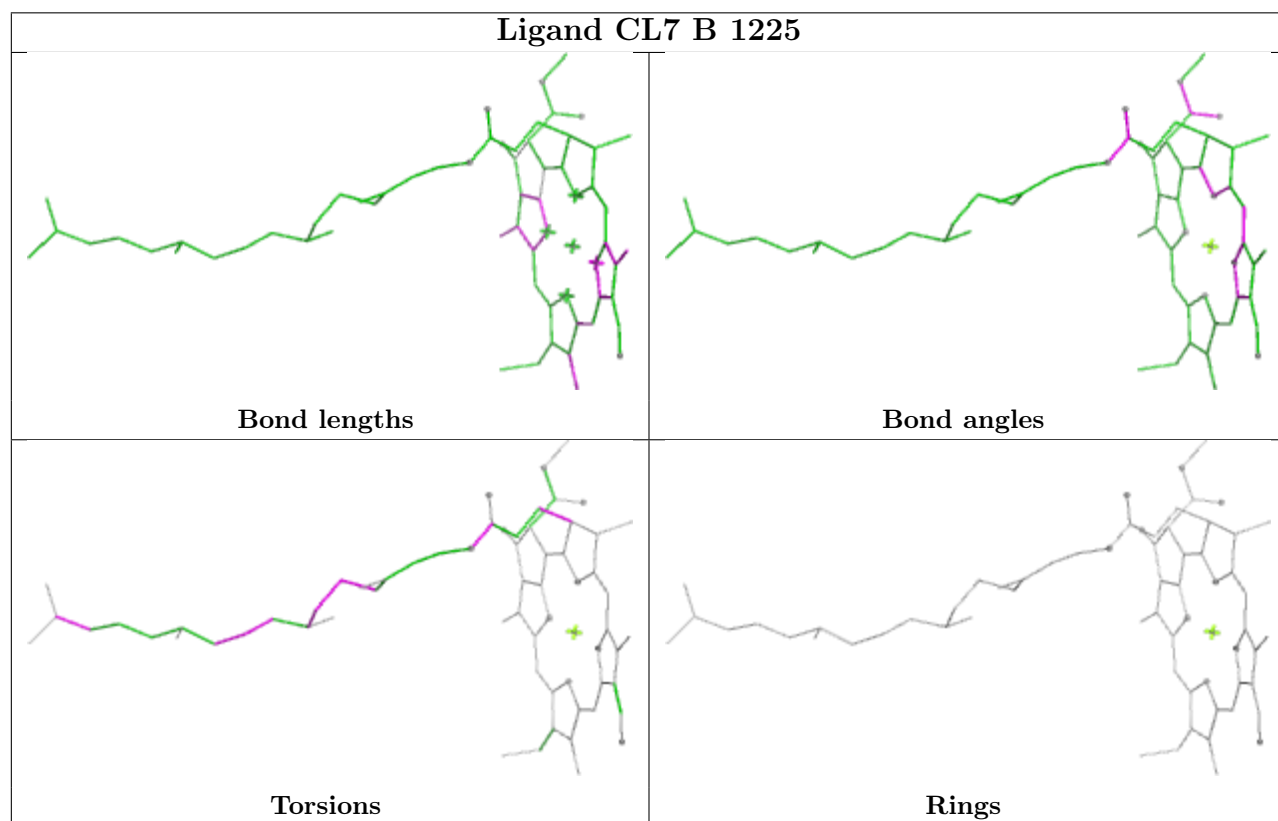
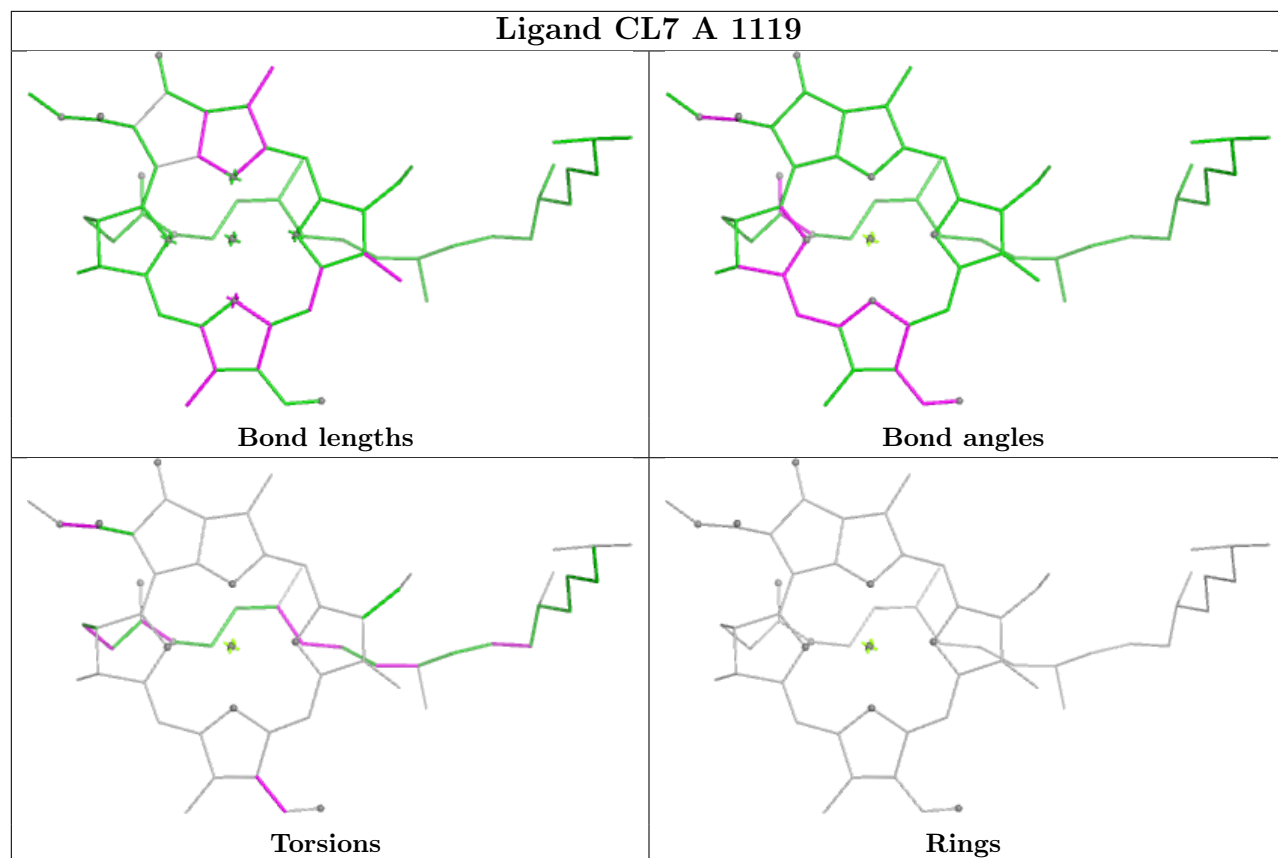


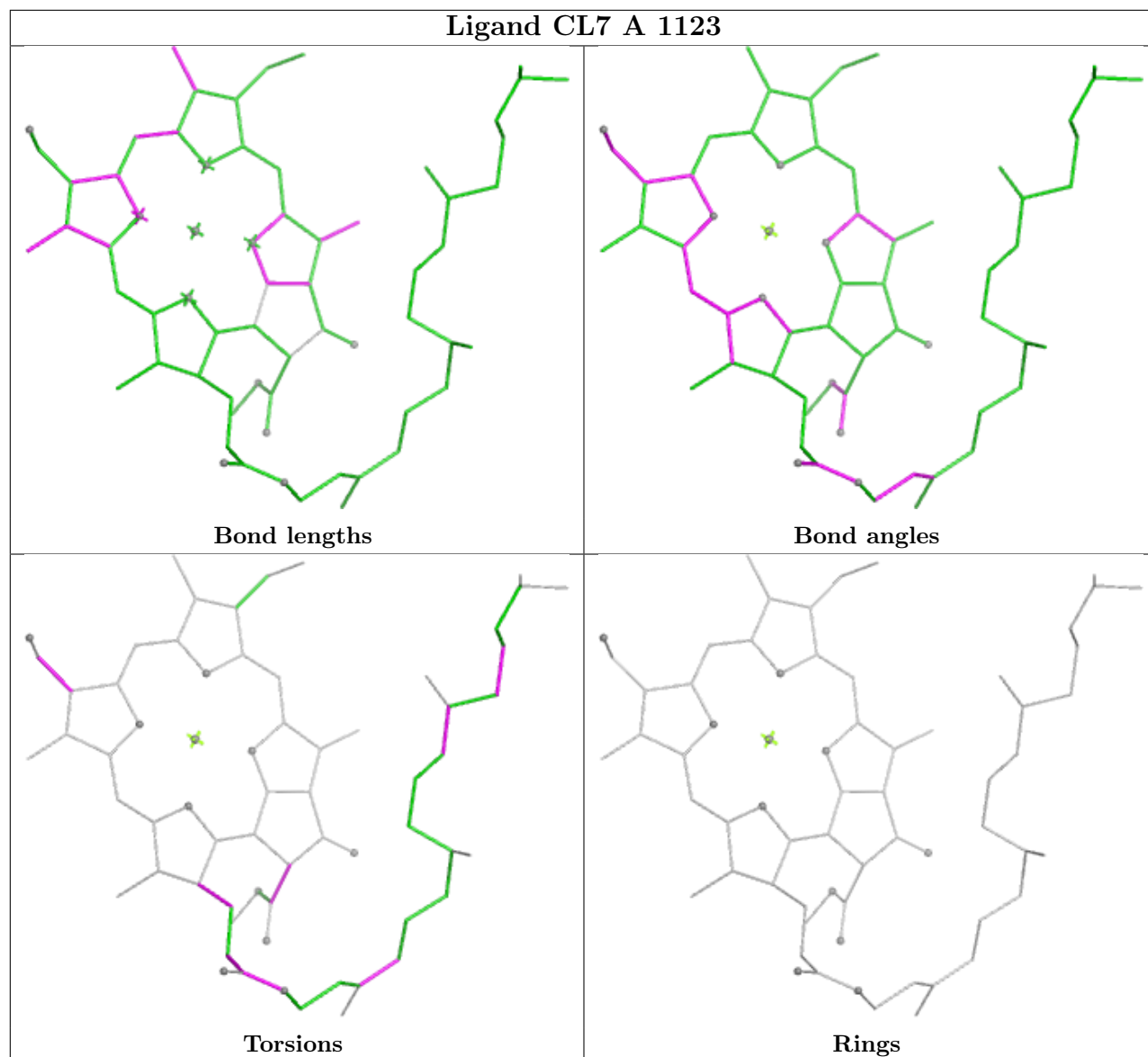


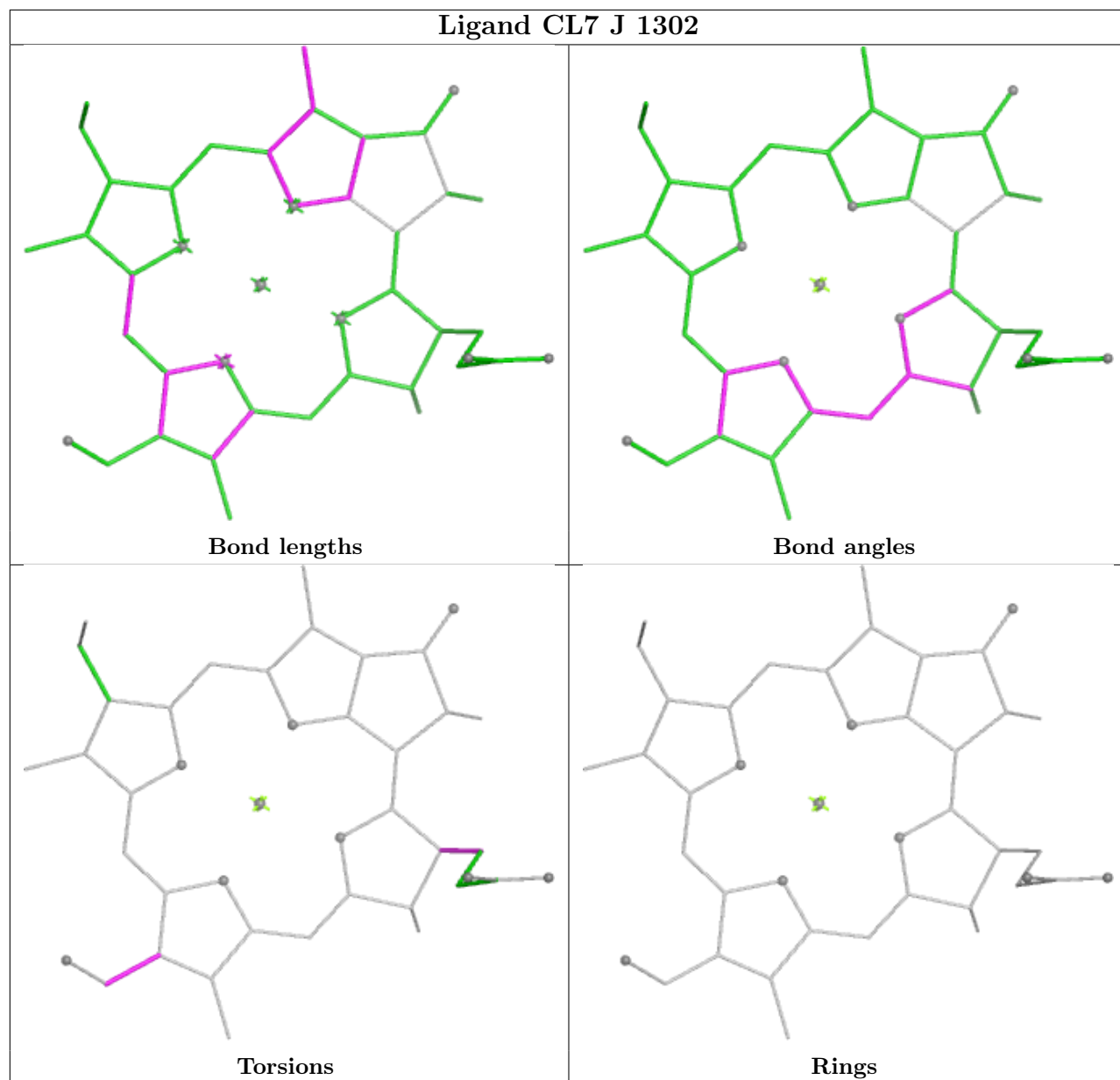


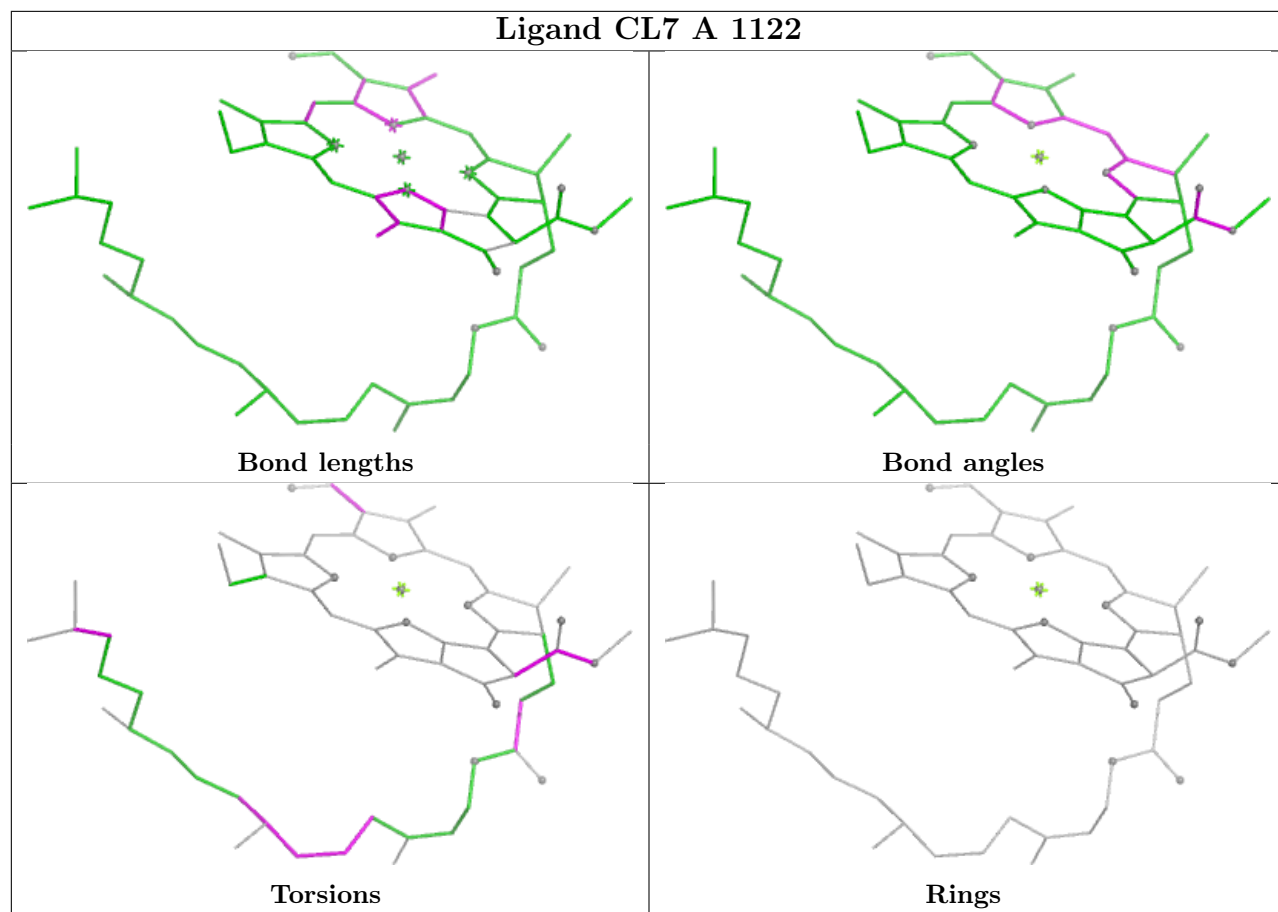


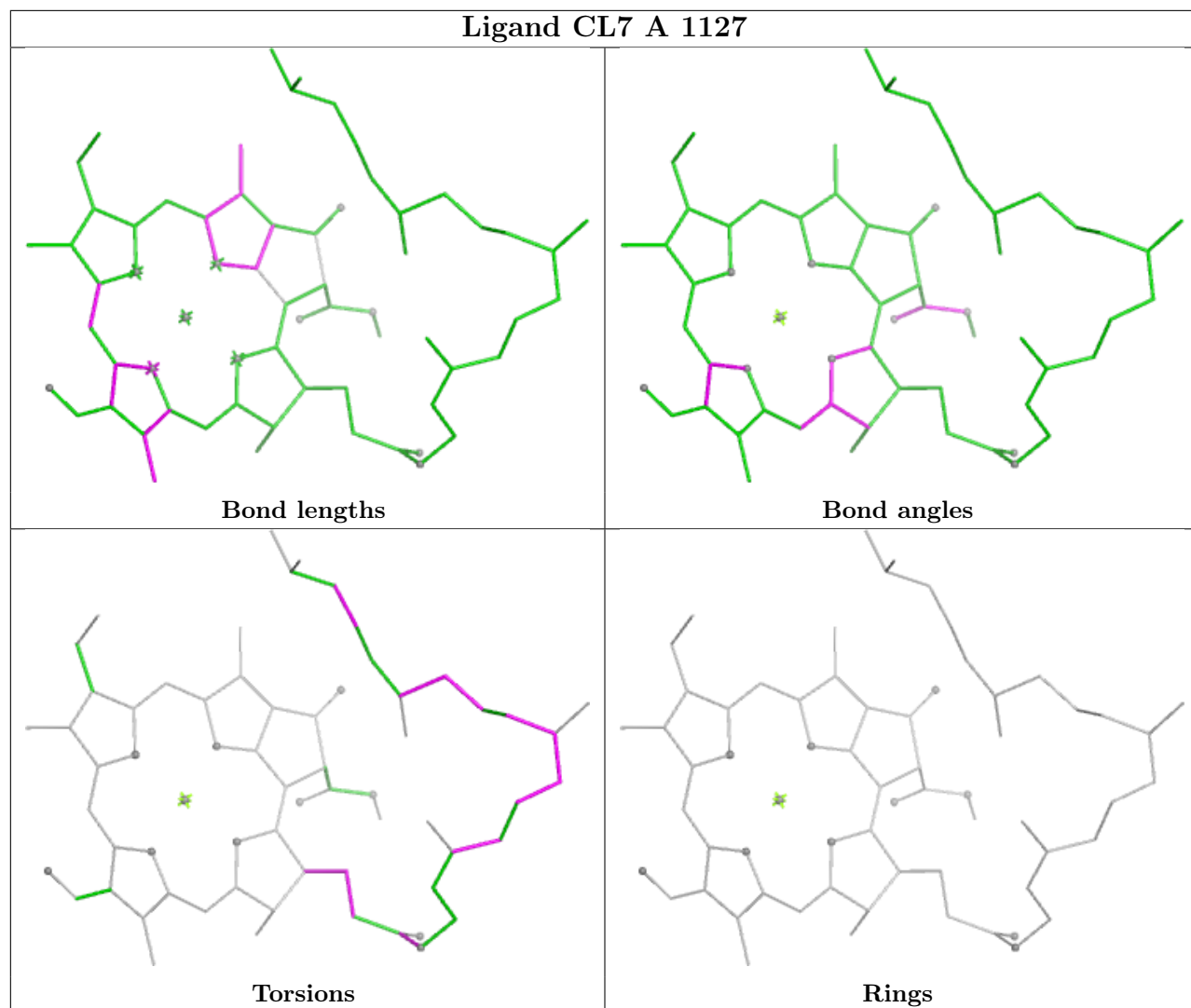


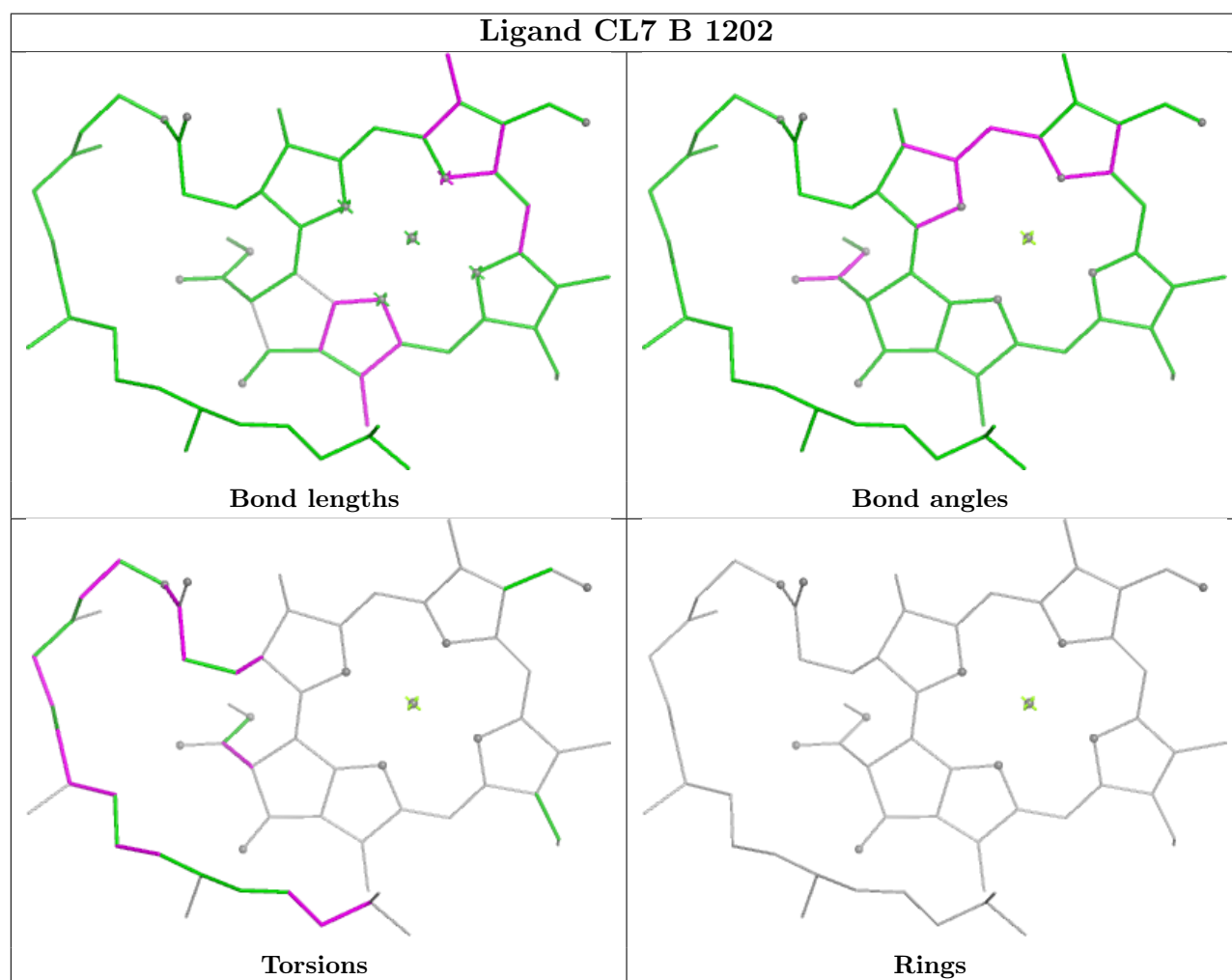
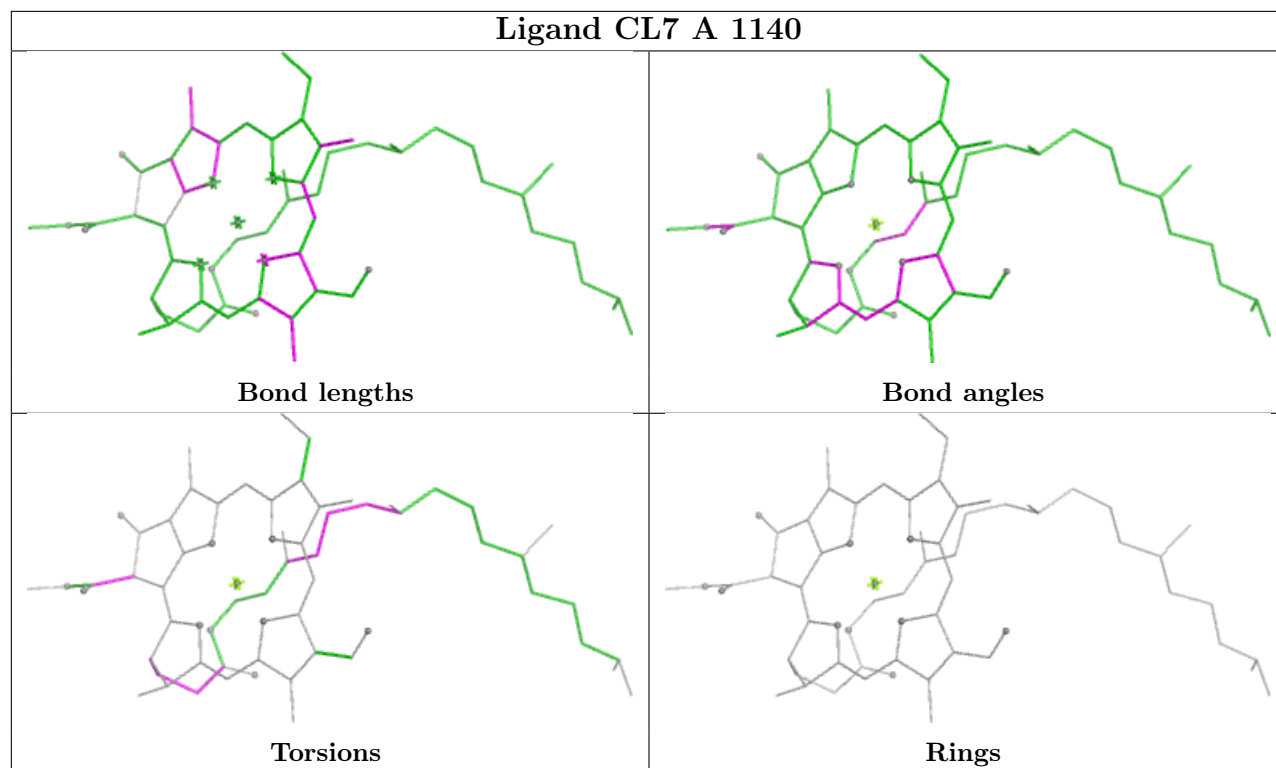


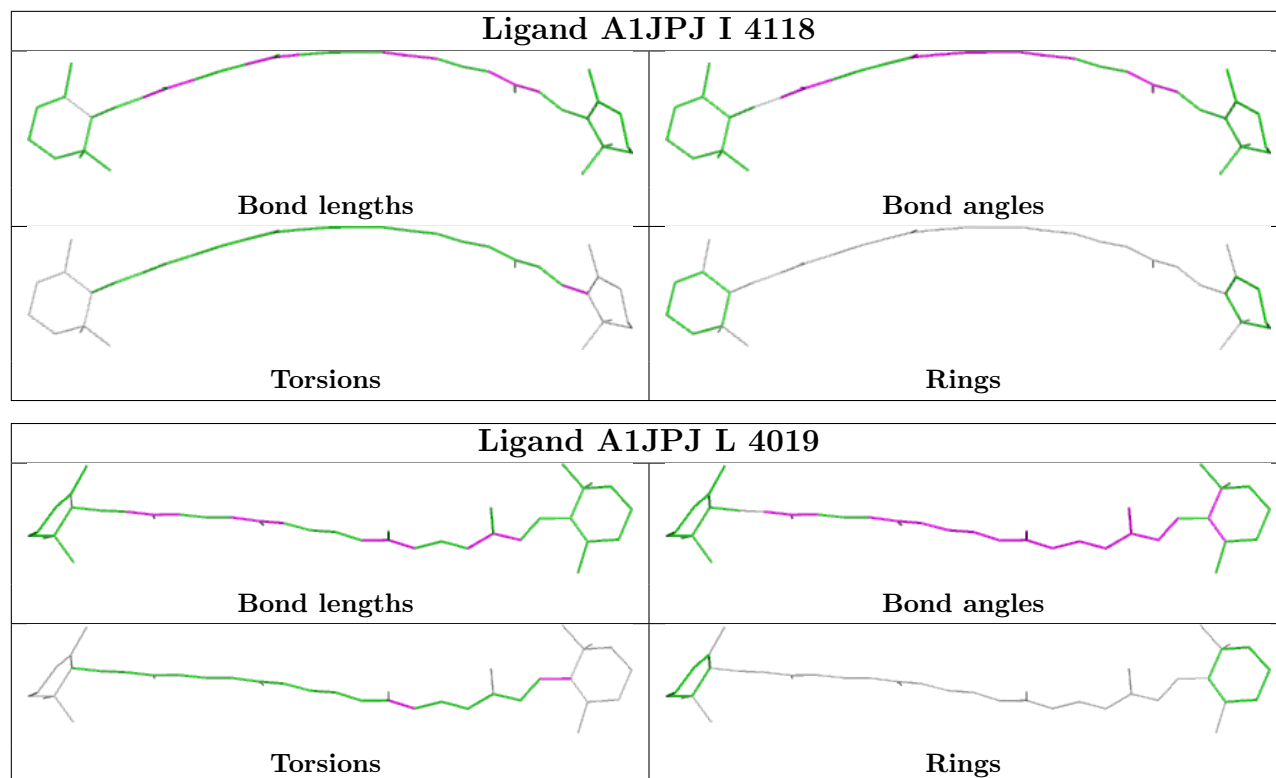


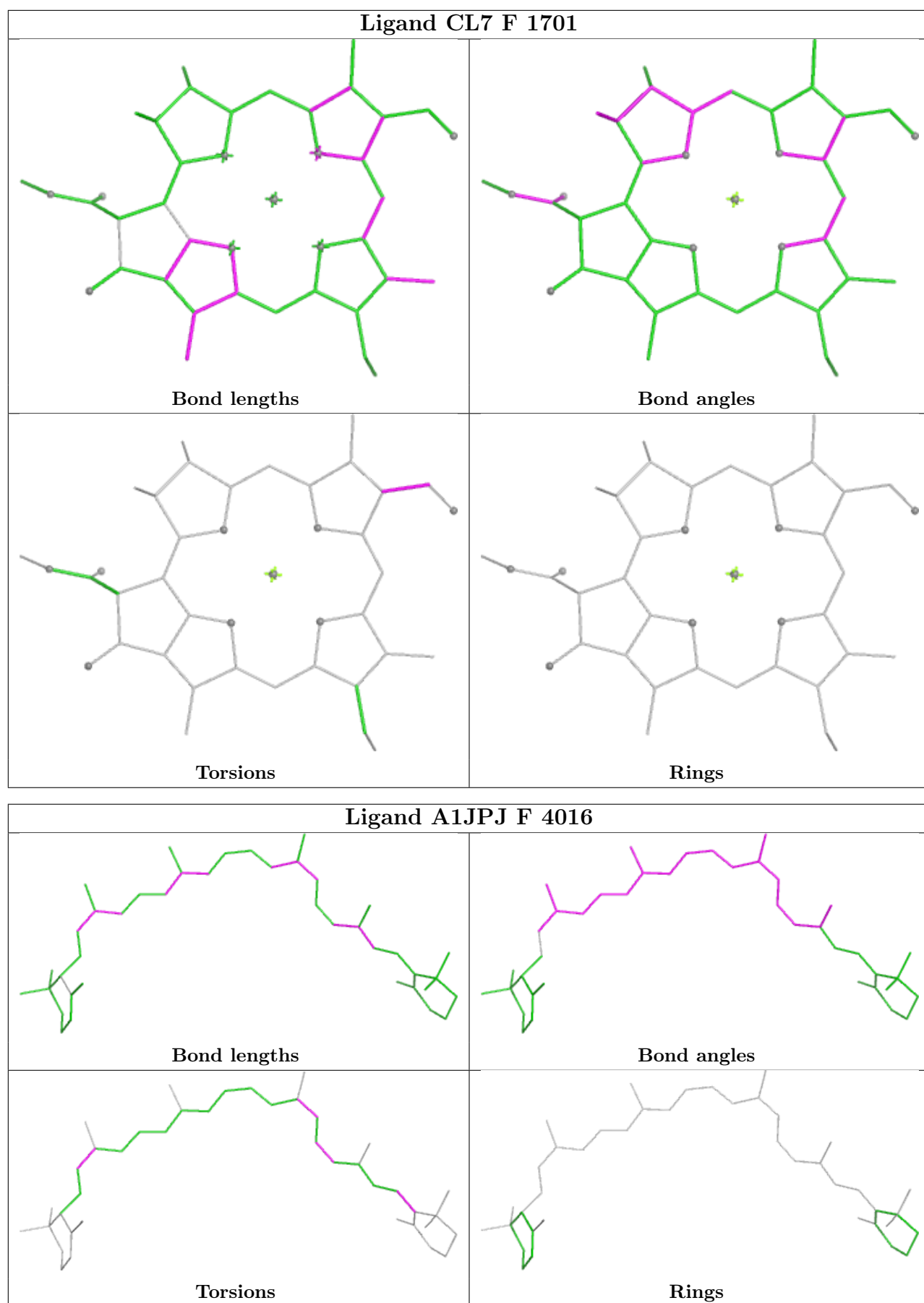


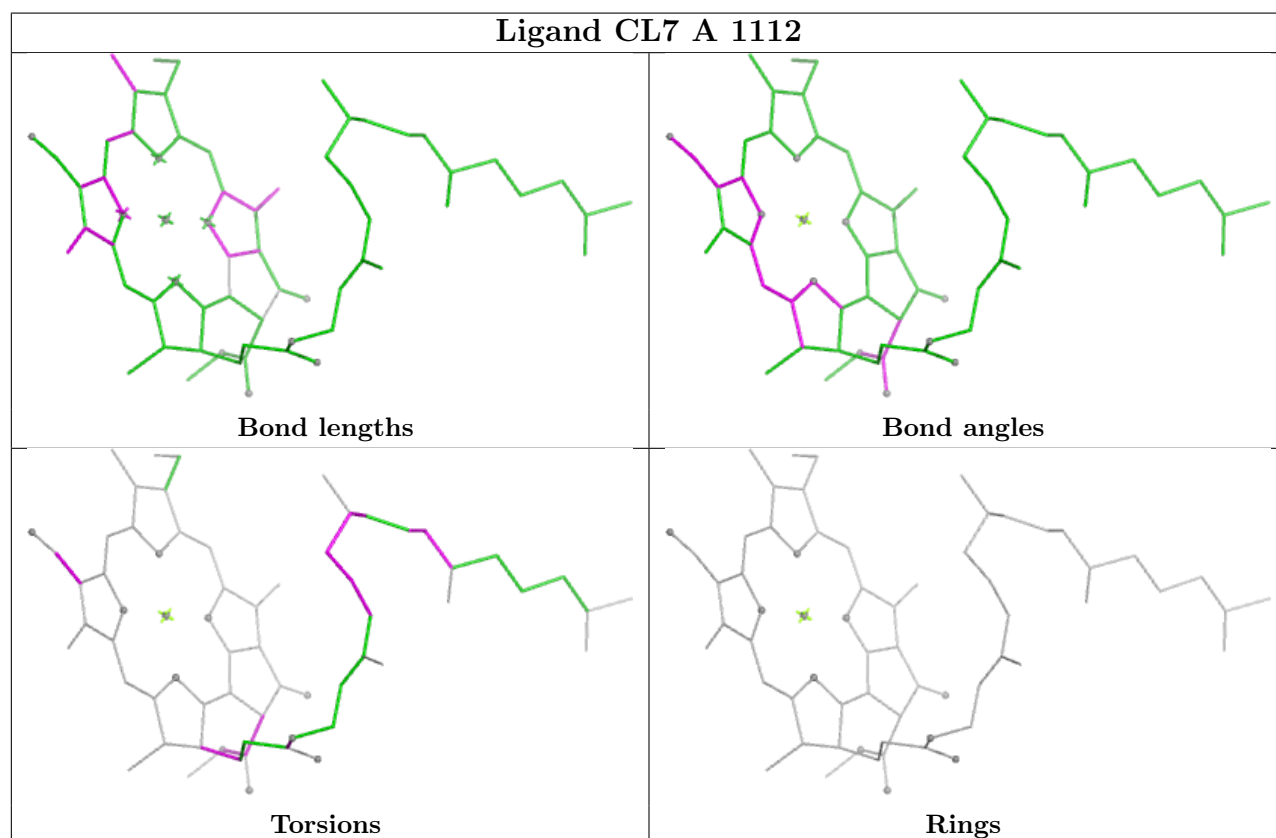
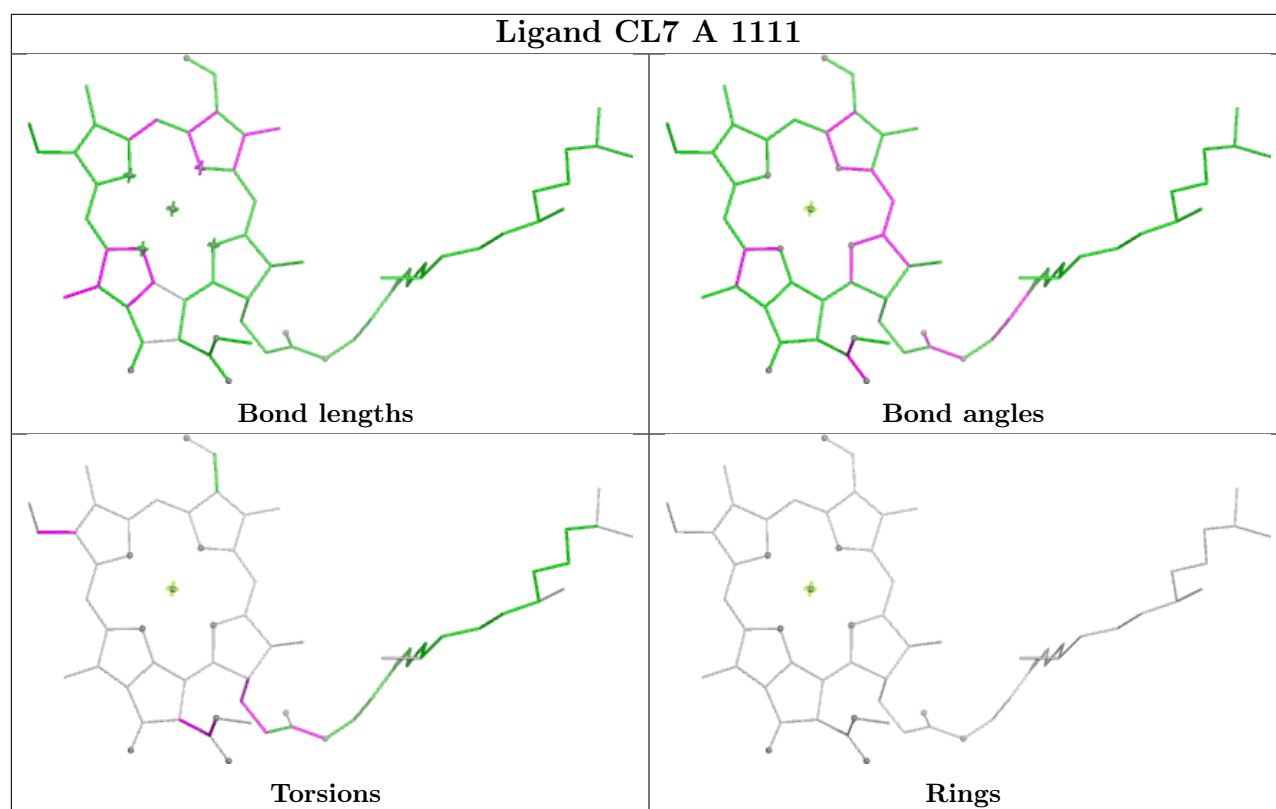


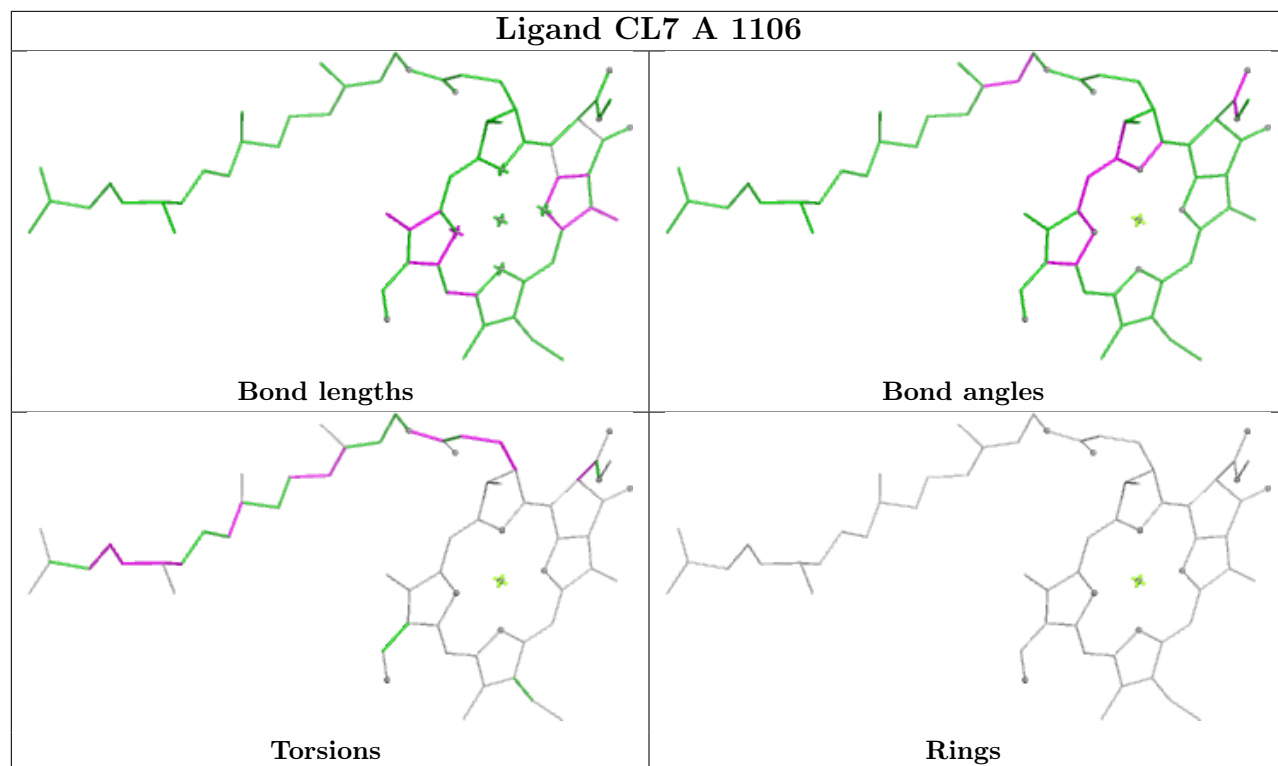


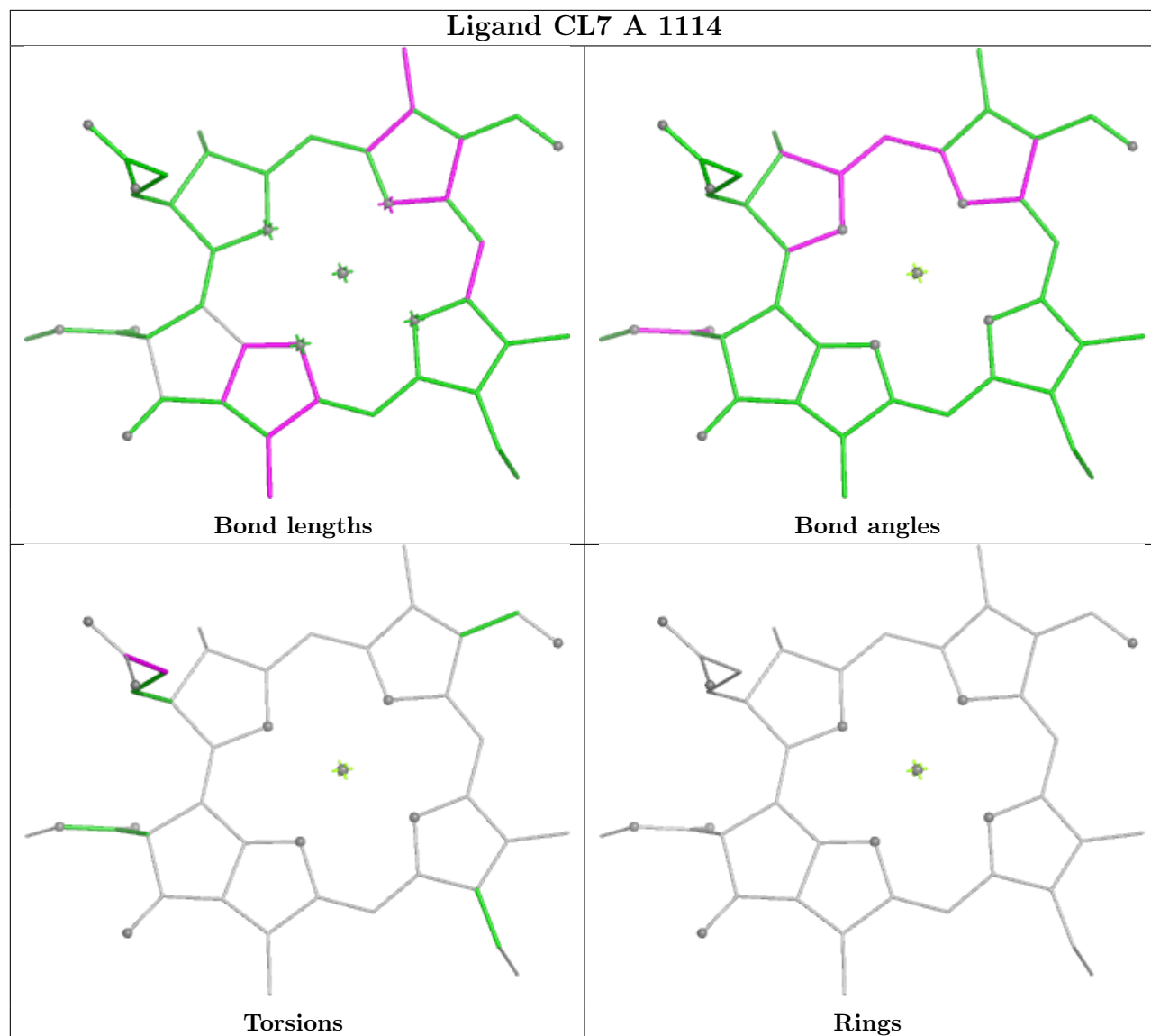


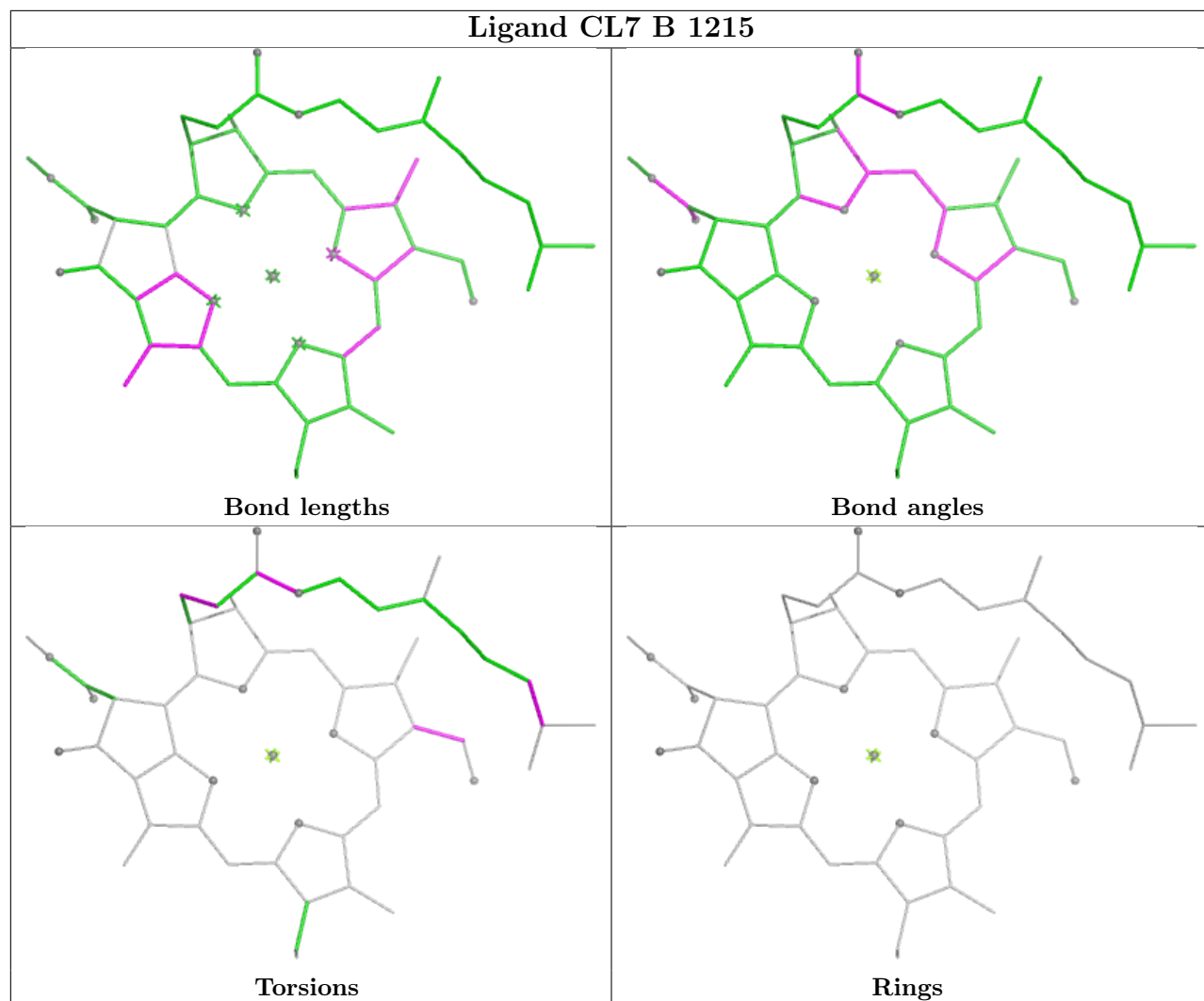


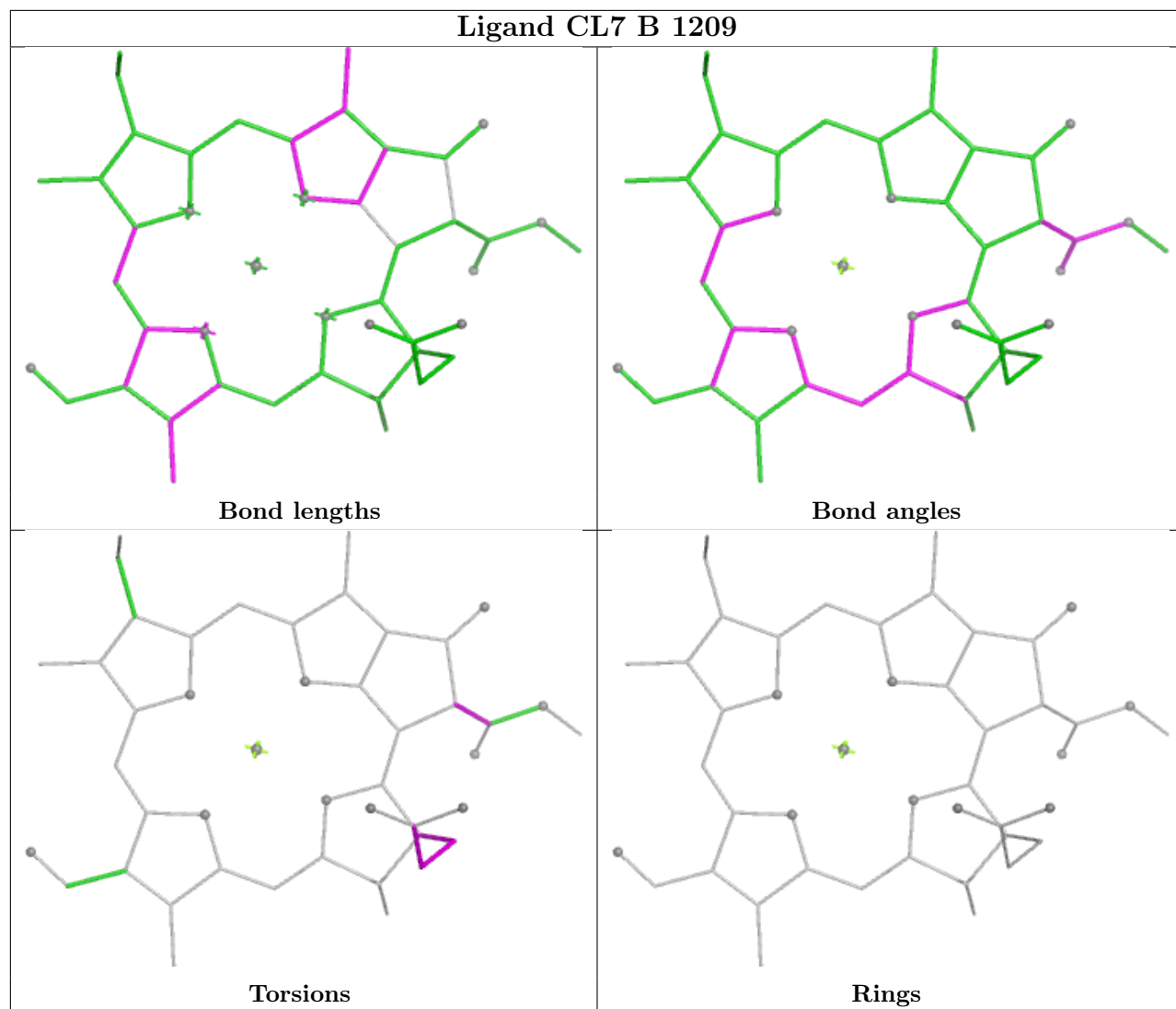


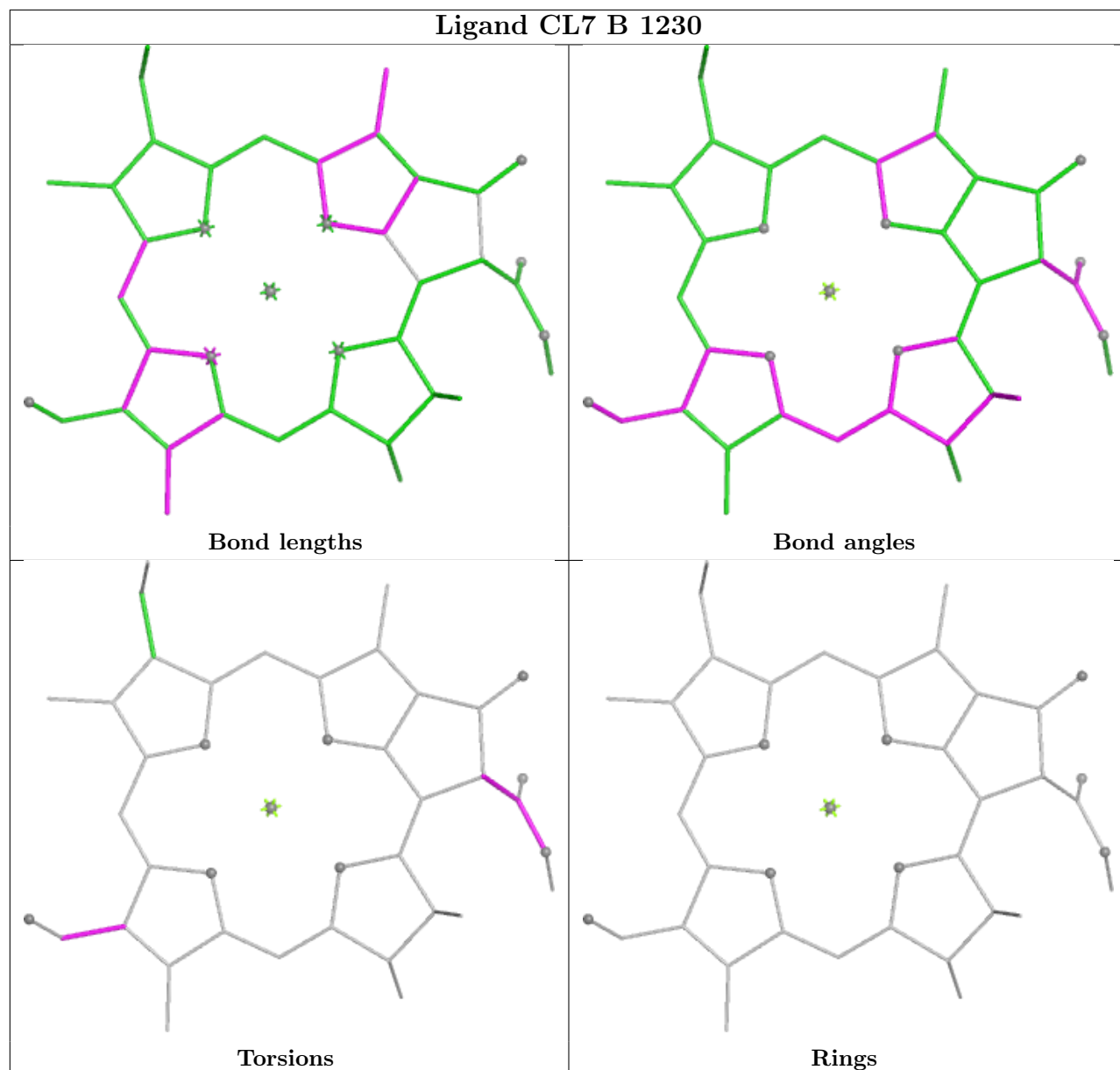


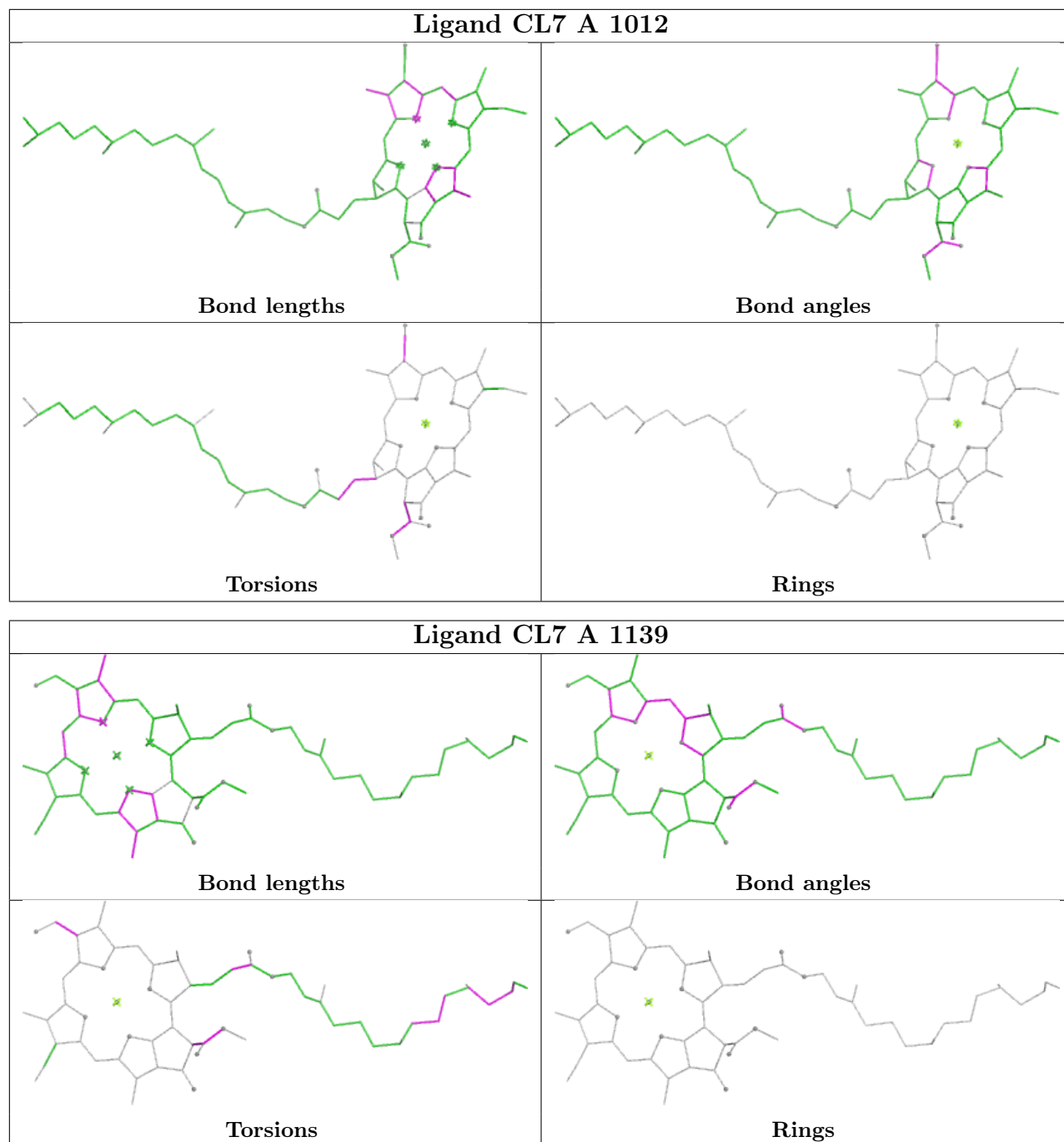


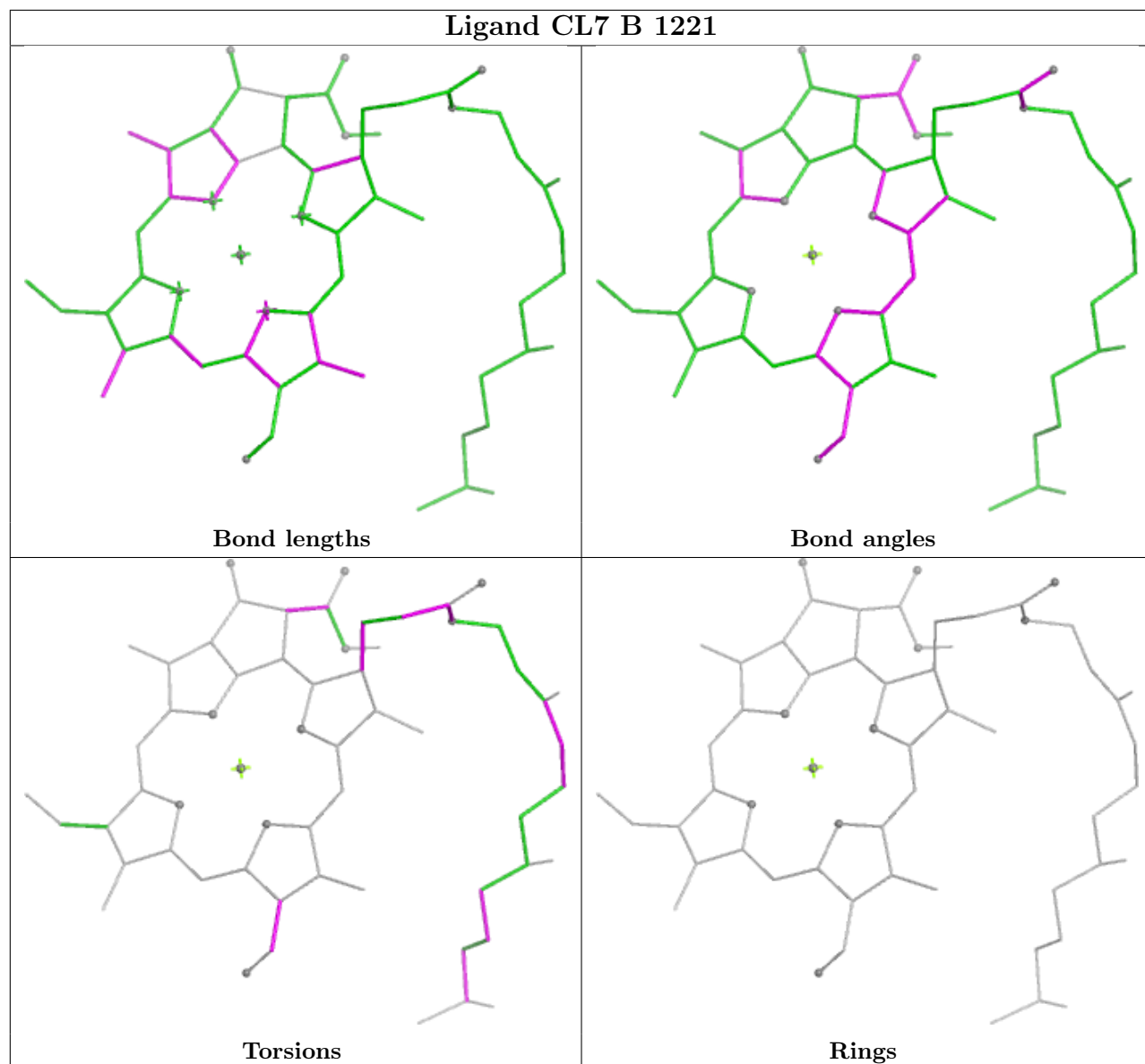


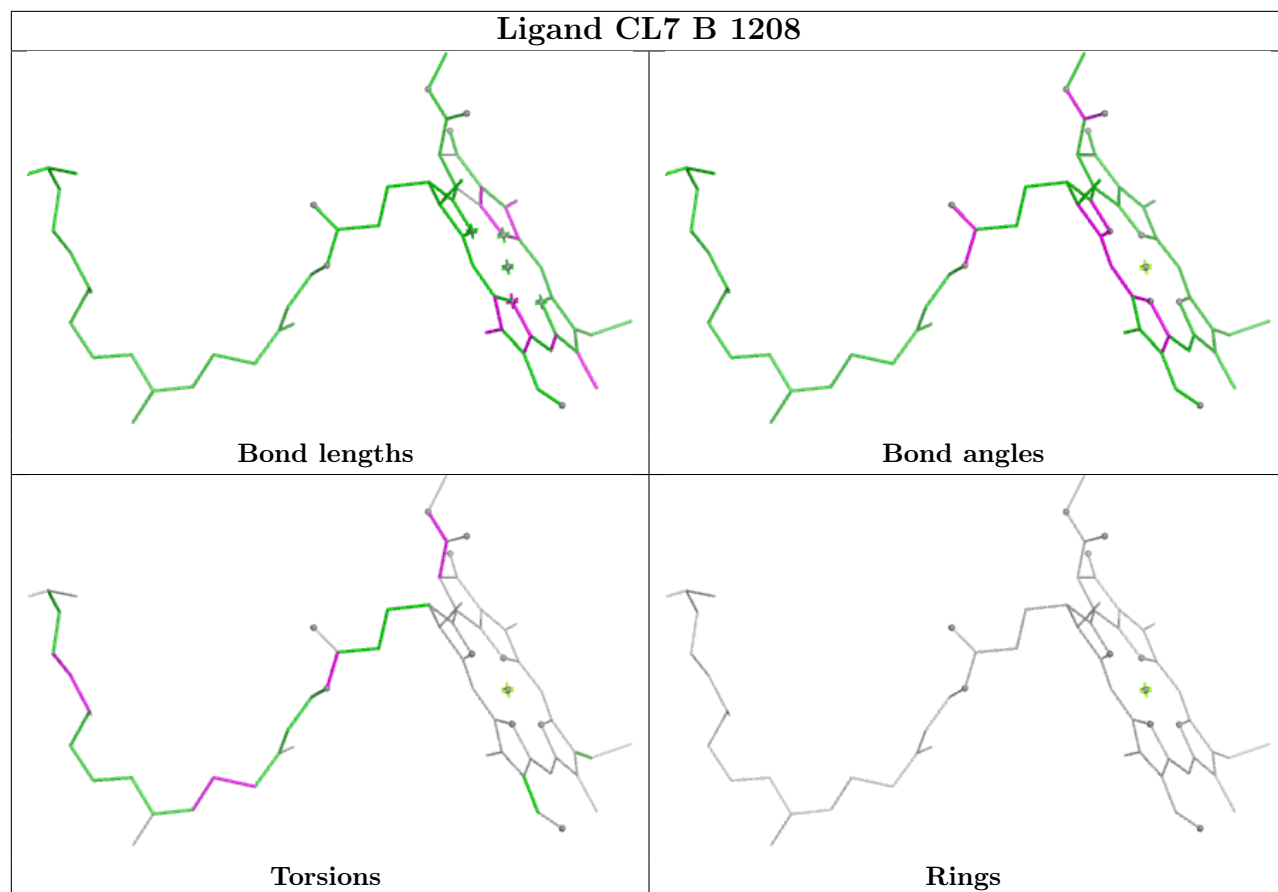


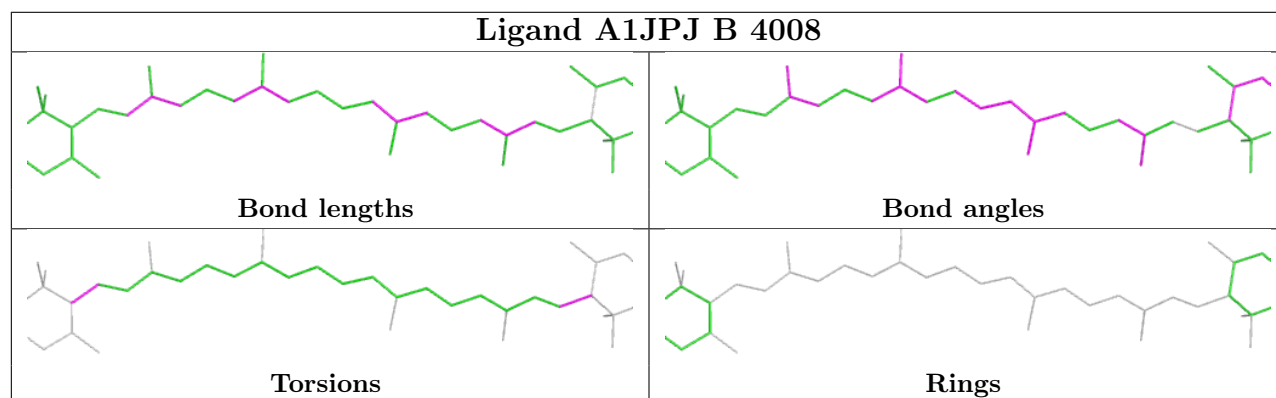
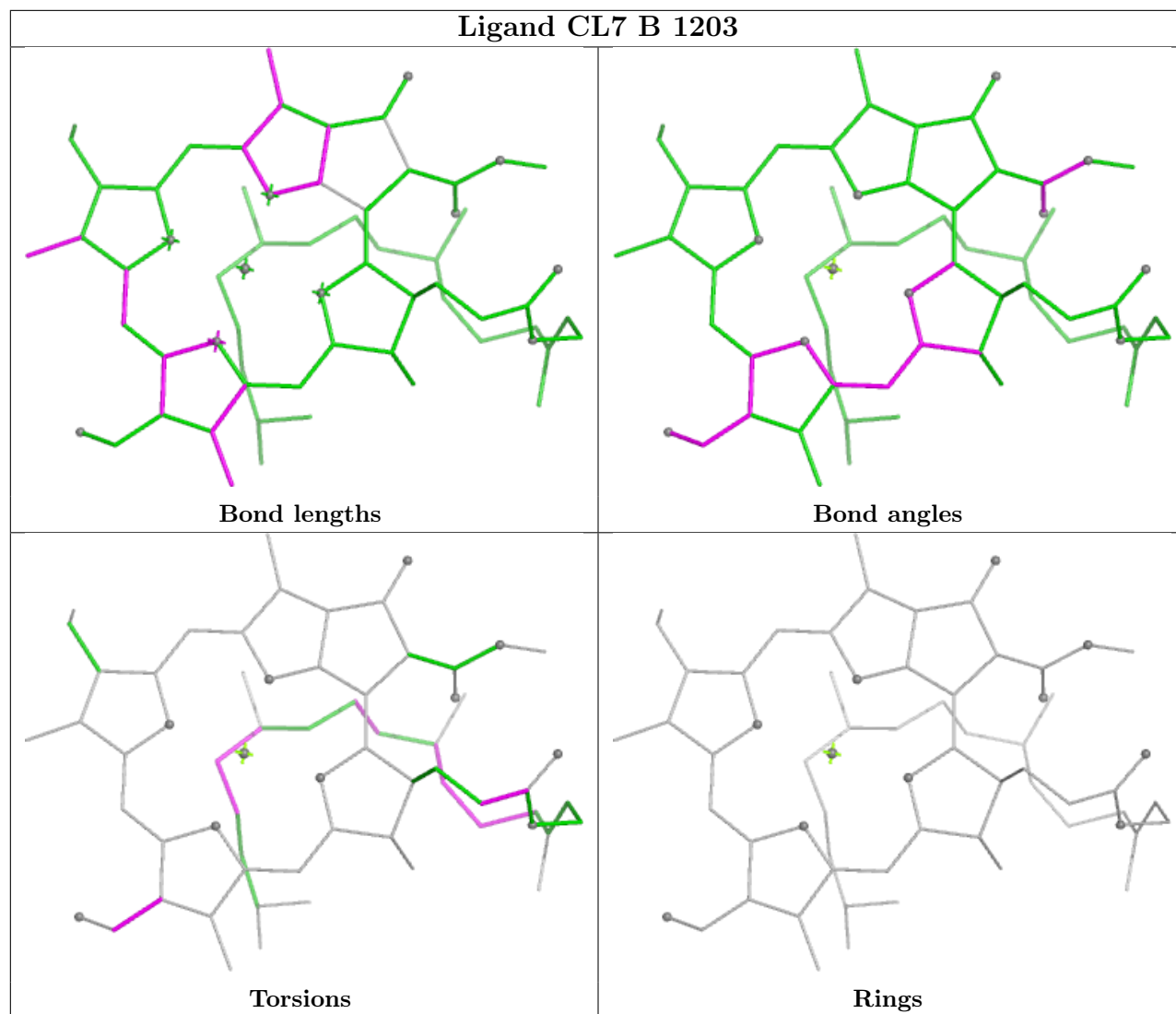


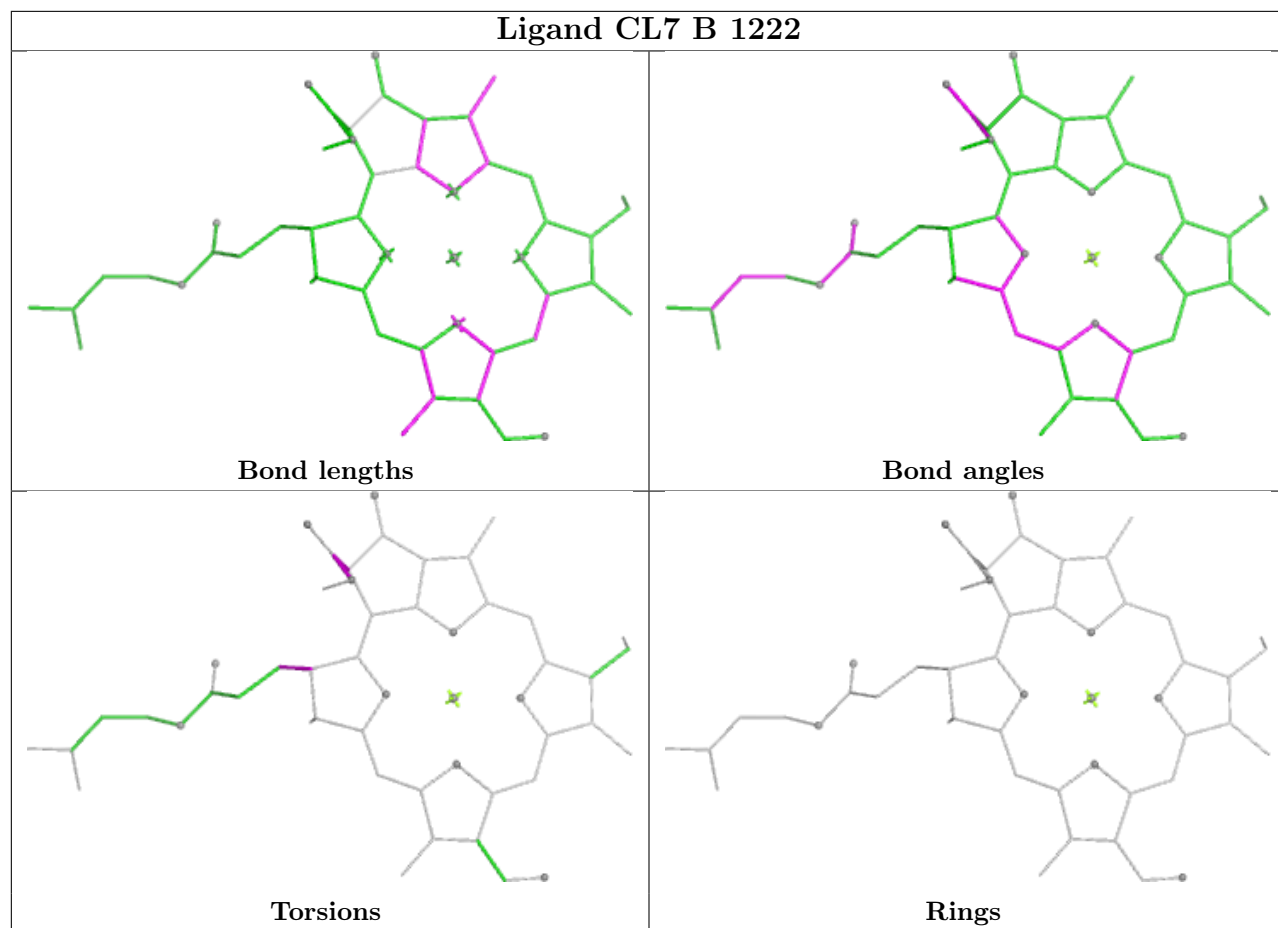


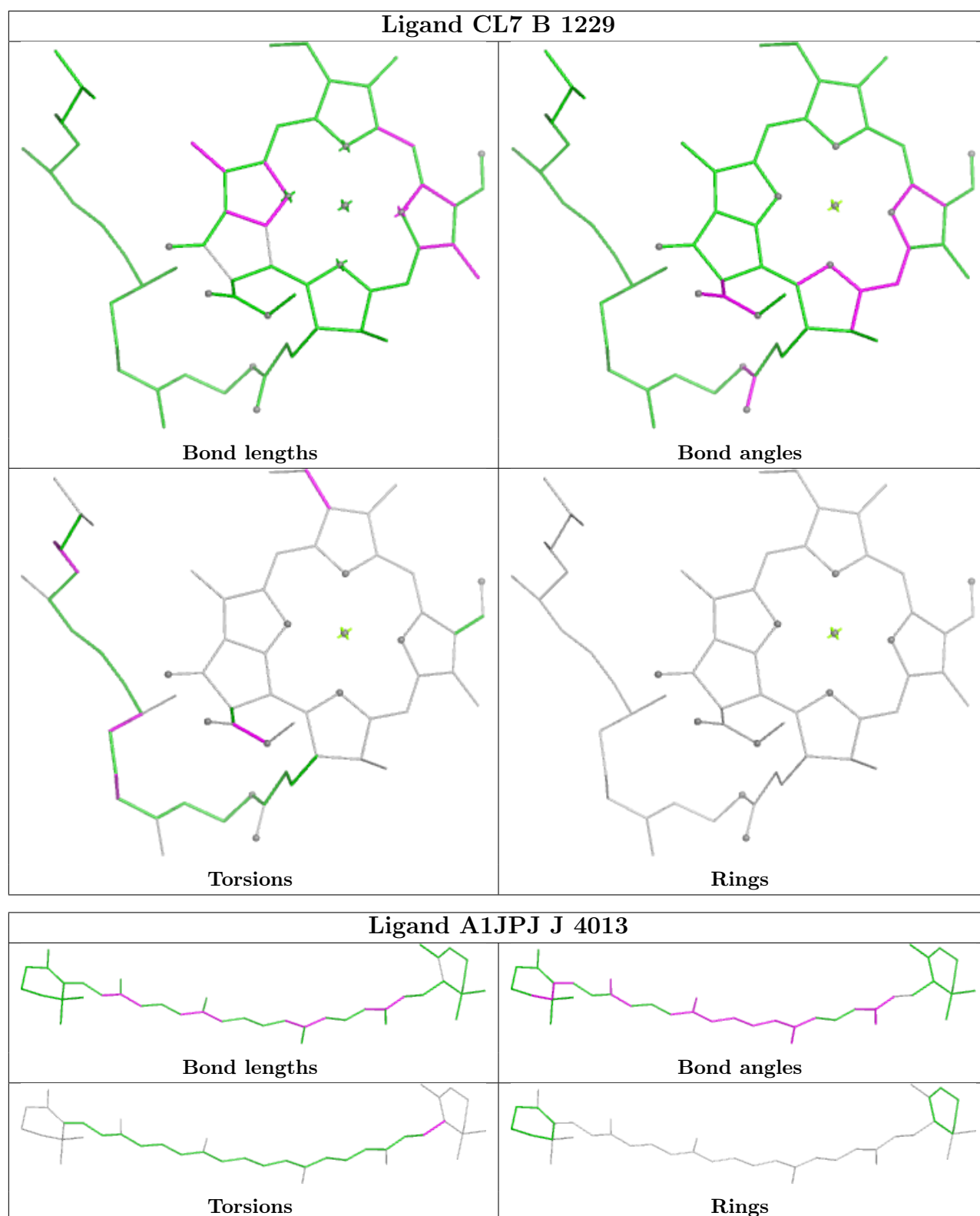


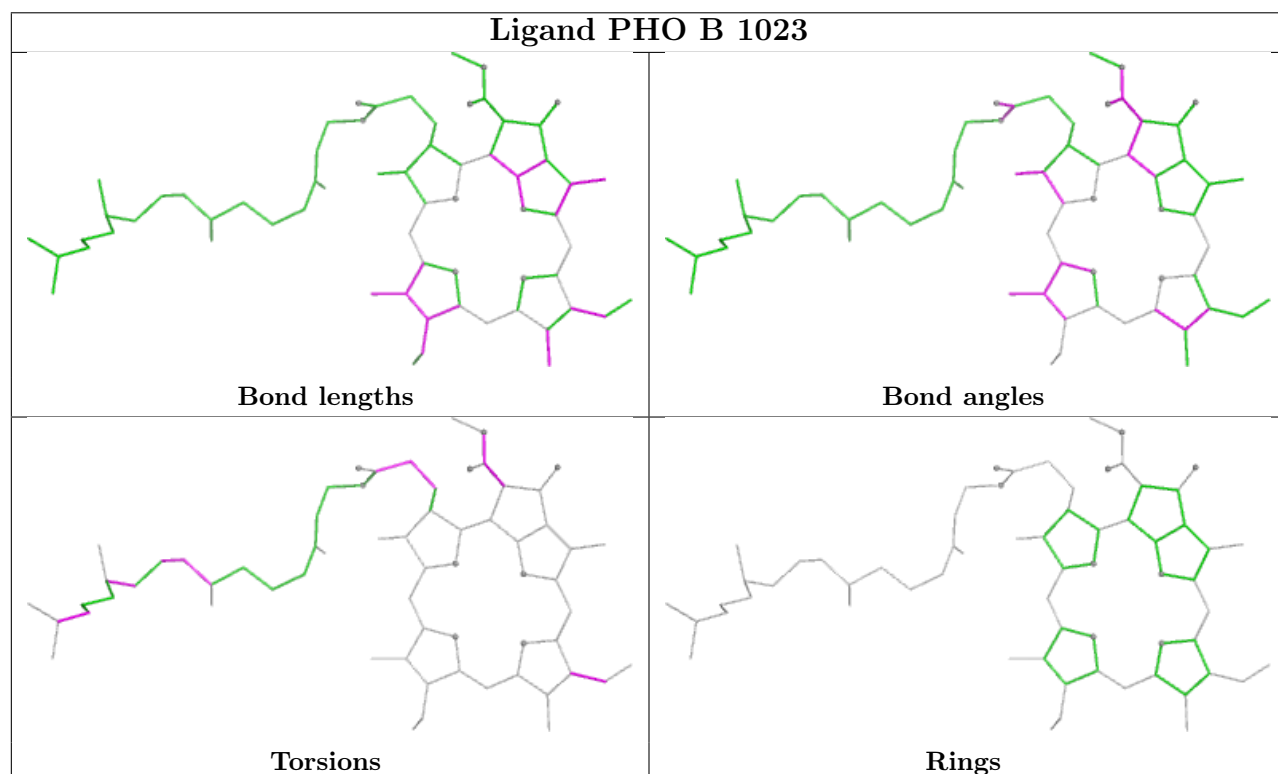
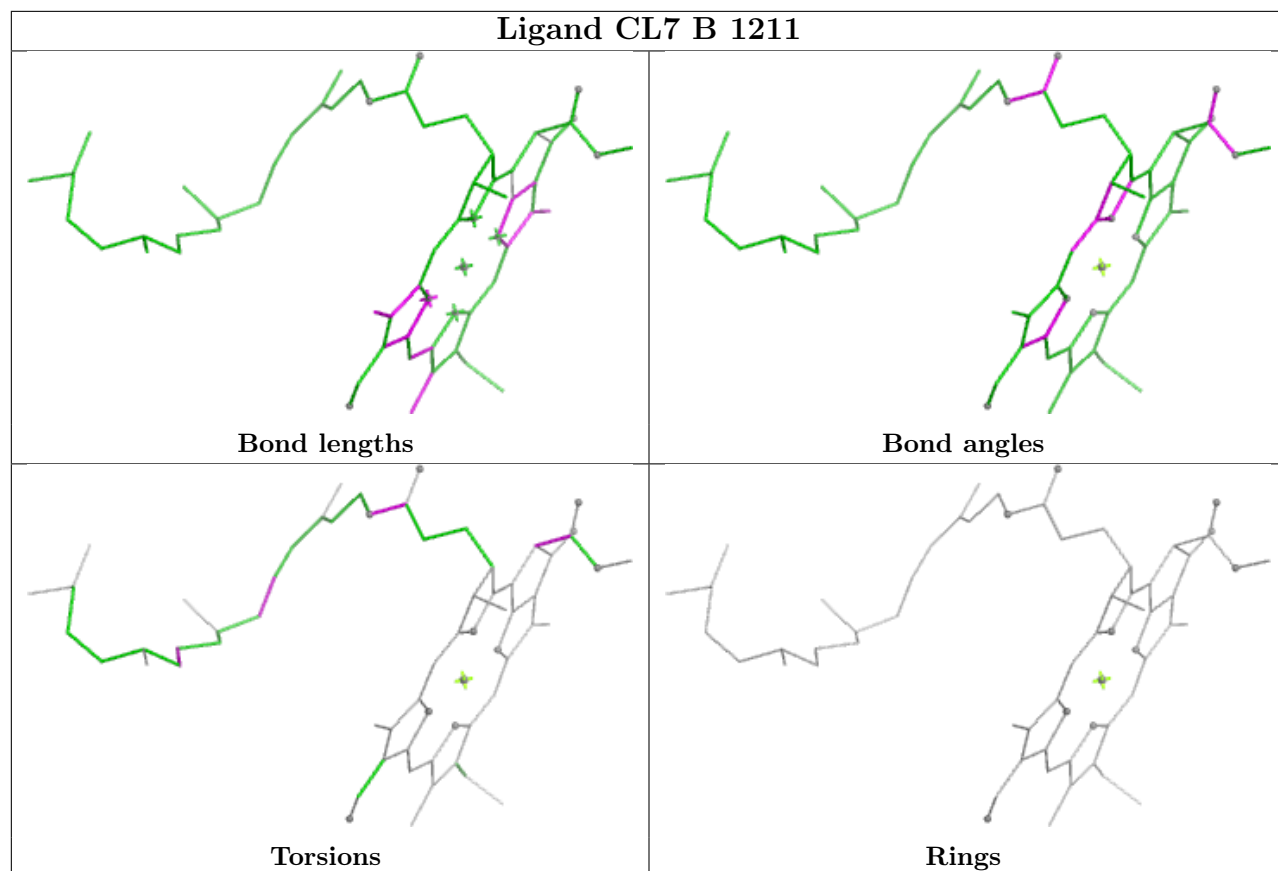


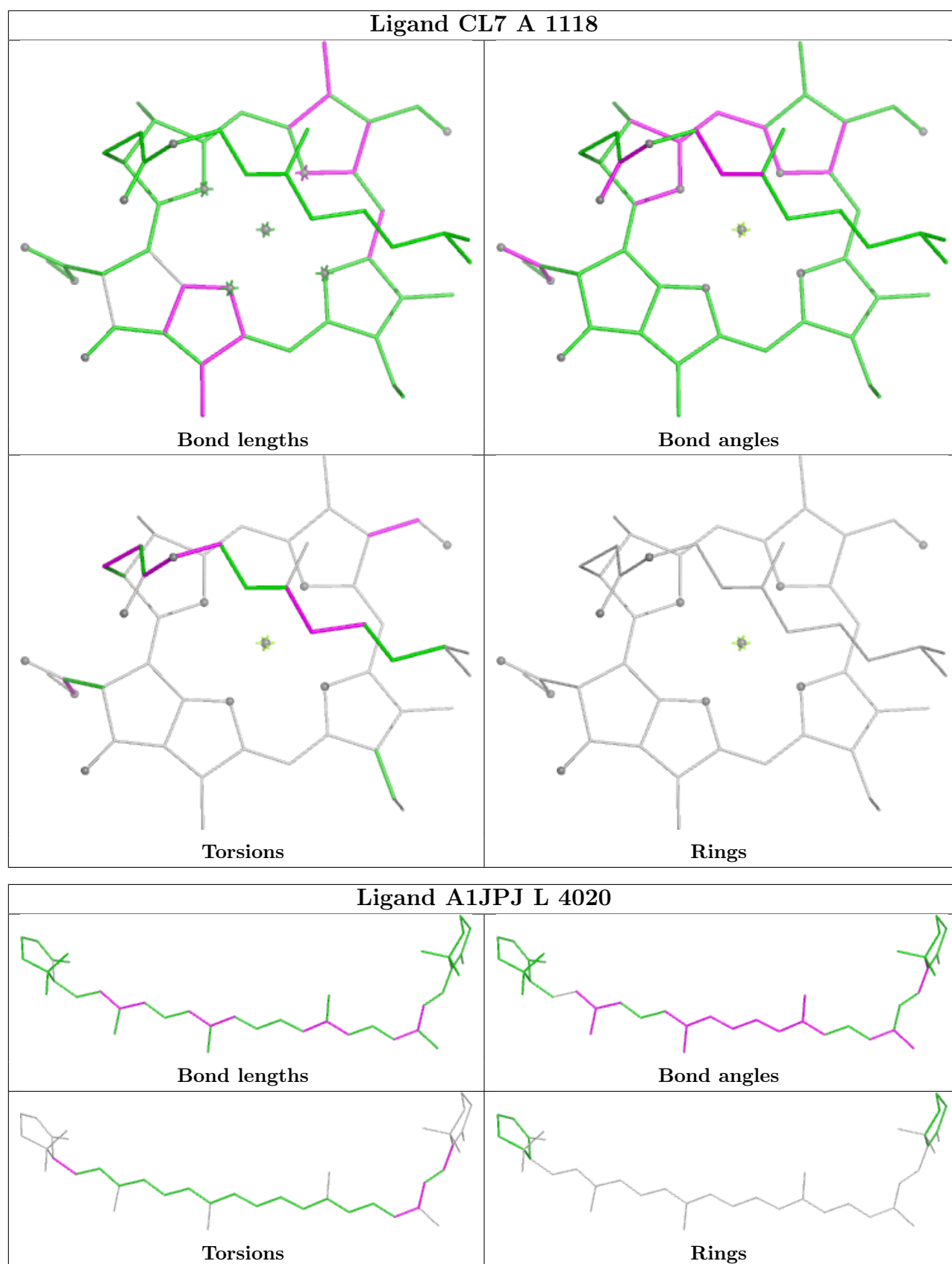


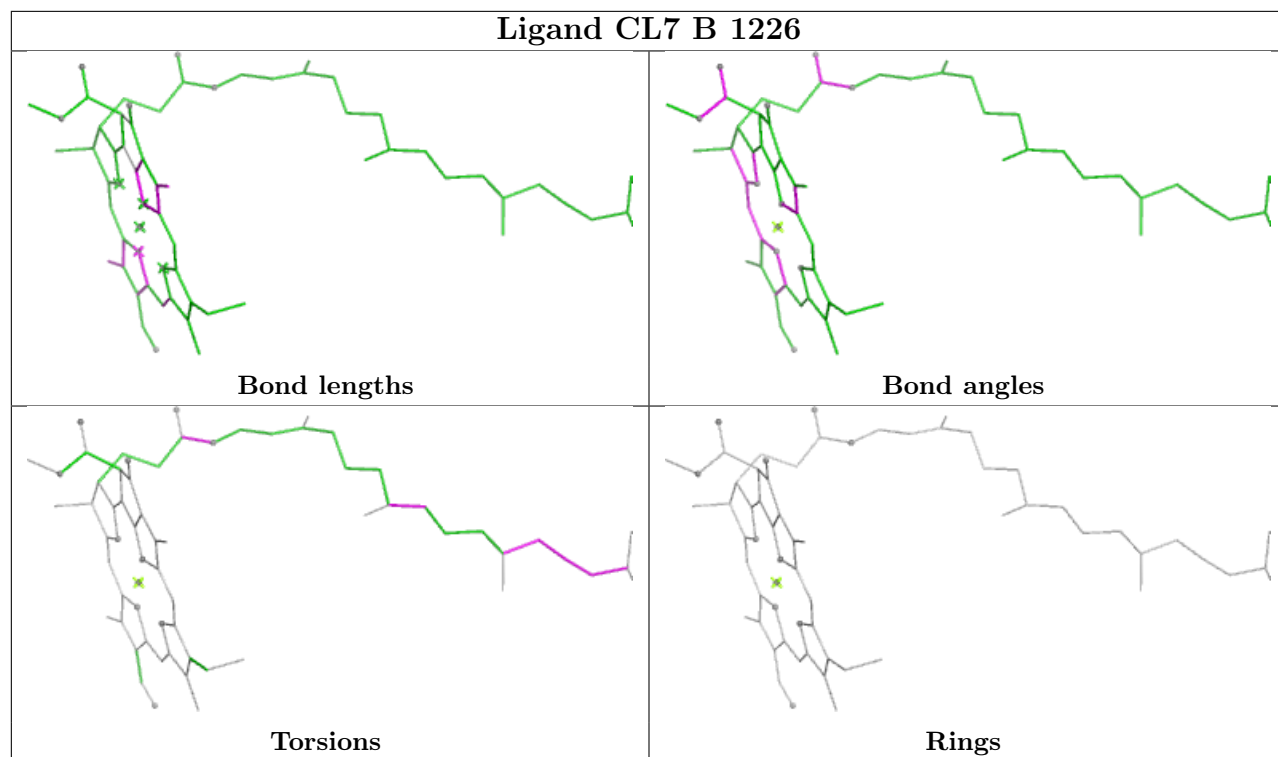


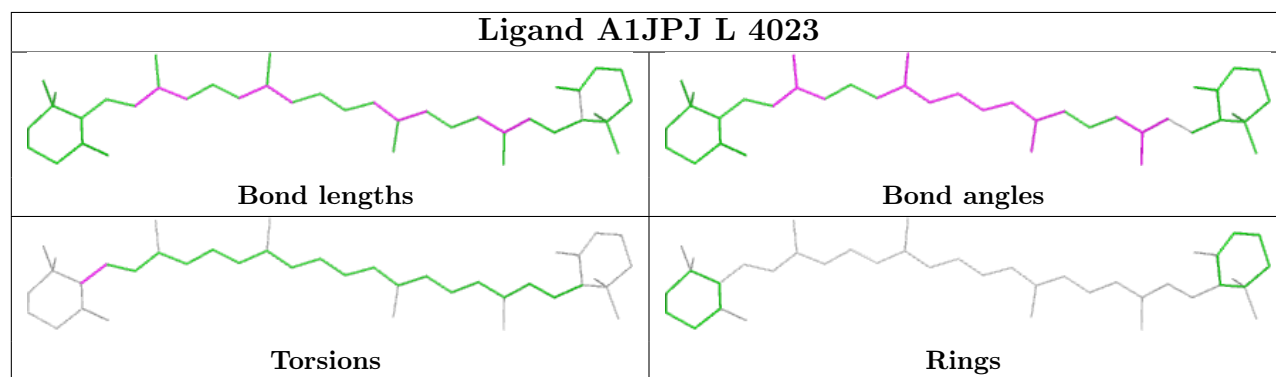
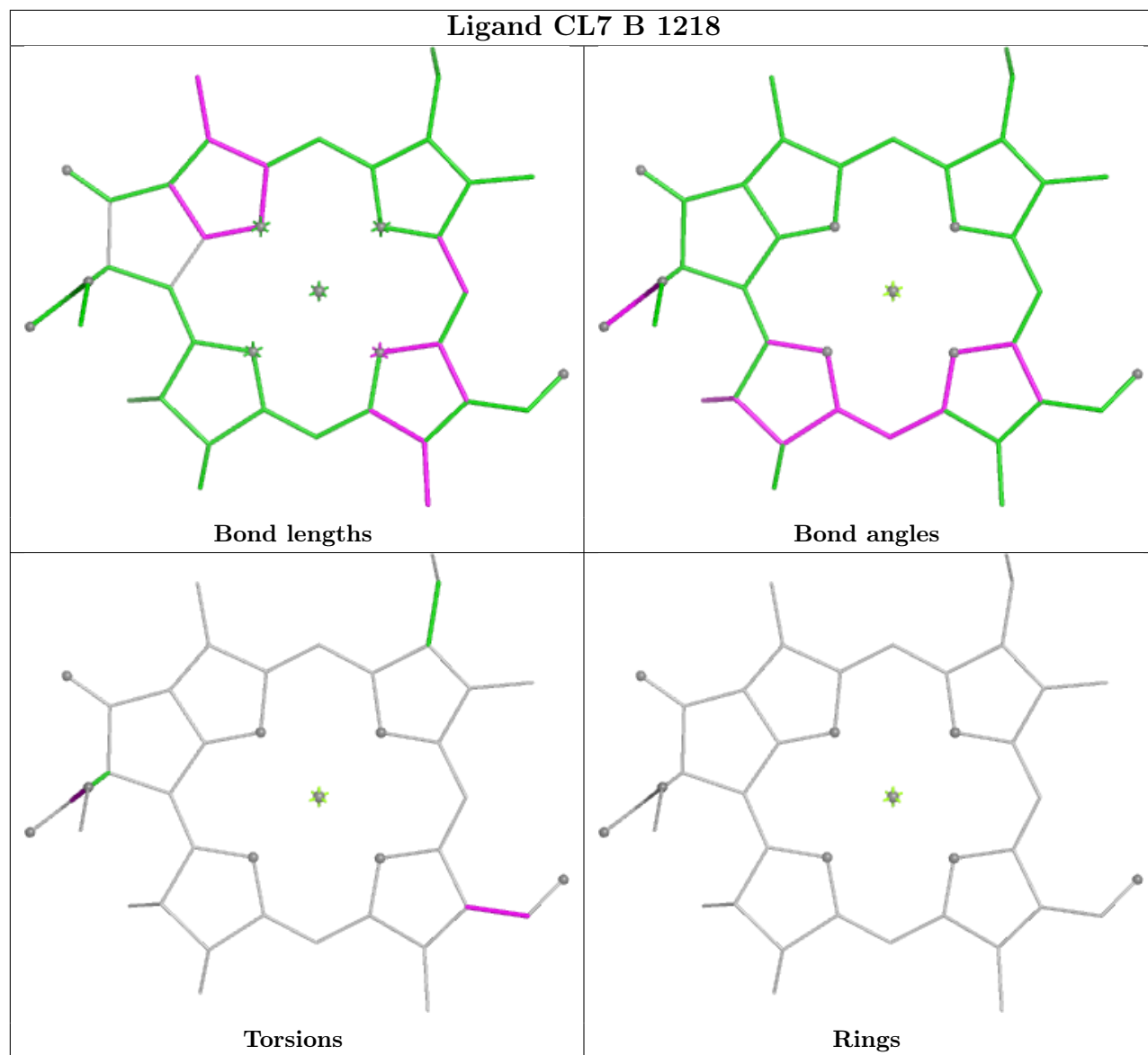


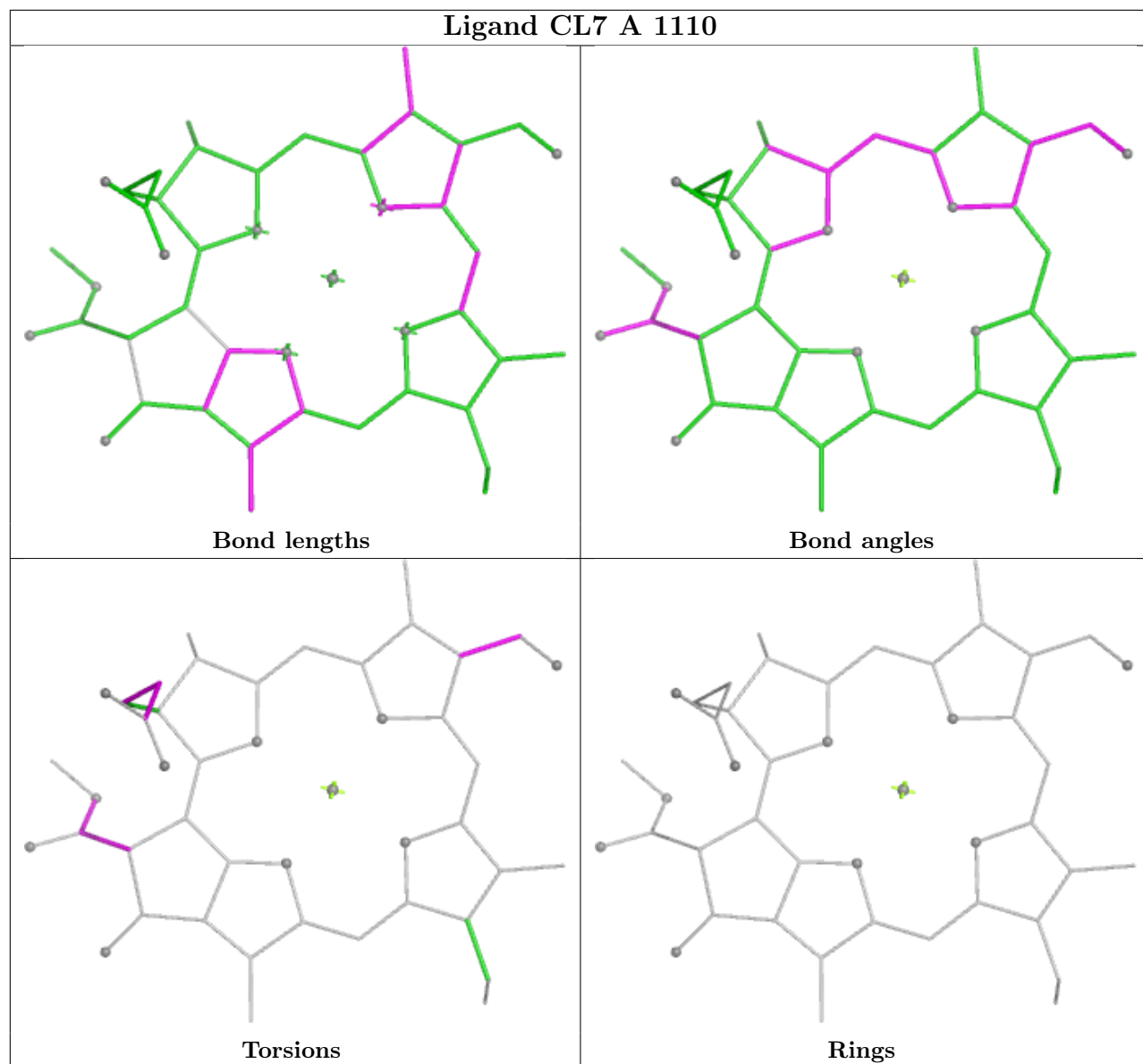


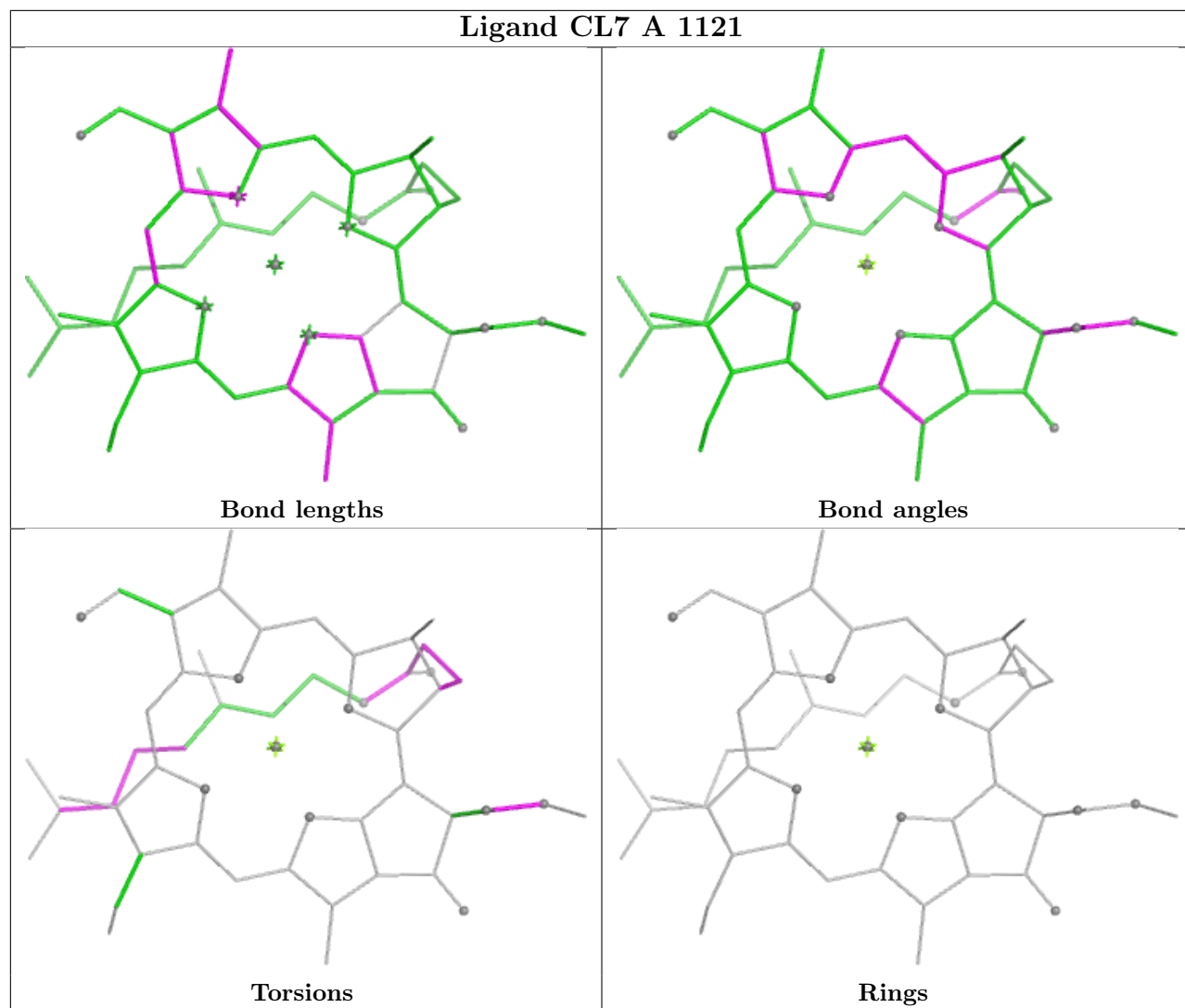


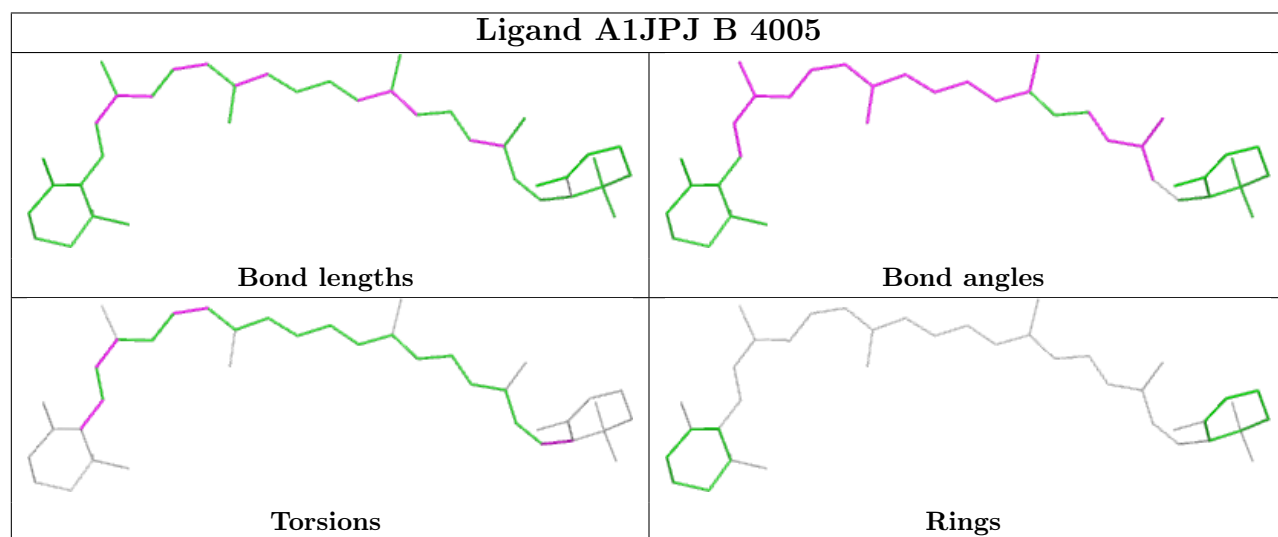
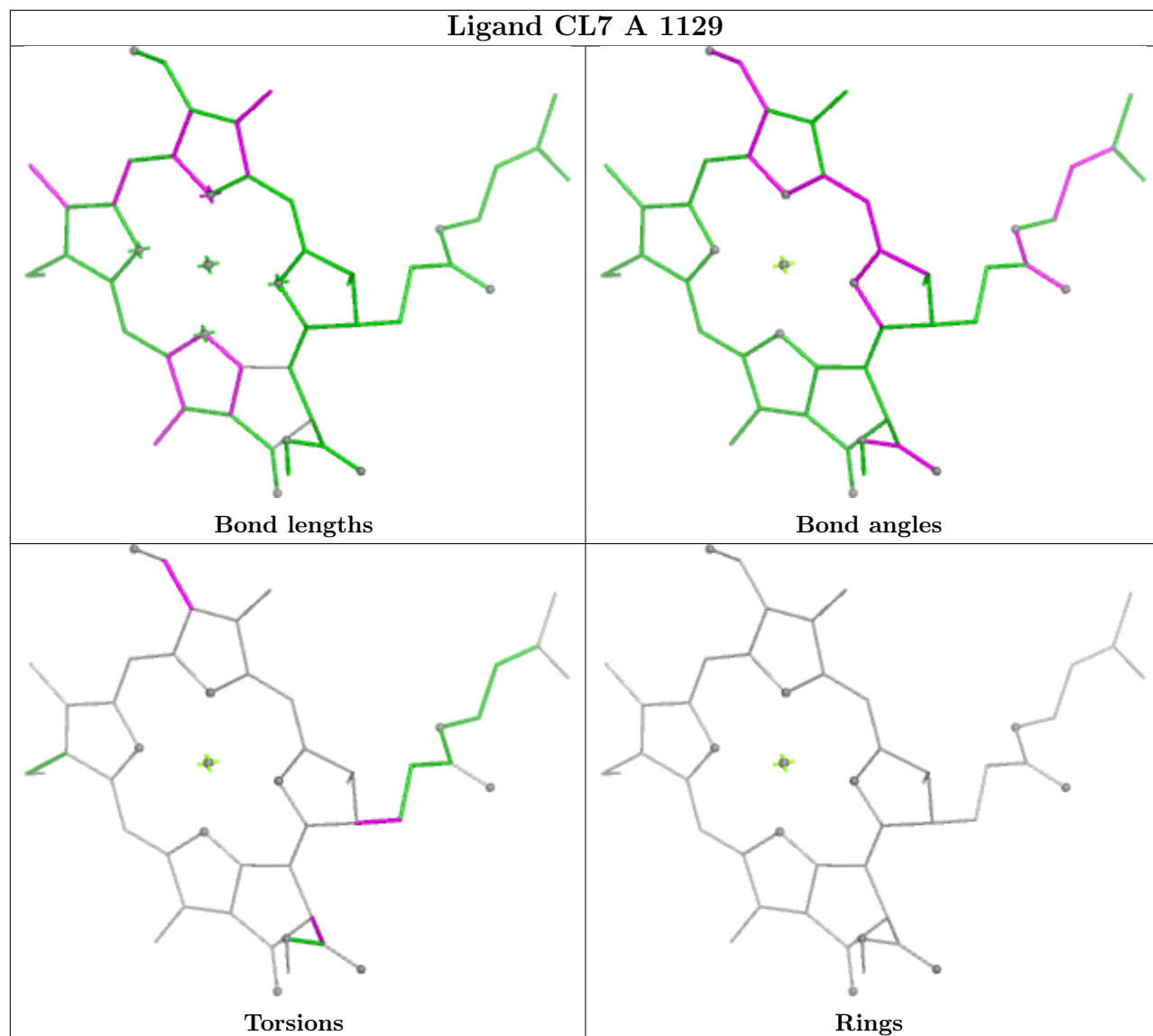


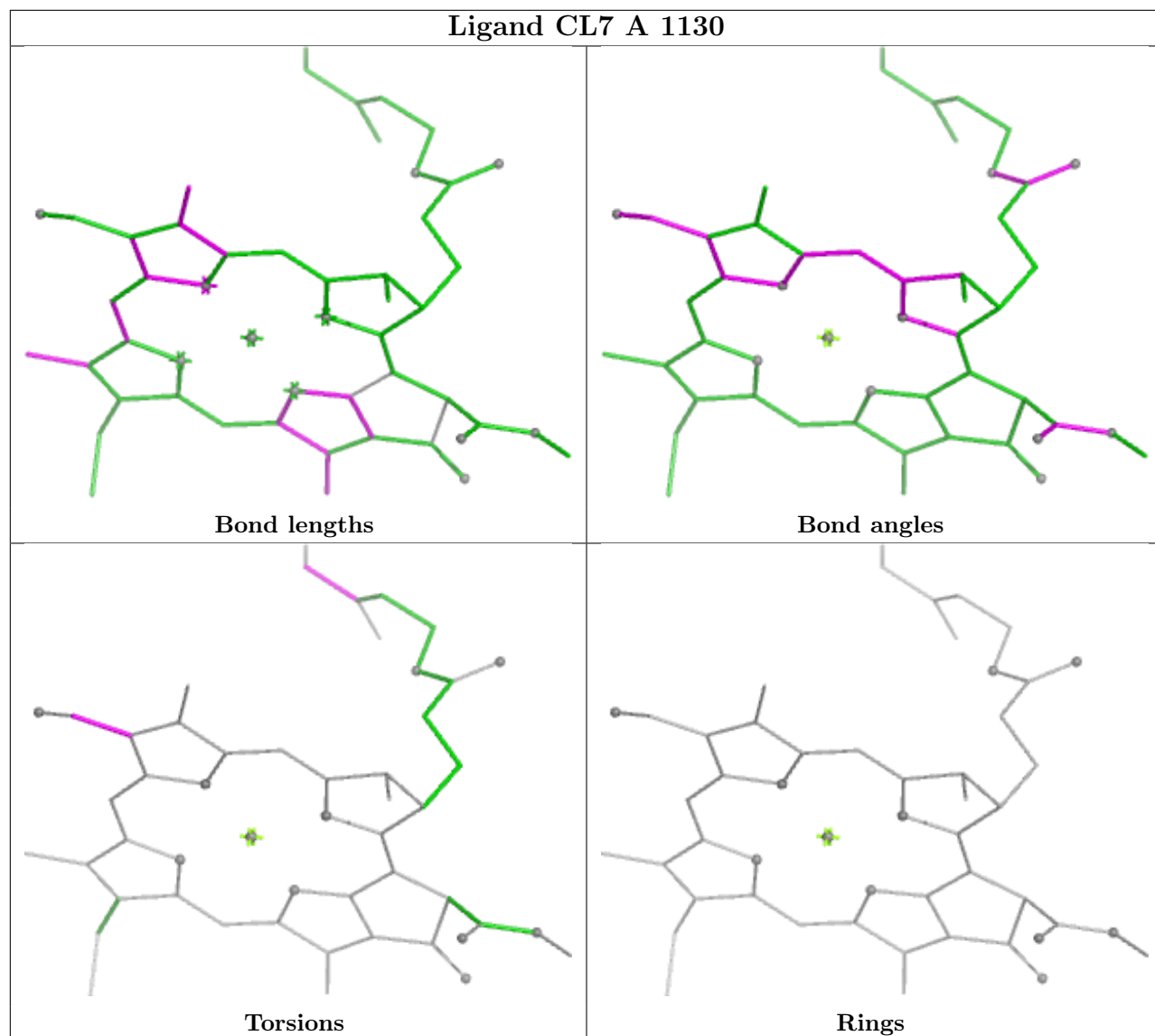


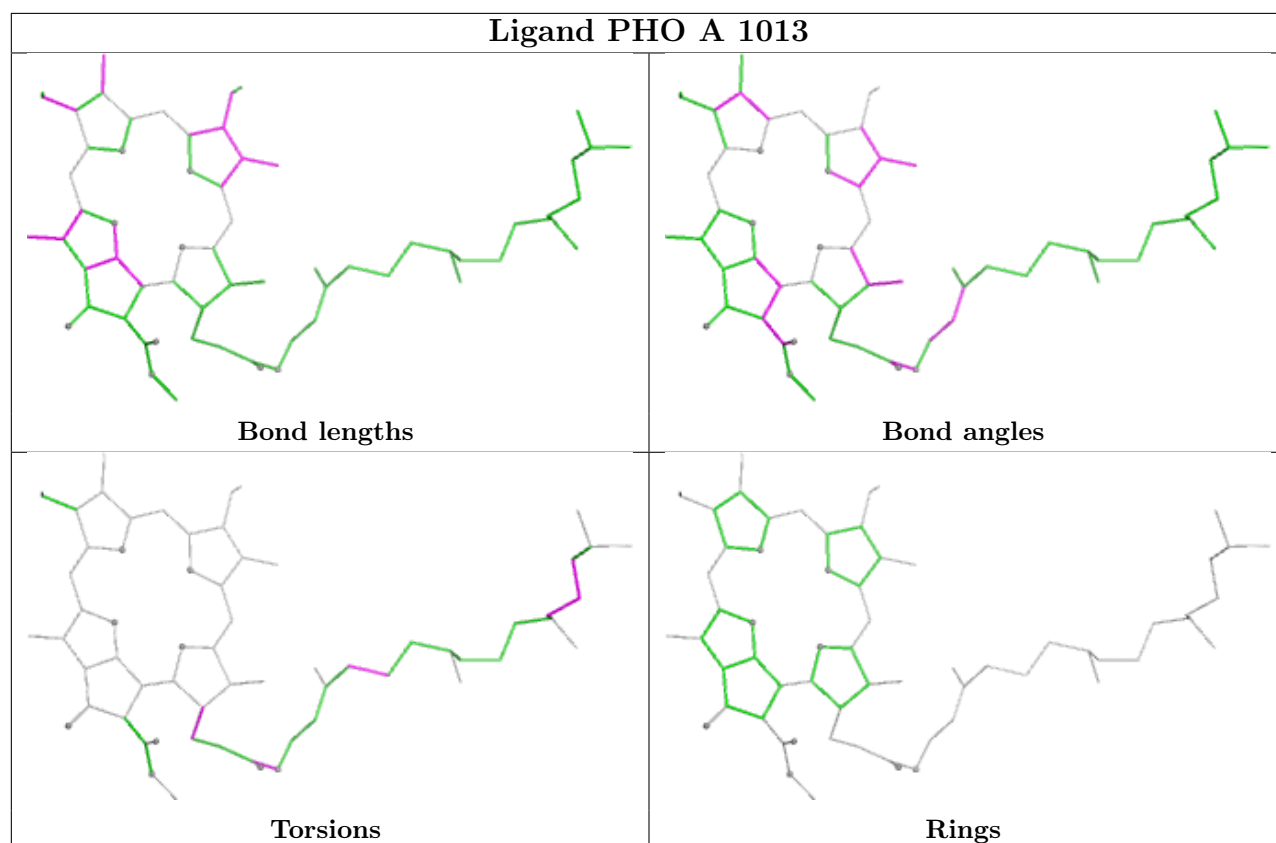
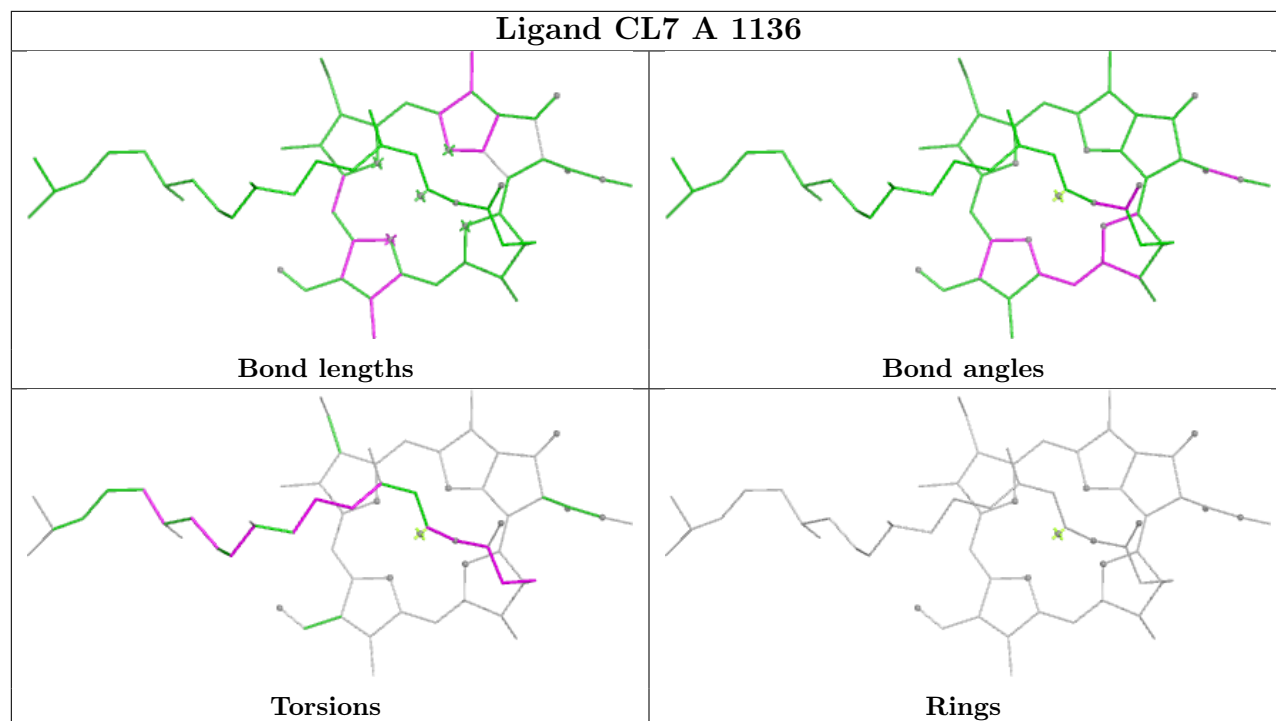


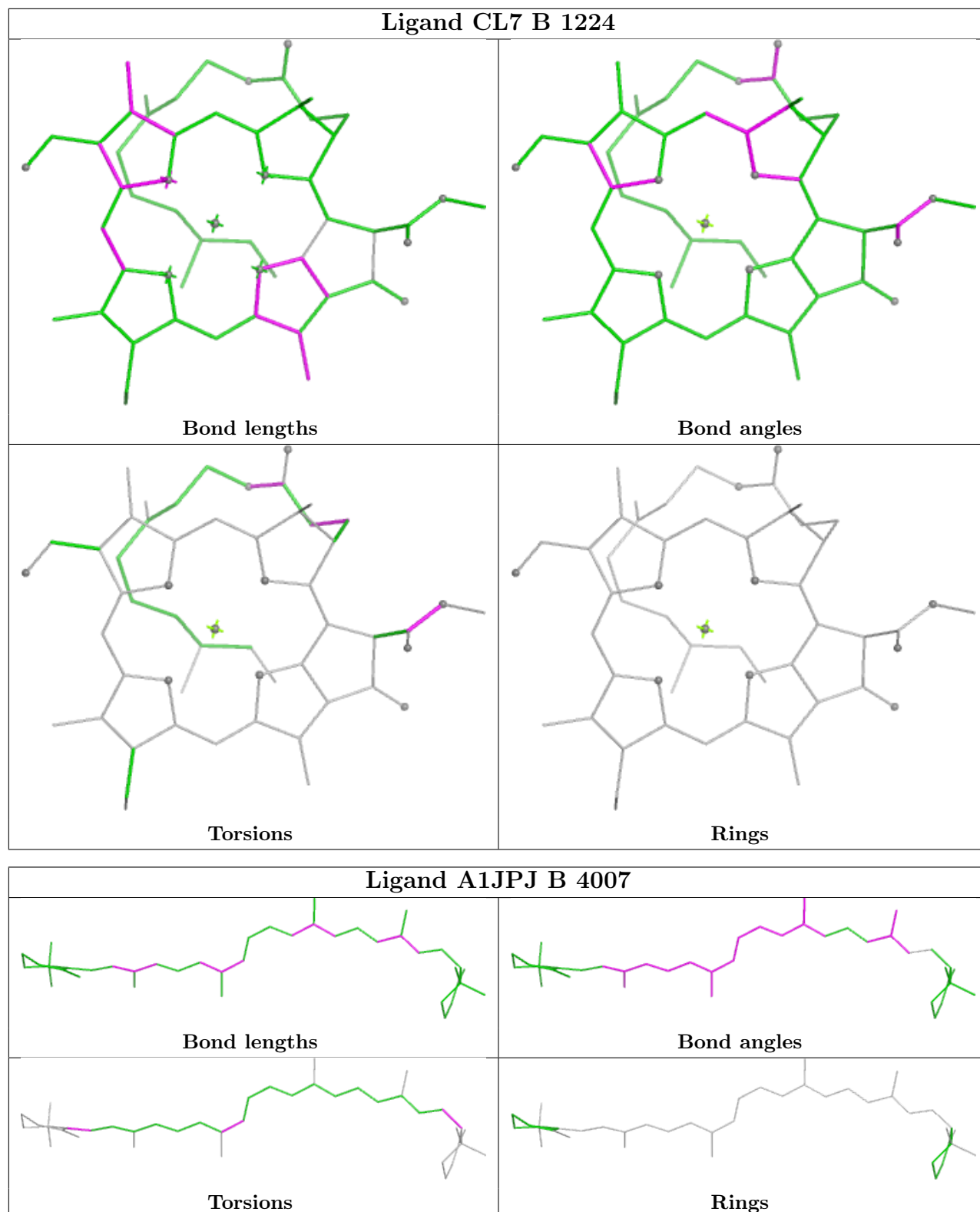


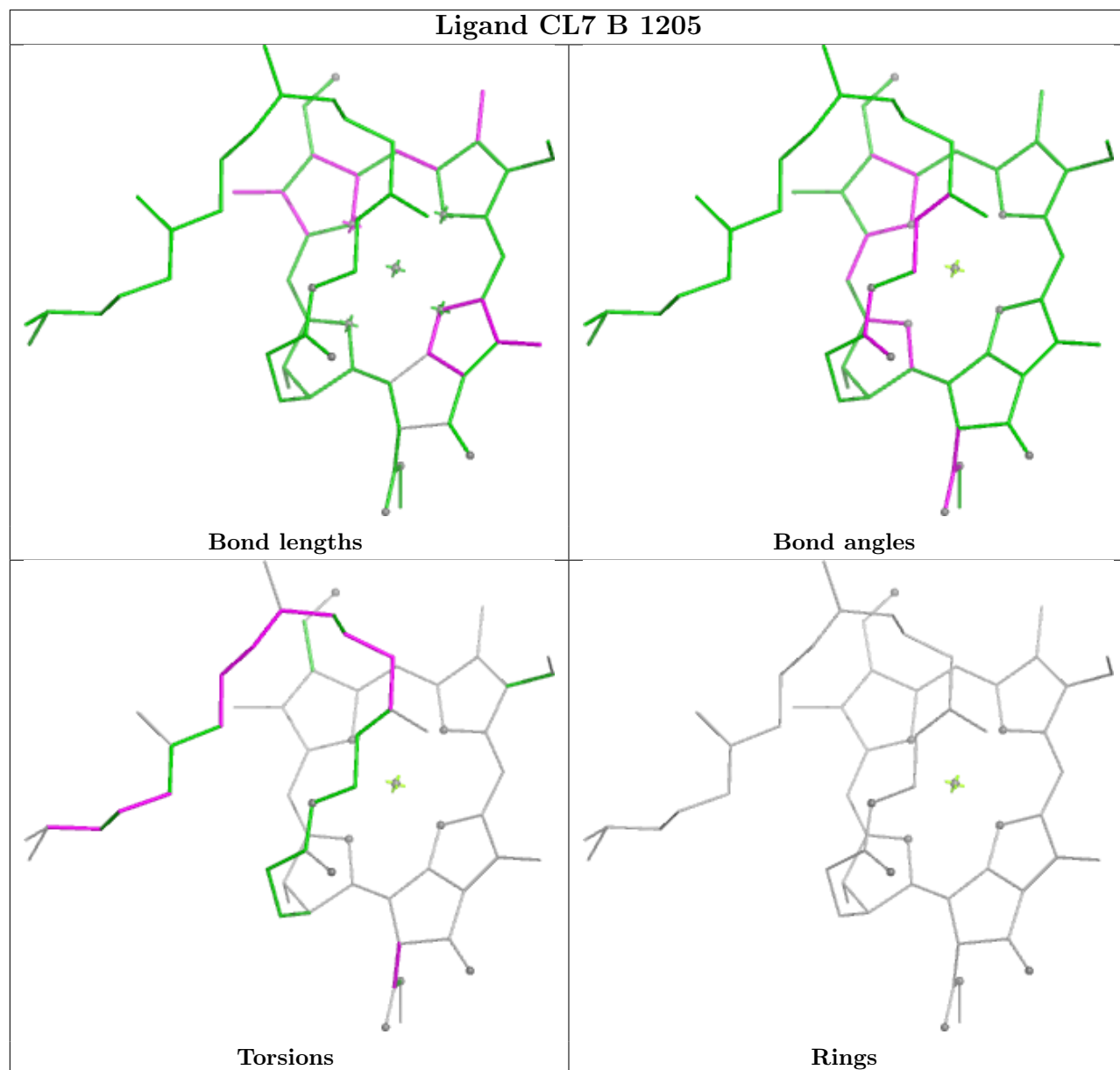


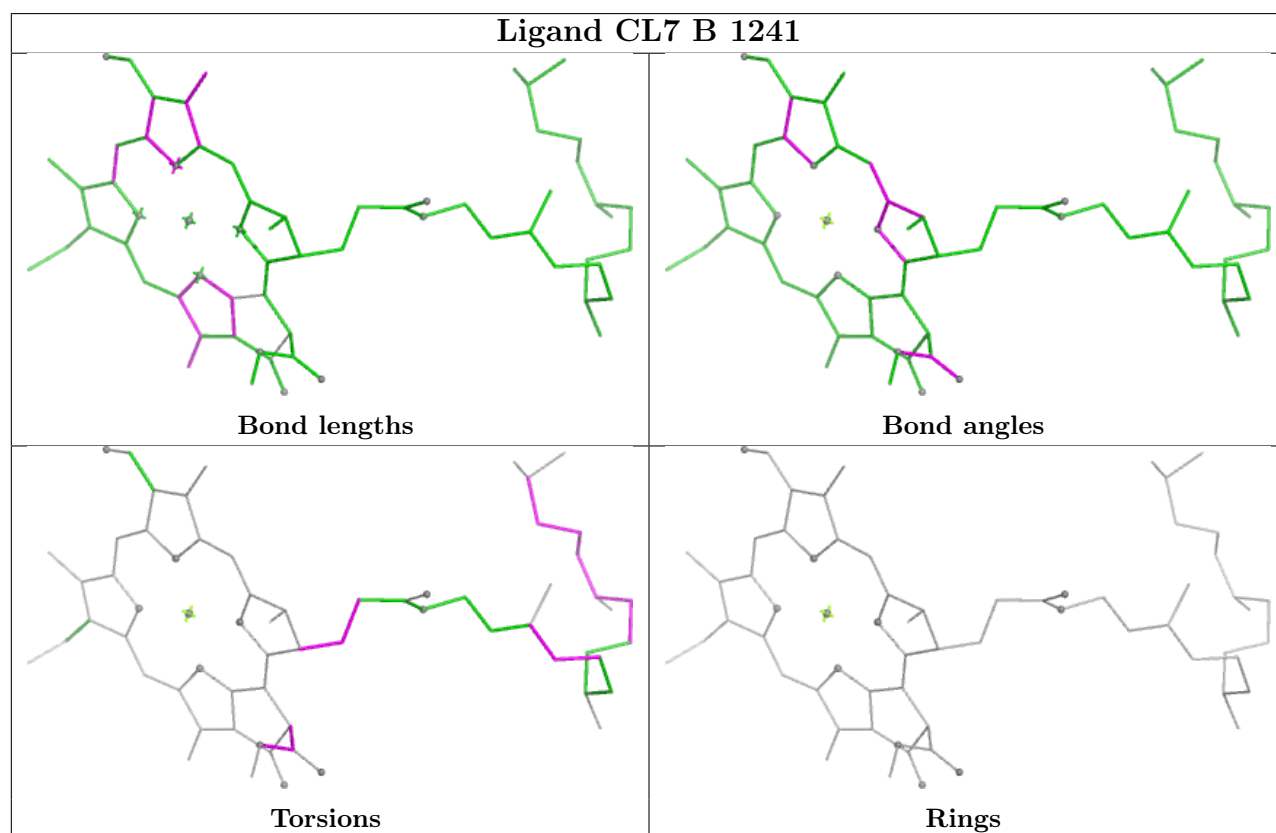
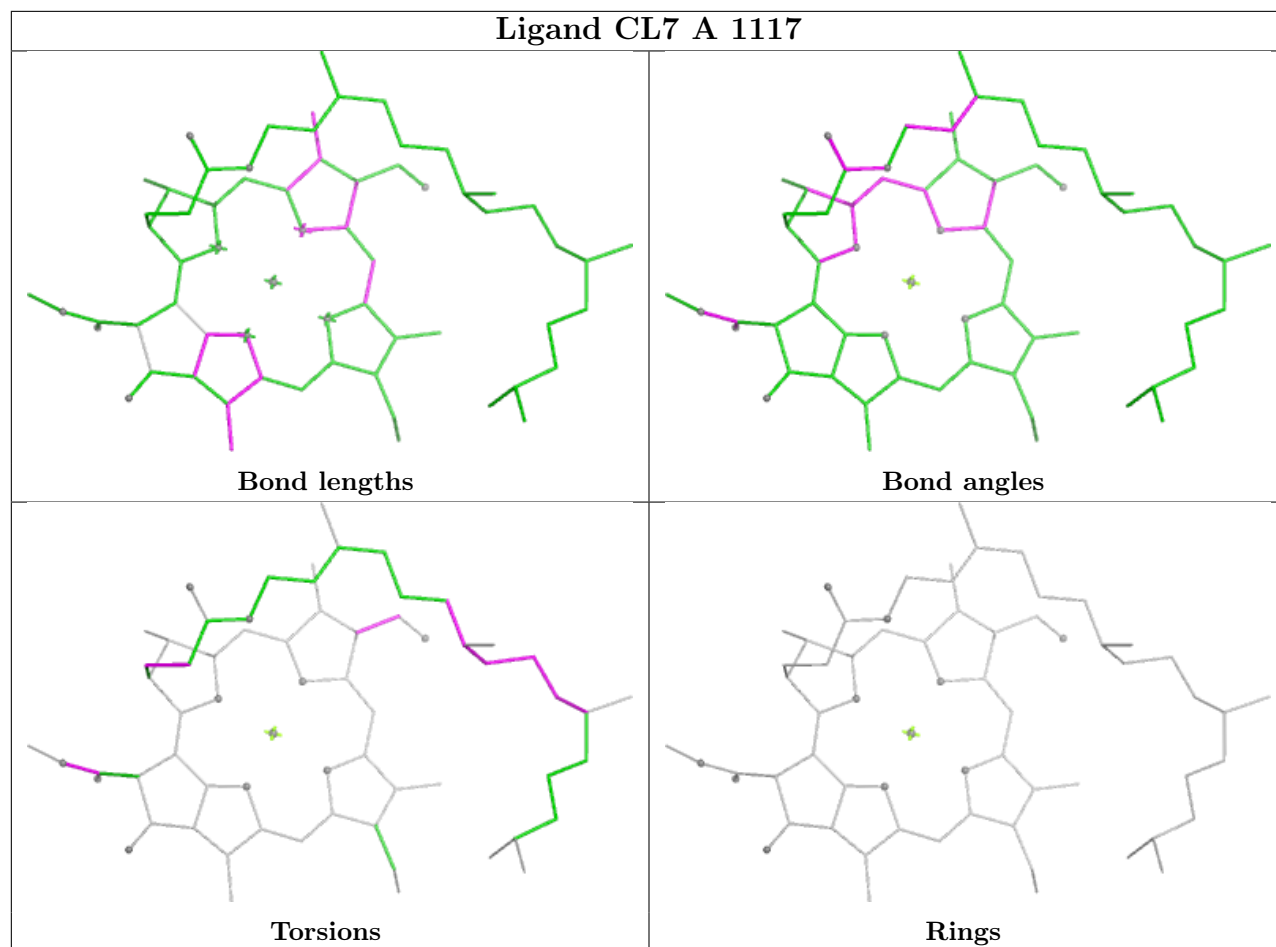


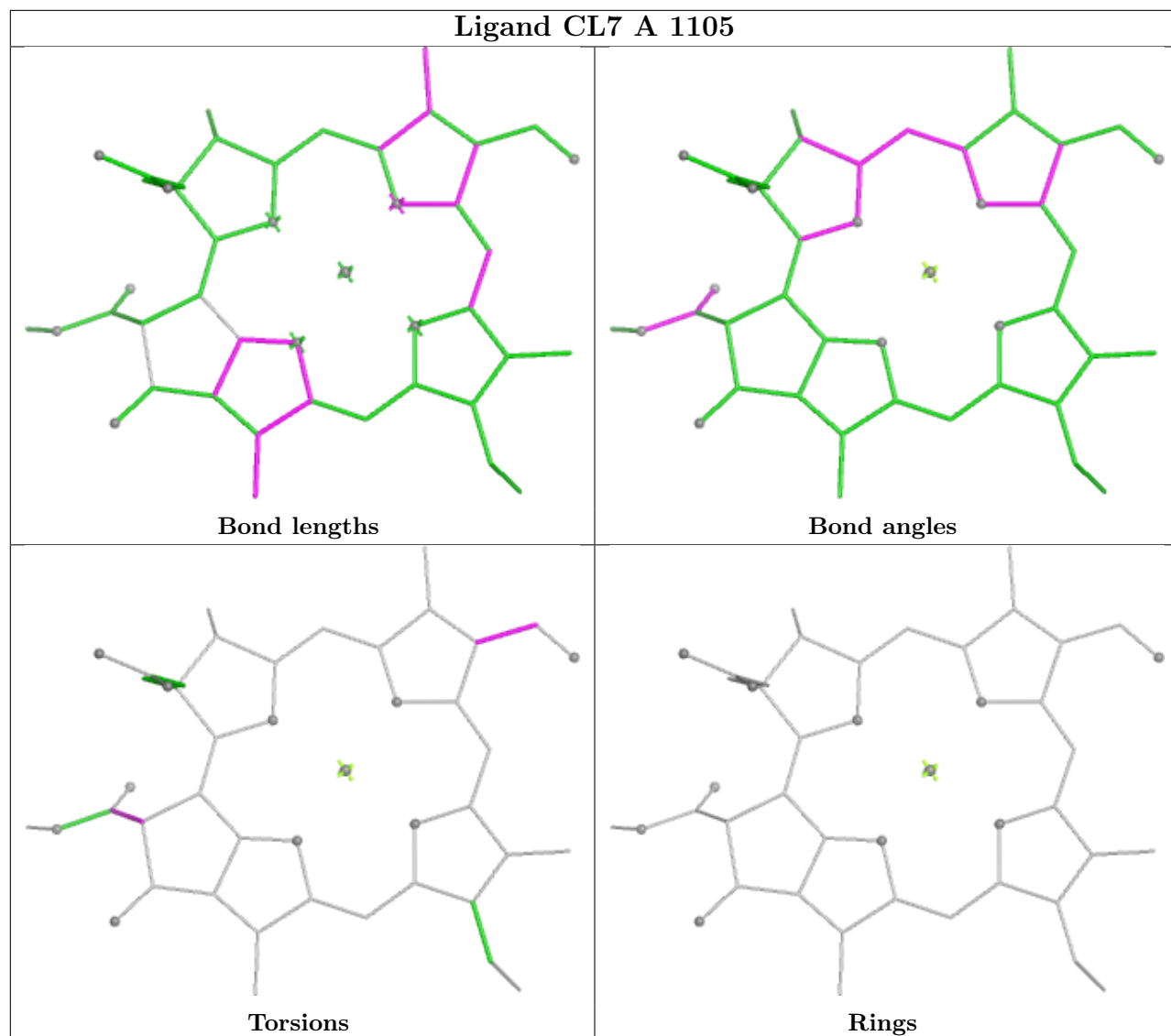


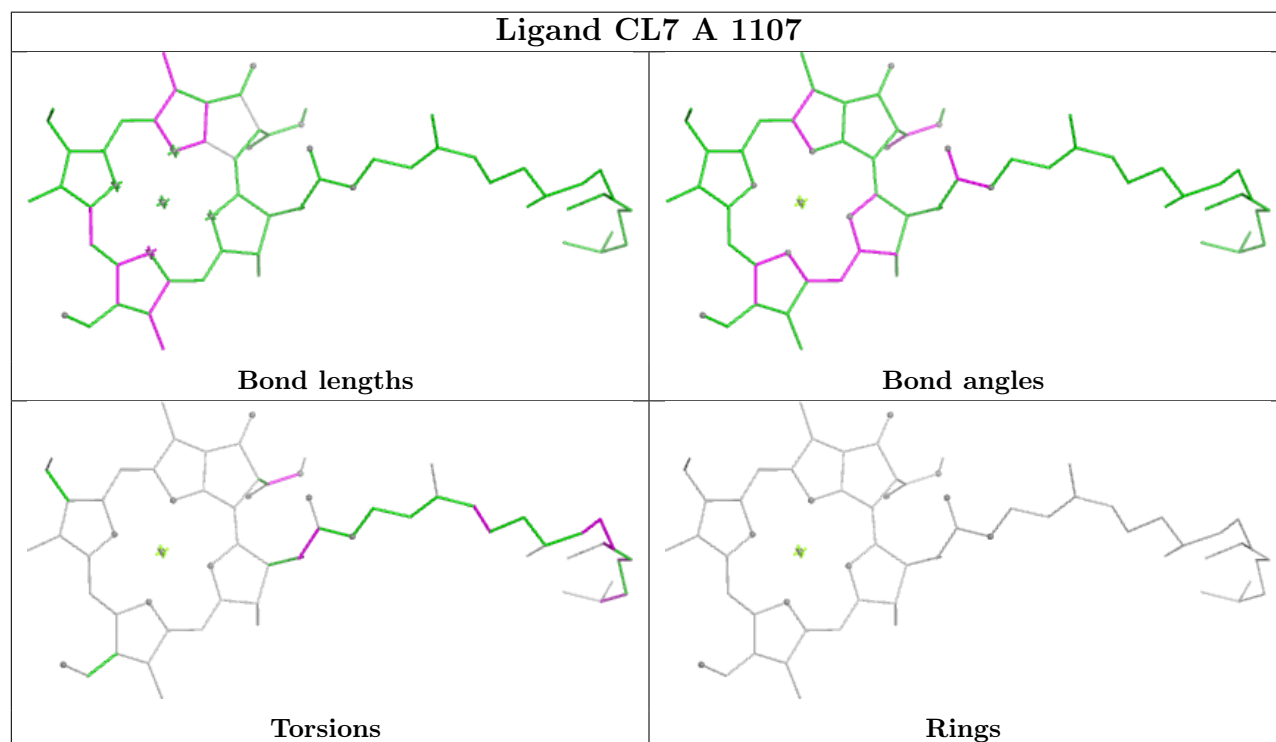
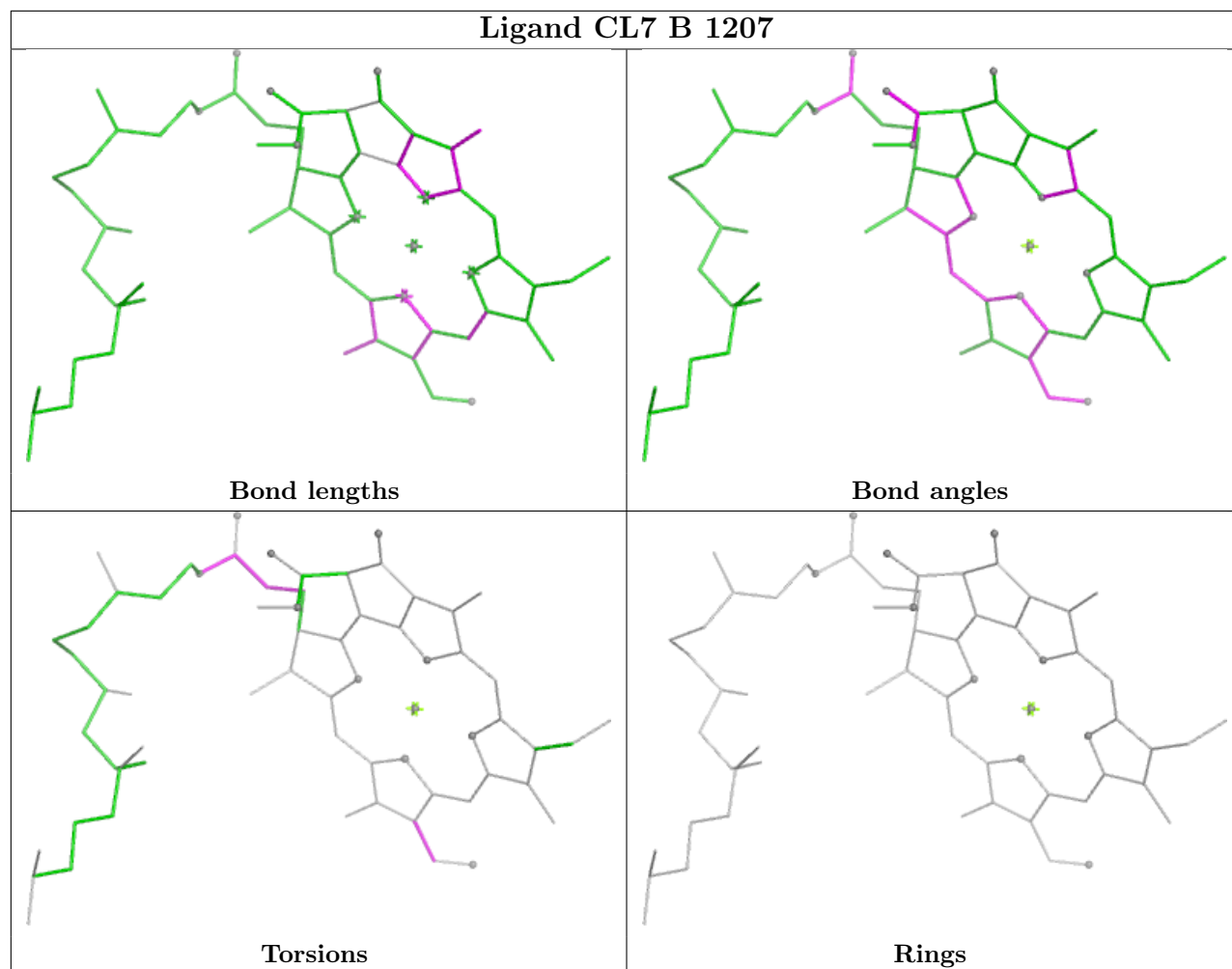


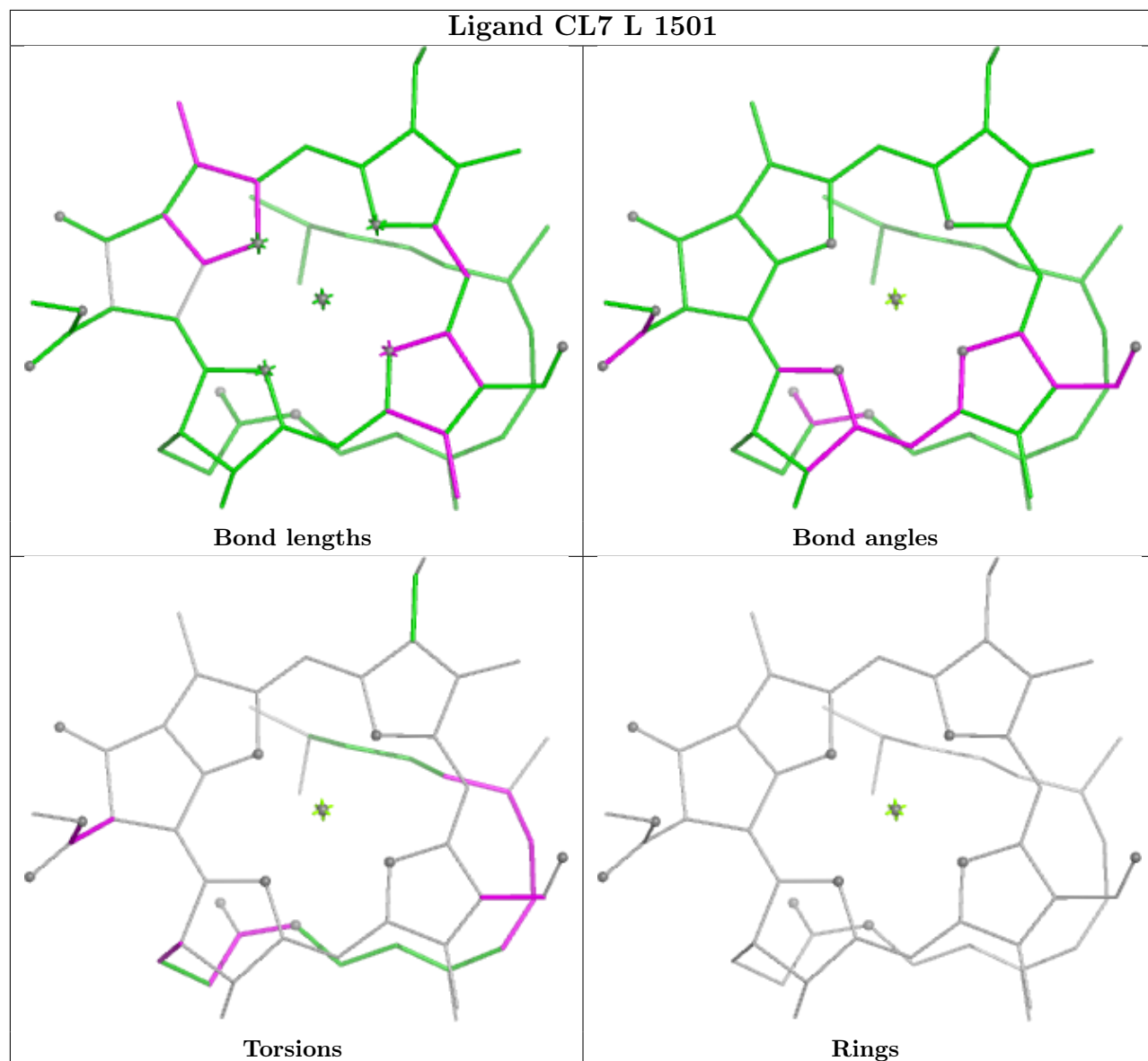


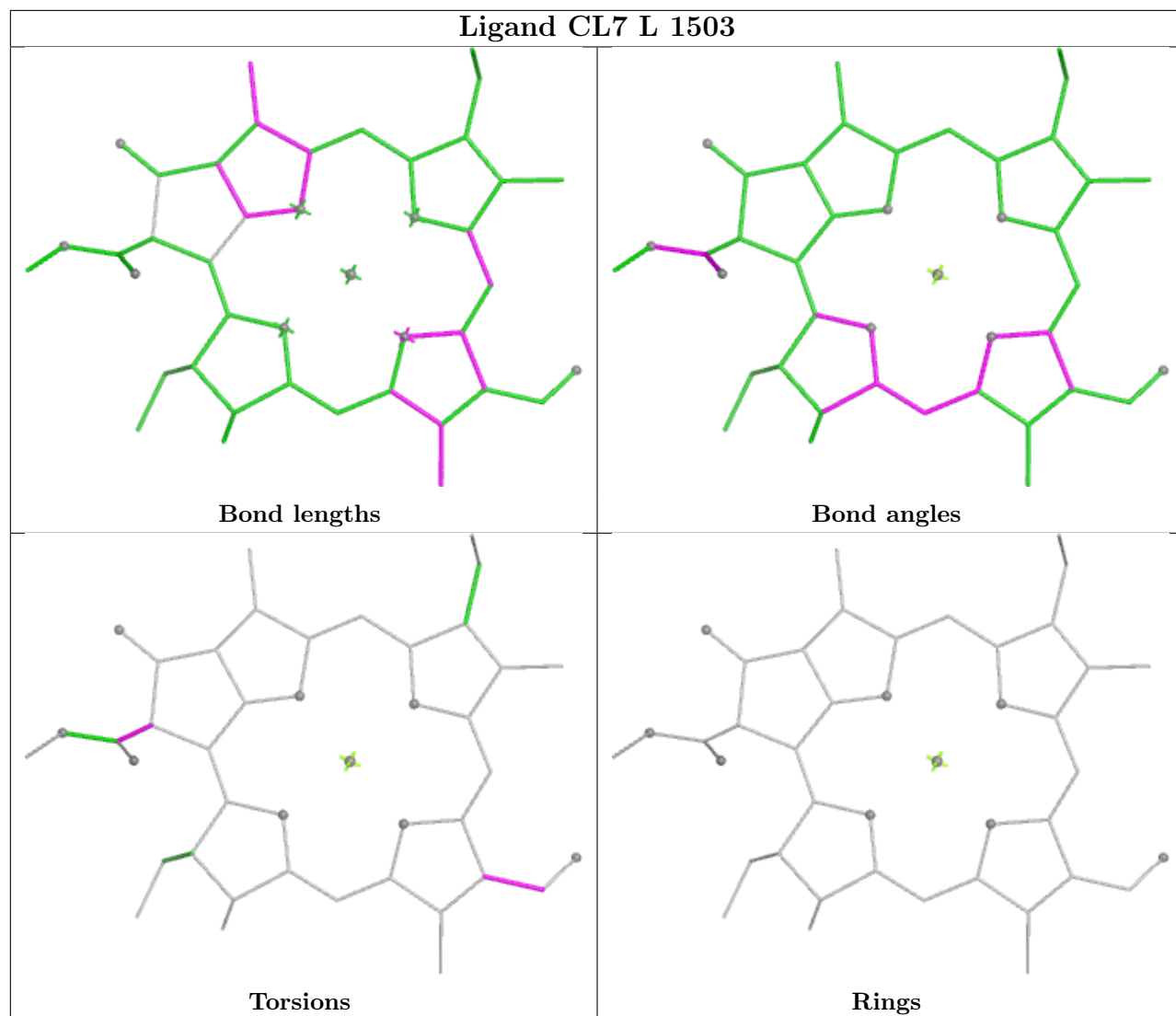


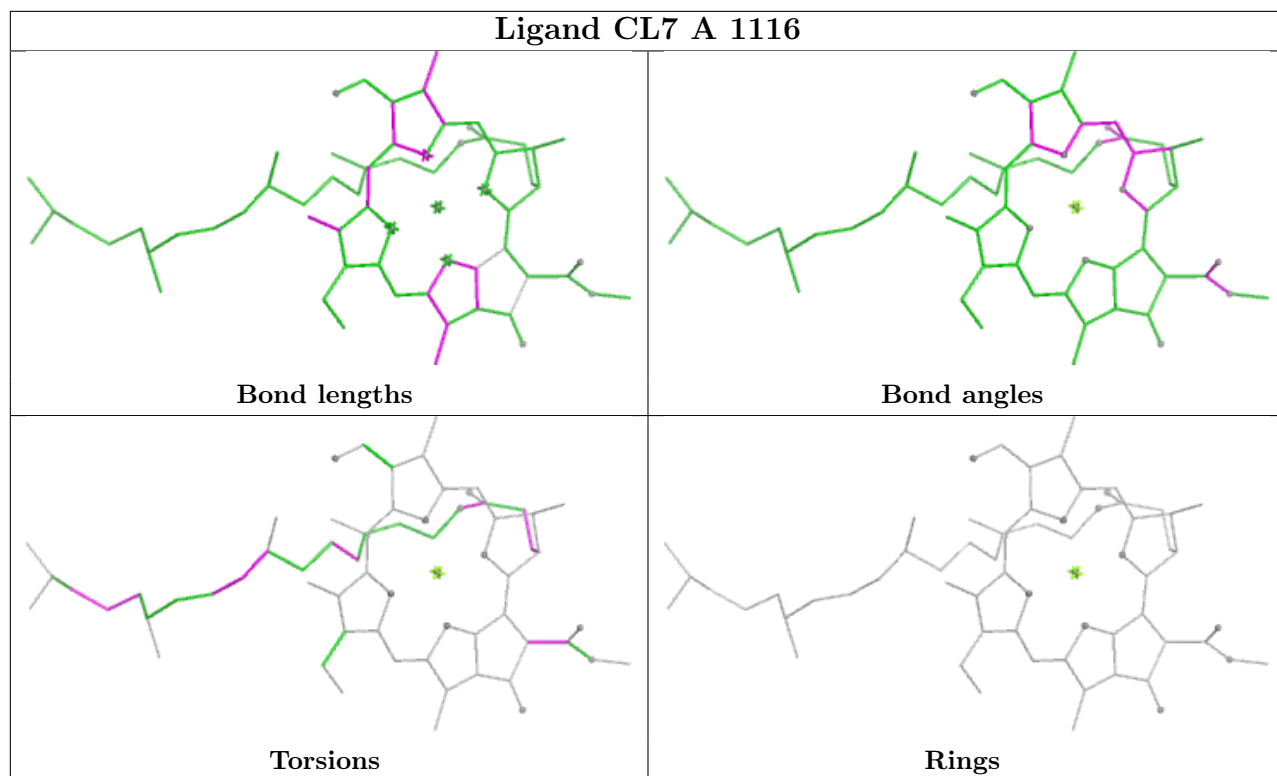


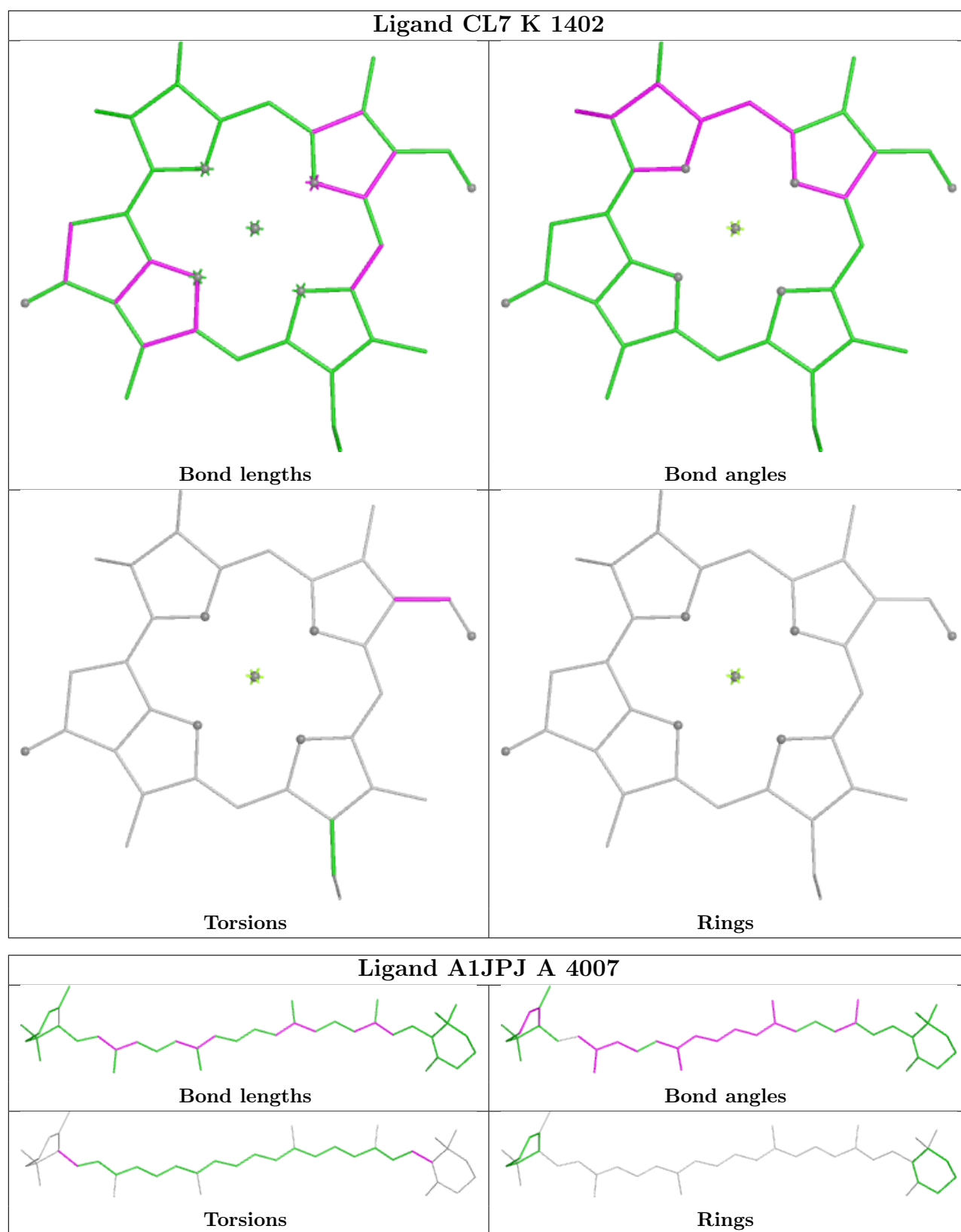


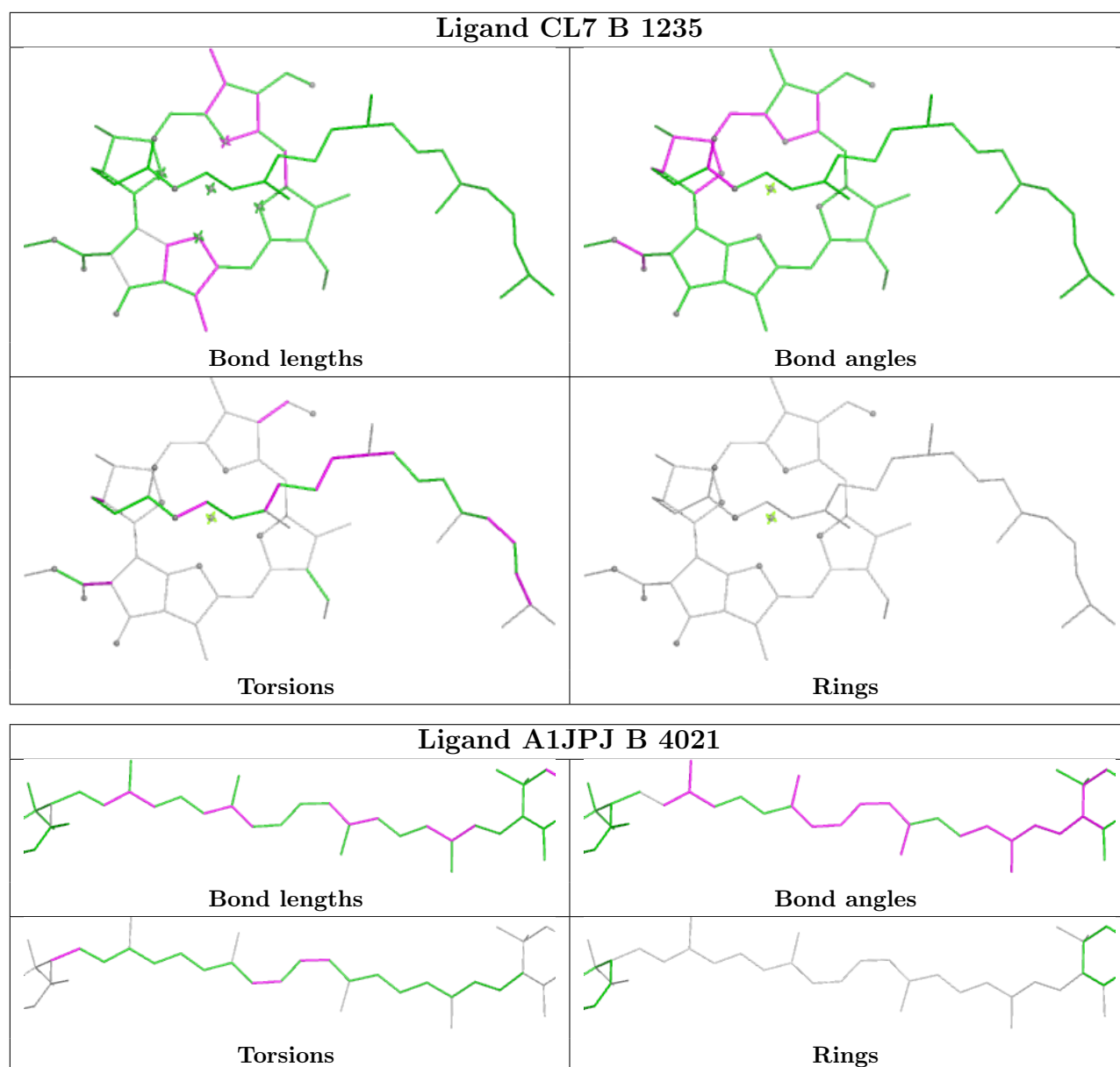


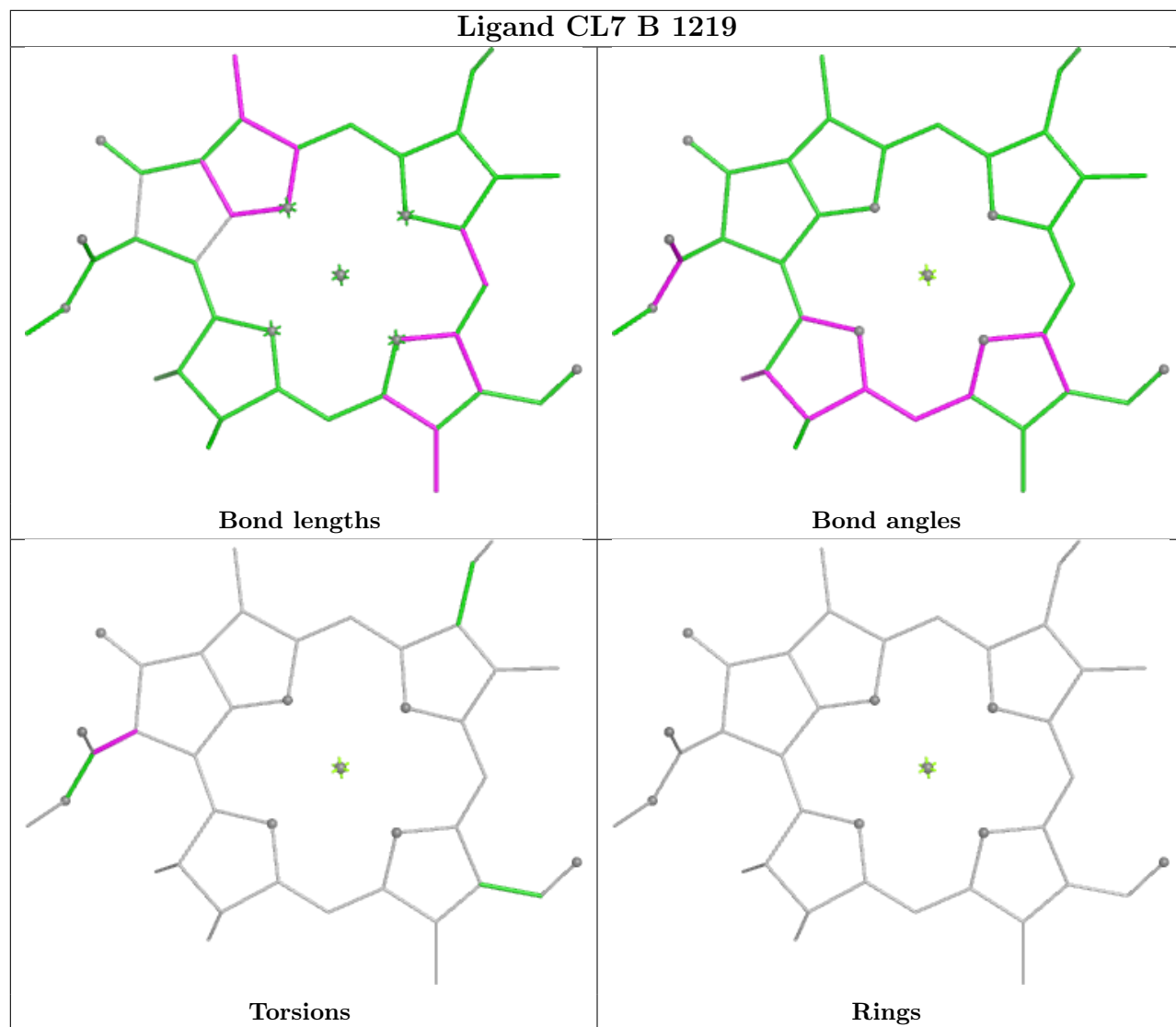


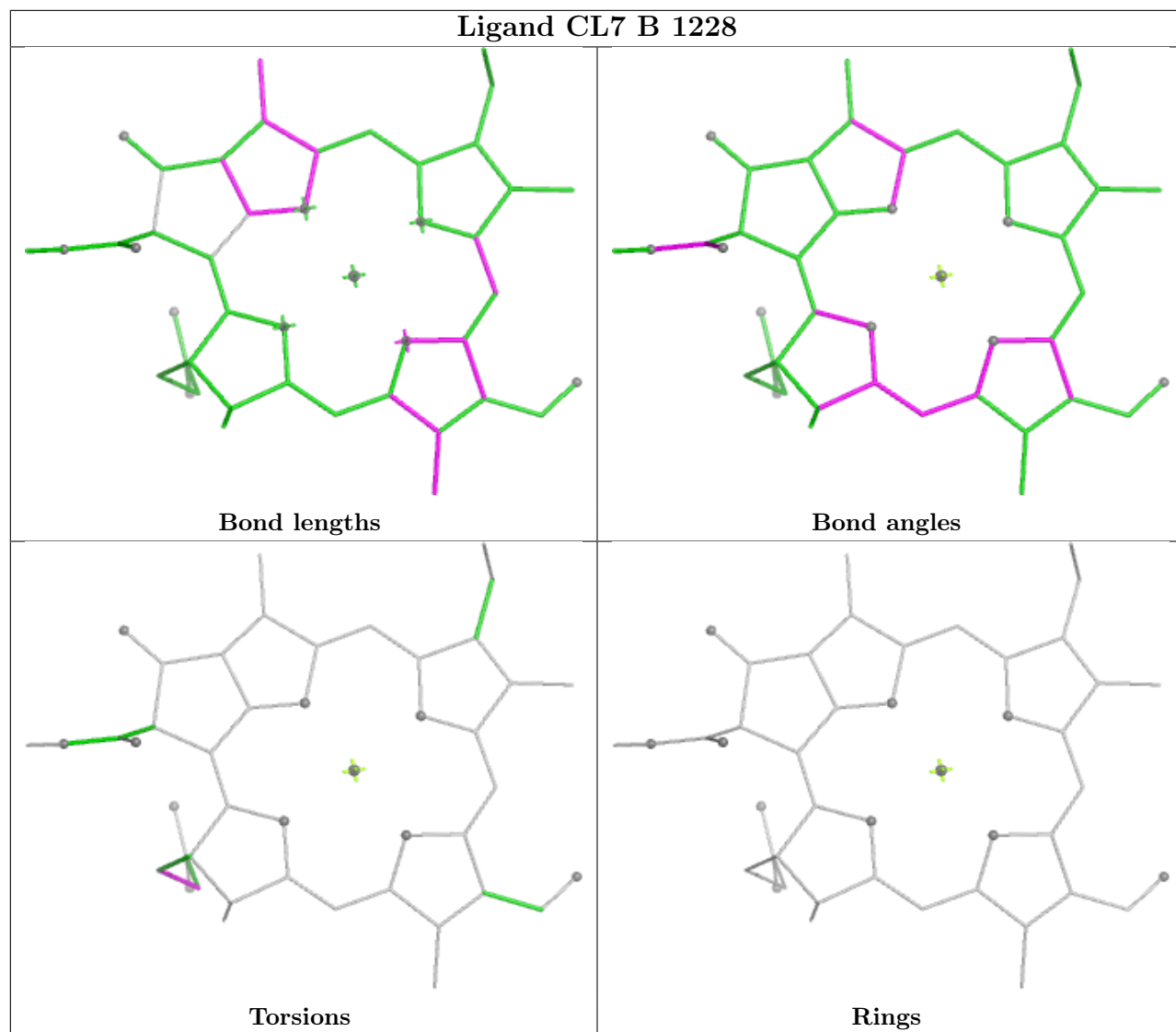


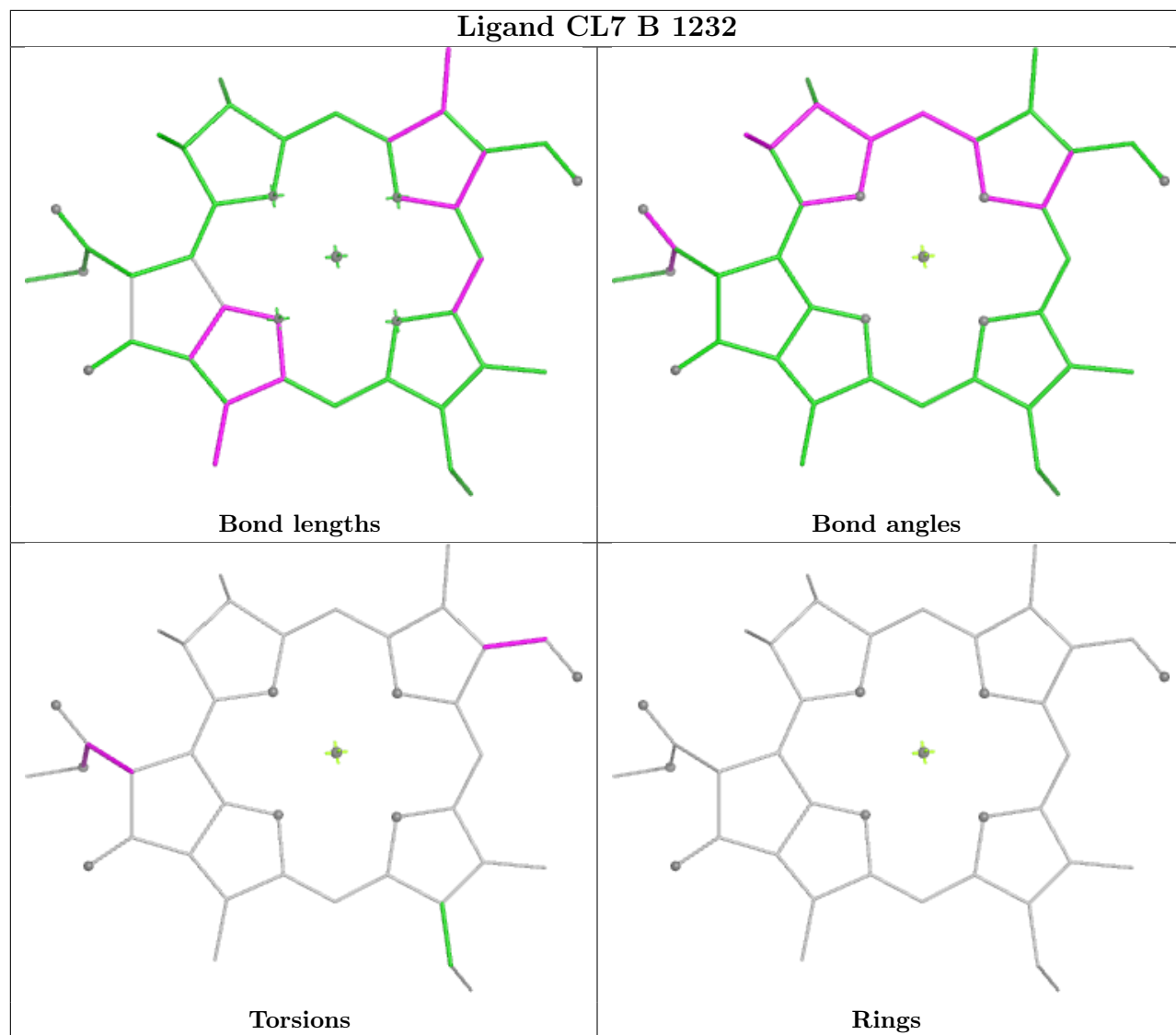


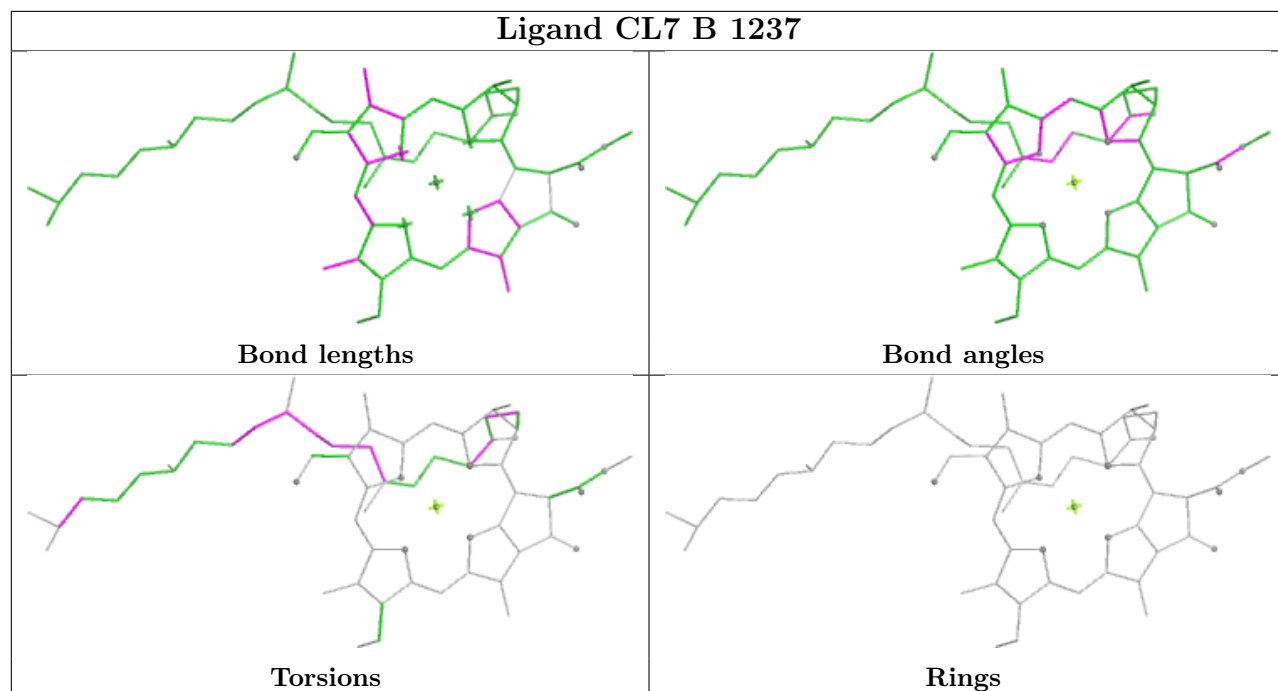


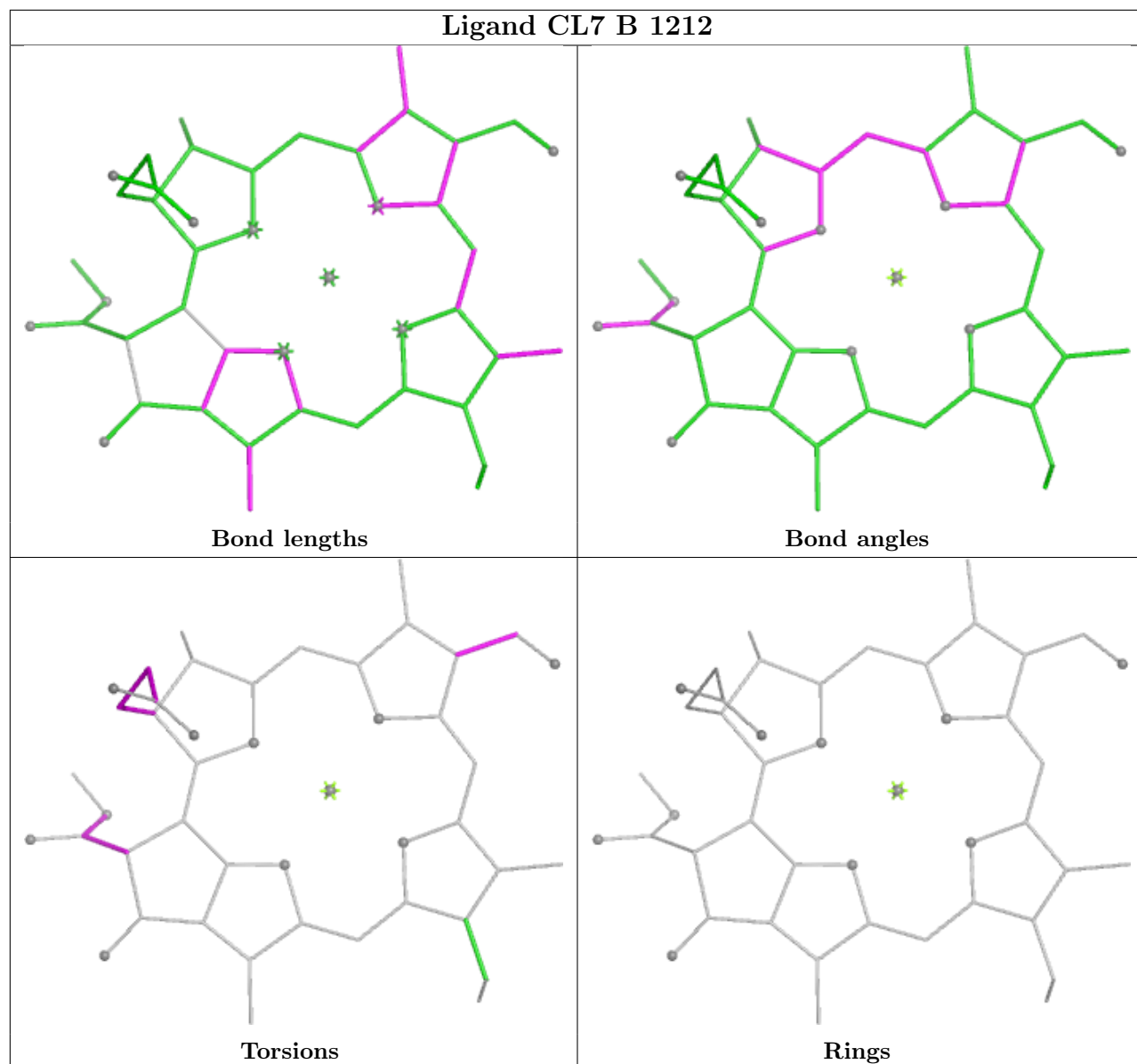


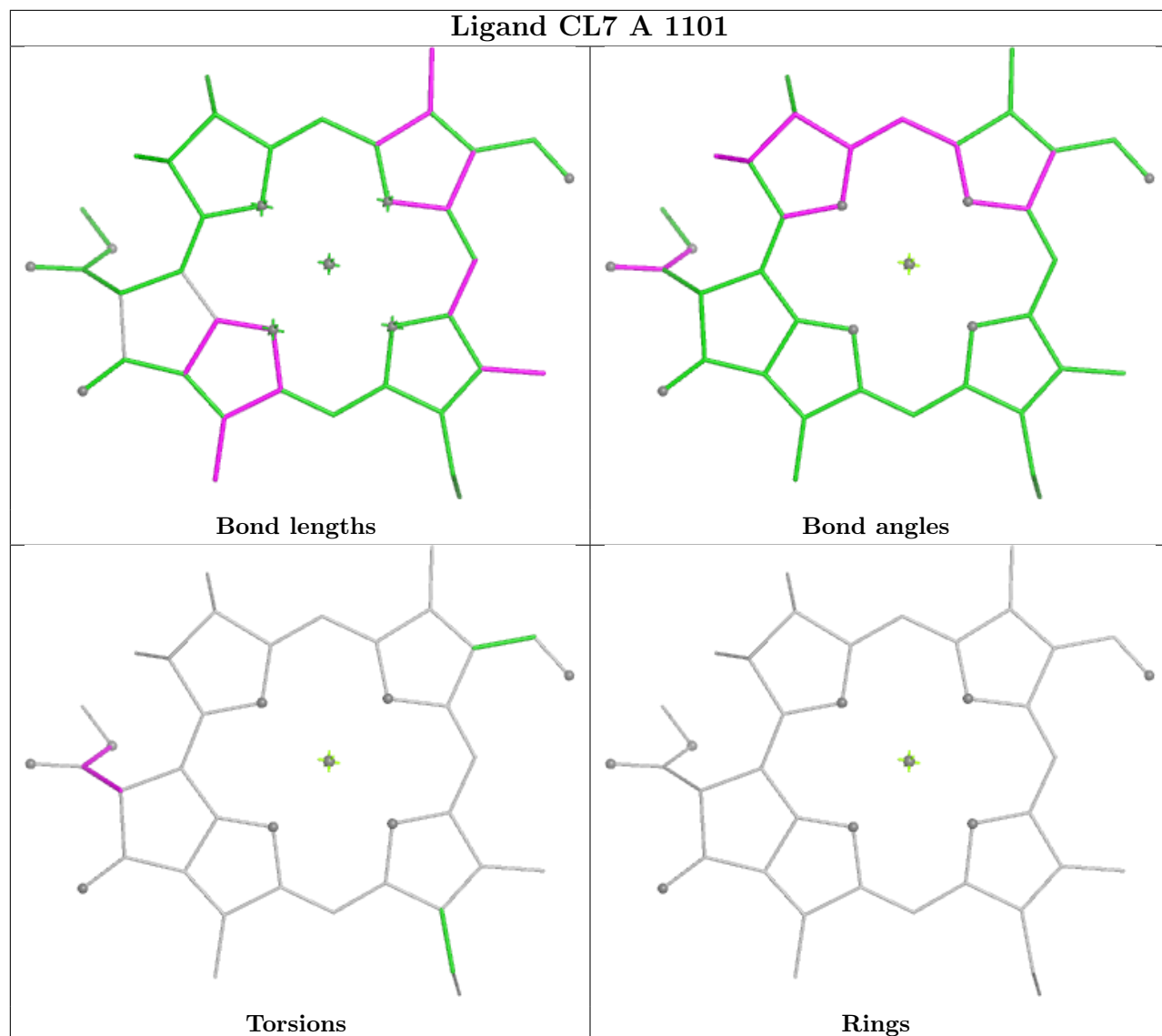


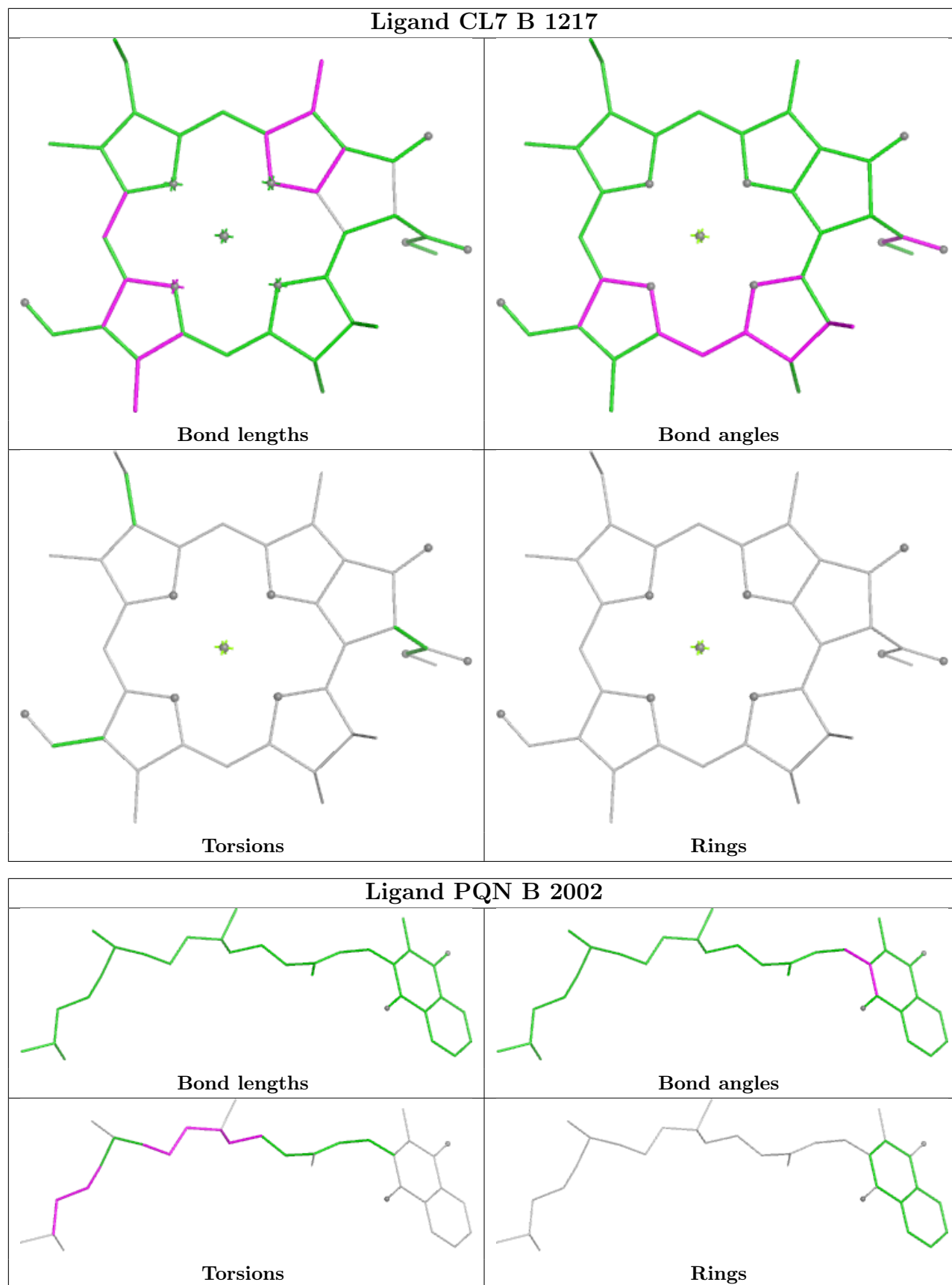


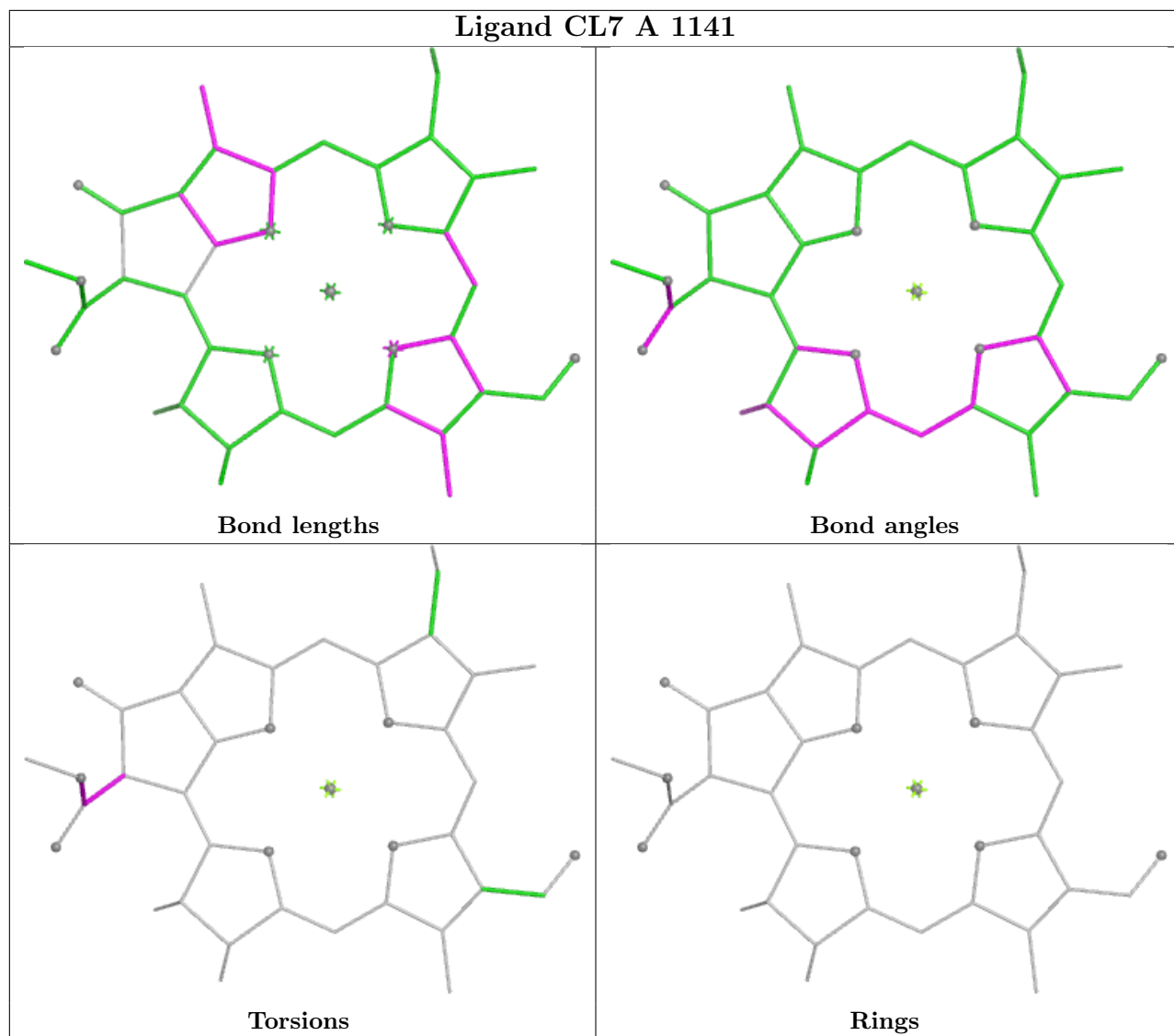


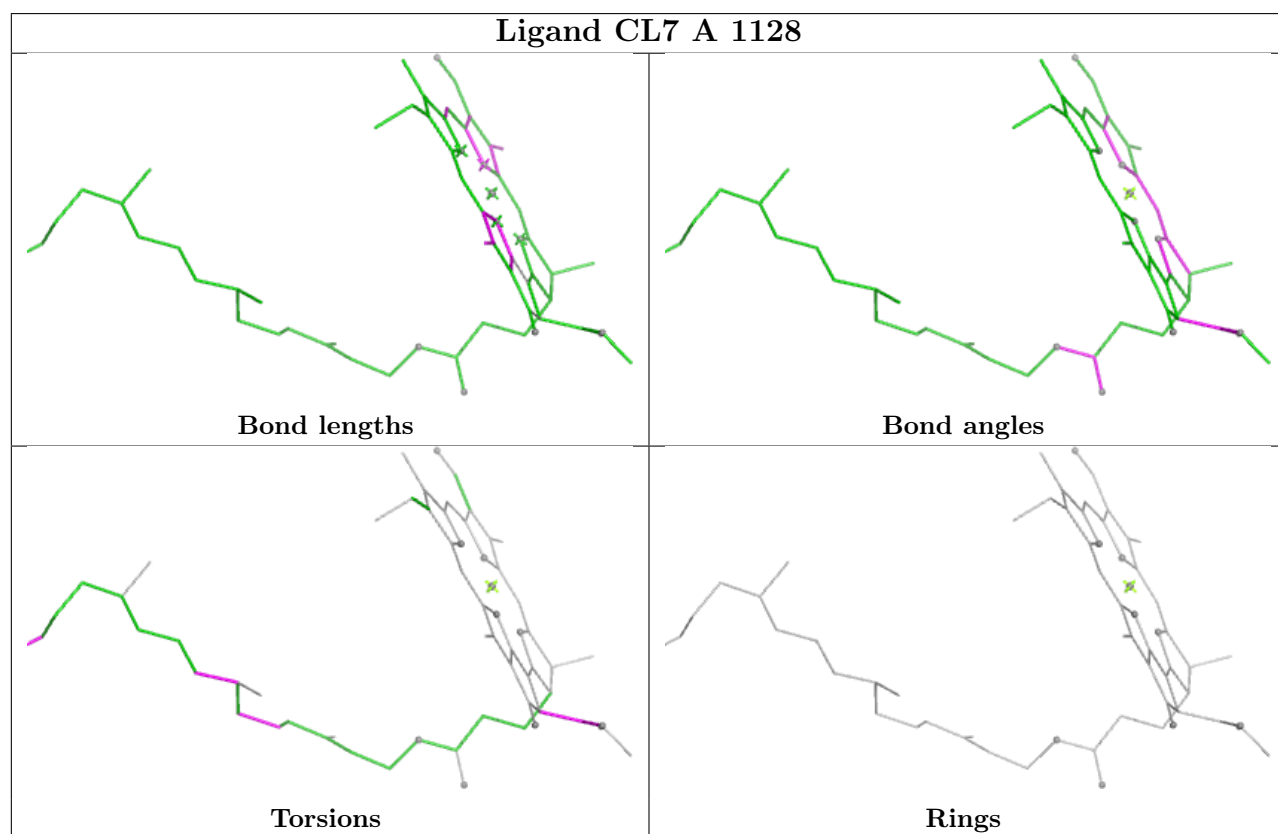
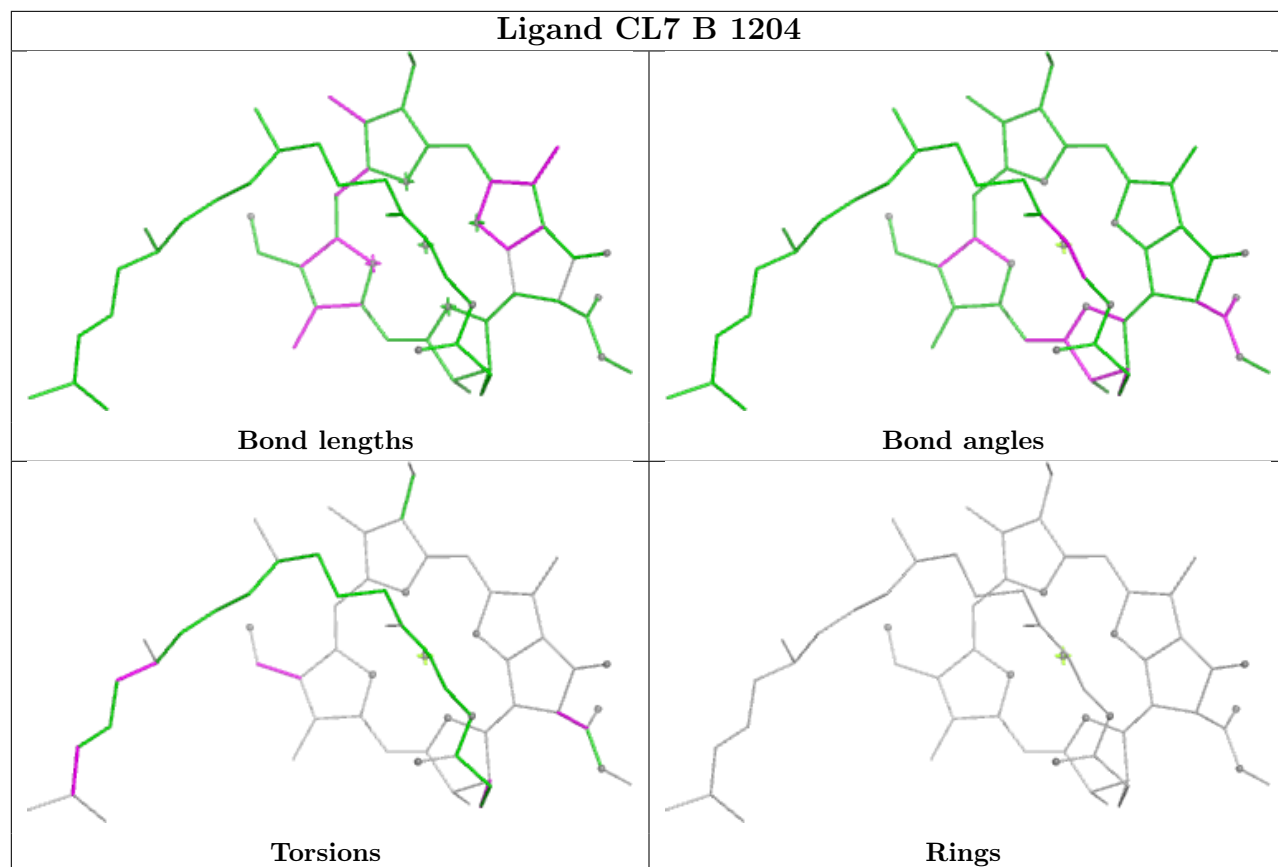


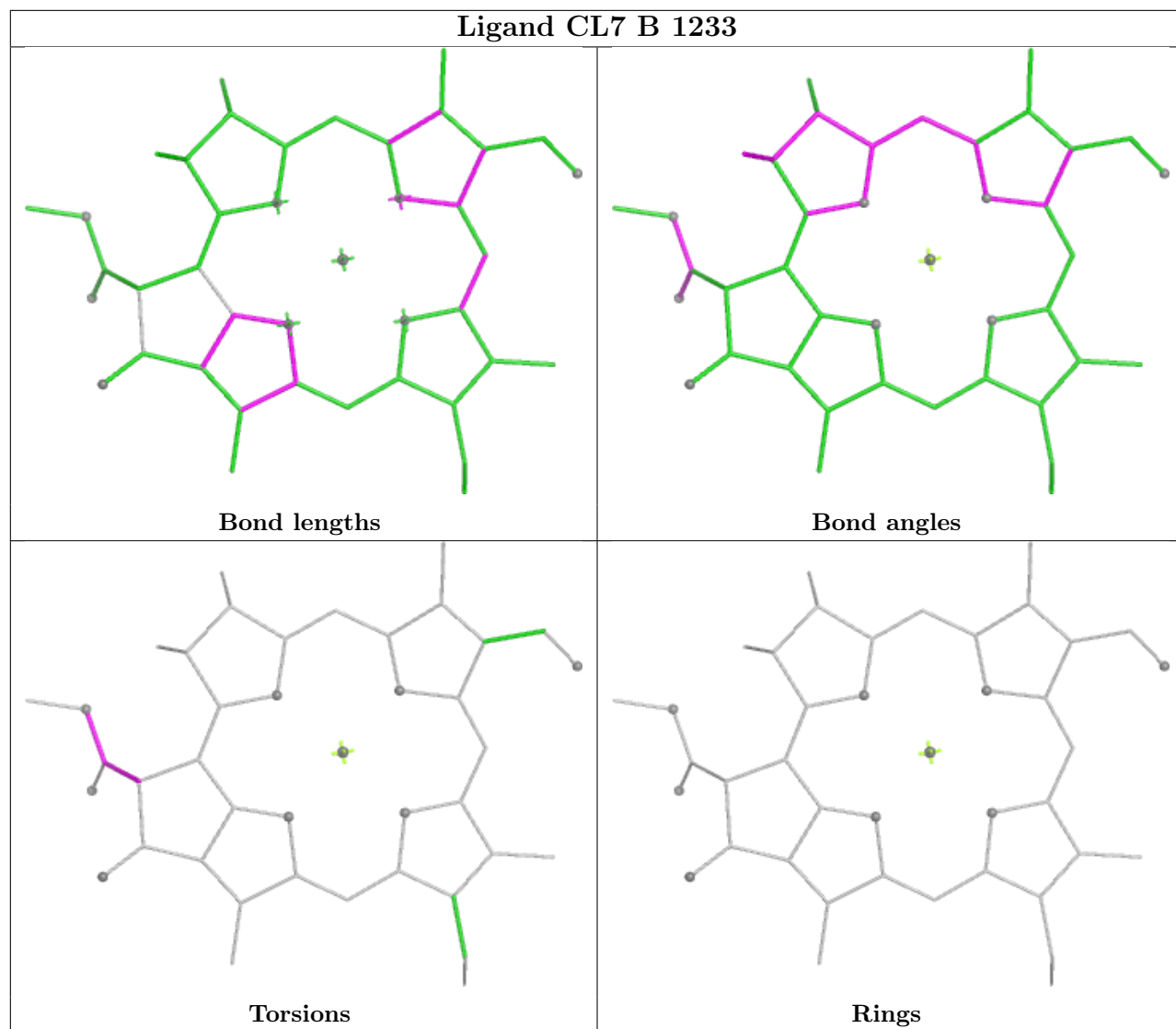


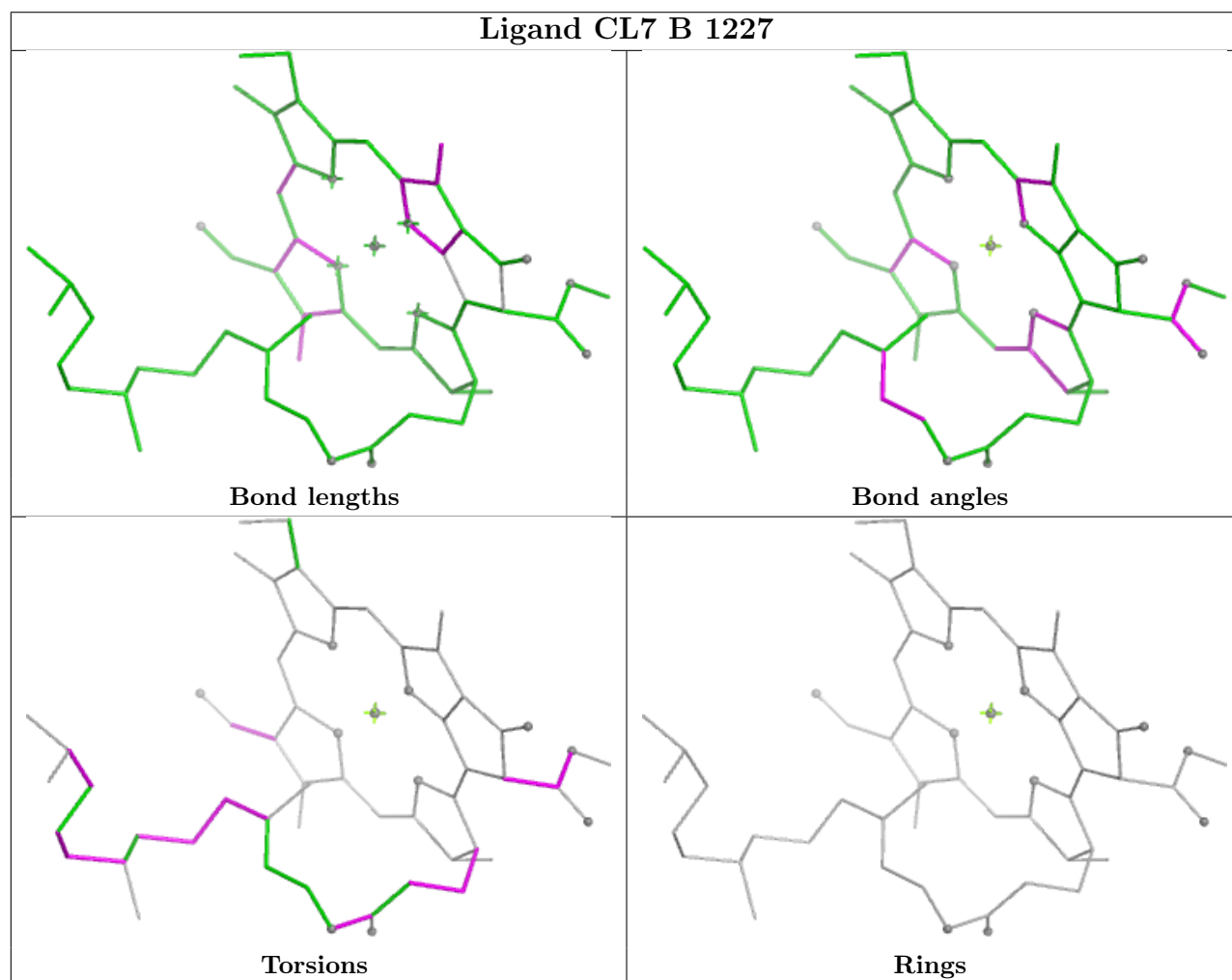
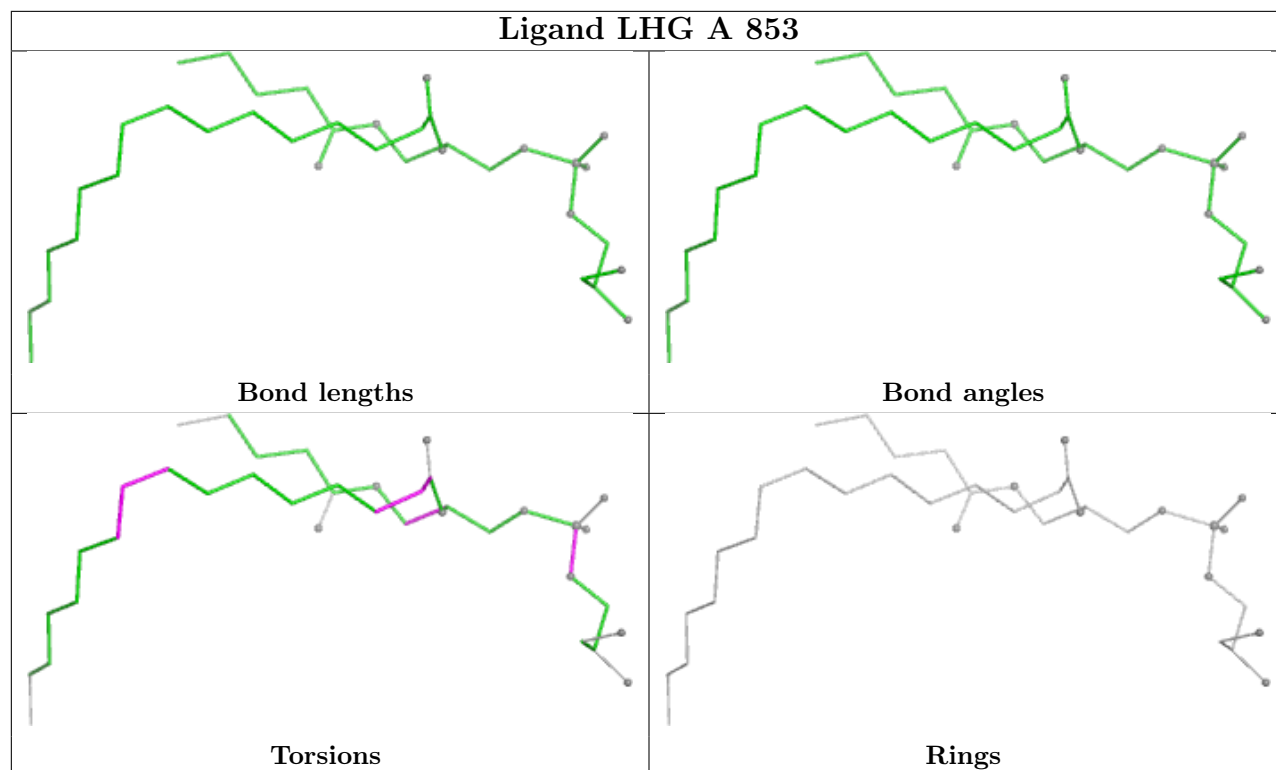


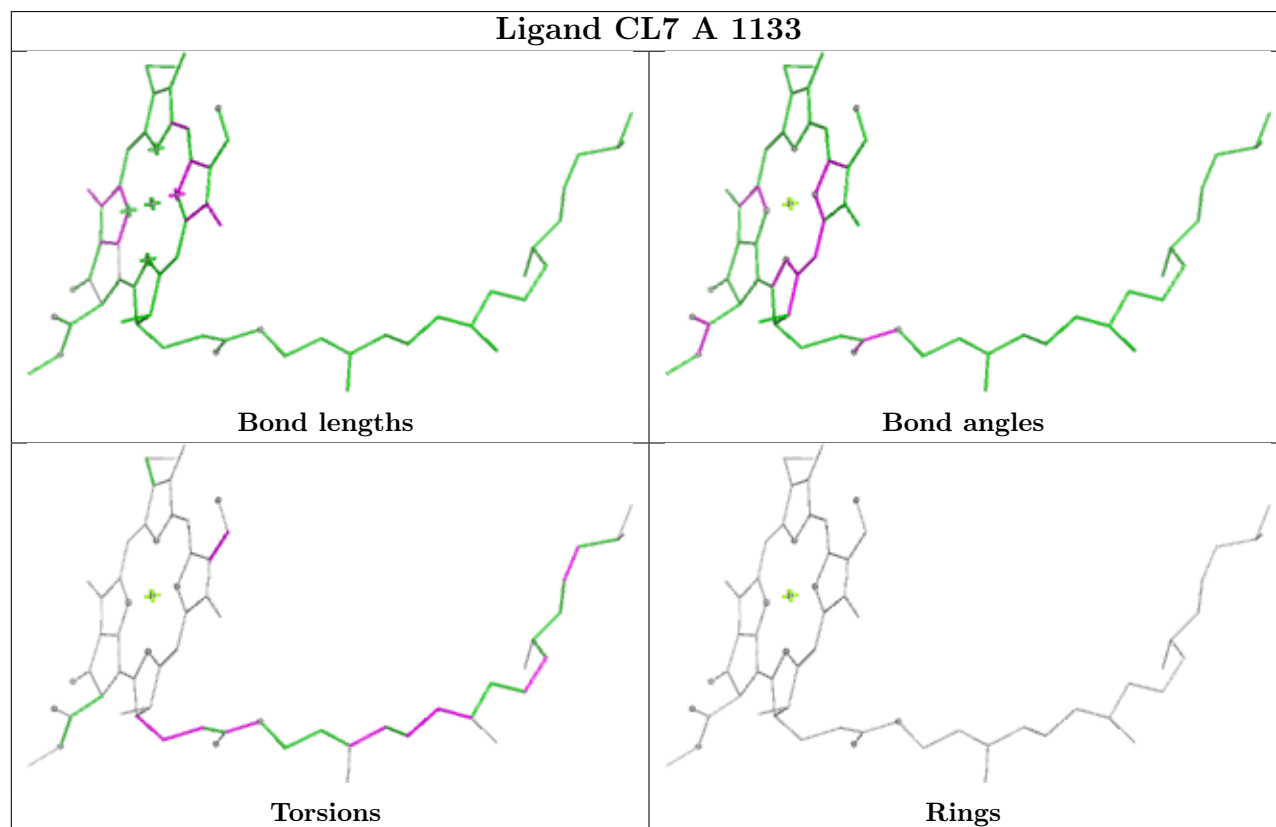
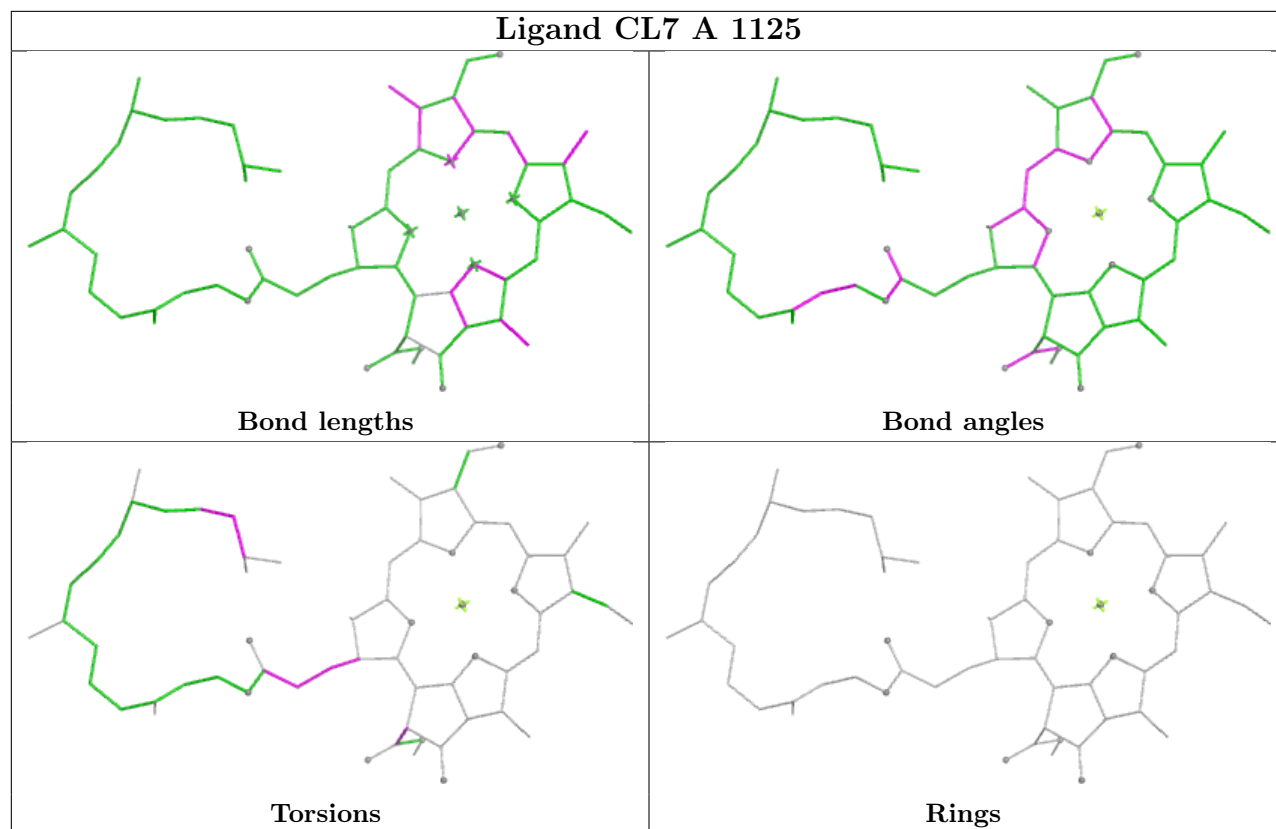


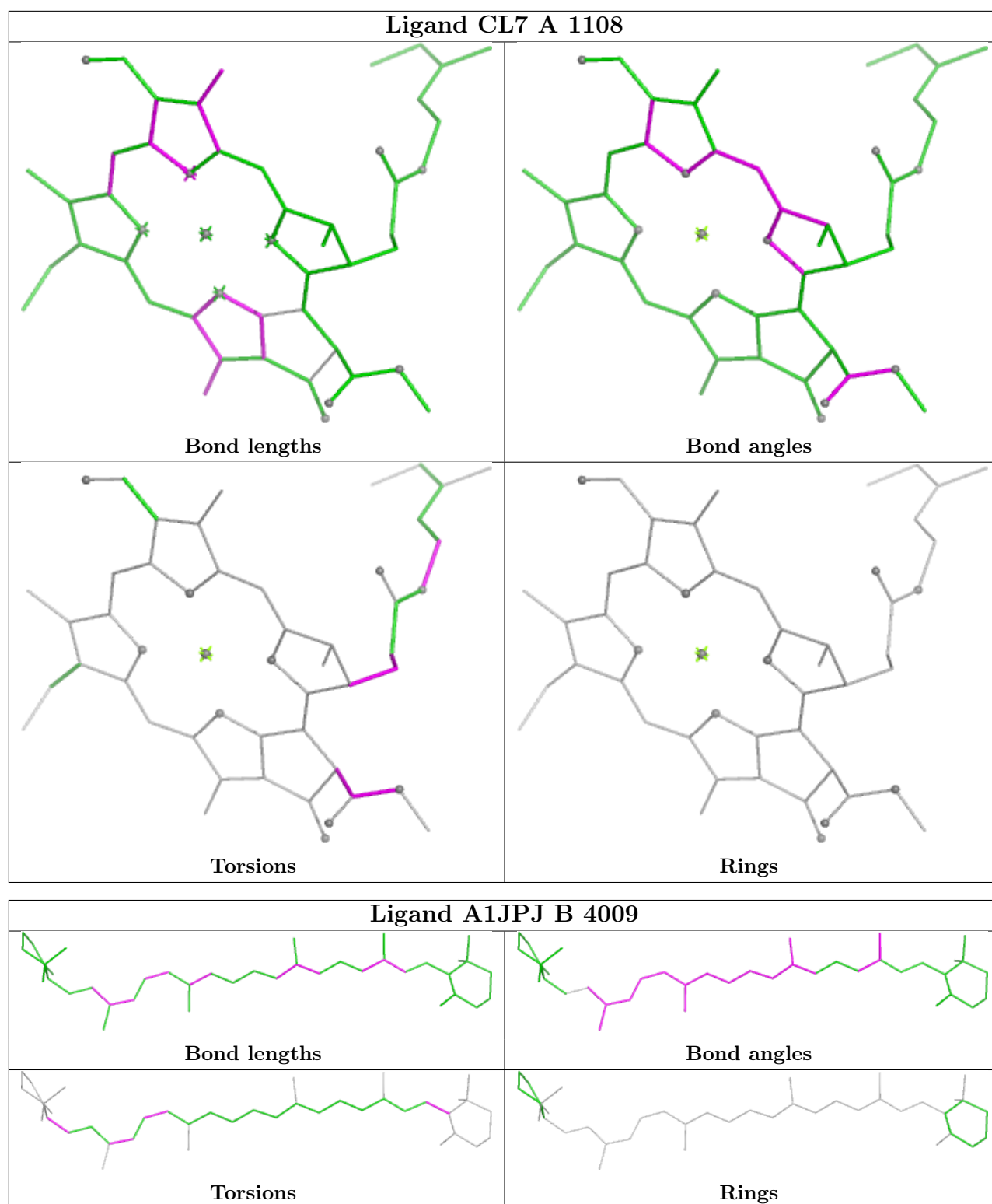


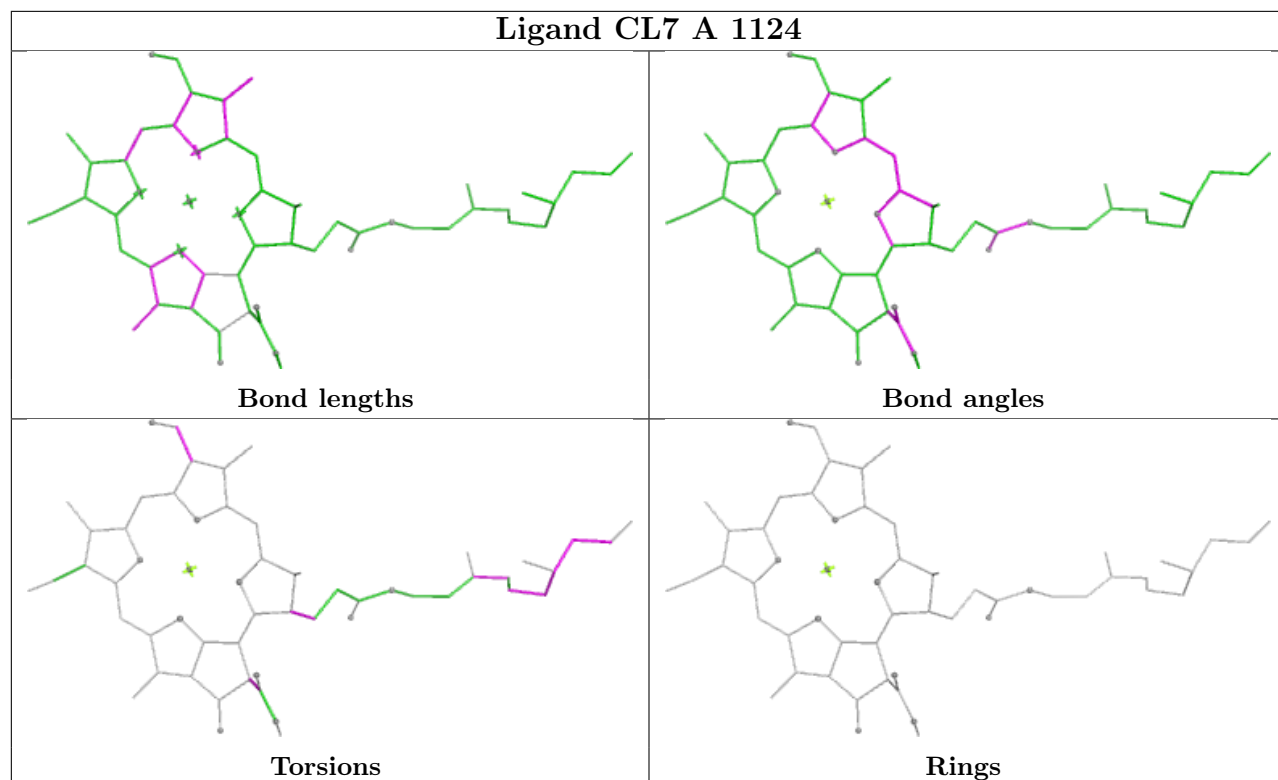


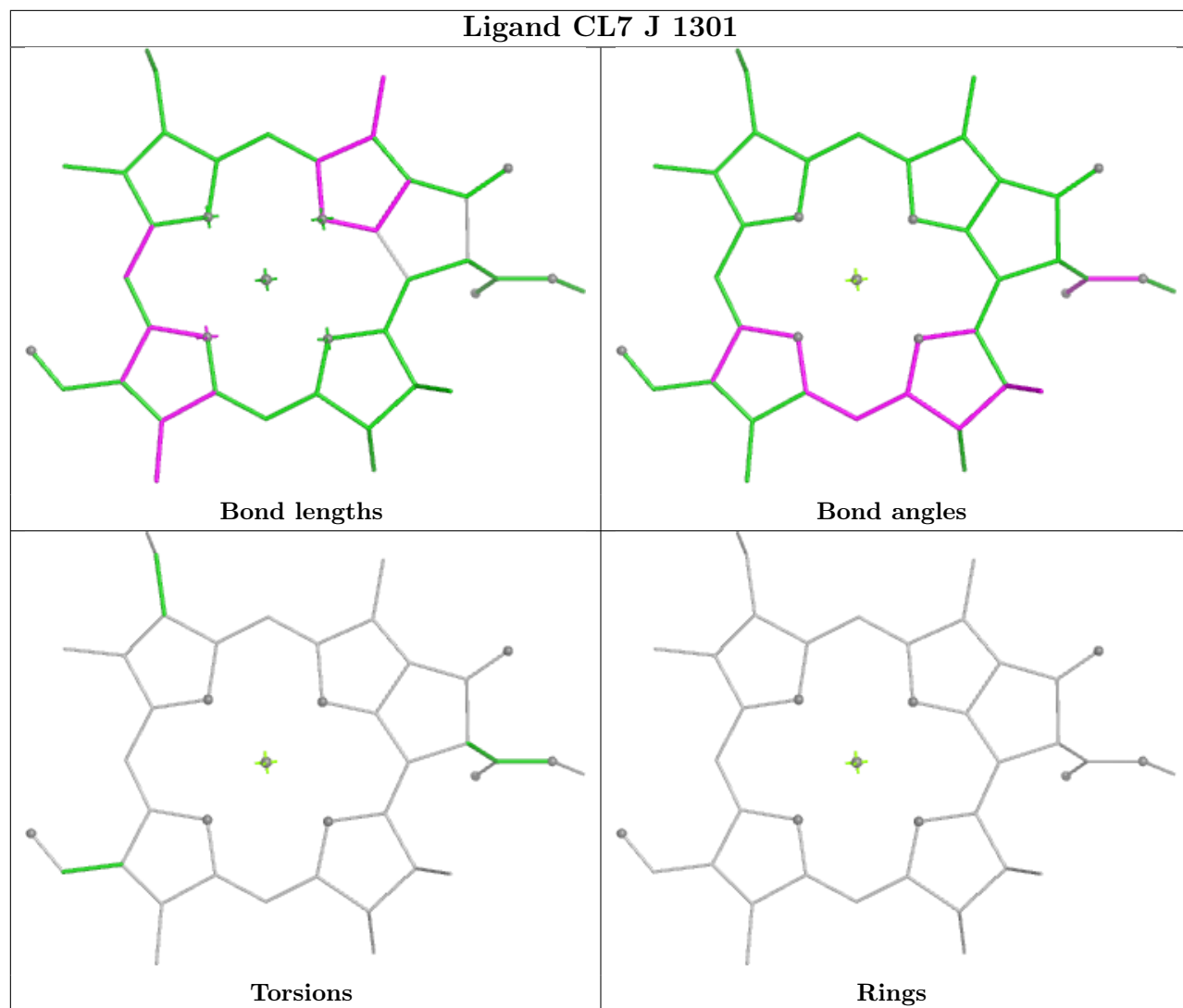


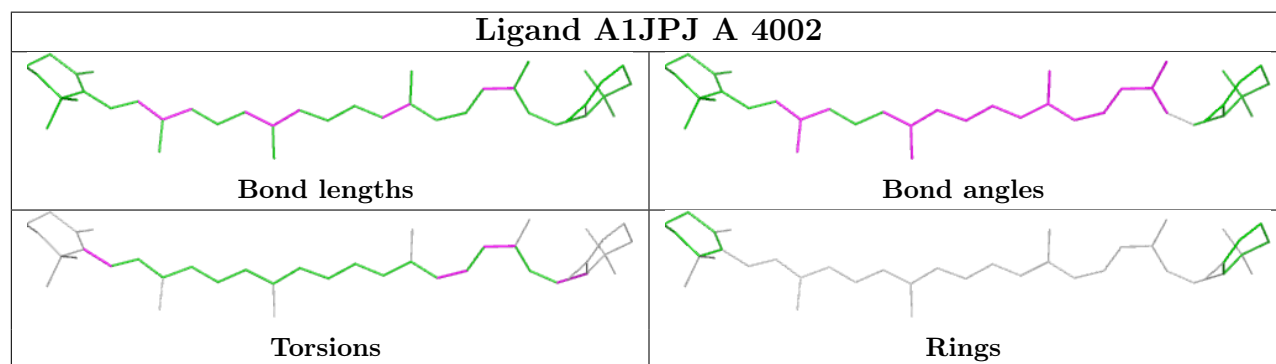
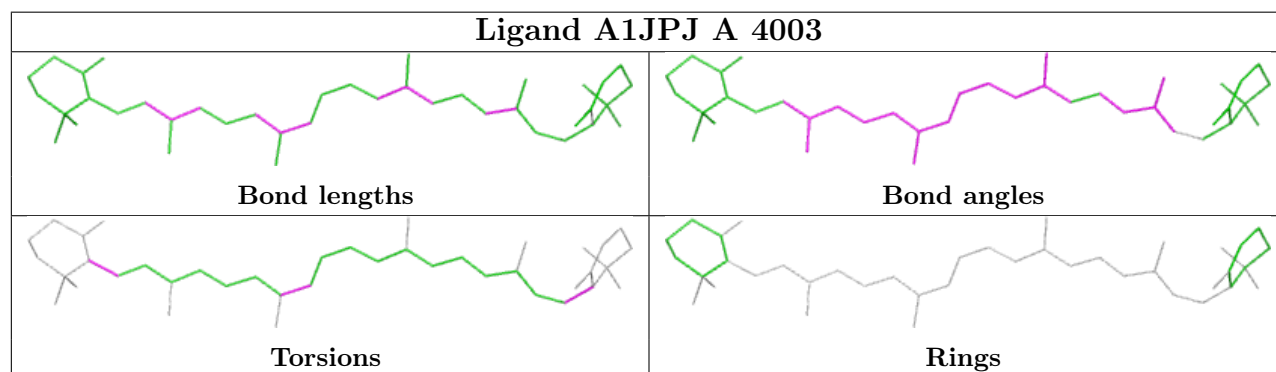
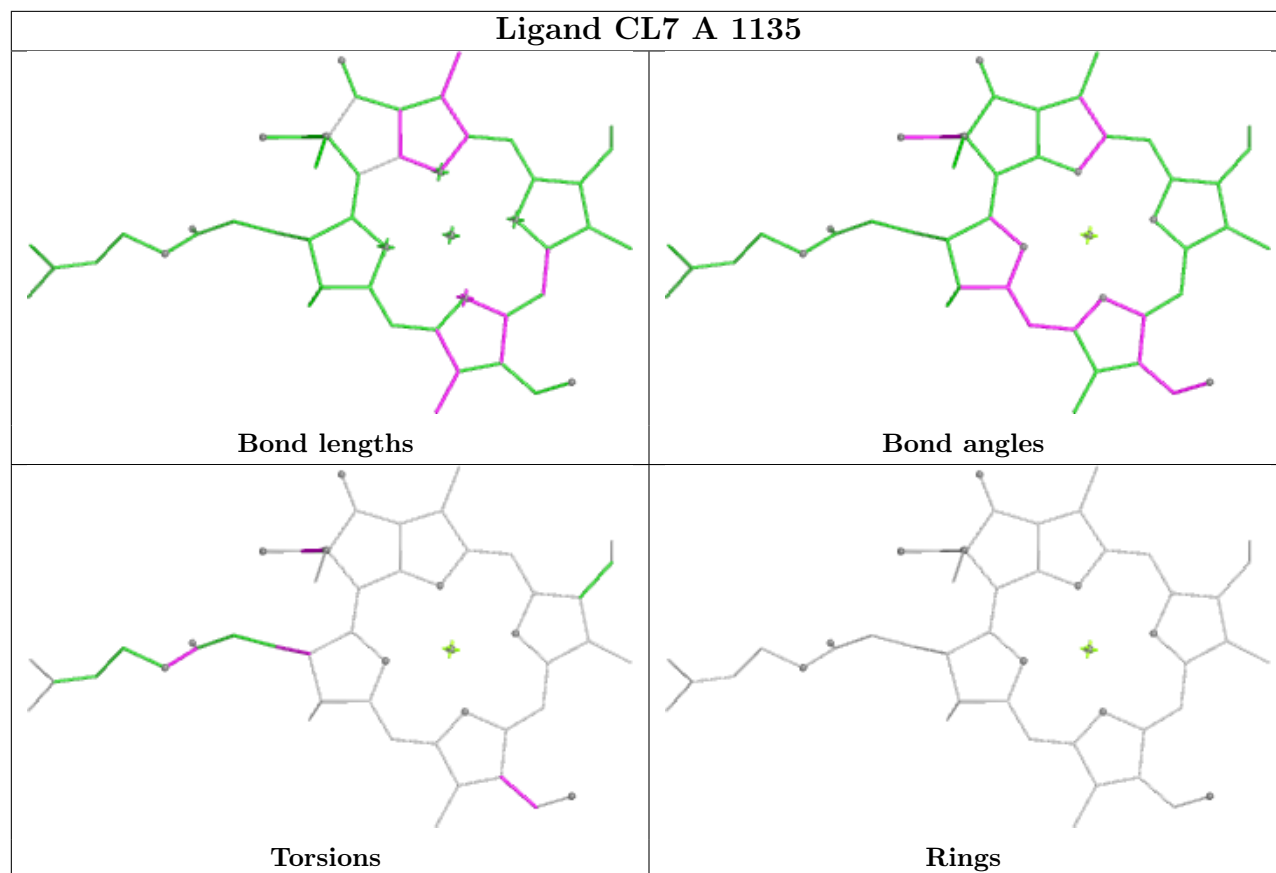


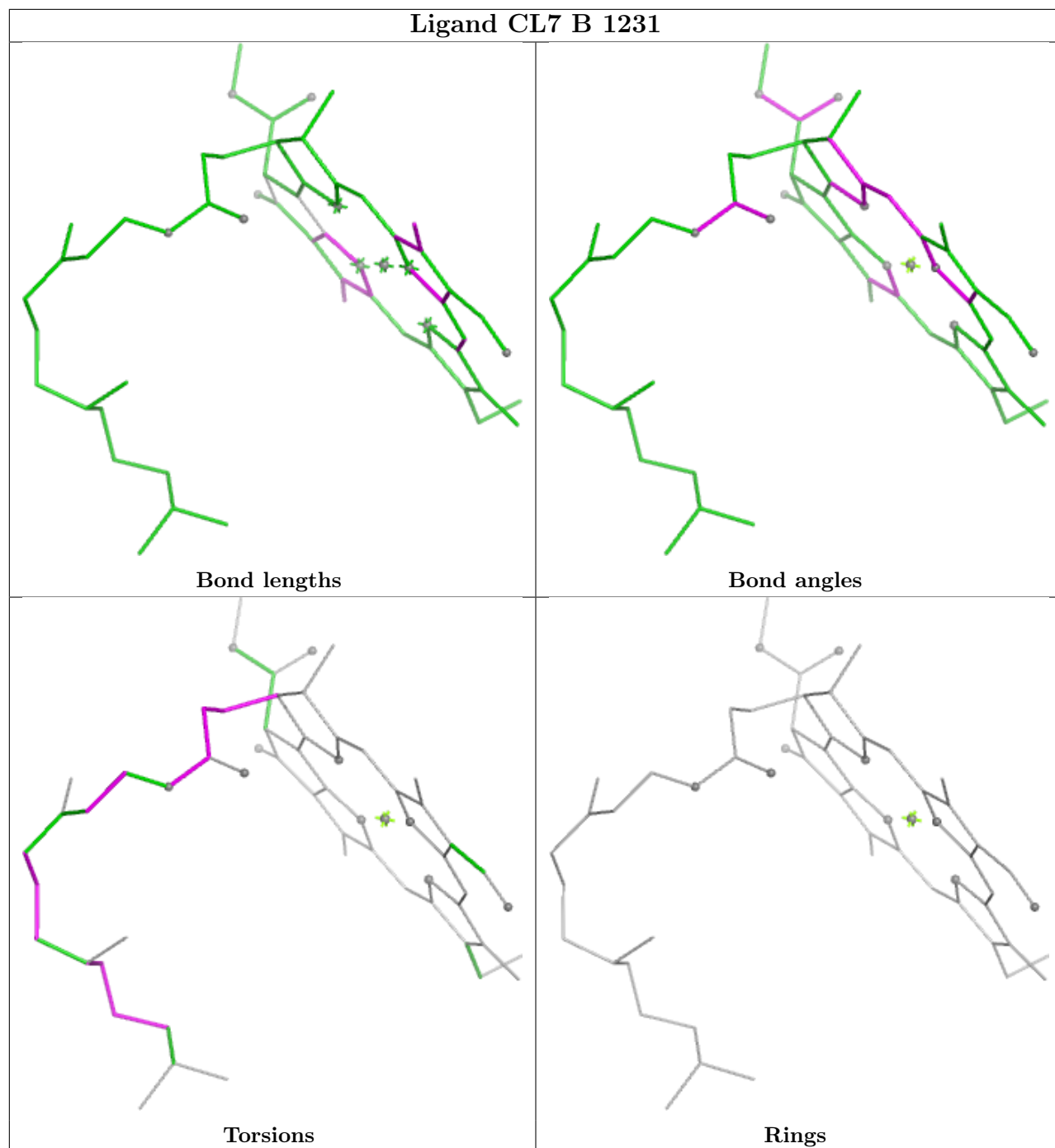


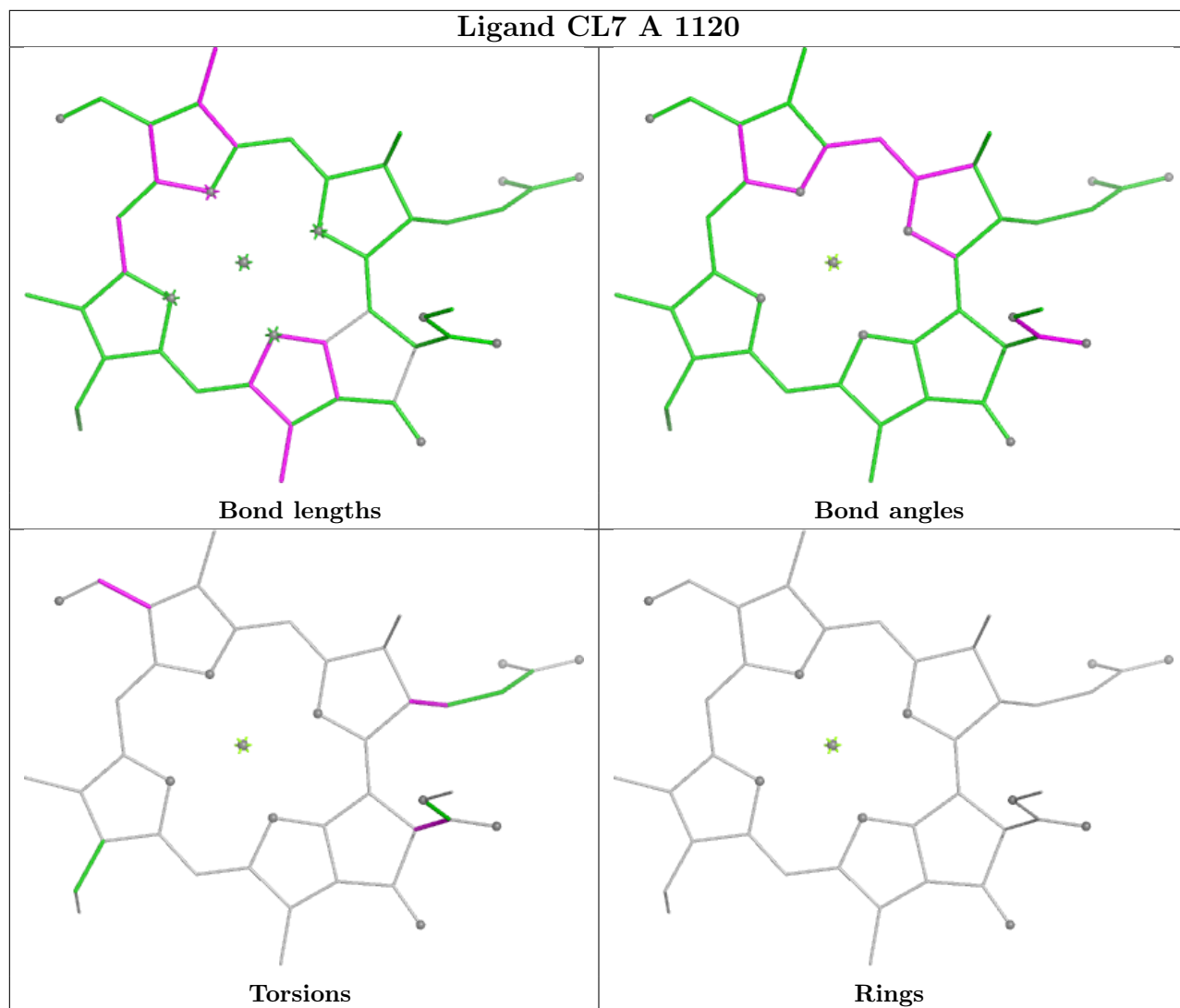


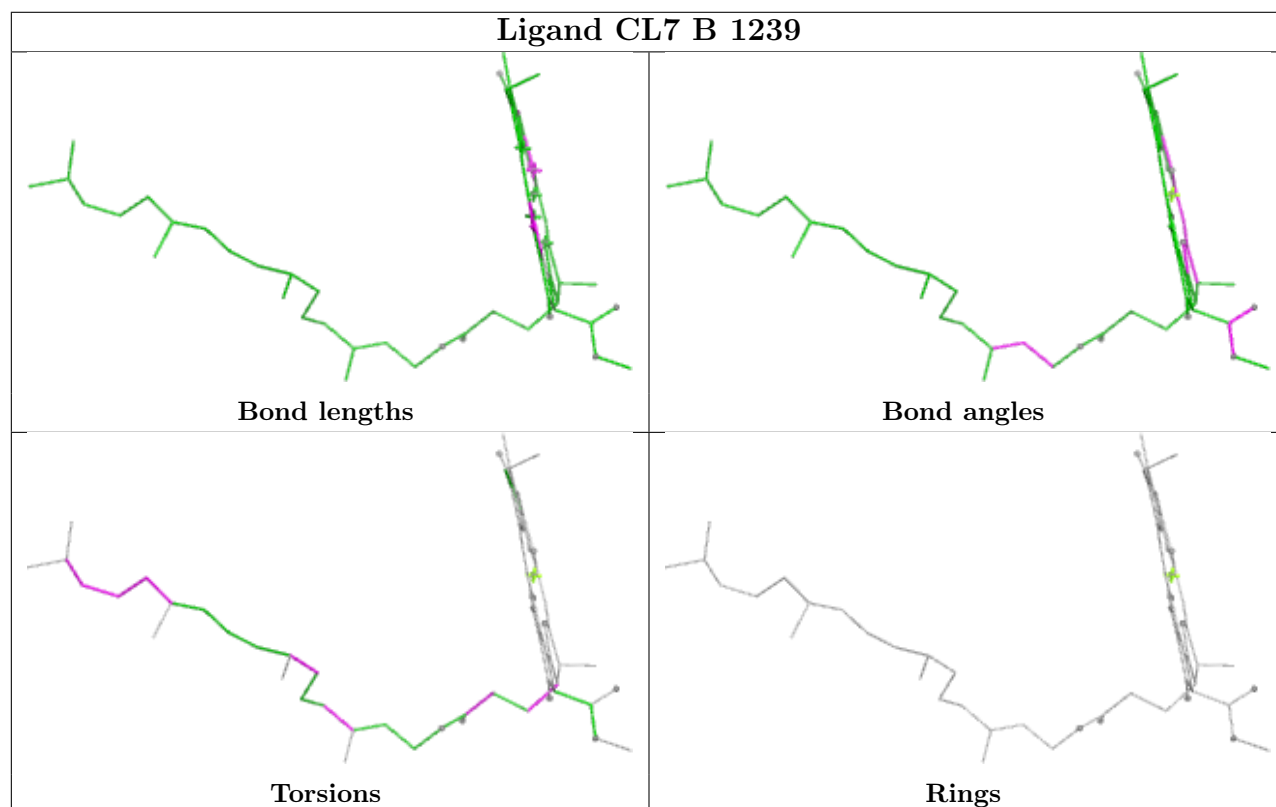
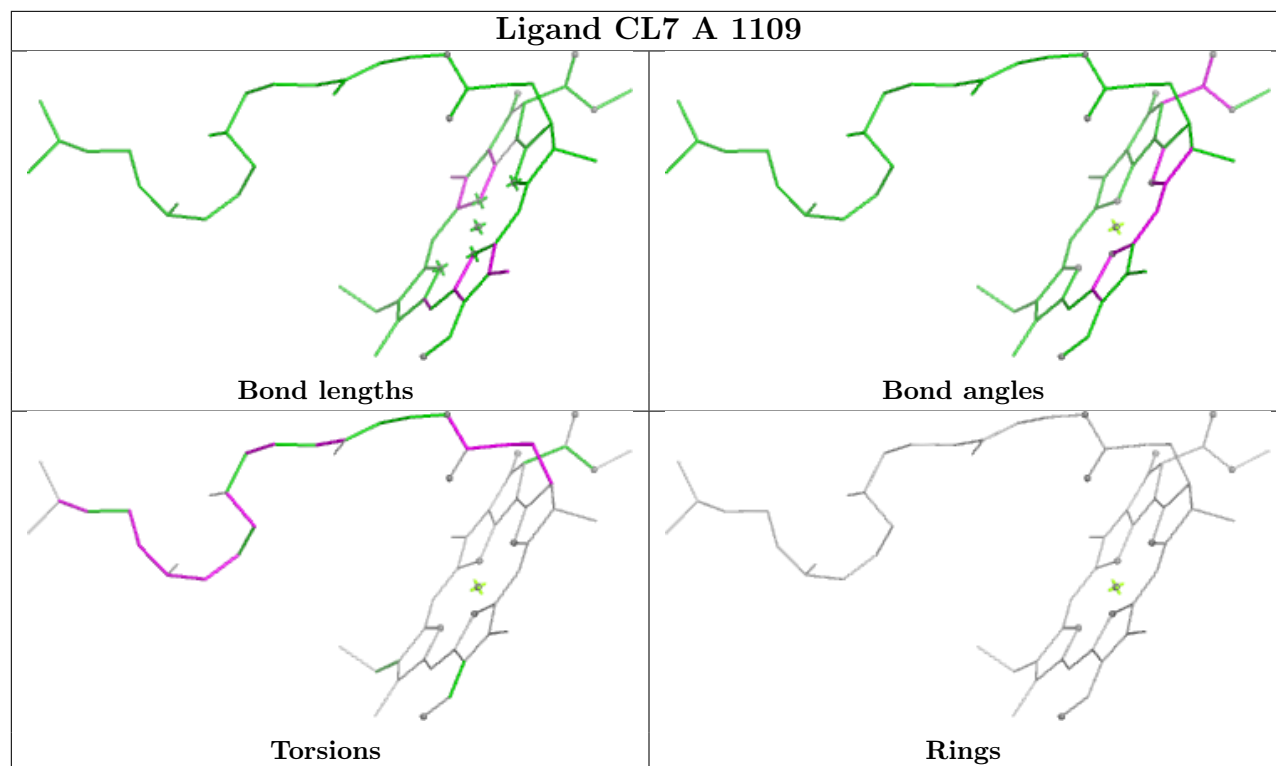


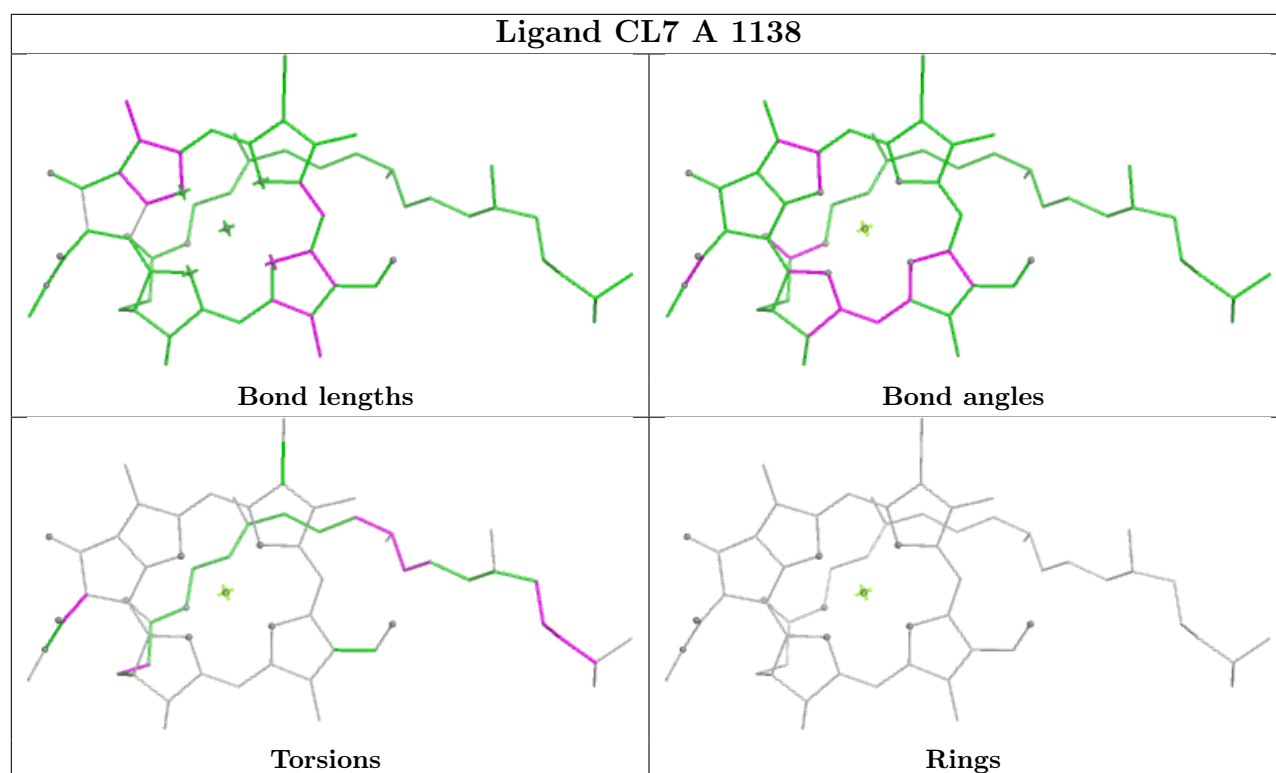












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

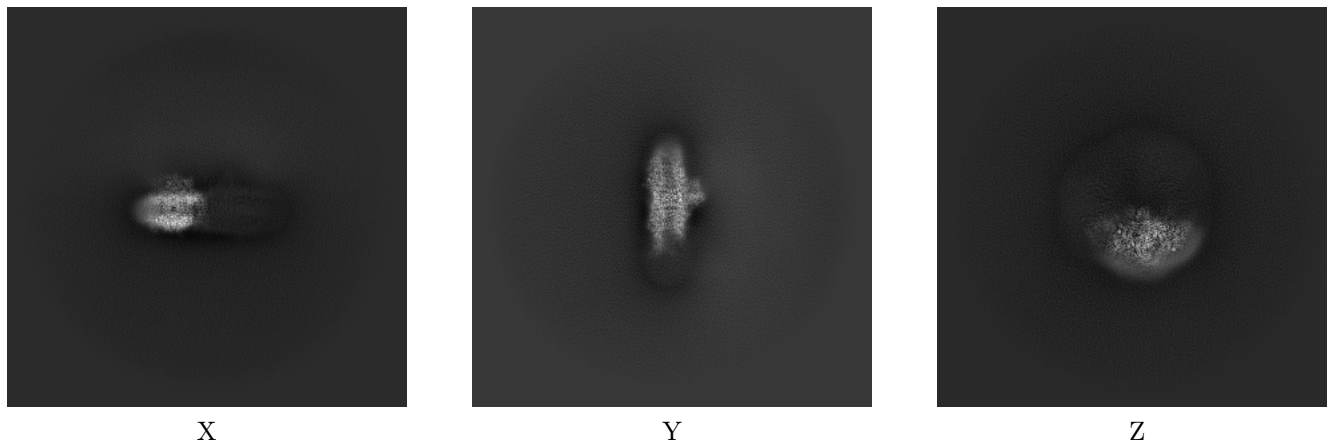
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54627. These allow visual inspection of the internal detail of the map and identification of artifacts.

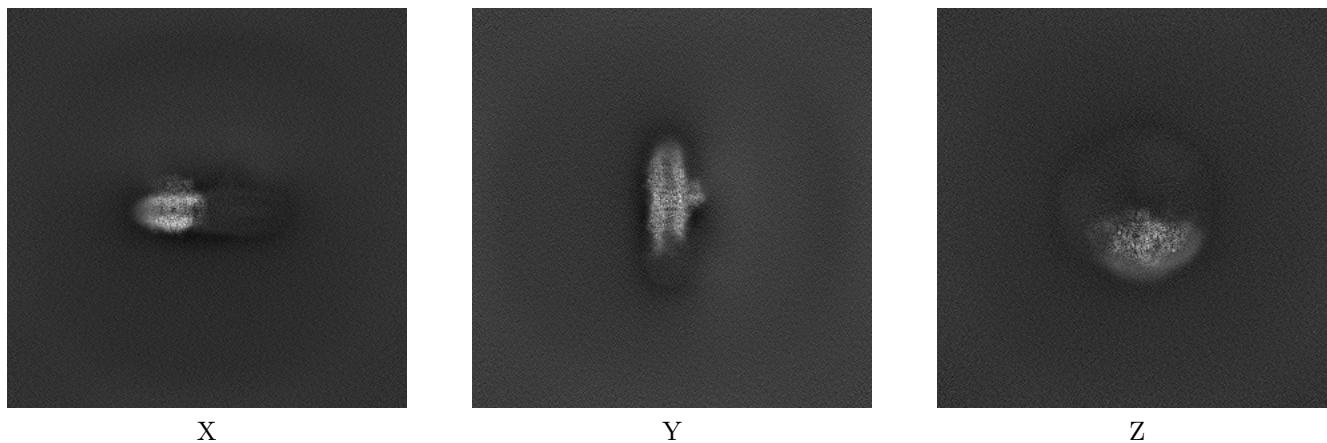
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



6.1.2 Raw map



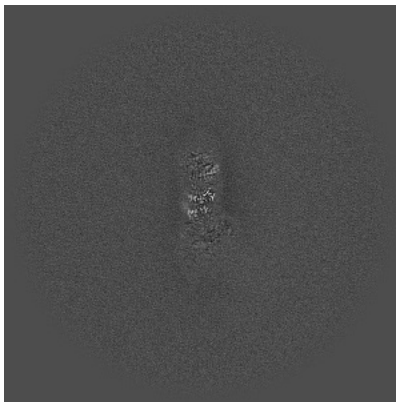
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

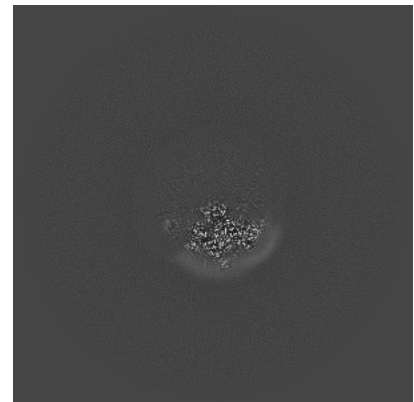
6.2.1 Primary map



X Index: 300



Y Index: 300



Z Index: 300

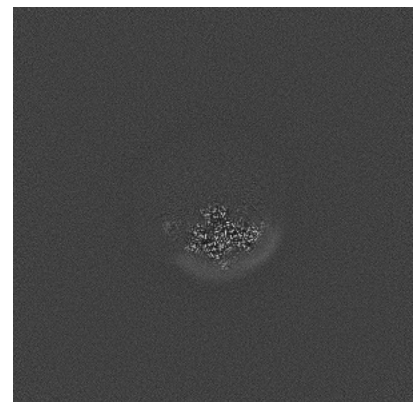
6.2.2 Raw map



X Index: 300



Y Index: 300

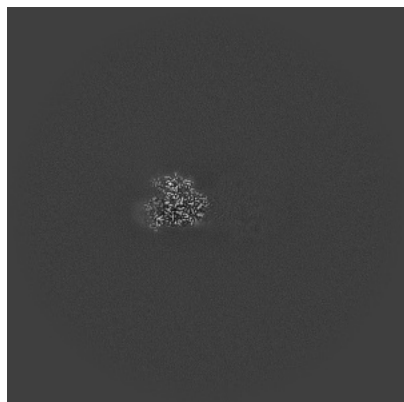


Z Index: 300

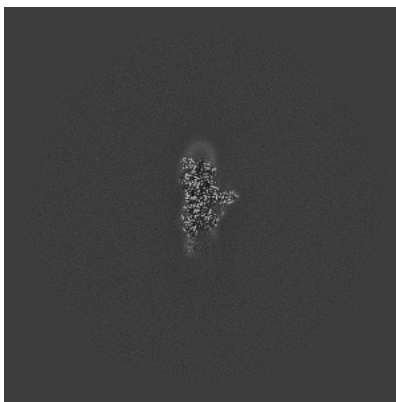
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

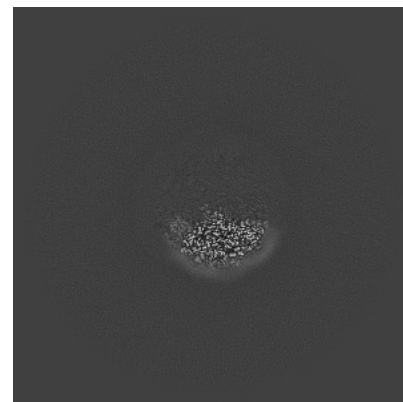
6.3.1 Primary map



X Index: 316

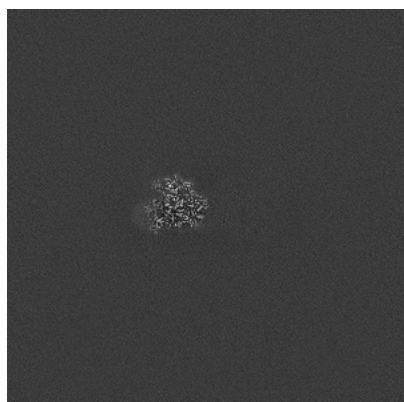


Y Index: 252

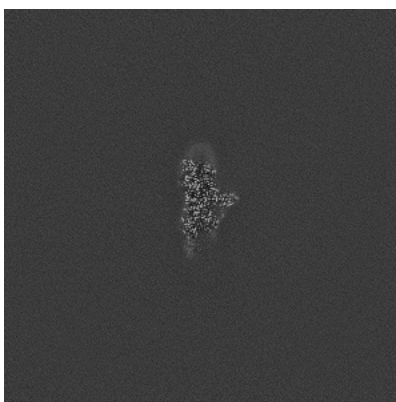


Z Index: 284

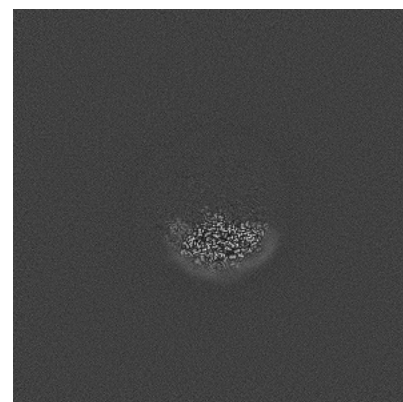
6.3.2 Raw map



X Index: 316



Y Index: 252

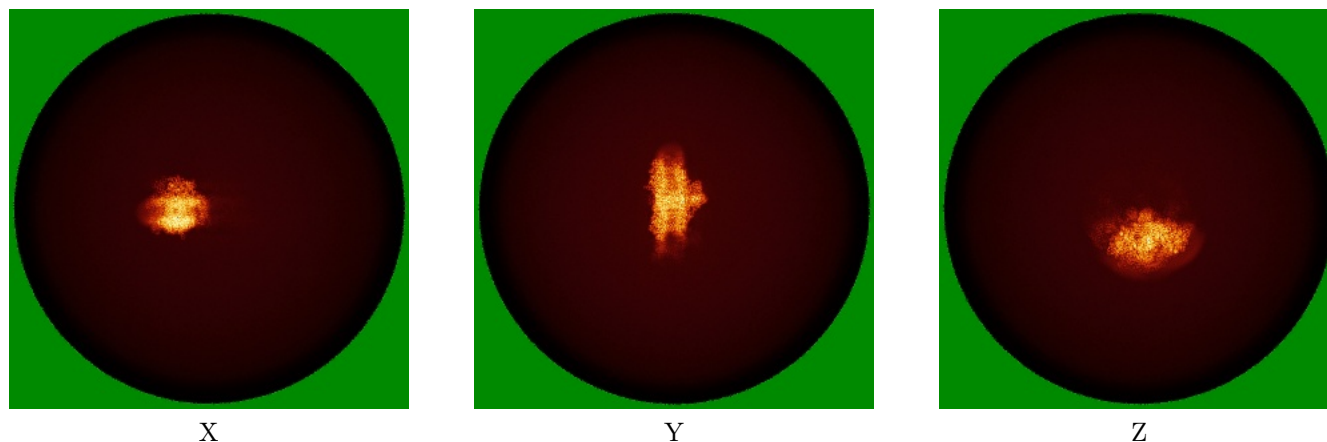


Z Index: 284

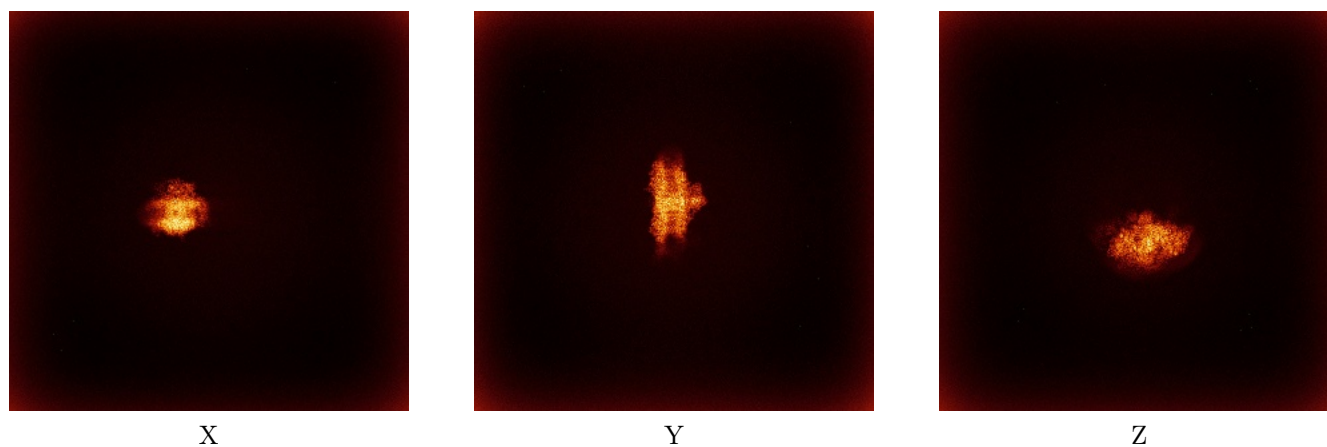
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



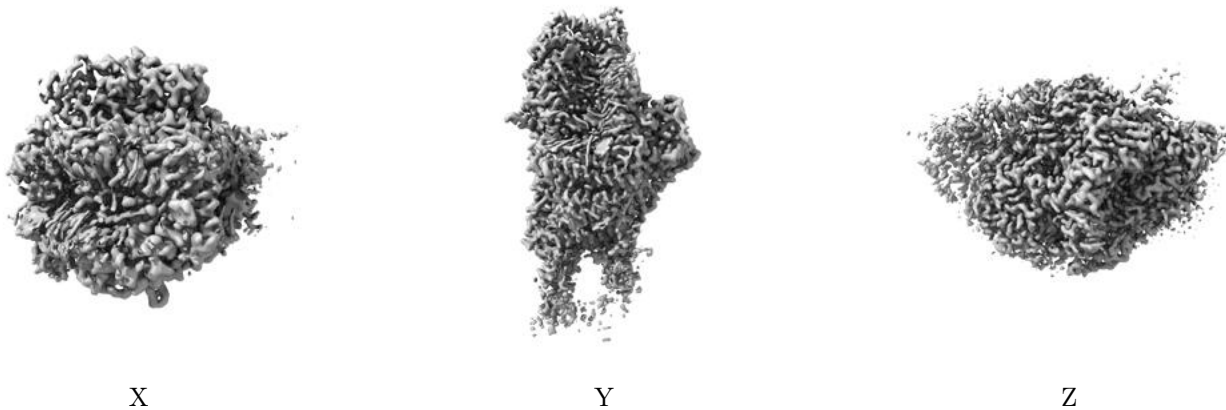
6.4.2 Raw map



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

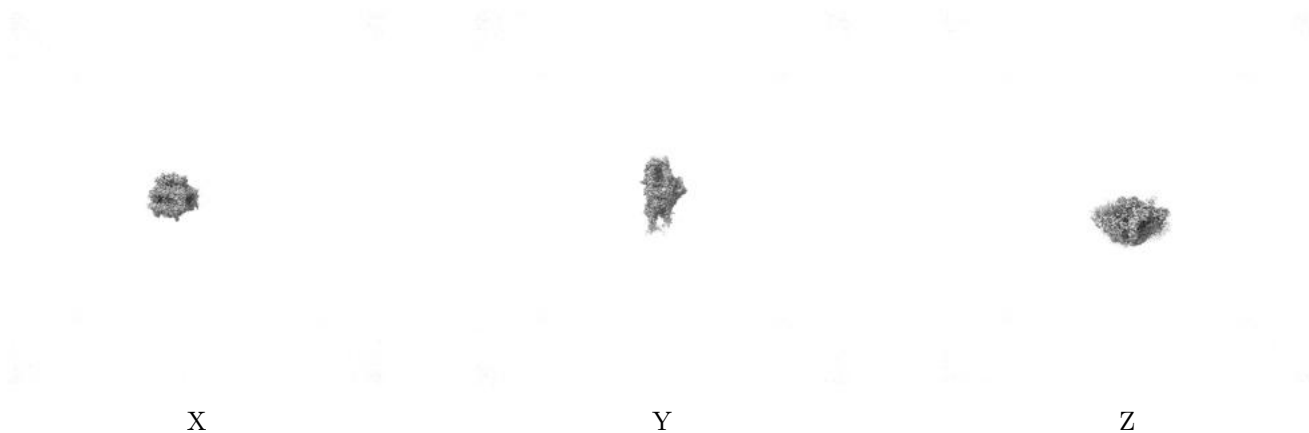
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

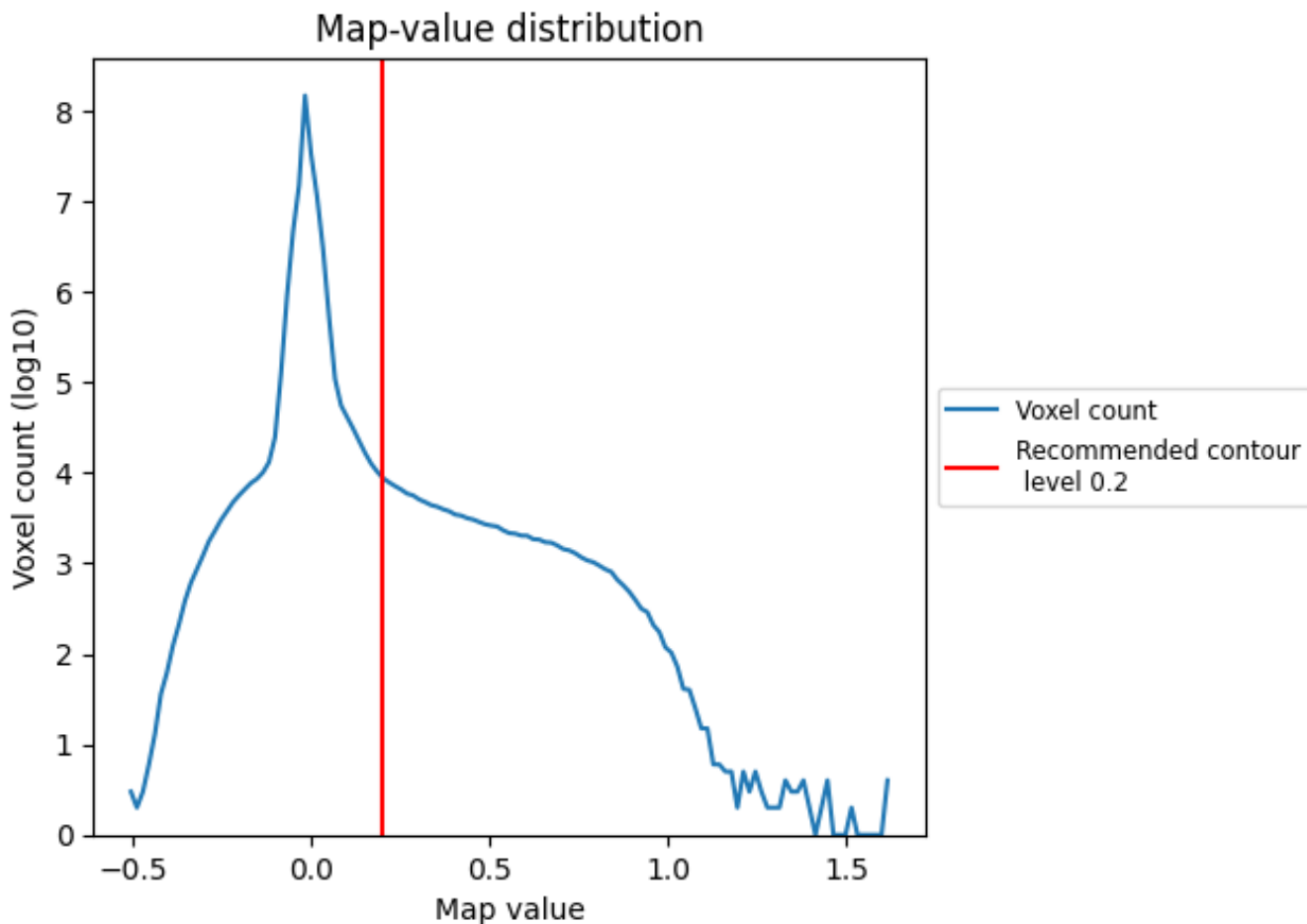
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

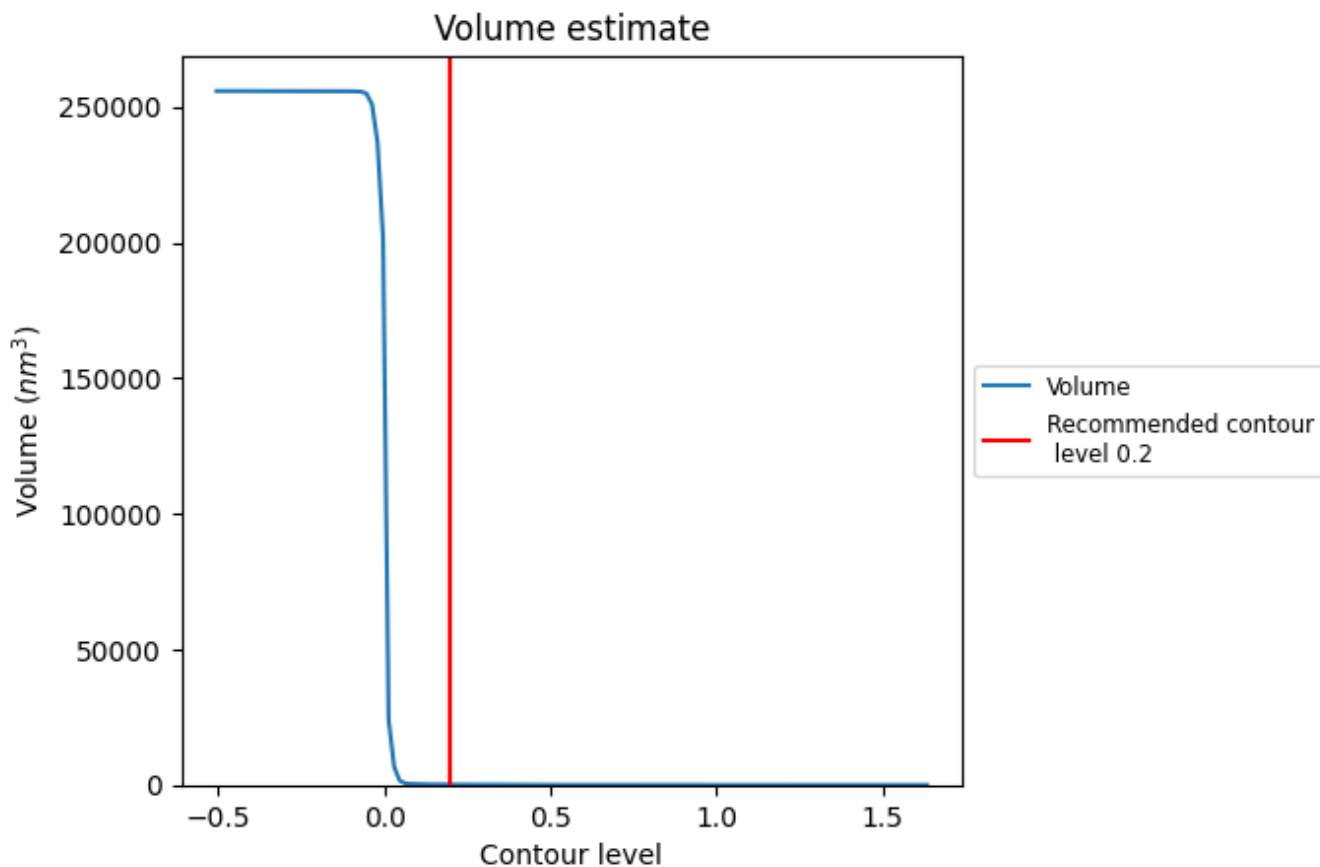
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

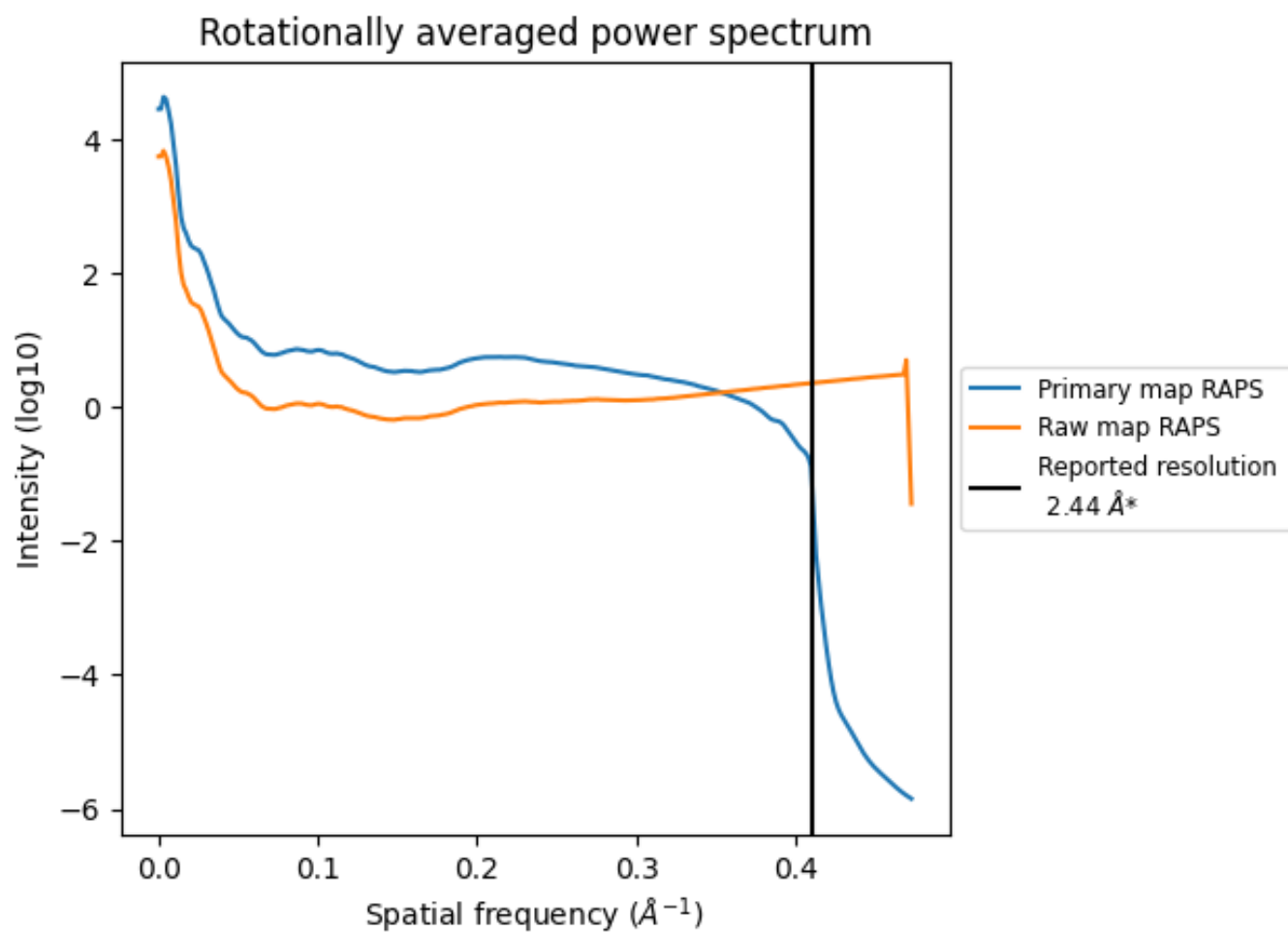
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 135 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

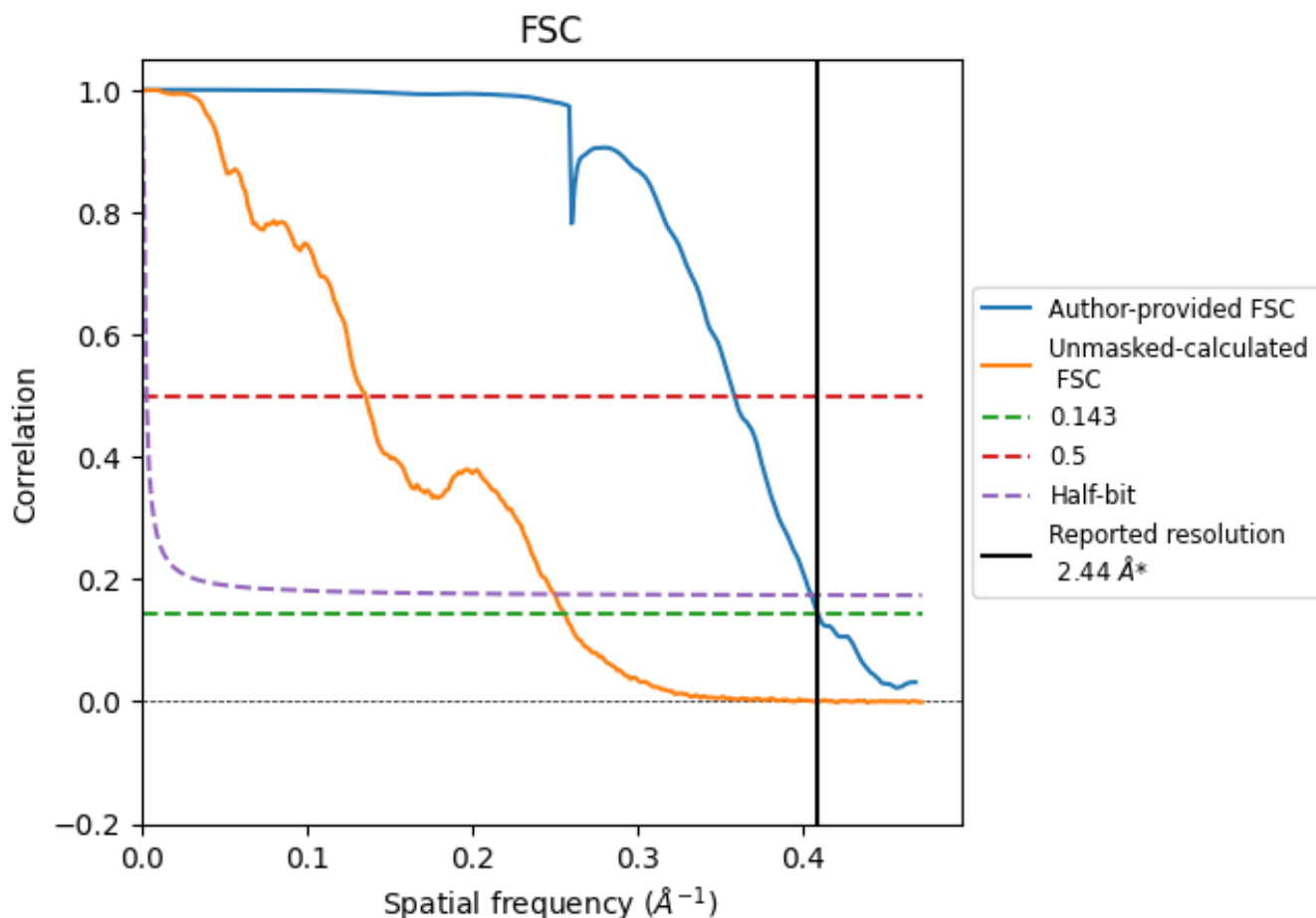


*Reported resolution corresponds to spatial frequency of 0.410 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.410\AA^{-1}

8.2 Resolution estimates [i](#)

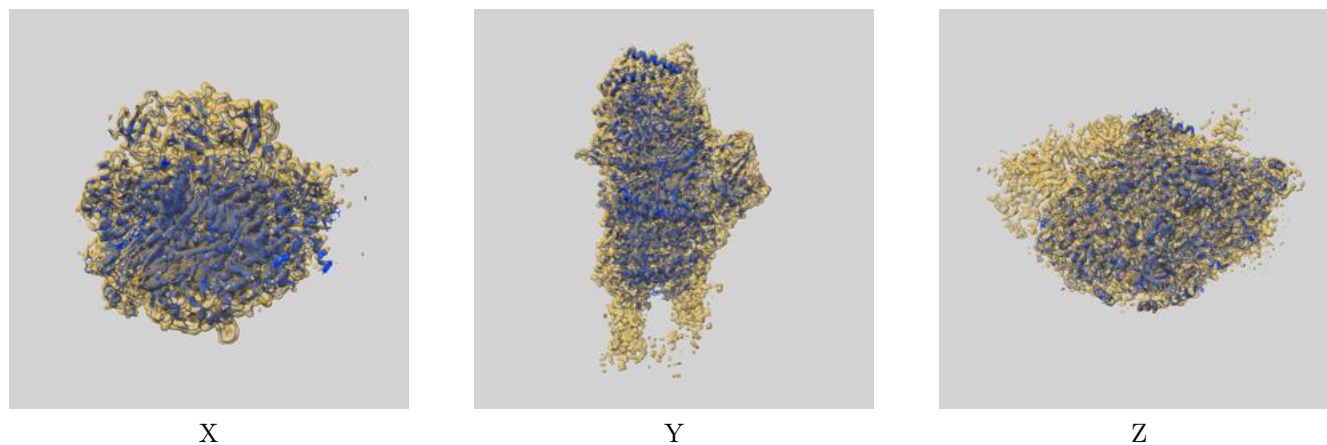
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.79	2.46
Unmasked-calculated*	3.90	7.37	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 2.44 by more than 10 %

9 Map-model fit [i](#)

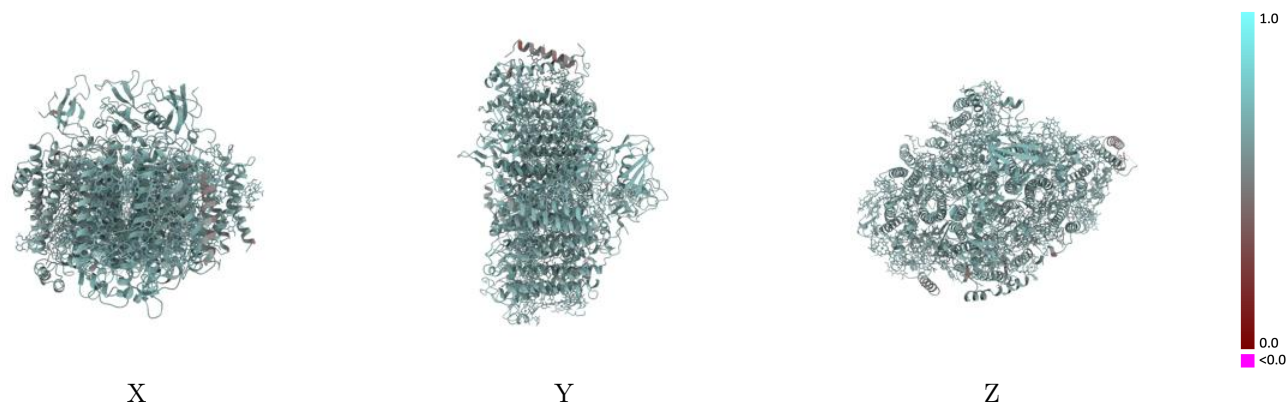
This section contains information regarding the fit between EMDB map EMD-54627 and PDB model 9S6P. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



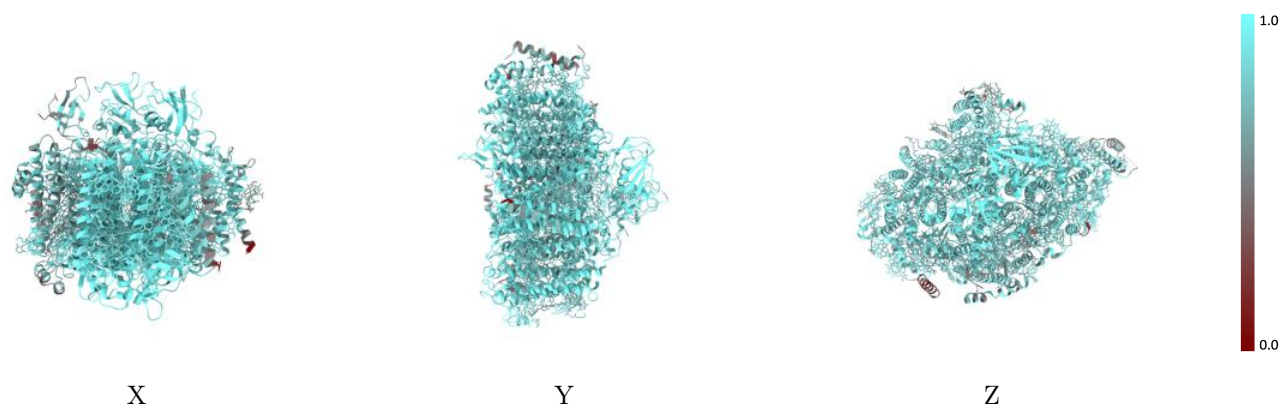
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



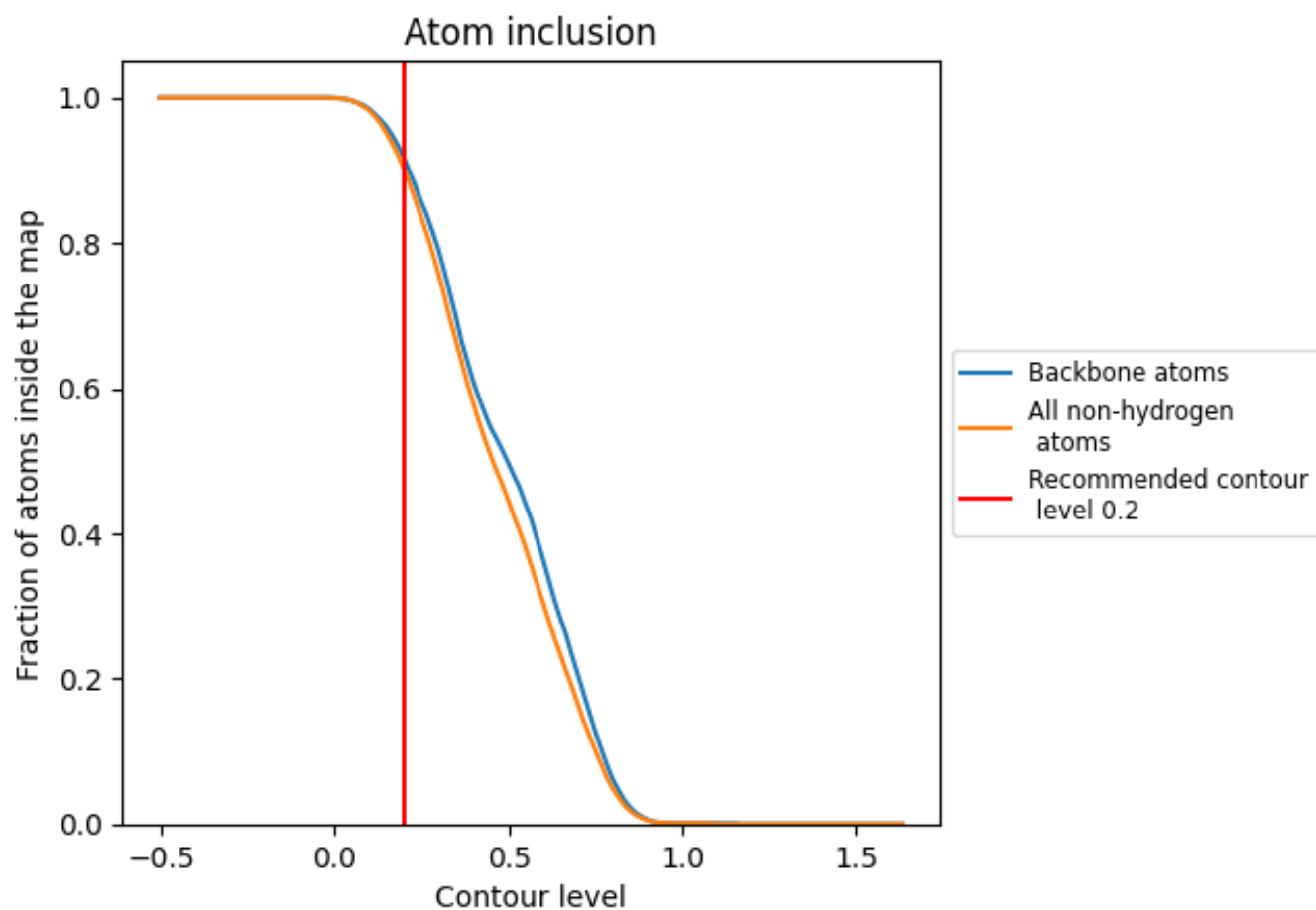
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.6220
A	 0.9370	 0.6330
B	 0.9360	 0.6300
C	 0.9830	 0.6360
D	 0.9460	 0.6230
E	 0.7450	 0.5970
F	 0.7490	 0.5880
I	 0.8130	 0.6040
J	 0.7050	 0.5750
K	 0.6370	 0.5240
L	 0.8420	 0.6160
M	 0.8340	 0.6020
X	 0.2790	 0.4850

