



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 06:45 AM JST

PDB ID : 7DWQ / pdb_00007dwq
EMDB ID : EMD-30882
Title : Photosystem I from a chlorophyll d-containing cyanobacterium *Acaryochloris marina*
Authors : Chen, J.H.; Zhang, X.; Shen, J.R.
Deposited on : 2021-01-17
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

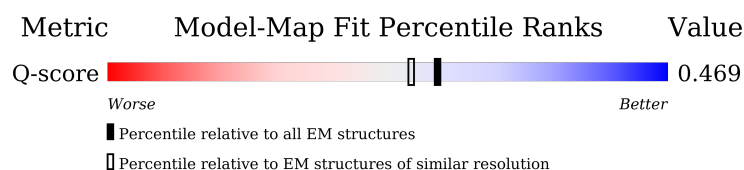
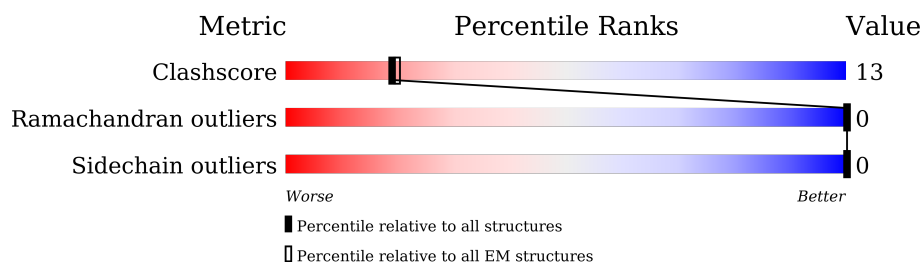
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



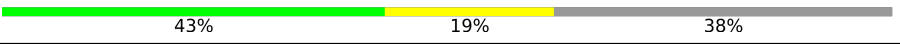
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	D	139	54% 14% 32%
2	A	753	71% 25% .
3	B	736	66% 24% 10%
4	C	81	78% 21% .

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Mol	Chain	Length	Quality of chain
5	E	89	
6	F	167	
7	J	51	
8	L	153	
9	M	31	
10	W	34	

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
11	CL7	A	1022	X	-	-	-
11	CL7	A	1101	X	-	-	-
11	CL7	A	1102	X	-	-	-
11	CL7	A	1103	X	-	-	-
11	CL7	A	1104	X	-	-	-
11	CL7	A	1105	X	-	-	-
11	CL7	A	1106	X	-	-	-
11	CL7	A	1107	X	-	-	-
11	CL7	A	1109	X	-	-	-
11	CL7	A	1110	X	-	-	-
11	CL7	A	1111	X	-	-	-
11	CL7	A	1112	X	-	-	-
11	CL7	A	1113	X	-	-	-
11	CL7	A	1114	X	-	-	-
11	CL7	A	1115	X	-	-	-
11	CL7	A	1116	X	-	-	-
11	CL7	A	1117	X	-	-	-
11	CL7	A	1118	X	-	-	-
11	CL7	A	1119	X	-	-	-
11	CL7	A	1120	X	-	-	-
11	CL7	A	1121	X	-	-	-
11	CL7	A	1122	X	-	-	-
11	CL7	A	1123	X	-	-	-
11	CL7	A	1124	X	-	-	-
11	CL7	A	1125	X	-	-	-
11	CL7	A	1126	X	-	-	-
11	CL7	A	1127	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CL7	A	1128	X	-	-	-
11	CL7	A	1129	X	-	-	-
11	CL7	A	1130	X	-	-	-
11	CL7	A	1131	X	-	-	-
11	CL7	A	1132	X	-	-	-
11	CL7	A	1135	X	-	-	-
11	CL7	A	1136	X	-	-	-
11	CL7	A	1137	X	-	-	-
11	CL7	A	1138	X	-	-	-
11	CL7	A	1139	X	-	-	-
11	CL7	A	1140	X	-	-	-
11	CL7	A	1237	X	-	-	-
11	CL7	A	1801	X	-	-	-
11	CL7	A	1802	X	-	-	-
11	CL7	B	1012	X	-	-	-
11	CL7	B	1021	X	-	-	-
11	CL7	B	1201	X	-	-	-
11	CL7	B	1202	X	-	-	-
11	CL7	B	1203	X	-	-	-
11	CL7	B	1204	X	-	-	-
11	CL7	B	1205	X	-	-	-
11	CL7	B	1206	X	-	-	-
11	CL7	B	1207	X	-	-	-
11	CL7	B	1208	X	-	-	-
11	CL7	B	1210	X	-	-	-
11	CL7	B	1211	X	-	-	-
11	CL7	B	1212	X	-	-	-
11	CL7	B	1213	X	-	-	-
11	CL7	B	1214	X	-	-	-
11	CL7	B	1215	X	-	-	-
11	CL7	B	1222	X	-	-	-
11	CL7	B	1223	X	-	-	-
11	CL7	B	1224	X	-	-	-
11	CL7	B	1225	X	-	-	-
11	CL7	B	1226	X	-	-	-
11	CL7	B	1228	X	-	-	-
11	CL7	B	1229	X	-	-	-
11	CL7	B	1230	X	-	-	-
11	CL7	B	1234	X	-	-	-
11	CL7	B	1235	X	-	-	-
11	CL7	B	1236	X	-	-	-
11	CL7	B	1238	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CL7	B	1239	X	-	-	-
11	CL7	F	1301	X	-	-	-
11	CL7	J	1302	X	-	-	-
11	CL7	L	1501	X	-	-	-
11	CL7	L	1502	X	-	-	-
11	CL7	L	1503	X	-	-	-
11	CL7	W	2601	X	-	-	-
14	LHG	A	5001	-	X	-	-
14	LHG	A	5003	-	X	-	-
15	G9R	A	1011	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 19961 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 protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	94	Total	C	N	O	S	0	0
			725	459	123	139	4		

- Molecule 2 is a protein called Photosystem I P740 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	726	Total	C	N	O	S	0	0
			5715	3734	977	975	29		

- Molecule 3 is a protein called Photosystem I P740 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	659	Total	C	N	O	S	0	0
			5252	3458	878	896	20		

- Molecule 4 is a protein called Photosystem I iron-sulfur center.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	58	Total	C	N	O	S	0	0
			452	283	83	85	1		

- Molecule 6 is a protein called Photosystem I protein PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			775	484	143	143	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	21	Total	C	N	O	0	0
			162	111	25	26		

- Molecule 8 is a protein called Photosystem I protein PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	144	Total	C	N	O	S	0	0
			1008	643	169	192	4		

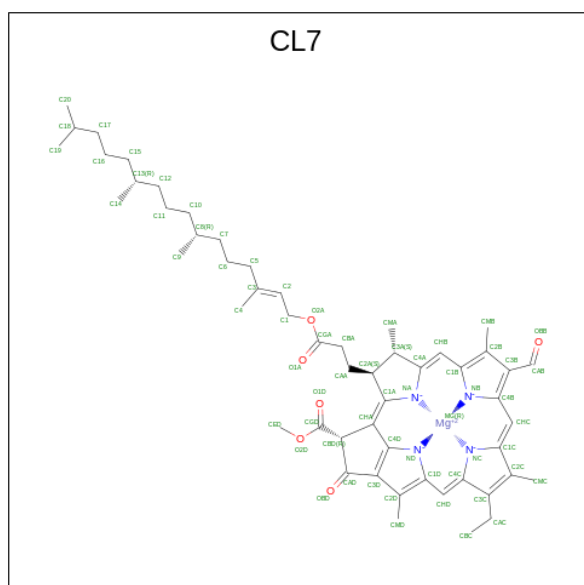
- Molecule 9 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	30	Total	C	N	O	S	0	0
			213	141	32	39	1		

- Molecule 10 is a protein called Photosystem I protein Psa27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	28	Total	C	N	O	S	0	0
			208	142	28	36	2		

- Molecule 11 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
11	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
11	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
11	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 65	C 54	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0
11	A	1	Total 45	C 34	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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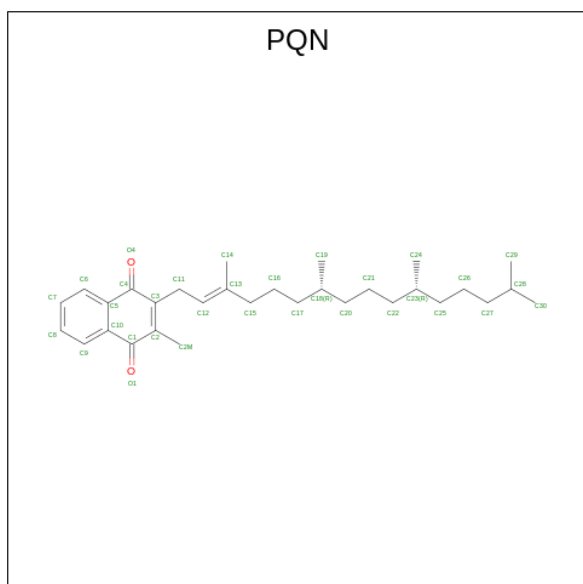
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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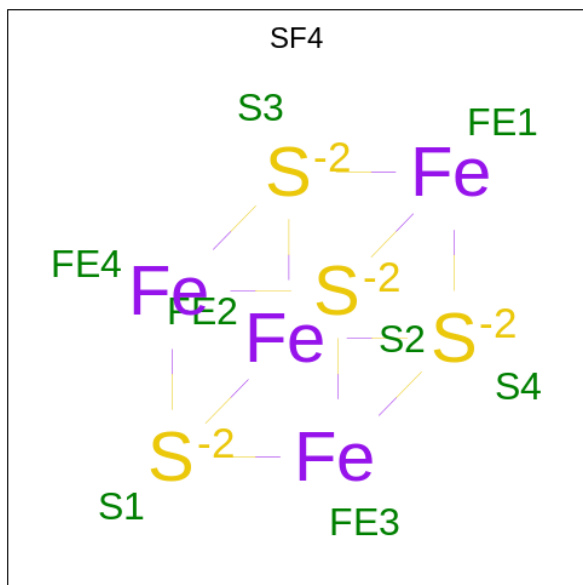
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	F	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	J	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	L	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	L	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
11	L	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
11	W	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

- Molecule 12 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



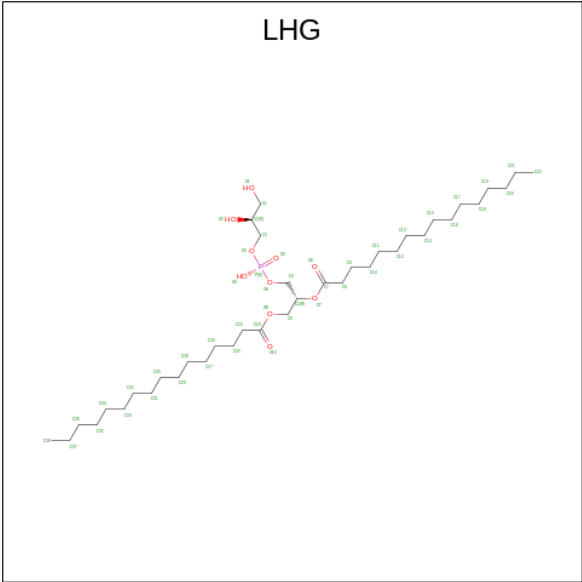
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			33	31	2	
12	B	1	Total	C	O	0
			33	31	2	

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



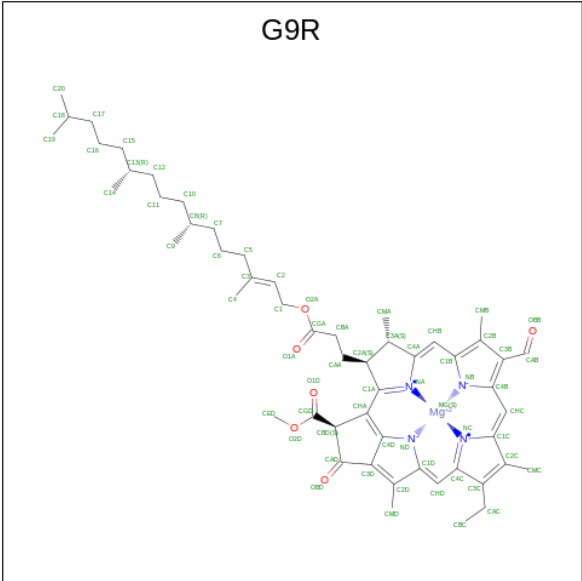
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	Fe	S	0
			8	4	4	
13	C	1	Total	Fe	S	0
			8	4	4	
13	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



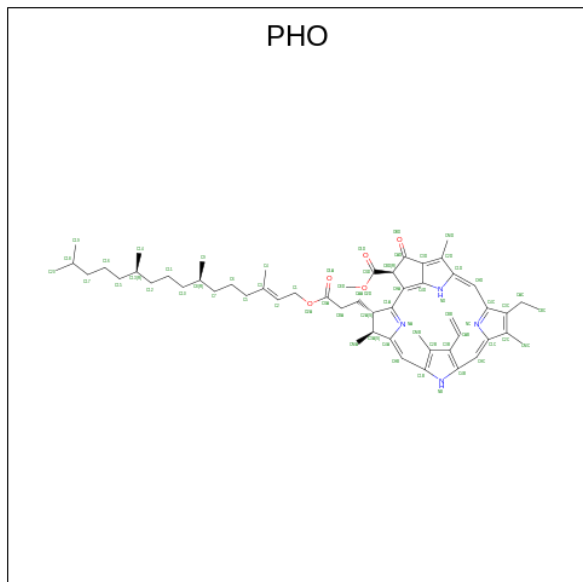
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			49	38	10	1	
14	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 15 is CHLOROPHYLL D ISOMER (CCD ID: G9R) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



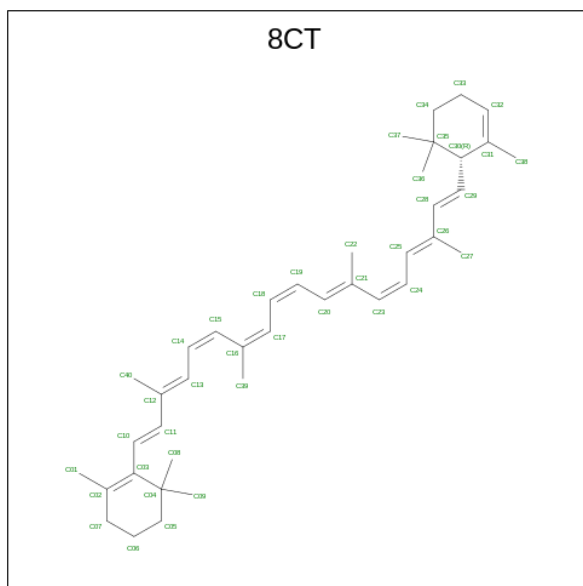
Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 16 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



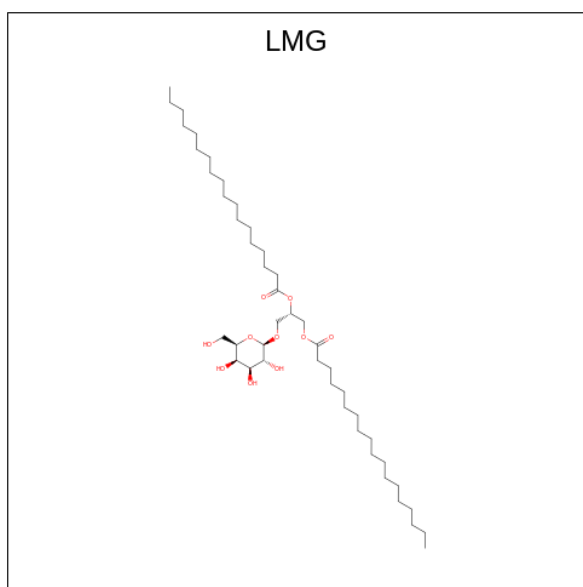
Mol	Chain	Residues	Atoms				AltConf
16	A	1	Total	C	N	O	0
			64	55	4	5	
16	B	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 17 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	W	1	Total C 40 40	0

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).

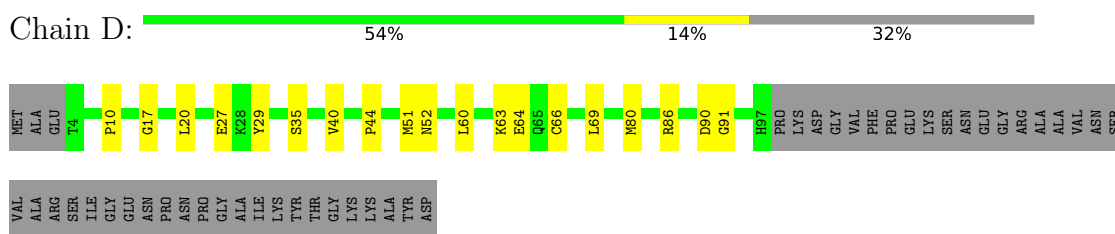


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	B	1	51	41	10	0

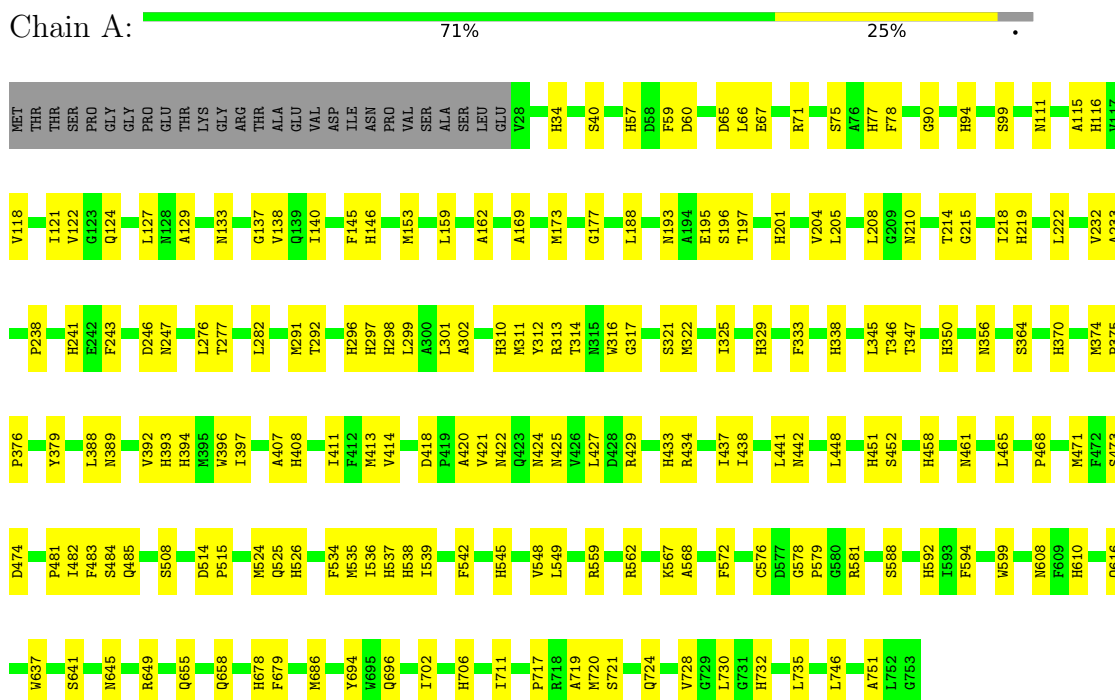
3 Residue-property plots

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

- Molecule 1: Photosystem I protein PsdA

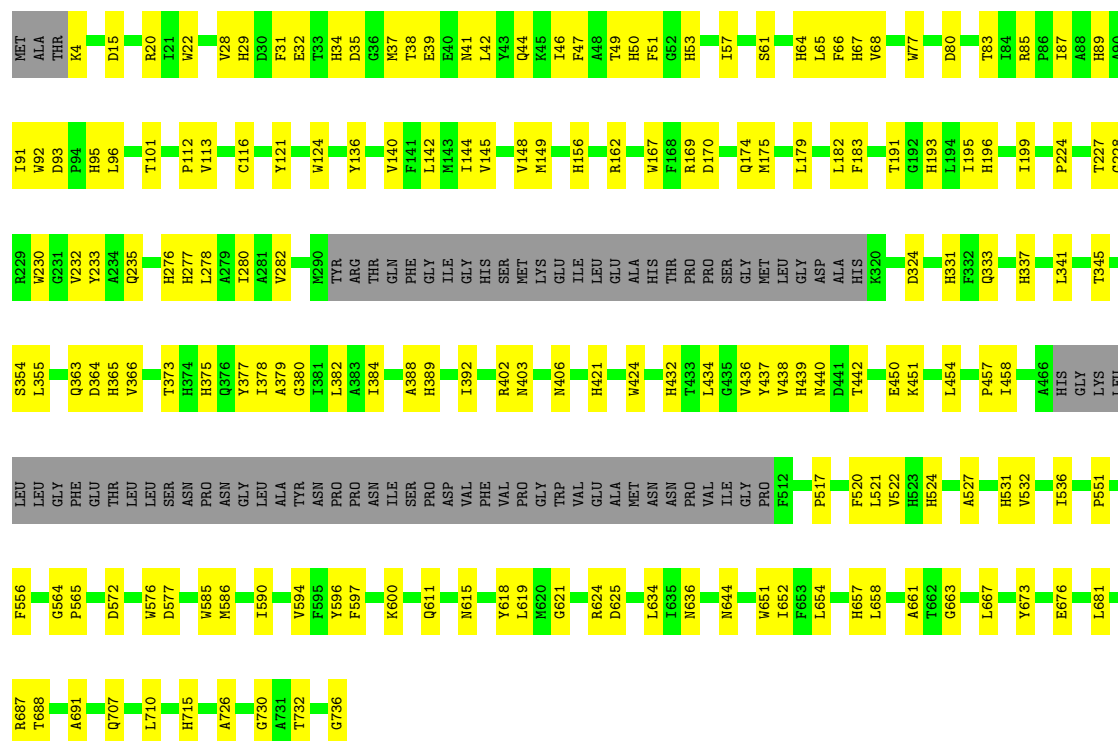


- Molecule 2: Photosystem I P740 chlorophyll a apoprotein A1



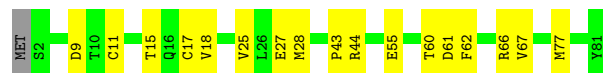
- Molecule 3: Photosystem I P740 chlorophyll a apoprotein A2





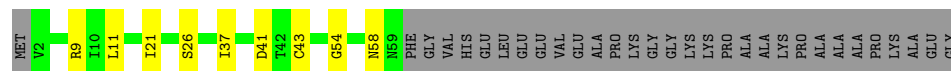
• Molecule 4: Photosystem I iron-sulfur center

Chain C: 78% 21% .



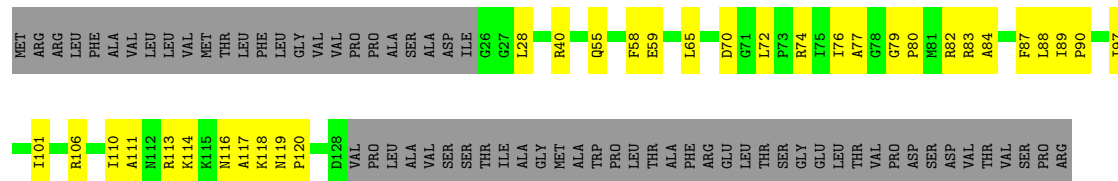
• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 55% 10% 35%



• Molecule 6: Photosystem I protein Psaf

Chain F: 43% 19% 38%

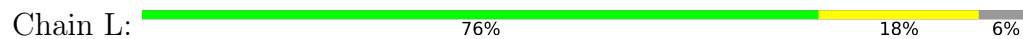


• Molecule 7: Photosystem I reaction center subunit IX

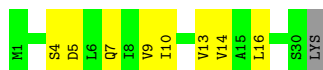
Chain J: 29% 12% 59%



• Molecule 8: Photosystem I protein PsaL



• Molecule 9: Photosystem I reaction center subunit XII



• Molecule 10: Photosystem I protein Psa27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	240880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	38244	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.061	Depositor
Minimum map value	-1.735	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.171	Depositor
Map size ($\text{\AA}$)	522.8, 522.8, 522.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3069999, 1.3069999, 1.3069999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, LHG, G9R, CL7, PHO, PQN, LMG, 8CT

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	D	0.10	0/737	0.26	0/995
2	A	0.14	0/5909	0.30	0/8049
3	B	0.13	0/5446	0.29	0/7439
4	C	0.12	0/609	0.30	0/825
5	E	0.11	0/460	0.29	0/623
6	F	0.17	0/790	0.40	0/1061
7	J	0.14	0/165	0.37	0/225
8	L	0.12	0/1030	0.27	0/1403
9	M	0.17	0/213	0.48	0/291
10	W	0.14	0/213	0.33	0/291
All	All	0.13	0/15572	0.30	0/21202

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

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	D	725	0	737	14	0
2	A	5715	0	5546	175	0
3	B	5252	0	5015	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	599	0	577	13	0
5	E	452	0	447	6	0
6	F	775	0	773	28	0
7	J	162	0	172	6	0
8	L	1008	0	1012	22	0
9	M	213	0	244	7	0
10	W	208	0	213	3	0
11	A	2145	0	1844	129	0
11	B	1445	0	1163	84	0
11	F	45	0	31	4	0
11	J	45	0	31	1	0
11	L	175	0	169	6	0
11	W	45	0	31	2	0
12	A	33	0	46	4	0
12	B	33	0	46	1	0
13	A	8	0	0	1	0
13	C	16	0	0	1	0
14	A	98	0	148	3	0
15	A	65	0	0	1	0
16	A	64	0	72	9	0
16	B	64	0	74	7	0
17	A	120	0	0	0	0
17	B	120	0	0	0	0
17	J	80	0	0	1	0
17	L	80	0	0	0	0
17	M	40	0	0	0	0
17	W	80	0	0	0	0
18	B	51	0	75	3	0
All	All	19961	0	18466	491	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (491) 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)
16:A:1013:PHO:H3A	16:A:1013:PHO:H2	1.33	1.06
2:A:408:HIS:HE1	11:A:1128:CL7:NA	1.65	0.94
2:A:57:HIS:HE1	11:A:1102:CL7:NB	1.69	0.90
2:A:706:HIS:HE1	11:A:1138:CL7:ND	1.78	0.80
2:A:721:SER:H	2:A:724:GLN:HE21	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:27:GLU:OE2	4:C:44:ARG:NH2	2.17	0.77
2:A:214:THR:HG21	2:A:299:LEU:HB2	1.67	0.77
3:B:91:ILE:HB	3:B:112:PRO:HB2	1.66	0.76
2:A:313:ARG:HH11	2:A:317:GLY:HA2	1.54	0.73
3:B:156:HIS:HE1	11:B:1208:CL7:NA	1.87	0.73
6:F:97:ILE:HG12	11:F:1301:CL7:HBA2	1.70	0.73
3:B:715:HIS:HE1	11:B:1239:CL7:ND	1.88	0.71
2:A:414:VAL:HG11	2:A:572:PHE:HB2	1.72	0.71
4:C:17:CYS:HB3	13:C:3003:SF4:S1	2.31	0.70
2:A:241:HIS:CD2	11:A:1114:CL7:CHD	2.72	0.70
4:C:15:THR:HG22	4:C:28:MET:HE3	1.74	0.70
3:B:389:HIS:HE1	11:B:1226:CL7:NA	1.89	0.69
6:F:114:LYS:HD3	6:F:118:LYS:HA	1.74	0.68
3:B:438:VAL:HG21	11:B:1012:CL7:H92C	1.76	0.67
2:A:222:LEU:HD22	2:A:291:MET:HB3	1.75	0.67
11:A:1131:CL7:HAB	11:A:1132:CL7:HHB	1.76	0.67
3:B:93:ASP:HB3	3:B:96:LEU:HG	1.75	0.67
3:B:380:GLY:HA3	3:B:590:ILE:HD11	1.74	0.67
3:B:451:LYS:HD3	11:B:1230:CL7:HED3	1.78	0.66
8:L:54:HIS:HE1	11:L:1502:CL7:ND	1.92	0.66
3:B:282:VAL:HG21	11:B:1213:CL7:HAB	1.76	0.66
2:A:616:GLN:OE1	2:A:655:GLN:NE2	2.29	0.66
2:A:329:HIS:HE1	11:A:1121:CL7:ND	1.94	0.65
3:B:710:LEU:HD11	18:B:5002:LMG:H301	1.79	0.65
3:B:277:HIS:HE1	11:B:1215:CL7:NA	1.95	0.65
11:B:1207:CL7:HBA2	8:L:67:PRO:HG2	1.79	0.65
11:A:1104:CL7:H2	14:A:5001:LHG:H252	1.80	0.64
2:A:314:THR:H	11:A:1118:CL7:HED1	1.62	0.64
11:A:1136:CL7:HBA2	11:A:1136:CL7:HBD	1.78	0.64
3:B:572:ASP:OD1	3:B:577:ASP:HB3	1.98	0.64
3:B:227:THR:HG22	3:B:228:GLY:H	1.62	0.63
3:B:611:GLN:O	3:B:615:ASN:HB2	1.98	0.63
6:F:79:GLY:HA2	6:F:88:LEU:HD11	1.81	0.63
8:L:48:LEU:O	8:L:52:MET:HG3	2.00	0.62
2:A:442:ASN:HD22	3:B:681:LEU:HD21	1.64	0.62
2:A:458:HIS:HE1	11:A:1132:CL7:C1A	2.05	0.62
2:A:169:ALA:O	2:A:173:MET:HG2	2.00	0.62
2:A:396:TRP:CD1	11:A:1126:CL7:HAB	2.35	0.61
2:A:215:GLY:HA3	11:A:1113:CL7:HAB	1.82	0.61
2:A:407:ALA:O	2:A:411:ILE:HD12	2.00	0.61
2:A:115:ALA:HB3	2:A:140:ILE:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:204:VAL:HA	2:A:208:LEU:HD13	1.81	0.61
3:B:53:HIS:HE1	11:B:1203:CL7:NC	1.98	0.61
1:D:64:GLU:OE2	2:A:581:ARG:NH2	2.31	0.61
2:A:67:GLU:OE2	2:A:71:ARG:NH2	2.33	0.61
11:A:1129:CL7:HBA1	14:A:5003:LHG:HC82	1.81	0.60
2:A:424:ASN:OD1	2:A:429:ARG:NH1	2.34	0.60
3:B:46:ILE:HG23	3:B:50:HIS:CE1	2.36	0.60
3:B:424:TRP:NE1	11:B:1229:CL7:OBD	2.34	0.60
3:B:341:LEU:HB3	3:B:382:LEU:HD23	1.83	0.60
8:L:103:LYS:HD2	8:L:104:PRO:HD2	1.84	0.60
2:A:484:SER:OG	11:A:1136:CL7:O2D	2.20	0.60
3:B:92:TRP:N	11:B:1206:CL7:O1D	2.29	0.60
2:A:241:HIS:HD2	11:A:1114:CL7:CHD	2.12	0.59
2:A:451:HIS:HE1	11:A:1131:CL7:C1A	2.15	0.59
2:A:702:ILE:HD13	11:A:1138:CL7:HMD1	1.84	0.59
6:F:40:ARG:NH2	6:F:70:ASP:O	2.33	0.59
2:A:121:ILE:HG12	2:A:122:VAL:H	1.67	0.59
5:E:9:ARG:HH21	5:E:21:ILE:HD11	1.65	0.59
3:B:615:ASN:ND2	3:B:625:ASP:OD2	2.28	0.59
2:A:111:ASN:OD1	2:A:133:ASN:ND2	2.31	0.59
3:B:95:HIS:HE1	11:B:1207:CL7:NB	1.96	0.59
2:A:376:PRO:HB2	11:A:1117:CL7:HAA1	1.85	0.59
3:B:657:HIS:HD2	11:B:1021:CL7:C1B	2.15	0.59
4:C:11:CYS:HA	4:C:60:THR:HG21	1.84	0.58
6:F:82:ARG:HG2	6:F:83:ARG:HG2	1.86	0.58
2:A:422:ASN:OD1	2:A:425:ASN:ND2	2.34	0.58
2:A:94:HIS:HE1	11:A:1105:CL7:NA	2.01	0.58
11:A:1131:CL7:HAB	11:A:1132:CL7:CHB	2.34	0.58
2:A:296:HIS:HE1	11:A:1115:CL7:C4D	2.08	0.58
2:A:374:MET:HE2	11:A:1116:CL7:HBD	1.85	0.58
2:A:218:ILE:HD12	2:A:222:LEU:HD12	1.85	0.58
11:B:1204:CL7:HAA1	11:B:1206:CL7:HED1	1.85	0.58
11:B:1201:CL7:HAB	11:B:1203:CL7:CAD	2.34	0.57
6:F:118:LYS:O	6:F:118:LYS:HD3	2.04	0.57
3:B:333:GLN:O	3:B:337:HIS:ND1	2.34	0.57
6:F:70:ASP:OD1	6:F:74:ARG:NH2	2.37	0.57
2:A:321:SER:O	2:A:325:ILE:HG12	2.05	0.57
11:A:1022:CL7:H2	3:B:654:LEU:HB3	1.87	0.57
2:A:451:HIS:HE1	11:A:1131:CL7:NA	2.00	0.57
2:A:205:LEU:HD11	11:A:1111:CL7:HBA2	1.87	0.57
11:L:1501:CL7:H11C	11:L:1501:CL7:H172	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:442:ASN:ND2	3:B:681:LEU:HD21	2.20	0.56
11:A:1138:CL7:HAA2	11:A:1138:CL7:HED3	1.86	0.56
3:B:44:GLN:OE1	3:B:162:ARG:NH1	2.38	0.56
3:B:377:TYR:CD2	11:B:1224:CL7:HAB	2.40	0.56
11:B:1230:CL7:HBA1	7:J:39:LEU:HD21	1.87	0.56
2:A:567:LYS:NZ	3:B:676:GLU:OE2	2.32	0.56
9:M:10:ILE:O	9:M:14:VAL:HG23	2.05	0.56
11:A:1135:CL7:H3A	11:A:1136:CL7:HAA2	1.88	0.56
3:B:156:HIS:HE1	11:B:1208:CL7:C1A	2.18	0.56
2:A:57:HIS:HE1	11:A:1102:CL7:C4B	2.18	0.56
3:B:61:SER:HB3	11:B:1225:CL7:H2	1.88	0.56
3:B:432:HIS:HE1	11:B:1229:CL7:ND	2.02	0.56
2:A:594:PHE:HD1	2:A:730:LEU:HD22	1.71	0.56
3:B:65:LEU:HD12	3:B:142:LEU:HD12	1.88	0.55
3:B:67:HIS:HE1	11:B:1204:CL7:C4D	2.20	0.55
3:B:170:ASP:O	3:B:174:GLN:NE2	2.39	0.55
2:A:296:HIS:HB3	11:A:1116:CL7:HMB2	1.88	0.55
3:B:365:HIS:ND1	3:B:736:GLY:O	2.37	0.55
6:F:82:ARG:O	6:F:83:ARG:NH1	2.39	0.55
3:B:621:GLY:O	3:B:625:ASP:HB2	2.06	0.55
6:F:89:ILE:HG13	6:F:90:PRO:HD3	1.88	0.55
1:D:27:GLU:OE2	1:D:86:ARG:HG2	2.07	0.55
3:B:31:PHE:HA	3:B:34:HIS:CD2	2.42	0.55
3:B:232:VAL:HA	3:B:235:GLN:HG2	1.88	0.55
2:A:116:HIS:HB2	2:A:138:VAL:HB	1.89	0.55
12:A:2001:PQN:H291	7:J:28:PHE:HZ	1.72	0.55
6:F:28:LEU:HB2	6:F:65:LEU:HD12	1.89	0.55
11:A:1122:CL7:HMC2	11:A:1129:CL7:HAC2	1.88	0.55
3:B:15:ASP:HB3	3:B:20:ARG:HB2	1.89	0.54
2:A:578:GLY:HA2	3:B:565:PRO:HD3	1.90	0.54
2:A:60:ASP:OD2	2:A:350:HIS:NE2	2.41	0.54
11:A:1132:CL7:HED1	8:L:67:PRO:HA	1.89	0.54
2:A:59:PHE:HE1	11:A:1102:CL7:HED1	1.72	0.54
16:A:1013:PHO:HHB	16:A:1013:PHO:H43	1.90	0.54
3:B:354:SER:HB2	11:B:1223:CL7:HBC3	1.90	0.54
3:B:454:LEU:HD23	3:B:517:PRO:HG2	1.89	0.54
2:A:232:VAL:HG23	2:A:233:ALA:H	1.73	0.54
3:B:191:THR:HG21	3:B:278:LEU:HB2	1.89	0.54
18:B:5002:LMG:O5	18:B:5002:LMG:O4	2.26	0.54
9:M:7:GLN:HA	9:M:10:ILE:HG22	1.89	0.54
11:A:1104:CL7:H121	11:A:1126:CL7:HBC1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1102:CL7:HBC3	11:A:1128:CL7:H41C	1.90	0.53
3:B:532:VAL:O	3:B:536:ILE:HD12	2.08	0.53
6:F:55:GLN:HA	6:F:58:PHE:HD2	1.73	0.53
2:A:481:PRO:HB3	2:A:534:PHE:HB2	1.91	0.53
3:B:87:ILE:HD12	3:B:113:VAL:HG21	1.89	0.53
2:A:277:THR:OG1	2:A:292:THR:OG1	2.26	0.53
11:A:1103:CL7:HMB2	11:A:1104:CL7:HAA1	1.91	0.53
1:D:40:VAL:HG11	2:A:420:ALA:HA	1.90	0.53
3:B:377:TYR:HD2	11:B:1224:CL7:HAB	1.74	0.53
11:B:1012:CL7:HED3	11:B:1012:CL7:HBA1	1.91	0.53
3:B:432:HIS:HE1	11:B:1229:CL7:C4D	2.21	0.53
3:B:434:LEU:O	3:B:438:VAL:HG12	2.09	0.53
8:L:91:VAL:HA	8:L:94:GLN:HG2	1.90	0.53
2:A:282:LEU:HD21	2:A:375:PRO:HD2	1.91	0.53
1:D:44:PRO:HD3	1:D:69:LEU:HD12	1.91	0.53
2:A:118:VAL:HA	11:A:1107:CL7:HED2	1.91	0.53
8:L:38:ARG:HB3	8:L:41:MET:HE3	1.91	0.53
2:A:468:PRO:HA	2:A:471:MET:HE2	1.91	0.52
2:A:686:MET:HG2	16:A:1013:PHO:NC	2.23	0.52
8:L:63:ALA:O	8:L:74:SER:OG	2.27	0.52
1:D:90:ASP:OD1	1:D:91:GLY:N	2.41	0.52
2:A:298:HIS:HE1	11:A:1117:CL7:C4D	2.15	0.52
2:A:645:ASN:OD1	2:A:649:ARG:NH1	2.42	0.52
3:B:590:ILE:O	3:B:594:VAL:HG22	2.08	0.52
2:A:536:ILE:HG21	2:A:610:HIS:CG	2.45	0.52
2:A:720:MET:HE1	2:A:728:VAL:HG21	1.91	0.52
16:A:1013:PHO:H51	3:B:434:LEU:HD23	1.90	0.52
11:B:1235:CL7:HAC2	6:F:77:ALA:HB1	1.92	0.52
2:A:205:LEU:HD12	11:A:1111:CL7:CHB	2.39	0.52
2:A:392:VAL:HG23	2:A:608:ASN:CG	2.35	0.52
2:A:538:HIS:HE1	11:A:1136:CL7:C4B	2.19	0.52
2:A:637:TRP:O	2:A:641:SER:OG	2.26	0.52
11:A:1132:CL7:H2	8:L:61:PRO:HB2	1.92	0.52
3:B:597:PHE:HB2	11:B:1234:CL7:HMC1	1.91	0.52
3:B:35:ASP:OD1	3:B:35:ASP:N	2.42	0.52
3:B:85:ARG:NH1	3:B:364:ASP:OD1	2.43	0.52
2:A:116:HIS:HE1	11:A:1106:CL7:C1B	2.19	0.52
8:L:83:SER:O	8:L:87:ILE:HG12	2.10	0.52
3:B:136:TYR:OH	9:M:7:GLN:O	2.26	0.52
2:A:333:PHE:O	2:A:429:ARG:NH2	2.43	0.51
2:A:535:MET:O	2:A:539:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:24:SER:HB2	8:L:27:VAL:HG12	1.92	0.51
2:A:364:SER:OG	2:A:394:HIS:O	2.27	0.51
3:B:618:TYR:OH	3:B:624:ARG:NH2	2.37	0.51
11:A:1104:CL7:H122	11:A:1104:CL7:H202	1.92	0.51
3:B:438:VAL:HG23	11:B:1012:CL7:H52C	1.92	0.51
3:B:673:TYR:OH	16:B:1023:PHO:OBD	2.28	0.51
2:A:392:VAL:HG13	11:A:1126:CL7:HMB2	1.92	0.51
9:M:5:ASP:O	9:M:9:VAL:HG23	2.10	0.51
2:A:721:SER:N	2:A:724:GLN:HE21	2.05	0.51
4:C:18:VAL:HG21	4:C:28:MET:HG2	1.92	0.51
2:A:78:PHE:HD2	2:A:177:GLY:HA2	1.76	0.51
8:L:103:LYS:HD2	8:L:104:PRO:CD	2.41	0.51
2:A:389:ASN:HB3	11:A:1126:CL7:HMA1	1.93	0.51
3:B:378:ILE:HD12	11:B:1203:CL7:H202	1.94	0.50
2:A:241:HIS:CE1	11:A:1114:CL7:CHA	2.87	0.50
6:F:101:ILE:HG12	11:F:1301:CL7:ND	2.26	0.50
3:B:657:HIS:CD2	11:B:1021:CL7:C1B	2.94	0.50
2:A:720:MET:HG2	12:A:2001:PQN:O4	2.11	0.50
5:E:41:ASP:OD2	5:E:41:ASP:N	2.45	0.50
2:A:356:ASN:ND2	11:A:1103:CL7:OBD	2.37	0.50
4:C:55:GLU:OE2	4:C:67:VAL:N	2.41	0.50
7:J:32:THR:O	7:J:36:LEU:HD23	2.12	0.50
3:B:652:ILE:HG22	3:B:726:ALA:HB2	1.93	0.50
9:M:10:ILE:HA	9:M:13:VAL:HG22	1.92	0.50
2:A:316:TRP:CZ3	11:A:1118:CL7:HBD	2.46	0.49
2:A:448:LEU:HB3	2:A:542:PHE:HB2	1.94	0.49
9:M:13:VAL:HA	9:M:16:LEU:HD23	1.94	0.49
3:B:51:PHE:HD1	3:B:149:MET:HG3	1.77	0.49
3:B:424:TRP:CE2	11:B:1228:CL7:HAB	2.46	0.49
2:A:210:ASN:HB3	2:A:302:ALA:HB2	1.94	0.49
2:A:473:SER:OG	2:A:474:ASP:N	2.46	0.49
3:B:276:HIS:HD1	11:B:1214:CL7:C1B	1.85	0.49
8:L:33:ASN:HB3	11:L:1501:CL7:HAC1	1.94	0.49
2:A:121:ILE:HG22	2:A:124:GLN:HG2	1.94	0.49
3:B:68:VAL:HG11	3:B:124:TRP:CZ3	2.48	0.49
3:B:89:HIS:CD2	11:B:1205:CL7:NA	2.80	0.49
3:B:324:ASP:OD2	3:B:402:ARG:NH2	2.46	0.49
2:A:679:PHE:HB2	11:B:1012:CL7:HAA2	1.95	0.49
3:B:32:GLU:OE2	3:B:331:HIS:NE2	2.45	0.49
3:B:29:HIS:HB2	11:B:1226:CL7:H11C	1.94	0.49
11:F:1301:CL7:CGA	11:F:1301:CL7:HBD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:241:HIS:HE1	11:A:1114:CL7:C1A	2.25	0.48
2:A:370:HIS:CD2	11:A:1125:CL7:NC	2.80	0.48
3:B:28:VAL:HG22	11:B:1226:CL7:H2	1.95	0.48
3:B:522:VAL:HG22	11:B:1021:CL7:H141	1.95	0.48
6:F:87:PHE:C	6:F:90:PRO:HD2	2.37	0.48
2:A:246:ASP:OD1	2:A:247:ASN:N	2.46	0.48
3:B:636:ASN:O	3:B:644:ASN:ND2	2.46	0.48
2:A:394:HIS:CD2	11:A:1127:CL7:NC	2.79	0.48
3:B:38:THR:OG1	3:B:41:ASN:OD1	2.29	0.48
5:E:11:LEU:HD23	5:E:11:LEU:H	1.77	0.48
3:B:101:THR:HG23	3:B:112:PRO:HG3	1.96	0.48
2:A:537:HIS:HD2	11:A:1135:CL7:C1B	2.27	0.48
2:A:297:HIS:ND1	11:A:1116:CL7:C1B	2.59	0.48
3:B:80:ASP:OD2	3:B:83:THR:OG1	2.31	0.48
8:L:54:HIS:HE1	11:L:1502:CL7:C4D	2.27	0.48
2:A:75:SER:HB3	11:A:1109:CL7:HAC2	1.96	0.48
2:A:413:MET:HE1	2:A:427:LEU:HD11	1.96	0.48
9:M:4:SER:H	9:M:7:GLN:NE2	2.10	0.48
16:A:1013:PHO:C1D	3:B:585:TRP:HE1	2.26	0.48
3:B:53:HIS:HE1	11:B:1203:CL7:C1C	2.26	0.48
3:B:373:THR:HG23	3:B:594:VAL:HG11	1.96	0.48
3:B:22:TRP:CG	3:B:707:GLN:HE22	2.32	0.47
7:J:33:ALA:HB1	11:J:1302:CL7:HHC	1.96	0.47
2:A:99:SER:HB2	2:A:145:PHE:HZ	1.79	0.47
2:A:392:VAL:CG1	11:A:1126:CL7:HMB2	2.44	0.47
2:A:515:PRO:HB3	2:A:525:GLN:HG3	1.96	0.47
3:B:688:THR:HG23	3:B:691:ALA:HB3	1.96	0.47
8:L:38:ARG:O	8:L:46:ARG:NH1	2.25	0.47
2:A:34:HIS:HA	2:A:40:SER:HB3	1.96	0.47
2:A:238:PRO:HG2	2:A:243:PHE:CE1	2.49	0.47
3:B:39:GLU:HA	3:B:42:LEU:HD12	1.96	0.47
3:B:224:PRO:HG2	3:B:233:TYR:CZ	2.49	0.47
3:B:457:PRO:HB3	3:B:520:PHE:HB2	1.95	0.47
11:B:1224:CL7:CGA	11:B:1224:CL7:H3A	2.45	0.47
2:A:728:VAL:HG22	11:A:1140:CL7:CAD	2.44	0.47
11:A:1111:CL7:HBA2	11:A:1111:CL7:H3A	1.57	0.47
3:B:196:HIS:HE1	11:B:1212:CL7:C1C	2.24	0.47
3:B:276:HIS:O	3:B:280:ILE:HG12	2.15	0.47
3:B:576:TRP:NE1	18:B:5002:LMG:O10	2.47	0.47
2:A:461:ASN:OD1	3:B:651:TRP:NE1	2.44	0.47
3:B:66:PHE:CD2	11:B:1204:CL7:HBC3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1215:CL7:CGA	11:B:1215:CL7:H3A	2.44	0.47
1:D:27:GLU:HA	1:D:27:GLU:OE1	2.15	0.47
2:A:277:THR:HA	11:A:1115:CL7:HED1	1.97	0.47
11:A:1106:CL7:CAD	11:A:1126:CL7:HBA2	2.45	0.47
3:B:366:VAL:HG22	3:B:732:THR:HG22	1.97	0.47
4:C:61:ASP:HA	4:C:62:PHE:HA	1.49	0.47
3:B:46:ILE:O	3:B:50:HIS:ND1	2.47	0.47
11:A:1237:CL7:H62C	11:A:1237:CL7:H41C	1.53	0.46
3:B:179:LEU:HA	3:B:183:PHE:HD2	1.80	0.46
3:B:442:THR:HG21	11:B:1230:CL7:HAC2	1.96	0.46
11:B:1238:CL7:H41C	11:B:1238:CL7:H62C	1.67	0.46
6:F:101:ILE:HG12	11:F:1301:CL7:C1D	2.46	0.46
2:A:67:GLU:OE1	2:A:188:LEU:N	2.47	0.46
11:A:1022:CL7:O1A	3:B:658:LEU:HD12	2.15	0.46
3:B:439:HIS:HE1	11:B:1230:CL7:C1A	2.10	0.46
2:A:193:ASN:HB3	2:A:196:SER:HB3	1.98	0.46
2:A:524:MET:HE3	2:A:524:MET:HA	1.96	0.46
16:B:1023:PHO:H3A	16:B:1023:PHO:H2	1.98	0.46
2:A:548:VAL:HG11	11:A:1137:CL7:HMB3	1.97	0.46
2:A:481:PRO:O	2:A:485:GLN:HG3	2.15	0.46
11:A:1101:CL7:H8	7:J:25:ALA:HA	1.98	0.46
11:B:1204:CL7:HBA1	11:B:1204:CL7:H3A	1.56	0.46
11:A:1126:CL7:HBA1	11:A:1126:CL7:H3A	1.48	0.46
3:B:277:HIS:HE1	11:B:1215:CL7:C1A	2.29	0.46
2:A:311:MET:HE3	2:A:312:TYR:CZ	2.50	0.46
6:F:89:ILE:CG1	6:F:90:PRO:HD3	2.46	0.46
2:A:297:HIS:HE2	11:A:1117:CL7:CMB	2.29	0.46
11:A:1129:CL7:HMA1	8:L:19:THR:HG21	1.97	0.46
11:A:1136:CL7:H8	11:A:1136:CL7:H52C	1.64	0.46
12:A:2001:PQN:H241	12:A:2001:PQN:H262	1.73	0.46
3:B:600:LYS:HD3	11:B:1234:CL7:HBC1	1.97	0.46
10:W:9:ILE:HG23	11:W:2601:CL7:HBA1	1.97	0.46
1:D:10:PRO:HB3	1:D:51:MET:HA	1.98	0.45
2:A:408:HIS:HE1	11:A:1128:CL7:C1A	2.25	0.45
2:A:452:SER:HB2	2:A:539:ILE:HD13	1.98	0.45
2:A:542:PHE:CZ	16:B:1023:PHO:HBA2	2.51	0.45
11:A:1112:CL7:HBA1	11:A:1112:CL7:H3A	1.43	0.45
10:W:30:VAL:HG23	10:W:31:GLU:OE1	2.16	0.45
2:A:433:HIS:CE1	2:A:437:ILE:HD11	2.51	0.45
11:A:1101:CL7:H71C	11:A:1101:CL7:H112	1.66	0.45
3:B:436:VAL:O	3:B:440:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:588:SER:O	2:A:592:HIS:ND1	2.43	0.45
3:B:230:TRP:HB2	11:B:1213:CL7:HBA1	1.99	0.45
1:D:20:LEU:HA	3:B:687:ARG:HH21	1.80	0.45
11:B:1206:CL7:HBA1	11:B:1206:CL7:H3A	1.81	0.45
2:A:162:ALA:HB2	11:A:1112:CL7:HBA2	1.97	0.45
3:B:169:ARG:HD3	3:B:169:ARG:HA	1.74	0.45
3:B:663:GLY:O	3:B:667:LEU:HD23	2.16	0.45
11:B:1213:CL7:HBA1	11:B:1213:CL7:H3A	1.66	0.45
4:C:25:VAL:O	4:C:43:PRO:HD2	2.17	0.45
2:A:195:GLU:HB3	2:A:312:TYR:HB3	1.97	0.45
5:E:43:CYS:HB2	5:E:54:GLY:HA3	1.97	0.45
1:D:60:LEU:HB2	1:D:66:CYS:SG	2.57	0.45
3:B:182:LEU:HD21	11:B:1225:CL7:H141	1.99	0.45
3:B:524:HIS:CD2	11:B:1235:CL7:NB	2.85	0.45
11:A:1123:CL7:HBA1	11:A:1123:CL7:H12C	1.69	0.45
2:A:735:LEU:HD22	11:A:1140:CL7:HMA3	1.99	0.44
11:B:1012:CL7:H41C	11:B:1012:CL7:H61C	1.56	0.44
5:E:26:SER:O	5:E:37:ILE:HG22	2.17	0.44
3:B:403:ASN:HB3	3:B:406:ASN:HD21	1.80	0.44
3:B:619:LEU:HD13	11:B:1012:CL7:H11C	2.00	0.44
2:A:599:TRP:CH2	11:A:1022:CL7:HAB	2.52	0.44
3:B:193:HIS:HB2	11:B:1211:CL7:C1C	2.48	0.44
3:B:384:ILE:CG1	3:B:586:MET:HG3	2.48	0.44
2:A:218:ILE:HG12	11:A:1113:CL7:HBC3	1.99	0.44
6:F:80:PRO:HG2	6:F:83:ARG:HB2	1.98	0.44
6:F:110:ILE:HA	6:F:113:ARG:HD3	1.99	0.44
10:W:11:THR:HB	10:W:12:PRO:HD3	1.99	0.44
2:A:374:MET:HG3	2:A:508:SER:HB2	2.00	0.44
11:A:1022:CL7:O1A	11:A:1022:CL7:H3A	2.17	0.44
3:B:49:THR:HG21	11:B:1202:CL7:CAB	2.47	0.44
2:A:241:HIS:CE1	11:A:1114:CL7:C1A	3.01	0.44
2:A:374:MET:CE	11:A:1116:CL7:HBD	2.48	0.44
2:A:441:LEU:HG	2:A:549:LEU:HB2	2.00	0.44
3:B:556:PHE:HZ	4:C:66:ARG:HD2	1.83	0.44
2:A:312:TYR:CZ	2:A:322:MET:HE1	2.52	0.44
3:B:47:PHE:CE2	3:B:51:PHE:HE2	2.35	0.44
3:B:458:ILE:HD11	6:F:76:ILE:HG23	2.00	0.44
11:L:1502:CL7:H62C	11:L:1502:CL7:H41C	1.76	0.44
2:A:458:HIS:CE1	11:A:1132:CL7:C4D	3.00	0.44
11:A:1106:CL7:C3D	11:A:1126:CL7:HBA2	2.48	0.44
4:C:9:ASP:OD1	4:C:9:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:SER:OG	1:D:52:ASN:O	2.34	0.43
2:A:338:HIS:CE1	14:A:5003:LHG:HC12	2.53	0.43
2:A:576:CYS:HB3	13:A:3001:SF4:S2	2.57	0.43
2:A:721:SER:H	2:A:724:GLN:NE2	2.08	0.43
11:A:1135:CL7:H3A	11:A:1136:CL7:CAA	2.48	0.43
3:B:450:GLU:HA	6:F:72:LEU:HD22	2.00	0.43
3:B:531:HIS:HE1	11:B:1236:CL7:C4D	2.29	0.43
11:B:1205:CL7:HBA1	11:B:1205:CL7:H3A	1.58	0.43
6:F:79:GLY:N	6:F:80:PRO:HD3	2.33	0.43
8:L:43:ALA:HB1	8:L:126:VAL:HG23	1.99	0.43
2:A:146:HIS:NE2	2:A:379:TYR:O	2.44	0.43
11:B:1021:CL7:H3A	11:B:1021:CL7:HBA2	1.37	0.43
11:B:1238:CL7:HAB	12:B:2002:PQN:H141	1.98	0.43
6:F:65:LEU:HD23	6:F:65:LEU:H	1.83	0.43
1:D:20:LEU:HD23	3:B:687:ARG:HH21	1.82	0.43
2:A:678:HIS:CD2	15:A:1011:G9R:NB	2.86	0.43
3:B:551:PRO:HD2	4:C:62:PHE:CE2	2.53	0.43
3:B:661:ALA:CB	16:B:1023:PHO:HBB2	2.48	0.43
2:A:153:MET:HE2	2:A:159:LEU:HD23	1.99	0.43
2:A:717:PRO:HB3	11:A:1139:CL7:C2C	2.48	0.43
11:A:1022:CL7:H162	16:B:1023:PHO:H202	2.00	0.43
11:A:1132:CL7:H141	11:A:1132:CL7:H161	1.70	0.43
2:A:59:PHE:CE1	11:A:1102:CL7:HED1	2.54	0.43
2:A:374:MET:SD	11:A:1125:CL7:HMC2	2.59	0.43
11:A:1119:CL7:HAA1	11:A:1123:CL7:C4B	2.49	0.43
11:A:1119:CL7:HAA2	11:A:1119:CL7:HBD	1.99	0.43
3:B:657:HIS:HD2	11:B:1021:CL7:CHB	2.32	0.43
6:F:113:ARG:HA	6:F:120:PRO:HB3	1.99	0.43
2:A:418:ASP:HB3	2:A:421:VAL:HG12	2.01	0.43
2:A:434:ARG:HA	2:A:437:ILE:HD12	1.99	0.43
11:A:1111:CL7:HED2	11:A:1111:CL7:HBD	1.71	0.43
11:A:1140:CL7:HBA1	11:A:1140:CL7:H3A	1.62	0.43
4:C:61:ASP:HB3	5:E:58:ASN:ND2	2.34	0.43
11:L:1501:CL7:HBD	11:L:1501:CL7:HED2	1.74	0.43
1:D:80:MET:SD	1:D:80:MET:N	2.92	0.43
2:A:686:MET:HE1	12:A:2001:PQN:H2M3	2.00	0.43
2:A:711:ILE:HG22	6:F:106:ARG:HG3	2.00	0.43
2:A:746:LEU:HA	2:A:746:LEU:HD23	1.71	0.43
2:A:408:HIS:HE1	11:A:1128:CL7:C4A	2.27	0.43
3:B:375:HIS:CD2	11:B:1225:CL7:NC	2.87	0.43
1:D:29:TYR:CE2	1:D:63:LYS:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:363:GLN:OE1	3:B:363:GLN:N	2.52	0.43
2:A:65:ASP:OD1	2:A:66:LEU:N	2.52	0.42
2:A:311:MET:HE3	2:A:312:TYR:CE1	2.54	0.42
2:A:706:HIS:CE1	11:A:1138:CL7:C4D	2.98	0.42
11:A:1022:CL7:C2	3:B:654:LEU:HB3	2.48	0.42
11:A:1110:CL7:CED	11:A:1110:CL7:H2A	2.49	0.42
3:B:345:THR:HB	3:B:379:ALA:HB2	2.00	0.42
2:A:121:ILE:HD11	7:J:36:LEU:HD12	1.99	0.42
11:B:1239:CL7:H61C	11:B:1239:CL7:H41C	1.61	0.42
2:A:219:HIS:HE1	11:A:1113:CL7:ND	2.18	0.42
2:A:345:LEU:HD23	2:A:345:LEU:HA	1.93	0.42
2:A:537:HIS:CD2	11:A:1135:CL7:C1B	3.03	0.42
2:A:545:HIS:HE1	11:A:1137:CL7:C4D	2.32	0.42
3:B:68:VAL:HG11	3:B:124:TRP:CH2	2.54	0.42
3:B:175:MET:SD	3:B:179:LEU:HD23	2.59	0.42
2:A:204:VAL:HG11	11:A:1110:CL7:HAC1	2.01	0.42
3:B:64:HIS:NE2	11:B:1205:CL7:HAA1	2.34	0.42
3:B:142:LEU:HA	3:B:145:VAL:HG12	2.01	0.42
3:B:276:HIS:HA	11:B:1214:CL7:C1B	2.50	0.42
3:B:522:VAL:HG11	3:B:596:TYR:CG	2.54	0.42
2:A:276:LEU:O	11:A:1115:CL7:HMA3	2.19	0.42
11:A:1022:CL7:H12C	3:B:658:LEU:HD12	2.00	0.42
3:B:140:VAL:O	3:B:144:ILE:HG12	2.20	0.42
3:B:437:TYR:CE1	3:B:521:LEU:HB3	2.55	0.42
6:F:111:ALA:O	6:F:116:ASN:ND2	2.52	0.42
8:L:20:PRO:O	8:L:24:SER:OG	2.37	0.42
2:A:525:GLN:HG2	2:A:526:HIS:H	1.85	0.42
3:B:355:LEU:HD11	11:B:1223:CL7:CAB	2.50	0.42
11:B:1213:CL7:HED3	11:B:1213:CL7:HBD	1.92	0.42
2:A:696:GLN:NE2	2:A:719:ALA:H	2.17	0.42
3:B:195:ILE:HD13	11:B:1212:CL7:HAC1	2.02	0.42
3:B:432:HIS:HB3	17:J:4015:8CT:C27	2.50	0.42
3:B:116:CYS:HA	11:B:1205:CL7:OBD	2.19	0.42
3:B:276:HIS:ND1	11:B:1214:CL7:C4A	2.81	0.42
11:B:1203:CL7:H93C	11:B:1203:CL7:H112	1.82	0.42
2:A:694:TYR:OH	16:A:1013:PHO:OBD	2.36	0.42
11:A:1130:CL7:HED1	8:L:17:LEU:HB2	2.02	0.42
11:A:1237:CL7:H143	11:A:1237:CL7:H111	1.76	0.42
11:B:1226:CL7:H41C	11:B:1226:CL7:H101	2.01	0.42
6:F:55:GLN:O	6:F:59:GLU:OE1	2.38	0.42
2:A:310:HIS:HD2	11:A:1118:CL7:C1A	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:465:LEU:HD22	3:B:96:LEU:HA	2.02	0.42
11:A:1103:CL7:H93C	11:A:1103:CL7:H112	1.95	0.42
11:A:1121:CL7:HBA2	11:A:1121:CL7:H3A	1.46	0.42
11:A:1122:CL7:O1A	11:A:1122:CL7:H3A	2.20	0.42
3:B:77:TRP:CZ3	3:B:121:TYR:HB3	2.55	0.42
3:B:522:VAL:HG11	3:B:596:TYR:HB2	2.02	0.42
2:A:116:HIS:NE2	11:A:1106:CL7:C4D	2.75	0.41
2:A:579:PRO:HD3	3:B:564:GLY:HA2	2.02	0.41
11:B:1021:CL7:H193	11:B:1021:CL7:H162	1.81	0.41
8:L:56:TYR:CD1	8:L:141:ALA:HB2	2.55	0.41
8:L:73:MET:HE3	8:L:73:MET:HB3	1.88	0.41
11:W:2601:CL7:H3A	11:W:2601:CL7:CGA	2.50	0.41
3:B:585:TRP:CH2	11:B:1012:CL7:HAB	2.55	0.41
2:A:129:ALA:N	2:A:137:GLY:O	2.53	0.41
2:A:316:TRP:HZ3	11:A:1118:CL7:HBD	1.84	0.41
11:A:1104:CL7:HBA1	11:A:1104:CL7:CGD	2.50	0.41
11:A:1140:CL7:H2	16:A:1013:PHO:H191	2.03	0.41
3:B:4:LYS:HE2	3:B:4:LYS:HB3	1.85	0.41
3:B:527:ALA:HB2	11:B:1236:CL7:HED2	2.02	0.41
8:L:91:VAL:O	8:L:95:ILE:HG12	2.20	0.41
2:A:77:HIS:HB3	11:A:1111:CL7:CGD	2.50	0.41
2:A:241:HIS:CE1	11:A:1114:CL7:NA	2.88	0.41
2:A:422:ASN:HA	2:A:425:ASN:HD21	1.85	0.41
2:A:732:HIS:HE1	11:A:1140:CL7:ND	2.14	0.41
11:A:1115:CL7:H2A	11:A:1115:CL7:CED	2.50	0.41
3:B:634:LEU:HD13	3:B:730:GLY:HA3	2.02	0.41
2:A:201:HIS:CD2	11:A:1111:CL7:NB	2.88	0.41
2:A:393:HIS:O	2:A:397:ILE:HG12	2.21	0.41
3:B:276:HIS:ND1	11:B:1214:CL7:C1B	2.68	0.41
3:B:384:ILE:HG13	3:B:586:MET:HG3	2.02	0.41
3:B:388:ALA:O	3:B:392:ILE:HG13	2.21	0.41
4:C:77:MET:HE2	4:C:77:MET:HB3	1.82	0.41
6:F:84:ALA:HA	6:F:88:LEU:HD13	2.02	0.41
2:A:448:LEU:HD11	11:A:1136:CL7:HMB2	2.02	0.41
2:A:471:MET:HE3	2:A:471:MET:HB2	1.89	0.41
11:A:1137:CL7:CED	11:A:1137:CL7:H2A	2.50	0.41
16:A:1013:PHO:H62	16:A:1013:PHO:H92	1.77	0.41
3:B:276:HIS:HA	11:B:1214:CL7:C2B	2.51	0.41
2:A:127:LEU:HD11	11:A:1107:CL7:HAC2	2.03	0.41
2:A:388:LEU:O	2:A:392:VAL:HG12	2.20	0.41
11:A:1104:CL7:H152	11:A:1127:CL7:HAB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:34:HIS:HB2	3:B:37:MET:HE3	2.03	0.41
3:B:144:ILE:O	3:B:148:VAL:HG23	2.21	0.41
3:B:421:HIS:HE1	11:B:1228:CL7:NA	2.19	0.41
16:B:1023:PHO:HED2	16:B:1023:PHO:HBD	1.87	0.41
2:A:301:LEU:CD2	11:A:1117:CL7:HAB	2.51	0.41
2:A:482:ILE:HG13	2:A:483:PHE:CD1	2.56	0.41
2:A:658:GLN:HG2	2:A:751:ALA:HB3	2.01	0.41
11:A:1802:CL7:HBA2	11:A:1802:CL7:H3A	1.66	0.41
3:B:195:ILE:HA	3:B:199:ILE:HD12	2.02	0.41
1:D:17:GLY:HA2	2:A:562:ARG:NH2	2.35	0.41
2:A:559:ARG:HG3	2:A:568:ALA:HB2	2.03	0.41
11:A:1102:CL7:H3A	11:A:1102:CL7:HBA2	1.66	0.41
11:A:1128:CL7:H162	11:A:1128:CL7:H141	1.71	0.41
3:B:53:HIS:O	3:B:57:ILE:HG13	2.21	0.41
3:B:524:HIS:HE1	11:B:1235:CL7:C4D	2.34	0.41
11:B:1238:CL7:H111	11:B:1238:CL7:H142	1.83	0.41
16:B:1023:PHO:H3A	16:B:1023:PHO:CGA	2.45	0.41
2:A:90:GLY:HA3	11:A:1105:CL7:HAB	2.03	0.41
2:A:197:THR:OG1	11:A:1111:CL7:HBC3	2.21	0.41
2:A:346:THR:HG23	2:A:347:THR:HG23	2.03	0.41
11:A:1101:CL7:H202	11:A:1126:CL7:H193	2.02	0.41
2:A:514:ASP:OD1	2:A:515:PRO:HD2	2.20	0.40
11:A:1130:CL7:HBA2	11:A:1130:CL7:H3A	1.85	0.40
3:B:167:TRP:HH2	11:B:1208:CL7:HMB1	1.86	0.40
11:B:1238:CL7:H162	11:B:1238:CL7:H121	1.82	0.40
2:A:458:HIS:HE1	11:A:1132:CL7:C4D	2.34	0.40
11:A:1131:CL7:H142	11:A:1131:CL7:H111	1.86	0.40
2:A:434:ARG:O	2:A:438:ILE:HG12	2.22	0.40
11:A:1022:CL7:H12C	11:A:1022:CL7:H52C	1.94	0.40
3:B:142:LEU:HA	3:B:142:LEU:HD23	1.92	0.40
2:A:448:LEU:HD13	2:A:542:PHE:HA	2.04	0.40
16:A:1013:PHO:CBB	16:A:1013:PHO:HHC	2.51	0.40
3:B:341:LEU:O	3:B:345:THR:OG1	2.26	0.40
3:B:586:MET:HG2	11:B:1222:CL7:HBC1	2.03	0.40
6:F:117:ALA:C	6:F:119:ASN:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	92/139 (66%)	90 (98%)	2 (2%)	0	100	100
2	A	724/753 (96%)	687 (95%)	37 (5%)	0	100	100
3	B	653/736 (89%)	631 (97%)	22 (3%)	0	100	100
4	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
5	E	56/89 (63%)	53 (95%)	3 (5%)	0	100	100
6	F	101/167 (60%)	96 (95%)	5 (5%)	0	100	100
7	J	19/51 (37%)	19 (100%)	0	0	100	100
8	L	142/153 (93%)	137 (96%)	5 (4%)	0	100	100
9	M	28/31 (90%)	28 (100%)	0	0	100	100
10	W	26/34 (76%)	23 (88%)	3 (12%)	0	100	100
All	All	1919/2234 (86%)	1838 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	78/112 (70%)	78 (100%)	0	100	100
2	A	584/606 (96%)	584 (100%)	0	100	100
3	B	531/594 (89%)	531 (100%)	0	100	100
4	C	68/69 (99%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	49/69 (71%)	49 (100%)	0	100	100
6	F	79/133 (59%)	79 (100%)	0	100	100
7	J	17/46 (37%)	17 (100%)	0	100	100
8	L	104/112 (93%)	104 (100%)	0	100	100
9	M	24/25 (96%)	24 (100%)	0	100	100
10	W	21/26 (81%)	21 (100%)	0	100	100
All	All	1555/1792 (87%)	1555 (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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	39	GLN
2	A	225	ASN
2	A	442	ASN
3	B	10	GLN
3	B	132	ASN
3	B	174	GLN
3	B	211	ASN
3	B	275	HIS
3	B	613	ASN
3	B	692	ASN
6	F	46	ASN
8	L	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

100 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$
11	CL7	A	1801	-	51,53,73	1.96	11 (21%)	56,89,113	2.67	18 (32%)
11	CL7	A	1109	11	51,53,73	1.96	11 (21%)	56,89,113	2.67	19 (33%)
11	CL7	A	1128	2	71,73,73	1.68	12 (16%)	80,113,113	2.42	20 (25%)
11	CL7	B	1206	3	51,53,73	1.96	12 (23%)	56,89,113	2.65	18 (32%)
15	G9R	A	1011	2	69,73,73	1.60	12 (17%)	83,113,113	2.17	23 (27%)
17	8CT	B	4017	-	40,41,41	4.73	25 (62%)	50,56,56	3.46	24 (48%)
16	PHO	A	1013	2	58,69,69	2.24	10 (17%)	56,99,99	1.47	8 (14%)
17	8CT	J	4015	-	40,41,41	4.74	25 (62%)	50,56,56	2.71	19 (38%)
11	CL7	B	1210	-	51,53,73	1.97	11 (21%)	56,89,113	2.70	18 (32%)
11	CL7	A	1132	2,8	71,73,73	1.67	13 (18%)	80,113,113	2.29	23 (28%)
17	8CT	A	4007	-	40,41,41	4.73	25 (62%)	50,56,56	3.21	21 (42%)
11	CL7	A	1129	2	51,53,73	1.94	11 (21%)	56,89,113	2.63	19 (33%)
11	CL7	B	1226	3	71,73,73	1.68	13 (18%)	80,113,113	2.43	22 (27%)
13	SF4	C	3003	4	0,12,12	-	-	-	-	-
17	8CT	W	4020	-	40,41,41	4.72	25 (62%)	50,56,56	2.46	18 (36%)
11	CL7	A	1123	-	71,73,73	1.69	12 (16%)	80,113,113	2.32	22 (27%)
11	CL7	A	1116	2	51,53,73	1.96	12 (23%)	56,89,113	2.65	18 (32%)
11	CL7	A	1136	2	71,73,73	1.70	12 (16%)	80,113,113	2.32	22 (27%)
11	CL7	A	1138	2	51,53,73	1.94	11 (21%)	56,89,113	2.68	19 (33%)
11	CL7	A	1107	2	51,53,73	1.95	11 (21%)	56,89,113	2.69	20 (35%)
11	CL7	W	2601	-	51,53,73	1.96	11 (21%)	56,89,113	2.70	18 (32%)
11	CL7	A	1110	2	51,53,73	1.95	12 (23%)	56,89,113	2.74	20 (35%)
11	CL7	A	1124	2	51,53,73	1.95	12 (23%)	56,89,113	2.67	20 (35%)
12	PQN	A	2001	-	34,34,34	3.52	17 (50%)	42,45,45	2.12	3 (7%)
17	8CT	L	4020	-	40,41,41	4.73	25 (62%)	50,56,56	2.55	17 (34%)
11	CL7	A	1111	2	51,53,73	1.97	12 (23%)	56,89,113	2.66	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CL7	A	1106	2	71,73,73	1.67	12 (16%)	80,113,113	2.31	21 (26%)
11	CL7	A	1105	2	51,53,73	1.97	11 (21%)	56,89,113	2.83	18 (32%)
11	CL7	J	1302	-	51,53,73	1.97	11 (21%)	56,89,113	2.67	19 (33%)
11	CL7	B	1236	3	51,53,73	1.96	11 (21%)	56,89,113	2.70	19 (33%)
11	CL7	B	1228	3	51,53,73	1.96	12 (23%)	56,89,113	2.64	19 (33%)
11	CL7	F	1301	-	51,53,73	1.98	11 (21%)	56,89,113	2.68	19 (33%)
13	SF4	C	3002	4	0,12,12	-	-	-		
11	CL7	B	1239	3	71,73,73	1.68	12 (16%)	80,113,113	2.33	20 (25%)
11	CL7	A	1140	2	71,73,73	1.68	12 (16%)	80,113,113	2.28	20 (25%)
11	CL7	L	1502	8	71,73,73	1.69	12 (16%)	80,113,113	2.31	21 (26%)
11	CL7	L	1503	-	51,53,73	1.95	12 (23%)	56,89,113	2.67	19 (33%)
11	CL7	A	1131	2	71,73,73	1.68	12 (16%)	80,113,113	2.32	21 (26%)
11	CL7	A	1119	-	51,53,73	1.95	12 (23%)	56,89,113	2.69	19 (33%)
11	CL7	A	1121	2	51,53,73	1.95	12 (23%)	56,89,113	2.67	18 (32%)
17	8CT	B	4014	-	40,41,41	4.75	25 (62%)	50,56,56	2.42	15 (30%)
11	CL7	A	1139	2	51,53,73	1.98	12 (23%)	56,89,113	2.66	18 (32%)
11	CL7	A	1102	11,2	51,53,73	1.95	11 (21%)	56,89,113	2.69	19 (33%)
11	CL7	A	1103	-	71,73,73	1.69	12 (16%)	80,113,113	2.29	20 (25%)
11	CL7	B	1229	3	51,53,73	1.96	12 (23%)	56,89,113	2.67	19 (33%)
11	CL7	B	1202	-	51,53,73	1.95	12 (23%)	56,89,113	2.67	17 (30%)
11	CL7	L	1501	8	71,73,73	1.68	12 (16%)	80,113,113	2.32	22 (27%)
11	CL7	B	1201	-	51,53,73	1.95	12 (23%)	56,89,113	2.66	20 (35%)
11	CL7	A	1101	-	71,73,73	1.69	11 (15%)	80,113,113	2.30	20 (25%)
11	CL7	A	1120	2	51,53,73	1.97	11 (21%)	56,89,113	2.69	20 (35%)
11	CL7	B	1207	3	51,53,73	1.95	12 (23%)	56,89,113	2.67	19 (33%)
11	CL7	B	1238	-	71,73,73	1.69	12 (16%)	80,113,113	2.31	21 (26%)
11	CL7	B	1021	11,3	71,73,73	1.65	12 (16%)	80,113,113	2.38	21 (26%)
17	8CT	A	4011	-	40,41,41	4.74	25 (62%)	50,56,56	2.86	18 (36%)
17	8CT	W	4018	-	40,41,41	4.76	25 (62%)	50,56,56	2.57	20 (40%)
11	CL7	B	1222	-	51,53,73	1.95	12 (23%)	56,89,113	2.66	20 (35%)
11	CL7	A	1104	-	71,73,73	1.70	13 (18%)	80,113,113	2.31	21 (26%)
11	CL7	B	1208	3	51,53,73	1.96	11 (21%)	56,89,113	2.66	20 (35%)
16	PHO	B	1023	-	58,69,69	2.21	10 (17%)	56,99,99	1.44	8 (14%)
11	CL7	B	1211	-	51,53,73	1.96	12 (23%)	56,89,113	2.64	17 (30%)
11	CL7	A	1127	11,2	51,53,73	1.97	12 (23%)	56,89,113	2.65	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	8CT	L	4019	-	40,41,41	4.76	24 (60%)	50,56,56	2.40	18 (36%)
11	CL7	A	1135	2	51,53,73	1.96	12 (23%)	56,89,113	2.71	19 (33%)
11	CL7	A	1118	2	51,53,73	1.96	11 (21%)	56,89,113	2.68	19 (33%)
11	CL7	B	1223	3	51,53,73	1.96	11 (21%)	56,89,113	2.69	19 (33%)
11	CL7	B	1212	3	51,53,73	1.97	11 (21%)	56,89,113	2.67	20 (35%)
11	CL7	B	1203	3	71,73,73	1.69	12 (16%)	80,113,113	2.31	22 (27%)
17	8CT	M	4021	-	40,41,41	4.76	25 (62%)	50,56,56	2.87	18 (36%)
11	CL7	B	1215	3	51,53,73	1.96	12 (23%)	56,89,113	2.69	20 (35%)
11	CL7	B	1213	-	51,53,73	1.97	11 (21%)	56,89,113	2.67	19 (33%)
12	PQN	B	2002	3	34,34,34	3.53	16 (47%)	42,45,45	2.20	3 (7%)
11	CL7	B	1204	3	51,53,73	1.95	12 (23%)	56,89,113	2.69	21 (37%)
11	CL7	B	1205	3	51,53,73	1.94	12 (23%)	56,89,113	2.69	17 (30%)
11	CL7	A	1113	2	51,53,73	1.96	11 (21%)	56,89,113	2.68	20 (35%)
14	LHG	A	5001	-	48,48,48	2.47	34 (70%)	51,54,54	1.62	7 (13%)
17	8CT	A	4008	-	40,41,41	4.72	24 (60%)	50,56,56	3.57	23 (46%)
11	CL7	A	1115	2	51,53,73	1.96	12 (23%)	56,89,113	2.71	19 (33%)
11	CL7	A	1237	-	71,73,73	1.68	12 (16%)	80,113,113	2.32	21 (26%)
14	LHG	A	5003	2	48,48,48	2.47	35 (72%)	51,54,54	1.62	7 (13%)
11	CL7	A	1130	2,8	51,53,73	1.95	12 (23%)	56,89,113	2.69	20 (35%)
11	CL7	A	1117	2	71,73,73	1.68	12 (16%)	80,113,113	2.29	20 (25%)
11	CL7	B	1225	3	71,73,73	1.68	13 (18%)	80,113,113	2.29	22 (27%)
17	8CT	J	4013	-	40,41,41	4.78	25 (62%)	50,56,56	2.53	18 (36%)
11	CL7	B	1230	3	51,53,73	1.95	12 (23%)	56,89,113	2.62	17 (30%)
11	CL7	A	1114	2	51,53,73	2.01	12 (23%)	56,89,113	2.62	20 (35%)
11	CL7	B	1214	3	51,53,73	1.97	12 (23%)	56,89,113	2.77	20 (35%)
11	CL7	B	1224	3	51,53,73	1.94	12 (23%)	56,89,113	2.64	17 (30%)
11	CL7	A	1022	11	71,73,73	1.69	13 (18%)	80,113,113	2.32	22 (27%)
11	CL7	A	1122	2	51,53,73	1.95	11 (21%)	56,89,113	2.67	19 (33%)
11	CL7	B	1012	-	71,73,73	1.68	11 (15%)	80,113,113	2.30	20 (25%)
11	CL7	A	1137	2	51,53,73	1.93	12 (23%)	56,89,113	2.72	21 (37%)
11	CL7	B	1235	3	51,53,73	1.95	11 (21%)	56,89,113	2.67	20 (35%)
17	8CT	B	4006	-	40,41,41	4.74	25 (62%)	50,56,56	2.58	16 (32%)
13	SF4	A	3001	2,3	0,12,12	-	-	-	-	-
11	CL7	A	1802	-	51,53,73	1.97	11 (21%)	56,89,113	2.68	20 (35%)
11	CL7	B	1234	3	51,53,73	1.96	12 (23%)	56,89,113	2.69	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CL7	A	1126	11,2	71,73,73	1.69	12 (16%)	80,113,113	2.26	19 (23%)
18	LMG	B	5002	-	51,51,55	2.84	30 (58%)	59,59,63	0.95	2 (3%)
11	CL7	A	1125	2	71,73,73	1.68	12 (16%)	80,113,113	2.34	22 (27%)
11	CL7	A	1112	-	51,53,73	1.96	11 (21%)	56,89,113	2.65	19 (33%)

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
11	CL7	A	1801	-	2/2/11/20	10/15/91/115	-
11	CL7	A	1109	11	2/2/11/20	7/15/91/115	-
11	CL7	A	1128	2	2/2/15/20	14/39/115/115	-
11	CL7	B	1206	3	2/2/11/20	10/15/91/115	-
15	G9R	A	1011	2	1/1/15/20	19/39/115/115	-
17	8CT	B	4017	-	-	9/29/63/63	0/2/2/2
16	PHO	A	1013	2	-	18/37/103/103	0/5/6/6
17	8CT	J	4015	-	-	11/29/63/63	0/2/2/2
11	CL7	B	1210	-	2/2/11/20	7/15/91/115	-
11	CL7	A	1132	2,8	2/2/15/20	16/39/115/115	-
17	8CT	A	4007	-	-	6/29/63/63	0/2/2/2
11	CL7	A	1129	2	2/2/11/20	8/15/91/115	-
11	CL7	B	1226	3	2/2/15/20	22/39/115/115	-
13	SF4	C	3003	4	-	-	0/6/5/5
17	8CT	W	4020	-	-	11/29/63/63	0/2/2/2
11	CL7	A	1123	-	2/2/15/20	14/39/115/115	-
11	CL7	A	1116	2	2/2/11/20	3/15/91/115	-
11	CL7	A	1136	2	2/2/15/20	18/39/115/115	-
11	CL7	A	1138	2	2/2/11/20	8/15/91/115	-
11	CL7	A	1107	2	2/2/11/20	5/15/91/115	-
11	CL7	W	2601	-	2/2/11/20	5/15/91/115	-
11	CL7	A	1110	2	2/2/11/20	5/15/91/115	-
11	CL7	A	1124	2	2/2/11/20	7/15/91/115	-
12	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
17	8CT	L	4020	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CL7	A	1111	2	2/2/11/20	9/15/91/115	-
11	CL7	A	1106	2	2/2/15/20	20/39/115/115	-
11	CL7	A	1105	2	2/2/11/20	9/15/91/115	-
11	CL7	J	1302	-	2/2/11/20	10/15/91/115	-
11	CL7	B	1236	3	2/2/11/20	7/15/91/115	-
11	CL7	B	1228	3	2/2/11/20	8/15/91/115	-
11	CL7	F	1301	-	2/2/11/20	7/15/91/115	-
13	SF4	C	3002	4	-	-	0/6/5/5
11	CL7	B	1239	3	2/2/15/20	15/39/115/115	-
11	CL7	A	1140	2	2/2/15/20	14/39/115/115	-
11	CL7	L	1502	8	2/2/15/20	15/39/115/115	-
11	CL7	L	1503	-	2/2/11/20	7/15/91/115	-
11	CL7	A	1131	2	2/2/15/20	20/39/115/115	-
11	CL7	A	1119	-	2/2/11/20	6/15/91/115	-
11	CL7	A	1121	2	2/2/11/20	7/15/91/115	-
17	8CT	B	4014	-	-	6/29/63/63	0/2/2/2
11	CL7	A	1139	2	2/2/11/20	5/15/91/115	-
11	CL7	A	1102	11,2	2/2/11/20	6/15/91/115	-
11	CL7	A	1103	-	2/2/15/20	16/39/115/115	-
11	CL7	B	1229	3	2/2/11/20	6/15/91/115	-
11	CL7	B	1202	-	2/2/11/20	8/15/91/115	-
11	CL7	L	1501	8	2/2/15/20	16/39/115/115	-
11	CL7	B	1201	-	2/2/11/20	6/15/91/115	-
11	CL7	A	1101	-	2/2/15/20	15/39/115/115	-
11	CL7	A	1120	2	2/2/11/20	5/15/91/115	-
11	CL7	B	1207	3	2/2/11/20	6/15/91/115	-
11	CL7	B	1238	-	2/2/15/20	16/39/115/115	-
11	CL7	B	1021	11,3	2/2/15/20	24/39/115/115	-
17	8CT	A	4011	-	-	14/29/63/63	0/2/2/2
17	8CT	W	4018	-	-	9/29/63/63	0/2/2/2
11	CL7	B	1222	-	2/2/11/20	7/15/91/115	-
11	CL7	A	1104	-	2/2/15/20	18/39/115/115	-
11	CL7	B	1208	3	2/2/11/20	7/15/91/115	-
16	PHO	B	1023	-	-	14/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CL7	B	1211	-	2/2/11/20	9/15/91/115	-
11	CL7	A	1127	11,2	2/2/11/20	7/15/91/115	-
17	8CT	L	4019	-	-	3/29/63/63	0/2/2/2
11	CL7	A	1135	2	2/2/11/20	11/15/91/115	-
11	CL7	A	1118	2	2/2/11/20	6/15/91/115	-
11	CL7	B	1223	3	2/2/11/20	8/15/91/115	-
11	CL7	B	1212	3	2/2/11/20	9/15/91/115	-
11	CL7	B	1203	3	2/2/15/20	25/39/115/115	-
17	8CT	M	4021	-	-	10/29/63/63	0/2/2/2
11	CL7	B	1215	3	2/2/11/20	6/15/91/115	-
11	CL7	B	1213	-	2/2/11/20	9/15/91/115	-
12	PQN	B	2002	3	-	13/23/43/43	0/2/2/2
11	CL7	B	1204	3	2/2/11/20	7/15/91/115	-
11	CL7	B	1205	3	2/2/11/20	5/15/91/115	-
11	CL7	A	1113	2	2/2/11/20	7/15/91/115	-
14	LHG	A	5001	-	-	21/53/53/53	-
17	8CT	A	4008	-	-	3/29/63/63	0/2/2/2
11	CL7	A	1115	2	2/2/11/20	9/15/91/115	-
11	CL7	A	1237	-	2/2/15/20	18/39/115/115	-
14	LHG	A	5003	2	-	30/53/53/53	-
11	CL7	A	1130	2,8	2/2/11/20	7/15/91/115	-
11	CL7	A	1117	2	2/2/15/20	19/39/115/115	-
11	CL7	B	1225	3	2/2/15/20	17/39/115/115	-
17	8CT	J	4013	-	-	11/29/63/63	0/2/2/2
11	CL7	B	1230	3	2/2/11/20	6/15/91/115	-
11	CL7	A	1114	2	2/2/11/20	6/15/91/115	-
11	CL7	B	1214	3	2/2/11/20	6/15/91/115	-
11	CL7	B	1224	3	2/2/11/20	7/15/91/115	-
11	CL7	A	1022	11	2/2/15/20	14/39/115/115	-
11	CL7	A	1122	2	2/2/11/20	6/15/91/115	-
11	CL7	B	1012	-	2/2/15/20	17/39/115/115	-
11	CL7	A	1137	2	2/2/11/20	8/15/91/115	-
11	CL7	B	1235	3	2/2/11/20	7/15/91/115	-
17	8CT	B	4006	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	A	3001	2,3	-	-	0/6/5/5
11	CL7	A	1802	-	2/2/11/20	9/15/91/115	-
11	CL7	B	1234	3	2/2/11/20	5/15/91/115	-
11	CL7	A	1126	11,2	2/2/15/20	18/39/115/115	-
18	LMG	B	5002	-	-	18/46/66/70	0/1/1/1
11	CL7	A	1125	2	2/2/15/20	17/39/115/115	-
11	CL7	A	1112	-	2/2/11/20	8/15/91/115	-

All (1379) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	4013	8CT	C02-C03	14.95	1.60	1.34
17	L	4019	8CT	C02-C03	14.91	1.60	1.34
17	W	4018	8CT	C02-C03	14.87	1.60	1.34
17	M	4021	8CT	C02-C03	14.86	1.60	1.34
17	A	4008	8CT	C02-C03	14.82	1.60	1.34
17	A	4011	8CT	C02-C03	14.81	1.60	1.34
17	B	4017	8CT	C02-C03	14.74	1.60	1.34
17	B	4006	8CT	C02-C03	14.73	1.60	1.34
17	L	4020	8CT	C02-C03	14.70	1.59	1.34
17	B	4014	8CT	C02-C03	14.68	1.59	1.34
17	J	4015	8CT	C02-C03	14.68	1.59	1.34
17	W	4020	8CT	C02-C03	14.57	1.59	1.34
17	A	4007	8CT	C02-C03	14.53	1.59	1.34
17	W	4018	8CT	C32-C31	13.75	1.59	1.32
17	M	4021	8CT	C32-C31	13.74	1.59	1.32
17	A	4011	8CT	C32-C31	13.72	1.59	1.32
17	A	4007	8CT	C32-C31	13.69	1.59	1.32
17	L	4020	8CT	C32-C31	13.66	1.59	1.32
17	A	4008	8CT	C32-C31	13.65	1.59	1.32
17	J	4013	8CT	C32-C31	13.65	1.59	1.32
17	W	4020	8CT	C32-C31	13.63	1.59	1.32
17	B	4006	8CT	C32-C31	13.61	1.59	1.32
17	B	4014	8CT	C32-C31	13.61	1.59	1.32
17	L	4019	8CT	C32-C31	13.61	1.59	1.32
17	B	4017	8CT	C32-C31	13.57	1.59	1.32
17	J	4015	8CT	C32-C31	13.44	1.59	1.32
17	A	4011	8CT	C34-C35	-9.37	1.34	1.54
17	W	4018	8CT	C34-C35	-9.34	1.35	1.54
17	W	4020	8CT	C34-C35	-9.28	1.35	1.54
17	L	4019	8CT	C34-C35	-9.25	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2002	PQN	O4-C4	9.25	1.42	1.23
12	A	2001	PQN	O4-C4	9.20	1.42	1.23
17	B	4017	8CT	C34-C35	-9.16	1.35	1.54
17	M	4021	8CT	C34-C35	-9.15	1.35	1.54
17	L	4020	8CT	C34-C35	-9.14	1.35	1.54
17	A	4007	8CT	C34-C35	-9.13	1.35	1.54
17	A	4008	8CT	C34-C35	-9.12	1.35	1.54
17	B	4014	8CT	C34-C35	-9.10	1.35	1.54
17	B	4006	8CT	C34-C35	-9.09	1.35	1.54
17	J	4015	8CT	C34-C35	-9.09	1.35	1.54
12	B	2002	PQN	O1-C1	9.09	1.42	1.23
17	J	4013	8CT	C34-C35	-9.08	1.35	1.54
16	A	1013	PHO	C1B-C2B	8.82	1.49	1.39
12	A	2001	PQN	O1-C1	8.75	1.41	1.23
16	B	1023	PHO	C1B-C2B	8.72	1.49	1.39
12	B	2002	PQN	C12-C13	8.18	1.52	1.33
12	A	2001	PQN	C12-C13	8.11	1.52	1.33
16	B	1023	PHO	C1D-C2D	7.75	1.48	1.39
16	A	1013	PHO	C1D-C2D	7.59	1.48	1.39
16	A	1013	PHO	C3B-C4B	7.48	1.50	1.41
17	A	4007	8CT	C04-C03	-7.11	1.44	1.53
17	W	4020	8CT	C04-C03	-7.06	1.44	1.53
17	B	4006	8CT	C04-C03	-7.01	1.44	1.53
16	B	1023	PHO	C3B-C4B	6.96	1.49	1.41
12	A	2001	PQN	C2M-C2	-6.95	1.36	1.50
17	L	4020	8CT	C04-C03	-6.92	1.44	1.53
17	B	4014	8CT	C04-C03	-6.90	1.44	1.53
17	J	4015	8CT	C04-C03	-6.87	1.44	1.53
17	A	4008	8CT	C04-C03	-6.86	1.44	1.53
17	W	4018	8CT	C04-C03	-6.86	1.44	1.53
17	L	4019	8CT	C04-C03	-6.82	1.44	1.53
12	B	2002	PQN	C2M-C2	-6.79	1.36	1.50
17	J	4013	8CT	C04-C03	-6.78	1.44	1.53
17	M	4021	8CT	C04-C03	-6.71	1.44	1.53
17	B	4017	8CT	C04-C03	-6.71	1.44	1.53
17	A	4011	8CT	C04-C03	-6.62	1.44	1.53
17	M	4021	8CT	C05-C06	-6.48	1.36	1.52
17	L	4019	8CT	C05-C06	-6.46	1.36	1.52
17	B	4017	8CT	C05-C06	-6.44	1.36	1.52
17	A	4008	8CT	C05-C06	-6.40	1.36	1.52
17	J	4013	8CT	C05-C06	-6.38	1.36	1.52
17	A	4011	8CT	C05-C06	-6.37	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	2001	PQN	C3-C2	6.34	1.46	1.35
17	W	4018	8CT	C05-C06	-6.32	1.37	1.52
12	B	2002	PQN	C3-C2	6.29	1.46	1.35
17	A	4007	8CT	C05-C06	-6.29	1.37	1.52
17	B	4014	8CT	C05-C06	-6.28	1.37	1.52
18	B	5002	LMG	O6-C1	6.28	1.57	1.41
17	J	4015	8CT	C05-C06	-6.26	1.37	1.52
17	W	4020	8CT	C05-C06	-6.26	1.37	1.52
17	L	4020	8CT	C05-C06	-6.25	1.37	1.52
17	B	4006	8CT	C05-C06	-6.22	1.37	1.52
17	J	4013	8CT	C15-C16	6.17	1.59	1.45
17	B	4017	8CT	C15-C16	6.16	1.59	1.45
17	A	4011	8CT	C15-C16	6.12	1.59	1.45
17	B	4006	8CT	C15-C16	6.12	1.59	1.45
17	L	4019	8CT	C15-C16	6.11	1.59	1.45
17	L	4020	8CT	C15-C16	6.07	1.59	1.45
17	W	4018	8CT	C15-C16	6.07	1.59	1.45
17	J	4015	8CT	C15-C16	6.05	1.58	1.45
17	M	4021	8CT	C15-C16	6.02	1.58	1.45
17	A	4007	8CT	C15-C16	6.01	1.58	1.45
17	B	4014	8CT	C15-C16	6.01	1.58	1.45
17	W	4020	8CT	C15-C16	5.89	1.58	1.45
18	B	5002	LMG	O8-C28	5.87	1.50	1.33
17	A	4008	8CT	C15-C16	5.81	1.58	1.45
17	B	4014	8CT	C11-C12	5.77	1.58	1.45
18	B	5002	LMG	O7-C10	5.76	1.50	1.34
17	B	4006	8CT	C11-C12	5.50	1.57	1.45
14	A	5001	LHG	O8-C23	5.31	1.48	1.33
17	L	4019	8CT	C11-C12	5.31	1.57	1.45
17	L	4020	8CT	C05-C04	5.30	1.66	1.54
17	J	4013	8CT	C11-C12	5.30	1.57	1.45
17	B	4006	8CT	C05-C04	5.29	1.66	1.54
17	W	4018	8CT	C05-C04	5.29	1.66	1.54
17	J	4015	8CT	C05-C04	5.29	1.66	1.54
17	W	4018	8CT	C11-C12	5.28	1.57	1.45
14	A	5003	LHG	O8-C23	5.28	1.48	1.33
17	B	4014	8CT	C05-C04	5.26	1.66	1.54
17	W	4020	8CT	C11-C12	5.26	1.57	1.45
17	J	4015	8CT	C11-C12	5.25	1.57	1.45
11	A	1114	CL7	CHD-C4C	5.25	1.48	1.38
17	A	4007	8CT	C11-C12	5.25	1.57	1.45
11	A	1126	CL7	CHD-C4C	5.25	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	4020	8CT	C11-C12	5.24	1.57	1.45
17	A	4011	8CT	C11-C12	5.24	1.57	1.45
11	A	1139	CL7	CHC-C1C	5.24	1.48	1.38
11	A	1111	CL7	CHD-C4C	5.23	1.48	1.38
17	M	4021	8CT	C11-C12	5.23	1.57	1.45
11	A	1128	CL7	CHC-C1C	5.23	1.48	1.38
14	A	5003	LHG	O7-C7	5.22	1.49	1.34
14	A	5001	LHG	O7-C7	5.22	1.49	1.34
17	W	4020	8CT	C05-C04	5.22	1.66	1.54
11	A	1132	CL7	CHD-C4C	5.22	1.48	1.38
17	J	4015	8CT	C34-C33	5.22	1.64	1.52
17	B	4017	8CT	C11-C12	5.21	1.57	1.45
17	A	4011	8CT	C05-C04	5.21	1.66	1.54
17	B	4017	8CT	C05-C04	5.21	1.66	1.54
11	B	1226	CL7	CHC-C1C	5.20	1.48	1.38
11	A	1105	CL7	CHC-C1C	5.20	1.48	1.38
17	J	4013	8CT	C05-C04	5.19	1.66	1.54
11	A	1114	CL7	CHC-C1C	5.19	1.48	1.38
11	A	1102	CL7	CHC-C1C	5.19	1.48	1.38
11	A	1135	CL7	CHC-C1C	5.19	1.48	1.38
11	A	1103	CL7	CHC-C1C	5.18	1.48	1.38
11	B	1205	CL7	CHD-C4C	5.18	1.48	1.38
17	M	4021	8CT	C05-C04	5.18	1.66	1.54
11	A	1129	CL7	CHD-C4C	5.18	1.48	1.38
11	B	1021	CL7	CHC-C1C	5.18	1.48	1.38
17	A	4008	8CT	C05-C04	5.18	1.66	1.54
11	B	1238	CL7	CHC-C1C	5.17	1.48	1.38
11	A	1125	CL7	CHC-C1C	5.17	1.48	1.38
17	A	4008	8CT	C11-C12	5.17	1.57	1.45
11	B	1211	CL7	CHC-C1C	5.16	1.48	1.38
11	B	1214	CL7	CHB-C1B	5.16	1.51	1.39
11	B	1212	CL7	CHD-C4C	5.16	1.48	1.38
17	B	4006	8CT	C34-C33	5.16	1.64	1.52
11	B	1222	CL7	CHC-C1C	5.16	1.48	1.38
11	B	1223	CL7	CHC-C1C	5.15	1.48	1.38
17	L	4019	8CT	C05-C04	5.15	1.66	1.54
17	B	4014	8CT	C34-C33	5.15	1.64	1.52
11	B	1208	CL7	CHD-C4C	5.15	1.48	1.38
11	J	1302	CL7	CHC-C1C	5.15	1.48	1.38
11	A	1115	CL7	CHC-C1C	5.15	1.48	1.38
11	A	1122	CL7	CHD-C4C	5.15	1.48	1.38
11	B	1213	CL7	CHC-C1C	5.15	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1106	CL7	CHC-C1C	5.14	1.48	1.38
11	B	1212	CL7	CHC-C1C	5.14	1.48	1.38
11	A	1801	CL7	CHC-C1C	5.14	1.48	1.38
17	A	4007	8CT	C05-C04	5.14	1.66	1.54
11	A	1120	CL7	CHC-C1C	5.14	1.48	1.38
11	B	1234	CL7	CHC-C1C	5.14	1.48	1.38
11	A	1111	CL7	CHC-C1C	5.14	1.48	1.38
11	A	1136	CL7	CHC-C1C	5.13	1.48	1.38
11	B	1213	CL7	CHD-C4C	5.13	1.48	1.38
11	B	1229	CL7	CHD-C4C	5.13	1.48	1.38
11	A	1118	CL7	CHC-C1C	5.13	1.48	1.38
11	A	1127	CL7	CHC-C1C	5.13	1.48	1.38
11	A	1802	CL7	CHC-C1C	5.13	1.48	1.38
11	A	1130	CL7	CHC-C1C	5.12	1.48	1.38
11	B	1228	CL7	CHC-C1C	5.12	1.48	1.38
11	F	1301	CL7	CHC-C1C	5.12	1.48	1.38
11	L	1502	CL7	CHD-C4C	5.12	1.48	1.38
11	A	1116	CL7	CHD-C4C	5.11	1.48	1.38
11	A	1126	CL7	CHC-C1C	5.11	1.48	1.38
11	B	1229	CL7	CHC-C1C	5.11	1.48	1.38
17	L	4020	8CT	C34-C33	5.11	1.64	1.52
11	A	1022	CL7	CHC-C1C	5.10	1.48	1.38
11	A	1139	CL7	CHD-C4C	5.10	1.48	1.38
11	B	1238	CL7	CHD-C4C	5.10	1.48	1.38
11	B	1210	CL7	CHD-C4C	5.09	1.48	1.38
11	A	1138	CL7	CHD-C4C	5.09	1.48	1.38
11	B	1228	CL7	CHD-C4C	5.09	1.48	1.38
17	A	4008	8CT	C34-C33	5.09	1.64	1.52
11	A	1101	CL7	CHC-C1C	5.09	1.48	1.38
11	L	1502	CL7	CHC-C1C	5.08	1.48	1.38
11	A	1107	CL7	CHD-C4C	5.08	1.48	1.38
11	A	1112	CL7	CHD-C4C	5.08	1.48	1.38
11	A	1237	CL7	CHC-C1C	5.08	1.48	1.38
11	B	1204	CL7	CHD-C4C	5.08	1.48	1.38
11	A	1113	CL7	CHC-C1C	5.08	1.48	1.38
11	A	1118	CL7	CHD-C4C	5.08	1.48	1.38
11	A	1121	CL7	CHD-C4C	5.08	1.48	1.38
11	A	1140	CL7	CHC-C1C	5.08	1.48	1.38
11	B	1234	CL7	CHD-C4C	5.08	1.48	1.38
11	F	1301	CL7	CHD-C4C	5.08	1.48	1.38
17	M	4021	8CT	C35-C30	5.08	1.70	1.56
11	A	1110	CL7	CHC-C1C	5.08	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1136	CL7	CHD-C4C	5.08	1.48	1.38
11	B	1201	CL7	CHC-C1C	5.08	1.48	1.38
11	B	1239	CL7	CHD-C4C	5.08	1.48	1.38
17	J	4015	8CT	C35-C30	5.08	1.70	1.56
11	A	1117	CL7	CHC-C1C	5.08	1.48	1.38
11	A	1124	CL7	CHC-C1C	5.08	1.48	1.38
11	B	1235	CL7	CHC-C1C	5.07	1.48	1.38
11	A	1802	CL7	CHD-C4C	5.07	1.48	1.38
11	A	1109	CL7	CHC-C1C	5.07	1.48	1.38
11	B	1012	CL7	CHC-C1C	5.07	1.48	1.38
17	A	4007	8CT	C35-C30	5.07	1.70	1.56
11	A	1123	CL7	CHC-C1C	5.07	1.48	1.38
11	B	1211	CL7	CHD-C4C	5.07	1.48	1.38
17	L	4019	8CT	C28-C26	5.07	1.56	1.45
11	A	1112	CL7	CHC-C1C	5.06	1.48	1.38
11	A	1121	CL7	CHC-C1C	5.06	1.48	1.38
11	B	1201	CL7	CHD-C4C	5.06	1.48	1.38
11	B	1205	CL7	CHC-C1C	5.06	1.48	1.38
11	B	1202	CL7	CHC-C1C	5.06	1.48	1.38
11	B	1215	CL7	CHC-C1C	5.06	1.48	1.38
11	B	1204	CL7	CHC-C1C	5.06	1.48	1.38
11	A	1102	CL7	CHD-C4C	5.06	1.48	1.38
11	B	1207	CL7	CHC-C1C	5.06	1.48	1.38
11	B	1236	CL7	CHD-C4C	5.06	1.48	1.38
17	J	4015	8CT	C28-C26	5.05	1.56	1.45
17	W	4020	8CT	C35-C30	5.05	1.70	1.56
11	A	1101	CL7	CHD-C4C	5.05	1.48	1.38
17	J	4013	8CT	C28-C26	5.05	1.56	1.45
11	L	1503	CL7	CHC-C1C	5.05	1.48	1.38
11	B	1203	CL7	CHC-C1C	5.05	1.48	1.38
11	B	1236	CL7	CHC-C1C	5.05	1.48	1.38
11	A	1109	CL7	CHD-C4C	5.05	1.48	1.38
11	W	2601	CL7	CHC-C1C	5.05	1.48	1.38
11	B	1225	CL7	CHD-C4C	5.05	1.48	1.38
11	A	1117	CL7	CHD-C4C	5.05	1.48	1.38
11	A	1127	CL7	CHD-C4C	5.05	1.48	1.38
11	B	1235	CL7	CHD-C4C	5.05	1.48	1.38
11	A	1116	CL7	CHC-C1C	5.05	1.48	1.38
11	A	1120	CL7	CHD-C4C	5.05	1.48	1.38
11	B	1224	CL7	CHD-C4C	5.04	1.48	1.38
11	B	1210	CL7	CHC-C1C	5.04	1.48	1.38
17	J	4013	8CT	C34-C33	5.04	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1124	CL7	CHD-C4C	5.04	1.48	1.38
11	A	1130	CL7	CHD-C4C	5.04	1.48	1.38
11	B	1222	CL7	CHD-C4C	5.04	1.48	1.38
17	A	4007	8CT	C34-C33	5.04	1.64	1.52
11	L	1501	CL7	CHC-C1C	5.03	1.48	1.38
11	A	1104	CL7	CHC-C1C	5.03	1.48	1.38
11	A	1801	CL7	CHD-C4C	5.03	1.48	1.38
11	A	1132	CL7	CHC-C1C	5.03	1.48	1.38
11	J	1302	CL7	CHD-C4C	5.03	1.48	1.38
11	A	1123	CL7	CHD-C4C	5.03	1.48	1.38
11	B	1206	CL7	CHD-C4C	5.03	1.48	1.38
17	B	4017	8CT	C14-C13	5.03	1.59	1.43
17	B	4014	8CT	C14-C13	5.03	1.59	1.43
11	B	1239	CL7	CHC-C1C	5.03	1.48	1.38
11	B	1207	CL7	CHD-C4C	5.03	1.48	1.38
11	A	1113	CL7	CHD-C4C	5.03	1.48	1.38
11	A	1103	CL7	CHD-C4C	5.03	1.48	1.38
11	A	1106	CL7	CHD-C4C	5.03	1.48	1.38
11	A	1129	CL7	CHC-C1C	5.03	1.48	1.38
11	B	1206	CL7	CHC-C1C	5.02	1.48	1.38
17	L	4019	8CT	C34-C33	5.02	1.64	1.52
17	J	4013	8CT	C14-C13	5.02	1.59	1.43
11	A	1140	CL7	CHD-C4C	5.02	1.48	1.38
11	L	1503	CL7	CHD-C4C	5.02	1.48	1.38
11	A	1237	CL7	CHD-C4C	5.02	1.48	1.38
11	B	1223	CL7	CHD-C4C	5.02	1.48	1.38
11	A	1138	CL7	CHC-C1C	5.02	1.48	1.38
11	B	1230	CL7	CHC-C1C	5.02	1.48	1.38
11	A	1107	CL7	CHC-C1C	5.01	1.48	1.38
11	B	1225	CL7	CHC-C1C	5.01	1.48	1.38
11	A	1131	CL7	CHD-C4C	5.01	1.48	1.38
11	A	1119	CL7	CHC-C1C	5.01	1.48	1.38
11	B	1203	CL7	CHD-C4C	5.01	1.48	1.38
11	A	1110	CL7	CHD-C4C	5.00	1.48	1.38
11	B	1224	CL7	CHC-C1C	5.00	1.48	1.38
17	A	4011	8CT	C35-C30	5.00	1.70	1.56
11	B	1012	CL7	CHD-C4C	4.99	1.48	1.38
11	A	1131	CL7	CHC-C1C	4.99	1.48	1.38
11	B	1226	CL7	CHB-C1B	4.99	1.50	1.39
11	A	1115	CL7	CHD-C4C	4.98	1.48	1.38
17	L	4019	8CT	C14-C13	4.98	1.58	1.43
11	B	1215	CL7	CHD-C4C	4.98	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1119	CL7	CHD-C4C	4.98	1.48	1.38
11	L	1501	CL7	CHD-C4C	4.98	1.48	1.38
11	W	2601	CL7	CHD-C4C	4.98	1.48	1.38
17	B	4006	8CT	C14-C13	4.97	1.58	1.43
11	B	1202	CL7	CHD-C4C	4.97	1.48	1.38
17	W	4018	8CT	C35-C30	4.97	1.70	1.56
11	A	1022	CL7	CHD-C4C	4.97	1.48	1.38
11	A	1137	CL7	CHD-C4C	4.97	1.48	1.38
17	A	4011	8CT	C14-C13	4.96	1.58	1.43
11	A	1104	CL7	CHD-C4C	4.96	1.48	1.38
11	B	1208	CL7	CHC-C1C	4.96	1.48	1.38
11	A	1135	CL7	CHD-C4C	4.94	1.48	1.38
17	W	4018	8CT	C14-C13	4.94	1.58	1.43
11	B	1214	CL7	CHD-C4C	4.94	1.48	1.38
11	A	1128	CL7	CHB-C1B	4.94	1.50	1.39
17	L	4020	8CT	C14-C13	4.94	1.58	1.43
11	A	1128	CL7	CHD-C4C	4.93	1.48	1.38
17	M	4021	8CT	C14-C13	4.93	1.58	1.43
11	B	1230	CL7	CHD-C4C	4.93	1.48	1.38
17	M	4021	8CT	C34-C33	4.92	1.64	1.52
11	A	1125	CL7	CHD-C4C	4.92	1.47	1.38
17	J	4013	8CT	C35-C30	4.92	1.70	1.56
11	A	1105	CL7	CHD-C4C	4.91	1.47	1.38
11	B	1021	CL7	CHB-C1B	4.91	1.50	1.39
17	A	4007	8CT	C14-C13	4.90	1.58	1.43
17	J	4015	8CT	C14-C13	4.90	1.58	1.43
11	A	1119	CL7	CHB-C1B	4.90	1.50	1.39
11	B	1208	CL7	CHB-C1B	4.89	1.50	1.39
17	B	4017	8CT	C34-C33	4.89	1.64	1.52
11	A	1137	CL7	CHC-C1C	4.89	1.47	1.38
11	B	1226	CL7	CHD-C4C	4.89	1.47	1.38
11	F	1301	CL7	CHB-C1B	4.88	1.50	1.39
17	B	4017	8CT	C35-C30	4.88	1.70	1.56
11	J	1302	CL7	CHB-C1B	4.88	1.50	1.39
11	A	1107	CL7	CHB-C1B	4.88	1.50	1.39
17	A	4011	8CT	C34-C33	4.87	1.64	1.52
11	B	1210	CL7	CHB-C1B	4.87	1.50	1.39
11	A	1136	CL7	CHB-C1B	4.86	1.50	1.39
17	B	4014	8CT	C35-C30	4.86	1.69	1.56
11	B	1213	CL7	CHB-C1B	4.86	1.50	1.39
11	A	1120	CL7	CHB-C1B	4.86	1.50	1.39
11	B	1206	CL7	CHB-C1B	4.85	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1212	CL7	CHB-C1B	4.85	1.50	1.39
11	A	1122	CL7	CHC-C1C	4.85	1.47	1.38
17	M	4021	8CT	C28-C26	4.85	1.56	1.45
11	A	1139	CL7	CHB-C1B	4.85	1.50	1.39
17	W	4020	8CT	C14-C13	4.84	1.58	1.43
11	B	1207	CL7	CHB-C1B	4.84	1.50	1.39
11	B	1223	CL7	CHB-C1B	4.84	1.50	1.39
11	A	1112	CL7	CHB-C1B	4.83	1.50	1.39
11	A	1802	CL7	CHB-C1B	4.83	1.50	1.39
11	A	1105	CL7	CHB-C1B	4.83	1.50	1.39
11	B	1204	CL7	CHB-C1B	4.83	1.50	1.39
11	L	1503	CL7	CHB-C1B	4.83	1.50	1.39
11	A	1113	CL7	CHB-C1B	4.83	1.50	1.39
11	W	2601	CL7	CHB-C1B	4.83	1.50	1.39
11	B	1238	CL7	CHB-C1B	4.83	1.50	1.39
17	W	4018	8CT	C34-C33	4.83	1.63	1.52
11	A	1114	CL7	CHB-C1B	4.83	1.50	1.39
11	B	1215	CL7	CHB-C1B	4.82	1.50	1.39
17	L	4019	8CT	C35-C30	4.82	1.69	1.56
11	B	1203	CL7	CHB-C1B	4.82	1.50	1.39
17	W	4020	8CT	C34-C33	4.82	1.63	1.52
11	B	1225	CL7	CHB-C1B	4.82	1.50	1.39
11	B	1201	CL7	CHB-C1B	4.82	1.50	1.39
11	A	1130	CL7	CHB-C1B	4.82	1.50	1.39
11	B	1214	CL7	CHC-C1C	4.82	1.47	1.38
17	A	4008	8CT	C35-C30	4.81	1.69	1.56
11	A	1237	CL7	CHB-C1B	4.81	1.50	1.39
11	A	1109	CL7	CHB-C1B	4.81	1.50	1.39
11	B	1202	CL7	CHB-C1B	4.81	1.50	1.39
17	A	4008	8CT	C14-C13	4.81	1.58	1.43
11	A	1116	CL7	CHB-C1B	4.81	1.50	1.39
11	A	1101	CL7	CHB-C1B	4.80	1.50	1.39
11	B	1236	CL7	CHB-C1B	4.80	1.50	1.39
11	A	1106	CL7	CHB-C1B	4.80	1.50	1.39
11	B	1228	CL7	CHB-C1B	4.80	1.50	1.39
11	A	1135	CL7	CHB-C1B	4.80	1.50	1.39
11	A	1121	CL7	CHB-C1B	4.80	1.50	1.39
11	A	1138	CL7	CHB-C1B	4.80	1.50	1.39
11	B	1211	CL7	CHB-C1B	4.80	1.50	1.39
11	B	1234	CL7	CHB-C1B	4.80	1.50	1.39
11	A	1125	CL7	CHB-C1B	4.80	1.50	1.39
11	A	1122	CL7	CHB-C1B	4.79	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1118	CL7	CHB-C1B	4.79	1.50	1.39
11	B	1230	CL7	CHB-C1B	4.79	1.50	1.39
11	A	1801	CL7	CHB-C1B	4.79	1.50	1.39
11	A	1102	CL7	CHB-C1B	4.79	1.50	1.39
11	A	1115	CL7	CHB-C1B	4.79	1.50	1.39
11	A	1129	CL7	CHB-C1B	4.78	1.50	1.39
11	A	1117	CL7	CHB-C1B	4.78	1.50	1.39
11	A	1131	CL7	CHB-C1B	4.78	1.50	1.39
11	B	1021	CL7	CHD-C4C	4.78	1.47	1.38
11	A	1110	CL7	CHB-C1B	4.77	1.50	1.39
17	L	4020	8CT	C35-C30	4.77	1.69	1.56
11	A	1124	CL7	CHB-C1B	4.76	1.50	1.39
11	B	1229	CL7	CHB-C1B	4.76	1.50	1.39
11	A	1111	CL7	CHB-C1B	4.76	1.50	1.39
11	B	1235	CL7	CHB-C1B	4.75	1.50	1.39
17	B	4006	8CT	C35-C30	4.75	1.69	1.56
11	A	1104	CL7	CHB-C1B	4.75	1.50	1.39
11	B	1222	CL7	CHB-C1B	4.75	1.50	1.39
11	L	1502	CL7	CHB-C1B	4.74	1.50	1.39
11	A	1140	CL7	CHB-C1B	4.74	1.50	1.39
11	A	1137	CL7	CHB-C1B	4.74	1.50	1.39
11	B	1239	CL7	CHB-C1B	4.74	1.50	1.39
11	L	1501	CL7	CHB-C1B	4.73	1.50	1.39
11	B	1205	CL7	CHB-C1B	4.73	1.50	1.39
11	B	1224	CL7	CHB-C1B	4.73	1.50	1.39
11	A	1123	CL7	CHB-C1B	4.72	1.50	1.39
11	A	1103	CL7	CHB-C1B	4.72	1.50	1.39
11	B	1012	CL7	CHB-C1B	4.69	1.49	1.39
17	L	4020	8CT	C28-C26	4.69	1.56	1.45
17	J	4013	8CT	C24-C25	4.69	1.58	1.43
11	A	1132	CL7	CHB-C1B	4.68	1.49	1.39
17	L	4019	8CT	C24-C25	4.68	1.58	1.43
11	A	1127	CL7	CHB-C1B	4.67	1.49	1.39
17	M	4021	8CT	C24-C25	4.66	1.57	1.43
17	B	4006	8CT	C24-C25	4.66	1.57	1.43
15	A	1011	G9R	CHB-C1B	4.66	1.49	1.39
17	B	4014	8CT	C28-C26	4.66	1.55	1.45
17	B	4014	8CT	C24-C25	4.66	1.57	1.43
17	A	4007	8CT	C24-C25	4.65	1.57	1.43
15	A	1011	G9R	CHC-C1C	4.65	1.48	1.38
17	A	4007	8CT	C28-C26	4.64	1.55	1.45
11	A	1126	CL7	CHB-C1B	4.64	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2002	PQN	C16-C15	-4.64	1.35	1.52
17	W	4018	8CT	C28-C26	4.64	1.55	1.45
17	W	4018	8CT	C24-C25	4.63	1.57	1.43
17	B	4017	8CT	C24-C25	4.63	1.57	1.43
17	L	4020	8CT	C24-C25	4.63	1.57	1.43
17	A	4011	8CT	C24-C25	4.62	1.57	1.43
12	A	2001	PQN	C16-C15	-4.61	1.35	1.52
17	B	4006	8CT	C28-C26	4.58	1.55	1.45
17	A	4008	8CT	C24-C25	4.58	1.57	1.43
17	W	4020	8CT	C28-C26	4.57	1.55	1.45
11	A	1022	CL7	CHB-C1B	4.57	1.49	1.39
16	B	1023	PHO	C3D-C4D	4.56	1.47	1.41
17	M	4021	8CT	C18-C17	4.55	1.57	1.43
17	A	4008	8CT	C28-C26	4.54	1.55	1.45
17	B	4017	8CT	C18-C17	4.53	1.57	1.43
17	J	4015	8CT	C24-C25	4.53	1.57	1.43
17	B	4017	8CT	C28-C26	4.53	1.55	1.45
16	A	1013	PHO	C3D-C4D	4.53	1.47	1.41
17	W	4020	8CT	C24-C25	4.53	1.57	1.43
17	J	4013	8CT	C18-C17	4.52	1.57	1.43
17	A	4011	8CT	C28-C26	4.51	1.55	1.45
17	L	4020	8CT	C18-C17	4.51	1.57	1.43
18	B	5002	LMG	C29-C28	4.51	1.63	1.50
17	B	4006	8CT	C18-C17	4.49	1.57	1.43
17	L	4019	8CT	C18-C17	4.47	1.57	1.43
17	W	4018	8CT	C18-C17	4.45	1.57	1.43
18	B	5002	LMG	O6-C5	4.45	1.55	1.44
17	J	4015	8CT	C18-C17	4.44	1.57	1.43
17	B	4014	8CT	C18-C17	4.44	1.57	1.43
17	A	4011	8CT	C18-C17	4.42	1.57	1.43
18	B	5002	LMG	O3-C3	4.42	1.53	1.43
17	A	4007	8CT	C18-C17	4.40	1.57	1.43
17	W	4020	8CT	C18-C17	4.37	1.57	1.43
17	A	4008	8CT	C18-C17	4.31	1.56	1.43
18	B	5002	LMG	C11-C10	4.25	1.63	1.50
14	A	5003	LHG	C8-C7	4.23	1.63	1.50
14	A	5001	LHG	C8-C7	4.18	1.62	1.50
14	A	5003	LHG	C24-C23	4.13	1.62	1.50
17	J	4013	8CT	C23-C21	4.12	1.54	1.45
17	L	4019	8CT	C23-C21	4.11	1.54	1.45
17	B	4006	8CT	C23-C21	4.08	1.54	1.45
14	A	5001	LHG	C24-C23	4.06	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	4007	8CT	C06-C07	4.06	1.65	1.52
17	L	4020	8CT	C06-C07	4.05	1.65	1.52
17	B	4006	8CT	C06-C07	4.04	1.65	1.52
17	J	4015	8CT	C06-C07	4.04	1.65	1.52
17	M	4021	8CT	C23-C21	4.03	1.54	1.45
17	W	4018	8CT	C23-C21	4.03	1.54	1.45
17	B	4014	8CT	C06-C07	4.01	1.65	1.52
17	B	4014	8CT	C23-C21	3.99	1.54	1.45
17	B	4017	8CT	C23-C21	3.99	1.54	1.45
17	A	4007	8CT	C23-C21	3.99	1.54	1.45
17	W	4020	8CT	C06-C07	3.98	1.65	1.52
17	W	4018	8CT	C06-C07	3.97	1.64	1.52
15	A	1011	G9R	CHD-C4C	3.95	1.48	1.39
17	L	4020	8CT	C23-C21	3.95	1.54	1.45
17	J	4013	8CT	C06-C07	3.95	1.64	1.52
17	A	4011	8CT	C23-C21	3.94	1.54	1.45
17	A	4008	8CT	C23-C21	3.93	1.54	1.45
17	B	4017	8CT	C06-C07	3.90	1.64	1.52
17	A	4011	8CT	C06-C07	3.90	1.64	1.52
17	A	4008	8CT	C06-C07	3.90	1.64	1.52
17	L	4019	8CT	C06-C07	3.88	1.64	1.52
17	W	4020	8CT	C23-C21	3.87	1.54	1.45
11	F	1301	CL7	C2A-C1A	3.87	1.56	1.50
17	M	4021	8CT	C06-C07	3.85	1.64	1.52
17	J	4015	8CT	C23-C21	3.83	1.54	1.45
11	A	1136	CL7	C2A-C1A	3.83	1.56	1.50
14	A	5001	LHG	P-O3	3.81	1.74	1.59
18	B	5002	LMG	C4-C5	3.79	1.61	1.53
11	A	1022	CL7	C2A-C1A	3.79	1.56	1.50
11	A	1115	CL7	C2A-C1A	3.78	1.56	1.50
14	A	5001	LHG	P-O6	3.77	1.74	1.59
16	B	1023	PHO	C4D-ND	-3.77	1.33	1.38
11	A	1127	CL7	C2A-C1A	3.77	1.56	1.50
14	A	5003	LHG	P-O3	3.76	1.74	1.59
16	A	1013	PHO	C4D-ND	-3.74	1.33	1.38
11	A	1104	CL7	C2A-C1A	3.74	1.56	1.50
14	A	5003	LHG	P-O6	3.73	1.74	1.59
11	B	1234	CL7	C2A-C1A	3.71	1.56	1.50
18	B	5002	LMG	O2-C2	3.70	1.51	1.43
11	A	1135	CL7	C2A-C1A	3.69	1.56	1.50
11	B	1214	CL7	C2A-C1A	3.66	1.56	1.50
11	A	1123	CL7	C2A-C1A	3.65	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1223	CL7	C2A-C1A	3.65	1.56	1.50
11	B	1206	CL7	C2A-C1A	3.64	1.56	1.50
11	F	1301	CL7	O2A-CGA	3.62	1.42	1.30
11	A	1116	CL7	O2A-CGA	3.62	1.42	1.30
11	J	1302	CL7	O2A-CGA	3.62	1.42	1.30
11	B	1212	CL7	O2A-CGA	3.62	1.42	1.30
11	A	1122	CL7	O2A-CGA	3.61	1.42	1.30
11	B	1228	CL7	C2A-C1A	3.61	1.56	1.50
11	B	1230	CL7	O2A-CGA	3.61	1.42	1.30
11	A	1109	CL7	O2A-CGA	3.61	1.42	1.30
11	A	1110	CL7	C2A-C1A	3.61	1.56	1.50
11	A	1121	CL7	O2A-CGA	3.61	1.42	1.30
11	B	1223	CL7	O2A-CGA	3.60	1.42	1.30
11	L	1503	CL7	O2A-CGA	3.60	1.42	1.30
11	B	1228	CL7	O2A-CGA	3.60	1.42	1.30
11	A	1115	CL7	O2A-CGA	3.60	1.42	1.30
11	W	2601	CL7	O2A-CGA	3.60	1.42	1.30
11	B	1207	CL7	O2A-CGA	3.60	1.42	1.30
11	A	1107	CL7	O2A-CGA	3.60	1.42	1.30
11	B	1210	CL7	O2A-CGA	3.60	1.42	1.30
11	A	1120	CL7	C2A-C1A	3.60	1.56	1.50
11	A	1801	CL7	O2A-CGA	3.60	1.42	1.30
11	B	1213	CL7	O2A-CGA	3.60	1.42	1.30
11	B	1229	CL7	O2A-CGA	3.60	1.42	1.30
11	A	1135	CL7	O2A-CGA	3.60	1.42	1.30
11	B	1201	CL7	O2A-CGA	3.59	1.42	1.30
11	B	1234	CL7	O2A-CGA	3.59	1.42	1.30
11	A	1124	CL7	O2A-CGA	3.59	1.42	1.30
11	B	1215	CL7	O2A-CGA	3.59	1.42	1.30
11	B	1235	CL7	O2A-CGA	3.59	1.42	1.30
11	A	1130	CL7	O2A-CGA	3.59	1.42	1.30
11	A	1102	CL7	O2A-CGA	3.59	1.42	1.30
11	A	1105	CL7	O2A-CGA	3.59	1.42	1.30
11	B	1208	CL7	O2A-CGA	3.59	1.42	1.30
11	A	1113	CL7	O2A-CGA	3.59	1.42	1.30
11	A	1118	CL7	O2A-CGA	3.59	1.42	1.30
11	A	1802	CL7	C2A-C1A	3.59	1.56	1.50
11	B	1210	CL7	C2A-C1A	3.59	1.56	1.50
11	A	1112	CL7	O2A-CGA	3.59	1.42	1.30
11	B	1236	CL7	O2A-CGA	3.59	1.42	1.30
11	B	1205	CL7	O2A-CGA	3.58	1.42	1.30
11	A	1802	CL7	O2A-CGA	3.58	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1222	CL7	O2A-CGA	3.58	1.42	1.30
11	A	1101	CL7	C2A-C1A	3.58	1.56	1.50
11	A	1111	CL7	O2A-CGA	3.58	1.42	1.30
11	A	1116	CL7	C2A-C1A	3.58	1.56	1.50
11	B	1206	CL7	O2A-CGA	3.58	1.42	1.30
11	A	1139	CL7	O2A-CGA	3.58	1.42	1.30
11	A	1114	CL7	O2A-CGA	3.58	1.42	1.30
11	B	1214	CL7	O2A-CGA	3.57	1.42	1.30
11	A	1103	CL7	C2A-C1A	3.57	1.56	1.50
11	A	1137	CL7	O2A-CGA	3.57	1.42	1.30
11	A	1120	CL7	O2A-CGA	3.57	1.42	1.30
11	A	1110	CL7	O2A-CGA	3.57	1.42	1.30
11	B	1203	CL7	C2A-C1A	3.57	1.56	1.50
11	A	1129	CL7	O2A-CGA	3.56	1.42	1.30
11	A	1138	CL7	O2A-CGA	3.56	1.42	1.30
11	A	1109	CL7	C2A-C1A	3.56	1.56	1.50
11	B	1213	CL7	C2A-C1A	3.56	1.56	1.50
11	A	1127	CL7	O2A-CGA	3.56	1.42	1.30
11	B	1204	CL7	O2A-CGA	3.55	1.42	1.30
11	A	1113	CL7	C2A-C1A	3.55	1.56	1.50
11	J	1302	CL7	C2A-C1A	3.55	1.56	1.50
11	A	1119	CL7	O2A-CGA	3.55	1.42	1.30
11	A	1105	CL7	O2D-CGD	3.55	1.41	1.33
11	B	1224	CL7	O2A-CGA	3.55	1.42	1.30
11	A	1113	CL7	O2D-CGD	3.55	1.41	1.33
11	A	1114	CL7	C2A-C1A	3.55	1.56	1.50
11	B	1202	CL7	O2A-CGA	3.55	1.42	1.30
11	F	1301	CL7	O2D-CGD	3.54	1.41	1.33
11	B	1202	CL7	C2A-C1A	3.54	1.56	1.50
11	A	1118	CL7	C2A-C1A	3.54	1.56	1.50
11	W	2601	CL7	O2D-CGD	3.54	1.41	1.33
11	B	1211	CL7	C2A-C1A	3.54	1.56	1.50
11	J	1302	CL7	O2D-CGD	3.54	1.41	1.33
11	A	1125	CL7	C2A-C1A	3.53	1.56	1.50
11	A	1120	CL7	O2D-CGD	3.53	1.41	1.33
11	B	1208	CL7	O2D-CGD	3.53	1.41	1.33
11	B	1229	CL7	C2A-C1A	3.53	1.56	1.50
11	A	1112	CL7	C2A-C1A	3.53	1.56	1.50
11	B	1223	CL7	O2D-CGD	3.53	1.41	1.33
11	B	1212	CL7	O2D-CGD	3.53	1.41	1.33
11	A	1124	CL7	O2D-CGD	3.53	1.41	1.33
11	B	1222	CL7	O2D-CGD	3.53	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1802	CL7	O2D-CGD	3.52	1.41	1.33
11	B	1211	CL7	O2A-CGA	3.52	1.42	1.30
11	B	1012	CL7	C2A-C1A	3.52	1.56	1.50
11	A	1118	CL7	O2D-CGD	3.52	1.41	1.33
11	A	1107	CL7	C2A-C1A	3.52	1.56	1.50
11	B	1236	CL7	C2A-C1A	3.52	1.56	1.50
11	A	1112	CL7	O2D-CGD	3.51	1.41	1.33
11	A	1121	CL7	O2D-CGD	3.51	1.41	1.33
11	A	1801	CL7	O2D-CGD	3.51	1.41	1.33
11	B	1234	CL7	O2D-CGD	3.51	1.41	1.33
11	B	1228	CL7	O2D-CGD	3.51	1.41	1.33
11	A	1801	CL7	C2A-C1A	3.51	1.56	1.50
11	A	1109	CL7	O2D-CGD	3.51	1.41	1.33
11	B	1230	CL7	O2D-CGD	3.51	1.41	1.33
11	A	1139	CL7	O2D-CGD	3.50	1.41	1.33
11	A	1114	CL7	O2D-CGD	3.50	1.41	1.33
11	B	1213	CL7	O2D-CGD	3.50	1.41	1.33
11	W	2601	CL7	C2A-C1A	3.50	1.56	1.50
11	A	1140	CL7	O2D-CGD	3.50	1.41	1.33
11	B	1229	CL7	O2D-CGD	3.50	1.41	1.33
18	B	5002	LMG	O1-C7	3.50	1.50	1.43
11	A	1111	CL7	O2D-CGD	3.50	1.41	1.33
11	A	1136	CL7	O2D-CGD	3.50	1.41	1.33
11	A	1138	CL7	O2D-CGD	3.49	1.41	1.33
11	B	1215	CL7	C2A-C1A	3.49	1.56	1.50
11	B	1214	CL7	O2D-CGD	3.49	1.41	1.33
11	B	1210	CL7	O2D-CGD	3.49	1.41	1.33
11	A	1237	CL7	O2D-CGD	3.49	1.41	1.33
11	B	1211	CL7	O2D-CGD	3.49	1.41	1.33
11	B	1212	CL7	C2A-C1A	3.49	1.56	1.50
15	A	1011	G9R	C3D-C4D	-3.49	1.36	1.44
11	A	1128	CL7	O2D-CGD	3.49	1.41	1.33
11	A	1131	CL7	C2A-C1A	3.49	1.56	1.50
11	A	1101	CL7	O2D-CGD	3.48	1.41	1.33
11	B	1226	CL7	O2D-CGD	3.48	1.41	1.33
11	L	1501	CL7	O2D-CGD	3.48	1.41	1.33
11	A	1117	CL7	O2D-CGD	3.48	1.41	1.33
11	B	1205	CL7	O2D-CGD	3.47	1.41	1.33
14	A	5003	LHG	C6-C5	3.47	1.61	1.50
11	A	1121	CL7	C2A-C1A	3.47	1.56	1.50
11	A	1119	CL7	O2D-CGD	3.47	1.41	1.33
11	A	1106	CL7	O2D-CGD	3.47	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1126	CL7	O2D-CGD	3.47	1.41	1.33
11	A	1104	CL7	O2D-CGD	3.47	1.41	1.33
11	A	1129	CL7	O2D-CGD	3.47	1.41	1.33
11	B	1224	CL7	O2D-CGD	3.47	1.41	1.33
11	B	1225	CL7	O2D-CGD	3.46	1.41	1.33
11	B	1230	CL7	C2A-C1A	3.46	1.56	1.50
11	L	1503	CL7	C2A-C1A	3.46	1.56	1.50
11	A	1122	CL7	O2D-CGD	3.45	1.41	1.33
11	B	1206	CL7	O2D-CGD	3.45	1.41	1.33
11	A	1102	CL7	C2A-C1A	3.45	1.56	1.50
11	A	1111	CL7	C2A-C1A	3.45	1.56	1.50
11	B	1201	CL7	O2D-CGD	3.45	1.41	1.33
11	A	1123	CL7	O2D-CGD	3.45	1.41	1.33
11	A	1135	CL7	O2D-CGD	3.45	1.41	1.33
14	A	5001	LHG	C4-C5	3.44	1.61	1.50
11	B	1236	CL7	O2D-CGD	3.44	1.41	1.33
11	A	1139	CL7	C2A-C1A	3.44	1.56	1.50
11	L	1503	CL7	O2D-CGD	3.44	1.41	1.33
11	B	1235	CL7	O2D-CGD	3.43	1.41	1.33
11	A	1116	CL7	O2D-CGD	3.43	1.41	1.33
11	L	1502	CL7	O2D-CGD	3.43	1.41	1.33
18	B	5002	LMG	C12-C11	3.43	1.64	1.52
14	A	5001	LHG	C6-C5	3.43	1.61	1.50
11	B	1239	CL7	O2D-CGD	3.43	1.41	1.33
11	A	1127	CL7	O2D-CGD	3.43	1.41	1.33
11	B	1207	CL7	O2D-CGD	3.43	1.41	1.33
11	L	1501	CL7	C2A-C1A	3.43	1.56	1.50
11	B	1204	CL7	O2D-CGD	3.43	1.41	1.33
11	B	1238	CL7	O2D-CGD	3.42	1.41	1.33
11	B	1203	CL7	O2D-CGD	3.42	1.41	1.33
14	A	5003	LHG	C4-C5	3.42	1.61	1.50
11	A	1115	CL7	O2D-CGD	3.42	1.41	1.33
11	A	1131	CL7	O2D-CGD	3.42	1.41	1.33
11	A	1103	CL7	O2D-CGD	3.42	1.41	1.33
11	A	1137	CL7	O2D-CGD	3.41	1.41	1.33
11	A	1237	CL7	C2A-C1A	3.41	1.56	1.50
11	B	1207	CL7	C2A-C1A	3.41	1.56	1.50
11	A	1105	CL7	C2A-C1A	3.41	1.56	1.50
11	A	1125	CL7	O2D-CGD	3.41	1.41	1.33
11	A	1130	CL7	O2D-CGD	3.41	1.41	1.33
11	B	1012	CL7	O2D-CGD	3.41	1.41	1.33
11	B	1208	CL7	C2A-C1A	3.40	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1130	CL7	C2A-C1A	3.40	1.56	1.50
11	A	1122	CL7	C2A-C1A	3.40	1.56	1.50
11	A	1110	CL7	O2D-CGD	3.40	1.41	1.33
11	B	1202	CL7	O2D-CGD	3.39	1.41	1.33
18	B	5002	LMG	C9-C8	3.39	1.61	1.50
11	B	1215	CL7	O2D-CGD	3.37	1.41	1.33
11	L	1502	CL7	C2A-C1A	3.37	1.55	1.50
15	A	1011	G9R	CHD-C1D	3.36	1.44	1.38
11	A	1107	CL7	O2D-CGD	3.36	1.41	1.33
11	A	1123	CL7	O2A-CGA	3.36	1.43	1.33
11	B	1201	CL7	C2A-C1A	3.35	1.55	1.50
11	B	1235	CL7	C2A-C1A	3.35	1.55	1.50
18	B	5002	LMG	C7-C8	3.34	1.61	1.50
11	A	1102	CL7	O2D-CGD	3.34	1.41	1.33
11	B	1021	CL7	O2D-CGD	3.33	1.41	1.33
11	A	1117	CL7	O2A-CGA	3.33	1.43	1.33
11	A	1129	CL7	C2A-C1A	3.31	1.55	1.50
11	A	1022	CL7	O2D-CGD	3.31	1.41	1.33
18	B	5002	LMG	C30-C29	3.31	1.64	1.52
11	B	1222	CL7	C2A-C1A	3.31	1.55	1.50
11	B	1225	CL7	C2A-C1A	3.30	1.55	1.50
11	B	1239	CL7	C2A-C1A	3.30	1.55	1.50
11	A	1137	CL7	C2A-C1A	3.29	1.55	1.50
11	A	1104	CL7	O2A-CGA	3.28	1.42	1.33
15	A	1011	G9R	O2D-CGD	3.28	1.41	1.33
11	B	1204	CL7	C2A-C1A	3.28	1.55	1.50
11	A	1101	CL7	O2A-CGA	3.27	1.42	1.33
11	B	1224	CL7	C2A-C1A	3.27	1.55	1.50
11	A	1124	CL7	C2A-C1A	3.27	1.55	1.50
17	J	4013	8CT	C19-C20	3.26	1.53	1.43
17	B	4017	8CT	C19-C20	3.26	1.53	1.43
11	B	1225	CL7	O2A-CGA	3.26	1.42	1.33
11	B	1012	CL7	O2A-CGA	3.26	1.42	1.33
11	B	1238	CL7	O2A-CGA	3.25	1.42	1.33
11	A	1132	CL7	O2D-CGD	3.25	1.41	1.33
11	A	1140	CL7	O2A-CGA	3.25	1.42	1.33
17	A	4007	8CT	C19-C20	3.24	1.53	1.43
11	A	1126	CL7	C2A-C1A	3.24	1.55	1.50
11	B	1021	CL7	O2A-CGA	3.24	1.42	1.33
11	A	1136	CL7	O2A-CGA	3.24	1.42	1.33
11	B	1203	CL7	O2A-CGA	3.24	1.42	1.33
11	A	1103	CL7	O2A-CGA	3.24	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1226	CL7	C2A-C1A	3.23	1.55	1.50
11	L	1501	CL7	O2A-CGA	3.22	1.42	1.33
11	B	1239	CL7	O2A-CGA	3.22	1.42	1.33
17	A	4008	8CT	C19-C20	3.22	1.53	1.43
15	A	1011	G9R	O2A-CGA	3.21	1.42	1.33
11	A	1132	CL7	O2A-CGA	3.21	1.42	1.33
17	B	4006	8CT	C19-C20	3.21	1.53	1.43
11	A	1106	CL7	O2A-CGA	3.20	1.42	1.33
11	L	1502	CL7	O2A-CGA	3.20	1.42	1.33
11	B	1238	CL7	C2A-C1A	3.20	1.55	1.50
11	A	1128	CL7	O2A-CGA	3.20	1.42	1.33
11	A	1131	CL7	O2A-CGA	3.20	1.42	1.33
11	A	1237	CL7	O2A-CGA	3.20	1.42	1.33
17	B	4014	8CT	C19-C20	3.20	1.53	1.43
11	A	1140	CL7	C2A-C1A	3.20	1.55	1.50
17	A	4011	8CT	C19-C20	3.20	1.53	1.43
17	M	4021	8CT	C19-C20	3.19	1.53	1.43
17	W	4020	8CT	C19-C20	3.19	1.53	1.43
11	A	1128	CL7	C2A-C1A	3.19	1.55	1.50
17	L	4020	8CT	C19-C20	3.18	1.53	1.43
17	L	4019	8CT	C19-C20	3.17	1.53	1.43
11	A	1126	CL7	O2A-CGA	3.17	1.42	1.33
11	A	1125	CL7	O2A-CGA	3.16	1.42	1.33
17	W	4018	8CT	C19-C20	3.16	1.53	1.43
11	A	1138	CL7	C2A-C1A	3.15	1.55	1.50
11	A	1022	CL7	O2A-CGA	3.15	1.42	1.33
12	B	2002	PQN	C10-C5	3.15	1.45	1.40
11	A	1119	CL7	C2A-C1A	3.14	1.55	1.50
11	A	1114	CL7	CHD-C1D	3.14	1.46	1.39
11	A	1132	CL7	C2A-C1A	3.14	1.55	1.50
17	J	4015	8CT	C19-C20	3.13	1.53	1.43
11	B	1226	CL7	O2A-CGA	3.11	1.42	1.33
11	A	1117	CL7	C2A-C1A	3.09	1.55	1.50
11	B	1205	CL7	C2A-C1A	3.09	1.55	1.50
11	A	1106	CL7	C2A-C1A	3.07	1.55	1.50
12	A	2001	PQN	C10-C5	3.04	1.45	1.40
12	A	2001	PQN	C11-C12	3.02	1.55	1.50
14	A	5003	LHG	C9-C8	3.01	1.63	1.52
18	B	5002	LMG	O4-C4	3.00	1.50	1.43
14	A	5001	LHG	C9-C8	2.97	1.63	1.52
11	B	1021	CL7	C2A-C1A	2.95	1.55	1.50
12	A	2001	PQN	C6-C5	2.95	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	2001	PQN	C10-C1	-2.94	1.42	1.48
12	B	2002	PQN	C6-C5	2.94	1.44	1.39
11	A	1128	CL7	CHC-C4B	2.91	1.45	1.39
14	A	5001	LHG	C25-C24	2.90	1.62	1.52
14	A	5001	LHG	C3-C2	2.90	1.61	1.51
17	W	4020	8CT	C07-C02	-2.90	1.45	1.51
17	B	4017	8CT	C07-C02	-2.90	1.45	1.51
14	A	5003	LHG	C25-C24	2.90	1.62	1.52
17	A	4008	8CT	C07-C02	-2.88	1.45	1.51
11	A	1139	CL7	CAB-C3B	2.88	1.51	1.45
17	W	4018	8CT	C07-C02	-2.87	1.45	1.51
11	B	1214	CL7	CAB-C3B	2.85	1.51	1.45
17	A	4007	8CT	C07-C02	-2.85	1.45	1.51
17	L	4020	8CT	C07-C02	-2.84	1.45	1.51
18	B	5002	LMG	C1-C2	2.83	1.60	1.52
17	B	4006	8CT	C07-C02	-2.83	1.45	1.51
17	B	4014	8CT	C07-C02	-2.82	1.45	1.51
17	J	4013	8CT	C07-C02	-2.82	1.45	1.51
11	A	1125	CL7	CHC-C4B	2.82	1.45	1.39
17	M	4021	8CT	C07-C02	-2.82	1.45	1.51
11	B	1226	CL7	CHC-C4B	2.82	1.45	1.39
17	A	4011	8CT	C07-C02	-2.82	1.45	1.51
17	J	4015	8CT	C07-C02	-2.81	1.45	1.51
11	A	1105	CL7	CHC-C4B	2.80	1.45	1.39
11	A	1135	CL7	CHC-C4B	2.79	1.45	1.39
14	A	5003	LHG	C3-C2	2.79	1.61	1.51
11	B	1226	CL7	C4C-C3C	-2.79	1.40	1.45
16	B	1023	PHO	CMC-C2C	-2.79	1.46	1.50
17	J	4015	8CT	C28-C29	2.78	1.38	1.32
11	B	1223	CL7	CHC-C4B	2.78	1.45	1.39
11	A	1116	CL7	CHC-C4B	2.78	1.45	1.39
11	A	1123	CL7	CHC-C4B	2.77	1.45	1.39
17	L	4019	8CT	C07-C02	-2.77	1.45	1.51
11	B	1222	CL7	CHC-C4B	2.77	1.45	1.39
11	A	1139	CL7	CHC-C4B	2.76	1.45	1.39
11	B	1202	CL7	CHC-C4B	2.76	1.45	1.39
11	A	1111	CL7	CHC-C4B	2.75	1.45	1.39
11	B	1229	CL7	CHC-C4B	2.75	1.45	1.39
11	A	1106	CL7	CHC-C4B	2.75	1.45	1.39
11	A	1102	CL7	CHC-C4B	2.75	1.45	1.39
11	B	1212	CL7	CHC-C4B	2.75	1.45	1.39
11	A	1130	CL7	CHC-C4B	2.75	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1213	CL7	CHC-C4B	2.75	1.45	1.39
11	A	1128	CL7	C4C-C3C	-2.74	1.40	1.45
11	B	1238	CL7	CHC-C4B	2.74	1.45	1.39
11	A	1114	CL7	CHC-C4B	2.73	1.45	1.39
11	A	1115	CL7	CHC-C4B	2.73	1.45	1.39
11	B	1021	CL7	CHC-C4B	2.73	1.45	1.39
11	A	1120	CL7	CHC-C4B	2.73	1.45	1.39
11	J	1302	CL7	CHC-C4B	2.72	1.45	1.39
11	A	1124	CL7	CHC-C4B	2.72	1.45	1.39
11	A	1103	CL7	CHC-C4B	2.72	1.45	1.39
11	B	1228	CL7	CHC-C4B	2.72	1.45	1.39
11	A	1801	CL7	CHC-C4B	2.72	1.45	1.39
11	A	1121	CL7	CHC-C4B	2.72	1.45	1.39
11	A	1237	CL7	CHC-C4B	2.71	1.45	1.39
11	B	1211	CL7	CHC-C4B	2.71	1.45	1.39
11	A	1113	CL7	CHC-C4B	2.71	1.45	1.39
12	B	2002	PQN	C11-C12	2.71	1.54	1.50
11	B	1230	CL7	CHC-C4B	2.71	1.45	1.39
11	A	1022	CL7	CHC-C4B	2.70	1.45	1.39
11	A	1127	CL7	CHC-C4B	2.70	1.45	1.39
11	A	1802	CL7	CHC-C4B	2.70	1.45	1.39
11	A	1118	CL7	CHC-C4B	2.69	1.45	1.39
11	A	1101	CL7	CHC-C4B	2.69	1.45	1.39
11	A	1136	CL7	CHC-C4B	2.69	1.45	1.39
11	F	1301	CL7	CHC-C4B	2.69	1.45	1.39
11	A	1117	CL7	CHC-C4B	2.69	1.45	1.39
11	B	1204	CL7	CHC-C4B	2.68	1.45	1.39
11	A	1138	CL7	CHC-C4B	2.68	1.45	1.39
17	J	4013	8CT	C28-C29	2.68	1.38	1.32
11	B	1215	CL7	CHC-C4B	2.68	1.45	1.39
11	B	1203	CL7	CHC-C4B	2.68	1.45	1.39
11	A	1125	CL7	C4C-C3C	-2.68	1.40	1.45
11	A	1112	CL7	CHC-C4B	2.68	1.45	1.39
11	A	1126	CL7	CHC-C4B	2.68	1.45	1.39
12	A	2001	PQN	C15-C13	2.67	1.56	1.51
11	L	1501	CL7	CHC-C4B	2.67	1.45	1.39
11	L	1503	CL7	CHC-C4B	2.67	1.45	1.39
17	A	4008	8CT	C22-C21	2.67	1.56	1.50
11	B	1234	CL7	CHC-C4B	2.67	1.45	1.39
11	B	1210	CL7	CHC-C4B	2.67	1.45	1.39
11	A	1140	CL7	CHC-C4B	2.67	1.45	1.39
11	A	1110	CL7	CHC-C4B	2.67	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1206	CL7	CHC-C4B	2.66	1.45	1.39
17	J	4015	8CT	C30-C29	2.66	1.54	1.50
11	B	1214	CL7	CHC-C4B	2.66	1.45	1.39
11	B	1239	CL7	CHC-C4B	2.65	1.45	1.39
17	J	4015	8CT	C01-C02	2.65	1.55	1.50
11	B	1201	CL7	CHC-C4B	2.65	1.45	1.39
15	A	1011	G9R	CHC-C4B	2.65	1.45	1.39
17	J	4013	8CT	C01-C02	2.65	1.55	1.50
11	A	1131	CL7	CHC-C4B	2.65	1.45	1.39
17	L	4019	8CT	C01-C02	2.65	1.55	1.50
11	B	1236	CL7	CHC-C4B	2.64	1.45	1.39
17	B	4006	8CT	C01-C02	2.64	1.55	1.50
17	A	4007	8CT	C22-C21	2.64	1.56	1.50
11	B	1224	CL7	CHC-C4B	2.63	1.45	1.39
11	A	1110	CL7	CAB-C3B	2.63	1.50	1.45
11	B	1205	CL7	CHC-C4B	2.63	1.45	1.39
11	B	1207	CL7	CHC-C4B	2.63	1.45	1.39
11	L	1502	CL7	CHC-C4B	2.62	1.45	1.39
11	W	2601	CL7	CHC-C4B	2.62	1.45	1.39
17	A	4011	8CT	C01-C02	2.62	1.55	1.50
11	B	1215	CL7	C4C-C3C	-2.62	1.40	1.45
11	B	1208	CL7	CHC-C4B	2.61	1.45	1.39
11	B	1235	CL7	CHC-C4B	2.61	1.45	1.39
11	B	1203	CL7	C4C-C3C	-2.61	1.40	1.45
11	A	1802	CL7	CAB-C3B	2.61	1.50	1.45
11	A	1119	CL7	CHC-C4B	2.61	1.45	1.39
17	J	4013	8CT	C22-C21	2.61	1.56	1.50
11	B	1230	CL7	CAB-C3B	2.61	1.50	1.45
17	B	4014	8CT	C01-C02	2.61	1.55	1.50
11	A	1109	CL7	CHC-C4B	2.61	1.45	1.39
11	W	2601	CL7	CAB-C3B	2.61	1.50	1.45
11	A	1104	CL7	CHC-C4B	2.61	1.45	1.39
11	A	1107	CL7	CHC-C4B	2.61	1.45	1.39
17	L	4020	8CT	C22-C21	2.61	1.56	1.50
17	B	4017	8CT	C01-C02	2.60	1.55	1.50
11	A	1022	CL7	C4C-C3C	-2.60	1.40	1.45
11	A	1102	CL7	CAB-C3B	2.60	1.50	1.45
11	B	1012	CL7	CHC-C4B	2.60	1.45	1.39
11	A	1114	CL7	CAB-C3B	2.60	1.50	1.45
11	A	1129	CL7	CHC-C4B	2.60	1.45	1.39
17	W	4018	8CT	C22-C21	2.60	1.56	1.50
17	W	4018	8CT	C01-C02	2.60	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1225	CL7	CHC-C4B	2.59	1.45	1.39
12	A	2001	PQN	C11-C3	2.59	1.55	1.51
12	B	2002	PQN	C15-C13	2.59	1.56	1.51
17	L	4020	8CT	C01-C02	2.58	1.55	1.50
11	F	1301	CL7	CAB-C3B	2.58	1.50	1.45
11	B	1210	CL7	CAB-C3B	2.57	1.50	1.45
17	A	4007	8CT	C01-C02	2.57	1.55	1.50
17	A	4008	8CT	C01-C02	2.57	1.55	1.50
11	A	1132	CL7	CHC-C4B	2.57	1.45	1.39
11	A	1126	CL7	CHD-C1D	2.57	1.45	1.39
11	J	1302	CL7	CAB-C3B	2.56	1.50	1.45
11	A	1111	CL7	OBD-CAD	2.56	1.26	1.22
16	A	1013	PHO	CMD-C2D	-2.56	1.46	1.51
11	A	1116	CL7	CAB-C3B	2.56	1.50	1.45
11	B	1213	CL7	CAB-C3B	2.56	1.50	1.45
11	A	1109	CL7	CAB-C3B	2.56	1.50	1.45
11	A	1801	CL7	C4C-C3C	-2.56	1.40	1.45
17	B	4014	8CT	C22-C21	2.56	1.56	1.50
17	M	4021	8CT	C22-C21	2.55	1.56	1.50
11	A	1130	CL7	C4C-C3C	-2.55	1.40	1.45
11	A	1120	CL7	CAB-C3B	2.55	1.50	1.45
11	B	1212	CL7	CAB-C3B	2.55	1.50	1.45
17	A	4011	8CT	C22-C21	2.55	1.56	1.50
11	A	1137	CL7	CHC-C4B	2.55	1.45	1.39
11	A	1105	CL7	CAB-C3B	2.55	1.50	1.45
17	B	4006	8CT	C22-C21	2.55	1.56	1.50
11	B	1211	CL7	CAB-C3B	2.55	1.50	1.45
17	W	4020	8CT	C22-C21	2.55	1.56	1.50
17	W	4020	8CT	C30-C29	2.54	1.54	1.50
11	B	1204	CL7	CAB-C3B	2.54	1.50	1.45
12	B	2002	PQN	C10-C1	-2.54	1.43	1.48
11	A	1117	CL7	CAB-C3B	2.54	1.50	1.45
17	J	4015	8CT	C22-C21	2.54	1.56	1.50
11	B	1205	CL7	CHD-C1D	2.54	1.45	1.39
11	A	1122	CL7	CHD-C1D	2.54	1.45	1.39
11	B	1206	CL7	CAB-C3B	2.54	1.50	1.45
17	W	4020	8CT	C01-C02	2.54	1.55	1.50
11	A	1135	CL7	C4C-C3C	-2.53	1.40	1.45
11	A	1113	CL7	CAB-C3B	2.53	1.50	1.45
11	A	1112	CL7	CAB-C3B	2.53	1.50	1.45
17	B	4017	8CT	C22-C21	2.53	1.56	1.50
11	A	1119	CL7	CAB-C3B	2.53	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1224	CL7	C4C-C3C	-2.52	1.40	1.45
11	B	1215	CL7	CAB-C3B	2.52	1.50	1.45
11	A	1132	CL7	CHD-C1D	2.52	1.45	1.39
11	L	1501	CL7	C4C-C3C	-2.52	1.40	1.45
11	A	1122	CL7	CAB-C3B	2.52	1.50	1.45
11	B	1222	CL7	CAB-C3B	2.52	1.50	1.45
11	A	1106	CL7	CAB-C3B	2.52	1.50	1.45
11	A	1104	CL7	C4C-C3C	-2.51	1.40	1.45
11	W	2601	CL7	C4C-C3C	-2.51	1.40	1.45
11	A	1136	CL7	CAB-C3B	2.51	1.50	1.45
11	A	1101	CL7	CAB-C3B	2.51	1.50	1.45
11	A	1118	CL7	CAB-C3B	2.51	1.50	1.45
11	A	1138	CL7	CAB-C3B	2.51	1.50	1.45
11	A	1102	CL7	C4C-C3C	-2.51	1.40	1.45
11	A	1103	CL7	CAB-C3B	2.50	1.50	1.45
11	A	1139	CL7	C4C-C3C	-2.50	1.40	1.45
18	B	5002	LMG	C37-C36	2.50	1.65	1.51
16	B	1023	PHO	CMD-C2D	-2.50	1.46	1.51
11	A	1115	CL7	C4C-C3C	-2.50	1.40	1.45
11	A	1140	CL7	C4C-C3C	-2.50	1.40	1.45
11	B	1202	CL7	CAB-C3B	2.50	1.50	1.45
11	B	1235	CL7	CAB-C3B	2.50	1.50	1.45
11	A	1129	CL7	CHD-C1D	2.49	1.45	1.39
11	A	1115	CL7	CAB-C3B	2.49	1.50	1.45
11	L	1502	CL7	CAB-C3B	2.49	1.50	1.45
16	A	1013	PHO	CMB-C2B	-2.49	1.46	1.51
11	B	1230	CL7	C4C-C3C	-2.49	1.40	1.45
11	B	1208	CL7	CHD-C1D	2.49	1.45	1.39
11	B	1222	CL7	C4C-C3C	-2.49	1.40	1.45
11	B	1210	CL7	CHD-C1D	2.49	1.45	1.39
17	M	4021	8CT	C01-C02	2.49	1.55	1.50
11	A	1126	CL7	CAB-C3B	2.48	1.50	1.45
11	B	1208	CL7	CAB-C3B	2.48	1.50	1.45
11	A	1123	CL7	C4C-C3C	-2.48	1.40	1.45
17	J	4013	8CT	C30-C29	2.48	1.53	1.50
11	B	1226	CL7	CAB-C3B	2.48	1.50	1.45
11	A	1136	CL7	C4C-C3C	-2.48	1.40	1.45
11	A	1124	CL7	C4C-C3C	-2.48	1.40	1.45
11	A	1131	CL7	C4C-C3C	-2.48	1.40	1.45
11	B	1229	CL7	C4C-C3C	-2.48	1.40	1.45
11	A	1128	CL7	CAB-C3B	2.48	1.50	1.45
11	B	1021	CL7	CAB-C3B	2.47	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	1503	CL7	CAB-C3B	2.47	1.50	1.45
15	A	1011	G9R	CAB-C3B	2.47	1.50	1.45
11	B	1224	CL7	CHD-C1D	2.47	1.45	1.39
15	A	1011	G9R	C4C-C3C	-2.47	1.40	1.45
11	A	1116	CL7	C4C-C3C	-2.47	1.40	1.45
11	B	1235	CL7	CHD-C1D	2.47	1.44	1.39
11	B	1203	CL7	CAB-C3B	2.47	1.50	1.45
11	A	1107	CL7	CAB-C3B	2.47	1.50	1.45
11	A	1104	CL7	CAB-C3B	2.47	1.50	1.45
17	L	4019	8CT	C28-C29	2.47	1.38	1.32
11	B	1012	CL7	C4C-C3C	-2.47	1.40	1.45
11	B	1236	CL7	CAB-C3B	2.46	1.50	1.45
11	A	1126	CL7	C4C-C3C	-2.46	1.40	1.45
11	A	1138	CL7	C4C-C3C	-2.46	1.40	1.45
11	A	1114	CL7	C4C-C3C	-2.46	1.40	1.45
11	B	1204	CL7	CHD-C1D	2.46	1.44	1.39
11	B	1225	CL7	C4C-C3C	-2.46	1.40	1.45
11	A	1802	CL7	CHD-C1D	2.46	1.44	1.39
11	B	1205	CL7	CAB-C3B	2.46	1.50	1.45
16	A	1013	PHO	CMC-C2C	-2.46	1.46	1.50
11	A	1103	CL7	C4C-C3C	-2.46	1.40	1.45
11	L	1503	CL7	C4C-C3C	-2.46	1.40	1.45
11	F	1301	CL7	C4C-C3C	-2.45	1.40	1.45
11	B	1238	CL7	C4C-C3C	-2.45	1.40	1.45
11	A	1137	CL7	CHD-C1D	2.45	1.44	1.39
11	B	1021	CL7	C4C-C3C	-2.45	1.40	1.45
17	L	4019	8CT	C22-C21	2.45	1.55	1.50
11	J	1302	CL7	CHD-C1D	2.45	1.44	1.39
11	A	1123	CL7	CAB-C3B	2.45	1.50	1.45
11	A	1125	CL7	CAB-C3B	2.45	1.50	1.45
11	A	1113	CL7	C4C-C3C	-2.45	1.40	1.45
11	A	1127	CL7	C4C-C3C	-2.45	1.40	1.45
11	A	1237	CL7	CAB-C3B	2.45	1.50	1.45
11	B	1228	CL7	CAB-C3B	2.44	1.50	1.45
11	B	1238	CL7	CAB-C3B	2.44	1.50	1.45
11	B	1211	CL7	C4C-C3C	-2.44	1.40	1.45
11	B	1235	CL7	C4C-C3C	-2.44	1.40	1.45
11	A	1131	CL7	CAB-C3B	2.44	1.50	1.45
11	A	1112	CL7	C4C-C3C	-2.44	1.40	1.45
11	B	1228	CL7	CHD-C1D	2.44	1.44	1.39
11	B	1225	CL7	CAB-C3B	2.44	1.50	1.45
11	B	1223	CL7	CAB-C3B	2.44	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1801	CL7	CAB-C3B	2.44	1.50	1.45
11	L	1501	CL7	CAB-C3B	2.44	1.50	1.45
11	A	1106	CL7	C4C-C3C	-2.44	1.40	1.45
11	A	1118	CL7	CHD-C1D	2.44	1.44	1.39
16	A	1013	PHO	C4D-CHA	2.44	1.43	1.39
11	A	1127	CL7	CAB-C3B	2.44	1.50	1.45
11	A	1127	CL7	CHD-C1D	2.44	1.44	1.39
11	B	1206	CL7	C4C-C3C	-2.44	1.40	1.45
11	A	1119	CL7	C4C-C3C	-2.43	1.40	1.45
11	B	1223	CL7	C4C-C3C	-2.43	1.40	1.45
11	A	1121	CL7	CHD-C1D	2.43	1.44	1.39
11	L	1502	CL7	CHD-C1D	2.43	1.44	1.39
11	A	1237	CL7	C4C-C3C	-2.43	1.40	1.45
11	A	1135	CL7	CAB-C3B	2.43	1.50	1.45
11	A	1136	CL7	CHD-C1D	2.43	1.44	1.39
11	A	1109	CL7	C4C-C3C	-2.43	1.40	1.45
11	B	1201	CL7	CAB-C3B	2.43	1.50	1.45
11	B	1212	CL7	CHD-C1D	2.43	1.44	1.39
11	F	1301	CL7	CHD-C1D	2.43	1.44	1.39
11	A	1121	CL7	CAB-C3B	2.42	1.50	1.45
11	A	1116	CL7	CHD-C1D	2.42	1.44	1.39
11	A	1139	CL7	CHD-C1D	2.42	1.44	1.39
11	A	1132	CL7	C4C-C3C	-2.42	1.40	1.45
11	B	1202	CL7	C4C-C3C	-2.42	1.40	1.45
11	B	1213	CL7	C4C-C3C	-2.42	1.40	1.45
11	A	1802	CL7	C4C-C3C	-2.42	1.40	1.45
11	B	1201	CL7	C4C-C3C	-2.42	1.40	1.45
11	A	1109	CL7	CHD-C1D	2.42	1.44	1.39
11	A	1101	CL7	C4C-C3C	-2.42	1.40	1.45
11	A	1124	CL7	CAB-C3B	2.42	1.50	1.45
11	A	1132	CL7	CAB-C3B	2.42	1.50	1.45
11	L	1503	CL7	CHD-C1D	2.42	1.44	1.39
11	A	1107	CL7	CHD-C1D	2.41	1.44	1.39
11	A	1111	CL7	CHD-C1D	2.41	1.44	1.39
12	B	2002	PQN	C5-C4	-2.41	1.43	1.48
11	A	1110	CL7	C4C-C3C	-2.41	1.40	1.45
11	B	1229	CL7	CHD-C1D	2.41	1.44	1.39
11	A	1130	CL7	CAB-C3B	2.41	1.50	1.45
11	B	1201	CL7	CHD-C1D	2.41	1.44	1.39
11	B	1213	CL7	CHD-C1D	2.41	1.44	1.39
11	A	1112	CL7	CHD-C1D	2.41	1.44	1.39
11	A	1107	CL7	C4C-C3C	-2.41	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1237	CL7	CHD-C1D	2.41	1.44	1.39
11	B	1236	CL7	CHD-C1D	2.41	1.44	1.39
11	A	1106	CL7	CHD-C1D	2.41	1.44	1.39
11	A	1130	CL7	CHD-C1D	2.41	1.44	1.39
11	A	1122	CL7	CHC-C4B	2.41	1.44	1.39
11	A	1137	CL7	CAB-C3B	2.41	1.50	1.45
11	B	1207	CL7	CAB-C3B	2.40	1.50	1.45
11	A	1801	CL7	CHD-C1D	2.40	1.44	1.39
11	A	1120	CL7	C4C-C3C	-2.40	1.40	1.45
11	A	1104	CL7	CHD-C1D	2.40	1.44	1.39
11	A	1131	CL7	CHD-C1D	2.40	1.44	1.39
11	A	1113	CL7	CHD-C1D	2.40	1.44	1.39
11	A	1138	CL7	CHD-C1D	2.40	1.44	1.39
11	A	1022	CL7	CHD-C1D	2.40	1.44	1.39
11	B	1206	CL7	CHD-C1D	2.40	1.44	1.39
11	B	1214	CL7	C4C-C3C	-2.40	1.40	1.45
11	B	1207	CL7	C4C-C3C	-2.40	1.40	1.45
17	W	4020	8CT	C28-C29	2.40	1.38	1.32
11	B	1203	CL7	CHD-C1D	2.40	1.44	1.39
16	B	1023	PHO	C4D-CHA	2.40	1.43	1.39
11	B	1211	CL7	CHD-C1D	2.40	1.44	1.39
11	A	1102	CL7	CHD-C1D	2.39	1.44	1.39
11	B	1207	CL7	CHD-C1D	2.39	1.44	1.39
11	B	1225	CL7	CHD-C1D	2.39	1.44	1.39
11	A	1140	CL7	CHD-C1D	2.39	1.44	1.39
11	A	1120	CL7	CHD-C1D	2.39	1.44	1.39
11	W	2601	CL7	CHD-C1D	2.39	1.44	1.39
11	A	1111	CL7	CAB-C3B	2.39	1.50	1.45
11	A	1121	CL7	C4C-C3C	-2.39	1.41	1.45
11	A	1137	CL7	C4C-C3C	-2.39	1.41	1.45
11	B	1228	CL7	C4C-C3C	-2.38	1.41	1.45
11	A	1101	CL7	CHD-C1D	2.38	1.44	1.39
11	B	1236	CL7	C4C-C3C	-2.38	1.41	1.45
11	A	1117	CL7	CHD-C1D	2.38	1.44	1.39
11	B	1208	CL7	C4C-C3C	-2.38	1.41	1.45
17	M	4021	8CT	C28-C29	2.37	1.37	1.32
11	B	1210	CL7	C4C-C3C	-2.37	1.41	1.45
11	B	1222	CL7	CHD-C1D	2.37	1.44	1.39
11	A	1110	CL7	CHD-C1D	2.37	1.44	1.39
16	B	1023	PHO	CAC-C3C	-2.37	1.47	1.51
11	B	1212	CL7	C4C-C3C	-2.37	1.41	1.45
11	J	1302	CL7	C4C-C3C	-2.36	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1129	CL7	CAB-C3B	2.36	1.50	1.45
11	B	1012	CL7	CHD-C1D	2.36	1.44	1.39
11	A	1123	CL7	CHD-C1D	2.36	1.44	1.39
16	B	1023	PHO	CMB-C2B	-2.36	1.46	1.51
11	A	1115	CL7	CHD-C1D	2.36	1.44	1.39
14	A	5001	LHG	C1-C2	2.36	1.61	1.51
11	B	1234	CL7	CAB-C3B	2.36	1.50	1.45
11	L	1501	CL7	CHD-C1D	2.35	1.44	1.39
11	A	1119	CL7	CHD-C1D	2.35	1.44	1.39
18	B	5002	LMG	C33-C32	2.35	1.64	1.51
11	A	1118	CL7	C4C-C3C	-2.35	1.41	1.45
11	B	1239	CL7	CHD-C1D	2.35	1.44	1.39
11	A	1124	CL7	CHD-C1D	2.34	1.44	1.39
11	L	1502	CL7	C4C-C3C	-2.34	1.41	1.45
11	B	1204	CL7	C4C-C3C	-2.34	1.41	1.45
11	B	1230	CL7	CHD-C1D	2.34	1.44	1.39
11	B	1238	CL7	CHD-C1D	2.34	1.44	1.39
11	A	1105	CL7	C4C-C3C	-2.34	1.41	1.45
11	B	1239	CL7	C4C-C3C	-2.34	1.41	1.45
11	B	1234	CL7	CHD-C1D	2.34	1.44	1.39
11	A	1103	CL7	CHD-C1D	2.34	1.44	1.39
11	B	1214	CL7	CHD-C1D	2.34	1.44	1.39
11	A	1126	CL7	C1B-C2B	-2.33	1.37	1.43
12	B	2002	PQN	C11-C3	2.33	1.55	1.51
14	A	5001	LHG	P-O5	2.33	1.59	1.50
17	B	4014	8CT	C10-C03	2.33	1.53	1.45
17	L	4020	8CT	C39-C16	2.33	1.55	1.50
16	A	1013	PHO	CAC-C3C	-2.33	1.47	1.51
11	A	1119	CL7	CMA-C3A	2.32	1.58	1.53
11	B	1210	CL7	OBD-CAD	2.32	1.26	1.22
11	B	1228	CL7	OBD-CAD	2.32	1.26	1.22
11	A	1117	CL7	C4C-C3C	-2.32	1.41	1.45
11	A	1112	CL7	OBD-CAD	2.32	1.26	1.22
11	B	1212	CL7	OBD-CAD	2.31	1.26	1.22
11	B	1202	CL7	CHD-C1D	2.31	1.44	1.39
11	B	1224	CL7	CAB-C3B	2.31	1.50	1.45
11	J	1302	CL7	OBD-CAD	2.31	1.26	1.22
17	M	4021	8CT	C30-C29	2.31	1.53	1.50
11	B	1215	CL7	CHD-C1D	2.31	1.44	1.39
11	B	1229	CL7	CAB-C3B	2.30	1.50	1.45
18	B	5002	LMG	C17-C16	2.30	1.64	1.51
11	B	1223	CL7	CHD-C1D	2.30	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1234	CL7	C4C-C3C	-2.30	1.41	1.45
11	A	1107	CL7	OBD-CAD	2.30	1.26	1.22
17	B	4017	8CT	C39-C16	2.30	1.55	1.50
11	A	1122	CL7	C4C-C3C	-2.29	1.41	1.45
11	B	1205	CL7	C4C-C3C	-2.29	1.41	1.45
11	B	1222	CL7	OBD-CAD	2.29	1.26	1.22
11	A	1114	CL7	OBD-CAD	2.28	1.26	1.22
11	A	1140	CL7	CAB-C3B	2.28	1.50	1.45
11	B	1213	CL7	OBD-CAD	2.28	1.26	1.22
11	A	1802	CL7	OBD-CAD	2.28	1.26	1.22
11	A	1139	CL7	OBD-CAD	2.28	1.26	1.22
17	B	4014	8CT	C30-C29	2.28	1.53	1.50
17	J	4013	8CT	C39-C16	2.28	1.55	1.50
11	A	1022	CL7	OBD-CAD	2.27	1.26	1.22
17	A	4007	8CT	C30-C29	2.27	1.53	1.50
14	A	5003	LHG	P-O5	2.27	1.59	1.50
11	A	1801	CL7	OBD-CAD	2.27	1.26	1.22
14	A	5003	LHG	C1-C2	2.27	1.61	1.51
17	M	4021	8CT	C39-C16	2.27	1.55	1.50
11	A	1129	CL7	C4C-C3C	-2.27	1.41	1.45
17	B	4006	8CT	C39-C16	2.27	1.55	1.50
11	A	1125	CL7	CHD-C1D	2.27	1.44	1.39
11	A	1135	CL7	CHD-C1D	2.26	1.44	1.39
11	A	1105	CL7	OBD-CAD	2.26	1.26	1.22
11	W	2601	CL7	OBD-CAD	2.26	1.26	1.22
18	B	5002	LMG	O8-C9	2.26	1.50	1.45
17	W	4018	8CT	C39-C16	2.26	1.55	1.50
17	B	4017	8CT	C28-C29	2.26	1.37	1.32
17	W	4018	8CT	C30-C29	2.25	1.53	1.50
11	A	1113	CL7	OBD-CAD	2.25	1.26	1.22
11	A	1132	CL7	OBD-CAD	2.25	1.26	1.22
11	B	1012	CL7	CAB-C3B	2.25	1.49	1.45
11	A	1102	CL7	OBD-CAD	2.25	1.26	1.22
11	F	1301	CL7	OBD-CAD	2.25	1.26	1.22
11	B	1236	CL7	OBD-CAD	2.24	1.26	1.22
17	J	4015	8CT	C39-C16	2.24	1.55	1.50
11	B	1239	CL7	OBD-CAD	2.24	1.26	1.22
11	B	1021	CL7	CHD-C1D	2.24	1.44	1.39
17	A	4007	8CT	C28-C29	2.24	1.37	1.32
17	A	4008	8CT	C28-C29	2.24	1.37	1.32
11	A	1131	CL7	OBD-CAD	2.24	1.26	1.22
11	A	1111	CL7	C4C-C3C	-2.24	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1208	CL7	OBD-CAD	2.23	1.26	1.22
11	A	1127	CL7	OBD-CAD	2.23	1.26	1.22
17	A	4011	8CT	C39-C16	2.23	1.55	1.50
11	B	1215	CL7	OBD-CAD	2.23	1.26	1.22
17	L	4019	8CT	C39-C16	2.23	1.55	1.50
11	A	1140	CL7	OBD-CAD	2.23	1.26	1.22
11	A	1118	CL7	OBD-CAD	2.23	1.26	1.22
11	A	1121	CL7	OBD-CAD	2.23	1.26	1.22
11	A	1022	CL7	C1B-C2B	-2.23	1.38	1.43
11	B	1214	CL7	OBD-CAD	2.23	1.26	1.22
17	B	4006	8CT	C10-C03	2.22	1.53	1.45
11	A	1128	CL7	OBD-CAD	2.22	1.26	1.22
11	A	1119	CL7	OBD-CAD	2.22	1.26	1.22
11	B	1201	CL7	OBD-CAD	2.22	1.26	1.22
11	A	1110	CL7	OBD-CAD	2.22	1.26	1.22
11	L	1502	CL7	OBD-CAD	2.22	1.26	1.22
11	B	1226	CL7	CHD-C1D	2.22	1.44	1.39
11	A	1128	CL7	CMB-C2B	2.22	1.55	1.50
11	A	1120	CL7	OBD-CAD	2.22	1.26	1.22
11	B	1224	CL7	OBD-CAD	2.22	1.26	1.22
11	B	1202	CL7	OBD-CAD	2.22	1.26	1.22
11	B	1230	CL7	OBD-CAD	2.22	1.26	1.22
11	B	1211	CL7	OBD-CAD	2.21	1.26	1.22
17	A	4007	8CT	C38-C31	2.21	1.54	1.50
17	A	4007	8CT	C39-C16	2.21	1.55	1.50
11	A	1127	CL7	C1B-C2B	-2.21	1.38	1.43
11	L	1503	CL7	OBD-CAD	2.21	1.26	1.22
11	B	1226	CL7	OBD-CAD	2.21	1.26	1.22
17	W	4018	8CT	C10-C03	2.21	1.52	1.45
11	B	1239	CL7	CAB-C3B	2.21	1.49	1.45
11	B	1235	CL7	OBD-CAD	2.20	1.26	1.22
17	J	4013	8CT	C38-C31	2.20	1.54	1.50
11	A	1128	CL7	CHD-C1D	2.20	1.44	1.39
11	L	1501	CL7	OBD-CAD	2.20	1.26	1.22
11	B	1229	CL7	OBD-CAD	2.20	1.26	1.22
11	A	1122	CL7	OBD-CAD	2.20	1.26	1.22
11	B	1234	CL7	OBD-CAD	2.20	1.26	1.22
11	A	1103	CL7	OBD-CAD	2.20	1.26	1.22
11	A	1138	CL7	OBD-CAD	2.20	1.26	1.22
11	A	1022	CL7	CAB-C3B	2.20	1.49	1.45
11	A	1115	CL7	OBD-CAD	2.19	1.26	1.22
12	B	2002	PQN	C8-C9	2.19	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1116	CL7	OBD-CAD	2.19	1.26	1.22
17	W	4018	8CT	C28-C29	2.19	1.37	1.32
11	A	1117	CL7	OBD-CAD	2.19	1.26	1.22
11	B	1238	CL7	OBD-CAD	2.19	1.26	1.22
17	A	4011	8CT	C10-C03	2.19	1.52	1.45
11	B	1204	CL7	OBD-CAD	2.19	1.26	1.22
11	A	1135	CL7	C1B-C2B	-2.19	1.38	1.43
11	A	1237	CL7	OBD-CAD	2.19	1.26	1.22
17	A	4011	8CT	C38-C31	2.19	1.54	1.50
12	A	2001	PQN	C5-C4	-2.18	1.44	1.48
17	L	4020	8CT	C10-C03	2.18	1.52	1.45
15	A	1011	G9R	OBD-CAD	2.18	1.26	1.22
11	B	1214	CL7	CHB-C4A	2.18	1.41	1.36
11	A	1104	CL7	OBD-CAD	2.18	1.26	1.22
11	A	1126	CL7	OBD-CAD	2.18	1.26	1.22
17	L	4019	8CT	C38-C31	2.18	1.54	1.50
11	A	1137	CL7	OBD-CAD	2.18	1.26	1.22
17	L	4019	8CT	C10-C03	2.18	1.52	1.45
12	B	2002	PQN	C8-C7	2.18	1.43	1.38
11	A	1101	CL7	OBD-CAD	2.18	1.26	1.22
17	J	4013	8CT	C10-C03	2.17	1.52	1.45
17	A	4007	8CT	C10-C03	2.17	1.52	1.45
17	J	4015	8CT	C10-C03	2.17	1.52	1.45
17	B	4006	8CT	C28-C29	2.17	1.37	1.32
17	A	4008	8CT	C38-C31	2.17	1.54	1.50
18	B	5002	LMG	C13-C12	2.17	1.63	1.51
12	A	2001	PQN	C8-C7	2.17	1.43	1.38
17	W	4020	8CT	C39-C16	2.17	1.55	1.50
11	A	1124	CL7	OBD-CAD	2.17	1.26	1.22
11	A	1117	CL7	C1B-C2B	-2.17	1.38	1.43
17	A	4011	8CT	C28-C29	2.17	1.37	1.32
11	A	1123	CL7	OBD-CAD	2.16	1.26	1.22
17	W	4020	8CT	C10-C03	2.16	1.52	1.45
11	B	1207	CL7	OBD-CAD	2.16	1.26	1.22
11	L	1502	CL7	C1B-C2B	-2.16	1.38	1.43
12	A	2001	PQN	C9-C10	2.16	1.43	1.39
12	A	2001	PQN	C8-C9	2.16	1.43	1.38
17	A	4008	8CT	C39-C16	2.16	1.55	1.50
11	A	1106	CL7	OBD-CAD	2.15	1.26	1.22
11	A	1105	CL7	CHD-C1D	2.15	1.44	1.39
11	B	1206	CL7	OBD-CAD	2.15	1.26	1.22
17	W	4018	8CT	C38-C31	2.15	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1203	CL7	OBD-CAD	2.15	1.26	1.22
11	B	1225	CL7	OBD-CAD	2.15	1.26	1.22
17	J	4015	8CT	C38-C31	2.14	1.54	1.50
11	A	1130	CL7	OBD-CAD	2.14	1.26	1.22
17	L	4020	8CT	C38-C31	2.14	1.54	1.50
11	A	1116	CL7	C1B-C2B	-2.14	1.38	1.43
17	L	4020	8CT	C30-C29	2.14	1.53	1.50
17	L	4020	8CT	C28-C29	2.14	1.37	1.32
11	B	1230	CL7	C1B-C2B	-2.13	1.38	1.43
17	B	4014	8CT	C28-C29	2.13	1.37	1.32
17	B	4017	8CT	C10-C03	2.13	1.52	1.45
17	B	4014	8CT	C38-C31	2.13	1.54	1.50
17	B	4017	8CT	C38-C31	2.13	1.54	1.50
11	A	1140	CL7	C1B-C2B	-2.13	1.38	1.43
12	B	2002	PQN	C9-C10	2.13	1.43	1.39
11	B	1226	CL7	CMB-C2B	2.12	1.55	1.50
17	A	4008	8CT	C10-C03	2.12	1.52	1.45
14	A	5003	LHG	C12-C11	2.12	1.63	1.51
11	A	1129	CL7	OBD-CAD	2.12	1.26	1.22
11	B	1223	CL7	OBD-CAD	2.12	1.26	1.22
11	A	1103	CL7	C1B-C2B	-2.11	1.38	1.43
14	A	5003	LHG	C31-C30	2.11	1.63	1.51
14	A	5003	LHG	C32-C31	2.11	1.63	1.51
14	A	5003	LHG	C36-C35	2.11	1.63	1.51
11	B	1205	CL7	C1B-C2B	-2.11	1.38	1.43
14	A	5003	LHG	C29-C28	2.11	1.63	1.51
11	A	1109	CL7	OBD-CAD	2.11	1.26	1.22
18	B	5002	LMG	C35-C34	2.11	1.63	1.51
14	A	5003	LHG	C34-C33	2.11	1.63	1.51
11	B	1224	CL7	C1B-C2B	-2.10	1.38	1.43
14	A	5003	LHG	C35-C34	2.10	1.63	1.51
14	A	5001	LHG	C31-C30	2.10	1.63	1.51
17	B	4006	8CT	C38-C31	2.10	1.54	1.50
17	M	4021	8CT	C10-C03	2.10	1.52	1.45
11	B	1012	CL7	C1B-C2B	-2.10	1.38	1.43
15	A	1011	G9R	C1B-C2B	-2.10	1.38	1.43
18	B	5002	LMG	C16-C15	2.10	1.63	1.51
11	A	1104	CL7	C1B-C2B	-2.10	1.38	1.43
14	A	5001	LHG	C32-C31	2.10	1.63	1.51
14	A	5003	LHG	C11-C10	2.10	1.63	1.51
14	A	5003	LHG	C27-C26	2.10	1.63	1.51
17	B	4017	8CT	C30-C29	2.10	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	5003	LHG	C28-C27	2.10	1.63	1.51
18	B	5002	LMG	C32-C31	2.09	1.63	1.51
14	A	5003	LHG	C10-C9	2.09	1.63	1.51
11	B	1239	CL7	C1B-C2B	-2.09	1.38	1.43
14	A	5001	LHG	C29-C28	2.09	1.63	1.51
17	M	4021	8CT	C38-C31	2.09	1.54	1.50
14	A	5001	LHG	C11-C10	2.09	1.63	1.51
17	A	4011	8CT	C30-C29	2.09	1.53	1.50
11	A	1132	CL7	C4C-NC	-2.09	1.35	1.37
14	A	5001	LHG	C34-C33	2.09	1.63	1.51
11	A	1111	CL7	C1B-C2B	-2.09	1.38	1.43
11	A	1124	CL7	C1B-C2B	-2.09	1.38	1.43
14	A	5001	LHG	C28-C27	2.09	1.63	1.51
14	A	5001	LHG	C35-C34	2.08	1.63	1.51
11	B	1238	CL7	C1B-C2B	-2.08	1.38	1.43
14	A	5001	LHG	C36-C35	2.08	1.63	1.51
14	A	5001	LHG	C12-C11	2.08	1.63	1.51
14	A	5003	LHG	C13-C12	2.08	1.63	1.51
11	A	1135	CL7	OBD-CAD	2.08	1.26	1.22
11	A	1130	CL7	C1B-C2B	-2.08	1.38	1.43
11	B	1234	CL7	C1B-C2B	-2.07	1.38	1.43
14	A	5003	LHG	C33-C32	2.07	1.63	1.51
14	A	5001	LHG	C10-C9	2.07	1.63	1.51
11	B	1021	CL7	CHB-C4A	2.07	1.41	1.36
14	A	5003	LHG	C14-C13	2.07	1.63	1.51
17	B	4014	8CT	C39-C16	2.07	1.55	1.50
11	B	1229	CL7	C1B-C2B	-2.07	1.38	1.43
14	A	5001	LHG	C27-C26	2.07	1.63	1.51
17	B	4006	8CT	C30-C29	2.07	1.53	1.50
11	A	1125	CL7	OBD-CAD	2.07	1.26	1.22
14	A	5001	LHG	C26-C25	2.07	1.63	1.51
11	A	1114	CL7	MG-NC	2.06	2.09	2.05
14	A	5003	LHG	C26-C25	2.06	1.63	1.51
18	B	5002	LMG	O1-C1	2.06	1.43	1.40
14	A	5001	LHG	C13-C12	2.06	1.63	1.51
14	A	5001	LHG	C16-C15	2.06	1.63	1.51
18	B	5002	LMG	C15-C14	2.06	1.63	1.51
11	B	1202	CL7	C1B-C2B	-2.06	1.38	1.43
17	W	4020	8CT	C38-C31	2.06	1.54	1.50
14	A	5003	LHG	C16-C15	2.06	1.63	1.51
14	A	5001	LHG	C14-C13	2.06	1.63	1.51
14	A	5001	LHG	C17-C16	2.05	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	5001	LHG	C33-C32	2.05	1.63	1.51
11	A	1123	CL7	C1B-C2B	-2.05	1.38	1.43
11	B	1228	CL7	C1B-C2B	-2.05	1.38	1.43
11	B	1207	CL7	C1B-C2B	-2.05	1.38	1.43
14	A	5001	LHG	C30-C29	2.05	1.63	1.51
14	A	5003	LHG	C30-C29	2.05	1.63	1.51
12	A	2001	PQN	C7-C6	2.05	1.43	1.38
11	B	1225	CL7	C4C-NC	-2.04	1.35	1.37
14	A	5003	LHG	C17-C16	2.04	1.63	1.51
11	A	1106	CL7	C1B-C2B	-2.04	1.38	1.43
18	B	5002	LMG	C18-C17	2.04	1.63	1.51
11	A	1136	CL7	OBD-CAD	2.04	1.26	1.22
14	A	5003	LHG	C15-C14	2.04	1.63	1.51
14	A	5003	LHG	C20-C19	2.04	1.63	1.51
11	A	1137	CL7	C1B-C2B	-2.04	1.38	1.43
11	B	1222	CL7	C1B-C2B	-2.03	1.38	1.43
18	B	5002	LMG	C4-C3	2.03	1.57	1.52
11	B	1211	CL7	C1B-C2B	-2.03	1.38	1.43
11	B	1201	CL7	C1B-C2B	-2.03	1.38	1.43
11	B	1215	CL7	C4C-NC	-2.03	1.35	1.37
11	A	1131	CL7	C1B-C2B	-2.03	1.38	1.43
14	A	5001	LHG	C15-C14	2.03	1.63	1.51
11	B	1205	CL7	OBD-CAD	2.03	1.26	1.22
14	A	5001	LHG	C20-C19	2.03	1.63	1.51
11	A	1132	CL7	C1B-C2B	-2.03	1.38	1.43
14	A	5003	LHG	C19-C18	2.03	1.63	1.51
11	B	1021	CL7	C1B-C2B	-2.02	1.38	1.43
11	A	1125	CL7	C1B-C2B	-2.02	1.38	1.43
11	B	1206	CL7	C1B-C2B	-2.02	1.38	1.43
14	A	5001	LHG	C18-C17	2.02	1.62	1.51
11	A	1110	CL7	C1B-C2B	-2.02	1.38	1.43
14	A	5003	LHG	C18-C17	2.02	1.62	1.51
11	A	1139	CL7	C1B-C2B	-2.02	1.38	1.43
18	B	5002	LMG	C21-C20	2.02	1.62	1.51
18	B	5002	LMG	C14-C13	2.02	1.62	1.51
11	B	1204	CL7	C1B-C2B	-2.02	1.38	1.43
11	A	1022	CL7	C4C-NC	-2.02	1.35	1.37
11	B	1225	CL7	C1B-C2B	-2.02	1.38	1.43
11	A	1121	CL7	C1B-C2B	-2.02	1.38	1.43
11	B	1226	CL7	CHB-C4A	2.02	1.41	1.36
11	A	1104	CL7	C4C-NC	-2.01	1.35	1.37
11	A	1136	CL7	C1B-C2B	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1115	CL7	C1B-C2B	-2.01	1.38	1.43
11	L	1503	CL7	C1B-C2B	-2.01	1.38	1.43
11	B	1203	CL7	C1B-C2B	-2.00	1.38	1.43
11	L	1501	CL7	C1B-C2B	-2.00	1.38	1.43
11	A	1237	CL7	C1B-C2B	-2.00	1.38	1.43

All (1797) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4008	8CT	C19-C20-C21	-10.91	111.73	127.31
17	A	4008	8CT	C24-C25-C26	-10.14	112.83	127.31
11	A	1105	CL7	C3C-C4C-NC	10.05	117.46	110.18
17	J	4015	8CT	C33-C32-C31	-9.65	115.60	124.85
11	B	1226	CL7	C3C-C4C-NC	9.49	117.05	110.18
11	A	1125	CL7	C3C-C4C-NC	9.45	117.03	110.18
11	A	1128	CL7	C3C-C4C-NC	9.44	117.02	110.18
11	A	1135	CL7	C3C-C4C-NC	9.38	116.98	110.18
11	B	1214	CL7	C3C-C4C-NC	9.37	116.97	110.18
11	B	1230	CL7	C3C-C4C-NC	9.27	116.89	110.18
17	A	4008	8CT	C18-C17-C16	-9.27	114.09	127.31
11	B	1234	CL7	C3C-C4C-NC	9.24	116.87	110.18
17	A	4011	8CT	C24-C25-C26	-9.23	114.13	127.31
11	B	1021	CL7	C3C-C4C-NC	9.23	116.87	110.18
11	A	1119	CL7	C3C-C4C-NC	9.18	116.83	110.18
11	A	1120	CL7	C3C-C4C-NC	9.18	116.83	110.18
11	B	1223	CL7	C3C-C4C-NC	9.18	116.83	110.18
17	A	4007	8CT	C19-C20-C21	-9.17	114.23	127.31
11	B	1238	CL7	C3C-C4C-NC	9.16	116.81	110.18
11	A	1113	CL7	C3C-C4C-NC	9.15	116.81	110.18
11	A	1110	CL7	C3C-C4C-NC	9.14	116.81	110.18
11	B	1202	CL7	C3C-C4C-NC	9.14	116.81	110.18
11	A	1104	CL7	C3C-C4C-NC	9.12	116.79	110.18
11	B	1012	CL7	C3C-C4C-NC	9.12	116.79	110.18
11	B	1213	CL7	C3C-C4C-NC	9.12	116.78	110.18
11	B	1206	CL7	C3C-C4C-NC	9.11	116.78	110.18
17	B	4017	8CT	C19-C20-C21	-9.10	114.32	127.31
11	A	1106	CL7	C3C-C4C-NC	9.09	116.77	110.18
11	A	1022	CL7	C3C-C4C-NC	9.09	116.77	110.18
11	B	1215	CL7	C3C-C4C-NC	9.09	116.77	110.18
11	A	1114	CL7	C3C-C4C-NC	9.09	116.76	110.18
11	A	1115	CL7	C3C-C4C-NC	9.08	116.76	110.18
11	A	1801	CL7	C3C-C4C-NC	9.08	116.76	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1123	CL7	C3C-C4C-NC	9.07	116.75	110.18
11	L	1501	CL7	C3C-C4C-NC	9.05	116.74	110.18
11	A	1131	CL7	C3C-C4C-NC	9.05	116.73	110.18
11	A	1102	CL7	C3C-C4C-NC	9.05	116.73	110.18
11	A	1124	CL7	C3C-C4C-NC	9.04	116.73	110.18
11	L	1503	CL7	C3C-C4C-NC	9.03	116.72	110.18
11	A	1802	CL7	C3C-C4C-NC	9.02	116.71	110.18
11	B	1236	CL7	C3C-C4C-NC	9.02	116.71	110.18
11	A	1137	CL7	C3C-C4C-NC	9.00	116.70	110.18
11	B	1203	CL7	C3C-C4C-NC	9.00	116.70	110.18
11	A	1237	CL7	C3C-C4C-NC	8.99	116.69	110.18
11	A	1116	CL7	C3C-C4C-NC	8.99	116.69	110.18
11	B	1207	CL7	C3C-C4C-NC	8.99	116.69	110.18
11	A	1101	CL7	C3C-C4C-NC	8.98	116.69	110.18
11	W	2601	CL7	C3C-C4C-NC	8.98	116.69	110.18
11	B	1229	CL7	C3C-C4C-NC	8.97	116.68	110.18
11	F	1301	CL7	C3C-C4C-NC	8.97	116.68	110.18
11	B	1210	CL7	C3C-C4C-NC	8.97	116.68	110.18
11	A	1140	CL7	C3C-C4C-NC	8.96	116.67	110.18
11	A	1103	CL7	C3C-C4C-NC	8.96	116.67	110.18
11	B	1212	CL7	C3C-C4C-NC	8.96	116.67	110.18
11	A	1127	CL7	C3C-C4C-NC	8.95	116.67	110.18
11	A	1136	CL7	C3C-C4C-NC	8.95	116.66	110.18
11	B	1204	CL7	C3C-C4C-NC	8.95	116.66	110.18
11	A	1118	CL7	C3C-C4C-NC	8.94	116.66	110.18
11	A	1138	CL7	C3C-C4C-NC	8.94	116.65	110.18
11	J	1302	CL7	C3C-C4C-NC	8.94	116.65	110.18
11	B	1239	CL7	C3C-C4C-NC	8.93	116.65	110.18
11	B	1208	CL7	C3C-C4C-NC	8.93	116.65	110.18
17	M	4021	8CT	C14-C13-C12	-8.93	114.57	127.31
11	A	1121	CL7	C3C-C4C-NC	8.92	116.64	110.18
11	A	1130	CL7	C3C-C4C-NC	8.92	116.64	110.18
11	A	1109	CL7	C3C-C4C-NC	8.92	116.64	110.18
11	A	1139	CL7	C3C-C4C-NC	8.91	116.64	110.18
11	B	1228	CL7	C3C-C4C-NC	8.88	116.62	110.18
11	B	1222	CL7	C3C-C4C-NC	8.86	116.60	110.18
11	B	1211	CL7	C3C-C4C-NC	8.86	116.60	110.18
17	B	4017	8CT	C24-C25-C26	-8.85	114.68	127.31
11	A	1117	CL7	C3C-C4C-NC	8.84	116.58	110.18
11	A	1107	CL7	C3C-C4C-NC	8.83	116.58	110.18
11	B	1201	CL7	C3C-C4C-NC	8.83	116.58	110.18
11	L	1502	CL7	C3C-C4C-NC	8.82	116.57	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1224	CL7	C3C-C4C-NC	8.80	116.56	110.18
11	A	1111	CL7	C3C-C4C-NC	8.79	116.55	110.18
11	B	1225	CL7	C3C-C4C-NC	8.79	116.55	110.18
11	A	1112	CL7	C3C-C4C-NC	8.74	116.51	110.18
11	B	1235	CL7	C3C-C4C-NC	8.70	116.49	110.18
11	A	1126	CL7	C3C-C4C-NC	8.61	116.42	110.18
17	B	4006	8CT	C33-C32-C31	-8.54	116.66	124.85
17	B	4014	8CT	C33-C32-C31	-8.50	116.70	124.85
17	B	4017	8CT	C33-C32-C31	-8.48	116.72	124.85
11	A	1129	CL7	C3C-C4C-NC	8.48	116.32	110.18
11	A	1122	CL7	C3C-C4C-NC	8.46	116.31	110.18
11	B	1205	CL7	C3C-C4C-NC	8.43	116.29	110.18
17	B	4017	8CT	C14-C13-C12	-8.32	115.44	127.31
11	A	1132	CL7	C3C-C4C-NC	8.31	116.20	110.18
11	B	1214	CL7	C2C-C1C-NC	8.28	116.20	110.10
17	A	4008	8CT	C33-C32-C31	-8.26	116.93	124.85
17	W	4020	8CT	C33-C32-C31	-8.25	116.94	124.85
17	J	4013	8CT	C33-C32-C31	-8.24	116.95	124.85
17	L	4019	8CT	C33-C32-C31	-8.18	117.01	124.85
17	L	4020	8CT	C33-C32-C31	-8.17	117.02	124.85
11	A	1137	CL7	C2C-C1C-NC	8.08	116.06	110.10
11	B	1208	CL7	C2C-C1C-NC	7.99	115.99	110.10
17	A	4007	8CT	C18-C17-C16	-7.97	115.94	127.31
11	A	1119	CL7	C2C-C1C-NC	7.95	115.97	110.10
11	A	1122	CL7	C2C-C1C-NC	7.94	115.95	110.10
17	M	4021	8CT	C33-C32-C31	-7.93	117.24	124.85
17	A	4007	8CT	C33-C32-C31	-7.93	117.25	124.85
11	A	1114	CL7	C2C-C1C-NC	7.87	115.90	110.10
11	A	1107	CL7	C2C-C1C-NC	7.85	115.89	110.10
17	A	4007	8CT	C24-C25-C26	-7.85	116.11	127.31
11	B	1210	CL7	C2C-C1C-NC	7.84	115.89	110.10
11	B	1204	CL7	C2C-C1C-NC	7.84	115.88	110.10
11	A	1131	CL7	C2C-C1C-NC	7.79	115.84	110.10
12	B	2002	PQN	C11-C12-C13	-7.77	113.85	126.79
11	B	1236	CL7	C2C-C1C-NC	7.77	115.83	110.10
11	A	1129	CL7	C2C-C1C-NC	7.77	115.83	110.10
11	A	1101	CL7	C2C-C1C-NC	7.76	115.82	110.10
11	A	1110	CL7	C2C-C1C-NC	7.76	115.82	110.10
11	A	1118	CL7	C2C-C1C-NC	7.75	115.81	110.10
11	B	1225	CL7	C2C-C1C-NC	7.75	115.81	110.10
11	B	1239	CL7	C2C-C1C-NC	7.73	115.80	110.10
11	B	1215	CL7	C2C-C1C-NC	7.72	115.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1207	CL7	C2C-C1C-NC	7.72	115.80	110.10
11	A	1104	CL7	C2C-C1C-NC	7.71	115.78	110.10
17	A	4011	8CT	C33-C32-C31	-7.68	117.48	124.85
11	A	1120	CL7	C2C-C1C-NC	7.68	115.76	110.10
11	B	1212	CL7	C2C-C1C-NC	7.67	115.75	110.10
11	A	1132	CL7	C2C-C1C-NC	7.66	115.75	110.10
11	A	1121	CL7	C2C-C1C-NC	7.65	115.74	110.10
11	B	1201	CL7	C2C-C1C-NC	7.64	115.73	110.10
11	A	1127	CL7	C2C-C1C-NC	7.64	115.73	110.10
11	A	1109	CL7	C2C-C1C-NC	7.63	115.73	110.10
11	L	1502	CL7	C2C-C1C-NC	7.63	115.73	110.10
11	B	1234	CL7	C2C-C1C-NC	7.63	115.73	110.10
11	A	1138	CL7	C2C-C1C-NC	7.63	115.73	110.10
11	A	1126	CL7	C2C-C1C-NC	7.63	115.72	110.10
11	B	1235	CL7	C2C-C1C-NC	7.62	115.72	110.10
11	F	1301	CL7	C2C-C1C-NC	7.62	115.72	110.10
11	L	1503	CL7	C2C-C1C-NC	7.62	115.72	110.10
11	A	1117	CL7	C2C-C1C-NC	7.62	115.72	110.10
11	B	1206	CL7	C2C-C1C-NC	7.62	115.72	110.10
11	B	1012	CL7	C2C-C1C-NC	7.61	115.71	110.10
11	L	1501	CL7	C2C-C1C-NC	7.61	115.71	110.10
11	J	1302	CL7	C2C-C1C-NC	7.61	115.71	110.10
11	B	1203	CL7	C2C-C1C-NC	7.60	115.71	110.10
11	A	1105	CL7	C2C-C1C-NC	7.60	115.70	110.10
11	A	1111	CL7	C2C-C1C-NC	7.60	115.70	110.10
11	B	1229	CL7	C2C-C1C-NC	7.60	115.70	110.10
11	A	1112	CL7	C2C-C1C-NC	7.60	115.70	110.10
11	A	1115	CL7	C2C-C1C-NC	7.59	115.70	110.10
11	A	1124	CL7	C2C-C1C-NC	7.59	115.69	110.10
11	A	1801	CL7	C2C-C1C-NC	7.58	115.69	110.10
11	A	1140	CL7	C2C-C1C-NC	7.57	115.69	110.10
11	B	1202	CL7	C2C-C1C-NC	7.57	115.69	110.10
11	B	1228	CL7	C2C-C1C-NC	7.57	115.69	110.10
11	B	1205	CL7	C2C-C1C-NC	7.57	115.68	110.10
11	A	1237	CL7	C2C-C1C-NC	7.57	115.68	110.10
11	B	1223	CL7	C2C-C1C-NC	7.57	115.68	110.10
11	B	1213	CL7	C2C-C1C-NC	7.56	115.67	110.10
11	A	1802	CL7	C2C-C1C-NC	7.55	115.67	110.10
11	A	1136	CL7	C2C-C1C-NC	7.54	115.66	110.10
11	A	1113	CL7	C2C-C1C-NC	7.53	115.65	110.10
11	A	1123	CL7	C2C-C1C-NC	7.53	115.65	110.10
11	B	1230	CL7	C2C-C1C-NC	7.52	115.65	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1238	CL7	C2C-C1C-NC	7.51	115.64	110.10
11	B	1211	CL7	C2C-C1C-NC	7.50	115.63	110.10
11	A	1106	CL7	C2C-C1C-NC	7.49	115.62	110.10
11	A	1116	CL7	C2C-C1C-NC	7.49	115.62	110.10
17	B	4017	8CT	C10-C11-C12	-7.49	114.92	126.23
11	A	1130	CL7	C2C-C1C-NC	7.47	115.61	110.10
12	A	2001	PQN	C15-C13-C12	-7.45	106.04	121.12
12	A	2001	PQN	C14-C13-C15	7.45	127.80	115.27
11	W	2601	CL7	C2C-C1C-NC	7.43	115.58	110.10
11	B	1224	CL7	C2C-C1C-NC	7.43	115.58	110.10
11	A	1103	CL7	C2C-C1C-NC	7.36	115.53	110.10
11	B	1222	CL7	C2C-C1C-NC	7.36	115.53	110.10
11	A	1102	CL7	C2C-C1C-NC	7.33	115.51	110.10
11	A	1022	CL7	C2C-C1C-NC	7.29	115.48	110.10
11	A	1135	CL7	C2C-C1C-NC	7.29	115.48	110.10
12	B	2002	PQN	C14-C13-C15	7.27	127.50	115.27
12	B	2002	PQN	C15-C13-C12	-7.26	106.42	121.12
11	A	1125	CL7	C2C-C1C-NC	7.24	115.44	110.10
11	B	1021	CL7	C2C-C1C-NC	7.24	115.44	110.10
11	B	1226	CL7	C2C-C1C-NC	7.23	115.43	110.10
11	A	1139	CL7	C2C-C1C-NC	7.22	115.42	110.10
11	A	1128	CL7	C2C-C1C-NC	7.21	115.42	110.10
14	A	5001	LHG	O4-P-O5	7.16	147.66	112.24
17	M	4021	8CT	C10-C11-C12	-7.16	115.41	126.23
14	A	5003	LHG	O4-P-O5	7.14	147.55	112.24
15	A	1011	G9R	C2B-C1B-NB	7.13	115.01	110.23
12	A	2001	PQN	C11-C12-C13	-6.88	115.33	126.79
11	L	1502	CL7	C2B-C1B-NB	6.81	114.80	110.23
11	A	1139	CL7	C2B-C1B-NB	6.77	114.77	110.23
11	A	1110	CL7	C2B-C1B-NB	6.76	114.77	110.23
11	A	1022	CL7	C2B-C1B-NB	6.75	114.76	110.23
11	A	1132	CL7	C2B-C1B-NB	6.74	114.75	110.23
11	B	1021	CL7	C1A-NA-C4A	6.74	110.38	106.30
11	A	1128	CL7	C2B-C1B-NB	6.67	114.70	110.23
11	B	1205	CL7	C2B-C1B-NB	6.67	114.70	110.23
11	A	1102	CL7	C2B-C1B-NB	6.67	114.70	110.23
11	A	1111	CL7	C2B-C1B-NB	6.66	114.70	110.23
11	W	2601	CL7	C2B-C1B-NB	6.66	114.70	110.23
11	B	1226	CL7	C2B-C1B-NB	6.66	114.70	110.23
11	A	1126	CL7	C2B-C1B-NB	6.59	114.65	110.23
11	B	1236	CL7	C2B-C1B-NB	6.57	114.64	110.23
11	B	1222	CL7	C2B-C1B-NB	6.56	114.63	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	W	4018	8CT	C24-C25-C26	-6.54	117.97	127.31
11	A	1104	CL7	C2B-C1B-NB	6.52	114.60	110.23
11	A	1124	CL7	C2B-C1B-NB	6.52	114.60	110.23
11	A	1123	CL7	C2B-C1B-NB	6.51	114.60	110.23
11	B	1212	CL7	C2B-C1B-NB	6.50	114.59	110.23
11	B	1203	CL7	C2B-C1B-NB	6.49	114.59	110.23
11	B	1201	CL7	C2B-C1B-NB	6.48	114.58	110.23
11	A	1114	CL7	C2B-C1B-NB	6.47	114.57	110.23
17	A	4011	8CT	C14-C13-C12	-6.45	118.10	127.31
11	B	1021	CL7	C2B-C1B-NB	6.45	114.56	110.23
11	B	1235	CL7	C2B-C1B-NB	6.45	114.55	110.23
11	A	1109	CL7	C2B-C1B-NB	6.44	114.55	110.23
11	A	1106	CL7	C2B-C1B-NB	6.44	114.55	110.23
11	A	1127	CL7	C2B-C1B-NB	6.43	114.54	110.23
11	B	1211	CL7	C2B-C1B-NB	6.41	114.53	110.23
11	L	1501	CL7	C2B-C1B-NB	6.41	114.53	110.23
11	A	1121	CL7	C2B-C1B-NB	6.41	114.53	110.23
11	A	1105	CL7	C2B-C1B-NB	6.40	114.52	110.23
11	B	1224	CL7	C2B-C1B-NB	6.40	114.52	110.23
11	A	1112	CL7	C2B-C1B-NB	6.39	114.52	110.23
11	J	1302	CL7	C2B-C1B-NB	6.39	114.52	110.23
11	B	1012	CL7	C2B-C1B-NB	6.39	114.52	110.23
11	A	1138	CL7	C2B-C1B-NB	6.38	114.51	110.23
11	B	1210	CL7	C2B-C1B-NB	6.38	114.51	110.23
11	A	1117	CL7	C2B-C1B-NB	6.38	114.51	110.23
11	B	1239	CL7	C2B-C1B-NB	6.37	114.50	110.23
11	A	1802	CL7	C2B-C1B-NB	6.36	114.50	110.23
11	B	1213	CL7	C2B-C1B-NB	6.36	114.50	110.23
11	B	1223	CL7	C2B-C1B-NB	6.34	114.48	110.23
17	W	4018	8CT	C33-C32-C31	-6.34	118.77	124.85
11	A	1116	CL7	C2B-C1B-NB	6.34	114.48	110.23
11	B	1228	CL7	C2B-C1B-NB	6.34	114.48	110.23
11	A	1118	CL7	C2B-C1B-NB	6.33	114.48	110.23
11	A	1801	CL7	C2B-C1B-NB	6.33	114.48	110.23
11	L	1503	CL7	C2B-C1B-NB	6.33	114.47	110.23
11	A	1129	CL7	C2B-C1B-NB	6.33	114.47	110.23
11	B	1229	CL7	C2B-C1B-NB	6.32	114.47	110.23
15	A	1011	G9R	C2C-C1C-NC	6.32	115.89	109.97
11	B	1238	CL7	C2B-C1B-NB	6.32	114.47	110.23
11	A	1131	CL7	C2B-C1B-NB	6.30	114.46	110.23
11	A	1130	CL7	C2B-C1B-NB	6.28	114.44	110.23
11	A	1115	CL7	C2B-C1B-NB	6.28	114.44	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1237	CL7	C2B-C1B-NB	6.27	114.43	110.23
11	B	1206	CL7	C2B-C1B-NB	6.27	114.43	110.23
11	A	1120	CL7	C2B-C1B-NB	6.27	114.43	110.23
11	B	1225	CL7	C2B-C1B-NB	6.26	114.43	110.23
11	A	1122	CL7	C2B-C1B-NB	6.26	114.43	110.23
11	B	1202	CL7	C2B-C1B-NB	6.25	114.42	110.23
11	A	1113	CL7	C2B-C1B-NB	6.25	114.42	110.23
11	A	1135	CL7	C2B-C1B-NB	6.25	114.42	110.23
11	A	1101	CL7	C2B-C1B-NB	6.22	114.40	110.23
11	A	1103	CL7	C2B-C1B-NB	6.21	114.39	110.23
11	B	1214	CL7	C1A-NA-C4A	6.21	110.06	106.30
11	B	1204	CL7	C2B-C1B-NB	6.19	114.38	110.23
11	B	1234	CL7	C2B-C1B-NB	6.18	114.37	110.23
11	A	1125	CL7	C2B-C1B-NB	6.17	114.37	110.23
11	A	1136	CL7	C2B-C1B-NB	6.16	114.36	110.23
11	F	1301	CL7	C2B-C1B-NB	6.16	114.36	110.23
11	B	1207	CL7	C2B-C1B-NB	6.15	114.36	110.23
11	B	1215	CL7	C2B-C1B-NB	6.14	114.34	110.23
17	B	4006	8CT	C18-C17-C16	-6.13	118.56	127.31
11	A	1137	CL7	C2B-C1B-NB	6.13	114.34	110.23
11	A	1107	CL7	C2B-C1B-NB	6.06	114.30	110.23
11	A	1140	CL7	C2B-C1B-NB	6.06	114.29	110.23
17	W	4018	8CT	C14-C13-C12	-6.05	118.67	127.31
11	A	1137	CL7	C1A-NA-C4A	6.02	109.95	106.30
11	A	1136	CL7	C1A-NA-C4A	5.97	109.91	106.30
11	B	1208	CL7	C2B-C1B-NB	5.96	114.23	110.23
17	A	4007	8CT	C14-C13-C12	-5.95	118.82	127.31
11	A	1110	CL7	C1A-NA-C4A	5.91	109.88	106.30
11	B	1230	CL7	C2B-C1B-NB	5.88	114.17	110.23
11	A	1138	CL7	C1A-NA-C4A	5.84	109.84	106.30
11	B	1226	CL7	C1A-NA-C4A	5.84	109.83	106.30
11	W	2601	CL7	C1A-NA-C4A	5.81	109.82	106.30
11	A	1122	CL7	C1A-NA-C4A	5.80	109.81	106.30
16	A	1013	PHO	C4D-CHA-CBD	-5.80	105.89	108.52
11	A	1128	CL7	C1A-NA-C4A	5.78	109.80	106.30
17	A	4008	8CT	C24-C23-C21	-5.76	110.24	126.42
11	A	1119	CL7	C1A-NA-C4A	5.75	109.78	106.30
11	B	1215	CL7	C1A-NA-C4A	5.74	109.77	106.30
15	A	1011	G9R	C4A-NA-C1A	5.73	109.28	106.71
11	A	1104	CL7	C1A-NA-C4A	5.72	109.77	106.30
16	B	1023	PHO	C4D-CHA-CBD	-5.71	105.93	108.52
11	A	1119	CL7	C2B-C1B-NB	5.71	114.06	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1115	CL7	C1A-NA-C4A	5.71	109.76	106.30
11	B	1214	CL7	C2B-C1B-NB	5.71	114.06	110.23
11	A	1105	CL7	C1A-NA-C4A	5.70	109.75	106.30
11	A	1102	CL7	C1A-NA-C4A	5.67	109.74	106.30
17	B	4006	8CT	C14-C13-C12	-5.66	119.24	127.31
11	A	1112	CL7	C1A-NA-C4A	5.65	109.72	106.30
17	A	4007	8CT	C04-C03-C02	-5.64	114.67	122.61
11	B	1236	CL7	C1A-NA-C4A	5.63	109.71	106.30
11	A	1107	CL7	C1A-NA-C4A	5.59	109.69	106.30
17	B	4014	8CT	C18-C17-C16	-5.59	119.33	127.31
17	J	4015	8CT	C27-C26-C25	-5.59	115.09	122.92
11	A	1106	CL7	C1A-NA-C4A	5.59	109.68	106.30
11	B	1207	CL7	C1A-NA-C4A	5.59	109.68	106.30
17	A	4011	8CT	C10-C11-C12	-5.59	117.80	126.23
11	F	1301	CL7	C1A-NA-C4A	5.58	109.68	106.30
11	A	1123	CL7	C1A-NA-C4A	5.57	109.67	106.30
11	A	1237	CL7	C1A-NA-C4A	5.57	109.67	106.30
11	B	1224	CL7	C1A-NA-C4A	5.57	109.67	106.30
11	B	1203	CL7	C1A-NA-C4A	5.56	109.67	106.30
15	A	1011	G9R	C3C-C4C-NC	5.56	116.81	110.57
11	B	1235	CL7	C1A-NA-C4A	5.56	109.67	106.30
11	B	1239	CL7	C1A-NA-C4A	5.56	109.67	106.30
11	A	1140	CL7	C1A-NA-C4A	5.56	109.67	106.30
11	A	1801	CL7	C1A-NA-C4A	5.54	109.66	106.30
11	A	1131	CL7	C1A-NA-C4A	5.54	109.66	106.30
11	A	1113	CL7	C1A-NA-C4A	5.54	109.66	106.30
17	L	4020	8CT	C04-C03-C02	-5.54	114.81	122.61
11	A	1109	CL7	C1A-NA-C4A	5.54	109.65	106.30
11	B	1204	CL7	C1A-NA-C4A	5.54	109.65	106.30
11	A	1116	CL7	C1A-NA-C4A	5.53	109.65	106.30
17	L	4020	8CT	C14-C13-C12	-5.52	119.43	127.31
11	B	1206	CL7	C1A-NA-C4A	5.52	109.64	106.30
11	A	1135	CL7	C1A-NA-C4A	5.52	109.64	106.30
11	A	1120	CL7	C1A-NA-C4A	5.51	109.64	106.30
11	B	1210	CL7	C1A-NA-C4A	5.51	109.64	106.30
11	J	1302	CL7	C1A-NA-C4A	5.49	109.63	106.30
11	A	1125	CL7	C1A-NA-C4A	5.49	109.62	106.30
11	B	1230	CL7	C1A-NA-C4A	5.49	109.62	106.30
11	L	1503	CL7	C1A-NA-C4A	5.49	109.62	106.30
11	L	1502	CL7	C1A-NA-C4A	5.48	109.62	106.30
17	W	4020	8CT	C19-C18-C17	-5.48	112.26	123.47
11	A	1101	CL7	C1A-NA-C4A	5.47	109.61	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1124	CL7	C1A-NA-C4A	5.47	109.61	106.30
11	A	1130	CL7	C1A-NA-C4A	5.46	109.61	106.30
11	B	1212	CL7	C1A-NA-C4A	5.46	109.60	106.30
11	B	1213	CL7	C1A-NA-C4A	5.45	109.60	106.30
11	B	1225	CL7	C1A-NA-C4A	5.45	109.60	106.30
11	B	1223	CL7	C1A-NA-C4A	5.44	109.59	106.30
11	A	1802	CL7	C1A-NA-C4A	5.43	109.59	106.30
11	B	1234	CL7	C1A-NA-C4A	5.43	109.59	106.30
11	B	1201	CL7	C1A-NA-C4A	5.42	109.58	106.30
11	L	1501	CL7	C1A-NA-C4A	5.42	109.58	106.30
11	A	1118	CL7	C1A-NA-C4A	5.42	109.58	106.30
11	A	1103	CL7	C1A-NA-C4A	5.41	109.58	106.30
11	B	1222	CL7	C1A-NA-C4A	5.41	109.58	106.30
17	J	4013	8CT	C14-C13-C12	-5.41	119.59	127.31
11	A	1121	CL7	C1A-NA-C4A	5.41	109.58	106.30
11	A	1139	CL7	C1A-NA-C4A	5.39	109.56	106.30
11	A	1111	CL7	C1A-NA-C4A	5.39	109.56	106.30
11	B	1211	CL7	C1A-NA-C4A	5.38	109.56	106.30
17	M	4021	8CT	C18-C17-C16	-5.38	119.63	127.31
17	J	4015	8CT	C18-C17-C16	-5.38	119.63	127.31
11	A	1129	CL7	C1A-NA-C4A	5.36	109.55	106.30
11	B	1202	CL7	C1A-NA-C4A	5.34	109.54	106.30
11	B	1208	CL7	C1A-NA-C4A	5.33	109.53	106.30
17	J	4013	8CT	C10-C11-C12	-5.32	118.19	126.23
11	A	1117	CL7	C1A-NA-C4A	5.32	109.52	106.30
11	B	1238	CL7	C1A-NA-C4A	5.30	109.51	106.30
11	A	1022	CL7	C1A-NA-C4A	5.30	109.51	106.30
11	B	1205	CL7	C1A-NA-C4A	5.30	109.51	106.30
11	A	1127	CL7	C1A-NA-C4A	5.29	109.50	106.30
11	B	1012	CL7	C1A-NA-C4A	5.29	109.50	106.30
11	A	1132	CL7	C1A-NA-C4A	5.28	109.50	106.30
11	B	1228	CL7	C1A-NA-C4A	5.26	109.49	106.30
17	L	4019	8CT	C18-C17-C16	-5.26	119.80	127.31
11	A	1128	CL7	C1D-ND-C4D	-5.26	102.60	106.33
11	A	1114	CL7	C1A-NA-C4A	5.24	109.47	106.30
17	W	4020	8CT	C24-C25-C26	-5.23	119.84	127.31
11	B	1229	CL7	C1A-NA-C4A	5.23	109.47	106.30
17	L	4019	8CT	C01-C02-C03	-5.12	118.78	124.53
17	M	4021	8CT	C01-C02-C03	-5.11	118.79	124.53
17	W	4018	8CT	C18-C17-C16	-5.11	120.02	127.31
11	A	1126	CL7	C1A-NA-C4A	5.09	109.38	106.30
11	A	1105	CL7	C1D-ND-C4D	-5.08	102.73	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1210	CL7	CMD-C2D-C1D	5.07	133.10	125.37
11	B	1226	CL7	C1D-ND-C4D	-5.07	102.73	106.33
11	A	1105	CL7	C2D-C1D-ND	5.07	113.63	110.23
17	J	4013	8CT	C19-C20-C21	-5.07	120.08	127.31
17	A	4011	8CT	C19-C20-C21	-5.06	120.09	127.31
17	J	4015	8CT	C14-C13-C12	-5.00	120.18	127.31
17	W	4018	8CT	C19-C20-C21	-4.99	120.19	127.31
17	B	4017	8CT	C24-C23-C21	-4.96	112.47	126.42
11	A	1107	CL7	CMD-C2D-C1D	4.92	132.86	125.37
11	A	1128	CL7	C2D-C1D-ND	4.90	113.52	110.23
17	B	4014	8CT	C40-C12-C13	-4.89	116.07	122.92
11	B	1226	CL7	C2D-C1D-ND	4.88	113.50	110.23
11	B	1021	CL7	C1D-ND-C4D	-4.85	102.89	106.33
11	A	1115	CL7	C1D-ND-C4D	-4.82	102.91	106.33
11	A	1117	CL7	C1D-ND-C4D	-4.81	102.92	106.33
11	A	1135	CL7	C1D-ND-C4D	-4.81	102.92	106.33
11	F	1301	CL7	C1D-ND-C4D	-4.79	102.93	106.33
11	A	1129	CL7	CMD-C2D-C1D	4.79	132.66	125.37
11	B	1211	CL7	CMD-C2D-C1D	4.78	132.65	125.37
11	A	1122	CL7	CMD-C2D-C1D	4.77	132.64	125.37
11	A	1135	CL7	C2D-C1D-ND	4.77	113.43	110.23
17	L	4020	8CT	C24-C25-C26	-4.76	120.51	127.31
17	B	4006	8CT	C04-C03-C02	-4.76	115.91	122.61
11	B	1214	CL7	C1D-ND-C4D	-4.76	102.95	106.33
17	B	4006	8CT	C01-C02-C03	-4.76	119.19	124.53
17	A	4011	8CT	C18-C17-C16	-4.76	120.52	127.31
11	A	1138	CL7	C1D-ND-C4D	-4.75	102.96	106.33
11	B	1205	CL7	C1D-ND-C4D	-4.74	102.97	106.33
11	B	1224	CL7	CMD-C2D-C1D	4.74	132.59	125.37
11	A	1109	CL7	CMD-C2D-C1D	4.73	132.58	125.37
11	A	1125	CL7	CMD-C2D-C1D	4.73	132.57	125.37
11	A	1111	CL7	C1D-ND-C4D	-4.72	102.98	106.33
11	B	1204	CL7	C1D-ND-C4D	-4.72	102.98	106.33
11	B	1203	CL7	CMD-C2D-C1D	4.72	132.56	125.37
17	W	4020	8CT	C01-C02-C03	-4.71	119.24	124.53
11	A	1136	CL7	C1D-ND-C4D	-4.71	102.99	106.33
11	B	1205	CL7	CMD-C2D-C1D	4.70	132.53	125.37
11	A	1113	CL7	C1D-ND-C4D	-4.69	103.00	106.33
11	A	1135	CL7	CMD-C2D-C1D	4.69	132.51	125.37
11	A	1802	CL7	C1D-ND-C4D	-4.68	103.01	106.33
11	A	1130	CL7	C1D-ND-C4D	-4.68	103.01	106.33
11	A	1237	CL7	C1D-ND-C4D	-4.68	103.01	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1234	CL7	C2D-C1D-ND	4.67	113.37	110.23
11	J	1302	CL7	CMD-C2D-C1D	4.67	132.49	125.37
11	A	1118	CL7	CMD-C2D-C1D	4.67	132.48	125.37
11	B	1226	CL7	CMD-C2D-C1D	4.67	132.48	125.37
11	A	1110	CL7	CMD-C2D-C1D	4.67	132.48	125.37
11	A	1139	CL7	CMD-C2D-C1D	4.66	132.47	125.37
11	B	1229	CL7	C1D-ND-C4D	-4.66	103.02	106.33
11	L	1501	CL7	CMD-C2D-C1D	4.66	132.47	125.37
11	B	1239	CL7	CMD-C2D-C1D	4.65	132.46	125.37
11	B	1234	CL7	C1D-ND-C4D	-4.65	103.03	106.33
11	A	1128	CL7	CMD-C2D-C1D	4.65	132.46	125.37
17	J	4015	8CT	C30-C31-C32	-4.65	115.75	121.47
11	B	1207	CL7	CMD-C2D-C1D	4.65	132.45	125.37
11	B	1222	CL7	C1D-ND-C4D	-4.65	103.03	106.33
11	A	1103	CL7	C1D-ND-C4D	-4.65	103.03	106.33
11	B	1021	CL7	C2D-C1D-ND	4.65	113.35	110.23
11	J	1302	CL7	C1D-ND-C4D	-4.65	103.03	106.33
11	A	1237	CL7	CMD-C2D-C1D	4.64	132.44	125.37
11	A	1116	CL7	C1D-ND-C4D	-4.64	103.04	106.33
11	B	1202	CL7	CMD-C2D-C1D	4.64	132.44	125.37
11	F	1301	CL7	CMD-C2D-C1D	4.64	132.43	125.37
11	B	1238	CL7	C1D-ND-C4D	-4.64	103.04	106.33
11	B	1239	CL7	C1D-ND-C4D	-4.63	103.05	106.33
11	A	1139	CL7	C1D-ND-C4D	-4.63	103.05	106.33
11	A	1125	CL7	C1D-ND-C4D	-4.63	103.05	106.33
11	A	1120	CL7	C1D-ND-C4D	-4.63	103.05	106.33
11	A	1119	CL7	C1D-ND-C4D	-4.62	103.05	106.33
11	A	1115	CL7	CMD-C2D-C1D	4.62	132.40	125.37
11	B	1213	CL7	C1D-ND-C4D	-4.62	103.06	106.33
11	B	1235	CL7	CMD-C2D-C1D	4.62	132.40	125.37
11	A	1115	CL7	C2D-C1D-ND	4.62	113.33	110.23
11	B	1229	CL7	CMD-C2D-C1D	4.62	132.40	125.37
11	A	1105	CL7	CMD-C2D-C1D	4.61	132.40	125.37
11	A	1113	CL7	CMD-C2D-C1D	4.61	132.40	125.37
11	W	2601	CL7	CMD-C2D-C1D	4.61	132.39	125.37
11	A	1127	CL7	CMD-C2D-C1D	4.61	132.39	125.37
11	B	1211	CL7	C1D-ND-C4D	-4.61	103.06	106.33
11	B	1223	CL7	CMD-C2D-C1D	4.61	132.38	125.37
11	A	1123	CL7	CMD-C2D-C1D	4.60	132.38	125.37
11	B	1222	CL7	CMD-C2D-C1D	4.60	132.38	125.37
11	B	1214	CL7	C2D-C1D-ND	4.60	113.32	110.23
11	W	2601	CL7	C1D-ND-C4D	-4.60	103.07	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1131	CL7	CMD-C2D-C1D	4.60	132.37	125.37
17	L	4020	8CT	C10-C11-C12	-4.59	119.30	126.23
11	A	1802	CL7	CMD-C2D-C1D	4.59	132.36	125.37
11	B	1212	CL7	CMD-C2D-C1D	4.58	132.35	125.37
11	A	1101	CL7	CMD-C2D-C1D	4.58	132.35	125.37
11	B	1225	CL7	CMD-C2D-C1D	4.58	132.35	125.37
11	A	1125	CL7	C2D-C1D-ND	4.58	113.30	110.23
11	A	1117	CL7	C2D-C1D-ND	4.58	113.30	110.23
11	A	1801	CL7	CMD-C2D-C1D	4.58	132.34	125.37
11	B	1208	CL7	CMD-C2D-C1D	4.57	132.34	125.37
11	B	1225	CL7	C1D-ND-C4D	-4.57	103.09	106.33
11	B	1235	CL7	C1D-ND-C4D	-4.57	103.09	106.33
11	A	1136	CL7	CMD-C2D-C1D	4.57	132.33	125.37
11	W	2601	CL7	C2D-C1D-ND	4.57	113.30	110.23
11	A	1103	CL7	CMD-C2D-C1D	4.57	132.32	125.37
11	A	1102	CL7	CMD-C2D-C1D	4.56	132.32	125.37
11	A	1121	CL7	C1D-ND-C4D	-4.56	103.09	106.33
11	F	1301	CL7	C2D-C1D-ND	4.56	113.29	110.23
11	A	1104	CL7	CMD-C2D-C1D	4.56	132.32	125.37
11	B	1228	CL7	CMD-C2D-C1D	4.56	132.32	125.37
11	B	1201	CL7	CMD-C2D-C1D	4.56	132.31	125.37
11	A	1140	CL7	C1D-ND-C4D	-4.55	103.10	106.33
11	A	1120	CL7	C2D-C1D-ND	4.55	113.28	110.23
11	B	1215	CL7	C1D-ND-C4D	-4.55	103.10	106.33
11	A	1109	CL7	C1D-ND-C4D	-4.55	103.10	106.33
17	W	4018	8CT	C35-C30-C29	-4.55	106.95	112.70
11	A	1102	CL7	C1D-ND-C4D	-4.55	103.10	106.33
11	B	1213	CL7	CMD-C2D-C1D	4.55	132.30	125.37
11	B	1205	CL7	C2D-C1D-ND	4.55	113.28	110.23
11	A	1124	CL7	CMD-C2D-C1D	4.54	132.28	125.37
11	A	1107	CL7	C1D-ND-C4D	-4.54	103.11	106.33
11	B	1214	CL7	CMD-C2D-C1D	4.54	132.28	125.37
11	B	1202	CL7	C1D-ND-C4D	-4.54	103.11	106.33
11	B	1210	CL7	C1D-ND-C4D	-4.54	103.11	106.33
11	B	1215	CL7	CMD-C2D-C1D	4.53	132.27	125.37
11	A	1118	CL7	C1D-ND-C4D	-4.53	103.12	106.33
11	A	1119	CL7	CMD-C2D-C1D	4.53	132.26	125.37
11	B	1238	CL7	CMD-C2D-C1D	4.53	132.26	125.37
11	B	1212	CL7	C1D-ND-C4D	-4.53	103.12	106.33
11	A	1130	CL7	CMD-C2D-C1D	4.52	132.26	125.37
11	L	1503	CL7	C1D-ND-C4D	-4.52	103.12	106.33
11	B	1223	CL7	C1D-ND-C4D	-4.52	103.13	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1112	CL7	CMD-C2D-C1D	4.52	132.25	125.37
11	A	1123	CL7	C1D-ND-C4D	-4.51	103.13	106.33
11	A	1113	CL7	C2D-C1D-ND	4.51	113.26	110.23
11	A	1132	CL7	C1D-ND-C4D	-4.51	103.13	106.33
11	A	1801	CL7	C1D-ND-C4D	-4.51	103.13	106.33
11	A	1119	CL7	C2D-C1D-ND	4.51	113.25	110.23
17	W	4020	8CT	C04-C03-C02	-4.51	116.27	122.61
11	A	1116	CL7	CMD-C2D-C1D	4.50	132.23	125.37
11	L	1501	CL7	C1D-ND-C4D	-4.50	103.14	106.33
11	B	1207	CL7	C1D-ND-C4D	-4.50	103.14	106.33
11	A	1801	CL7	C2D-C1D-ND	4.50	113.25	110.23
11	B	1234	CL7	CMD-C2D-C1D	4.50	132.22	125.37
11	B	1236	CL7	C1D-ND-C4D	-4.50	103.14	106.33
11	B	1202	CL7	C2D-C1D-ND	4.50	113.25	110.23
11	L	1502	CL7	CMD-C2D-C1D	4.49	132.21	125.37
11	A	1131	CL7	C1D-ND-C4D	-4.49	103.15	106.33
17	A	4008	8CT	C23-C21-C20	4.49	125.83	118.94
11	B	1230	CL7	C1D-ND-C4D	-4.49	103.15	106.33
11	A	1112	CL7	C1D-ND-C4D	-4.48	103.15	106.33
17	M	4021	8CT	C14-C15-C16	-4.48	113.82	126.42
11	B	1239	CL7	C2D-C1D-ND	4.48	113.24	110.23
11	A	1802	CL7	C2D-C1D-ND	4.48	113.24	110.23
17	L	4019	8CT	C14-C13-C12	-4.48	120.92	127.31
11	B	1204	CL7	CMD-C2D-C1D	4.48	132.19	125.37
17	B	4017	8CT	C01-C02-C03	-4.48	119.50	124.53
11	A	1106	CL7	C1D-ND-C4D	-4.48	103.16	106.33
11	A	1120	CL7	CMD-C2D-C1D	4.47	132.18	125.37
11	B	1222	CL7	C2D-C1D-ND	4.47	113.23	110.23
11	A	1101	CL7	C1D-ND-C4D	-4.47	103.16	106.33
11	A	1136	CL7	C2D-C1D-ND	4.46	113.22	110.23
11	B	1230	CL7	C2D-C1D-ND	4.46	113.22	110.23
17	B	4017	8CT	C04-C03-C02	-4.46	116.34	122.61
11	A	1111	CL7	C2D-C1D-ND	4.45	113.22	110.23
11	A	1140	CL7	C2D-C1D-ND	4.45	113.22	110.23
17	B	4006	8CT	C07-C02-C03	-4.45	116.27	122.73
11	L	1503	CL7	CMD-C2D-C1D	4.45	132.14	125.37
17	A	4007	8CT	C10-C11-C12	-4.45	119.52	126.23
11	A	1102	CL7	C2D-C1D-ND	4.45	113.21	110.23
17	B	4014	8CT	C30-C31-C32	-4.44	116.01	121.47
11	A	1103	CL7	C2D-C1D-ND	4.44	113.21	110.23
11	B	1201	CL7	C1D-ND-C4D	-4.44	103.18	106.33
17	L	4020	8CT	C07-C02-C03	-4.43	116.30	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1104	CL7	C2D-C1D-ND	4.43	113.20	110.23
11	A	1137	CL7	CMD-C2D-C1D	4.43	132.11	125.37
11	A	1123	CL7	C2D-C1D-ND	4.43	113.20	110.23
11	B	1223	CL7	C2D-C1D-ND	4.43	113.20	110.23
11	A	1122	CL7	C1D-ND-C4D	-4.42	103.19	106.33
11	B	1208	CL7	C1D-ND-C4D	-4.42	103.19	106.33
11	A	1106	CL7	CMD-C2D-C1D	4.42	132.10	125.37
11	B	1228	CL7	C1D-ND-C4D	-4.41	103.20	106.33
11	A	1132	CL7	CMD-C2D-C1D	4.41	132.09	125.37
11	A	1114	CL7	CMD-C2D-C1D	4.41	132.09	125.37
11	L	1503	CL7	C2D-C1D-ND	4.41	113.19	110.23
11	A	1110	CL7	C2D-C1D-ND	4.40	113.18	110.23
11	B	1206	CL7	C2D-C1D-ND	4.40	113.18	110.23
11	A	1121	CL7	C2D-C1D-ND	4.40	113.18	110.23
11	B	1238	CL7	C2D-C1D-ND	4.40	113.18	110.23
17	A	4008	8CT	C14-C13-C12	-4.39	121.04	127.31
15	A	1011	G9R	CMD-C2D-C1D	4.39	132.46	124.71
11	B	1236	CL7	C2D-C1D-ND	4.39	113.18	110.23
11	A	1237	CL7	C2D-C1D-ND	4.39	113.17	110.23
11	B	1213	CL7	C2D-C1D-ND	4.39	113.17	110.23
11	A	1118	CL7	C2D-C1D-ND	4.39	113.17	110.23
11	L	1501	CL7	C2D-C1D-ND	4.39	113.17	110.23
11	A	1124	CL7	C1D-ND-C4D	-4.38	103.22	106.33
11	B	1215	CL7	C2D-C1D-ND	4.38	113.17	110.23
11	A	1106	CL7	C2D-C1D-ND	4.38	113.17	110.23
17	A	4008	8CT	C35-C30-C29	-4.38	107.16	112.70
11	A	1104	CL7	C1D-ND-C4D	-4.38	103.22	106.33
11	B	1224	CL7	C1D-ND-C4D	-4.38	103.22	106.33
11	B	1212	CL7	C2D-C1D-ND	4.38	113.17	110.23
11	B	1207	CL7	C2D-C1D-ND	4.37	113.16	110.23
17	A	4007	8CT	C24-C23-C21	-4.37	114.14	126.42
11	A	1130	CL7	C2D-C1D-ND	4.37	113.16	110.23
11	A	1117	CL7	CMD-C2D-C1D	4.37	132.02	125.37
17	A	4011	8CT	C01-C02-C03	-4.37	119.62	124.53
11	A	1111	CL7	CMD-C2D-C1D	4.37	132.02	125.37
11	J	1302	CL7	C2D-C1D-ND	4.36	113.16	110.23
11	A	1022	CL7	C2D-C1D-ND	4.36	113.16	110.23
11	A	1109	CL7	C2D-C1D-ND	4.36	113.15	110.23
11	A	1116	CL7	C2D-C1D-ND	4.36	113.15	110.23
11	L	1502	CL7	C1D-ND-C4D	-4.35	103.24	106.33
11	B	1206	CL7	C1D-ND-C4D	-4.35	103.24	106.33
11	A	1127	CL7	C1D-ND-C4D	-4.35	103.25	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1229	CL7	C2D-C1D-ND	4.34	113.14	110.23
11	A	1137	CL7	C1D-ND-C4D	-4.33	103.26	106.33
11	A	1101	CL7	C2D-C1D-ND	4.33	113.14	110.23
17	A	4008	8CT	C01-C02-C03	-4.33	119.67	124.53
11	A	1121	CL7	CMD-C2D-C1D	4.33	131.96	125.37
11	A	1126	CL7	CMD-C2D-C1D	4.32	131.96	125.37
11	A	1110	CL7	C1D-ND-C4D	-4.32	103.26	106.33
17	L	4020	8CT	C01-C02-C03	-4.32	119.67	124.53
11	B	1012	CL7	C2D-C1D-ND	4.32	113.13	110.23
11	A	1140	CL7	CMD-C2D-C1D	4.32	131.95	125.37
11	B	1206	CL7	CMD-C2D-C1D	4.32	131.95	125.37
11	A	1022	CL7	C1D-ND-C4D	-4.31	103.27	106.33
11	A	1107	CL7	C2D-C1D-ND	4.31	113.12	110.23
11	B	1012	CL7	C1D-ND-C4D	-4.31	103.27	106.33
11	B	1203	CL7	C1D-ND-C4D	-4.30	103.28	106.33
11	A	1139	CL7	C2D-C1D-ND	4.30	113.11	110.23
11	B	1235	CL7	C2D-C1D-ND	4.30	113.11	110.23
11	B	1021	CL7	CMD-C2D-C1D	4.29	131.91	125.37
11	B	1204	CL7	C2D-C1D-ND	4.29	113.11	110.23
11	A	1138	CL7	CMD-C2D-C1D	4.29	131.90	125.37
11	A	1112	CL7	C2D-C1D-ND	4.28	113.10	110.23
11	A	1131	CL7	C2D-C1D-ND	4.28	113.10	110.23
11	B	1230	CL7	CMD-C2D-C1D	4.28	131.89	125.37
15	A	1011	G9R	C1D-ND-C4D	-4.27	103.30	106.33
11	A	1137	CL7	C2D-C1D-ND	4.27	113.09	110.23
11	B	1236	CL7	CMD-C2D-C1D	4.26	131.86	125.37
11	A	1129	CL7	C1D-ND-C4D	-4.26	103.31	106.33
11	A	1138	CL7	C2D-C1D-ND	4.25	113.08	110.23
11	B	1203	CL7	C2D-C1D-ND	4.25	113.08	110.23
11	A	1126	CL7	C1D-ND-C4D	-4.25	103.31	106.33
11	B	1210	CL7	C2D-C1D-ND	4.25	113.08	110.23
11	B	1225	CL7	C2D-C1D-ND	4.25	113.08	110.23
11	A	1022	CL7	CMD-C2D-C1D	4.25	131.84	125.37
11	B	1228	CL7	C2D-C1D-ND	4.21	113.06	110.23
17	L	4020	8CT	C19-C20-C21	-4.21	121.30	127.31
11	A	1124	CL7	C2D-C1D-ND	4.21	113.06	110.23
11	B	1201	CL7	C2D-C1D-ND	4.21	113.05	110.23
11	A	1127	CL7	C2D-C1D-ND	4.20	113.05	110.23
11	B	1224	CL7	C2D-C1D-ND	4.19	113.04	110.23
11	B	1208	CL7	C2D-C1D-ND	4.16	113.02	110.23
11	L	1502	CL7	C2D-C1D-ND	4.16	113.02	110.23
11	B	1211	CL7	C2D-C1D-ND	4.15	113.01	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1022	CL7	C3A-C4A-CHB	-4.15	117.54	123.70
17	B	4014	8CT	C01-C02-C03	-4.14	119.88	124.53
11	A	1122	CL7	C2D-C1D-ND	4.14	113.00	110.23
17	J	4013	8CT	C18-C17-C16	-4.13	121.42	127.31
17	W	4020	8CT	C07-C02-C03	-4.11	116.77	122.73
17	A	4007	8CT	C07-C02-C03	-4.10	116.78	122.73
17	J	4015	8CT	C01-C02-C03	-4.08	119.94	124.53
11	A	1114	CL7	C1D-ND-C4D	-4.08	103.44	106.33
17	J	4015	8CT	C04-C03-C02	-4.07	116.87	122.61
17	B	4014	8CT	C07-C02-C03	-4.07	116.83	122.73
11	B	1012	CL7	CMD-C2D-C1D	4.06	131.56	125.37
11	A	1132	CL7	C2D-C1D-ND	4.05	112.95	110.23
17	J	4013	8CT	C01-C02-C03	-4.01	120.02	124.53
14	A	5003	LHG	O6-P-O5	-4.01	93.42	109.07
17	B	4017	8CT	C18-C17-C16	-4.00	121.60	127.31
17	L	4020	8CT	C30-C31-C32	-3.99	116.56	121.47
11	A	1126	CL7	C2D-C1D-ND	3.98	112.90	110.23
17	A	4008	8CT	C30-C31-C32	-3.98	116.57	121.47
18	B	5002	LMG	O7-C10-C11	3.97	120.07	111.50
17	L	4019	8CT	C10-C11-C12	-3.97	120.24	126.23
17	J	4015	8CT	C10-C11-C12	-3.93	120.29	126.23
17	J	4015	8CT	C07-C02-C03	-3.92	117.04	122.73
17	M	4021	8CT	C24-C25-C26	-3.91	121.72	127.31
17	B	4014	8CT	C04-C03-C02	-3.91	117.10	122.61
11	A	1129	CL7	C2D-C1D-ND	3.91	112.85	110.23
17	B	4006	8CT	C24-C25-C26	-3.88	121.78	127.31
11	A	1104	CL7	C3A-C4A-CHB	-3.86	117.98	123.70
17	J	4013	8CT	C27-C26-C25	-3.85	117.53	122.92
17	A	4008	8CT	C22-C21-C20	-3.82	117.56	122.92
14	A	5001	LHG	O7-C7-C8	3.82	119.74	111.50
11	A	1127	CL7	C3A-C4A-CHB	-3.82	118.03	123.70
14	A	5003	LHG	O3-P-O5	-3.82	94.15	109.07
17	M	4021	8CT	C18-C19-C20	-3.81	115.68	123.47
11	A	1110	CL7	C3A-C4A-CHB	-3.80	118.06	123.70
17	B	4006	8CT	C30-C31-C32	-3.80	116.79	121.47
11	B	1012	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
14	A	5001	LHG	O6-P-O5	-3.76	94.39	109.07
11	A	1131	CL7	C3A-C4A-CHB	-3.75	118.14	123.70
15	A	1011	G9R	C2D-C1D-ND	3.74	112.86	110.10
11	A	1123	CL7	C3A-C4A-CHB	-3.74	118.15	123.70
14	A	5001	LHG	O3-P-O5	-3.73	94.49	109.07
17	B	4014	8CT	C40-C12-C11	3.73	123.95	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1226	CL7	CHD-C4C-C3C	-3.70	118.95	124.94
17	L	4019	8CT	C35-C30-C29	-3.69	108.03	112.70
11	A	1103	CL7	C3A-C4A-CHB	-3.69	118.23	123.70
17	B	4017	8CT	C23-C21-C20	3.68	124.59	118.94
11	A	1126	CL7	C3A-C4A-CHB	-3.68	118.24	123.70
11	A	1102	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
11	A	1128	CL7	CMB-C2B-C1B	3.66	130.95	125.37
15	A	1011	G9R	CHB-C4A-NA	3.66	129.58	124.51
11	A	1115	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
11	A	1137	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
16	B	1023	PHO	CMB-C2B-C3B	3.65	131.50	124.68
11	B	1224	CL7	C3A-C4A-CHB	-3.65	118.29	123.70
17	B	4017	8CT	C07-C02-C03	-3.65	117.44	122.73
15	A	1011	G9R	CHD-C1D-ND	-3.64	121.11	124.45
11	A	1124	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
11	A	1128	CL7	CHD-C4C-C3C	-3.64	119.04	124.94
11	A	1128	CL7	CHB-C1B-NB	-3.64	120.41	124.26
11	L	1502	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
17	A	4011	8CT	C28-C26-C25	3.63	124.51	118.94
11	B	1239	CL7	C3A-C4A-CHB	-3.63	118.32	123.70
11	B	1226	CL7	CHB-C1B-NB	-3.63	120.42	124.26
17	J	4013	8CT	C04-C03-C02	-3.62	117.51	122.61
11	A	1116	CL7	C3A-C4A-CHB	-3.62	118.33	123.70
14	A	5003	LHG	O7-C7-C8	3.61	119.27	111.50
11	B	1228	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
11	A	1132	CL7	O2D-CGD-O1D	-3.60	116.80	123.84
17	A	4008	8CT	C07-C02-C03	-3.60	117.51	122.73
11	B	1206	CL7	C3A-C4A-CHB	-3.57	118.39	123.70
11	B	1203	CL7	C3A-C4A-CHB	-3.57	118.40	123.70
17	A	4007	8CT	C01-C02-C07	3.56	120.46	113.62
11	A	1132	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
11	A	1125	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
11	B	1222	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
11	A	1114	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
11	A	1122	CL7	C3A-C4A-CHB	-3.55	118.43	123.70
11	B	1229	CL7	C3A-C4A-CHB	-3.55	118.43	123.70
11	A	1112	CL7	C3A-C4A-CHB	-3.55	118.44	123.70
17	B	4017	8CT	C22-C21-C20	-3.54	117.97	122.92
11	A	1135	CL7	C3A-C4A-CHB	-3.54	118.45	123.70
17	B	4014	8CT	C18-C19-C20	-3.54	116.23	123.47
11	A	1118	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
11	A	1101	CL7	C3A-C4A-CHB	-3.53	118.46	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1121	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
11	W	2601	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
11	A	1105	CL7	CHD-C4C-C3C	-3.53	119.22	124.94
11	A	1139	CL7	C3A-C4A-CHB	-3.52	118.47	123.70
11	B	1210	CL7	C3A-C4A-CHB	-3.52	118.47	123.70
11	B	1205	CL7	CHD-C1D-ND	-3.52	120.53	124.26
17	W	4020	8CT	C10-C11-C12	-3.52	120.92	126.23
11	A	1801	CL7	C3A-C4A-CHB	-3.51	118.49	123.70
11	B	1223	CL7	C3A-C4A-CHB	-3.51	118.50	123.70
11	L	1501	CL7	C3A-C4A-CHB	-3.50	118.50	123.70
11	A	1125	CL7	CHD-C4C-C3C	-3.50	119.26	124.94
11	A	1109	CL7	C3A-C4A-CHB	-3.50	118.51	123.70
11	B	1236	CL7	C3A-C4A-CHB	-3.50	118.51	123.70
17	W	4018	8CT	C04-C03-C02	-3.50	117.69	122.61
11	B	1211	CL7	C3A-C4A-CHB	-3.50	118.51	123.70
17	B	4006	8CT	C19-C20-C21	-3.49	122.33	127.31
11	A	1237	CL7	C3A-C4A-CHB	-3.49	118.53	123.70
11	B	1234	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
17	L	4019	8CT	C27-C26-C28	3.48	123.56	118.08
11	A	1129	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
17	B	4017	8CT	C19-C18-C17	-3.48	116.35	123.47
11	B	1202	CL7	C3A-C4A-CHB	-3.48	118.54	123.70
11	A	1110	CL7	O2D-CGD-O1D	-3.48	117.04	123.84
11	B	1201	CL7	C3A-C4A-CHB	-3.48	118.54	123.70
11	B	1213	CL7	C3A-C4A-CHB	-3.48	118.54	123.70
11	B	1205	CL7	C3A-C4A-CHB	-3.47	118.54	123.70
17	W	4018	8CT	C10-C11-C12	-3.47	120.99	126.23
17	A	4007	8CT	C14-C15-C16	-3.47	116.67	126.42
11	A	1105	CL7	C3A-C4A-CHB	-3.47	118.55	123.70
11	A	1130	CL7	C3A-C4A-CHB	-3.47	118.55	123.70
11	A	1111	CL7	C3A-C4A-CHB	-3.47	118.55	123.70
11	J	1302	CL7	C3A-C4A-CHB	-3.47	118.56	123.70
17	M	4021	8CT	C35-C30-C29	-3.47	108.32	112.70
11	B	1235	CL7	C3A-C4A-CHB	-3.46	118.56	123.70
11	A	1113	CL7	C3A-C4A-CHB	-3.46	118.56	123.70
11	F	1301	CL7	C3A-C4A-CHB	-3.46	118.56	123.70
11	A	1117	CL7	C3A-C4A-CHB	-3.46	118.57	123.70
11	A	1802	CL7	C3A-C4A-CHB	-3.45	118.58	123.70
11	L	1503	CL7	C3A-C4A-CHB	-3.44	118.59	123.70
15	A	1011	G9R	CHD-C4C-C3C	-3.44	119.78	124.84
11	A	1106	CL7	C3A-C4A-CHB	-3.44	118.60	123.70
11	B	1215	CL7	C3A-C4A-CHB	-3.42	118.62	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1204	CL7	C3A-C4A-CHB	-3.42	118.62	123.70
17	W	4018	8CT	C14-C15-C16	-3.42	116.80	126.42
17	A	4007	8CT	C01-C02-C03	-3.42	120.69	124.53
11	B	1021	CL7	CHB-C1B-NB	-3.42	120.64	124.26
17	W	4020	8CT	C18-C17-C16	-3.42	122.43	127.31
11	B	1207	CL7	C3A-C4A-CHB	-3.42	118.63	123.70
17	A	4011	8CT	C27-C26-C25	-3.41	118.15	122.92
11	B	1212	CL7	C3A-C4A-CHB	-3.41	118.64	123.70
11	A	1107	CL7	C3A-C4A-CHB	-3.40	118.65	123.70
11	A	1126	CL7	CHD-C1D-ND	-3.40	120.66	124.26
11	A	1120	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
11	A	1140	CL7	C3A-C4A-CHB	-3.39	118.66	123.70
11	A	1114	CL7	CHD-C4C-C3C	-3.38	119.46	124.94
17	J	4013	8CT	C24-C25-C26	-3.37	122.50	127.31
11	A	1138	CL7	C3A-C4A-CHB	-3.37	118.70	123.70
11	B	1238	CL7	C3A-C4A-CHB	-3.37	118.70	123.70
17	A	4007	8CT	C22-C21-C20	-3.36	118.21	122.92
11	B	1208	CL7	C3A-C4A-CHB	-3.36	118.71	123.70
11	A	1136	CL7	C3A-C4A-CHB	-3.35	118.73	123.70
17	J	4015	8CT	C01-C02-C07	3.35	120.04	113.62
11	A	1128	CL7	CHC-C1C-NC	-3.34	121.38	124.45
17	L	4019	8CT	C19-C20-C21	-3.34	122.54	127.31
17	J	4013	8CT	C35-C30-C29	-3.33	108.49	112.70
11	B	1225	CL7	C3A-C4A-CHB	-3.32	118.77	123.70
11	A	1105	CL7	CAC-C3C-C2C	3.32	133.20	127.53
11	B	1230	CL7	C3A-C4A-CHB	-3.32	118.78	123.70
17	A	4007	8CT	C23-C21-C20	3.31	124.03	118.94
11	A	1132	CL7	CHD-C1D-ND	-3.31	120.75	124.26
11	A	1135	CL7	CHD-C4C-C3C	-3.30	119.58	124.94
11	B	1021	CL7	CHD-C4C-C3C	-3.30	119.58	124.94
17	A	4008	8CT	C28-C26-C25	3.30	124.01	118.94
11	B	1215	CL7	CHD-C4C-C3C	-3.29	119.60	124.94
11	A	1129	CL7	CHD-C1D-ND	-3.29	120.78	124.26
17	B	4017	8CT	C40-C12-C13	-3.28	118.32	122.92
17	W	4018	8CT	C01-C02-C07	3.28	119.92	113.62
17	B	4017	8CT	C35-C30-C29	-3.27	108.57	112.70
15	A	1011	G9R	C7-C6-C5	-3.26	104.50	113.36
11	B	1203	CL7	CHD-C4C-C3C	-3.24	119.68	124.94
11	B	1223	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
15	A	1011	G9R	CHB-C1B-NB	-3.24	120.83	124.26
17	W	4018	8CT	C07-C02-C03	-3.23	118.03	122.73
11	B	1226	CL7	CMB-C2B-C1B	3.23	130.29	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	4015	8CT	C25-C24-C23	-3.23	113.14	123.22
11	A	1111	CL7	CHD-C1D-ND	-3.23	120.84	124.26
11	B	1214	CL7	CHD-C4C-C3C	-3.23	119.71	124.94
11	A	1102	CL7	O2D-CGD-O1D	-3.23	117.53	123.84
11	A	1119	CL7	CHD-C4C-C3C	-3.22	119.71	124.94
11	B	1226	CL7	C7-C6-C5	-3.22	104.61	113.36
11	A	1105	CL7	C4C-C3C-C2C	-3.22	102.93	107.13
11	A	1102	CL7	CHD-C4C-C3C	-3.22	119.72	124.94
11	A	1115	CL7	O2D-CGD-O1D	-3.22	117.55	123.84
11	A	1113	CL7	CHD-C4C-C3C	-3.22	119.72	124.94
11	A	1115	CL7	CHD-C4C-C3C	-3.21	119.73	124.94
11	B	1226	CL7	CHC-C1C-NC	-3.21	121.51	124.45
11	B	1210	CL7	CHD-C1D-ND	-3.20	120.87	124.26
11	F	1301	CL7	CHD-C1D-ND	-3.20	120.87	124.26
11	B	1230	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
11	A	1022	CL7	CHD-C4C-C3C	-3.20	119.76	124.94
11	B	1212	CL7	CHD-C1D-ND	-3.20	120.87	124.26
11	B	1224	CL7	CHD-C1D-ND	-3.19	120.88	124.26
11	B	1226	CL7	C3B-C2B-C1B	-3.19	103.31	107.16
11	A	1107	CL7	CHD-C1D-ND	-3.18	120.89	124.26
11	A	1122	CL7	CHD-C1D-ND	-3.18	120.89	124.26
11	A	1136	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
11	A	1104	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
11	B	1213	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
11	W	2601	CL7	CHD-C4C-C3C	-3.17	119.79	124.94
17	B	4014	8CT	C01-C02-C07	3.17	119.71	113.62
17	B	4017	8CT	C39-C16-C15	3.17	123.08	118.08
11	A	1136	CL7	CHD-C1D-ND	-3.17	120.90	124.26
11	L	1501	CL7	CHD-C1D-ND	-3.17	120.90	124.26
11	A	1802	CL7	CHD-C4C-C3C	-3.17	119.80	124.94
11	A	1139	CL7	CHD-C1D-ND	-3.17	120.90	124.26
11	B	1214	CL7	CHB-C1B-NB	-3.17	120.90	124.26
11	A	1136	CL7	O2D-CGD-O1D	-3.17	117.65	123.84
11	A	1130	CL7	CHD-C4C-C3C	-3.17	119.81	124.94
11	B	1235	CL7	CHD-C1D-ND	-3.16	120.91	124.26
11	A	1139	CL7	CHD-C4C-C3C	-3.16	119.81	124.94
11	B	1222	CL7	CHD-C4C-C3C	-3.16	119.81	124.94
11	A	1107	CL7	CMB-C2B-C1B	3.16	130.18	125.37
17	W	4018	8CT	C01-C02-C03	-3.16	120.98	124.53
11	B	1229	CL7	CHD-C4C-C3C	-3.15	119.83	124.94
11	A	1802	CL7	CHD-C1D-ND	-3.15	120.92	124.26
11	F	1301	CL7	CHD-C4C-C3C	-3.15	119.83	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1211	CL7	CHD-C1D-ND	-3.15	120.92	124.26
11	A	1801	CL7	CHD-C4C-C3C	-3.15	119.83	124.94
11	A	1116	CL7	CHD-C1D-ND	-3.15	120.92	124.26
11	A	1123	CL7	CHD-C4C-C3C	-3.15	119.83	124.94
11	A	1140	CL7	CHD-C4C-C3C	-3.15	119.83	124.94
11	B	1239	CL7	CHD-C1D-ND	-3.15	120.92	124.26
11	A	1128	CL7	C3B-C2B-C1B	-3.15	103.36	107.16
11	B	1225	CL7	CHD-C1D-ND	-3.15	120.92	124.26
11	B	1204	CL7	CHD-C1D-ND	-3.15	120.93	124.26
11	L	1501	CL7	CHD-C4C-C3C	-3.14	119.84	124.94
11	B	1214	CL7	C3A-C4A-CHB	-3.14	119.03	123.70
11	B	1206	CL7	CHD-C4C-C3C	-3.14	119.85	124.94
11	A	1120	CL7	CHD-C4C-C3C	-3.14	119.85	124.94
11	B	1201	CL7	CHD-C1D-ND	-3.14	120.93	124.26
11	B	1226	CL7	C3A-C4A-CHB	-3.14	119.04	123.70
11	B	1012	CL7	CHD-C4C-C3C	-3.14	119.86	124.94
11	A	1138	CL7	CHD-C1D-ND	-3.14	120.94	124.26
11	B	1222	CL7	CHD-C1D-ND	-3.14	120.94	124.26
11	A	1137	CL7	O2D-CGD-O1D	-3.13	117.72	123.84
11	B	1228	CL7	CHD-C1D-ND	-3.13	120.94	124.26
11	B	1229	CL7	CHD-C1D-ND	-3.13	120.94	124.26
15	A	1011	G9R	O2D-CGD-O1D	-3.13	117.72	123.84
11	A	1117	CL7	CHD-C1D-ND	-3.13	120.95	124.26
11	B	1213	CL7	CHD-C1D-ND	-3.13	120.95	124.26
11	A	1106	CL7	CHD-C4C-C3C	-3.13	119.87	124.94
11	J	1302	CL7	CHD-C4C-C3C	-3.12	119.87	124.94
11	A	1122	CL7	CHB-C1B-NB	-3.12	120.95	124.26
17	W	4020	8CT	C13-C14-C15	-3.12	113.47	123.22
11	A	1118	CL7	CHD-C1D-ND	-3.12	120.95	124.26
11	B	1236	CL7	O2D-CGD-O1D	-3.12	117.74	123.84
11	A	1105	CL7	CHD-C1D-ND	-3.12	120.95	124.26
11	A	1128	CL7	CHD-C1D-ND	-3.12	120.96	124.26
11	A	1109	CL7	CHD-C1D-ND	-3.11	120.96	124.26
11	B	1205	CL7	O2D-CGD-O1D	-3.11	117.75	123.84
11	A	1130	CL7	CHD-C1D-ND	-3.11	120.96	124.26
11	L	1502	CL7	C7-C6-C5	-3.11	104.91	113.36
17	A	4008	8CT	C27-C26-C25	-3.11	118.56	122.92
11	A	1120	CL7	CHD-C1D-ND	-3.11	120.97	124.26
11	B	1212	CL7	CHD-C4C-C3C	-3.11	119.90	124.94
11	A	1102	CL7	CHD-C1D-ND	-3.11	120.97	124.26
11	B	1238	CL7	CHD-C4C-C3C	-3.11	119.90	124.94
11	L	1503	CL7	CHD-C4C-C3C	-3.10	119.91	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1112	CL7	CHD-C1D-ND	-3.10	120.97	124.26
17	L	4020	8CT	C35-C30-C29	-3.10	108.78	112.70
11	B	1202	CL7	CHD-C4C-C3C	-3.10	119.91	124.94
11	J	1302	CL7	CHD-C1D-ND	-3.10	120.98	124.26
11	A	1109	CL7	CHD-C4C-C3C	-3.09	119.92	124.94
11	A	1124	CL7	CHD-C4C-C3C	-3.09	119.92	124.94
11	A	1121	CL7	CHD-C1D-ND	-3.09	120.98	124.26
17	A	4008	8CT	C11-C10-C03	-3.09	118.52	127.20
11	A	1114	CL7	C2D-C1D-ND	3.09	112.30	110.23
11	A	1127	CL7	CHD-C4C-C3C	-3.09	119.94	124.94
17	L	4020	8CT	C01-C02-C07	3.09	119.54	113.62
11	B	1226	CL7	CHD-C1D-ND	-3.09	120.99	124.26
11	A	1101	CL7	CHD-C4C-C3C	-3.08	119.94	124.94
11	A	1110	CL7	CHD-C4C-C3C	-3.08	119.94	124.94
11	B	1204	CL7	O2D-CGD-O1D	-3.08	117.81	123.84
11	A	1123	CL7	CHD-C1D-ND	-3.08	120.99	124.26
11	A	1237	CL7	CHD-C4C-C3C	-3.08	119.94	124.94
11	A	1127	CL7	CHD-C1D-ND	-3.08	121.00	124.26
11	B	1021	CL7	O2D-CGD-O1D	-3.08	117.82	123.84
11	B	1214	CL7	O2D-CGD-O1D	-3.08	117.82	123.84
11	B	1235	CL7	O2D-CGD-O1D	-3.08	117.82	123.84
11	B	1236	CL7	CHD-C4C-C3C	-3.08	119.95	124.94
11	B	1238	CL7	CHD-C1D-ND	-3.07	121.00	124.26
11	B	1225	CL7	CHD-C4C-C3C	-3.07	119.96	124.94
11	A	1135	CL7	CHD-C1D-ND	-3.07	121.00	124.26
11	B	1234	CL7	CHD-C1D-ND	-3.07	121.00	124.26
17	A	4008	8CT	C14-C15-C16	-3.07	117.79	126.42
17	A	4011	8CT	C24-C23-C21	-3.07	117.79	126.42
11	A	1113	CL7	CHD-C1D-ND	-3.07	121.01	124.26
11	B	1214	CL7	CHC-C1C-NC	-3.07	121.63	124.45
11	A	1116	CL7	CHD-C4C-C3C	-3.07	119.97	124.94
17	A	4011	8CT	C01-C02-C07	3.07	119.51	113.62
11	B	1203	CL7	CHD-C1D-ND	-3.07	121.01	124.26
11	A	1237	CL7	CHD-C1D-ND	-3.07	121.01	124.26
11	B	1207	CL7	CHD-C4C-C3C	-3.06	119.98	124.94
11	A	1103	CL7	CHD-C1D-ND	-3.06	121.02	124.26
11	A	1128	CL7	C3A-C4A-CHB	-3.06	119.16	123.70
11	W	2601	CL7	CHB-C1B-NB	-3.06	121.02	124.26
11	A	1131	CL7	CHD-C4C-C3C	-3.06	119.98	124.94
11	L	1501	CL7	C7-C6-C5	-3.06	105.06	113.36
11	A	1103	CL7	CHD-C4C-C3C	-3.06	119.98	124.94
17	B	4017	8CT	C01-C02-C07	3.06	119.49	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	4017	8CT	C27-C26-C25	-3.06	118.64	122.92
11	A	1128	CL7	C7-C6-C5	-3.05	105.07	113.36
11	W	2601	CL7	CHD-C1D-ND	-3.05	121.03	124.26
11	A	1123	CL7	C7-C6-C5	-3.05	105.07	113.36
11	A	1125	CL7	CHC-C1C-NC	-3.05	121.65	124.45
11	B	1202	CL7	O2D-CGD-O1D	-3.05	117.87	123.84
17	M	4021	8CT	C19-C20-C21	-3.05	122.96	127.31
17	B	4017	8CT	C11-C12-C13	3.05	123.62	118.94
11	B	1207	CL7	O2D-CGD-O1D	-3.05	117.88	123.84
11	A	1125	CL7	O2D-CGD-O1D	-3.05	117.88	123.84
11	A	1135	CL7	CHC-C1C-NC	-3.05	121.65	124.45
11	A	1130	CL7	O2D-CGD-O1D	-3.05	117.88	123.84
17	M	4021	8CT	C40-C12-C13	-3.04	118.66	122.92
11	A	1112	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
11	L	1503	CL7	CHD-C1D-ND	-3.04	121.04	124.26
11	B	1211	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
11	B	1239	CL7	O2D-CGD-O1D	-3.04	117.89	123.84
11	B	1228	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
11	A	1121	CL7	CHD-C4C-C3C	-3.04	120.02	124.94
11	B	1234	CL7	CHD-C4C-C3C	-3.04	120.02	124.94
11	A	1138	CL7	CHD-C4C-C3C	-3.04	120.02	124.94
11	B	1239	CL7	C7-C6-C5	-3.04	105.11	113.36
11	B	1201	CL7	CHD-C4C-C3C	-3.03	120.02	124.94
11	A	1130	CL7	CAA-CBA-CGA	-3.03	104.46	112.51
17	B	4017	8CT	C28-C26-C25	3.03	123.59	118.94
11	B	1210	CL7	CHB-C1B-NB	-3.03	121.05	124.26
11	A	1131	CL7	C7-C6-C5	-3.03	105.13	113.36
11	B	1207	CL7	CHD-C1D-ND	-3.03	121.05	124.26
11	A	1137	CL7	CHD-C4C-C3C	-3.03	120.03	124.94
11	A	1107	CL7	CHB-C1B-NB	-3.02	121.06	124.26
11	A	1117	CL7	C7-C6-C5	-3.02	105.15	113.36
17	B	4006	8CT	C35-C30-C29	-3.02	108.89	112.70
15	A	1011	G9R	C1C-C2C-C3C	-3.02	103.78	106.96
16	A	1013	PHO	CMD-C2D-C3D	3.01	130.32	124.68
11	A	1101	CL7	O2D-CGD-O1D	-3.01	117.95	123.84
16	A	1013	PHO	O2D-CGD-O1D	-3.01	117.95	123.84
11	B	1208	CL7	CMB-C2B-C1B	3.01	129.95	125.37
11	B	1202	CL7	CHD-C1D-ND	-3.01	121.07	124.26
11	A	1237	CL7	O2D-CGD-O1D	-3.01	117.96	123.84
11	L	1502	CL7	CHD-C1D-ND	-3.01	121.07	124.26
11	A	1137	CL7	CMB-C2B-C1B	3.01	129.95	125.37
11	A	1124	CL7	CHD-C1D-ND	-3.00	121.08	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1801	CL7	CHD-C1D-ND	-3.00	121.08	124.26
11	A	1104	CL7	CHB-C1B-NB	-3.00	121.08	124.26
11	A	1101	CL7	CHD-C1D-ND	-2.99	121.09	124.26
11	B	1208	CL7	CHD-C1D-ND	-2.99	121.09	124.26
11	B	1223	CL7	CHD-C1D-ND	-2.99	121.09	124.26
11	A	1022	CL7	CHD-C1D-ND	-2.99	121.09	124.26
11	A	1106	CL7	CHD-C1D-ND	-2.99	121.09	124.26
11	A	1103	CL7	O2D-CGD-O1D	-2.99	117.99	123.84
11	A	1120	CL7	O2D-CGD-O1D	-2.99	117.99	123.84
11	A	1106	CL7	O2D-CGD-O1D	-2.99	117.99	123.84
17	A	4008	8CT	C10-C11-C12	-2.99	121.72	126.23
11	A	1140	CL7	CHD-C1D-ND	-2.99	121.09	124.26
11	B	1223	CL7	CHC-C1C-NC	-2.99	121.71	124.45
11	B	1224	CL7	CHD-C4C-C3C	-2.98	120.10	124.94
11	A	1125	CL7	CHD-C1D-ND	-2.98	121.10	124.26
11	A	1118	CL7	CHD-C4C-C3C	-2.98	120.11	124.94
11	B	1210	CL7	CHD-C4C-C3C	-2.98	120.11	124.94
11	B	1215	CL7	CHD-C1D-ND	-2.98	121.10	124.26
11	B	1239	CL7	CHD-C4C-C3C	-2.98	120.11	124.94
11	A	1122	CL7	O2D-CGD-O1D	-2.98	118.02	123.84
11	A	1106	CL7	CHC-C1C-NC	-2.98	121.72	124.45
11	A	1132	CL7	CHB-C1B-NB	-2.98	121.11	124.26
11	A	1136	CL7	CHB-C1B-NB	-2.97	121.11	124.26
11	A	1119	CL7	C3A-C4A-CHB	-2.97	119.29	123.70
11	L	1503	CL7	O2D-CGD-O1D	-2.97	118.03	123.84
11	A	1119	CL7	CHD-C1D-ND	-2.97	121.11	124.26
11	A	1138	CL7	CHB-C1B-NB	-2.97	121.11	124.26
17	J	4013	8CT	C07-C02-C03	-2.97	118.42	122.73
11	B	1238	CL7	O2D-CGD-O1D	-2.97	118.03	123.84
11	A	1126	CL7	C7-C6-C5	-2.97	105.30	113.36
11	L	1502	CL7	CHD-C4C-C3C	-2.97	120.13	124.94
17	J	4015	8CT	C19-C20-C21	-2.96	123.08	127.31
11	A	1137	CL7	CHB-C1B-NB	-2.96	121.12	124.26
11	A	1110	CL7	O2D-CGD-CBD	2.96	116.53	111.27
11	B	1215	CL7	O2D-CGD-O1D	-2.96	118.06	123.84
11	A	1110	CL7	CHB-C1B-NB	-2.96	121.13	124.26
11	A	1140	CL7	O2D-CGD-O1D	-2.95	118.06	123.84
11	B	1204	CL7	CHD-C4C-C3C	-2.95	120.15	124.94
17	J	4013	8CT	C01-C02-C07	2.95	119.29	113.62
11	A	1135	CL7	CHB-C1B-NB	-2.95	121.13	124.26
11	A	1107	CL7	CHD-C4C-C3C	-2.95	120.16	124.94
11	B	1235	CL7	CHD-C4C-C3C	-2.95	120.16	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4011	8CT	C04-C03-C02	-2.95	118.46	122.61
11	A	1110	CL7	CHD-C1D-ND	-2.94	121.14	124.26
11	B	1203	CL7	CHC-C1C-NC	-2.94	121.75	124.45
11	B	1234	CL7	O2D-CGD-O1D	-2.94	118.09	123.84
11	A	1106	CL7	CHB-C1B-NB	-2.94	121.14	124.26
11	A	1135	CL7	O2D-CGD-O1D	-2.94	118.09	123.84
11	A	1115	CL7	CHC-C1C-NC	-2.94	121.76	124.45
16	B	1023	PHO	C3D-C4D-ND	2.93	111.72	107.72
17	B	4017	8CT	C39-C16-C17	-2.93	118.81	122.92
11	A	1105	CL7	CHB-C1B-NB	-2.93	121.15	124.26
11	A	1126	CL7	O2D-CGD-O1D	-2.93	118.11	123.84
11	B	1238	CL7	CHC-C1C-NC	-2.93	121.76	124.45
11	A	1109	CL7	CHB-C1B-NB	-2.93	121.16	124.26
11	B	1235	CL7	CHB-C1B-NB	-2.93	121.16	124.26
11	B	1210	CL7	O2D-CGD-O1D	-2.93	118.12	123.84
11	A	1117	CL7	CHD-C4C-C3C	-2.92	120.20	124.94
11	B	1208	CL7	CHB-C1B-NB	-2.92	121.16	124.26
11	B	1223	CL7	O2D-CGD-O1D	-2.92	118.12	123.84
11	A	1131	CL7	CHD-C1D-ND	-2.92	121.17	124.26
11	B	1215	CL7	CHB-C1B-NB	-2.92	121.17	124.26
11	B	1206	CL7	CHD-C1D-ND	-2.92	121.17	124.26
11	B	1208	CL7	CHD-C4C-C3C	-2.92	120.21	124.94
11	B	1205	CL7	C4D-C3D-CAD	-2.92	105.46	107.42
15	A	1011	G9R	C3D-C2D-C1D	-2.92	101.85	105.83
11	A	1121	CL7	O2D-CGD-O1D	-2.91	118.14	123.84
11	B	1239	CL7	CMB-C2B-C1B	2.91	129.80	125.37
11	A	1802	CL7	O2D-CGD-O1D	-2.91	118.15	123.84
11	A	1112	CL7	CHB-C1B-NB	-2.91	121.18	124.26
17	W	4020	8CT	C01-C02-C07	2.90	119.19	113.62
17	M	4021	8CT	C05-C04-C03	2.90	114.94	110.48
11	A	1802	CL7	CHB-C1B-NB	-2.90	121.19	124.26
11	B	1229	CL7	CHC-C1C-NC	-2.89	121.80	124.45
11	A	1237	CL7	C7-C6-C5	-2.89	105.50	113.36
11	B	1203	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
11	B	1203	CL7	C7-C6-C5	-2.89	105.51	113.36
11	B	1201	CL7	O2D-CGD-O1D	-2.89	118.19	123.84
11	A	1129	CL7	CHB-C1B-NB	-2.89	121.20	124.26
11	B	1012	CL7	CHC-C1C-NC	-2.88	121.80	124.45
11	A	1116	CL7	O2D-CGD-O1D	-2.88	118.20	123.84
11	B	1239	CL7	CHC-C1C-NC	-2.88	121.81	124.45
11	B	1214	CL7	CHD-C1D-ND	-2.88	121.21	124.26
11	A	1115	CL7	CHB-C1B-NB	-2.88	121.21	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1201	CL7	CHB-C1B-NB	-2.88	121.21	124.26
11	A	1114	CL7	O2D-CGD-O1D	-2.88	118.21	123.84
11	A	1103	CL7	C7-C6-C5	-2.88	105.55	113.36
11	B	1203	CL7	CHB-C1B-NB	-2.88	121.21	124.26
11	B	1238	CL7	C7-C6-C5	-2.87	105.55	113.36
11	A	1107	CL7	O2D-CGD-O1D	-2.87	118.22	123.84
11	B	1205	CL7	CHD-C4C-C3C	-2.87	120.28	124.94
11	A	1104	CL7	CHD-C1D-ND	-2.87	121.22	124.26
11	A	1136	CL7	C7-C6-C5	-2.87	105.56	113.36
17	M	4021	8CT	C01-C02-C07	2.87	119.13	113.62
11	L	1501	CL7	CHB-C1B-NB	-2.87	121.22	124.26
11	B	1202	CL7	CHC-C1C-NC	-2.87	121.82	124.45
11	A	1106	CL7	C7-C6-C5	-2.87	105.57	113.36
11	L	1503	CL7	CHB-C1B-NB	-2.87	121.22	124.26
11	B	1201	CL7	CHC-C1C-NC	-2.87	121.82	124.45
11	A	1102	CL7	CHB-C1B-NB	-2.87	121.22	124.26
11	B	1236	CL7	CHB-C1B-NB	-2.87	121.22	124.26
11	A	1119	CL7	O2D-CGD-O1D	-2.87	118.23	123.84
15	A	1011	G9R	C4D-C3D-CAD	-2.86	104.72	108.10
11	A	1115	CL7	CHD-C1D-ND	-2.86	121.23	124.26
11	A	1237	CL7	CHB-C1B-NB	-2.86	121.23	124.26
11	A	1118	CL7	O2D-CGD-O1D	-2.86	118.25	123.84
11	A	1118	CL7	CHB-C1B-NB	-2.86	121.23	124.26
11	A	1801	CL7	O2D-CGD-O1D	-2.86	118.26	123.84
17	J	4013	8CT	C27-C26-C28	2.85	122.58	118.08
11	B	1021	CL7	C3A-C4A-CHB	-2.85	119.47	123.70
11	B	1224	CL7	CHB-C1B-NB	-2.85	121.24	124.26
11	L	1502	CL7	O2D-CGD-O1D	-2.85	118.26	123.84
11	B	1226	CL7	O2D-CGD-O1D	-2.85	118.26	123.84
17	L	4019	8CT	C05-C04-C03	2.85	114.87	110.48
11	B	1213	CL7	CHC-C1C-NC	-2.85	121.83	124.45
11	W	2601	CL7	O2D-CGD-O1D	-2.85	118.26	123.84
11	A	1120	CL7	CHC-C1C-NC	-2.85	121.83	124.45
14	A	5001	LHG	O4-P-O6	-2.85	94.51	107.75
11	B	1225	CL7	CHB-C1B-NB	-2.85	121.24	124.26
11	J	1302	CL7	CHB-C1B-NB	-2.85	121.24	124.26
11	A	1130	CL7	CHC-C1C-NC	-2.85	121.84	124.45
11	A	1101	CL7	CHB-C1B-NB	-2.85	121.24	124.26
11	A	1123	CL7	CHC-C1C-NC	-2.84	121.84	124.45
11	A	1140	CL7	C7-C6-C5	-2.84	105.64	113.36
11	B	1012	CL7	CHB-C1B-NB	-2.84	121.25	124.26
11	B	1211	CL7	CHB-C1B-NB	-2.84	121.25	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1204	CL7	CMB-C2B-C1B	2.84	129.69	125.37
11	A	1131	CL7	CHB-C1B-NB	-2.84	121.25	124.26
11	B	1021	CL7	C7-C6-C5	-2.84	105.65	113.36
11	B	1212	CL7	O2D-CGD-O1D	-2.84	118.29	123.84
11	A	1119	CL7	CHC-C1C-NC	-2.84	121.85	124.45
11	A	1111	CL7	CHB-C1B-NB	-2.84	121.25	124.26
11	B	1204	CL7	CHB-C1B-NB	-2.84	121.25	124.26
11	A	1137	CL7	CHD-C1D-ND	-2.83	121.26	124.26
17	A	4011	8CT	C07-C02-C03	-2.83	118.62	122.73
11	A	1131	CL7	CHC-C1C-NC	-2.83	121.85	124.45
11	B	1236	CL7	CHD-C1D-ND	-2.83	121.26	124.26
11	A	1104	CL7	O2D-CGD-O1D	-2.83	118.30	123.84
11	A	1113	CL7	CHC-C1C-NC	-2.83	121.85	124.45
11	A	1123	CL7	O2D-CGD-O1D	-2.83	118.30	123.84
17	B	4006	8CT	C01-C02-C07	2.83	119.05	113.62
11	B	1206	CL7	CHB-C1B-NB	-2.83	121.26	124.26
11	A	1119	CL7	CHB-C1B-NB	-2.83	121.26	124.26
11	B	1212	CL7	CHB-C1B-NB	-2.83	121.26	124.26
11	A	1111	CL7	CHD-C4C-C3C	-2.83	120.36	124.94
11	A	1022	CL7	O2D-CGD-O1D	-2.83	118.31	123.84
11	A	1131	CL7	O2D-CGD-O1D	-2.83	118.31	123.84
11	F	1301	CL7	O2D-CGD-O1D	-2.83	118.31	123.84
11	B	1207	CL7	CHB-C1B-NB	-2.83	121.27	124.26
11	B	1208	CL7	O2D-CGD-O1D	-2.82	118.32	123.84
11	A	1124	CL7	CHC-C1C-NC	-2.82	121.86	124.45
11	A	1113	CL7	O2D-CGD-O1D	-2.82	118.32	123.84
11	A	1237	CL7	CMB-C2B-C1B	2.82	129.66	125.37
17	M	4021	8CT	C11-C12-C13	2.82	123.26	118.94
11	A	1129	CL7	O2D-CGD-O1D	-2.82	118.33	123.84
11	B	1012	CL7	CHD-C1D-ND	-2.81	121.28	124.26
11	B	1212	CL7	CHC-C1C-NC	-2.81	121.87	124.45
11	L	1501	CL7	CHC-C1C-NC	-2.81	121.87	124.45
11	F	1301	CL7	CHC-C1C-NC	-2.81	121.87	124.45
11	A	1139	CL7	CHB-C1B-NB	-2.81	121.28	124.26
11	B	1012	CL7	O2D-CGD-O1D	-2.81	118.35	123.84
17	J	4015	8CT	C27-C26-C28	2.81	122.50	118.08
11	F	1301	CL7	CHB-C1B-NB	-2.81	121.29	124.26
11	A	1101	CL7	CHC-C1C-NC	-2.81	121.88	124.45
11	B	1213	CL7	O2D-CGD-O1D	-2.81	118.35	123.84
11	B	1215	CL7	CHC-C1C-NC	-2.81	121.88	124.45
11	A	1140	CL7	CHC-C1C-NC	-2.80	121.88	124.45
11	B	1012	CL7	CMB-C2B-C1B	2.80	129.64	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1101	CL7	C7-C6-C5	-2.80	105.75	113.36
11	B	1206	CL7	CHC-C1C-NC	-2.80	121.88	124.45
11	A	1109	CL7	O2D-CGD-O1D	-2.80	118.37	123.84
11	A	1111	CL7	O2D-CGD-O1D	-2.80	118.37	123.84
16	B	1023	PHO	O2D-CGD-O1D	-2.80	118.37	123.84
11	A	1121	CL7	CHB-C1B-NB	-2.80	121.30	124.26
11	A	1123	CL7	CHB-C1B-NB	-2.79	121.30	124.26
11	A	1132	CL7	CMB-C2B-C1B	2.79	129.62	125.37
11	A	1129	CL7	CMB-C2B-C1B	2.79	129.62	125.37
11	A	1117	CL7	O2D-CGD-O1D	-2.79	118.38	123.84
11	B	1239	CL7	C3B-C2B-C1B	-2.79	103.79	107.16
11	B	1225	CL7	O2D-CGD-O1D	-2.79	118.38	123.84
11	A	1801	CL7	CHB-C1B-NB	-2.79	121.30	124.26
11	A	1105	CL7	CHC-C1C-NC	-2.79	121.89	124.45
11	B	1236	CL7	CHC-C1C-NC	-2.79	121.89	124.45
11	L	1501	CL7	O2D-CGD-O1D	-2.79	118.39	123.84
11	B	1228	CL7	O2D-CGD-O1D	-2.79	118.39	123.84
11	J	1302	CL7	O2D-CGD-O1D	-2.79	118.39	123.84
11	A	1022	CL7	C7-C6-C5	-2.79	105.79	113.36
11	B	1229	CL7	CMB-C2B-C1B	2.79	129.61	125.37
11	A	1237	CL7	CHC-C1C-NC	-2.79	121.89	124.45
11	B	1205	CL7	CHB-C1B-NB	-2.79	121.31	124.26
17	L	4019	8CT	C07-C02-C03	-2.78	118.69	122.73
11	B	1234	CL7	CHC-C1C-NC	-2.78	121.89	124.45
11	B	1225	CL7	C7-C6-C5	-2.78	105.80	113.36
11	A	1124	CL7	O2D-CGD-O1D	-2.78	118.40	123.84
11	A	1132	CL7	C4D-C3D-CAD	-2.78	105.55	107.42
11	A	1121	CL7	CHC-C1C-NC	-2.78	121.90	124.45
11	B	1224	CL7	O2D-CGD-O1D	-2.78	118.41	123.84
11	A	1110	CL7	CHC-C1C-NC	-2.78	121.90	124.45
11	A	1114	CL7	CHB-C1B-NB	-2.78	121.32	124.26
11	A	1117	CL7	CHC-C1C-NC	-2.78	121.90	124.45
11	J	1302	CL7	CHC-C1C-NC	-2.78	121.90	124.45
11	A	1113	CL7	CHB-C1B-NB	-2.78	121.32	124.26
11	A	1132	CL7	CHD-C4C-C3C	-2.77	120.44	124.94
11	A	1138	CL7	C4D-C3D-CAD	-2.77	105.56	107.42
14	A	5001	LHG	O4-P-O3	-2.77	94.87	107.75
14	A	5003	LHG	O4-P-O3	-2.77	94.88	107.75
11	A	1126	CL7	CHD-C4C-C3C	-2.77	120.45	124.94
17	J	4015	8CT	C18-C19-C20	-2.77	117.80	123.47
11	A	1802	CL7	CHC-C1C-NC	-2.77	121.91	124.45
11	A	1111	CL7	C3B-C2B-C1B	-2.77	103.82	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1215	CL7	CMB-C2B-C1B	2.77	129.58	125.37
11	A	1801	CL7	CHC-C1C-NC	-2.77	121.91	124.45
11	B	1230	CL7	CHD-C1D-ND	-2.76	121.33	124.26
11	A	1125	CL7	C7-C6-C5	-2.76	105.86	113.36
11	A	1128	CL7	O2D-CGD-O1D	-2.76	118.44	123.84
11	A	1120	CL7	CHB-C1B-NB	-2.76	121.34	124.26
11	A	1125	CL7	CMB-C2B-C1B	2.76	129.57	125.37
11	A	1112	CL7	O2D-CGD-O1D	-2.76	118.45	123.84
11	B	1230	CL7	O2D-CGD-O1D	-2.76	118.45	123.84
11	B	1223	CL7	CHB-C1B-NB	-2.76	121.34	124.26
11	B	1213	CL7	CHB-C1B-NB	-2.76	121.34	124.26
11	B	1234	CL7	CHB-C1B-NB	-2.76	121.34	124.26
11	B	1204	CL7	CHC-C1C-NC	-2.76	121.92	124.45
11	A	1139	CL7	O2D-CGD-O1D	-2.76	118.45	123.84
11	B	1206	CL7	O2D-CGD-O1D	-2.76	118.45	123.84
11	B	1211	CL7	O2D-CGD-O1D	-2.75	118.45	123.84
11	A	1022	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
11	B	1236	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
11	L	1503	CL7	CHC-C1C-NC	-2.75	121.92	124.45
11	B	1222	CL7	O2D-CGD-O1D	-2.75	118.46	123.84
11	A	1118	CL7	CMB-C2B-C1B	2.75	129.56	125.37
11	B	1222	CL7	CHC-C1C-NC	-2.75	121.93	124.45
16	A	1013	PHO	C3D-C4D-ND	2.75	111.47	107.72
11	B	1021	CL7	CHD-C1D-ND	-2.75	121.34	124.26
11	B	1229	CL7	O2D-CGD-O1D	-2.75	118.46	123.84
11	A	1125	CL7	CHB-C1B-NB	-2.75	121.35	124.26
17	L	4019	8CT	C30-C31-C32	-2.75	118.08	121.47
11	B	1239	CL7	CHB-C1B-NB	-2.75	121.35	124.26
11	A	1124	CL7	CHB-C1B-NB	-2.75	121.35	124.26
11	A	1122	CL7	CHD-C4C-C3C	-2.75	120.49	124.94
18	B	5002	LMG	O8-C28-C29	2.75	120.53	111.91
17	A	4007	8CT	C27-C26-C25	-2.74	119.08	122.92
17	A	4008	8CT	C39-C16-C17	-2.74	119.08	122.92
11	A	1119	CL7	CMB-C2B-C1B	2.74	129.55	125.37
11	B	1012	CL7	C7-C6-C5	-2.74	105.92	113.36
11	A	1105	CL7	O2D-CGD-O1D	-2.74	118.48	123.84
11	A	1127	CL7	O2D-CGD-O1D	-2.74	118.48	123.84
11	A	1122	CL7	CMB-C2B-C1B	2.74	129.54	125.37
11	B	1222	CL7	CHB-C1B-NB	-2.73	121.36	124.26
11	B	1238	CL7	CHB-C1B-NB	-2.73	121.36	124.26
11	A	1118	CL7	CHC-C1C-NC	-2.73	121.94	124.45
11	W	2601	CL7	C3B-C2B-C1B	-2.73	103.86	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1022	CL7	CHC-C1C-NC	-2.73	121.94	124.45
11	B	1228	CL7	CHC-C1C-NC	-2.73	121.95	124.45
11	B	1012	CL7	C4D-C3D-CAD	-2.72	105.59	107.42
17	B	4014	8CT	C24-C25-C26	-2.72	123.43	127.31
11	A	1111	CL7	CHC-C1C-NC	-2.72	121.96	124.45
11	A	1129	CL7	CHD-C4C-C3C	-2.72	120.54	124.94
11	B	1224	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
17	W	4020	8CT	C11-C10-C03	-2.71	119.58	127.20
11	A	1127	CL7	CHC-C1C-NC	-2.71	121.96	124.45
11	L	1502	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
17	W	4018	8CT	C24-C23-C21	-2.71	118.80	126.42
15	A	1011	G9R	C3B-C2B-C1B	-2.71	103.89	107.16
11	B	1223	CL7	CMB-C2B-C1B	2.71	129.49	125.37
11	A	1132	CL7	C7-C6-C5	-2.71	106.01	113.36
11	B	1234	CL7	CMB-C2B-C1B	2.71	129.49	125.37
11	L	1502	CL7	CHC-C1C-NC	-2.71	121.97	124.45
11	B	1205	CL7	CMB-C2B-C1B	2.70	129.49	125.37
11	A	1801	CL7	CMB-C2B-C1B	2.70	129.49	125.37
11	A	1131	CL7	C4-C3-C5	2.70	119.82	115.27
11	B	1202	CL7	CHB-C1B-NB	-2.70	121.39	124.26
11	A	1101	CL7	CMB-C2B-C1B	2.70	129.49	125.37
11	B	1021	CL7	C4C-C3C-C2C	-2.70	103.61	107.13
11	A	1107	CL7	CHC-C1C-NC	-2.70	121.98	124.45
11	A	1022	CL7	CHB-C1B-NB	-2.70	121.40	124.26
17	L	4020	8CT	C18-C19-C20	-2.70	117.95	123.47
17	J	4015	8CT	C11-C10-C03	-2.69	119.64	127.20
11	L	1502	CL7	C4-C3-C5	2.69	119.80	115.27
17	W	4018	8CT	C11-C10-C03	-2.69	119.64	127.20
11	A	1130	CL7	CHB-C1B-NB	-2.69	121.41	124.26
17	A	4008	8CT	C01-C02-C07	2.69	118.78	113.62
11	A	1116	CL7	CHC-C1C-NC	-2.68	121.99	124.45
11	B	1226	CL7	CAC-C3C-C2C	2.68	132.11	127.53
11	B	1021	CL7	CMA-C3A-C2A	-2.68	103.02	113.83
11	B	1228	CL7	CHB-C1B-NB	-2.68	121.42	124.26
11	B	1234	CL7	C4C-C3C-C2C	-2.67	103.64	107.13
11	A	1104	CL7	CHC-C1C-NC	-2.67	122.00	124.45
16	A	1013	PHO	CMB-C2B-C3B	2.67	129.68	124.68
11	B	1229	CL7	CHB-C1B-NB	-2.67	121.43	124.26
11	A	1116	CL7	CHB-C1B-NB	-2.67	121.43	124.26
11	B	1207	CL7	CHC-C1C-NC	-2.67	122.00	124.45
11	A	1138	CL7	O2D-CGD-O1D	-2.67	118.62	123.84
11	A	1124	CL7	C3B-C2B-C1B	-2.67	103.94	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1126	CL7	C4D-C3D-CAD	-2.66	105.63	107.42
11	A	1140	CL7	CHB-C1B-NB	-2.66	121.44	124.26
11	A	1115	CL7	CMB-C2B-C1B	2.66	129.42	125.37
11	B	1224	CL7	CMB-C2B-C1B	2.66	129.42	125.37
17	A	4007	8CT	C39-C16-C17	-2.66	119.19	122.92
17	A	4011	8CT	C05-C04-C03	2.66	114.58	110.48
17	B	4006	8CT	C14-C15-C16	-2.66	118.94	126.42
11	A	1132	CL7	C3B-C2B-C1B	-2.66	103.95	107.16
11	B	1235	CL7	CHC-C1C-NC	-2.65	122.02	124.45
11	A	1022	CL7	O2A-CGA-O1A	-2.65	116.91	123.59
14	A	5003	LHG	O4-P-O6	-2.65	95.45	107.75
11	B	1210	CL7	CHC-C1C-NC	-2.65	122.02	124.45
11	A	1112	CL7	CHC-C1C-NC	-2.64	122.02	124.45
11	A	1114	CL7	CHC-C1C-NC	-2.64	122.03	124.45
11	B	1211	CL7	CHC-C1C-NC	-2.64	122.03	124.45
11	A	1121	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
11	A	1123	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
11	B	1012	CL7	C3B-C2B-C1B	-2.64	103.98	107.16
11	A	1103	CL7	CHC-C1C-NC	-2.63	122.03	124.45
11	A	1102	CL7	CHC-C1C-NC	-2.63	122.04	124.45
11	A	1117	CL7	CHB-C1B-NB	-2.63	121.47	124.26
11	A	1131	CL7	CMB-C2B-C1B	2.63	129.37	125.37
14	A	5003	LHG	O8-C23-C24	2.63	120.15	111.91
11	B	1201	CL7	C3B-C2B-C1B	-2.62	103.99	107.16
11	A	1022	CL7	CMB-C2B-C1B	2.62	129.37	125.37
17	B	4006	8CT	C18-C19-C20	-2.62	118.10	123.47
11	A	1105	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
11	B	1230	CL7	C4C-C3C-C2C	-2.62	103.71	107.13
11	B	1225	CL7	CHC-C1C-NC	-2.62	122.05	124.45
11	A	1138	CL7	CMB-C2B-C1B	2.62	129.35	125.37
11	A	1135	CL7	C4C-C3C-C2C	-2.62	103.72	107.13
11	A	1138	CL7	CHC-C1C-NC	-2.61	122.05	124.45
17	B	4006	8CT	C40-C12-C13	-2.61	119.26	122.92
11	L	1501	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
11	B	1222	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
11	A	1128	CL7	C4-C3-C5	2.61	119.66	115.27
11	B	1202	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
11	A	1103	CL7	CHB-C1B-NB	-2.61	121.50	124.26
11	B	1203	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
11	A	1127	CL7	CMB-C2B-C1B	2.60	129.34	125.37
11	A	1122	CL7	C3B-C4B-NB	2.60	112.93	110.52
17	J	4013	8CT	C05-C04-C03	2.60	114.48	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1801	CL7	C3B-C2B-C1B	-2.60	104.02	107.16
11	A	1139	CL7	CHC-C1C-NC	-2.60	122.07	124.45
11	A	1130	CL7	CMB-C2B-C1B	2.60	129.33	125.37
11	A	1125	CL7	C3B-C2B-C1B	-2.60	104.03	107.16
11	J	1302	CL7	C3B-C2B-C1B	-2.60	104.03	107.16
11	B	1205	CL7	C3B-C2B-C1B	-2.59	104.03	107.16
11	B	1226	CL7	C4-C3-C5	2.59	119.63	115.27
11	B	1235	CL7	C3B-C2B-C1B	-2.59	104.03	107.16
11	A	1138	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
11	W	2601	CL7	CHC-C1C-NC	-2.59	122.08	124.45
11	A	1110	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
11	B	1212	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
11	B	1223	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
11	B	1229	CL7	C3B-C2B-C1B	-2.58	104.04	107.16
15	A	1011	G9R	C4-C3-C5	2.58	119.61	115.27
11	L	1502	CL7	CHB-C1B-NB	-2.58	121.53	124.26
11	A	1132	CL7	O2D-CGD-CBD	2.58	115.85	111.27
11	A	1126	CL7	C4-C3-C5	2.58	119.61	115.27
11	B	1213	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
11	A	1102	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
11	A	1129	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
14	A	5001	LHG	O8-C23-C24	2.57	119.98	111.91
11	A	1125	CL7	C4-C3-C5	2.57	119.60	115.27
11	B	1214	CL7	C3B-C4B-NB	2.57	112.90	110.52
11	A	1128	CL7	C4C-C3C-C2C	-2.57	103.78	107.13
11	A	1117	CL7	C4C-C3C-C2C	-2.57	103.78	107.13
11	A	1114	CL7	C3B-C2B-C1B	-2.56	104.07	107.16
17	B	4006	8CT	C27-C26-C25	-2.56	119.33	122.92
15	A	1011	G9R	CMB-C2B-C1B	2.56	129.27	125.37
11	A	1135	CL7	C3B-C2B-C1B	-2.56	104.07	107.16
11	B	1225	CL7	CMB-C2B-C1B	2.56	129.27	125.37
11	A	1125	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
17	W	4018	8CT	C35-C30-C31	2.56	116.00	111.42
11	A	1104	CL7	C3B-C2B-C1B	-2.56	104.08	107.16
11	A	1135	CL7	CMB-C2B-C1B	2.55	129.26	125.37
17	A	4011	8CT	C35-C30-C31	2.55	115.99	111.42
11	B	1234	CL7	C3B-C2B-C1B	-2.55	104.08	107.16
11	A	1136	CL7	CHC-C1C-NC	-2.55	122.11	124.45
11	A	1112	CL7	C3B-C2B-C1B	-2.55	104.08	107.16
11	A	1137	CL7	C4D-C3D-CAD	-2.55	105.71	107.42
11	A	1128	CL7	CAC-C3C-C2C	2.55	131.89	127.53
11	B	1238	CL7	C3B-C2B-C1B	-2.55	104.08	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	1503	CL7	C3B-C2B-C1B	-2.55	104.08	107.16
16	B	1023	PHO	CMD-C2D-C3D	2.55	129.44	124.68
11	B	1236	CL7	C4D-C3D-CAD	-2.55	105.71	107.42
11	A	1109	CL7	C3B-C2B-C1B	-2.55	104.09	107.16
11	A	1113	CL7	C3B-C2B-C1B	-2.54	104.09	107.16
11	B	1202	CL7	C4C-C3C-C2C	-2.54	103.81	107.13
11	A	1137	CL7	CHC-C1C-NC	-2.54	122.12	124.45
11	A	1106	CL7	C3B-C2B-C1B	-2.54	104.10	107.16
11	B	1210	CL7	C3B-C2B-C1B	-2.54	104.10	107.16
11	A	1104	CL7	C7-C6-C5	-2.54	106.47	113.36
11	B	1211	CL7	C3B-C2B-C1B	-2.54	104.10	107.16
11	B	1230	CL7	CHC-C1C-NC	-2.54	122.12	124.45
11	J	1302	CL7	CMB-C2B-C1B	2.54	129.23	125.37
11	A	1103	CL7	CMB-C2B-C1B	2.53	129.23	125.37
11	A	1130	CL7	C3B-C2B-C1B	-2.53	104.11	107.16
11	B	1225	CL7	C3B-C2B-C1B	-2.53	104.11	107.16
11	B	1208	CL7	CHC-C1C-NC	-2.53	122.13	124.45
11	B	1238	CL7	CMB-C2B-C1B	2.53	129.22	125.37
11	A	1109	CL7	C4C-C3C-C2C	-2.53	103.83	107.13
11	A	1118	CL7	C3B-C2B-C1B	-2.53	104.11	107.16
11	F	1301	CL7	C3B-C2B-C1B	-2.52	104.12	107.16
11	B	1224	CL7	CHC-C1C-NC	-2.52	122.14	124.45
11	A	1802	CL7	C3B-C2B-C1B	-2.52	104.12	107.16
11	A	1103	CL7	C4C-C3C-C2C	-2.52	103.85	107.13
11	A	1113	CL7	CMB-C2B-C1B	2.51	129.20	125.37
11	B	1235	CL7	CMB-C2B-C1B	2.51	129.20	125.37
11	L	1501	CL7	CMB-C2B-C1B	2.51	129.19	125.37
11	B	1021	CL7	C3B-C2B-C1B	-2.51	104.13	107.16
11	A	1121	CL7	CMB-C2B-C1B	2.51	129.19	125.37
11	A	1122	CL7	C3B-C2B-C1B	-2.51	104.13	107.16
11	A	1131	CL7	C3B-C2B-C1B	-2.51	104.13	107.16
17	A	4008	8CT	C05-C04-C03	2.51	114.34	110.48
11	A	1111	CL7	CMB-C2B-C1B	2.51	129.19	125.37
11	A	1120	CL7	C3B-C2B-C1B	-2.51	104.14	107.16
11	A	1120	CL7	C4C-C3C-C2C	-2.50	103.86	107.13
11	B	1226	CL7	C4C-C3C-C2C	-2.50	103.86	107.13
17	L	4019	8CT	C11-C10-C03	-2.50	120.18	127.20
17	A	4008	8CT	C04-C03-C02	-2.50	119.09	122.61
17	A	4007	8CT	C11-C10-C03	-2.50	120.19	127.20
11	A	1116	CL7	C4C-C3C-C2C	-2.50	103.87	107.13
11	A	1140	CL7	C3B-C2B-C1B	-2.50	104.15	107.16
11	B	1207	CL7	CMB-C2B-C1B	2.49	129.17	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1113	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
11	B	1228	CL7	C3B-C2B-C1B	-2.49	104.15	107.16
11	B	1239	CL7	C4-C3-C5	2.49	119.46	115.27
11	B	1206	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
11	W	2601	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
11	B	1238	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
11	A	1129	CL7	CHC-C1C-NC	-2.49	122.17	124.45
17	W	4018	8CT	C27-C26-C25	-2.49	119.44	122.92
11	B	1215	CL7	C3B-C2B-C1B	-2.49	104.16	107.16
11	B	1236	CL7	C4C-C3C-C2C	-2.48	103.89	107.13
11	A	1117	CL7	C4D-C3D-CAD	-2.48	105.75	107.42
11	L	1503	CL7	CMB-C2B-C1B	2.48	129.15	125.37
11	A	1237	CL7	C3B-C2B-C1B	-2.48	104.17	107.16
11	B	1207	CL7	C3B-C2B-C1B	-2.48	104.17	107.16
11	B	1214	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
11	B	1210	CL7	CMB-C2B-C1B	2.48	129.14	125.37
11	A	1136	CL7	C4D-C3D-CAD	-2.47	105.76	107.42
11	B	1012	CL7	C4C-C3C-C2C	-2.47	103.91	107.13
11	A	1115	CL7	C3B-C2B-C1B	-2.47	104.19	107.16
11	B	1021	CL7	CMB-C2B-C1B	2.46	129.12	125.37
11	A	1107	CL7	C3B-C2B-C1B	-2.46	104.19	107.16
17	J	4013	8CT	C30-C31-C32	-2.46	118.44	121.47
11	A	1101	CL7	C3B-C2B-C1B	-2.46	104.19	107.16
11	A	1102	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
11	B	1206	CL7	C3B-C2B-C1B	-2.46	104.20	107.16
17	M	4021	8CT	C04-C03-C02	-2.45	119.16	122.61
11	A	1106	CL7	C4-C3-C5	2.45	119.40	115.27
11	A	1802	CL7	CMB-C2B-C1B	2.45	129.11	125.37
11	A	1109	CL7	CMB-C2B-C1B	2.45	129.10	125.37
11	A	1123	CL7	C4-C3-C5	2.45	119.39	115.27
17	B	4014	8CT	C25-C24-C23	-2.45	115.57	123.22
11	B	1214	CL7	CAA-CBA-CGA	-2.45	106.01	112.51
11	A	1139	CL7	C3B-C2B-C1B	-2.45	104.21	107.16
11	B	1212	CL7	CMB-C2B-C1B	2.45	129.10	125.37
11	B	1204	CL7	C4C-C3C-C2C	-2.44	103.94	107.13
11	A	1105	CL7	CMB-C2B-C1B	2.44	129.09	125.37
11	B	1223	CL7	C4C-C3C-C2C	-2.44	103.94	107.13
11	A	1122	CL7	C4C-C3C-C2C	-2.44	103.94	107.13
11	A	1111	CL7	C4C-C3C-C2C	-2.44	103.94	107.13
11	B	1204	CL7	C4D-C3D-CAD	-2.44	105.78	107.42
11	L	1503	CL7	C4C-C3C-C2C	-2.44	103.95	107.13
11	B	1021	CL7	CHC-C1C-NC	-2.44	122.21	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1115	CL7	O2D-CGD-CBD	2.44	115.59	111.27
11	A	1112	CL7	CMB-C2B-C1B	2.43	129.08	125.37
11	A	1104	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
11	A	1123	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
11	B	1012	CL7	C4-C3-C5	2.43	119.36	115.27
11	A	1121	CL7	C4D-C3D-CAD	-2.43	105.78	107.42
11	A	1127	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
11	A	1237	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
11	B	1213	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
11	A	1124	CL7	CMB-C2B-C1B	2.43	129.06	125.37
11	A	1119	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
11	A	1117	CL7	C3B-C2B-C1B	-2.42	104.23	107.16
11	B	1021	CL7	C4D-C3D-CAD	-2.42	105.79	107.42
11	B	1207	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
11	A	1116	CL7	CMB-C2B-C1B	2.42	129.06	125.37
11	A	1137	CL7	C3B-C2B-C1B	-2.42	104.24	107.16
16	A	1013	PHO	O2D-CGD-CBD	2.42	114.06	111.00
11	A	1101	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
11	A	1124	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
11	A	1802	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
11	A	1127	CL7	CHB-C1B-NB	-2.42	121.70	124.26
11	B	1239	CL7	C4C-C3C-C2C	-2.42	103.98	107.13
11	A	1104	CL7	CMB-C2B-C1B	2.42	129.05	125.37
11	A	1136	CL7	CMB-C2B-C1B	2.42	129.05	125.37
17	L	4020	8CT	C11-C10-C03	-2.41	120.42	127.20
11	A	1132	CL7	CHC-C1C-NC	-2.41	122.23	124.45
11	B	1211	CL7	CMB-C2B-C1B	2.41	129.04	125.37
11	B	1214	CL7	C3B-C2B-C1B	-2.41	104.25	107.16
11	B	1230	CL7	CHB-C1B-NB	-2.41	121.71	124.26
11	A	1103	CL7	C3B-C2B-C1B	-2.41	104.25	107.16
11	A	1120	CL7	CMB-C2B-C1B	2.41	129.04	125.37
11	J	1302	CL7	C4C-C3C-C2C	-2.41	103.99	107.13
11	B	1234	CL7	C4D-C3D-CAD	-2.41	105.80	107.42
11	A	1109	CL7	CHC-C1C-NC	-2.40	122.24	124.45
11	A	1106	CL7	CMB-C2B-C1B	2.40	129.03	125.37
11	B	1236	CL7	CMB-C2B-C1B	2.40	129.03	125.37
11	A	1139	CL7	C4C-C3C-C2C	-2.40	103.99	107.13
11	A	1114	CL7	C4C-C3C-C2C	-2.40	104.00	107.13
11	B	1205	CL7	C4C-C3C-C2C	-2.40	104.00	107.13
11	B	1213	CL7	CMB-C2B-C1B	2.40	129.03	125.37
11	A	1022	CL7	C4C-C3C-C2C	-2.40	104.00	107.13
11	L	1501	CL7	C4C-C3C-C2C	-2.40	104.00	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	1502	CL7	C4C-C3C-C2C	-2.40	104.00	107.13
11	A	1110	CL7	C4C-C3C-C2C	-2.40	104.00	107.13
11	A	1801	CL7	C4C-C3C-C2C	-2.40	104.00	107.13
11	L	1501	CL7	C4-C3-C5	2.40	119.30	115.27
17	A	4011	8CT	C40-C12-C13	-2.40	119.57	122.92
11	B	1224	CL7	C4C-C3C-C2C	-2.40	104.00	107.13
17	A	4007	8CT	C35-C30-C29	-2.40	109.67	112.70
11	A	1137	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
11	A	1106	CL7	C4D-C3D-CAD	-2.39	105.81	107.42
11	A	1106	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
11	B	1202	CL7	CMB-C2B-C1B	2.39	129.01	125.37
11	A	1123	CL7	CMB-C2B-C1B	2.39	129.00	125.37
17	A	4008	8CT	C18-C19-C20	2.39	128.36	123.47
11	A	1115	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
11	A	1121	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
11	B	1212	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
11	A	1114	CL7	CMB-C2B-C1B	2.39	129.00	125.37
11	B	1228	CL7	CMB-C2B-C1B	2.39	129.00	125.37
11	B	1210	CL7	C4C-C3C-C2C	-2.38	104.02	107.13
11	A	1140	CL7	CMB-C2B-C1B	2.38	129.00	125.37
11	B	1235	CL7	C4D-C3D-CAD	-2.38	105.82	107.42
11	F	1301	CL7	C4C-C3C-C2C	-2.38	104.02	107.13
11	B	1208	CL7	C4C-C3C-C2C	-2.38	104.03	107.13
11	B	1228	CL7	C4C-C3C-C2C	-2.38	104.03	107.13
11	A	1116	CL7	C3B-C2B-C1B	-2.37	104.30	107.16
11	A	1118	CL7	C4C-C3C-C2C	-2.37	104.03	107.13
11	A	1127	CL7	C3B-C2B-C1B	-2.37	104.30	107.16
11	A	1131	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
11	B	1206	CL7	C4D-C3D-CAD	-2.37	105.83	107.42
11	B	1204	CL7	C3B-C2B-C1B	-2.36	104.31	107.16
11	A	1126	CL7	C3B-C2B-C1B	-2.36	104.31	107.16
11	A	1136	CL7	C3B-C2B-C1B	-2.36	104.31	107.16
11	B	1239	CL7	C4D-C3D-CAD	-2.36	105.83	107.42
17	L	4020	8CT	C18-C17-C16	-2.36	123.94	127.31
17	L	4019	8CT	C01-C02-C07	2.36	118.15	113.62
11	A	1136	CL7	C4-C3-C5	2.36	119.24	115.27
11	A	1125	CL7	C4D-C3D-CAD	-2.36	105.83	107.42
11	A	1136	CL7	C4C-C3C-C2C	-2.36	104.05	107.13
11	B	1205	CL7	CHC-C1C-NC	-2.36	122.29	124.45
11	A	1130	CL7	C4C-C3C-C2C	-2.36	104.06	107.13
17	L	4019	8CT	C25-C24-C23	-2.36	115.86	123.22
17	B	4006	8CT	C39-C16-C17	-2.36	119.62	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1140	CL7	C4C-C3C-C2C	-2.36	104.06	107.13
11	A	1140	CL7	C4D-C3D-CAD	-2.35	105.84	107.42
17	B	4017	8CT	C10-C03-C02	-2.35	115.76	121.46
11	B	1238	CL7	C4-C3-C5	2.35	119.22	115.27
11	A	1129	CL7	C4D-C3D-CAD	-2.35	105.84	107.42
11	B	1229	CL7	C4C-C3C-C2C	-2.35	104.07	107.13
11	A	1126	CL7	CHC-C1C-NC	-2.34	122.30	124.45
11	A	1120	CL7	C4D-C3D-CAD	-2.34	105.84	107.42
11	B	1021	CL7	CGD-CBD-CAD	2.34	118.33	110.73
11	W	2601	CL7	C3B-C4B-NB	2.34	112.69	110.52
11	B	1215	CL7	C4C-C3C-C2C	-2.34	104.07	107.13
11	B	1211	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
11	A	1102	CL7	O2D-CGD-CBD	2.34	115.43	111.27
11	A	1103	CL7	C4-C3-C5	2.34	119.21	115.27
17	M	4021	8CT	C35-C30-C31	2.34	115.61	111.42
11	L	1502	CL7	C4D-C3D-CAD	-2.34	105.85	107.42
11	A	1138	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
11	A	1139	CL7	C3B-C4B-NB	2.33	112.68	110.52
11	B	1208	CL7	C3B-C2B-C1B	-2.33	104.35	107.16
11	L	1503	CL7	C4D-C3D-CAD	-2.33	105.86	107.42
11	A	1237	CL7	C4-C3-C5	2.33	119.19	115.27
11	B	1214	CL7	CMB-C2B-C1B	2.33	128.91	125.37
15	A	1011	G9R	C3B-C4B-NB	2.33	112.67	110.52
17	B	4017	8CT	C05-C04-C03	2.33	114.06	110.48
11	B	1222	CL7	CAA-CBA-CGA	-2.33	106.34	112.51
11	F	1301	CL7	CMB-C2B-C1B	2.32	128.91	125.37
17	W	4018	8CT	C40-C12-C13	-2.32	119.67	122.92
11	A	1126	CL7	C4C-C3C-C2C	-2.32	104.10	107.13
17	J	4015	8CT	C14-C15-C16	-2.32	119.91	126.42
11	A	1119	CL7	C3B-C2B-C1B	-2.32	104.37	107.16
11	B	1222	CL7	C4C-C3C-C2C	-2.32	104.11	107.13
17	W	4020	8CT	C24-C23-C21	-2.31	119.92	126.42
11	A	1126	CL7	CHB-C1B-NB	-2.31	121.81	124.26
11	B	1201	CL7	CMB-C2B-C1B	2.31	128.88	125.37
11	A	1116	CL7	C4D-C3D-CAD	-2.31	105.87	107.42
11	B	1225	CL7	C4C-C3C-C2C	-2.31	104.12	107.13
11	A	1107	CL7	C4C-C3C-C2C	-2.30	104.12	107.13
11	B	1229	CL7	C4D-C3D-CAD	-2.30	105.87	107.42
11	B	1230	CL7	CMB-C2B-C1B	2.30	128.87	125.37
17	J	4015	8CT	C35-C30-C29	-2.30	109.79	112.70
11	B	1201	CL7	C4C-C3C-C2C	-2.30	104.13	107.13
11	B	1235	CL7	C4C-C3C-C2C	-2.30	104.14	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1112	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
11	A	1101	CL7	C4-C3-C5	2.29	119.13	115.27
11	B	1222	CL7	CMB-C2B-C1B	2.29	128.86	125.37
11	B	1021	CL7	O1D-CGD-CBD	2.29	129.16	124.48
17	L	4020	8CT	C40-C12-C13	-2.29	119.72	122.92
11	L	1501	CL7	C4D-C3D-CAD	-2.28	105.89	107.42
11	B	1203	CL7	C4C-C3C-C2C	-2.28	104.16	107.13
11	B	1203	CL7	CMB-C2B-C1B	2.28	128.84	125.37
15	A	1011	G9R	CAA-CBA-CGA	-2.27	106.61	113.25
11	B	1201	CL7	C4D-C3D-CAD	-2.27	105.89	107.42
11	B	1207	CL7	C4D-C3D-CAD	-2.27	105.89	107.42
11	B	1203	CL7	C4-C3-C5	2.27	119.09	115.27
11	A	1110	CL7	C3B-C4B-NB	2.27	112.62	110.52
16	A	1013	PHO	C1C-C2C-C3C	-2.26	106.73	108.61
11	B	1230	CL7	C4D-C3D-CAD	-2.26	105.90	107.42
11	A	1129	CL7	C4C-C3C-C2C	-2.25	104.19	107.13
16	A	1013	PHO	C4D-ND-C1D	-2.25	106.54	108.83
11	A	1237	CL7	CAA-CBA-CGA	-2.25	106.68	113.25
11	A	1109	CL7	C3B-C4B-NB	2.25	112.60	110.52
11	A	1129	CL7	C3B-C4B-NB	2.25	112.60	110.52
11	A	1128	CL7	CAA-CBA-CGA	-2.25	106.69	113.25
11	B	1206	CL7	CMB-C2B-C1B	2.25	128.79	125.37
17	A	4011	8CT	C22-C21-C20	-2.24	119.78	122.92
17	J	4015	8CT	C28-C26-C25	2.24	122.38	118.94
17	J	4015	8CT	C22-C21-C23	2.24	121.61	118.08
17	B	4014	8CT	C39-C16-C17	-2.24	119.78	122.92
11	A	1109	CL7	C4D-C3D-CAD	-2.24	105.92	107.42
11	A	1124	CL7	C4D-C3D-CAD	-2.23	105.92	107.42
11	B	1225	CL7	C4-C3-C5	2.23	119.03	115.27
11	B	1214	CL7	C4D-C3D-CAD	-2.23	105.92	107.42
11	B	1203	CL7	C4D-C3D-CAD	-2.23	105.92	107.42
11	B	1238	CL7	C4D-C3D-CAD	-2.23	105.92	107.42
17	J	4013	8CT	C40-C12-C13	-2.23	119.80	122.92
11	B	1214	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
11	A	1112	CL7	C4D-C3D-CAD	-2.23	105.92	107.42
11	A	1022	CL7	C4-C3-C5	2.22	119.01	115.27
11	A	1140	CL7	C4-C3-C5	2.22	119.01	115.27
11	A	1102	CL7	C3B-C4B-NB	2.22	112.58	110.52
17	A	4007	8CT	C40-C12-C13	-2.22	119.81	122.92
17	W	4018	8CT	C18-C19-C20	-2.22	118.94	123.47
11	A	1125	CL7	CAA-CBA-CGA	-2.21	106.78	113.25
11	B	1210	CL7	C3B-C4B-NB	2.21	112.57	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	4014	8CT	C22-C21-C23	2.21	121.56	118.08
11	B	1202	CL7	C4D-C3D-CAD	-2.21	105.93	107.42
11	A	1104	CL7	C4D-C3D-CAD	-2.21	105.93	107.42
11	A	1137	CL7	CAA-CBA-CGA	-2.21	106.64	112.51
17	A	4008	8CT	C15-C16-C17	2.20	122.32	118.94
11	W	2601	CL7	C4D-C3D-CAD	-2.20	105.94	107.42
11	A	1137	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
11	A	1114	CL7	C4D-C3D-CAD	-2.20	105.94	107.42
11	A	1137	CL7	O2D-CGD-CBD	2.20	115.18	111.27
11	A	1118	CL7	C4D-C3D-CAD	-2.20	105.94	107.42
11	A	1127	CL7	C4D-C3D-CAD	-2.20	105.94	107.42
17	W	4020	8CT	C27-C26-C25	-2.20	119.84	122.92
11	B	1203	CL7	CAC-C3C-C2C	2.20	131.29	127.53
17	A	4007	8CT	C28-C26-C25	2.19	122.30	118.94
17	W	4020	8CT	C18-C19-C20	2.19	127.96	123.47
11	B	1208	CL7	C4D-C3D-CAD	-2.19	105.95	107.42
17	M	4021	8CT	C07-C02-C03	-2.19	119.56	122.73
11	B	1225	CL7	C1C-C2C-C3C	-2.18	103.75	106.94
17	A	4011	8CT	C39-C16-C17	-2.18	119.87	122.92
11	A	1132	CL7	C4-C3-C5	2.18	118.94	115.27
11	A	1107	CL7	CAA-CBA-CGA	-2.18	106.72	112.51
11	A	1122	CL7	C4D-C3D-CAD	-2.18	105.96	107.42
11	A	1132	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
11	B	1208	CL7	C1C-C2C-C3C	-2.17	103.77	106.94
11	B	1215	CL7	C1C-C2C-C3C	-2.17	103.77	106.94
11	A	1119	CL7	C3B-C4B-NB	2.17	112.53	110.52
11	B	1201	CL7	C3B-C4B-NB	2.17	112.53	110.52
11	A	1802	CL7	C4D-C3D-CAD	-2.17	105.96	107.42
17	J	4013	8CT	C19-C18-C17	-2.17	119.03	123.47
11	L	1502	CL7	C3B-C4B-NB	2.17	112.53	110.52
11	A	1136	CL7	O2D-CGD-CBD	2.17	115.12	111.27
11	A	1125	CL7	CAC-C3C-C2C	2.17	131.23	127.53
17	W	4020	8CT	C40-C12-C11	2.16	121.49	118.08
17	B	4017	8CT	C30-C31-C32	-2.16	118.81	121.47
17	M	4021	8CT	C27-C26-C25	-2.16	119.89	122.92
11	A	1114	CL7	CHD-C1D-ND	-2.16	121.97	124.26
11	A	1137	CL7	C3B-C4B-NB	2.16	112.52	110.52
11	A	1117	CL7	CMB-C2B-C1B	2.16	128.66	125.37
11	A	1022	CL7	C4D-C3D-CAD	-2.16	105.97	107.42
11	A	1123	CL7	C4D-C3D-CAD	-2.16	105.97	107.42
11	B	1208	CL7	C3B-C4B-NB	2.16	112.52	110.52
11	B	1206	CL7	C3B-C4B-NB	2.16	112.52	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	4014	8CT	C04-C03-C10	2.16	121.88	115.78
11	A	1101	CL7	C4D-C3D-CAD	-2.15	105.97	107.42
11	B	1226	CL7	CAA-CBA-CGA	-2.15	106.98	113.25
11	B	1203	CL7	C1C-C2C-C3C	-2.14	103.81	106.94
11	A	1119	CL7	C4D-C3D-CAD	-2.14	105.98	107.42
11	A	1102	CL7	CAC-C3C-C2C	2.14	131.19	127.53
17	A	4007	8CT	C15-C16-C17	2.14	122.23	118.94
11	B	1225	CL7	C4D-C3D-CAD	-2.14	105.98	107.42
11	B	1228	CL7	C4D-C3D-CAD	-2.14	105.98	107.42
17	L	4020	8CT	C24-C23-C21	-2.14	120.40	126.42
11	B	1225	CL7	C3B-C4B-NB	2.14	112.50	110.52
11	A	1107	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
11	A	1138	CL7	C3B-C4B-NB	2.14	112.50	110.52
17	W	4020	8CT	C35-C30-C29	-2.14	110.00	112.70
11	A	1119	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
11	B	1215	CL7	C3B-C4B-NB	2.14	112.50	110.52
11	B	1210	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
11	A	1135	CL7	C4D-C3D-CAD	-2.13	105.99	107.42
11	B	1235	CL7	C3B-C4B-NB	2.13	112.49	110.52
11	A	1131	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
17	W	4020	8CT	C14-C13-C12	-2.13	124.27	127.31
11	B	1229	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
11	A	1124	CL7	CAA-CBA-CGA	-2.13	106.86	112.51
11	B	1204	CL7	CAC-C3C-C2C	2.13	131.17	127.53
11	B	1223	CL7	C4D-C3D-CAD	-2.13	105.99	107.42
11	A	1110	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
11	A	1125	CL7	C4D-C3D-C2D	2.13	110.07	107.30
11	A	1131	CL7	CAA-CBA-CGA	-2.13	107.04	113.25
17	W	4018	8CT	C22-C21-C20	-2.13	119.94	122.92
11	A	1131	CL7	C4D-C3D-CAD	-2.12	105.99	107.42
11	B	1212	CL7	C4D-C3D-CAD	-2.12	105.99	107.42
11	A	1132	CL7	C3B-C4B-NB	2.12	112.48	110.52
11	A	1114	CL7	C3B-C4B-NB	2.12	112.48	110.52
11	A	1136	CL7	C3B-C4B-NB	2.12	112.48	110.52
11	A	1104	CL7	CAC-C3C-C2C	2.12	131.15	127.53
17	L	4019	8CT	C39-C16-C17	-2.12	119.96	122.92
11	A	1127	CL7	CAC-C3C-C2C	2.11	131.15	127.53
11	A	1237	CL7	C4D-C3D-CAD	-2.11	106.00	107.42
11	A	1112	CL7	C3B-C4B-NB	2.11	112.47	110.52
11	A	1132	CL7	C4C-C3C-C2C	-2.11	104.37	107.13
11	B	1222	CL7	CAC-C3C-C2C	2.11	131.14	127.53
11	A	1139	CL7	C4D-C3D-CAD	-2.11	106.00	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1204	CL7	C1C-C2C-C3C	-2.11	103.86	106.94
11	B	1213	CL7	C4D-C3D-CAD	-2.11	106.00	107.42
17	J	4013	8CT	C22-C21-C20	-2.11	119.97	122.92
17	W	4020	8CT	C35-C30-C31	2.10	115.19	111.42
11	A	1103	CL7	CAA-CBA-CGA	-2.10	107.11	113.25
11	F	1301	CL7	C3B-C4B-NB	2.10	112.47	110.52
11	B	1208	CL7	CAA-CBA-CGA	-2.10	106.93	112.51
11	A	1107	CL7	C3B-C4B-NB	2.10	112.46	110.52
11	L	1501	CL7	CAA-CBA-CGA	-2.10	107.12	113.25
11	A	1115	CL7	C4D-C3D-CAD	-2.10	106.01	107.42
11	A	1118	CL7	C1C-C2C-C3C	-2.10	103.88	106.94
11	B	1236	CL7	C3B-C4B-NB	2.10	112.46	110.52
11	J	1302	CL7	C4D-C3D-CAD	-2.10	106.01	107.42
11	A	1138	CL7	C1C-C2C-C3C	-2.10	103.88	106.94
11	B	1201	CL7	C1C-C2C-C3C	-2.10	103.88	106.94
11	A	1112	CL7	C1C-C2C-C3C	-2.09	103.88	106.94
11	B	1213	CL7	CAC-C3C-C2C	2.09	131.11	127.53
17	W	4018	8CT	C39-C16-C17	-2.09	119.99	122.92
11	A	1126	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
11	B	1215	CL7	CAC-C3C-C2C	2.09	131.10	127.53
11	A	1130	CL7	C4D-C3D-CAD	-2.09	106.02	107.42
17	L	4019	8CT	C22-C21-C23	2.09	121.37	118.08
11	A	1111	CL7	C4D-C3D-CAD	-2.09	106.02	107.42
11	B	1212	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
11	A	1802	CL7	CAA-CBA-CGA	-2.09	106.97	112.51
15	A	1011	G9R	C4C-C3C-C2C	-2.09	103.86	106.90
11	B	1215	CL7	C4D-C3D-CAD	-2.08	106.02	107.42
11	A	1120	CL7	C3B-C4B-NB	2.08	112.45	110.52
11	A	1103	CL7	CAC-C3C-C2C	2.08	131.09	127.53
11	A	1101	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
11	A	1129	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
11	A	1104	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
11	B	1203	CL7	C3B-C4B-NB	2.08	112.44	110.52
11	A	1113	CL7	CAA-CBA-CGA	-2.08	106.99	112.51
11	A	1115	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
11	F	1301	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
11	A	1135	CL7	CAC-C3C-C2C	2.08	131.08	127.53
11	A	1022	CL7	CAC-C3C-C2C	2.07	131.08	127.53
11	A	1127	CL7	C1C-C2C-C3C	-2.07	103.91	106.94
11	J	1302	CL7	C3B-C4B-NB	2.07	112.44	110.52
11	B	1239	CL7	C1C-C2C-C3C	-2.07	103.91	106.94
11	B	1223	CL7	C1C-C2C-C3C	-2.07	103.92	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	4019	8CT	C18-C19-C20	-2.07	119.23	123.47
11	B	1222	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
15	A	1011	G9R	CAC-C3C-C2C	2.07	131.07	127.53
11	B	1238	CL7	CAA-CBA-CGA	-2.07	107.21	113.25
11	A	1113	CL7	C4D-C3D-CAD	-2.07	106.03	107.42
11	A	1802	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
11	A	1121	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
11	A	1801	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
11	L	1501	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
11	B	1211	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
11	B	1228	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
11	A	1105	CL7	C4D-C3D-CAD	-2.06	106.04	107.42
11	B	1212	CL7	CAC-C3C-C2C	2.06	131.05	127.53
11	B	1226	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
11	B	1212	CL7	C3B-C4B-NB	2.06	112.42	110.52
11	A	1140	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
11	B	1235	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
11	L	1502	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
11	A	1118	CL7	C3B-C4B-NB	2.06	112.42	110.52
11	A	1104	CL7	C3B-C4B-NB	2.05	112.42	110.52
11	W	2601	CL7	CMB-C2B-C1B	2.05	128.50	125.37
11	L	1502	CL7	CAA-CBA-CGA	-2.05	107.25	113.25
11	B	1213	CL7	C1C-C2C-C3C	-2.05	103.94	106.94
11	A	1113	CL7	CAC-C3C-C2C	2.05	131.03	127.53
11	J	1302	CL7	C1C-C2C-C3C	-2.05	103.95	106.94
11	A	1139	CL7	CAA-CBA-CGA	-2.05	107.07	112.51
11	A	1124	CL7	C1C-C2C-C3C	-2.05	103.95	106.94
11	A	1120	CL7	C1C-C2C-C3C	-2.05	103.95	106.94
11	A	1130	CL7	C1C-C2C-C3C	-2.05	103.95	106.94
11	A	1802	CL7	C3B-C4B-NB	2.05	112.41	110.52
16	B	1023	PHO	C4D-ND-C1D	-2.05	106.75	108.83
11	A	1117	CL7	C4-C3-C5	2.05	118.71	115.27
11	L	1503	CL7	C3B-C4B-NB	2.05	112.41	110.52
11	A	1124	CL7	CAC-C3C-C2C	2.04	131.03	127.53
11	B	1207	CL7	C1C-C2C-C3C	-2.04	103.96	106.94
11	B	1224	CL7	C4D-C3D-CAD	-2.04	106.05	107.42
11	A	1117	CL7	C3B-C4B-NB	2.04	112.41	110.52
11	B	1235	CL7	O2D-CGD-CBD	2.04	114.90	111.27
11	A	1114	CL7	C1C-C2C-C3C	-2.04	103.96	106.94
11	B	1012	CL7	C1C-C2C-C3C	-2.04	103.96	106.94
11	A	1801	CL7	C4D-C3D-CAD	-2.04	106.05	107.42
11	A	1114	CL7	CAC-C3C-C2C	2.04	131.02	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1236	CL7	C1C-C2C-C3C	-2.04	103.97	106.94
11	A	1110	CL7	C4D-C3D-C2D	2.03	109.95	107.30
11	L	1503	CL7	C1C-C2C-C3C	-2.03	103.97	106.94
11	B	1230	CL7	C3B-C2B-C1B	-2.03	104.71	107.16
11	B	1225	CL7	CAC-C3C-C2C	2.03	131.00	127.53
11	A	1106	CL7	C1C-C2C-C3C	-2.03	103.97	106.94
11	A	1120	CL7	CAC-C3C-C2C	2.03	131.00	127.53
11	B	1229	CL7	CAC-C3C-C2C	2.03	131.00	127.53
11	A	1123	CL7	C1C-C2C-C3C	-2.03	103.98	106.94
11	F	1301	CL7	C4D-C3D-CAD	-2.03	106.06	107.42
11	A	1106	CL7	C3B-C4B-NB	2.03	112.40	110.52
11	A	1122	CL7	CHC-C1C-NC	-2.03	122.59	124.45
11	A	1122	CL7	C1C-C2C-C3C	-2.03	103.98	106.94
11	B	1226	CL7	C4D-C3D-CAD	-2.02	106.06	107.42
11	B	1223	CL7	CAC-C3C-C2C	2.02	130.99	127.53
11	B	1222	CL7	C4D-C3D-CAD	-2.02	106.06	107.42
11	B	1204	CL7	C3B-C4B-NB	2.02	112.39	110.52
11	A	1130	CL7	CAC-C3C-C2C	2.02	130.98	127.53
11	A	1123	CL7	CAA-CBA-CGA	-2.02	107.35	113.25
11	A	1116	CL7	CAC-C3C-C2C	2.02	130.98	127.53
11	A	1022	CL7	C1C-C2C-C3C	-2.02	103.99	106.94
11	B	1204	CL7	CAA-CBA-CGA	-2.02	107.15	112.51
11	A	1109	CL7	CAC-C3C-C2C	2.02	130.98	127.53
11	B	1228	CL7	CAC-C3C-C2C	2.02	130.98	127.53
11	A	1132	CL7	CAA-CBA-CGA	-2.01	107.37	113.25
11	L	1501	CL7	CAC-C3C-C2C	2.01	130.97	127.53
11	A	1110	CL7	C4D-C3D-CAD	-2.01	106.07	107.42
16	B	1023	PHO	O2D-CGD-CBD	2.01	113.54	111.00
11	A	1107	CL7	C4D-C3D-CAD	-2.01	106.07	107.42
11	A	1102	CL7	C1C-C2C-C3C	-2.01	104.01	106.94
11	B	1238	CL7	CAC-C3C-C2C	2.01	130.97	127.53
11	A	1237	CL7	C1C-C2C-C3C	-2.01	104.01	106.94
11	B	1207	CL7	C3B-C4B-NB	2.01	112.38	110.52
11	A	1127	CL7	CAA-CBA-CGA	-2.01	107.18	112.51
11	A	1113	CL7	C3B-C4B-NB	2.01	112.38	110.52
16	B	1023	PHO	O1D-CGD-CBD	2.01	128.08	124.74
11	A	1136	CL7	C1C-C2C-C3C	-2.01	104.01	106.94
17	L	4020	8CT	C27-C26-C25	-2.01	120.11	122.92
11	B	1201	CL7	CAA-CBA-CGA	-2.00	107.19	112.51
11	A	1135	CL7	C4D-C3D-C2D	2.00	109.91	107.30
17	L	4019	8CT	C27-C26-C25	-2.00	120.12	122.92
11	A	1123	CL7	CAC-C3C-C2C	2.00	130.96	127.53

All (153) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	1022	CL7	NC
11	A	1022	CL7	NA
11	A	1101	CL7	NC
11	A	1101	CL7	NA
11	A	1102	CL7	NC
11	A	1102	CL7	NA
11	A	1103	CL7	NC
11	A	1103	CL7	NA
11	A	1104	CL7	NC
11	A	1104	CL7	NA
11	A	1105	CL7	NC
11	A	1105	CL7	NA
11	A	1106	CL7	NC
11	A	1106	CL7	NA
11	A	1107	CL7	NC
11	A	1107	CL7	NA
11	A	1109	CL7	NC
11	A	1109	CL7	NA
11	A	1110	CL7	NC
11	A	1110	CL7	NA
11	A	1111	CL7	NC
11	A	1111	CL7	NA
11	A	1112	CL7	NC
11	A	1112	CL7	NA
11	A	1113	CL7	NC
11	A	1113	CL7	NA
11	A	1114	CL7	NC
11	A	1114	CL7	NA
11	A	1115	CL7	NC
11	A	1115	CL7	NA
11	A	1116	CL7	NC
11	A	1116	CL7	NA
11	A	1117	CL7	NC
11	A	1117	CL7	NA
11	A	1118	CL7	NC
11	A	1118	CL7	NA
11	A	1119	CL7	NC
11	A	1119	CL7	NA
11	A	1120	CL7	NC
11	A	1120	CL7	NA
11	A	1121	CL7	NC
11	A	1121	CL7	NA

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Mol	Chain	Res	Type	Atom
11	A	1122	CL7	NC
11	A	1122	CL7	NA
11	A	1123	CL7	NC
11	A	1123	CL7	NA
11	A	1124	CL7	NC
11	A	1124	CL7	NA
11	A	1125	CL7	NC
11	A	1125	CL7	NA
11	A	1126	CL7	NC
11	A	1126	CL7	NA
11	A	1127	CL7	NC
11	A	1127	CL7	NA
11	A	1128	CL7	NC
11	A	1128	CL7	NA
11	A	1129	CL7	NC
11	A	1129	CL7	NA
11	A	1130	CL7	NC
11	A	1130	CL7	NA
11	A	1131	CL7	NC
11	A	1131	CL7	NA
11	A	1132	CL7	NC
11	A	1132	CL7	NA
11	A	1135	CL7	NC
11	A	1135	CL7	NA
11	A	1136	CL7	NC
11	A	1136	CL7	NA
11	A	1137	CL7	NC
11	A	1137	CL7	NA
11	A	1138	CL7	NC
11	A	1138	CL7	NA
11	A	1139	CL7	NC
11	A	1139	CL7	NA
11	A	1140	CL7	NC
11	A	1140	CL7	NA
11	A	1237	CL7	NC
11	A	1237	CL7	NA
11	A	1801	CL7	NC
11	A	1801	CL7	NA
11	A	1802	CL7	NC
11	A	1802	CL7	NA
11	B	1012	CL7	NC
11	B	1012	CL7	NA

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Mol	Chain	Res	Type	Atom
11	B	1021	CL7	NC
11	B	1021	CL7	NA
11	B	1201	CL7	NC
11	B	1201	CL7	NA
11	B	1202	CL7	NC
11	B	1202	CL7	NA
11	B	1203	CL7	NC
11	B	1203	CL7	NA
11	B	1204	CL7	NC
11	B	1204	CL7	NA
11	B	1205	CL7	NC
11	B	1205	CL7	NA
11	B	1206	CL7	NC
11	B	1206	CL7	NA
11	B	1207	CL7	NC
11	B	1207	CL7	NA
11	B	1208	CL7	NC
11	B	1208	CL7	NA
11	B	1210	CL7	NC
11	B	1210	CL7	NA
11	B	1211	CL7	NC
11	B	1211	CL7	NA
11	B	1212	CL7	NC
11	B	1212	CL7	NA
11	B	1213	CL7	NC
11	B	1213	CL7	NA
11	B	1214	CL7	NC
11	B	1214	CL7	NA
11	B	1215	CL7	NC
11	B	1215	CL7	NA
11	B	1222	CL7	NC
11	B	1222	CL7	NA
11	B	1223	CL7	NC
11	B	1223	CL7	NA
11	B	1224	CL7	NC
11	B	1224	CL7	NA
11	B	1225	CL7	NC
11	B	1225	CL7	NA
11	B	1226	CL7	NC
11	B	1226	CL7	NA
11	B	1228	CL7	NC
11	B	1228	CL7	NA

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Mol	Chain	Res	Type	Atom
11	B	1229	CL7	NC
11	B	1229	CL7	NA
11	B	1230	CL7	NC
11	B	1230	CL7	NA
11	B	1234	CL7	NC
11	B	1234	CL7	NA
11	B	1235	CL7	NC
11	B	1235	CL7	NA
11	B	1236	CL7	NC
11	B	1236	CL7	NA
11	B	1238	CL7	NC
11	B	1238	CL7	NA
11	B	1239	CL7	NC
11	B	1239	CL7	NA
11	F	1301	CL7	NC
11	F	1301	CL7	NA
11	J	1302	CL7	NC
11	J	1302	CL7	NA
11	L	1501	CL7	NC
11	L	1501	CL7	NA
11	L	1502	CL7	NC
11	L	1502	CL7	NA
11	L	1503	CL7	NC
11	L	1503	CL7	NA
11	W	2601	CL7	NC
11	W	2601	CL7	NA
15	A	1011	G9R	ND

All (1040) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1022	CL7	C2B-C3B-CAB-OBB
11	A	1022	CL7	C4B-C3B-CAB-OBB
11	A	1101	CL7	C1A-C2A-CAA-CBA
11	A	1101	CL7	C3A-C2A-CAA-CBA
11	A	1102	CL7	C1A-C2A-CAA-CBA
11	A	1103	CL7	C4-C3-C5-C6
11	A	1103	CL7	C4B-C3B-CAB-OBB
11	A	1104	CL7	C1A-C2A-CAA-CBA
11	A	1104	CL7	C3A-C2A-CAA-CBA
11	A	1104	CL7	C2B-C3B-CAB-OBB
11	A	1104	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
11	A	1105	CL7	CBD-CGD-O2D-CED
11	A	1105	CL7	C2B-C3B-CAB-OBB
11	A	1105	CL7	C4B-C3B-CAB-OBB
11	A	1106	CL7	C3A-C2A-CAA-CBA
11	A	1106	CL7	CHA-CBD-CGD-O2D
11	A	1106	CL7	CHA-CBD-CGD-O1D
11	A	1106	CL7	CAD-CBD-CGD-O1D
11	A	1106	CL7	C2B-C3B-CAB-OBB
11	A	1106	CL7	C4B-C3B-CAB-OBB
11	A	1107	CL7	C2B-C3B-CAB-OBB
11	A	1107	CL7	C4B-C3B-CAB-OBB
11	A	1109	CL7	CBD-CGD-O2D-CED
11	A	1109	CL7	C2B-C3B-CAB-OBB
11	A	1109	CL7	C4B-C3B-CAB-OBB
11	A	1111	CL7	C1A-C2A-CAA-CBA
11	A	1111	CL7	C3A-C2A-CAA-CBA
11	A	1111	CL7	CBD-CGD-O2D-CED
11	A	1111	CL7	C2B-C3B-CAB-OBB
11	A	1111	CL7	C4B-C3B-CAB-OBB
11	A	1112	CL7	C3A-C2A-CAA-CBA
11	A	1112	CL7	C2B-C3B-CAB-OBB
11	A	1112	CL7	C4B-C3B-CAB-OBB
11	A	1113	CL7	CBD-CGD-O2D-CED
11	A	1113	CL7	C2B-C3B-CAB-OBB
11	A	1113	CL7	C4B-C3B-CAB-OBB
11	A	1114	CL7	C2B-C3B-CAB-OBB
11	A	1114	CL7	C4B-C3B-CAB-OBB
11	A	1115	CL7	CHA-CBD-CGD-O2D
11	A	1115	CL7	CHA-CBD-CGD-O1D
11	A	1115	CL7	C4B-C3B-CAB-OBB
11	A	1117	CL7	C4B-C3B-CAB-OBB
11	A	1118	CL7	C2B-C3B-CAB-OBB
11	A	1118	CL7	C4B-C3B-CAB-OBB
11	A	1119	CL7	C2B-C3B-CAB-OBB
11	A	1119	CL7	C4B-C3B-CAB-OBB
11	A	1120	CL7	C2B-C3B-CAB-OBB
11	A	1120	CL7	C4B-C3B-CAB-OBB
11	A	1121	CL7	C3A-C2A-CAA-CBA
11	A	1121	CL7	C2B-C3B-CAB-OBB
11	A	1121	CL7	C4B-C3B-CAB-OBB
11	A	1122	CL7	C2B-C3B-CAB-OBB
11	A	1122	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
11	A	1123	CL7	O1A-CGA-O2A-C1
11	A	1123	CL7	CBA-CGA-O2A-C1
11	A	1123	CL7	C2B-C3B-CAB-OBB
11	A	1123	CL7	C4B-C3B-CAB-OBB
11	A	1124	CL7	C2B-C3B-CAB-OBB
11	A	1124	CL7	C4B-C3B-CAB-OBB
11	A	1125	CL7	C1A-C2A-CAA-CBA
11	A	1125	CL7	C3A-C2A-CAA-CBA
11	A	1125	CL7	CHA-CBD-CGD-O2D
11	A	1125	CL7	CHA-CBD-CGD-O1D
11	A	1125	CL7	C2B-C3B-CAB-OBB
11	A	1125	CL7	C4B-C3B-CAB-OBB
11	A	1126	CL7	C1A-C2A-CAA-CBA
11	A	1126	CL7	C3A-C2A-CAA-CBA
11	A	1126	CL7	CBD-CGD-O2D-CED
11	A	1126	CL7	C2B-C3B-CAB-OBB
11	A	1126	CL7	C4B-C3B-CAB-OBB
11	A	1128	CL7	C11-C12-C13-C14
11	A	1129	CL7	CBD-CGD-O2D-CED
11	A	1129	CL7	C2B-C3B-CAB-OBB
11	A	1129	CL7	C4B-C3B-CAB-OBB
11	A	1130	CL7	C1A-C2A-CAA-CBA
11	A	1130	CL7	C3A-C2A-CAA-CBA
11	A	1130	CL7	C2B-C3B-CAB-OBB
11	A	1130	CL7	C4B-C3B-CAB-OBB
11	A	1131	CL7	C2-C3-C5-C6
11	A	1131	CL7	C4-C3-C5-C6
11	A	1132	CL7	C6-C7-C8-C9
11	A	1132	CL7	C2B-C3B-CAB-OBB
11	A	1132	CL7	C4B-C3B-CAB-OBB
11	A	1135	CL7	C2A-CAA-CBA-CGA
11	A	1135	CL7	C2B-C3B-CAB-OBB
11	A	1135	CL7	C4B-C3B-CAB-OBB
11	A	1136	CL7	C1A-C2A-CAA-CBA
11	A	1136	CL7	C3A-C2A-CAA-CBA
11	A	1136	CL7	C2B-C3B-CAB-OBB
11	A	1136	CL7	C4B-C3B-CAB-OBB
11	A	1137	CL7	C2B-C3B-CAB-OBB
11	A	1137	CL7	C4B-C3B-CAB-OBB
11	A	1138	CL7	CBD-CGD-O2D-CED
11	A	1138	CL7	C2B-C3B-CAB-OBB
11	A	1138	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
11	A	1139	CL7	CBD-CGD-O2D-CED
11	A	1140	CL7	C1A-C2A-CAA-CBA
11	A	1140	CL7	C3A-C2A-CAA-CBA
11	A	1140	CL7	C2B-C3B-CAB-OBB
11	A	1140	CL7	C4B-C3B-CAB-OBB
11	A	1801	CL7	C2A-CAA-CBA-CGA
11	A	1801	CL7	C1A-C2A-CAA-CBA
11	A	1801	CL7	C3A-C2A-CAA-CBA
11	A	1801	CL7	C4B-C3B-CAB-OBB
11	A	1802	CL7	C1A-C2A-CAA-CBA
11	A	1802	CL7	C3A-C2A-CAA-CBA
11	A	1802	CL7	C2B-C3B-CAB-OBB
11	A	1802	CL7	C4B-C3B-CAB-OBB
11	B	1012	CL7	C4-C3-C5-C6
11	B	1012	CL7	C2B-C3B-CAB-OBB
11	B	1012	CL7	C4B-C3B-CAB-OBB
11	B	1021	CL7	C2-C3-C5-C6
11	B	1021	CL7	C4-C3-C5-C6
11	B	1021	CL7	C2A-CAA-CBA-CGA
11	B	1021	CL7	C1A-C2A-CAA-CBA
11	B	1021	CL7	C3A-C2A-CAA-CBA
11	B	1202	CL7	CHA-CBD-CGD-O2D
11	B	1202	CL7	CHA-CBD-CGD-O1D
11	B	1202	CL7	C2B-C3B-CAB-OBB
11	B	1202	CL7	C4B-C3B-CAB-OBB
11	B	1203	CL7	CBA-CGA-O2A-C1
11	B	1203	CL7	CHA-CBD-CGD-O1D
11	B	1203	CL7	CBD-CGD-O2D-CED
11	B	1203	CL7	C2B-C3B-CAB-OBB
11	B	1203	CL7	C4B-C3B-CAB-OBB
11	B	1204	CL7	C1A-C2A-CAA-CBA
11	B	1204	CL7	C3A-C2A-CAA-CBA
11	B	1205	CL7	C1A-C2A-CAA-CBA
11	B	1205	CL7	C3A-C2A-CAA-CBA
11	B	1206	CL7	C1A-C2A-CAA-CBA
11	B	1206	CL7	C3A-C2A-CAA-CBA
11	B	1206	CL7	CHA-CBD-CGD-O2D
11	B	1206	CL7	CHA-CBD-CGD-O1D
11	B	1206	CL7	CBD-CGD-O2D-CED
11	B	1206	CL7	C4B-C3B-CAB-OBB
11	B	1207	CL7	C2B-C3B-CAB-OBB
11	B	1207	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
11	B	1210	CL7	C2B-C3B-CAB-OBB
11	B	1210	CL7	C4B-C3B-CAB-OBB
11	B	1211	CL7	CBD-CGD-O2D-CED
11	B	1211	CL7	C2B-C3B-CAB-OBB
11	B	1211	CL7	C4B-C3B-CAB-OBB
11	B	1212	CL7	CBD-CGD-O2D-CED
11	B	1212	CL7	C2B-C3B-CAB-OBB
11	B	1212	CL7	C4B-C3B-CAB-OBB
11	B	1213	CL7	C1A-C2A-CAA-CBA
11	B	1213	CL7	C3A-C2A-CAA-CBA
11	B	1213	CL7	CBD-CGD-O2D-CED
11	B	1213	CL7	C2B-C3B-CAB-OBB
11	B	1213	CL7	C4B-C3B-CAB-OBB
11	B	1214	CL7	C4B-C3B-CAB-OBB
11	B	1215	CL7	C1A-C2A-CAA-CBA
11	B	1215	CL7	C3A-C2A-CAA-CBA
11	B	1215	CL7	C2B-C3B-CAB-OBB
11	B	1215	CL7	C4B-C3B-CAB-OBB
11	B	1222	CL7	C2B-C3B-CAB-OBB
11	B	1222	CL7	C4B-C3B-CAB-OBB
11	B	1223	CL7	C4B-C3B-CAB-OBB
11	B	1224	CL7	C1A-C2A-CAA-CBA
11	B	1224	CL7	CBD-CGD-O2D-CED
11	B	1224	CL7	C2B-C3B-CAB-OBB
11	B	1224	CL7	C4B-C3B-CAB-OBB
11	B	1225	CL7	CHA-CBD-CGD-O2D
11	B	1225	CL7	CHA-CBD-CGD-O1D
11	B	1225	CL7	C2B-C3B-CAB-OBB
11	B	1225	CL7	C4B-C3B-CAB-OBB
11	B	1226	CL7	CBD-CGD-O2D-CED
11	B	1226	CL7	C2B-C3B-CAB-OBB
11	B	1226	CL7	C4B-C3B-CAB-OBB
11	B	1228	CL7	CBD-CGD-O2D-CED
11	B	1228	CL7	C2B-C3B-CAB-OBB
11	B	1228	CL7	C4B-C3B-CAB-OBB
11	B	1229	CL7	CBD-CGD-O2D-CED
11	B	1234	CL7	C2B-C3B-CAB-OBB
11	B	1234	CL7	C4B-C3B-CAB-OBB
11	B	1235	CL7	C1A-C2A-CAA-CBA
11	B	1235	CL7	C3A-C2A-CAA-CBA
11	B	1235	CL7	C2B-C3B-CAB-OBB
11	B	1235	CL7	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
11	B	1236	CL7	C2B-C3B-CAB-OBB
11	B	1236	CL7	C4B-C3B-CAB-OBB
11	B	1238	CL7	C2-C3-C5-C6
11	B	1238	CL7	C4-C3-C5-C6
11	B	1238	CL7	C2B-C3B-CAB-OBB
11	B	1238	CL7	C4B-C3B-CAB-OBB
11	B	1239	CL7	C2-C3-C5-C6
11	B	1239	CL7	C4-C3-C5-C6
11	B	1239	CL7	C4B-C3B-CAB-OBB
11	F	1301	CL7	C2A-CAA-CBA-CGA
11	F	1301	CL7	C2B-C3B-CAB-OBB
11	F	1301	CL7	C4B-C3B-CAB-OBB
11	J	1302	CL7	CBD-CGD-O2D-CED
11	J	1302	CL7	C2B-C3B-CAB-OBB
11	J	1302	CL7	C4B-C3B-CAB-OBB
11	L	1501	CL7	CBD-CGD-O2D-CED
11	L	1501	CL7	C2B-C3B-CAB-OBB
11	L	1501	CL7	C4B-C3B-CAB-OBB
11	L	1502	CL7	C4-C3-C5-C6
11	L	1503	CL7	C2B-C3B-CAB-OBB
11	L	1503	CL7	C4B-C3B-CAB-OBB
14	A	5001	LHG	C3-O3-P-O4
14	A	5003	LHG	O1-C1-C2-C3
14	A	5003	LHG	C3-O3-P-O4
14	A	5003	LHG	C4-O6-P-O5
14	A	5003	LHG	C8-C7-O7-C5
15	A	1011	G9R	C1A-C2A-CAA-CBA
15	A	1011	G9R	C3A-C2A-CAA-CBA
15	A	1011	G9R	C4B-C3B-CAB-OBB
15	A	1011	G9R	C2-C3-C5-C6
15	A	1011	G9R	C4-C3-C5-C6
16	B	1023	PHO	C1A-C2A-CAA-CBA
16	B	1023	PHO	C3A-C2A-CAA-CBA
16	B	1023	PHO	CBD-CGD-O2D-CED
16	B	1023	PHO	O1D-CGD-O2D-CED
17	A	4007	8CT	C14-C15-C16-C17
17	A	4007	8CT	C14-C15-C16-C39
17	A	4007	8CT	C28-C29-C30-C31
17	A	4007	8CT	C28-C29-C30-C35
17	A	4008	8CT	C14-C15-C16-C17
17	A	4008	8CT	C14-C15-C16-C39
17	A	4011	8CT	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	A	4011	8CT	C10-C11-C12-C40
17	A	4011	8CT	C20-C21-C23-C24
17	A	4011	8CT	C22-C21-C23-C24
17	A	4011	8CT	C23-C24-C25-C26
17	A	4011	8CT	C28-C29-C30-C31
17	A	4011	8CT	C28-C29-C30-C35
17	B	4006	8CT	C14-C15-C16-C17
17	B	4006	8CT	C14-C15-C16-C39
17	B	4006	8CT	C25-C26-C28-C29
17	B	4006	8CT	C27-C26-C28-C29
17	B	4014	8CT	C25-C26-C28-C29
17	B	4014	8CT	C27-C26-C28-C29
17	B	4017	8CT	C14-C15-C16-C17
17	B	4017	8CT	C14-C15-C16-C39
17	B	4017	8CT	C25-C26-C28-C29
17	B	4017	8CT	C27-C26-C28-C29
17	J	4013	8CT	C14-C15-C16-C17
17	J	4013	8CT	C14-C15-C16-C39
17	J	4013	8CT	C23-C24-C25-C26
17	J	4013	8CT	C25-C26-C28-C29
17	J	4013	8CT	C27-C26-C28-C29
17	J	4015	8CT	C25-C26-C28-C29
17	J	4015	8CT	C27-C26-C28-C29
17	L	4020	8CT	C16-C17-C18-C19
17	L	4020	8CT	C23-C24-C25-C26
17	L	4019	8CT	C25-C26-C28-C29
17	L	4019	8CT	C27-C26-C28-C29
17	M	4021	8CT	C22-C21-C23-C24
17	W	4018	8CT	C28-C29-C30-C35
17	W	4020	8CT	C10-C11-C12-C13
17	W	4020	8CT	C10-C11-C12-C40
17	W	4020	8CT	C20-C21-C23-C24
17	W	4020	8CT	C22-C21-C23-C24
17	W	4020	8CT	C25-C26-C28-C29
17	W	4020	8CT	C27-C26-C28-C29
18	B	5002	LMG	O6-C1-O1-C7
11	A	1126	CL7	O1D-CGD-O2D-CED
11	A	1138	CL7	O1D-CGD-O2D-CED
11	B	1213	CL7	O1D-CGD-O2D-CED
11	B	1226	CL7	O1D-CGD-O2D-CED
11	B	1230	CL7	O1D-CGD-O2D-CED
11	A	1109	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	A	1113	CL7	O1D-CGD-O2D-CED
11	A	1129	CL7	O1D-CGD-O2D-CED
11	B	1203	CL7	O1D-CGD-O2D-CED
11	L	1501	CL7	O1D-CGD-O2D-CED
11	A	1106	CL7	CBD-CGD-O2D-CED
11	A	1110	CL7	CBD-CGD-O2D-CED
11	A	1114	CL7	CBD-CGD-O2D-CED
11	A	1124	CL7	CBD-CGD-O2D-CED
11	A	1127	CL7	CBD-CGD-O2D-CED
11	A	1131	CL7	CBD-CGD-O2D-CED
11	B	1021	CL7	CBD-CGD-O2D-CED
11	B	1202	CL7	CBD-CGD-O2D-CED
11	B	1208	CL7	CBD-CGD-O2D-CED
11	B	1210	CL7	CBD-CGD-O2D-CED
11	B	1230	CL7	CBD-CGD-O2D-CED
11	W	2601	CL7	CBD-CGD-O2D-CED
16	A	1013	PHO	CBD-CGD-O2D-CED
11	A	1128	CL7	O1A-CGA-O2A-C1
11	B	1203	CL7	O1A-CGA-O2A-C1
11	A	1111	CL7	O1D-CGD-O2D-CED
11	A	1131	CL7	O1D-CGD-O2D-CED
11	B	1021	CL7	O1D-CGD-O2D-CED
11	B	1202	CL7	O1D-CGD-O2D-CED
11	B	1210	CL7	O1D-CGD-O2D-CED
11	B	1212	CL7	O1D-CGD-O2D-CED
11	W	2601	CL7	O1D-CGD-O2D-CED
11	B	1226	CL7	C8-C10-C11-C12
11	A	1124	CL7	O1D-CGD-O2D-CED
11	A	1139	CL7	O1D-CGD-O2D-CED
11	B	1206	CL7	O1D-CGD-O2D-CED
11	B	1211	CL7	O1D-CGD-O2D-CED
11	B	1224	CL7	O1D-CGD-O2D-CED
11	J	1302	CL7	O1D-CGD-O2D-CED
11	A	1128	CL7	CBA-CGA-O2A-C1
11	A	1115	CL7	CBD-CGD-O2D-CED
11	A	1117	CL7	CBD-CGD-O2D-CED
11	A	1119	CL7	CBD-CGD-O2D-CED
11	A	1137	CL7	CBD-CGD-O2D-CED
11	A	1140	CL7	CBD-CGD-O2D-CED
11	B	1012	CL7	CBD-CGD-O2D-CED
11	L	1502	CL7	CBD-CGD-O2D-CED
11	L	1503	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	B	1226	CL7	O1A-CGA-O2A-C1
11	L	1501	CL7	O1A-CGA-O2A-C1
11	B	1228	CL7	O1D-CGD-O2D-CED
11	B	1229	CL7	O1D-CGD-O2D-CED
11	A	1105	CL7	O1D-CGD-O2D-CED
11	A	1801	CL7	CBD-CGD-O2D-CED
11	B	1205	CL7	CBD-CGD-O2D-CED
11	A	1106	CL7	O1D-CGD-O2D-CED
14	A	5003	LHG	O9-C7-O7-C5
11	A	1022	CL7	C3-C5-C6-C7
11	A	1104	CL7	C3-C5-C6-C7
11	A	1126	CL7	C3-C5-C6-C7
11	A	1132	CL7	C3-C5-C6-C7
11	A	1237	CL7	C3-C5-C6-C7
11	B	1012	CL7	C3-C5-C6-C7
11	B	1226	CL7	C3-C5-C6-C7
11	B	1239	CL7	C3-C5-C6-C7
12	A	2001	PQN	C13-C15-C16-C17
12	B	2002	PQN	C13-C15-C16-C17
11	A	1101	CL7	CBA-CGA-O2A-C1
11	A	1132	CL7	CBA-CGA-O2A-C1
11	B	1226	CL7	CBA-CGA-O2A-C1
11	A	1118	CL7	CBD-CGD-O2D-CED
11	A	1103	CL7	C2-C3-C5-C6
11	B	1012	CL7	C2-C3-C5-C6
11	L	1502	CL7	C2-C3-C5-C6
11	A	1112	CL7	C2A-CAA-CBA-CGA
11	A	1114	CL7	C2A-CAA-CBA-CGA
11	B	1225	CL7	C2A-CAA-CBA-CGA
11	B	1230	CL7	C2A-CAA-CBA-CGA
11	A	1103	CL7	O1A-CGA-O2A-C1
11	B	1225	CL7	C3-C5-C6-C7
11	A	1125	CL7	CBA-CGA-O2A-C1
11	B	1021	CL7	CBA-CGA-O2A-C1
11	L	1501	CL7	CBA-CGA-O2A-C1
11	A	1114	CL7	O1D-CGD-O2D-CED
11	A	1127	CL7	O1D-CGD-O2D-CED
16	A	1013	PHO	O1D-CGD-O2D-CED
11	A	1101	CL7	O1A-CGA-O2A-C1
11	A	1106	CL7	O1A-CGA-O2A-C1
11	A	1125	CL7	O1A-CGA-O2A-C1
17	J	4013	8CT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
17	M	4021	8CT	C16-C17-C18-C19
17	W	4020	8CT	C18-C19-C20-C21
11	A	1022	CL7	CBD-CGD-O2D-CED
11	A	1130	CL7	CBD-CGD-O2D-CED
11	A	1135	CL7	CBD-CGD-O2D-CED
11	B	1201	CL7	CBD-CGD-O2D-CED
11	B	1236	CL7	CBD-CGD-O2D-CED
11	A	1103	CL7	CBA-CGA-O2A-C1
11	A	1106	CL7	CBA-CGA-O2A-C1
14	A	5001	LHG	C24-C23-O8-C6
11	A	1132	CL7	O1A-CGA-O2A-C1
14	A	5003	LHG	C10-C11-C12-C13
11	A	1110	CL7	O1D-CGD-O2D-CED
14	A	5001	LHG	C13-C14-C15-C16
11	B	1214	CL7	CBD-CGD-O2D-CED
11	L	1502	CL7	C3-C5-C6-C7
11	B	1021	CL7	O1A-CGA-O2A-C1
11	A	1237	CL7	C4-C3-C5-C6
11	A	1237	CL7	C2-C3-C5-C6
11	A	1105	CL7	C2A-CAA-CBA-CGA
11	B	1212	CL7	C2A-CAA-CBA-CGA
11	B	1208	CL7	O1D-CGD-O2D-CED
14	A	5001	LHG	O10-C23-O8-C6
16	B	1023	PHO	CBA-CGA-O2A-C1
11	A	1119	CL7	O1D-CGD-O2D-CED
11	A	1137	CL7	O1D-CGD-O2D-CED
11	B	1225	CL7	CBA-CGA-O2A-C1
11	B	1204	CL7	CBD-CGD-O2D-CED
18	B	5002	LMG	C4-C5-C6-O5
17	B	4014	8CT	C12-C13-C14-C15
11	A	1022	CL7	C10-C11-C12-C13
14	A	5003	LHG	O6-C4-C5-O7
11	A	1128	CL7	C13-C15-C16-C17
11	A	1140	CL7	C5-C6-C7-C8
11	B	1238	CL7	C8-C10-C11-C12
16	B	1023	PHO	C3-C5-C6-C7
11	A	1117	CL7	C14-C13-C15-C16
11	A	1123	CL7	C11-C10-C8-C9
11	A	1125	CL7	C11-C10-C8-C9
11	A	1131	CL7	C11-C10-C8-C9
11	A	1136	CL7	C11-C10-C8-C9
11	A	1237	CL7	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
11	B	1203	CL7	C11-C10-C8-C9
11	B	1226	CL7	C6-C7-C8-C9
11	B	1226	CL7	C14-C13-C15-C16
12	A	2001	PQN	C21-C22-C23-C24
15	A	1011	G9R	C11-C10-C8-C9
15	A	1011	G9R	C14-C13-C15-C16
11	A	1140	CL7	O1D-CGD-O2D-CED
11	A	1125	CL7	C10-C11-C12-C13
11	B	1021	CL7	C5-C6-C7-C8
11	B	1238	CL7	C2A-CAA-CBA-CGA
17	A	4011	8CT	C27-C26-C28-C29
17	J	4013	8CT	C10-C11-C12-C40
17	J	4015	8CT	C14-C15-C16-C39
17	L	4020	8CT	C14-C15-C16-C39
17	W	4018	8CT	C10-C11-C12-C40
17	W	4018	8CT	C27-C26-C28-C29
17	W	4020	8CT	C14-C15-C16-C39
17	J	4013	8CT	C10-C11-C12-C13
17	J	4015	8CT	C14-C15-C16-C17
17	L	4020	8CT	C14-C15-C16-C17
17	M	4021	8CT	C20-C21-C23-C24
17	W	4018	8CT	C10-C11-C12-C13
17	W	4018	8CT	C25-C26-C28-C29
17	W	4020	8CT	C14-C15-C16-C17
11	A	1101	CL7	C13-C15-C16-C17
11	B	1238	CL7	C10-C11-C12-C13
11	L	1502	CL7	C13-C15-C16-C17
11	A	1115	CL7	O1D-CGD-O2D-CED
11	A	1117	CL7	O1D-CGD-O2D-CED
11	B	1012	CL7	O1D-CGD-O2D-CED
11	B	1223	CL7	CBD-CGD-O2D-CED
11	A	1128	CL7	C3-C5-C6-C7
11	A	1237	CL7	CBA-CGA-O2A-C1
11	A	1022	CL7	C13-C15-C16-C17
11	A	1117	CL7	C5-C6-C7-C8
11	B	1021	CL7	C10-C11-C12-C13
11	B	1021	CL7	C15-C16-C17-C18
11	A	1123	CL7	C10-C11-C12-C13
11	A	1131	CL7	C13-C15-C16-C17
11	B	1239	CL7	C10-C11-C12-C13
11	B	1239	CL7	C15-C16-C17-C18
11	L	1501	CL7	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	B	5002	LMG	C28-C29-C30-C31
11	A	1126	CL7	C15-C16-C17-C18
12	A	2001	PQN	C18-C20-C21-C22
15	A	1011	G9R	CBA-CGA-O2A-C1
14	A	5003	LHG	C5-C6-O8-C23
11	L	1502	CL7	O1D-CGD-O2D-CED
16	B	1023	PHO	C2-C1-O2A-CGA
11	A	1123	CL7	C13-C15-C16-C17
11	L	1502	CL7	C10-C11-C12-C13
11	B	1222	CL7	CBD-CGD-O2D-CED
11	A	1237	CL7	C10-C11-C12-C13
11	L	1502	CL7	C8-C10-C11-C12
11	A	1101	CL7	C11-C10-C8-C7
11	A	1103	CL7	C11-C12-C13-C15
11	A	1104	CL7	C12-C13-C15-C16
11	A	1126	CL7	C12-C13-C15-C16
11	B	1021	CL7	C12-C13-C15-C16
11	B	1226	CL7	C6-C7-C8-C10
15	A	1011	G9R	C12-C13-C15-C16
17	B	4006	8CT	C12-C13-C14-C15
11	A	1121	CL7	C2A-CAA-CBA-CGA
11	A	1129	CL7	C2A-CAA-CBA-CGA
11	A	1802	CL7	C2A-CAA-CBA-CGA
11	B	1211	CL7	C2A-CAA-CBA-CGA
11	J	1302	CL7	C2A-CAA-CBA-CGA
11	A	1801	CL7	O1D-CGD-O2D-CED
11	B	1205	CL7	O1D-CGD-O2D-CED
11	L	1503	CL7	O1D-CGD-O2D-CED
11	A	1101	CL7	C8-C10-C11-C12
12	B	2002	PQN	C20-C21-C22-C23
15	A	1011	G9R	C13-C15-C16-C17
16	B	1023	PHO	C5-C6-C7-C8
14	A	5003	LHG	C15-C16-C17-C18
14	A	5001	LHG	C9-C10-C11-C12
11	A	1122	CL7	CBD-CGD-O2D-CED
11	A	1126	CL7	C10-C11-C12-C13
11	A	1237	CL7	O1A-CGA-O2A-C1
11	B	1225	CL7	O1A-CGA-O2A-C1
16	B	1023	PHO	O1A-CGA-O2A-C1
11	A	1103	CL7	C8-C10-C11-C12
11	A	1104	CL7	C8-C10-C11-C12
11	A	1104	CL7	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	A	1132	CL7	C5-C6-C7-C8
11	B	1012	CL7	C13-C15-C16-C17
15	A	1011	G9R	C10-C11-C12-C13
11	A	1118	CL7	O1D-CGD-O2D-CED
11	B	1226	CL7	C10-C11-C12-C13
11	L	1502	CL7	C5-C6-C7-C8
16	A	1013	PHO	C8-C10-C11-C12
14	A	5001	LHG	C3-O3-P-O6
14	A	5003	LHG	C3-O3-P-O6
14	A	5003	LHG	C4-O6-P-O3
11	A	1117	CL7	C3-C5-C6-C7
14	A	5003	LHG	C24-C23-O8-C6
11	A	1123	CL7	C8-C10-C11-C12
11	A	1131	CL7	C10-C11-C12-C13
11	A	1132	CL7	C13-C15-C16-C17
12	B	2002	PQN	C23-C25-C26-C27
11	A	1104	CL7	C15-C16-C17-C18
11	A	1119	CL7	C2A-CAA-CBA-CGA
14	A	5001	LHG	C15-C16-C17-C18
14	A	5001	LHG	C24-C25-C26-C27
11	B	1238	CL7	C16-C17-C18-C19
14	A	5001	LHG	C28-C29-C30-C31
14	A	5001	LHG	O6-C4-C5-O7
14	A	5003	LHG	C17-C18-C19-C20
14	A	5003	LHG	C7-C8-C9-C10
11	A	1022	CL7	O1D-CGD-O2D-CED
14	A	5003	LHG	C28-C29-C30-C31
15	A	1011	G9R	O1A-CGA-O2A-C1
11	B	1236	CL7	O1D-CGD-O2D-CED
18	B	5002	LMG	O6-C5-C6-O5
11	B	1021	CL7	C11-C10-C8-C9
11	L	1502	CL7	C11-C10-C8-C9
14	A	5003	LHG	C24-C25-C26-C27
11	L	1502	CL7	C2A-CAA-CBA-CGA
14	A	5003	LHG	O10-C23-O8-C6
17	A	4011	8CT	C14-C15-C16-C39
17	B	4006	8CT	C10-C11-C12-C40
17	J	4015	8CT	C10-C11-C12-C40
17	L	4020	8CT	C27-C26-C28-C29
17	M	4021	8CT	C27-C26-C28-C29
17	W	4018	8CT	C14-C15-C16-C39
18	B	5002	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
14	A	5001	LHG	O1-C1-C2-C3
17	A	4011	8CT	C14-C15-C16-C17
17	B	4006	8CT	C10-C11-C12-C13
17	J	4015	8CT	C10-C11-C12-C13
17	L	4020	8CT	C25-C26-C28-C29
17	M	4021	8CT	C25-C26-C28-C29
17	W	4018	8CT	C14-C15-C16-C17
11	A	1104	CL7	C16-C17-C18-C19
11	B	1012	CL7	C10-C11-C12-C13
11	L	1501	CL7	C15-C16-C17-C18
14	A	5001	LHG	C25-C26-C27-C28
18	B	5002	LMG	C30-C31-C32-C33
11	B	1201	CL7	O1D-CGD-O2D-CED
11	B	1203	CL7	C8-C10-C11-C12
16	B	1023	PHO	C13-C15-C16-C17
14	A	5003	LHG	C13-C14-C15-C16
11	A	1140	CL7	CBA-CGA-O2A-C1
11	A	1102	CL7	C3A-C2A-CAA-CBA
11	A	1135	CL7	C3A-C2A-CAA-CBA
11	B	1012	CL7	C3A-C2A-CAA-CBA
11	B	1202	CL7	C3A-C2A-CAA-CBA
11	B	1203	CL7	C3A-C2A-CAA-CBA
11	B	1207	CL7	C3A-C2A-CAA-CBA
11	B	1224	CL7	C3A-C2A-CAA-CBA
16	A	1013	PHO	C3A-C2A-CAA-CBA
11	A	1123	CL7	C15-C16-C17-C18
11	A	1131	CL7	C15-C16-C17-C18
16	A	1013	PHO	C15-C16-C17-C18
14	A	5003	LHG	C30-C31-C32-C33
18	B	5002	LMG	C19-C20-C21-C22
11	A	1130	CL7	O1D-CGD-O2D-CED
14	A	5001	LHG	C12-C13-C14-C15
14	A	5003	LHG	C26-C27-C28-C29
16	A	1013	PHO	C3-C5-C6-C7
14	A	5001	LHG	O1-C1-C2-O2
14	A	5003	LHG	O1-C1-C2-O2
11	B	1012	CL7	C5-C6-C7-C8
11	A	1123	CL7	C3-C5-C6-C7
11	A	1136	CL7	C3-C5-C6-C7
14	A	5001	LHG	C10-C11-C12-C13
11	A	1101	CL7	C3-C5-C6-C7
17	A	4007	8CT	C04-C03-C10-C11

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Mol	Chain	Res	Type	Atoms
17	B	4017	8CT	C02-C03-C10-C11
17	J	4013	8CT	C02-C03-C10-C11
17	L	4020	8CT	C04-C03-C10-C11
17	M	4021	8CT	C02-C03-C10-C11
17	W	4020	8CT	C02-C03-C10-C11
11	A	1140	CL7	C13-C15-C16-C17
11	B	1239	CL7	C5-C6-C7-C8
12	B	2002	PQN	C18-C20-C21-C22
18	B	5002	LMG	C11-C10-O7-C8
11	A	1135	CL7	O1D-CGD-O2D-CED
11	B	1238	CL7	C13-C15-C16-C17
11	A	1106	CL7	C11-C10-C8-C7
11	A	1131	CL7	C6-C7-C8-C10
11	A	1136	CL7	C6-C7-C8-C10
11	A	1140	CL7	C6-C7-C8-C10
11	A	1237	CL7	C11-C12-C13-C15
11	B	1021	CL7	C11-C10-C8-C7
11	B	1226	CL7	C12-C13-C15-C16
15	A	1011	G9R	C11-C10-C8-C7
16	A	1013	PHO	C11-C10-C8-C7
11	A	1140	CL7	O1A-CGA-O2A-C1
11	A	1136	CL7	C5-C6-C7-C8
17	A	4011	8CT	C12-C13-C14-C15
11	A	1101	CL7	C16-C17-C18-C20
11	B	1238	CL7	C16-C17-C18-C20
11	A	1122	CL7	C2A-CAA-CBA-CGA
11	A	1237	CL7	C2A-CAA-CBA-CGA
15	A	1011	G9R	C8-C10-C11-C12
18	B	5002	LMG	C34-C35-C36-C37
11	B	1203	CL7	C3-C5-C6-C7
14	A	5003	LHG	C25-C26-C27-C28
11	A	1136	CL7	CBA-CGA-O2A-C1
18	B	5002	LMG	O9-C10-O7-C8
11	A	1117	CL7	C15-C16-C17-C18
16	A	1013	PHO	C16-C17-C18-C20
11	A	1022	CL7	C11-C10-C8-C9
11	A	1131	CL7	C6-C7-C8-C9
11	A	1140	CL7	C6-C7-C8-C9
11	A	1237	CL7	C11-C10-C8-C9
11	B	1021	CL7	C14-C13-C15-C16
11	B	1239	CL7	C14-C13-C15-C16
16	B	1023	PHO	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
11	A	1802	CL7	CBD-CGD-O2D-CED
11	A	1106	CL7	C1A-C2A-CAA-CBA
11	A	1109	CL7	C1A-C2A-CAA-CBA
11	A	1110	CL7	C1A-C2A-CAA-CBA
11	A	1112	CL7	C1A-C2A-CAA-CBA
11	A	1114	CL7	C1A-C2A-CAA-CBA
11	A	1115	CL7	C1A-C2A-CAA-CBA
11	A	1116	CL7	C1A-C2A-CAA-CBA
11	A	1120	CL7	C1A-C2A-CAA-CBA
11	A	1121	CL7	C1A-C2A-CAA-CBA
11	A	1122	CL7	C1A-C2A-CAA-CBA
11	A	1135	CL7	C1A-C2A-CAA-CBA
11	A	1138	CL7	C1A-C2A-CAA-CBA
11	B	1202	CL7	C1A-C2A-CAA-CBA
11	B	1207	CL7	C1A-C2A-CAA-CBA
11	B	1211	CL7	C1A-C2A-CAA-CBA
11	B	1214	CL7	C1A-C2A-CAA-CBA
11	B	1222	CL7	C1A-C2A-CAA-CBA
11	B	1229	CL7	C1A-C2A-CAA-CBA
11	B	1230	CL7	C1A-C2A-CAA-CBA
11	F	1301	CL7	C1A-C2A-CAA-CBA
11	A	1104	CL7	C16-C17-C18-C20
14	A	5001	LHG	C11-C12-C13-C14
17	W	4018	8CT	C12-C13-C14-C15
17	W	4020	8CT	C16-C17-C18-C19
11	B	1214	CL7	O1D-CGD-O2D-CED
14	A	5001	LHG	O6-C4-C5-C6
14	A	5003	LHG	O6-C4-C5-C6
11	B	1225	CL7	C10-C11-C12-C13
11	A	1101	CL7	C16-C17-C18-C19
11	B	1226	CL7	C5-C6-C7-C8
15	A	1011	G9R	C2A-CAA-CBA-CGA
11	A	1104	CL7	C10-C11-C12-C13
11	A	1101	CL7	C2B-C3B-CAB-OBB
11	A	1103	CL7	C2B-C3B-CAB-OBB
11	A	1115	CL7	C2B-C3B-CAB-OBB
11	A	1131	CL7	C2B-C3B-CAB-OBB
11	A	1237	CL7	C2B-C3B-CAB-OBB
11	A	1801	CL7	C2B-C3B-CAB-OBB
11	B	1021	CL7	C2B-C3B-CAB-OBB
11	B	1204	CL7	C2B-C3B-CAB-OBB
11	B	1214	CL7	C2B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
11	B	1223	CL7	C2B-C3B-CAB-OBB
11	B	1239	CL7	C2B-C3B-CAB-OBB
15	A	1011	G9R	C2B-C3B-CAB-OBB
11	A	1126	CL7	C4-C3-C5-C6
11	B	1204	CL7	O1D-CGD-O2D-CED
11	A	1136	CL7	C16-C17-C18-C19
16	A	1013	PHO	C16-C17-C18-C19
11	A	1131	CL7	C4B-C3B-CAB-OBB
11	B	1021	CL7	C4B-C3B-CAB-OBB
11	B	1201	CL7	C4B-C3B-CAB-OBB
11	A	1138	CL7	C2A-CAA-CBA-CGA
11	B	1226	CL7	C15-C16-C17-C18
16	A	1013	PHO	C2-C1-O2A-CGA
11	B	1223	CL7	O1D-CGD-O2D-CED
11	B	1222	CL7	O1D-CGD-O2D-CED
11	A	1136	CL7	C16-C17-C18-C20
11	A	1022	CL7	C5-C6-C7-C8
11	A	1117	CL7	C8-C10-C11-C12
11	A	1136	CL7	C8-C10-C11-C12
11	A	1136	CL7	O1A-CGA-O2A-C1
14	A	5001	LHG	C17-C18-C19-C20
18	B	5002	LMG	O1-C7-C8-O7
11	A	1022	CL7	C11-C12-C13-C15
11	A	1117	CL7	C12-C13-C15-C16
11	A	1126	CL7	C2-C3-C5-C6
11	A	1132	CL7	C6-C7-C8-C10
11	A	1237	CL7	C11-C10-C8-C7
11	B	1203	CL7	C11-C10-C8-C7
11	B	1203	CL7	C11-C12-C13-C15
11	B	1238	CL7	C12-C13-C15-C16
11	B	1239	CL7	C12-C13-C15-C16
12	A	2001	PQN	C21-C22-C23-C25
12	B	2002	PQN	C22-C23-C25-C26
16	B	1023	PHO	C11-C10-C8-C7
11	A	1022	CL7	C11-C12-C13-C14
11	A	1132	CL7	C11-C10-C8-C9
11	A	1136	CL7	C6-C7-C8-C9
11	A	1237	CL7	C14-C13-C15-C16
12	B	2002	PQN	C16-C17-C18-C19
12	B	2002	PQN	C21-C22-C23-C24
12	B	2002	PQN	C24-C23-C25-C26
16	A	1013	PHO	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	A	1013	PHO	C14-C13-C15-C16
11	A	1122	CL7	O1D-CGD-O2D-CED
14	A	5001	LHG	C31-C32-C33-C34
11	A	1106	CL7	C8-C10-C11-C12
12	A	2001	PQN	C14-C13-C15-C16
11	A	1103	CL7	C5-C6-C7-C8
11	B	1222	CL7	C3A-C2A-CAA-CBA
14	A	5003	LHG	C4-C5-C6-O8
11	B	1224	CL7	C2A-CAA-CBA-CGA
14	A	5003	LHG	C11-C10-C9-C8
11	B	1225	CL7	C13-C15-C16-C17
11	A	1126	CL7	CAA-CBA-CGA-O2A
18	B	5002	LMG	O7-C8-C9-O8
11	A	1104	CL7	C2-C1-O2A-CGA
12	A	2001	PQN	C24-C23-C25-C26
14	A	5003	LHG	C5-C4-O6-P
16	A	1013	PHO	C1A-C2A-CAA-CBA
11	A	1103	CL7	C2A-CAA-CBA-CGA
11	L	1501	CL7	C3-C5-C6-C7
17	B	4014	8CT	C02-C03-C10-C11
17	A	4011	8CT	C25-C26-C28-C29
11	A	1103	CL7	C15-C16-C17-C18
11	A	1126	CL7	C5-C6-C7-C8
11	L	1501	CL7	C10-C11-C12-C13
15	A	1011	G9R	C3-C5-C6-C7
11	B	1225	CL7	C8-C10-C11-C12
11	A	1131	CL7	C11-C10-C8-C7
11	B	1012	CL7	C12-C13-C15-C16
11	B	1203	CL7	C6-C7-C8-C10
12	B	2002	PQN	C16-C17-C18-C20
12	B	2002	PQN	C21-C22-C23-C25
16	A	1013	PHO	C12-C13-C15-C16
16	B	1023	PHO	C12-C13-C15-C16
17	M	4021	8CT	C18-C19-C20-C21
17	M	4021	8CT	C23-C24-C25-C26
11	B	1234	CL7	C2A-CAA-CBA-CGA
14	A	5001	LHG	C26-C27-C28-C29
11	A	1105	CL7	CAD-CBD-CGD-O2D
11	A	1106	CL7	CAD-CBD-CGD-O2D
11	A	1107	CL7	CAD-CBD-CGD-O2D
11	A	1112	CL7	CAD-CBD-CGD-O2D
11	A	1117	CL7	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	A	1118	CL7	CAD-CBD-CGD-O2D
11	A	1123	CL7	CAD-CBD-CGD-O2D
11	A	1130	CL7	CAD-CBD-CGD-O2D
11	A	1139	CL7	CAD-CBD-CGD-O2D
11	B	1208	CL7	CAD-CBD-CGD-O2D
11	B	1212	CL7	CAD-CBD-CGD-O2D
11	B	1213	CL7	CAD-CBD-CGD-O2D
11	B	1215	CL7	CAD-CBD-CGD-O2D
11	B	1222	CL7	CAD-CBD-CGD-O2D
11	J	1302	CL7	CAD-CBD-CGD-O2D
12	B	2002	PQN	C14-C13-C15-C16
11	B	1203	CL7	C10-C11-C12-C13
18	B	5002	LMG	O1-C7-C8-C9
11	B	1226	CL7	C13-C15-C16-C17
11	A	1106	CL7	C2A-CAA-CBA-CGA
11	A	1101	CL7	CHA-CBD-CGD-O2D
11	A	1101	CL7	CHA-CBD-CGD-O1D
11	A	1103	CL7	CHA-CBD-CGD-O2D
11	A	1103	CL7	CHA-CBD-CGD-O1D
11	A	1110	CL7	CHA-CBD-CGD-O2D
11	A	1110	CL7	CHA-CBD-CGD-O1D
11	A	1135	CL7	CHA-CBD-CGD-O2D
11	A	1135	CL7	CHA-CBD-CGD-O1D
11	A	1137	CL7	CHA-CBD-CGD-O2D
11	A	1137	CL7	CHA-CBD-CGD-O1D
11	B	1203	CL7	CHA-CBD-CGD-O2D
14	A	5003	LHG	O7-C5-C6-O8
11	A	1131	CL7	C16-C17-C18-C20
18	B	5002	LMG	C33-C34-C35-C36
11	B	1012	CL7	C14-C13-C15-C16
11	B	1203	CL7	C6-C7-C8-C9
17	J	4015	8CT	C22-C21-C23-C24
11	A	1117	CL7	C1A-C2A-CAA-CBA
11	B	1012	CL7	C1A-C2A-CAA-CBA
11	B	1203	CL7	C1A-C2A-CAA-CBA
11	B	1225	CL7	C1A-C2A-CAA-CBA
11	A	1237	CL7	C16-C17-C18-C20
11	A	1802	CL7	O1D-CGD-O2D-CED
14	A	5003	LHG	C4-O6-P-O4
11	A	1126	CL7	C2C-C3C-CAC-CBC
11	A	1104	CL7	CBD-CGD-O2D-CED
11	A	1128	CL7	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
11	B	1238	CL7	C3-C5-C6-C7
11	A	1132	CL7	C16-C17-C18-C19
11	A	1123	CL7	C11-C10-C8-C7
11	A	1136	CL7	C11-C10-C8-C7
11	B	1012	CL7	C11-C10-C8-C7
11	B	1226	CL7	C11-C10-C8-C7
11	B	1239	CL7	C11-C10-C8-C7
11	J	1302	CL7	C3A-C2A-CAA-CBA
17	B	4017	8CT	C28-C29-C30-C31
17	W	4018	8CT	C28-C29-C30-C31
11	B	1226	CL7	C2A-CAA-CBA-CGA
11	A	1237	CL7	O2A-C1-C2-C3
11	A	1103	CL7	C11-C12-C13-C14
11	A	1103	CL7	C14-C13-C15-C16
11	A	1104	CL7	C14-C13-C15-C16
11	A	1106	CL7	C11-C10-C8-C9
11	A	1128	CL7	C14-C13-C15-C16
11	B	1203	CL7	C11-C12-C13-C14
17	A	4011	8CT	C13-C14-C15-C16
17	B	4017	8CT	C13-C14-C15-C16
11	A	1117	CL7	C2B-C3B-CAB-OBB
11	B	1206	CL7	C2B-C3B-CAB-OBB
11	A	1101	CL7	C4B-C3B-CAB-OBB
11	A	1127	CL7	C4B-C3B-CAB-OBB
11	A	1237	CL7	C4B-C3B-CAB-OBB
11	B	1204	CL7	C4B-C3B-CAB-OBB
11	B	1208	CL7	C4B-C3B-CAB-OBB
11	A	1111	CL7	C2A-CAA-CBA-CGA
11	B	1207	CL7	C2A-CAA-CBA-CGA
11	A	1125	CL7	C2-C1-O2A-CGA
11	B	1203	CL7	C2-C1-O2A-CGA
15	A	1011	G9R	C5-C6-C7-C8
11	A	1117	CL7	C13-C15-C16-C17
17	A	4008	8CT	C02-C03-C10-C11
17	A	4011	8CT	C02-C03-C10-C11
17	B	4006	8CT	C02-C03-C10-C11
12	B	2002	PQN	C12-C13-C15-C16
18	B	5002	LMG	C29-C30-C31-C32
11	B	1235	CL7	CBD-CGD-O2D-CED
11	L	1501	CL7	C2A-CAA-CBA-CGA
11	A	1104	CL7	O1D-CGD-O2D-CED
11	A	1131	CL7	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	A	1101	CL7	C11-C10-C8-C9
11	A	1126	CL7	C14-C13-C15-C16
11	B	1012	CL7	C11-C10-C8-C9
11	B	1226	CL7	C11-C10-C8-C9
11	B	1239	CL7	C11-C10-C8-C9
16	B	1023	PHO	C14-C13-C15-C16
17	B	4006	8CT	C23-C24-C25-C26
11	B	1203	CL7	C16-C17-C18-C20
11	A	1132	CL7	C15-C16-C17-C18
14	A	5003	LHG	C19-C20-C21-C22
11	A	1132	CL7	C8-C10-C11-C12
11	A	1117	CL7	C2A-CAA-CBA-CGA
17	B	4006	8CT	C16-C17-C18-C19
11	A	1136	CL7	C13-C15-C16-C17
11	A	1106	CL7	C3-C5-C6-C7
11	B	1021	CL7	C3-C5-C6-C7
11	A	1117	CL7	C4-C3-C5-C6
11	A	1117	CL7	C2-C3-C5-C6
11	B	1021	CL7	C13-C15-C16-C17
11	L	1502	CL7	C3A-C2A-CAA-CBA
11	A	1137	CL7	CAA-CBA-CGA-O1A
11	A	1128	CL7	C4-C3-C5-C6
11	B	1225	CL7	C11-C10-C8-C9
11	A	1111	CL7	CAA-CBA-CGA-O1A
11	A	1111	CL7	CAA-CBA-CGA-O2A
17	B	4006	8CT	C24-C25-C26-C27
17	B	4014	8CT	C40-C12-C13-C14
17	B	4017	8CT	C39-C16-C17-C18
17	J	4013	8CT	C24-C25-C26-C27
17	J	4015	8CT	C24-C25-C26-C27
11	A	1126	CL7	C4C-C3C-CAC-CBC
11	B	1206	CL7	CAA-CBA-CGA-O1A
11	A	1104	CL7	O2A-C1-C2-C3
11	B	1021	CL7	O2A-C1-C2-C3
11	A	1115	CL7	CAA-CBA-CGA-O2A
17	M	4021	8CT	C10-C11-C12-C40
11	A	1105	CL7	C1A-C2A-CAA-CBA
11	A	1128	CL7	C1A-C2A-CAA-CBA
11	B	1210	CL7	C1A-C2A-CAA-CBA
11	J	1302	CL7	C1A-C2A-CAA-CBA
11	L	1503	CL7	C1A-C2A-CAA-CBA
11	A	1115	CL7	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
11	A	1137	CL7	CAA-CBA-CGA-O2A
11	B	1203	CL7	C5-C6-C7-C8
11	A	1109	CL7	CAA-CBA-CGA-O1A
11	A	1128	CL7	C2-C3-C5-C6
11	A	1103	CL7	C10-C11-C12-C13
17	B	4006	8CT	C24-C25-C26-C28
17	B	4014	8CT	C11-C12-C13-C14
17	B	4017	8CT	C15-C16-C17-C18
17	J	4013	8CT	C24-C25-C26-C28
17	J	4015	8CT	C24-C25-C26-C28
11	B	1201	CL7	CAA-CBA-CGA-O2A
11	A	1237	CL7	C16-C17-C18-C19
11	A	1106	CL7	C2-C1-O2A-CGA
11	L	1502	CL7	C2-C1-O2A-CGA
11	B	1206	CL7	CAA-CBA-CGA-O2A
11	B	1238	CL7	C11-C12-C13-C14
16	A	1013	PHO	O1A-CGA-O2A-C1
11	A	1120	CL7	CAA-CBA-CGA-O2A
11	B	1215	CL7	C2A-CAA-CBA-CGA
11	A	1109	CL7	CAA-CBA-CGA-O2A
11	B	1229	CL7	CAA-CBA-CGA-O1A
17	J	4015	8CT	C04-C03-C10-C11
18	B	5002	LMG	C7-C8-C9-O8
11	A	1102	CL7	CAA-CBA-CGA-O2A
17	A	4007	8CT	C16-C17-C18-C19
11	B	1235	CL7	O1D-CGD-O2D-CED
11	A	1116	CL7	CAA-CBA-CGA-O2A
11	B	1229	CL7	CAA-CBA-CGA-O2A
16	A	1013	PHO	CBA-CGA-O2A-C1
11	A	1802	CL7	CAA-CBA-CGA-O2A
11	A	1802	CL7	CAA-CBA-CGA-O1A
11	B	1236	CL7	CAA-CBA-CGA-O1A
11	B	1236	CL7	CAA-CBA-CGA-O2A
11	J	1302	CL7	CAA-CBA-CGA-O2A
11	W	2601	CL7	CAA-CBA-CGA-O2A
11	A	1120	CL7	CAA-CBA-CGA-O1A
11	A	1801	CL7	CAA-CBA-CGA-O2A
11	B	1201	CL7	CAA-CBA-CGA-O1A
11	A	1140	CL7	C16-C17-C18-C20
11	B	1238	CL7	C5-C6-C7-C8
11	A	1125	CL7	C11-C10-C8-C7
11	L	1502	CL7	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
11	A	1135	CL7	CAA-CBA-CGA-O1A
11	A	1135	CL7	CAA-CBA-CGA-O2A
11	B	1230	CL7	CAA-CBA-CGA-O2A
11	A	1131	CL7	C16-C17-C18-C19
11	A	1127	CL7	C2B-C3B-CAB-OBB
11	B	1208	CL7	C2B-C3B-CAB-OBB
11	A	1124	CL7	C2A-CAA-CBA-CGA
11	A	1125	CL7	C16-C17-C18-C20
11	A	1139	CL7	CAA-CBA-CGA-O2A
11	B	1223	CL7	CAA-CBA-CGA-O2A
11	B	1205	CL7	C4B-C3B-CAB-OBB
11	B	1229	CL7	C4B-C3B-CAB-OBB
11	B	1210	CL7	C3A-C2A-CAA-CBA
11	L	1503	CL7	C3A-C2A-CAA-CBA
11	A	1121	CL7	CAA-CBA-CGA-O2A
11	A	1801	CL7	CAA-CBA-CGA-O1A
11	A	1113	CL7	CAD-CBD-CGD-O2D
11	A	1124	CL7	CAD-CBD-CGD-O2D
11	A	1127	CL7	CAD-CBD-CGD-O2D
11	A	1128	CL7	CAD-CBD-CGD-O2D
11	A	1129	CL7	CAD-CBD-CGD-O2D
11	A	1131	CL7	CAD-CBD-CGD-O2D
11	A	1132	CL7	CAD-CBD-CGD-O2D
11	A	1801	CL7	CAD-CBD-CGD-O2D
11	B	1201	CL7	CAD-CBD-CGD-O2D
11	B	1210	CL7	CAD-CBD-CGD-O2D
11	B	1211	CL7	CAD-CBD-CGD-O2D
11	B	1214	CL7	CAD-CBD-CGD-O2D
11	B	1226	CL7	CAD-CBD-CGD-O2D
11	B	1228	CL7	CAD-CBD-CGD-O2D
11	F	1301	CL7	CAD-CBD-CGD-O2D
11	L	1502	CL7	CAD-CBD-CGD-O2D
11	L	1503	CL7	CAD-CBD-CGD-O2D
11	A	1125	CL7	C16-C17-C18-C19
14	A	5001	LHG	C19-C20-C21-C22
11	A	1022	CL7	C15-C16-C17-C18
11	A	1105	CL7	CAA-CBA-CGA-O2A
11	J	1302	CL7	CAA-CBA-CGA-O1A
11	A	1106	CL7	C4-C3-C5-C6
11	A	1102	CL7	CAA-CBA-CGA-O1A
11	A	1113	CL7	CAA-CBA-CGA-O2A
11	W	2601	CL7	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	J	4015	8CT	C20-C21-C23-C24
17	M	4021	8CT	C10-C11-C12-C13
11	A	1138	CL7	CAA-CBA-CGA-O2A
11	A	1139	CL7	CAA-CBA-CGA-O1A
11	B	1213	CL7	CAA-CBA-CGA-O2A
11	B	1223	CL7	CAA-CBA-CGA-O1A
11	F	1301	CL7	CAA-CBA-CGA-O2A
16	A	1013	PHO	CAA-CBA-CGA-O2A
11	A	1107	CL7	CAA-CBA-CGA-O1A
11	A	1107	CL7	CAA-CBA-CGA-O2A
11	A	1116	CL7	CAA-CBA-CGA-O1A
11	A	1127	CL7	CAA-CBA-CGA-O1A
11	A	1127	CL7	CAA-CBA-CGA-O2A
11	A	1125	CL7	O2A-C1-C2-C3
11	B	1203	CL7	O2A-C1-C2-C3
11	B	1236	CL7	C2A-CAA-CBA-CGA
11	A	1121	CL7	CAA-CBA-CGA-O1A
11	B	1213	CL7	CAA-CBA-CGA-O1A
11	B	1238	CL7	C15-C16-C17-C18
11	B	1225	CL7	C16-C17-C18-C20
11	A	1102	CL7	CHA-CBD-CGD-O2D
11	A	1102	CL7	CHA-CBD-CGD-O1D
11	B	1223	CL7	CHA-CBD-CGD-O2D
11	B	1223	CL7	CHA-CBD-CGD-O1D
11	B	1234	CL7	CHA-CBD-CGD-O2D
11	B	1234	CL7	CHA-CBD-CGD-O1D
11	L	1501	CL7	CHA-CBD-CGD-O2D
11	L	1501	CL7	CHA-CBD-CGD-O1D
11	A	1112	CL7	CAA-CBA-CGA-O2A
11	F	1301	CL7	CAA-CBA-CGA-O1A
11	A	1131	CL7	C3-C5-C6-C7
11	A	1117	CL7	C16-C17-C18-C20
11	A	1105	CL7	CAA-CBA-CGA-O1A
11	B	1212	CL7	CAA-CBA-CGA-O2A
11	B	1230	CL7	CAA-CBA-CGA-O1A
11	A	1131	CL7	CAA-CBA-CGA-O2A
12	B	2002	PQN	C25-C26-C27-C28
11	A	1126	CL7	CAA-CBA-CGA-O1A
11	B	1021	CL7	CAA-CBA-CGA-O2A
18	B	5002	LMG	O8-C28-C29-C30
11	A	1113	CL7	CAA-CBA-CGA-O1A
11	A	1128	CL7	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
11	B	1225	CL7	C11-C10-C8-C7
11	B	1012	CL7	C8-C10-C11-C12
11	A	1129	CL7	CAA-CBA-CGA-O2A
11	A	1140	CL7	CAA-CBA-CGA-O2A
11	B	1225	CL7	C16-C17-C18-C19
11	B	1208	CL7	CAA-CBA-CGA-O2A
11	A	1128	CL7	C2A-CAA-CBA-CGA
11	B	1235	CL7	C2A-CAA-CBA-CGA
11	A	1117	CL7	C16-C17-C18-C19
12	A	2001	PQN	C12-C13-C15-C16
11	A	1022	CL7	C1A-C2A-CAA-CBA
11	A	1118	CL7	C1A-C2A-CAA-CBA
11	A	1124	CL7	C1A-C2A-CAA-CBA
11	B	1212	CL7	C1A-C2A-CAA-CBA
11	B	1228	CL7	C1A-C2A-CAA-CBA
11	B	1239	CL7	C1A-C2A-CAA-CBA
11	A	1138	CL7	CAA-CBA-CGA-O1A
16	A	1013	PHO	CAA-CBA-CGA-O1A
11	W	2601	CL7	C2A-CAA-CBA-CGA
11	B	1021	CL7	CAA-CBA-CGA-O1A
12	A	2001	PQN	C15-C16-C17-C18
11	B	1228	CL7	CAA-CBA-CGA-O2A
11	A	1112	CL7	CAA-CBA-CGA-O1A
11	B	1204	CL7	CAA-CBA-CGA-O2A
11	A	1237	CL7	C13-C15-C16-C17
11	L	1501	CL7	C13-C15-C16-C17
11	B	1021	CL7	C8-C10-C11-C12
11	B	1212	CL7	CAA-CBA-CGA-O1A
14	A	5003	LHG	O7-C7-C8-C9
11	A	1129	CL7	CAA-CBA-CGA-O1A
11	A	1131	CL7	CAA-CBA-CGA-O1A
11	A	1022	CL7	C6-C7-C8-C9
11	A	1125	CL7	C11-C12-C13-C14
11	B	1238	CL7	C14-C13-C15-C16
18	B	5002	LMG	O10-C28-C29-C30
11	A	1136	CL7	CAA-CBA-CGA-O2A
11	B	1226	CL7	CAA-CBA-CGA-O2A
11	A	1104	CL7	C5-C6-C7-C8
11	B	1239	CL7	CAA-CBA-CGA-O2A
11	L	1501	CL7	CAA-CBA-CGA-O2A
11	B	1208	CL7	CAA-CBA-CGA-O1A
11	B	1203	CL7	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	A	1106	CL7	C12-C13-C15-C16
11	A	1125	CL7	C11-C12-C13-C15
11	B	1203	CL7	C12-C13-C15-C16
11	A	1132	CL7	CAA-CBA-CGA-O1A
11	B	1211	CL7	CAA-CBA-CGA-O2A
11	A	1123	CL7	CAA-CBA-CGA-O2A
11	A	1132	CL7	CAA-CBA-CGA-O2A
17	L	4019	8CT	C10-C11-C12-C13
11	B	1228	CL7	CAA-CBA-CGA-O1A
15	A	1011	G9R	CAA-CBA-CGA-O2A
11	B	1225	CL7	C5-C6-C7-C8
11	A	1119	CL7	CAA-CBA-CGA-O1A
11	B	1239	CL7	C8-C10-C11-C12
11	A	1117	CL7	CAA-CBA-CGA-O2A
11	A	1123	CL7	CAA-CBA-CGA-O1A
11	A	1136	CL7	CAA-CBA-CGA-O1A
11	A	1128	CL7	C8-C10-C11-C12
11	B	1226	CL7	CAA-CBA-CGA-O1A
11	L	1501	CL7	CAA-CBA-CGA-O1A
11	B	1207	CL7	CAA-CBA-CGA-O2A
11	B	1211	CL7	CAA-CBA-CGA-O1A

There are no ring outliers.

82 monomers are involved in 252 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1109	CL7	1	0
11	A	1128	CL7	5	0
11	B	1206	CL7	3	0
15	A	1011	G9R	1	0
16	A	1013	PHO	9	0
17	J	4015	8CT	1	0
11	A	1132	CL7	8	0
11	A	1129	CL7	3	0
11	B	1226	CL7	4	0
13	C	3003	SF4	1	0
11	A	1123	CL7	2	0
11	A	1116	CL7	4	0
11	A	1136	CL7	7	0
11	A	1138	CL7	4	0
11	A	1107	CL7	2	0
11	W	2601	CL7	2	0

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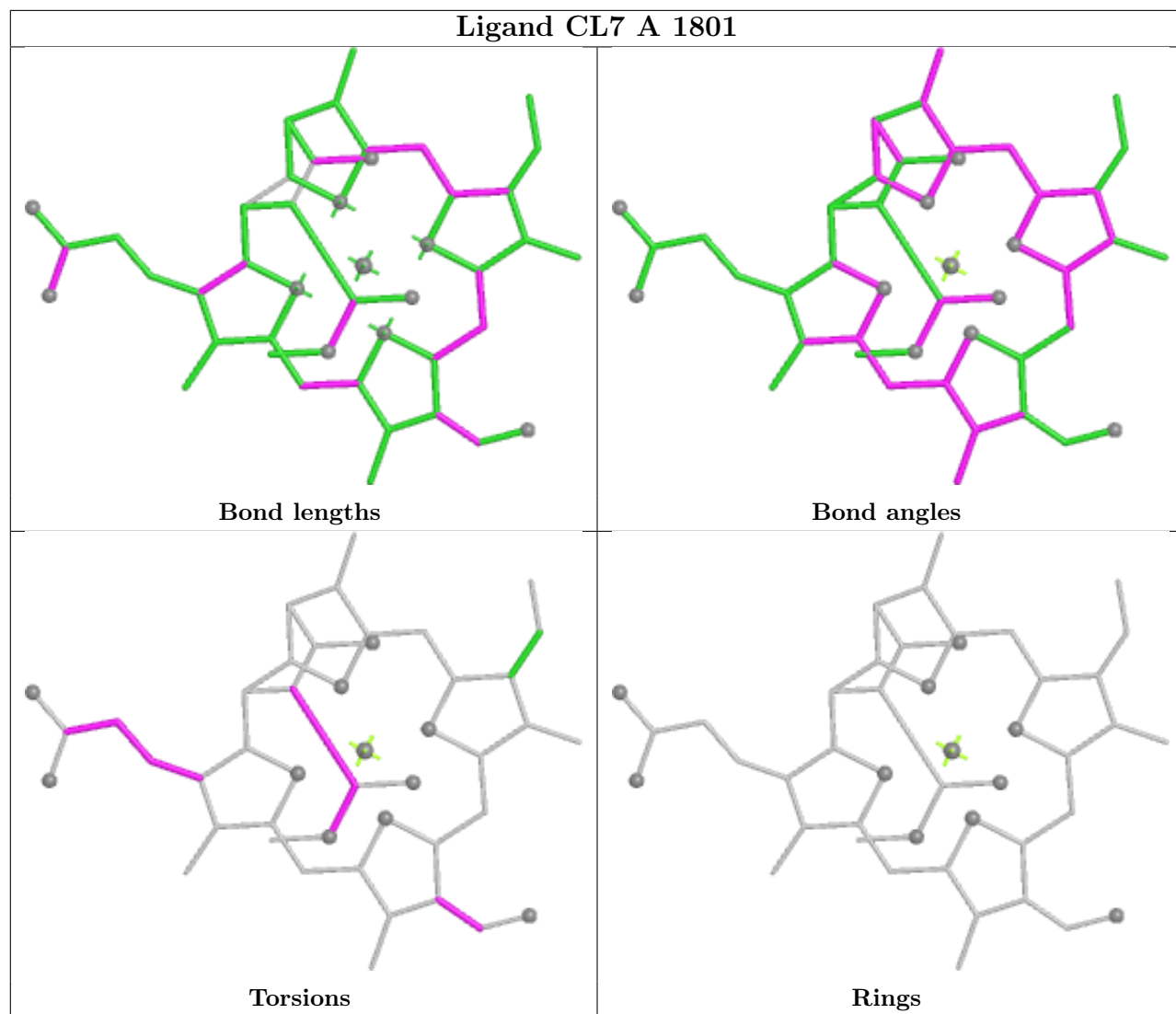
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1110	CL7	2	0
12	A	2001	PQN	4	0
11	A	1111	CL7	7	0
11	A	1106	CL7	4	0
11	A	1105	CL7	2	0
11	J	1302	CL7	1	0
11	B	1236	CL7	2	0
11	B	1228	CL7	2	0
11	F	1301	CL7	4	0
11	B	1239	CL7	2	0
11	A	1140	CL7	5	0
11	L	1502	CL7	3	0
11	A	1131	CL7	5	0
11	A	1119	CL7	2	0
11	A	1121	CL7	2	0
11	A	1139	CL7	1	0
11	A	1102	CL7	6	0
11	A	1103	CL7	3	0
11	B	1229	CL7	3	0
11	B	1202	CL7	1	0
11	L	1501	CL7	3	0
11	B	1201	CL7	1	0
11	A	1101	CL7	3	0
11	B	1207	CL7	2	0
11	B	1238	CL7	4	0
11	B	1021	CL7	6	0
11	B	1222	CL7	1	0
11	A	1104	CL7	6	0
11	B	1208	CL7	3	0
16	B	1023	PHO	7	0
11	B	1211	CL7	1	0
11	A	1127	CL7	2	0
11	A	1135	CL7	4	0
11	A	1118	CL7	4	0
11	B	1223	CL7	2	0
11	B	1212	CL7	2	0
11	B	1203	CL7	5	0
11	B	1215	CL7	3	0
11	B	1213	CL7	4	0
12	B	2002	PQN	1	0
11	B	1204	CL7	4	0
11	B	1205	CL7	4	0

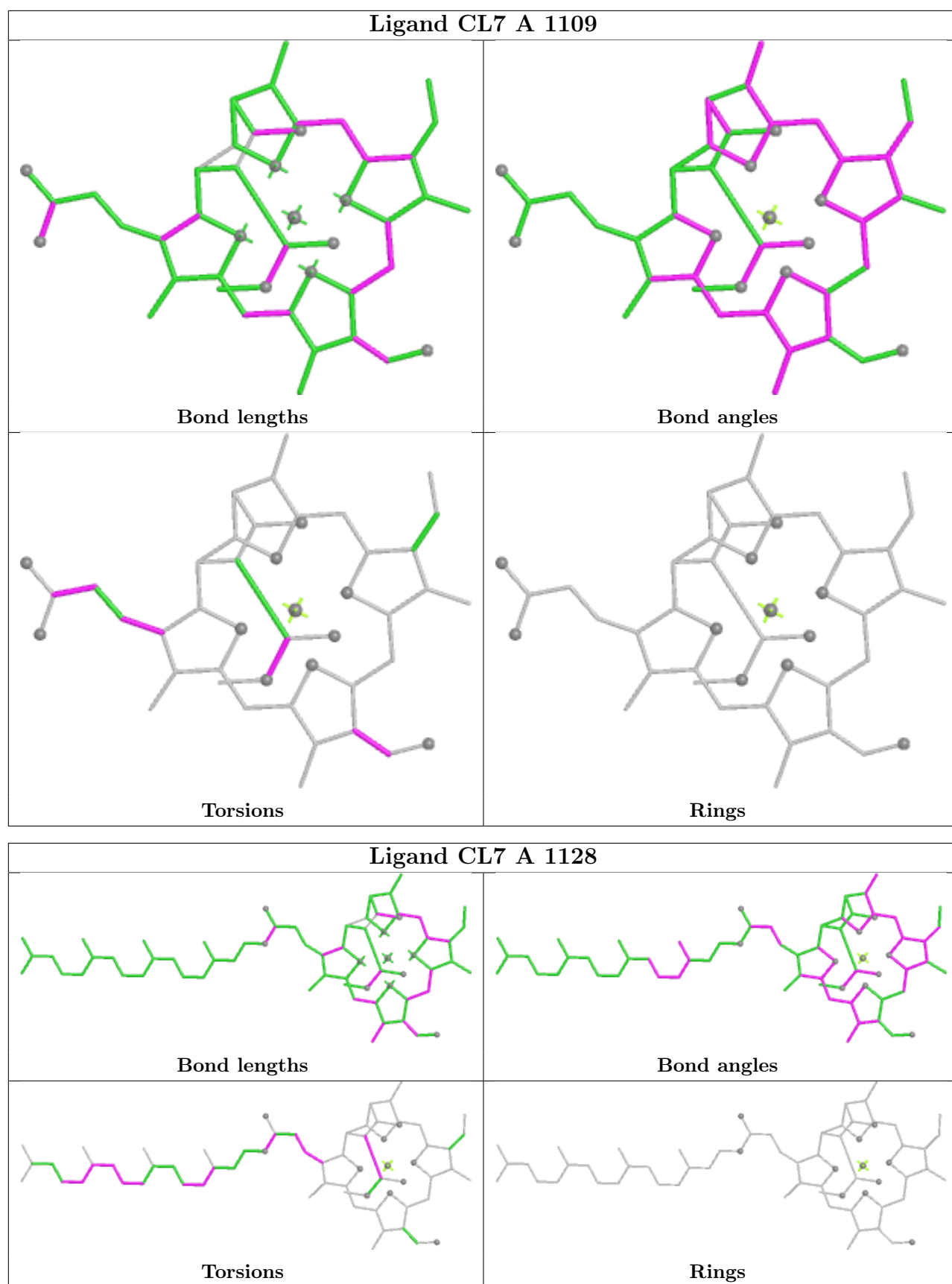
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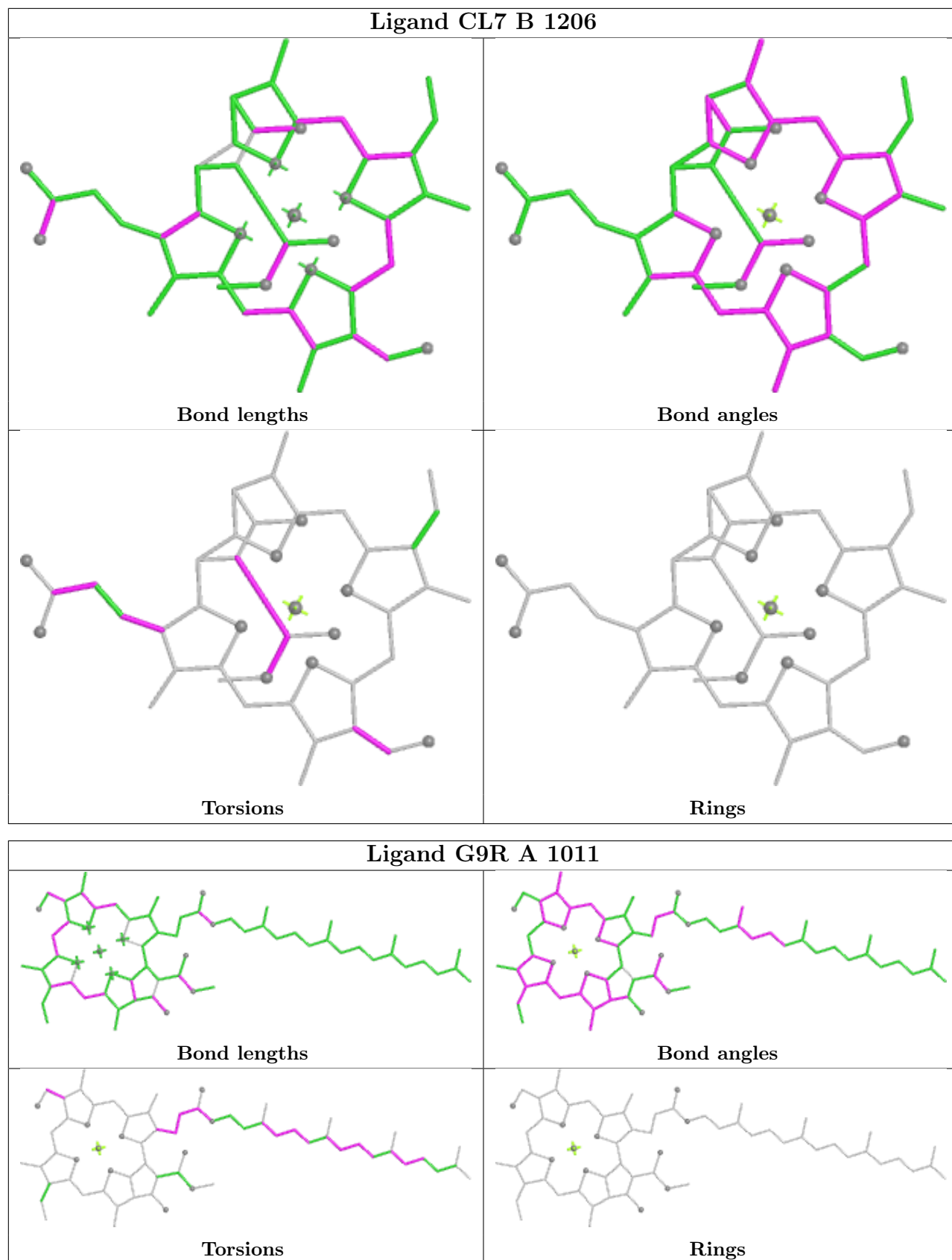
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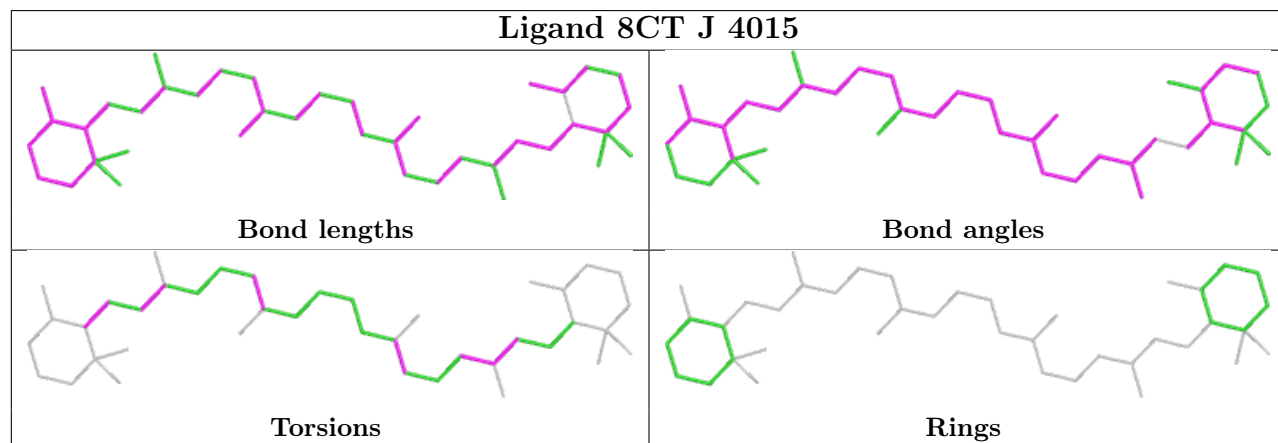
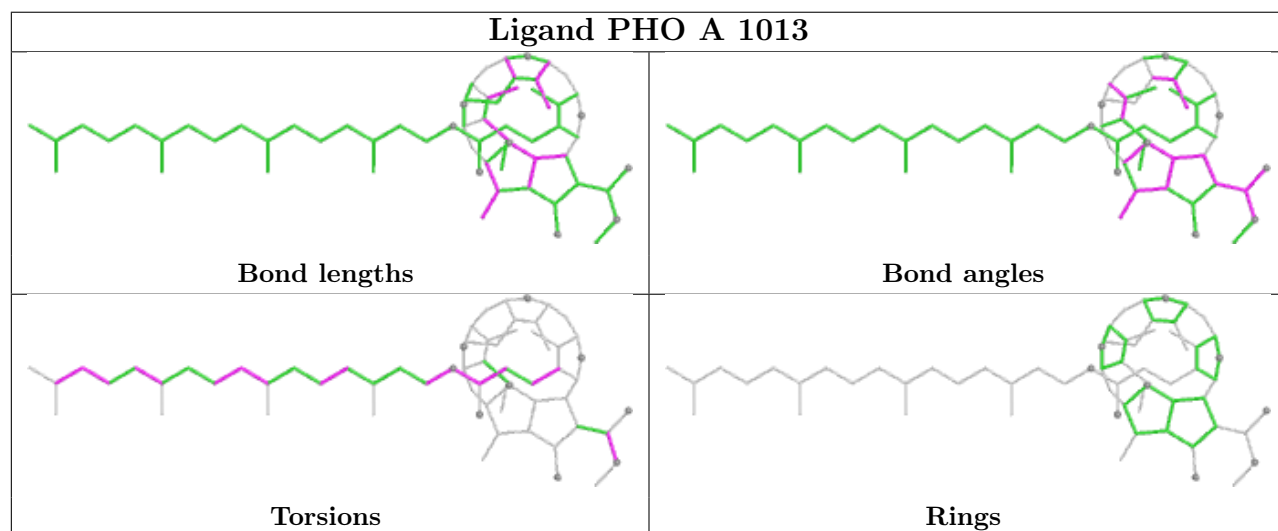
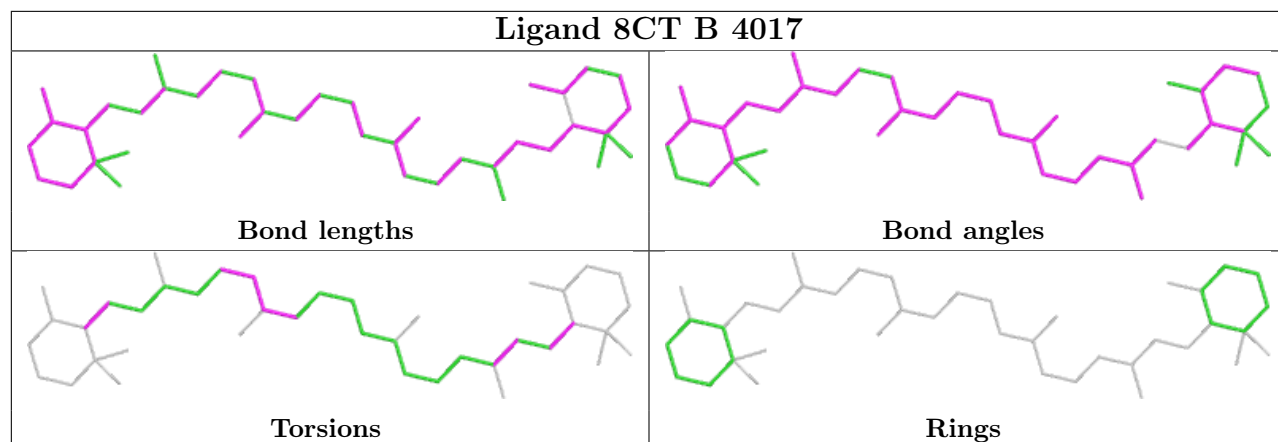
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1113	CL7	3	0
14	A	5001	LHG	1	0
11	A	1115	CL7	4	0
11	A	1237	CL7	2	0
14	A	5003	LHG	2	0
11	A	1130	CL7	2	0
11	A	1117	CL7	4	0
11	B	1225	CL7	3	0
11	B	1230	CL7	4	0
11	A	1114	CL7	6	0
11	B	1214	CL7	5	0
11	B	1224	CL7	3	0
11	A	1022	CL7	8	0
11	A	1122	CL7	2	0
11	B	1012	CL7	7	0
11	A	1137	CL7	3	0
11	B	1235	CL7	3	0
13	A	3001	SF4	1	0
11	A	1802	CL7	1	0
11	B	1234	CL7	2	0
11	A	1126	CL7	9	0
18	B	5002	LMG	3	0
11	A	1125	CL7	2	0
11	A	1112	CL7	2	0

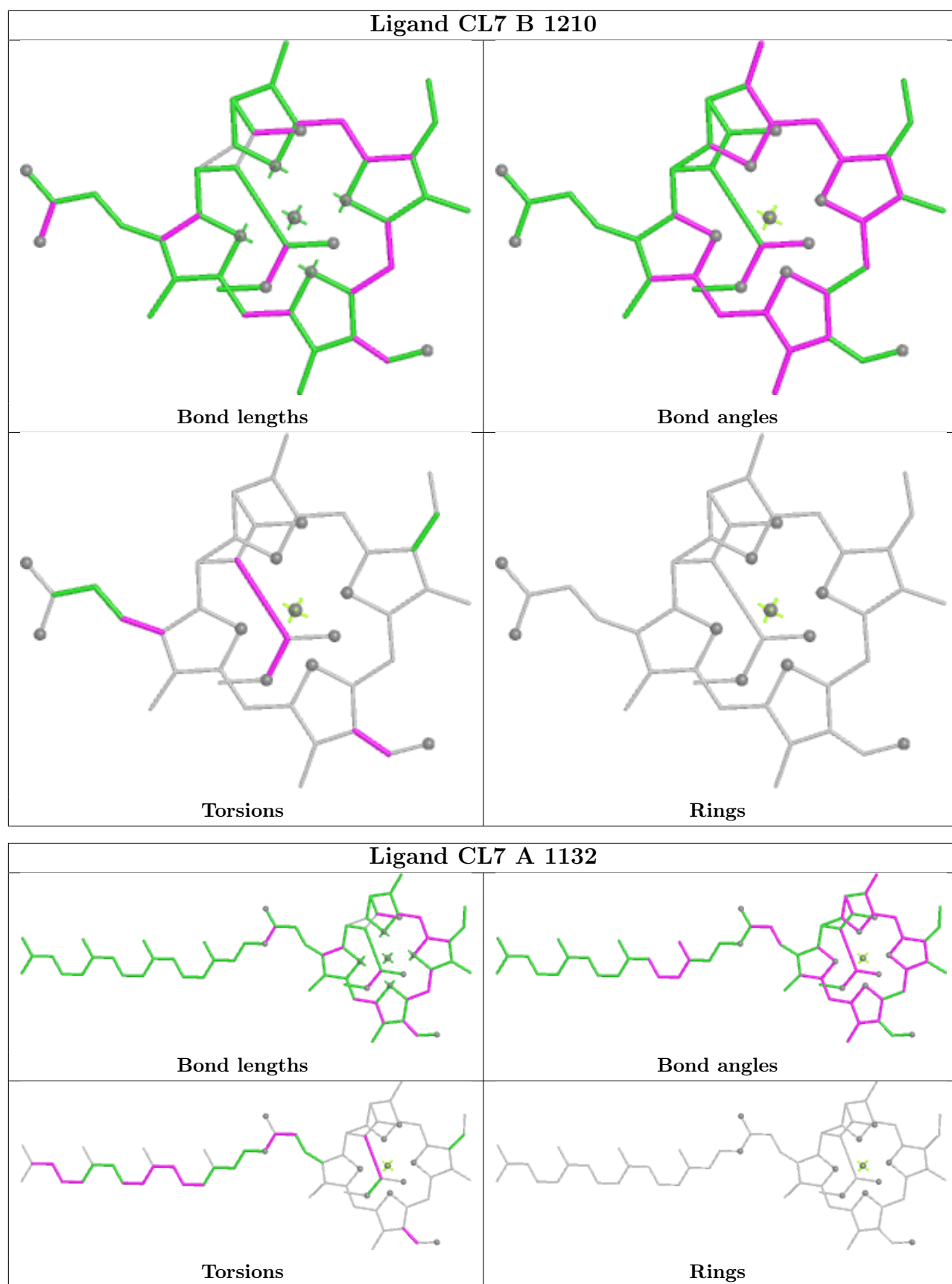
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

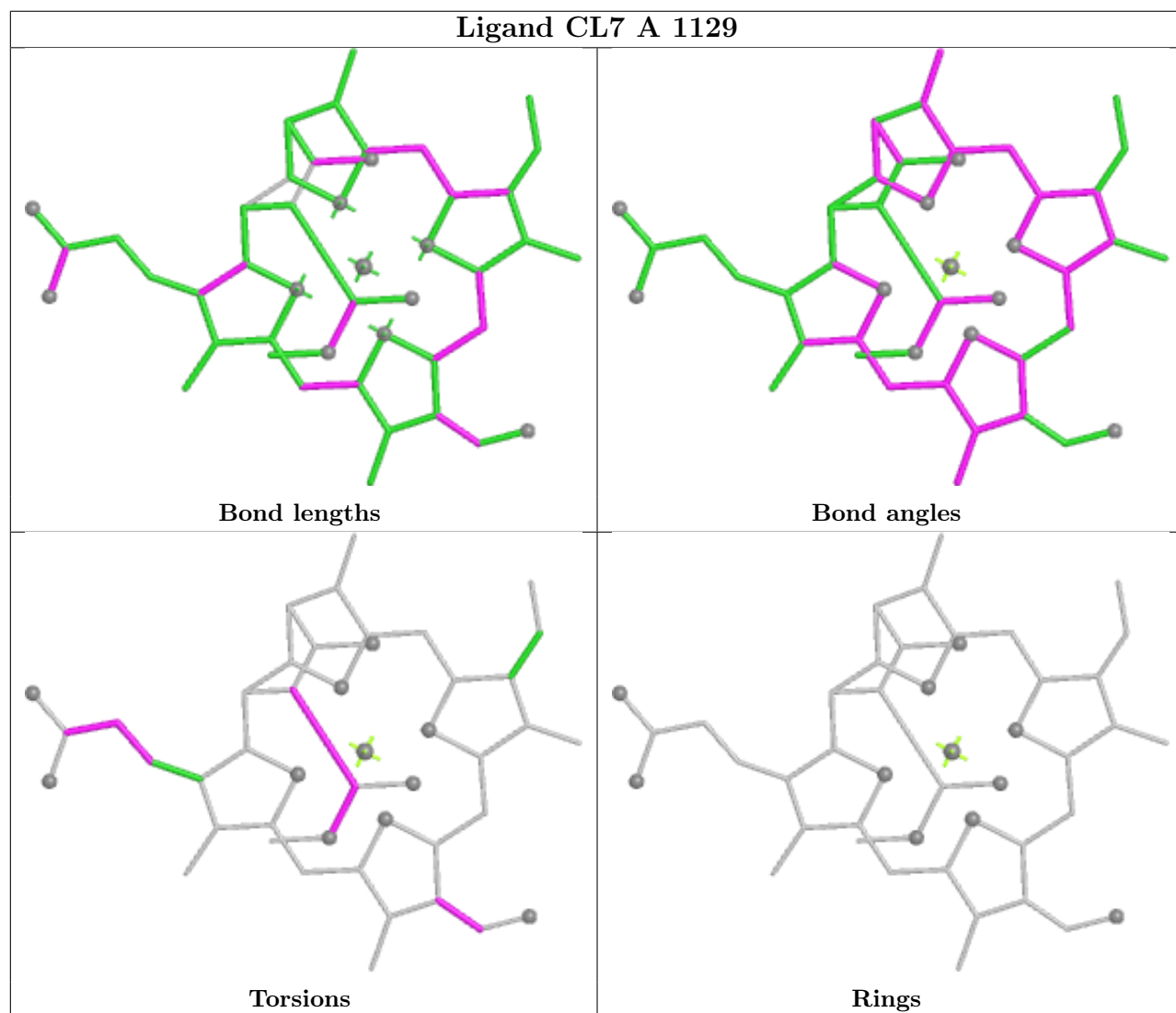
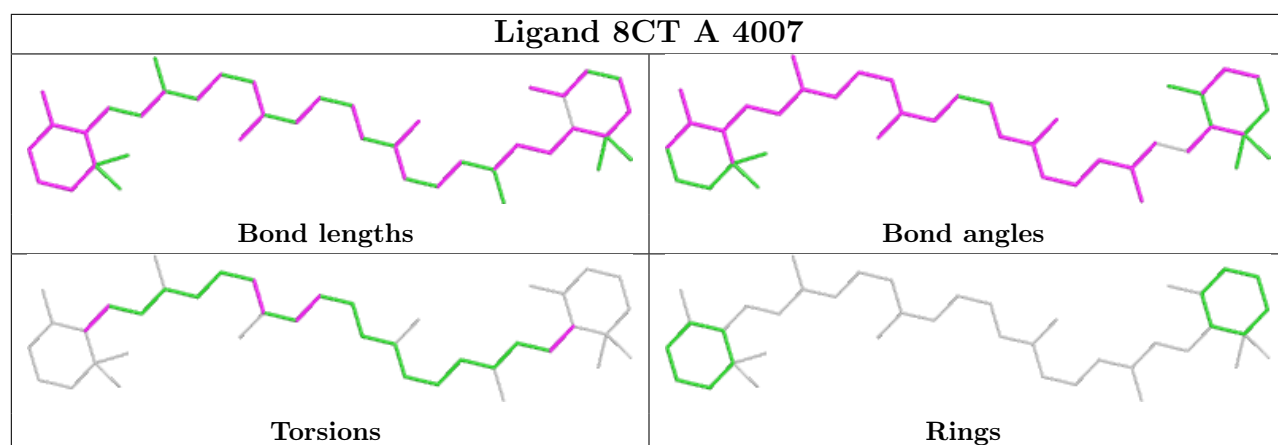


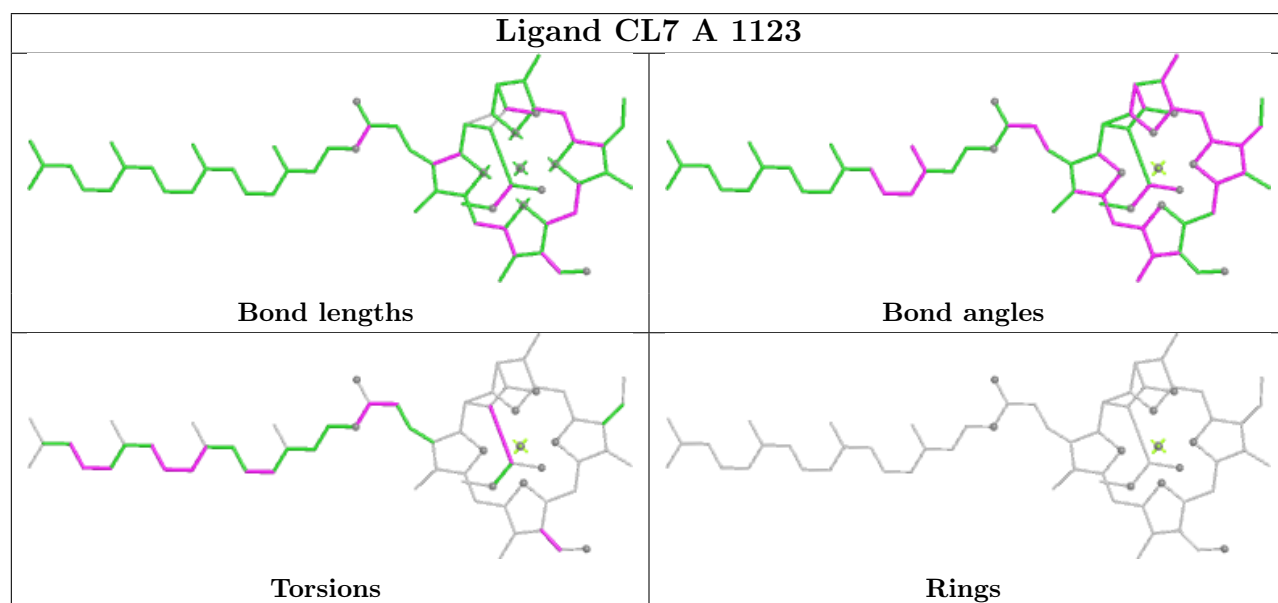
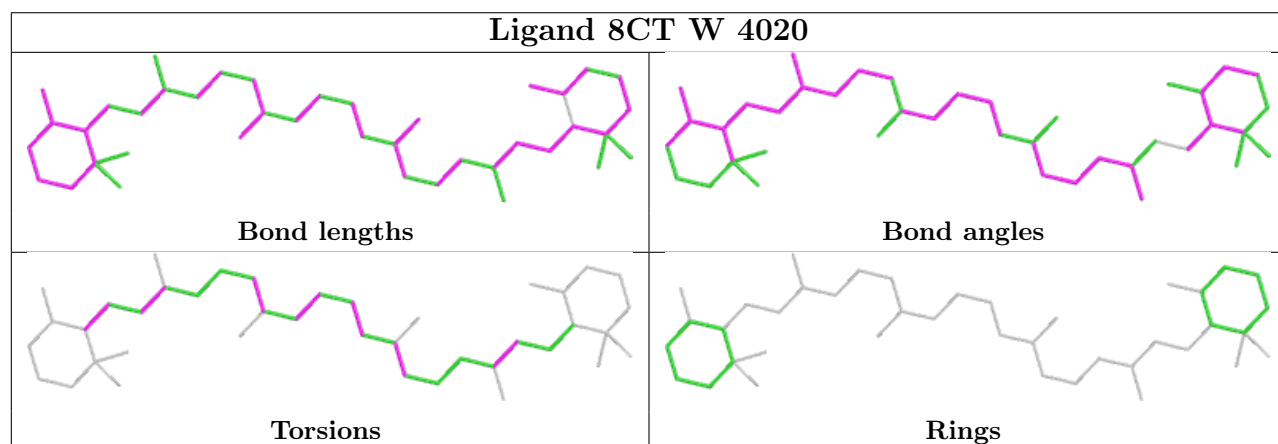
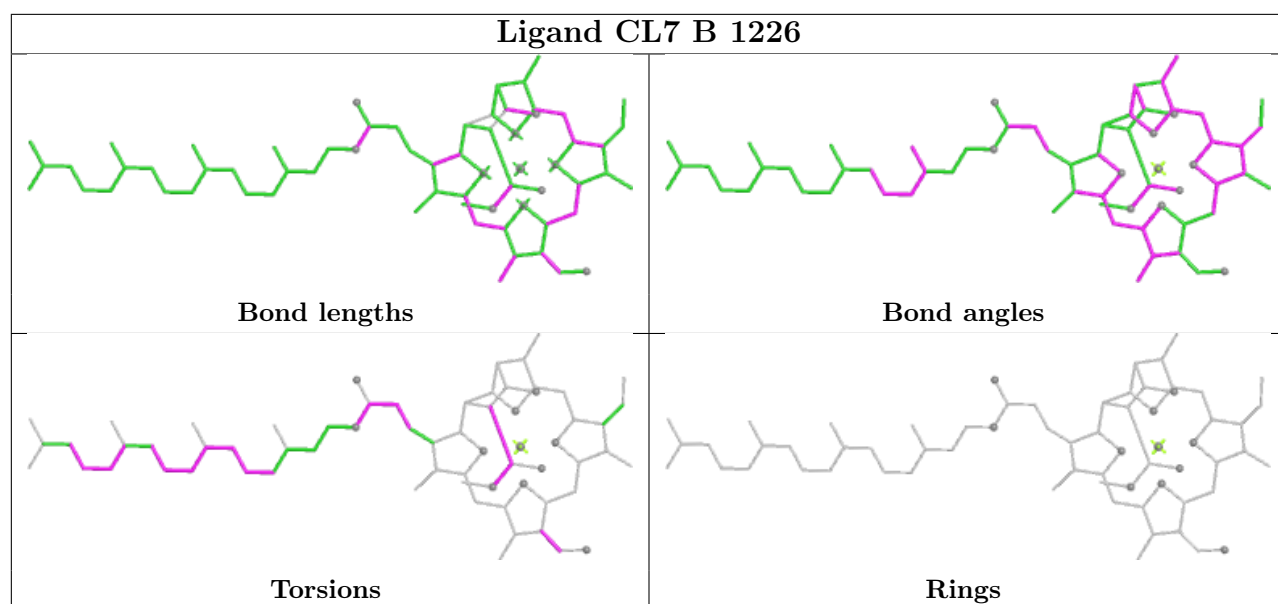


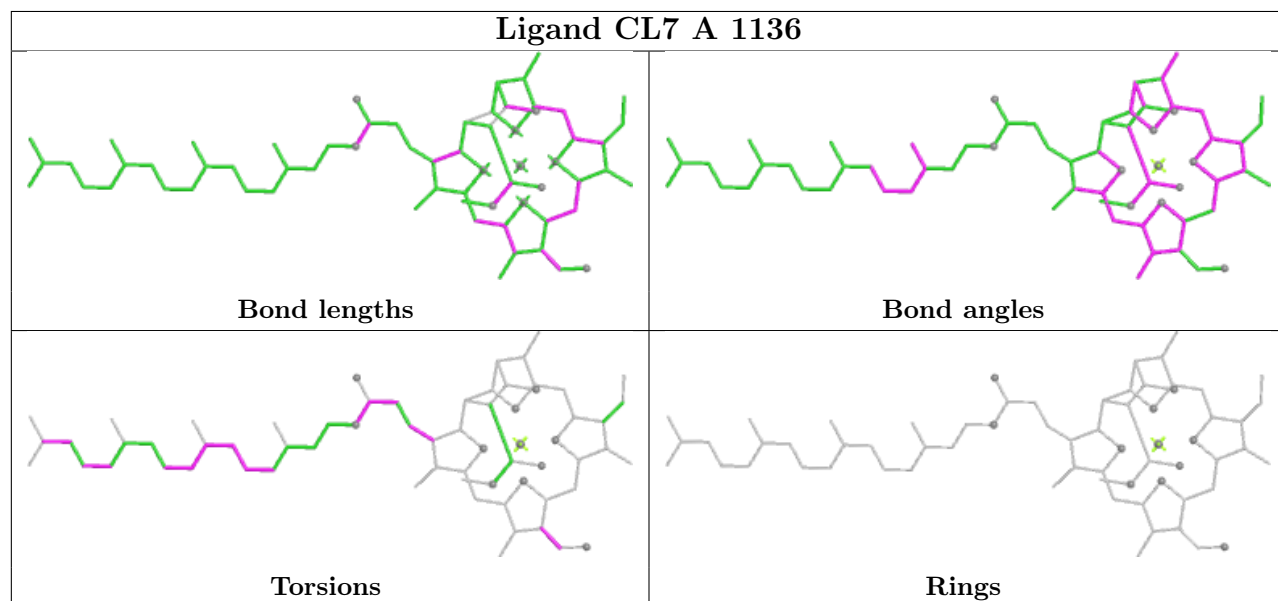
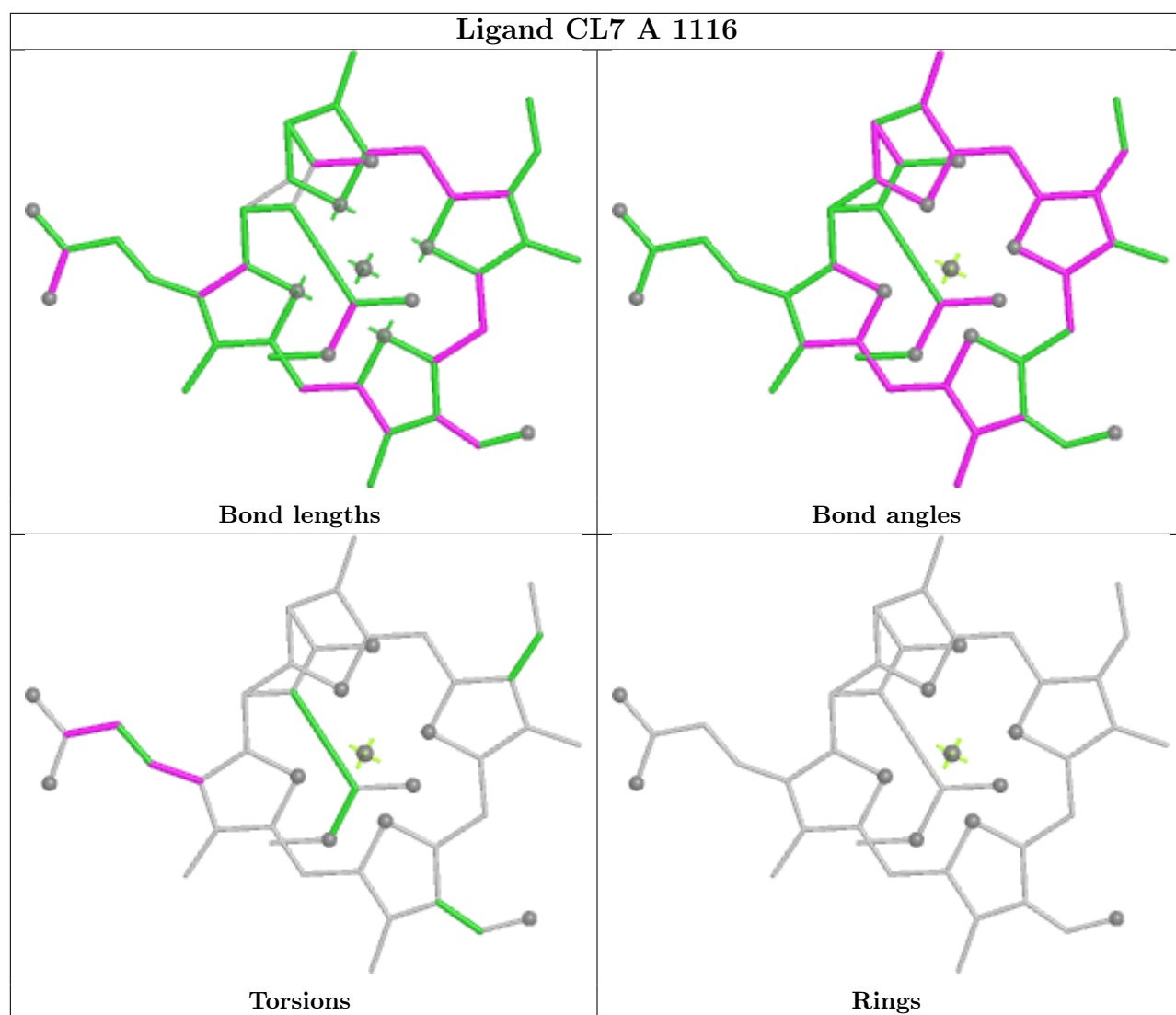


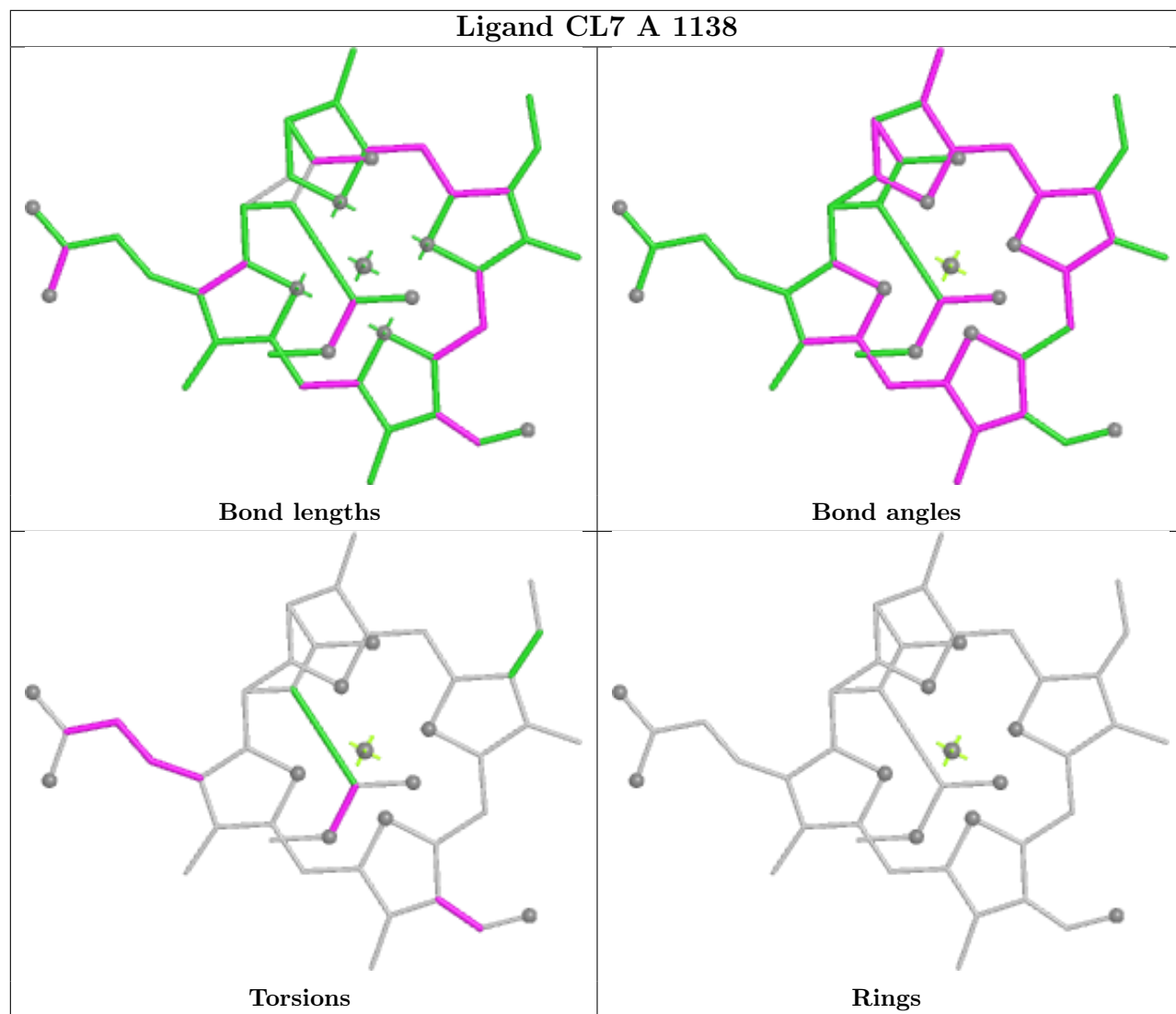


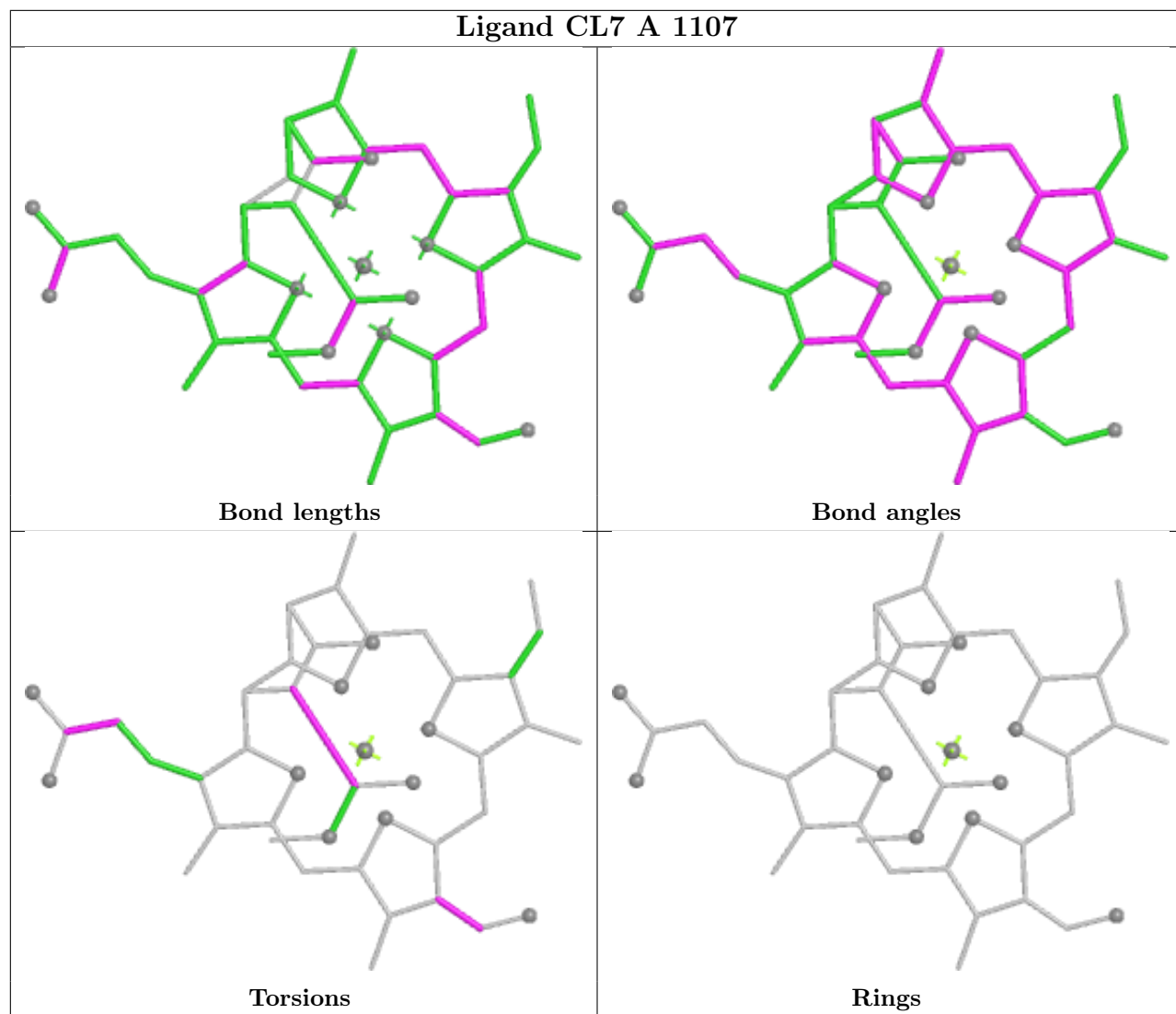


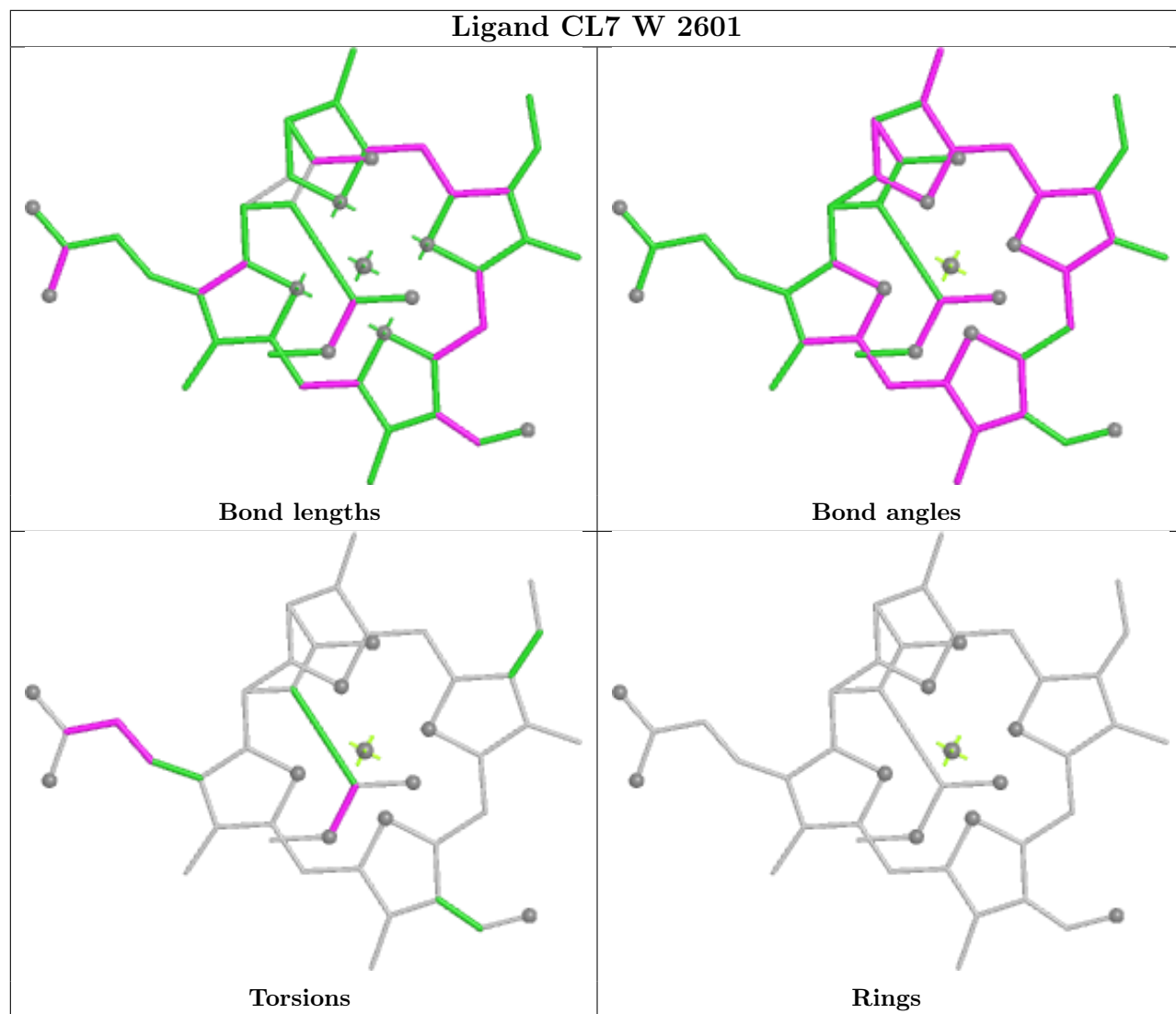


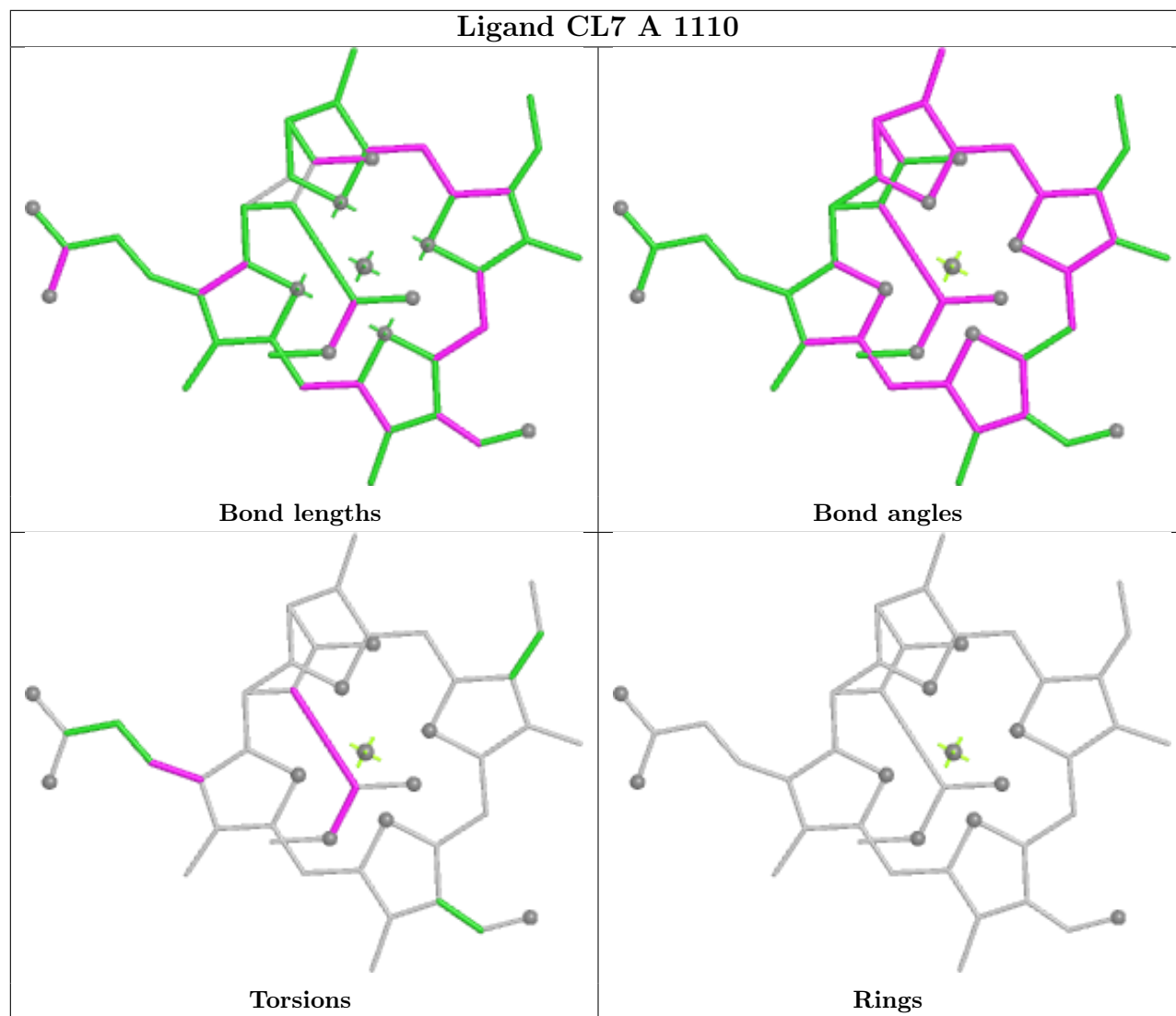


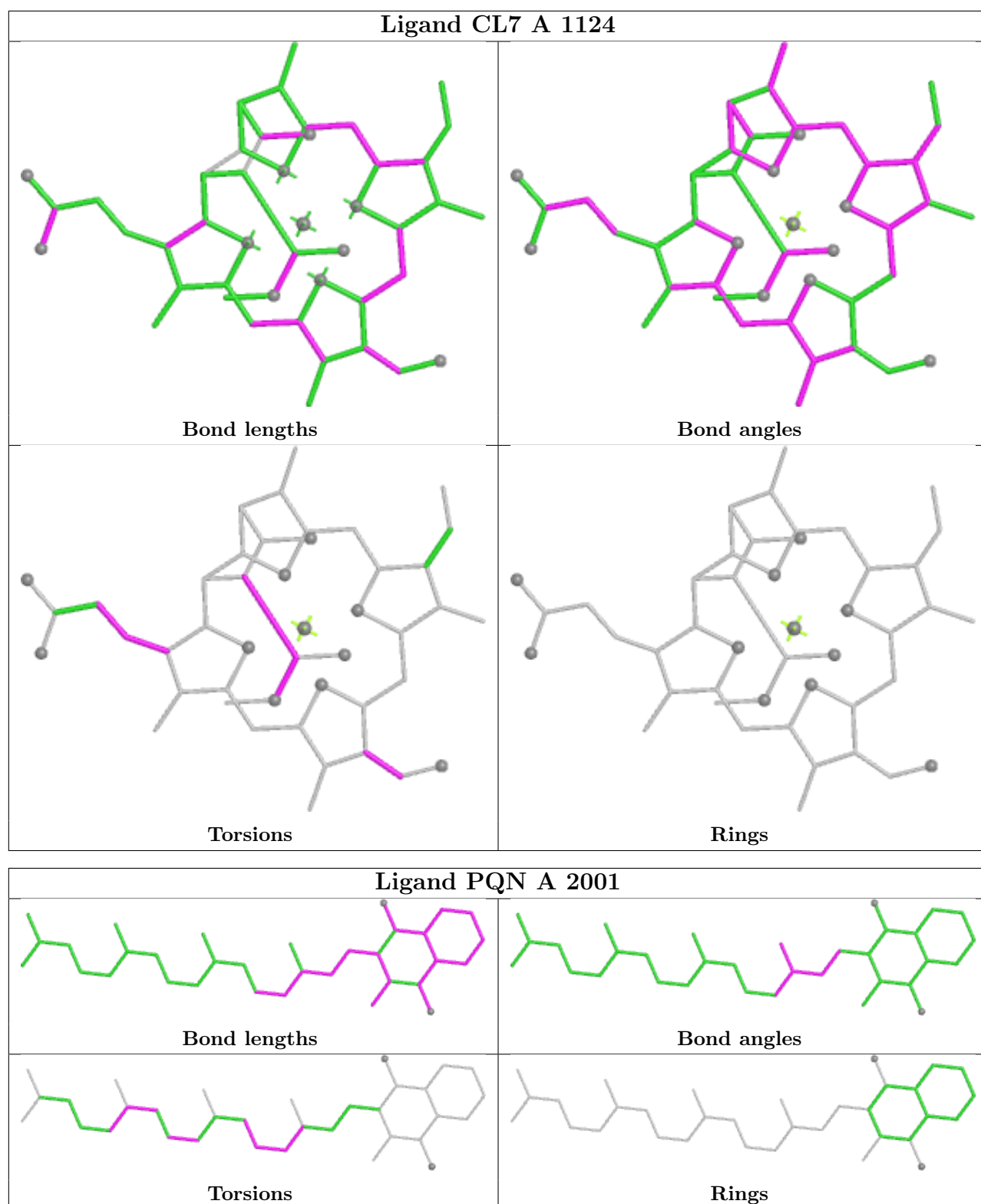


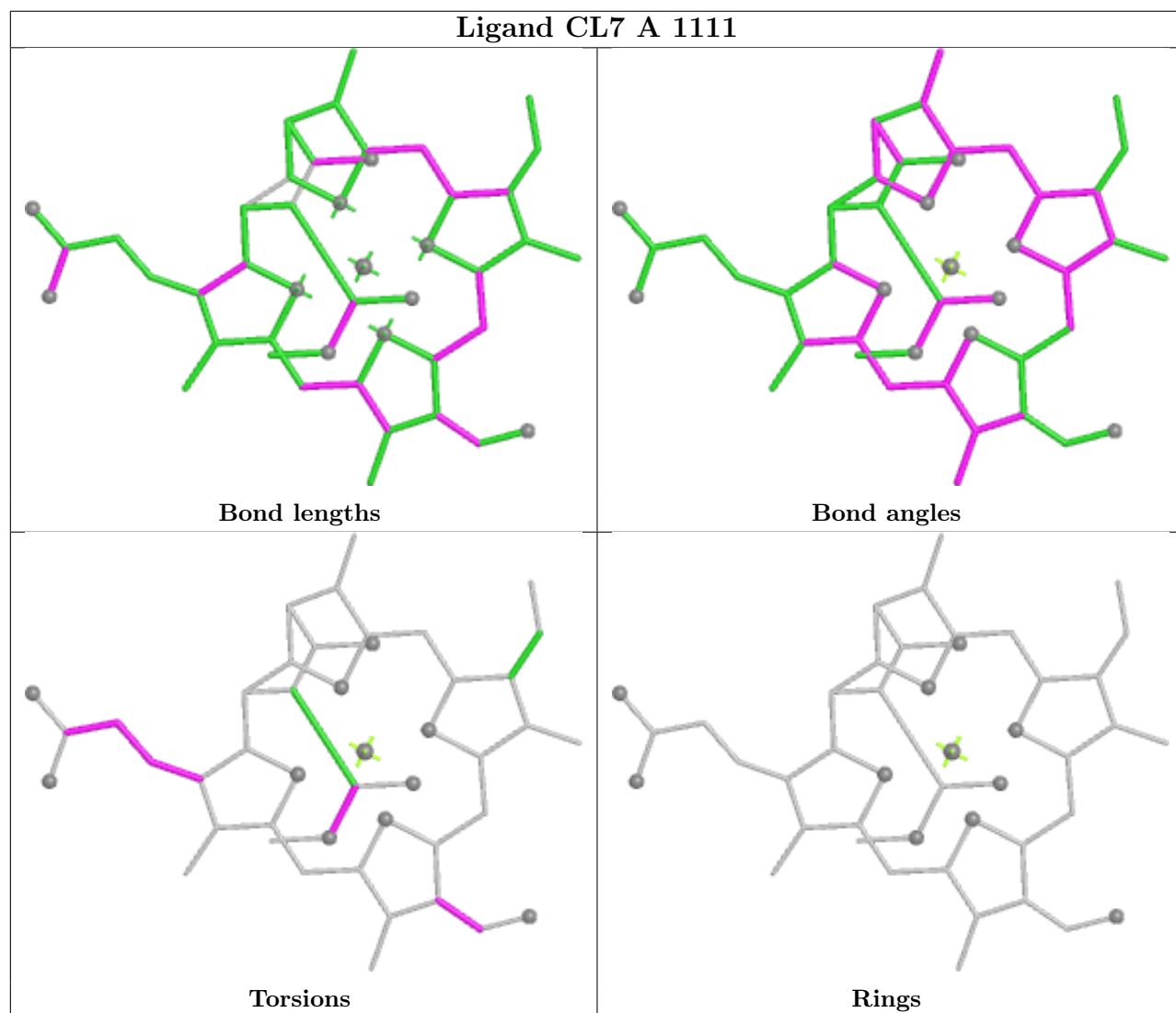
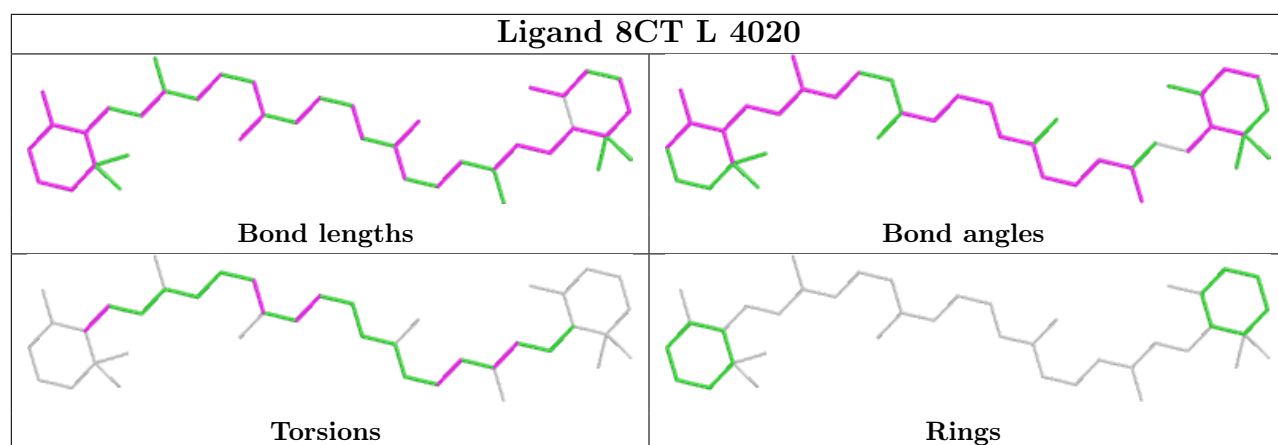


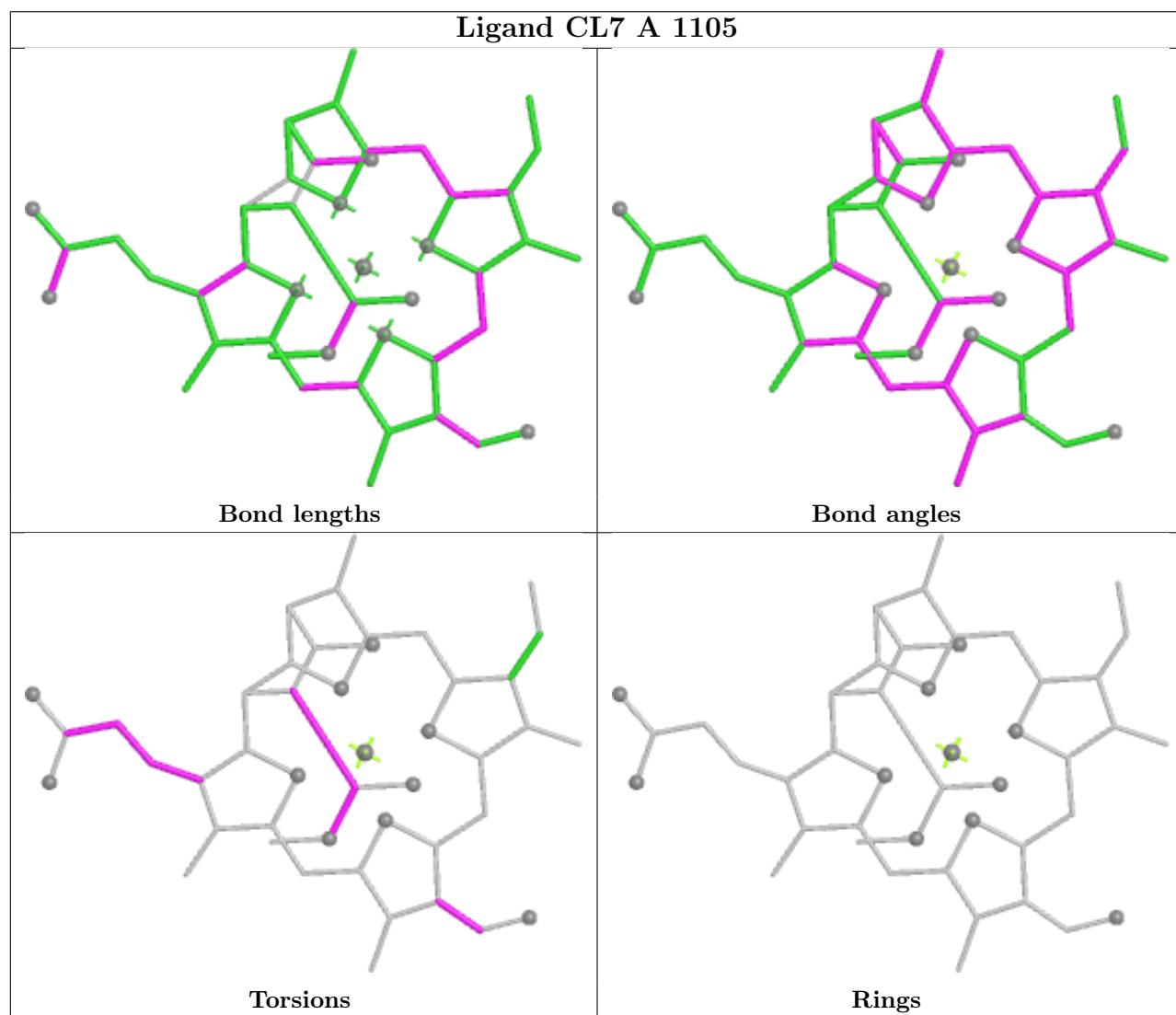
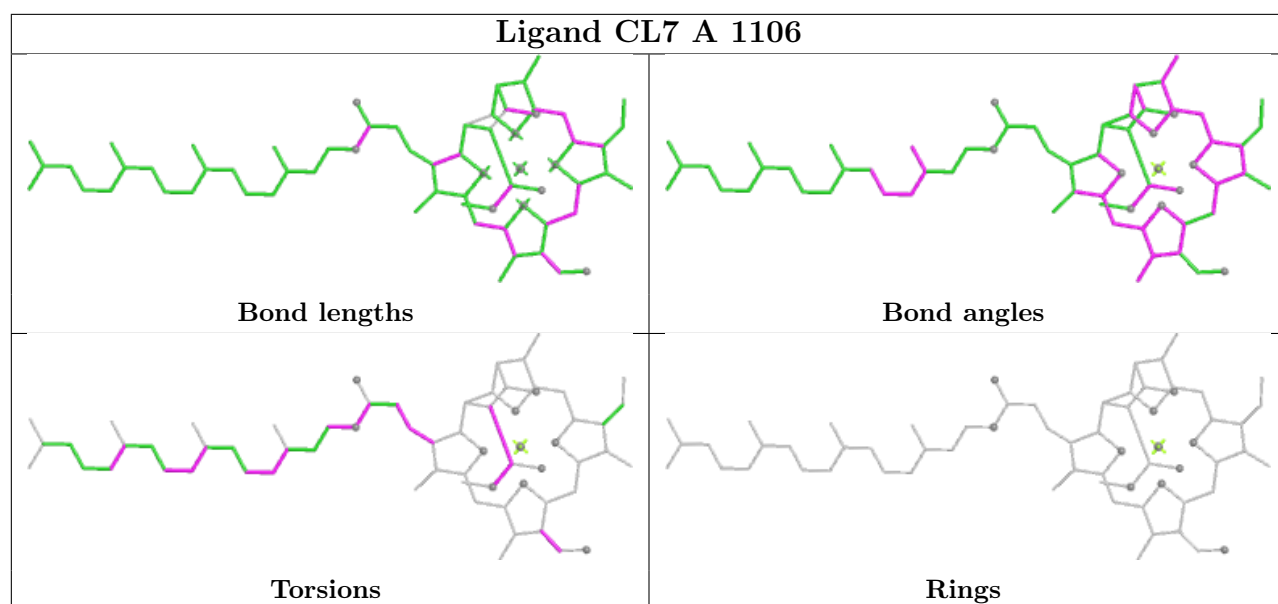




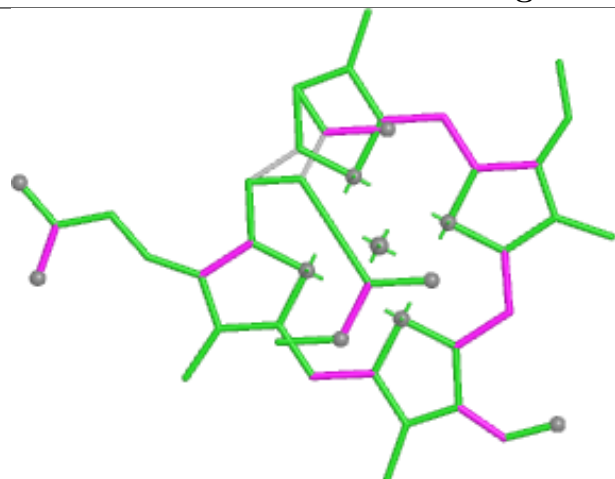




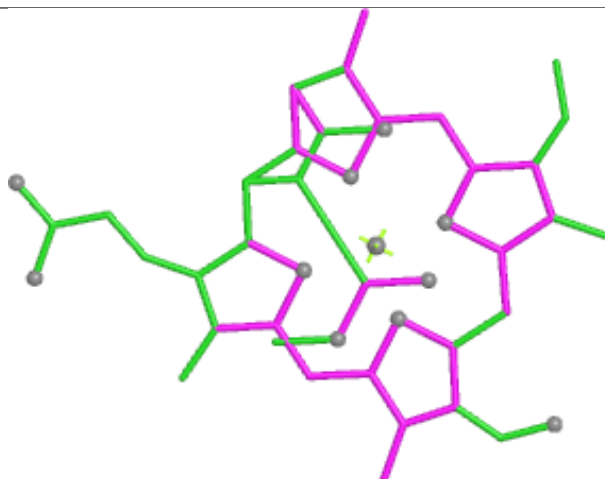




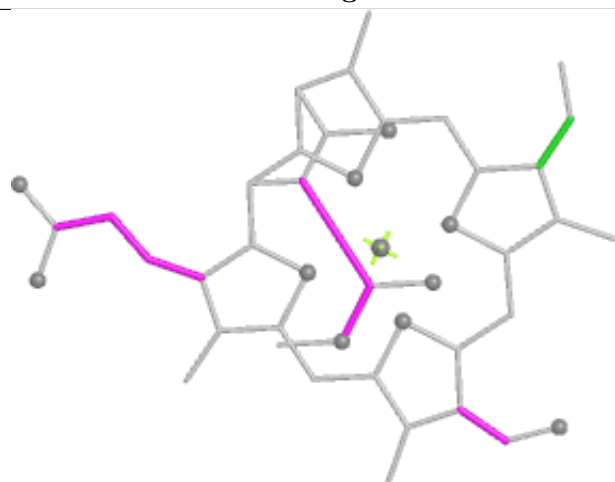
Ligand CL7 J 1302



Bond lengths



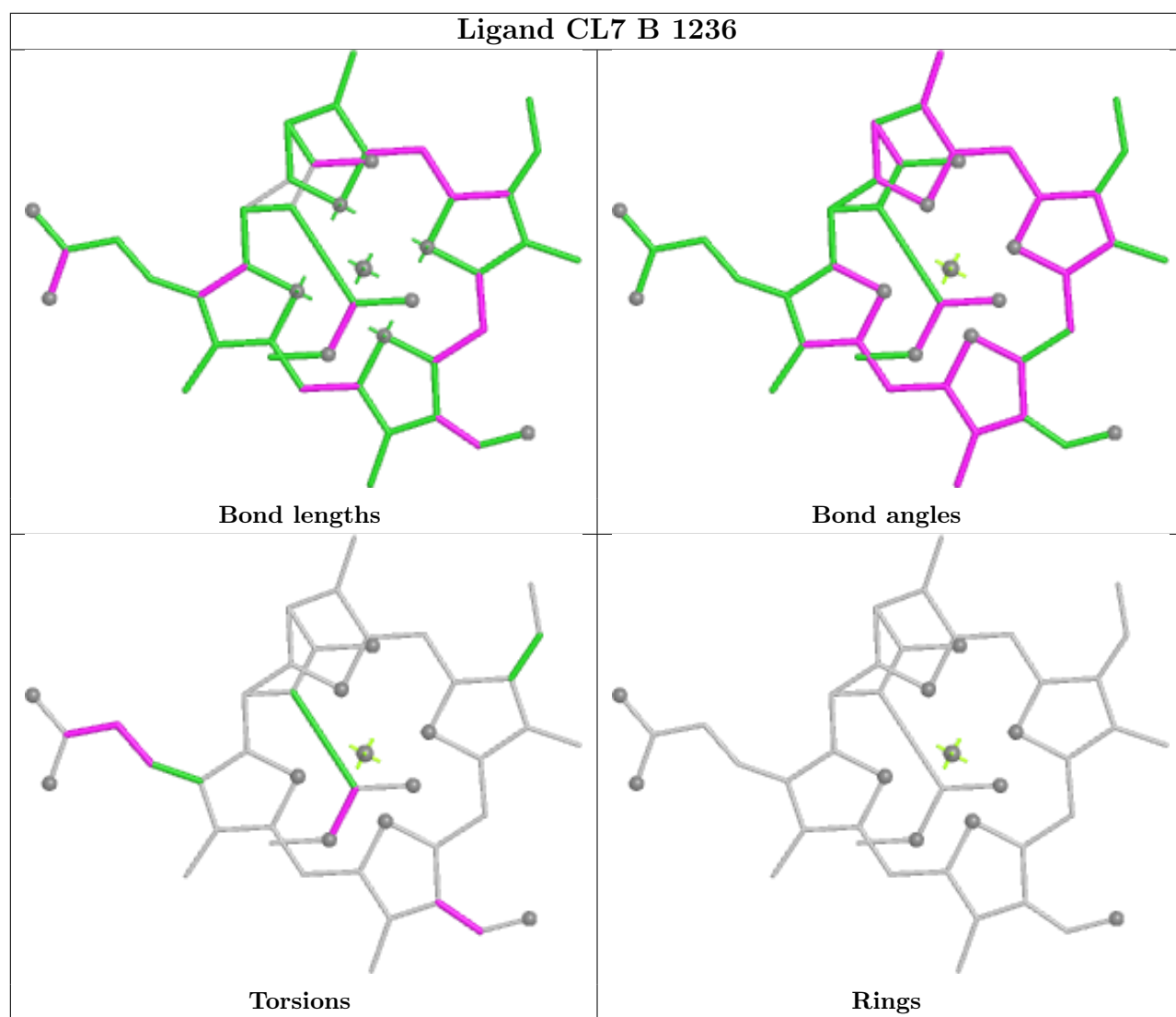
Bond angles

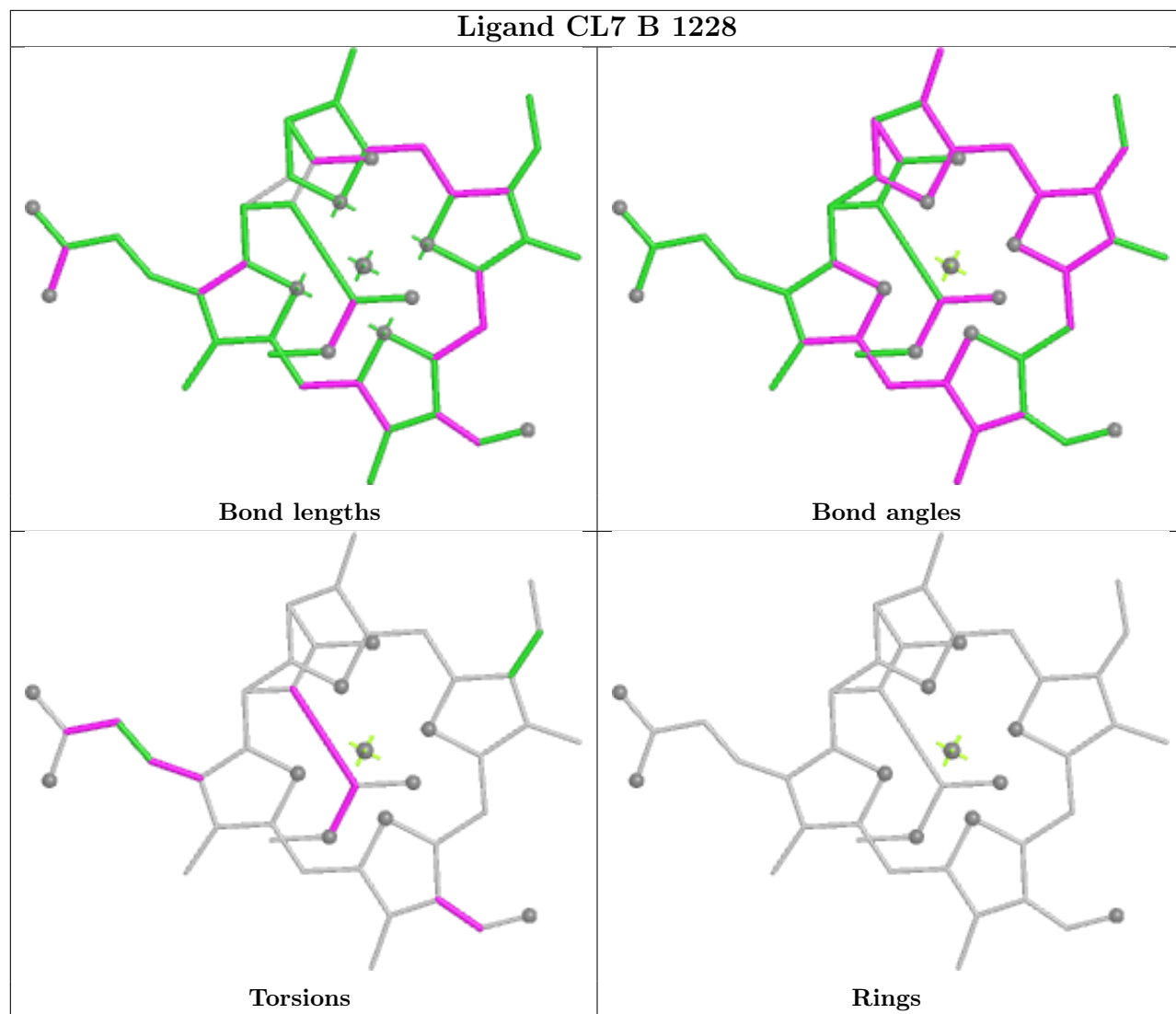


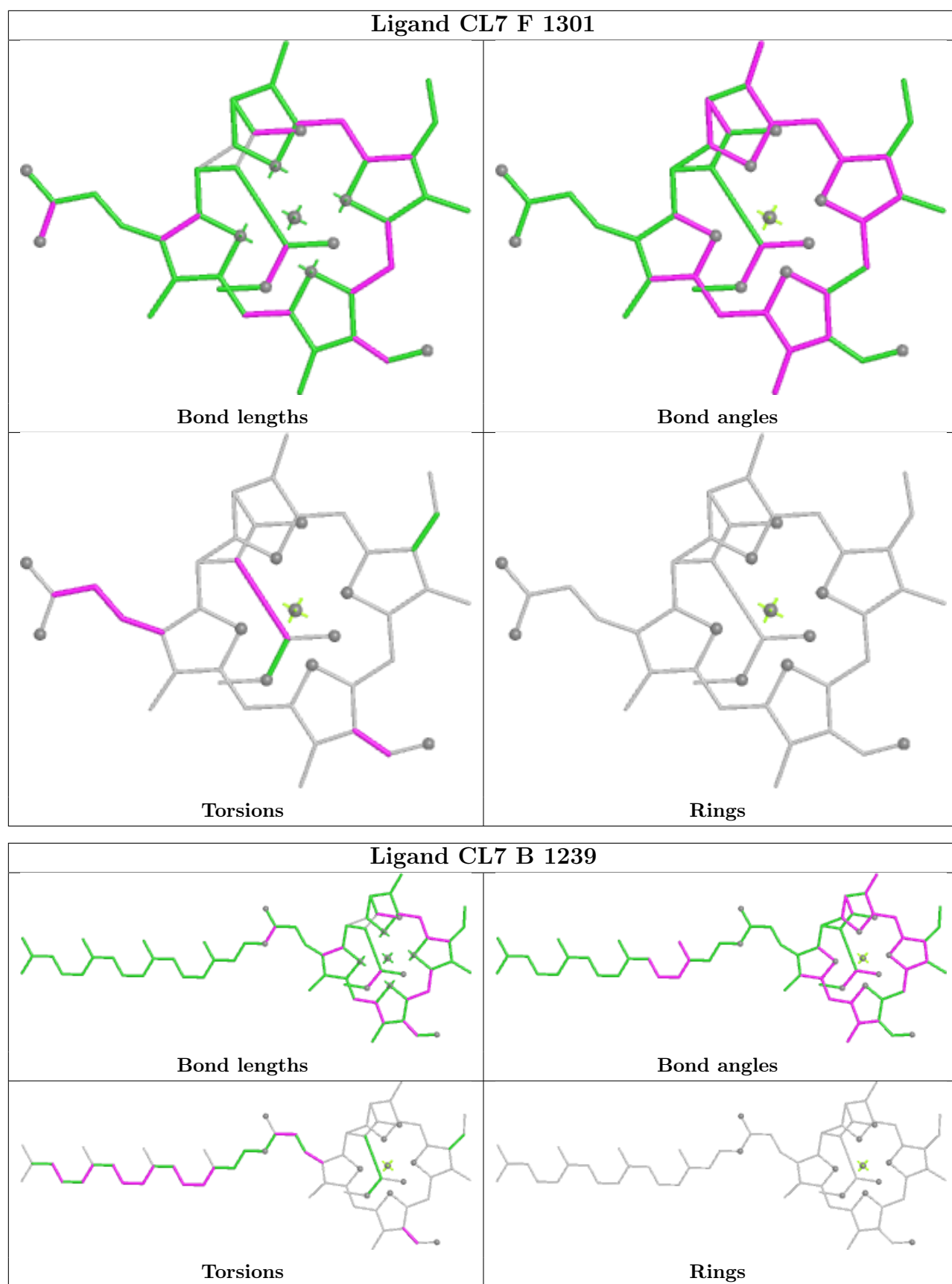
Torsions

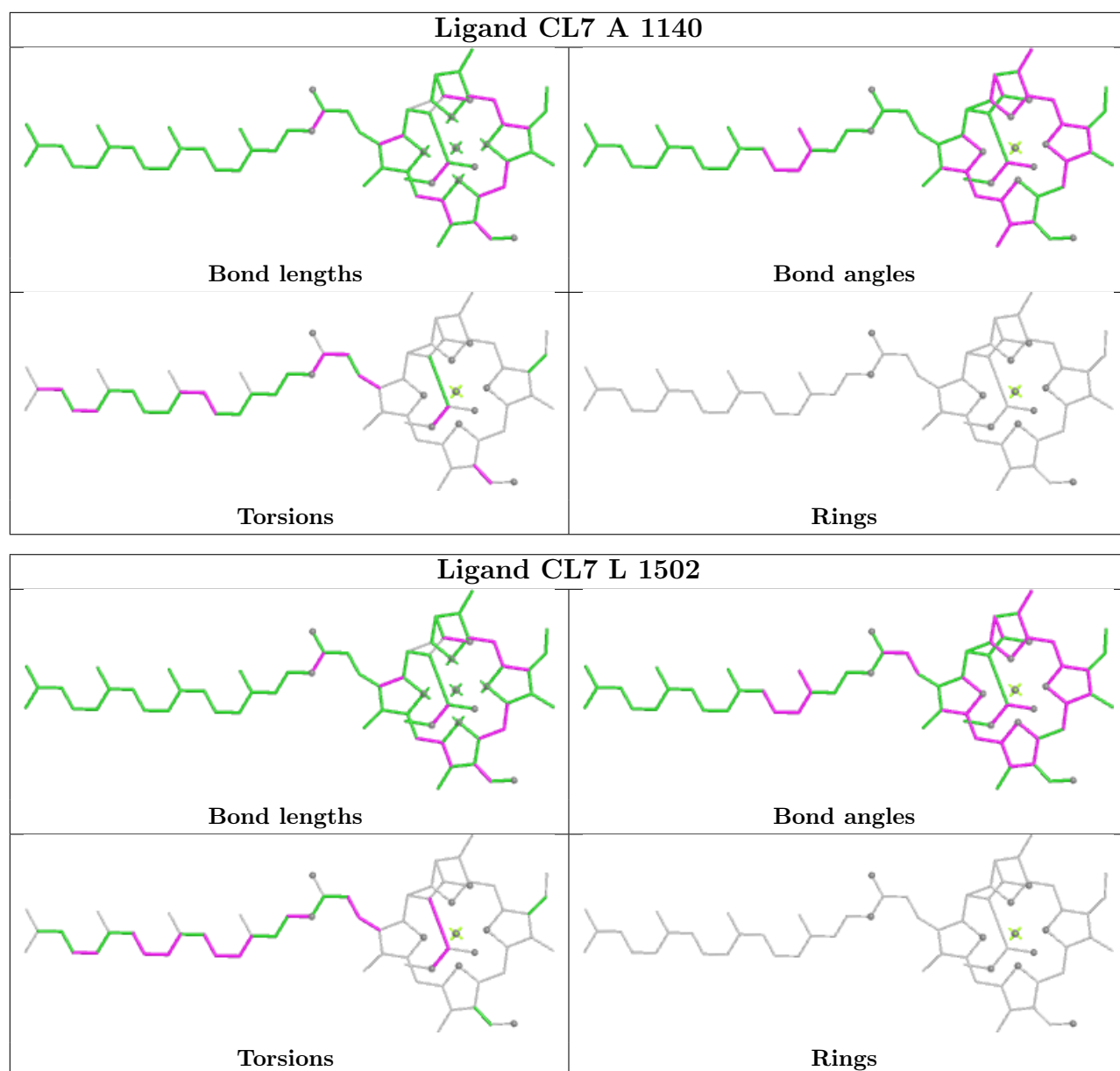


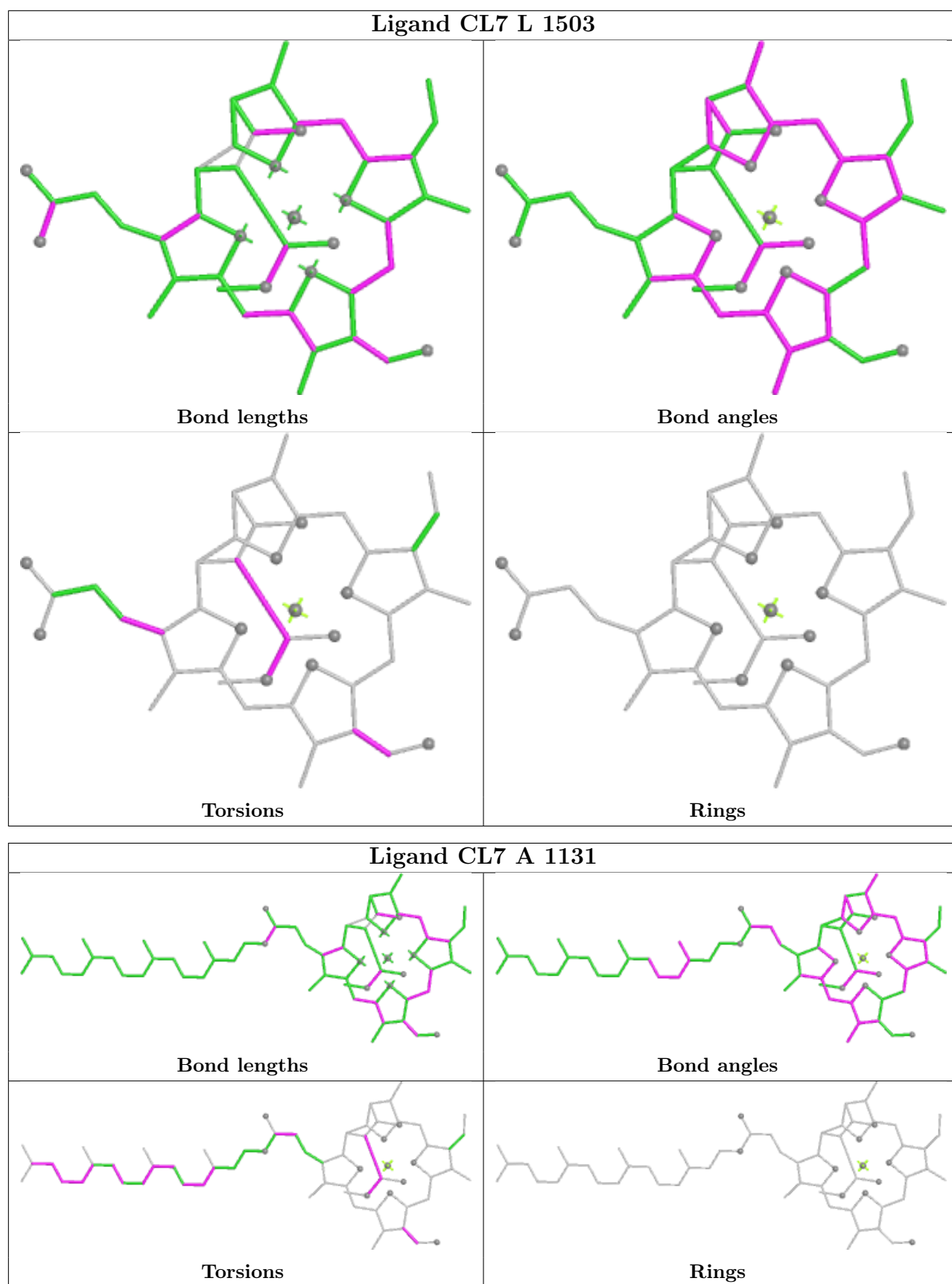
Rings

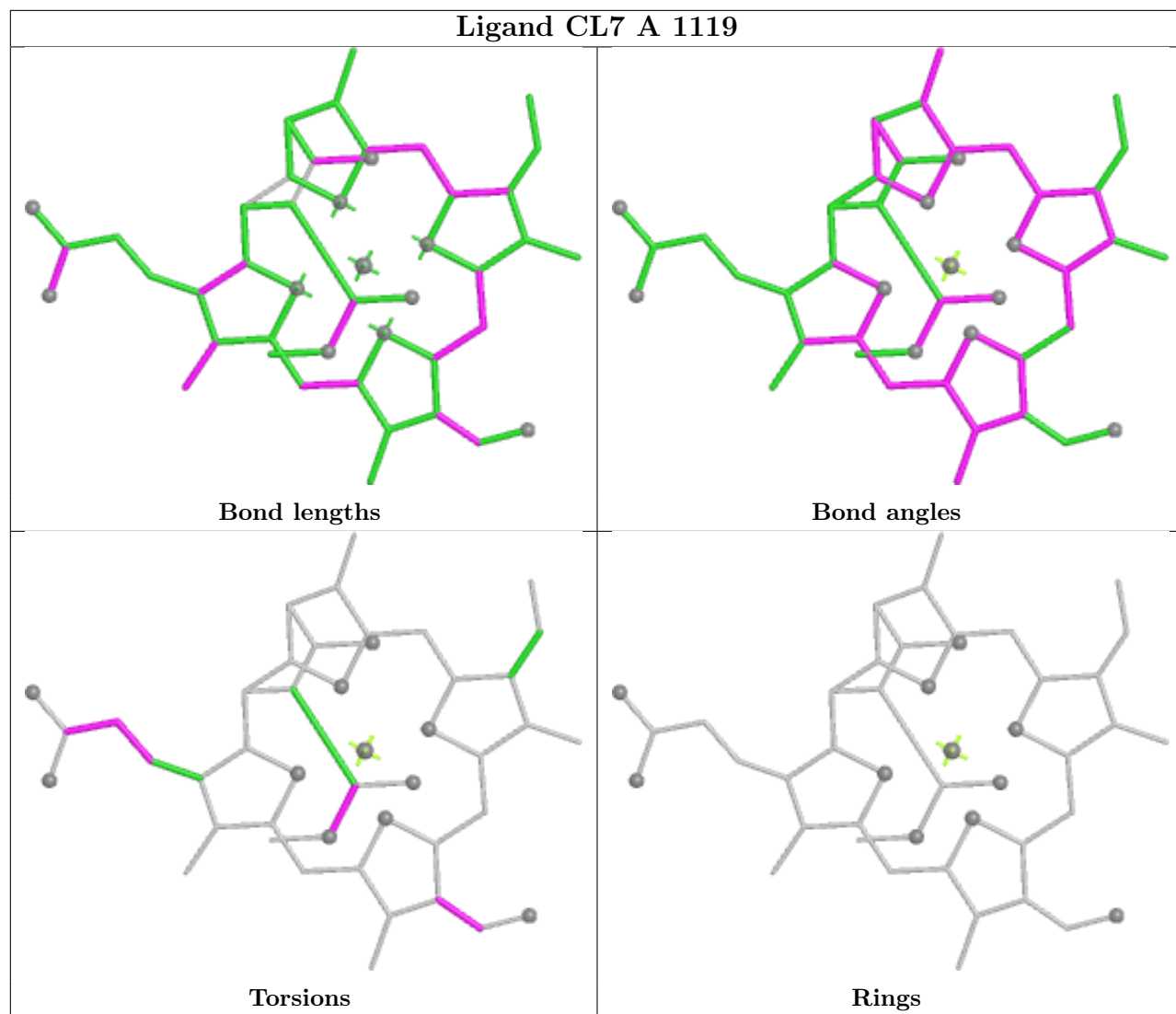


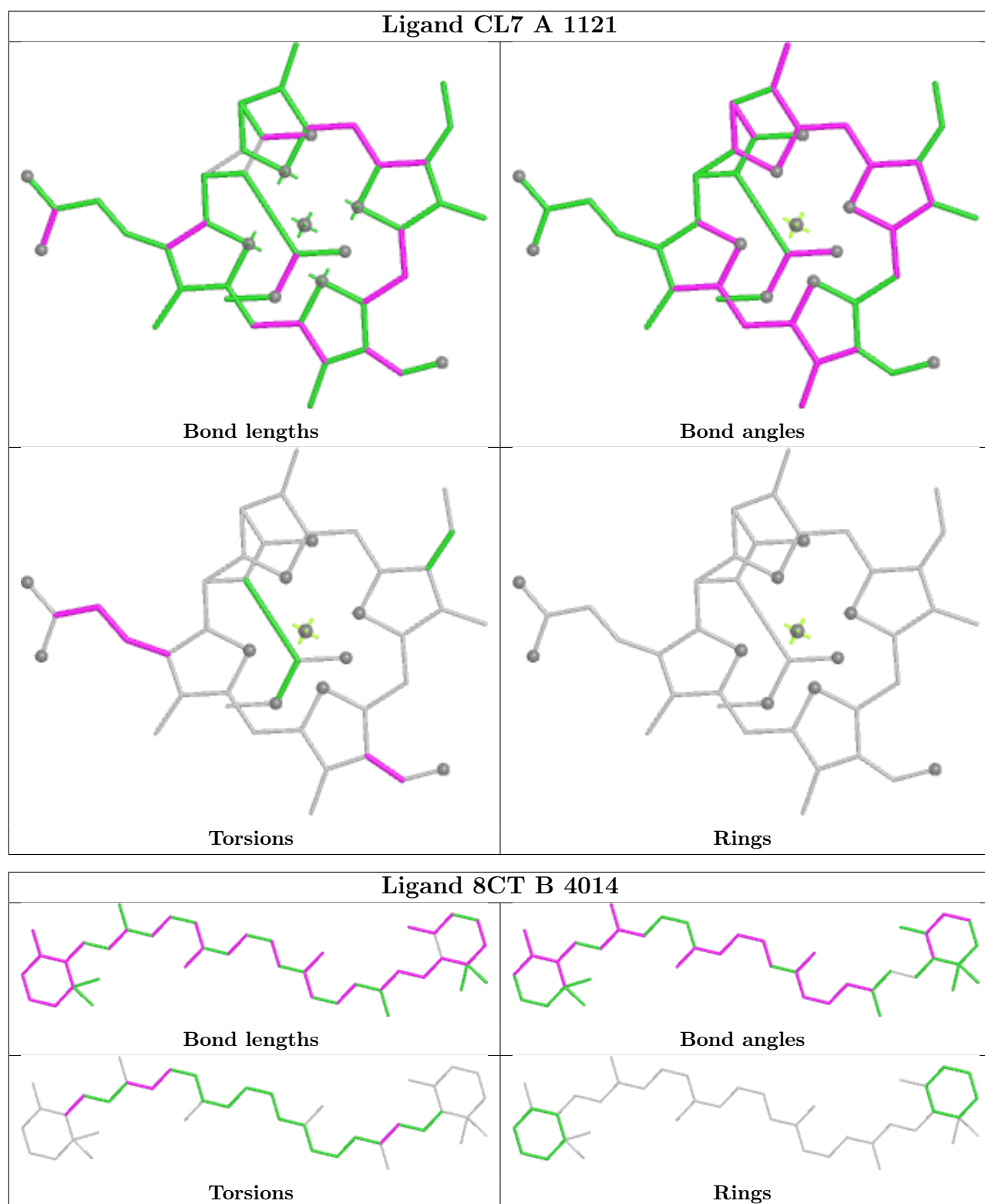


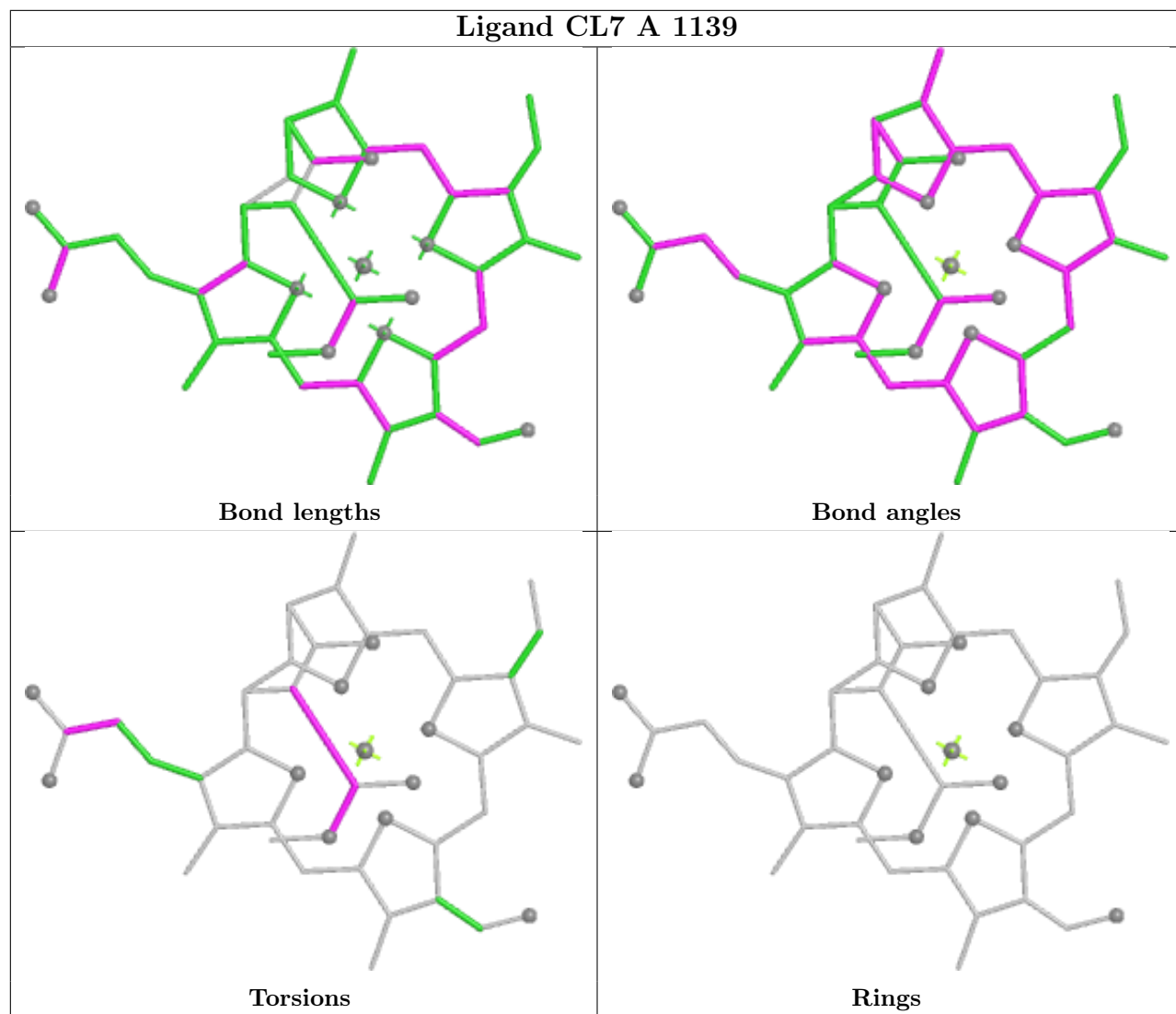


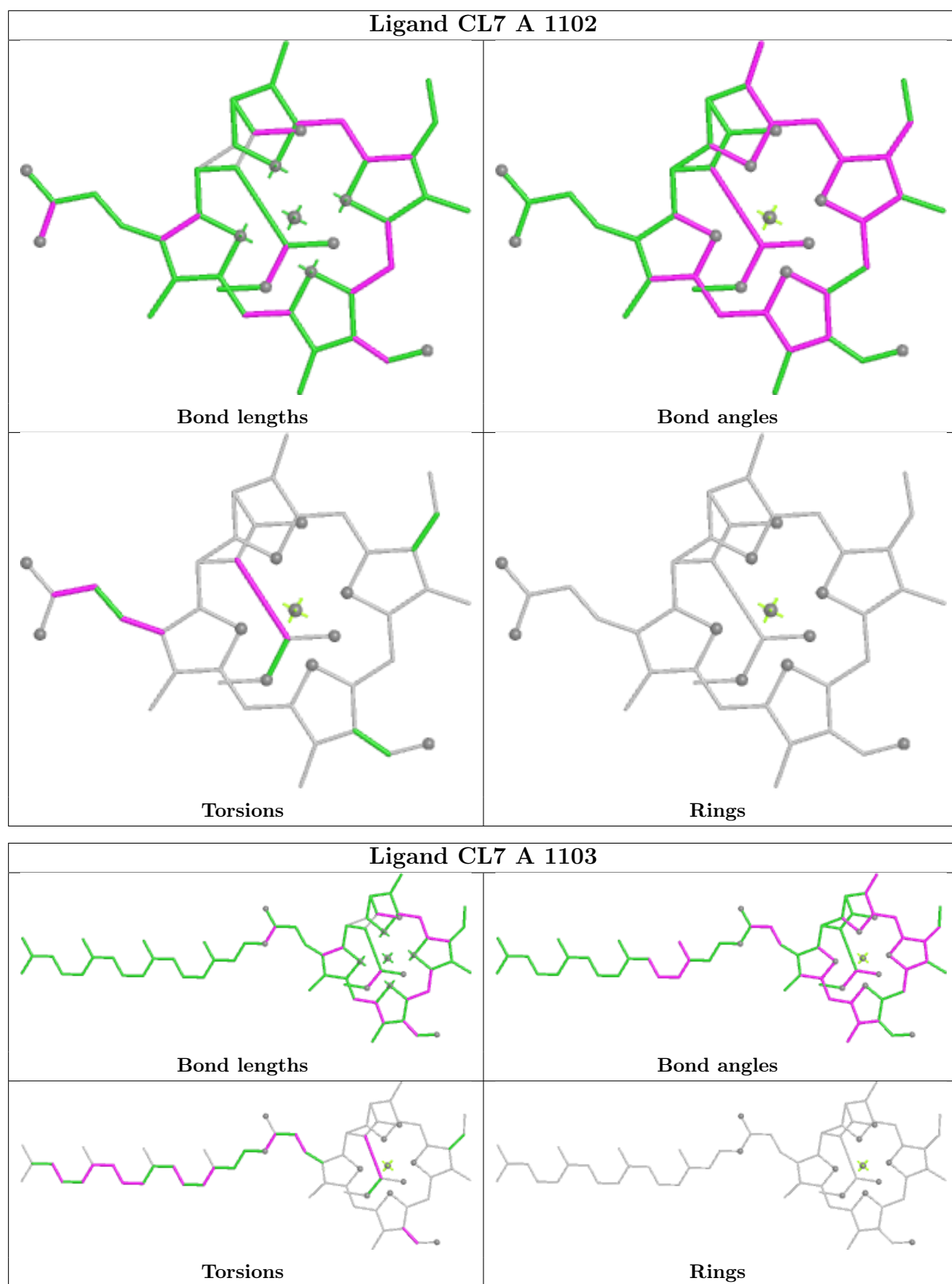


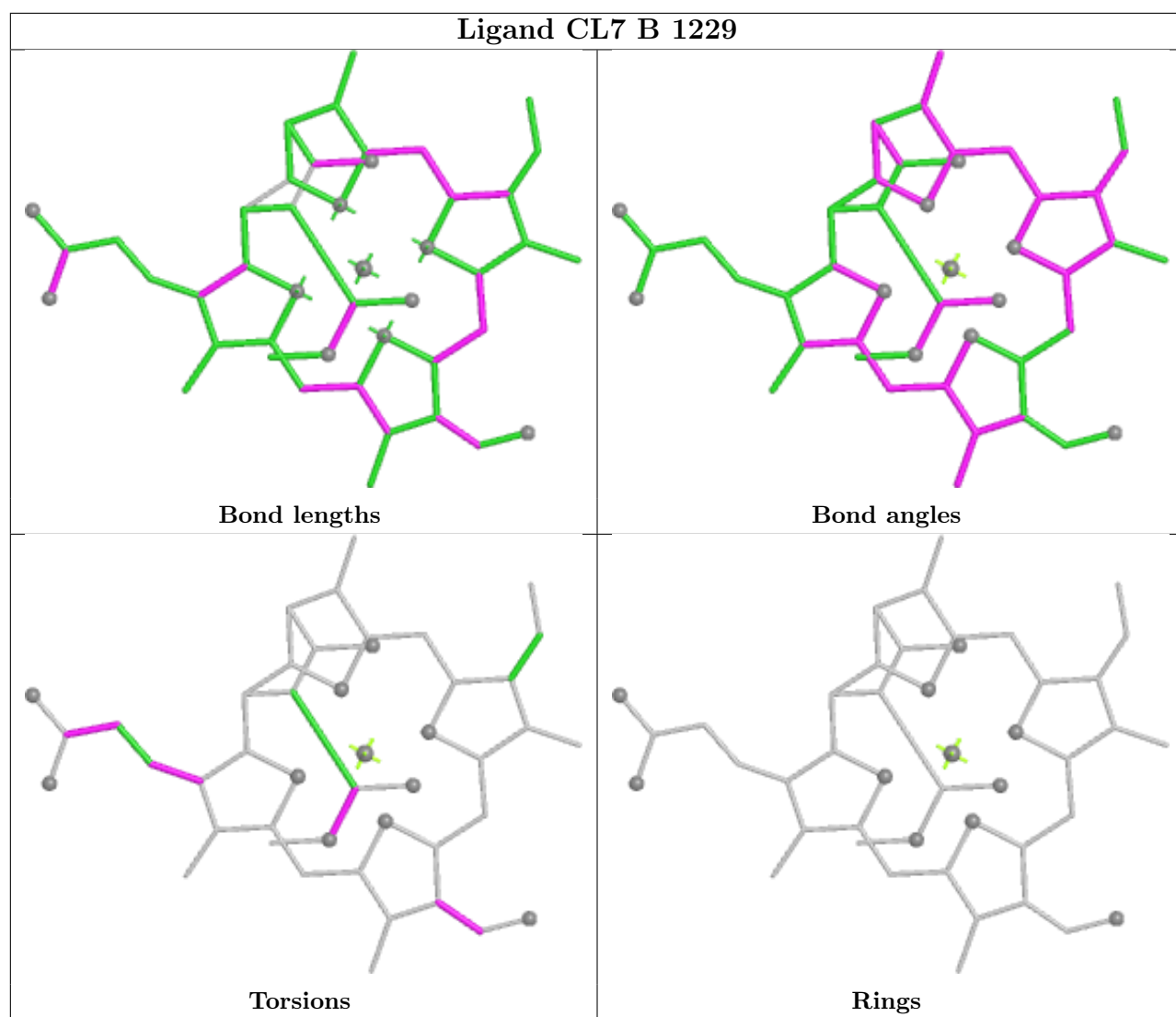


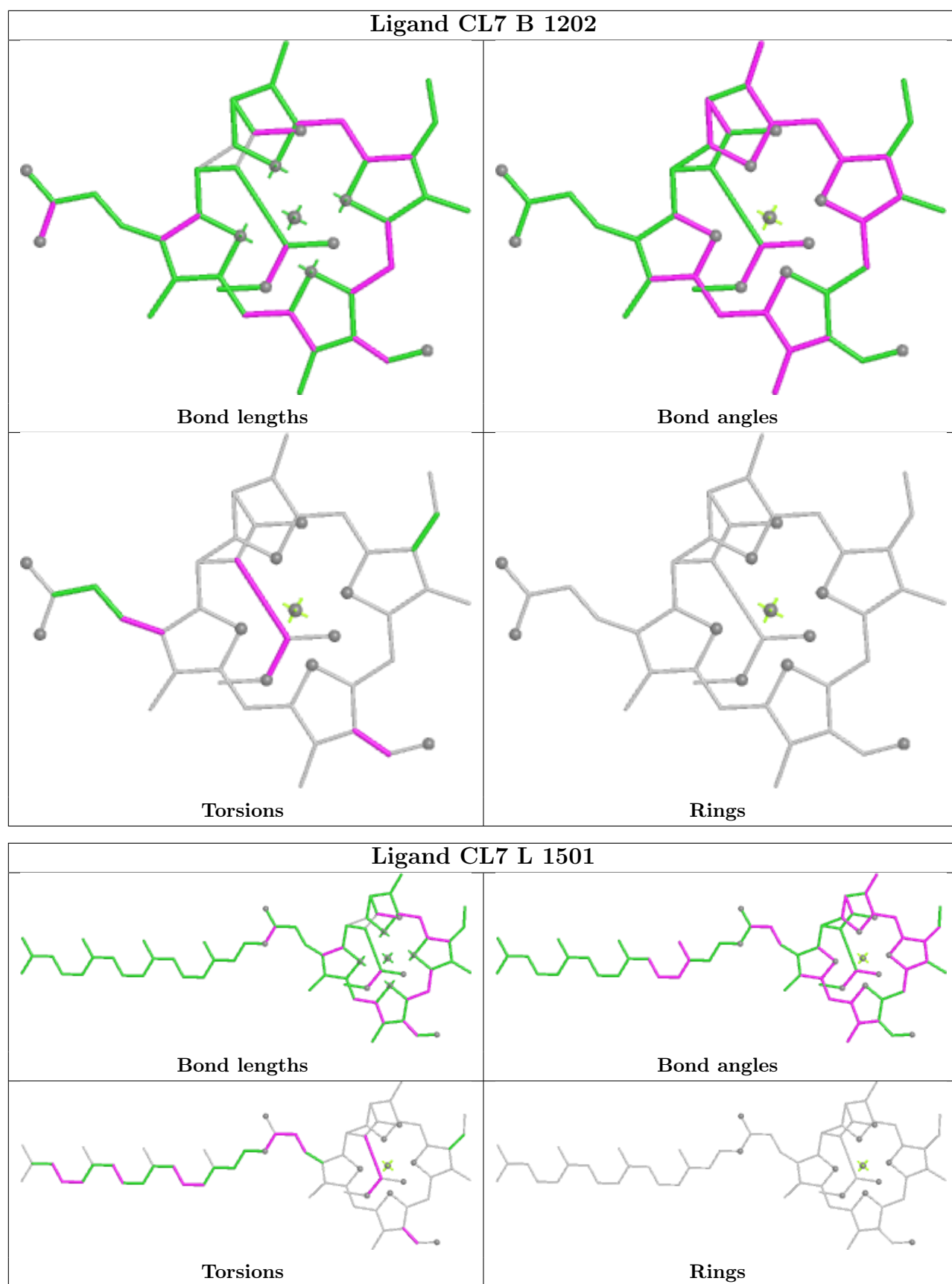


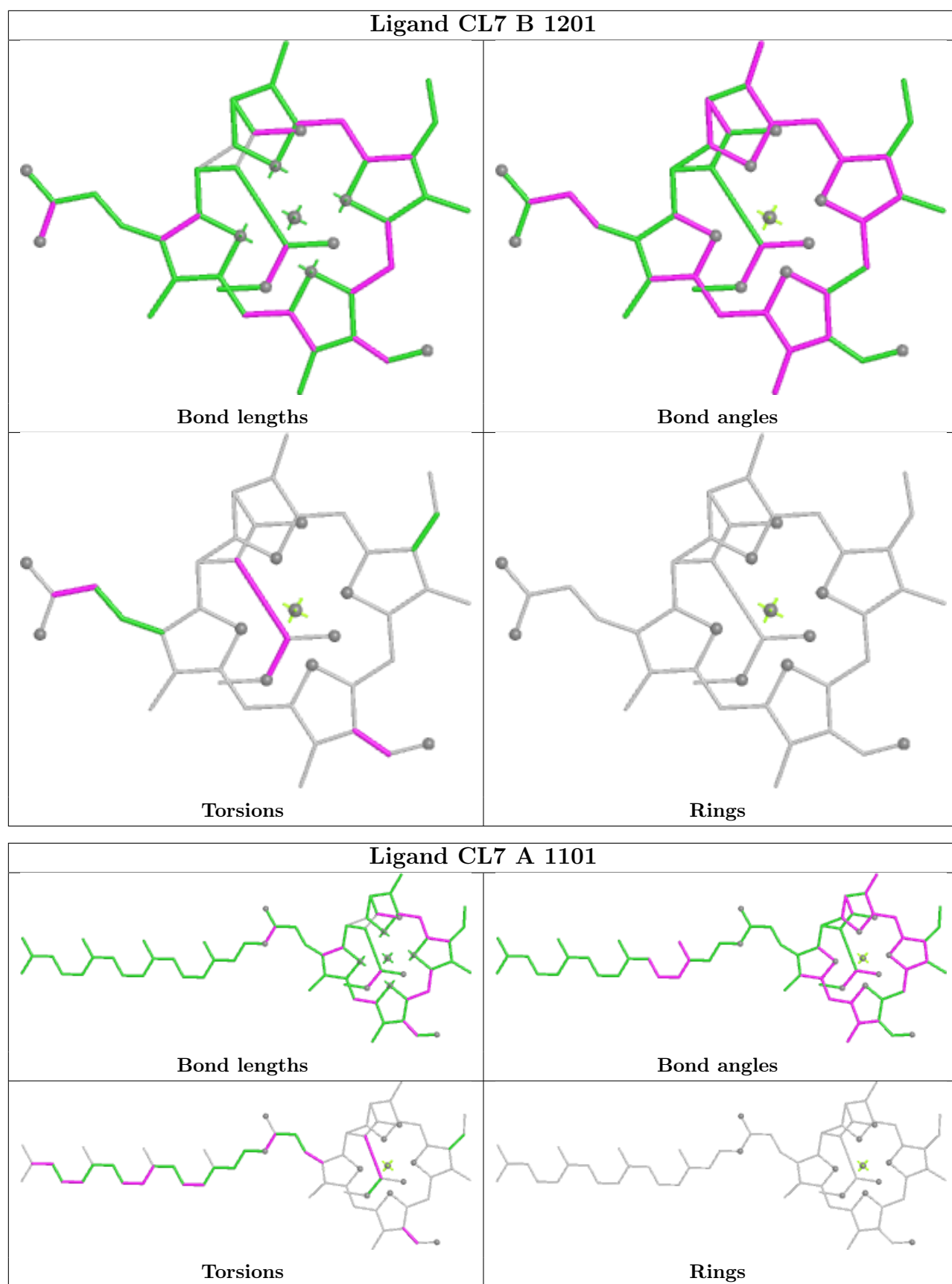


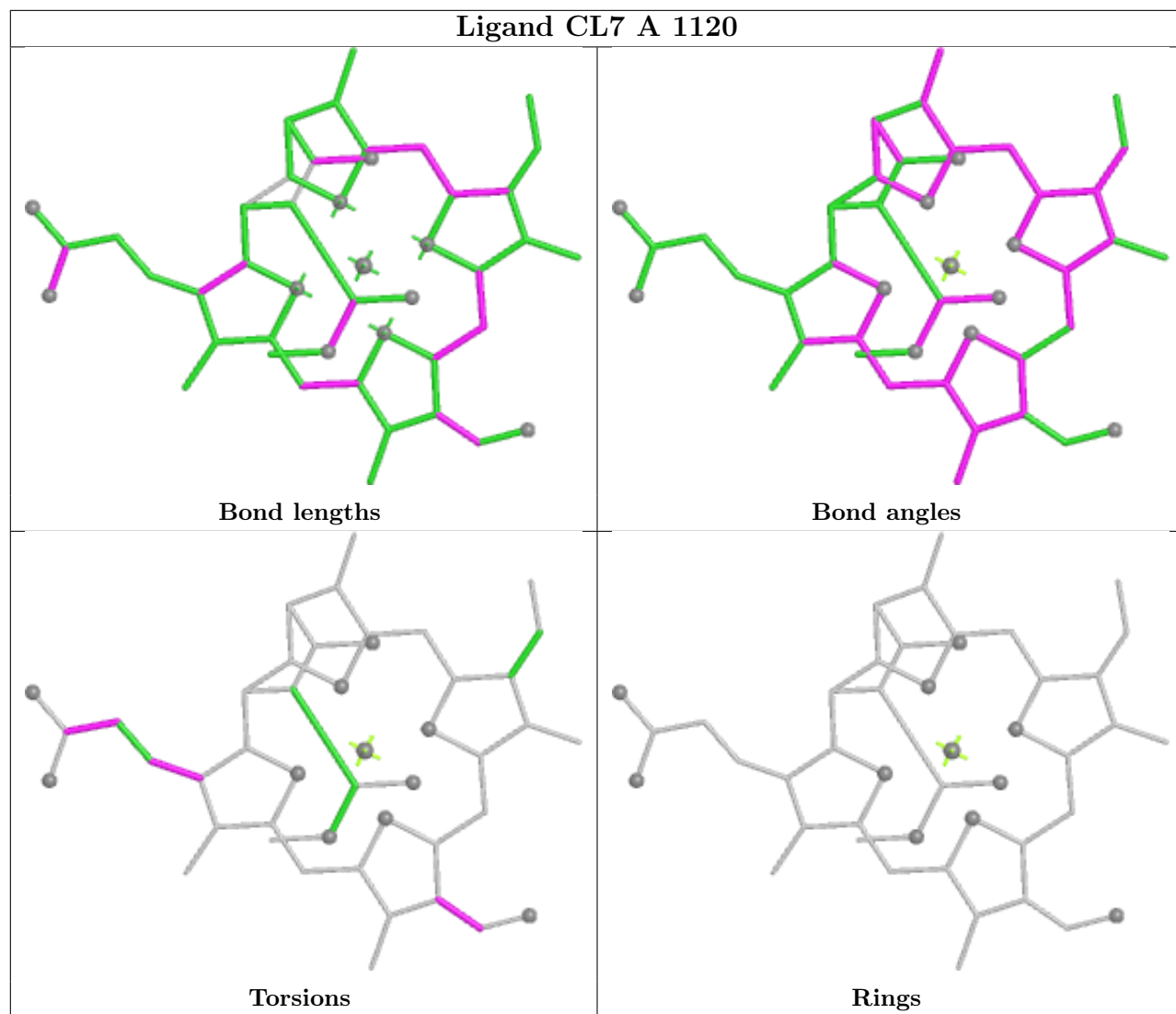


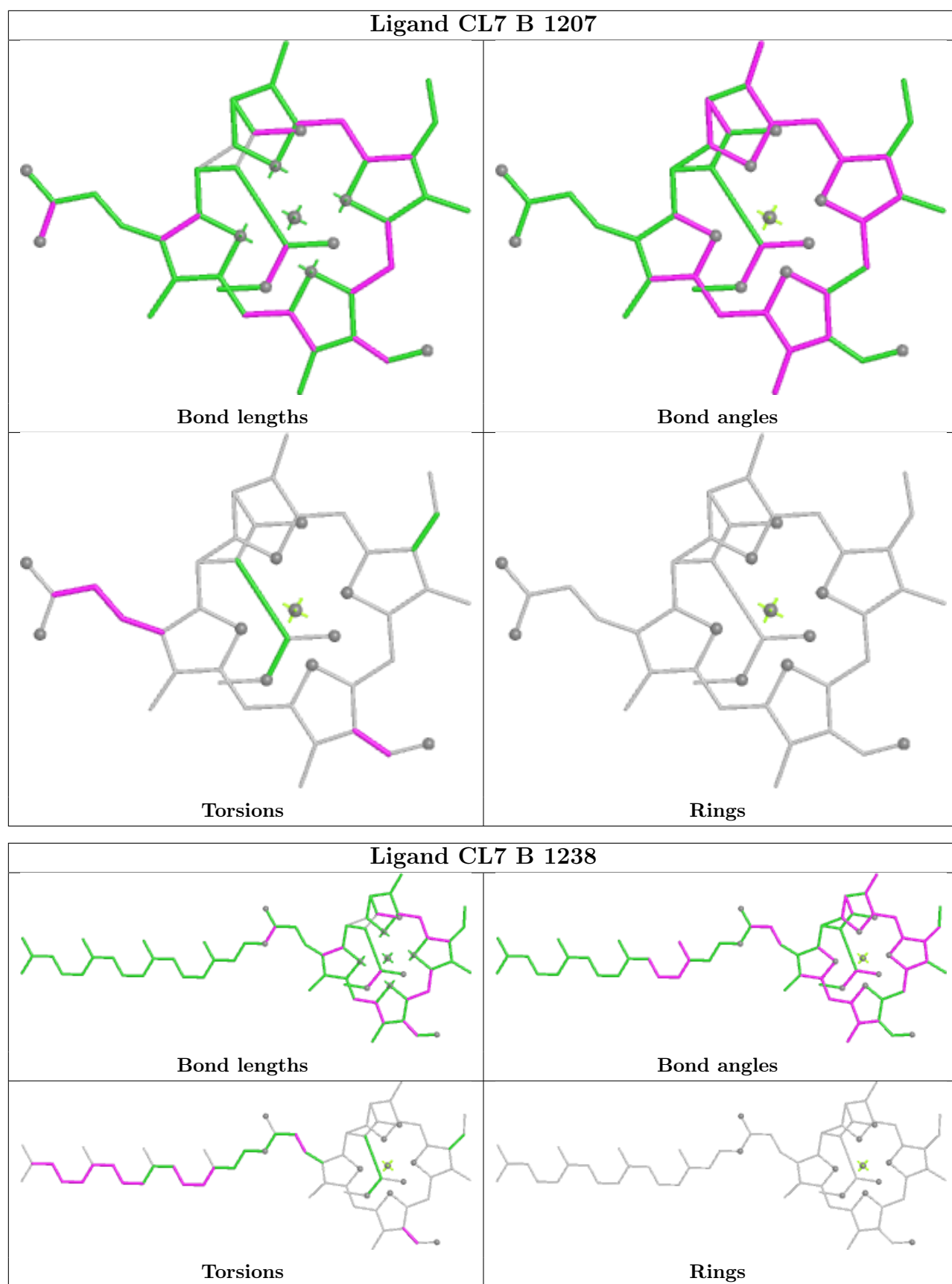


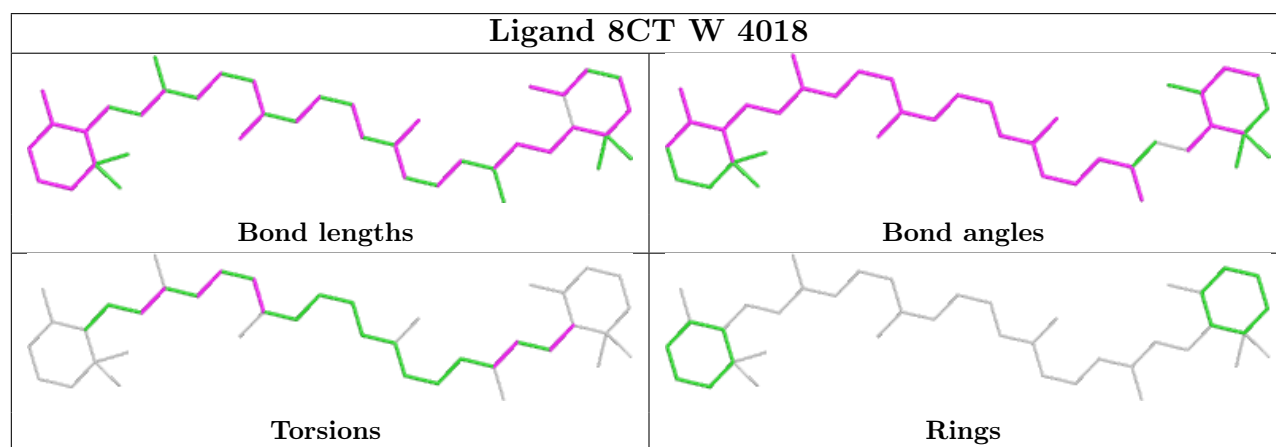
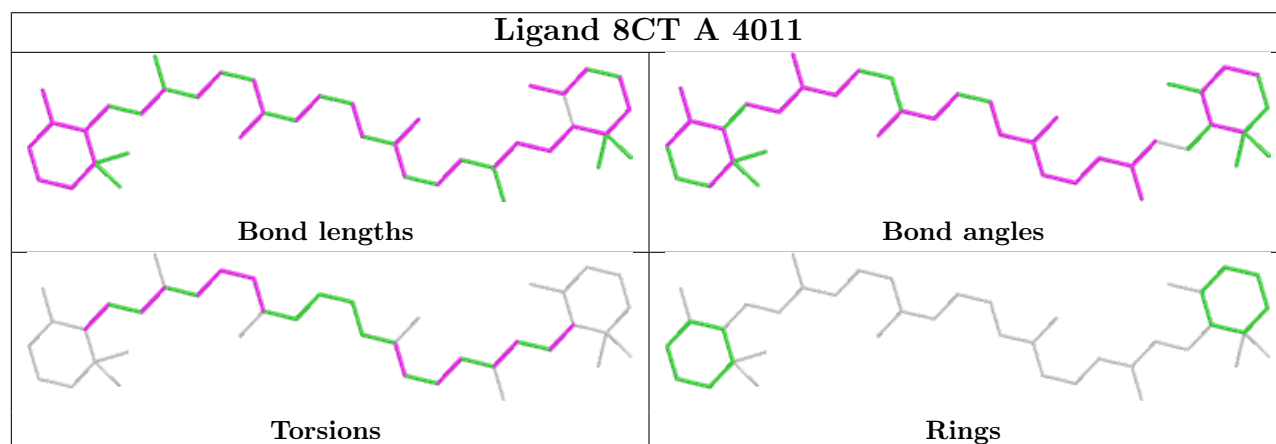
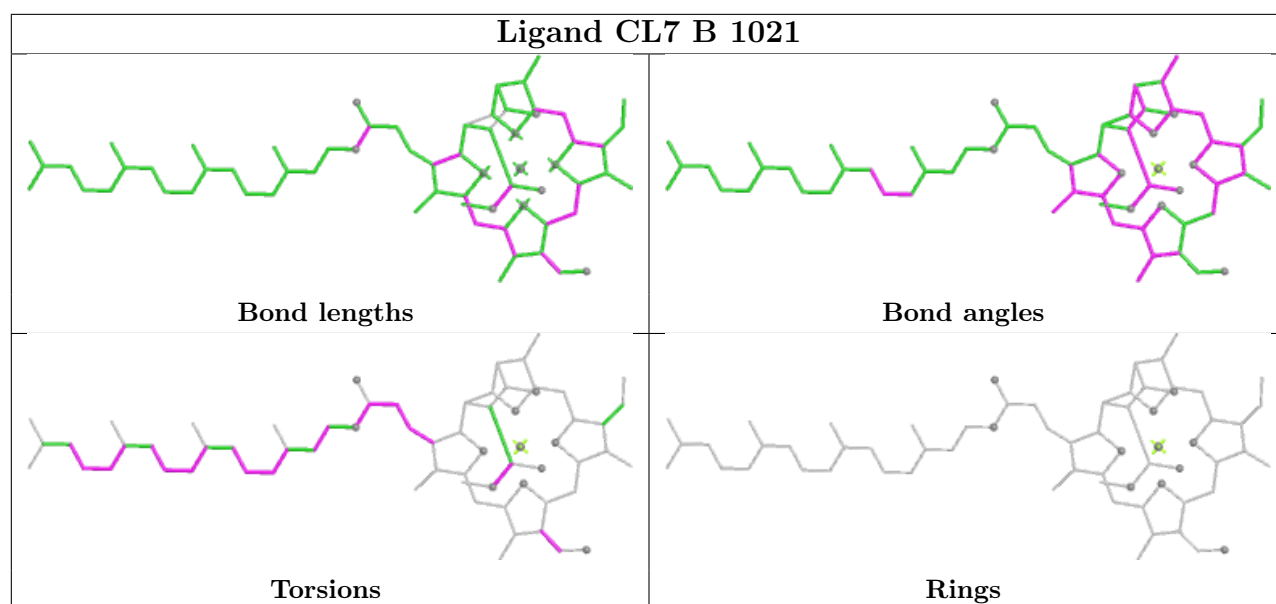


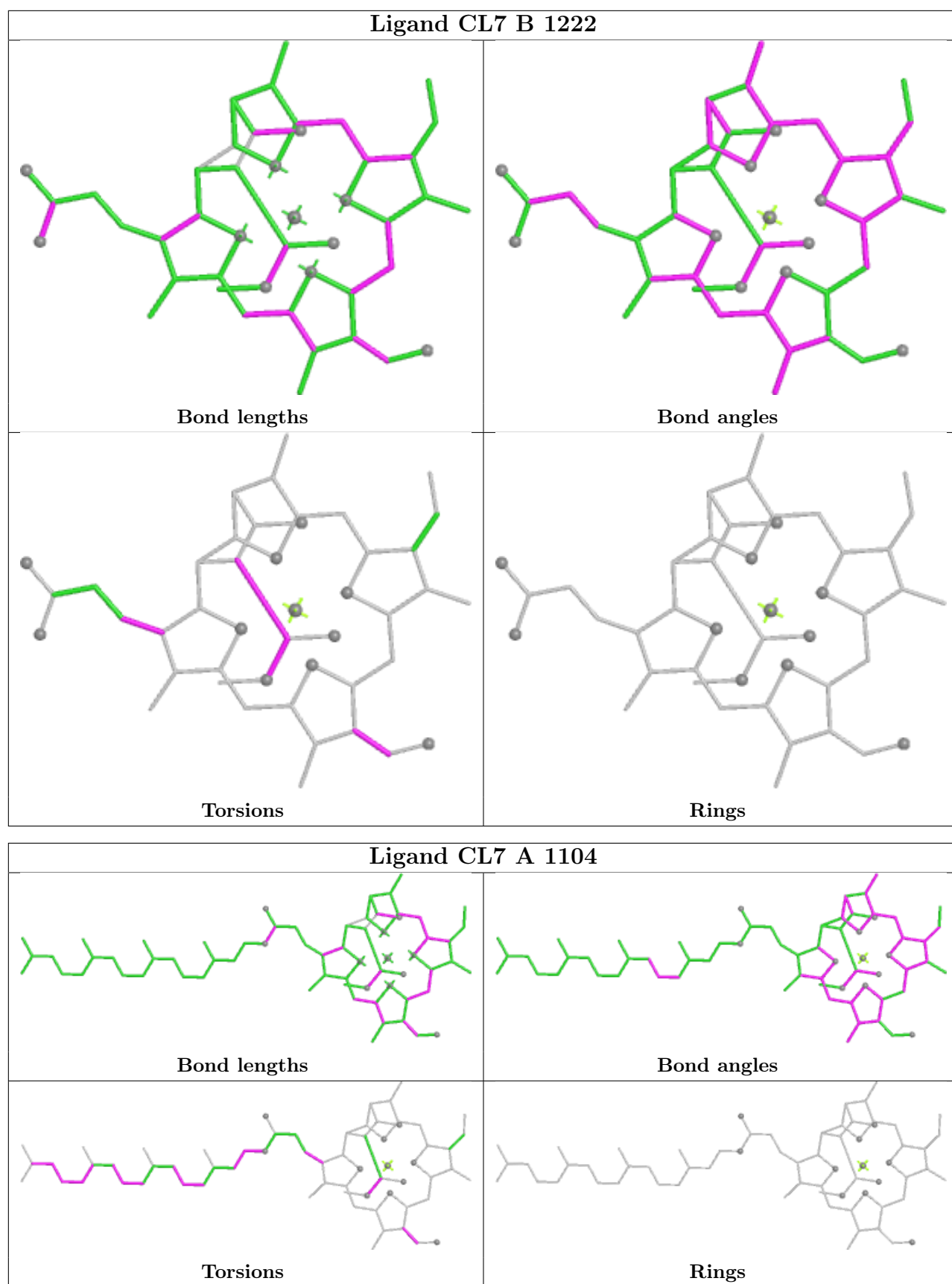


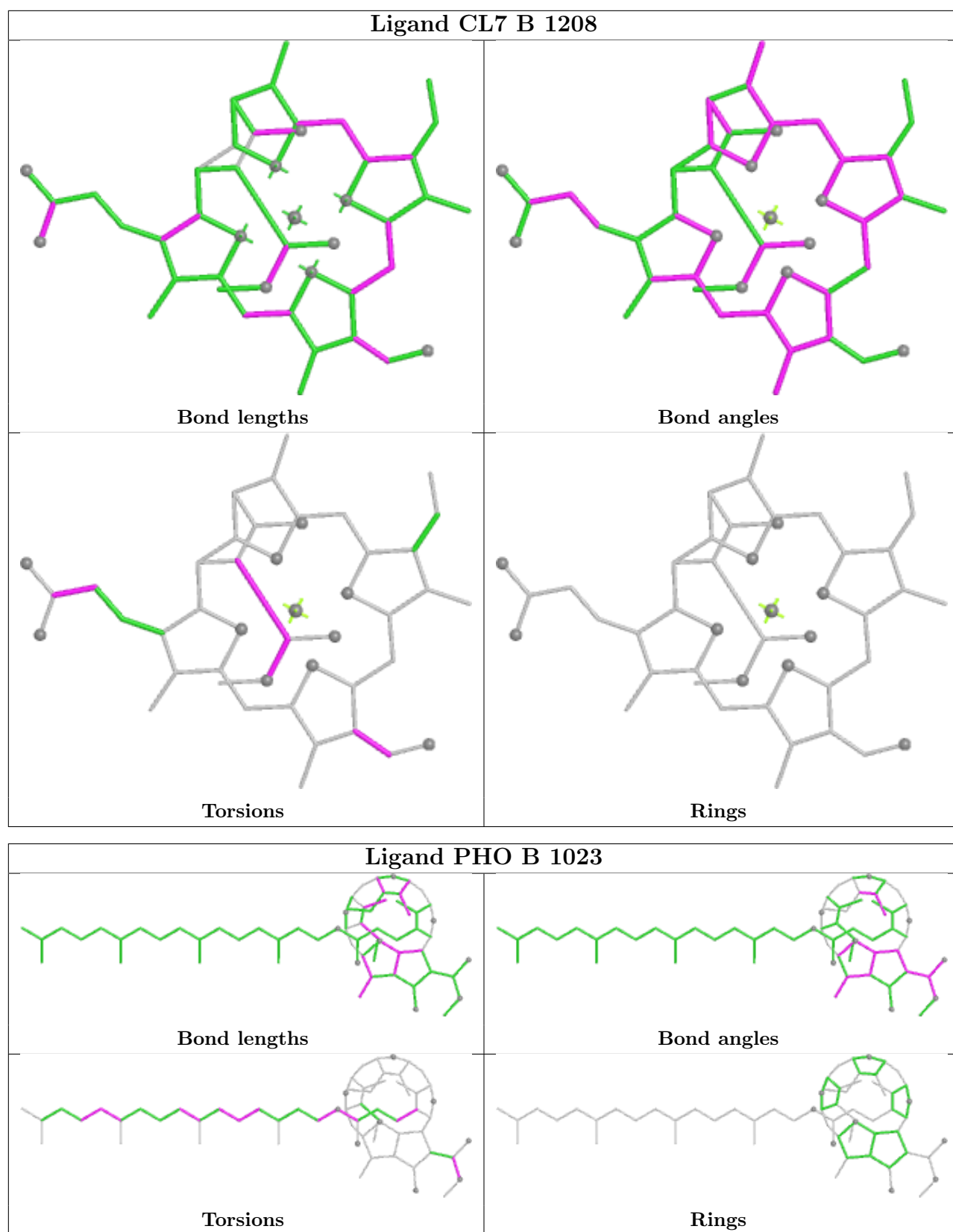


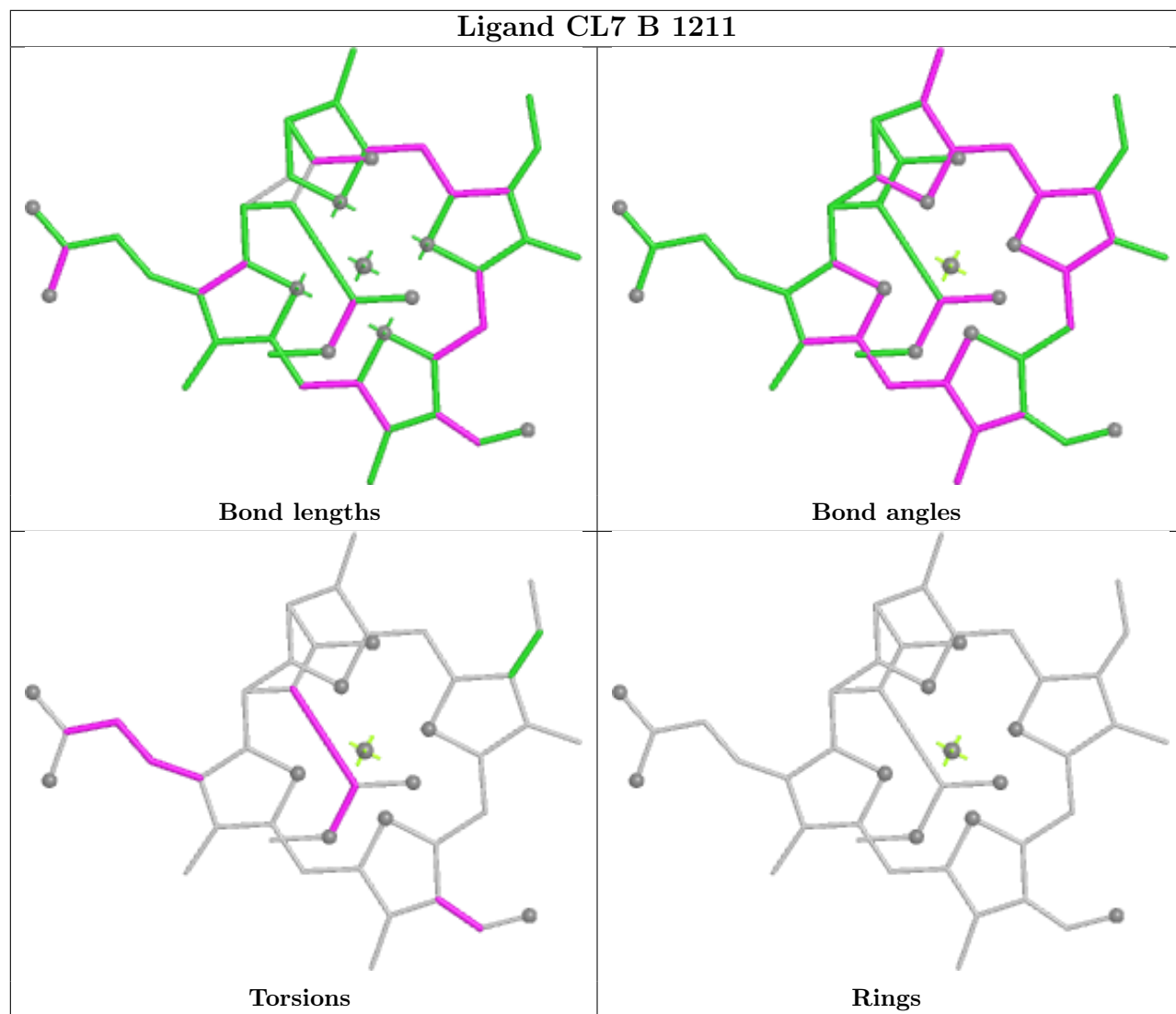


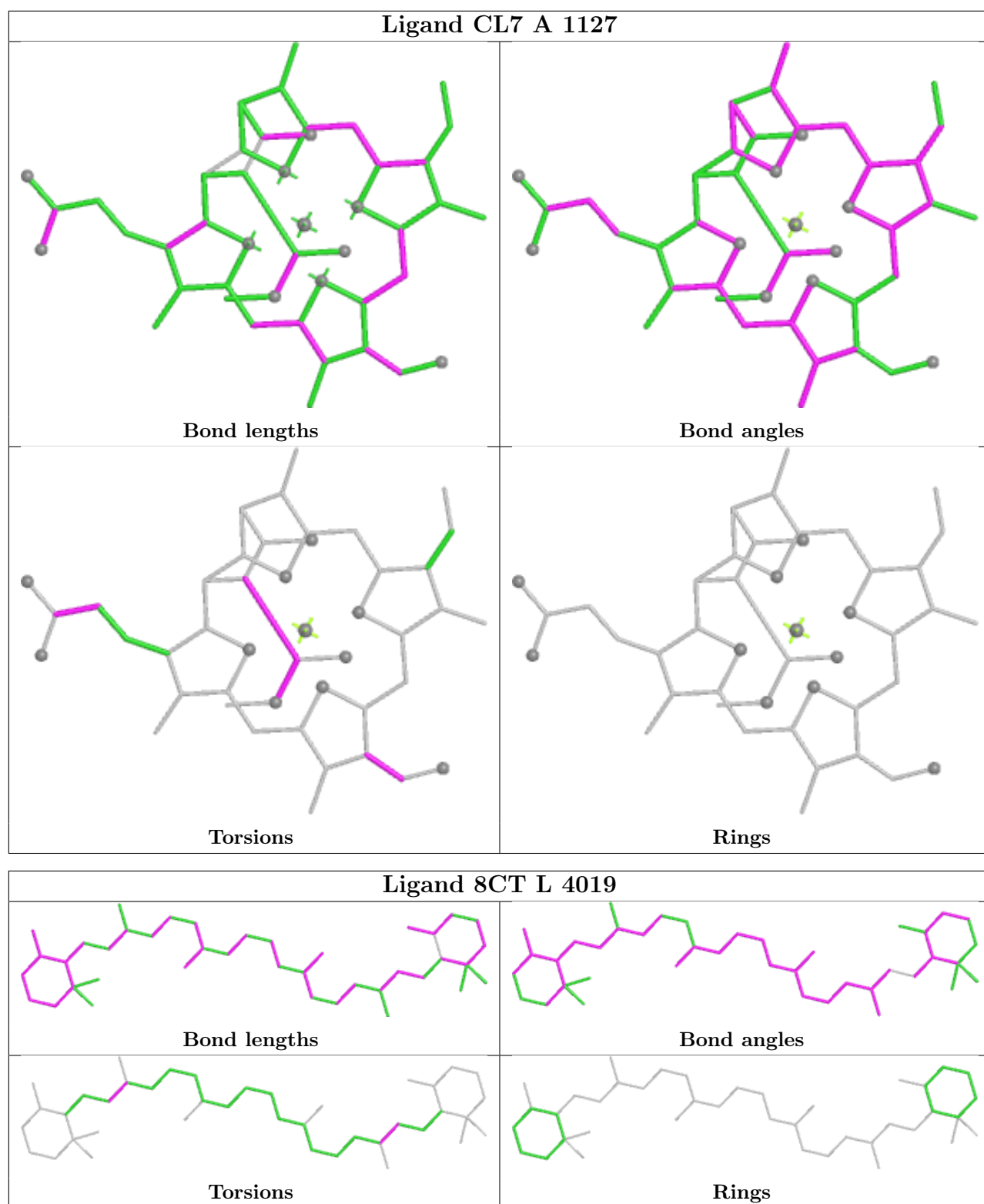


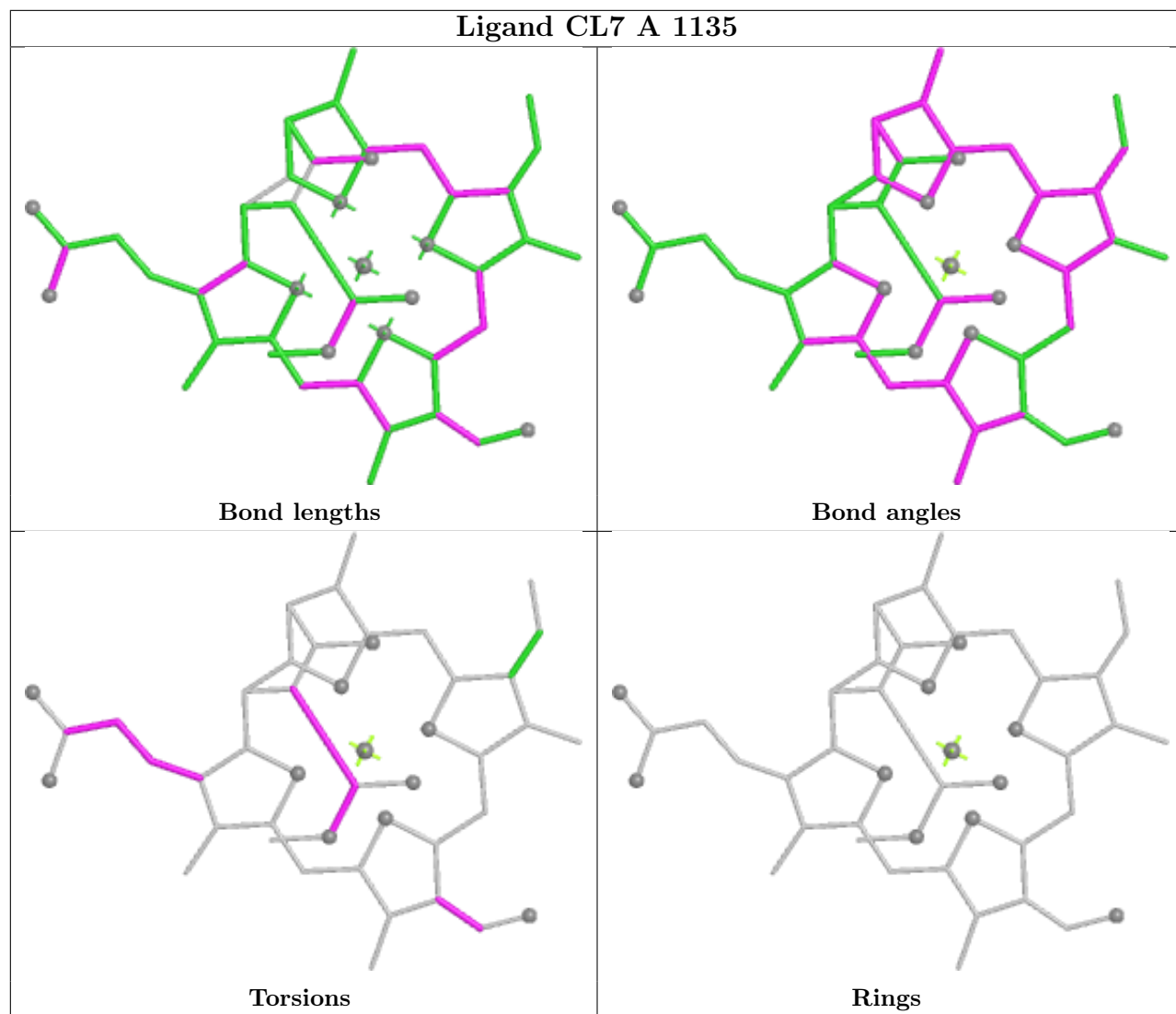


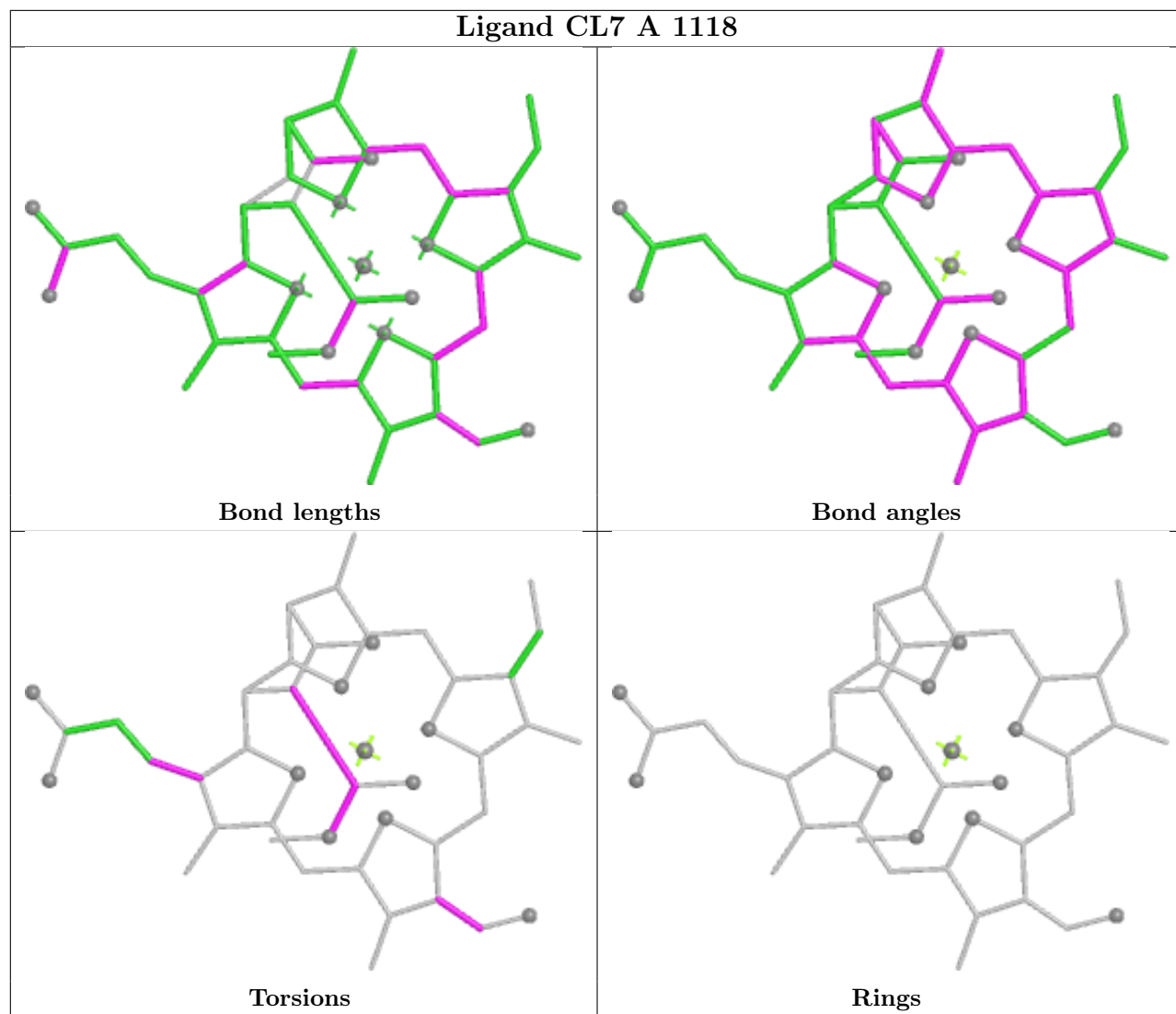


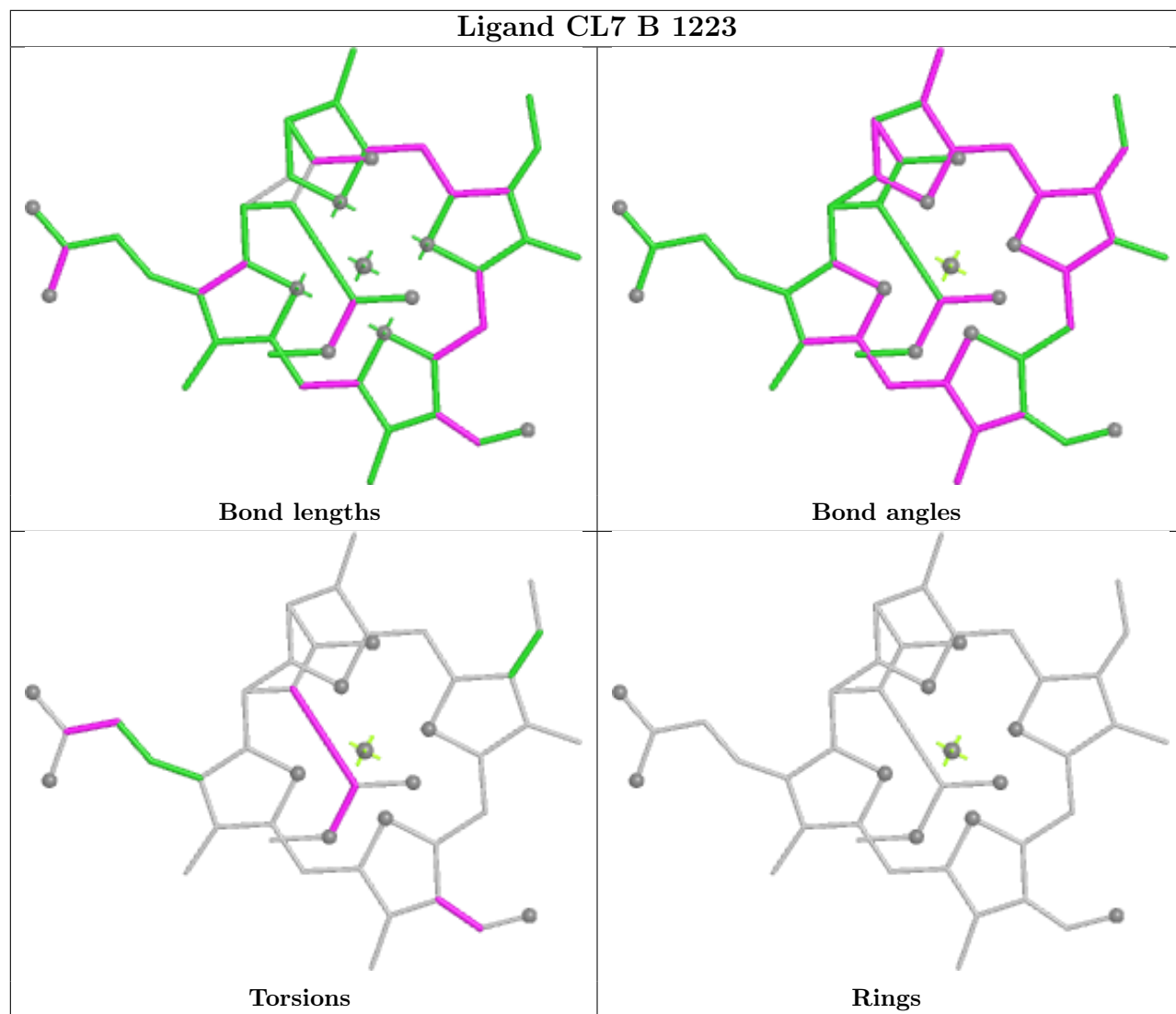


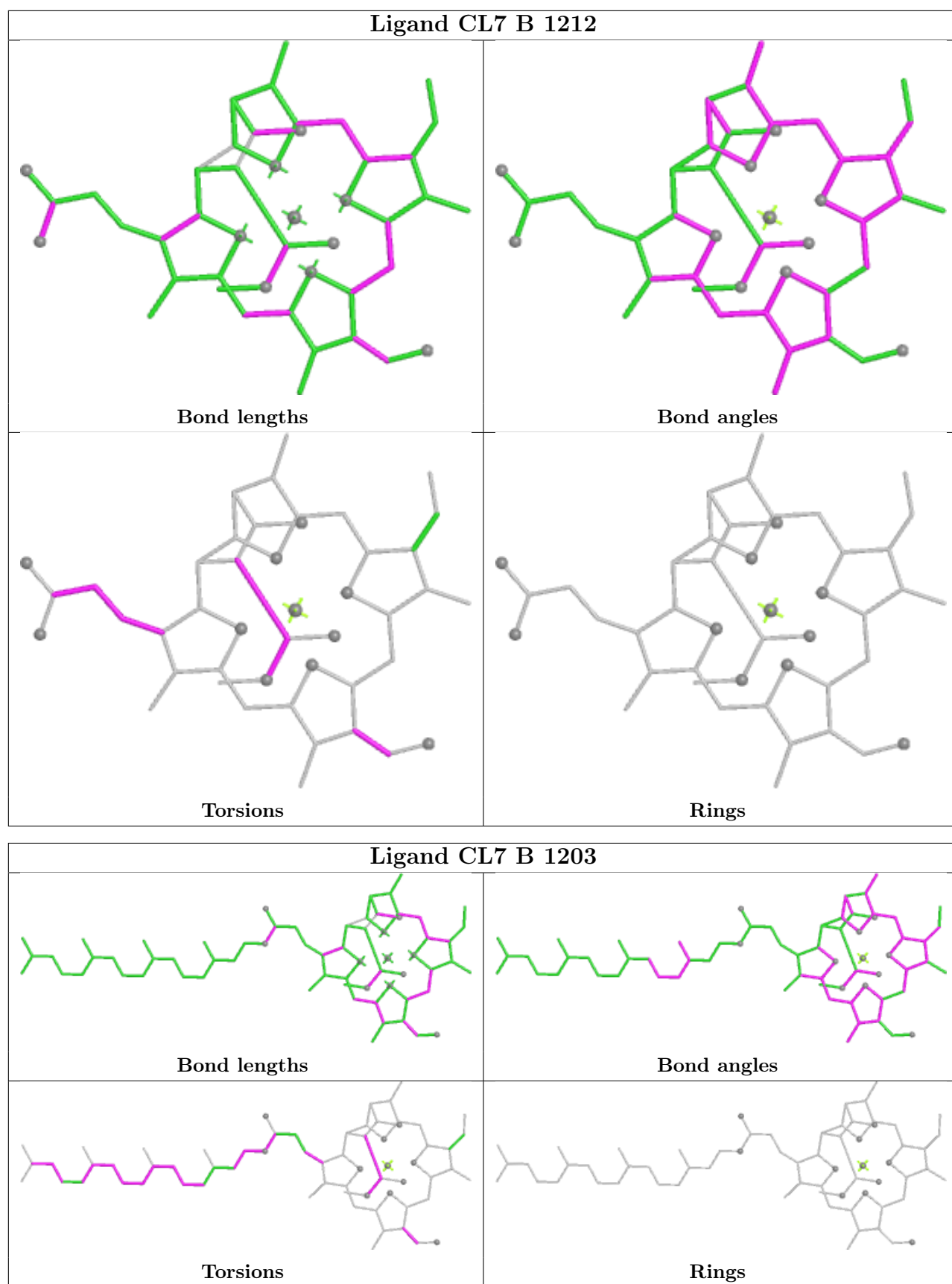


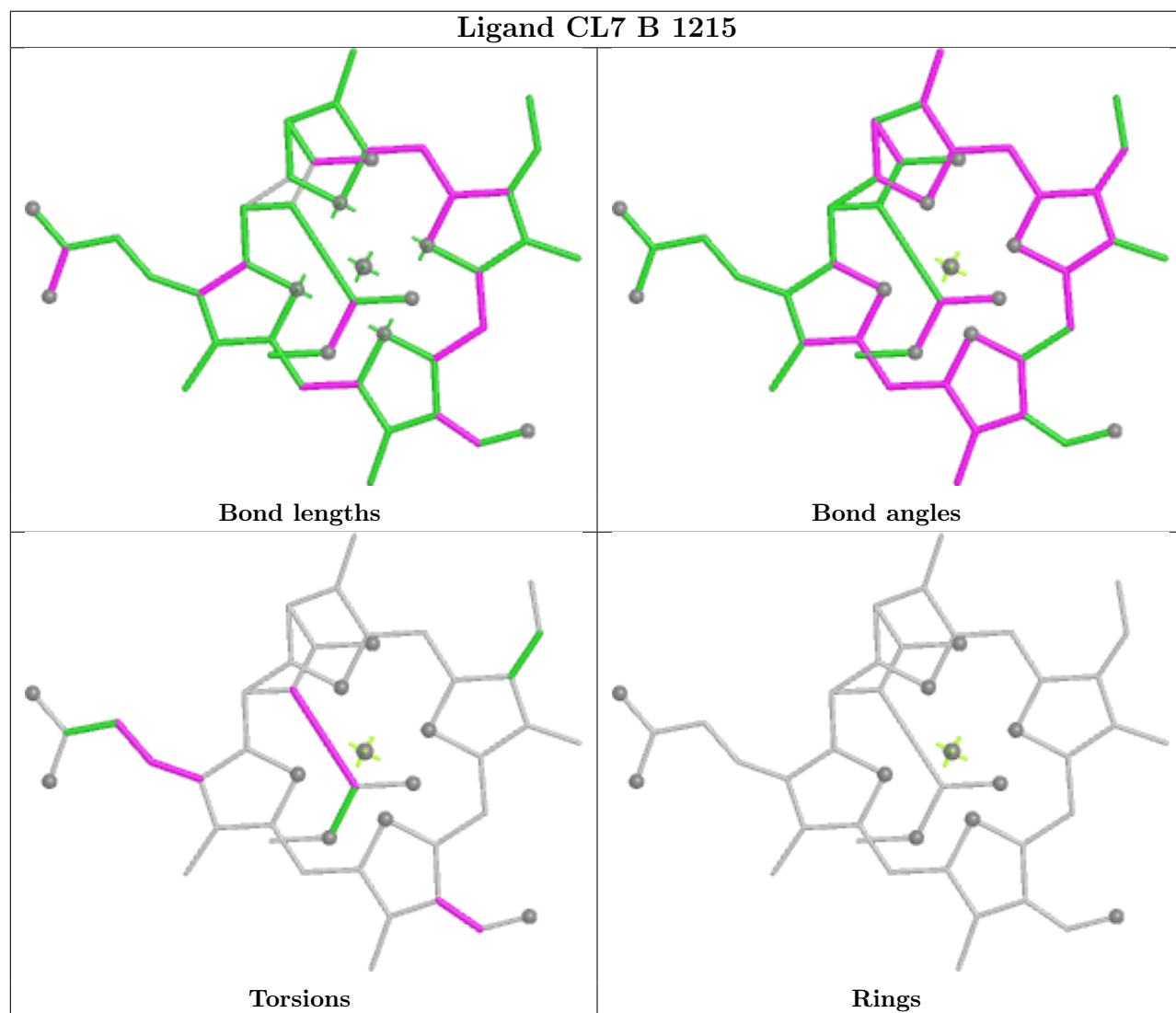
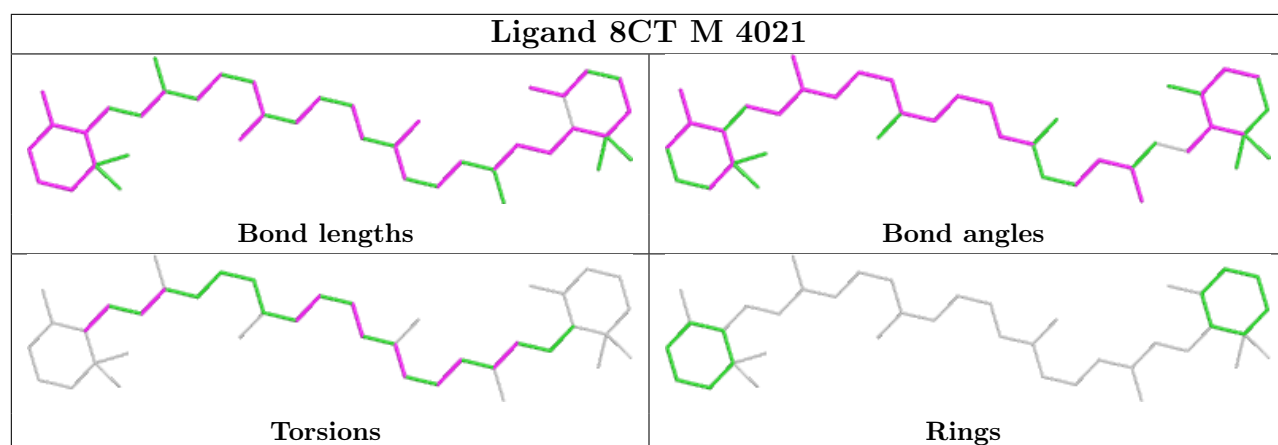


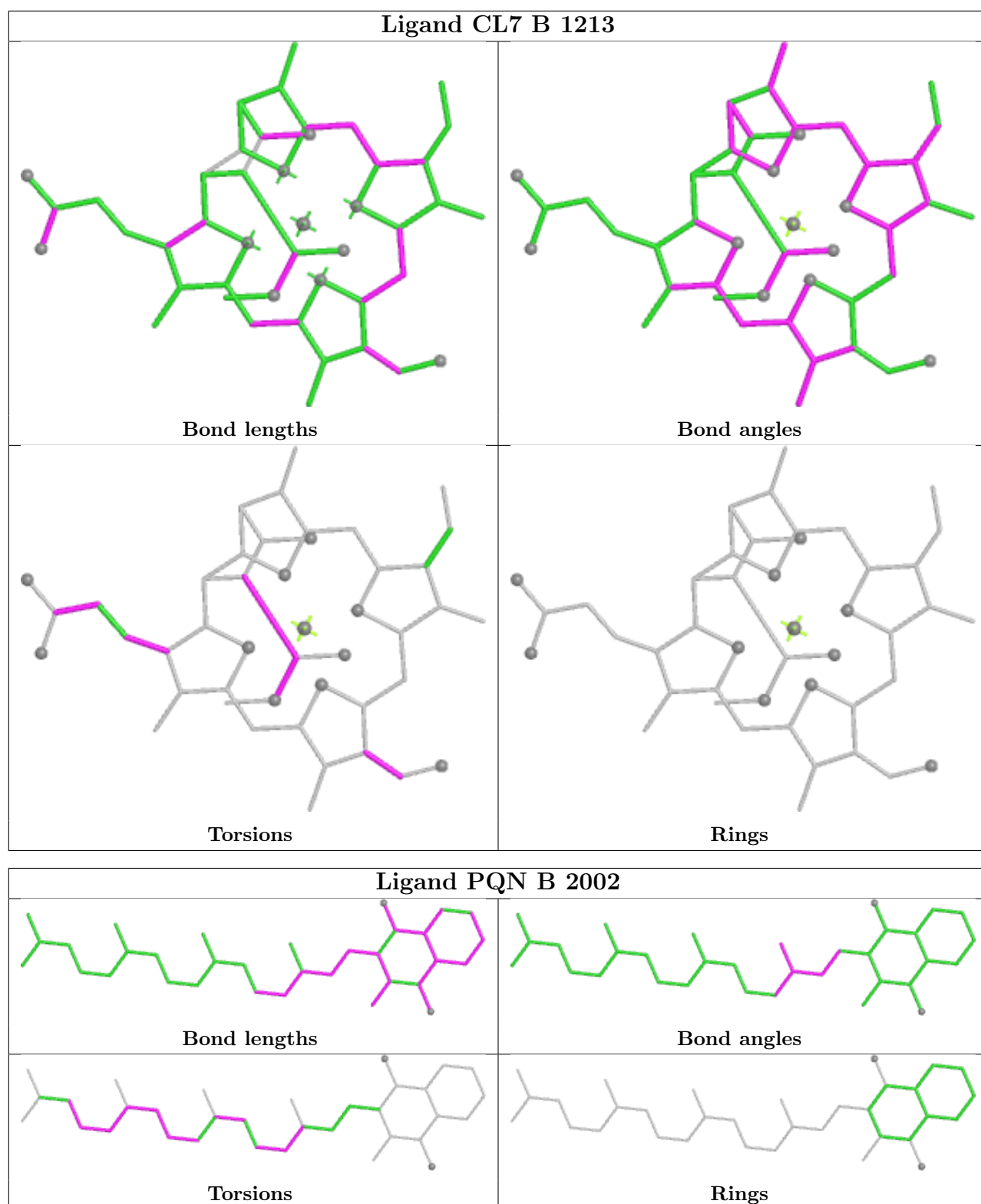


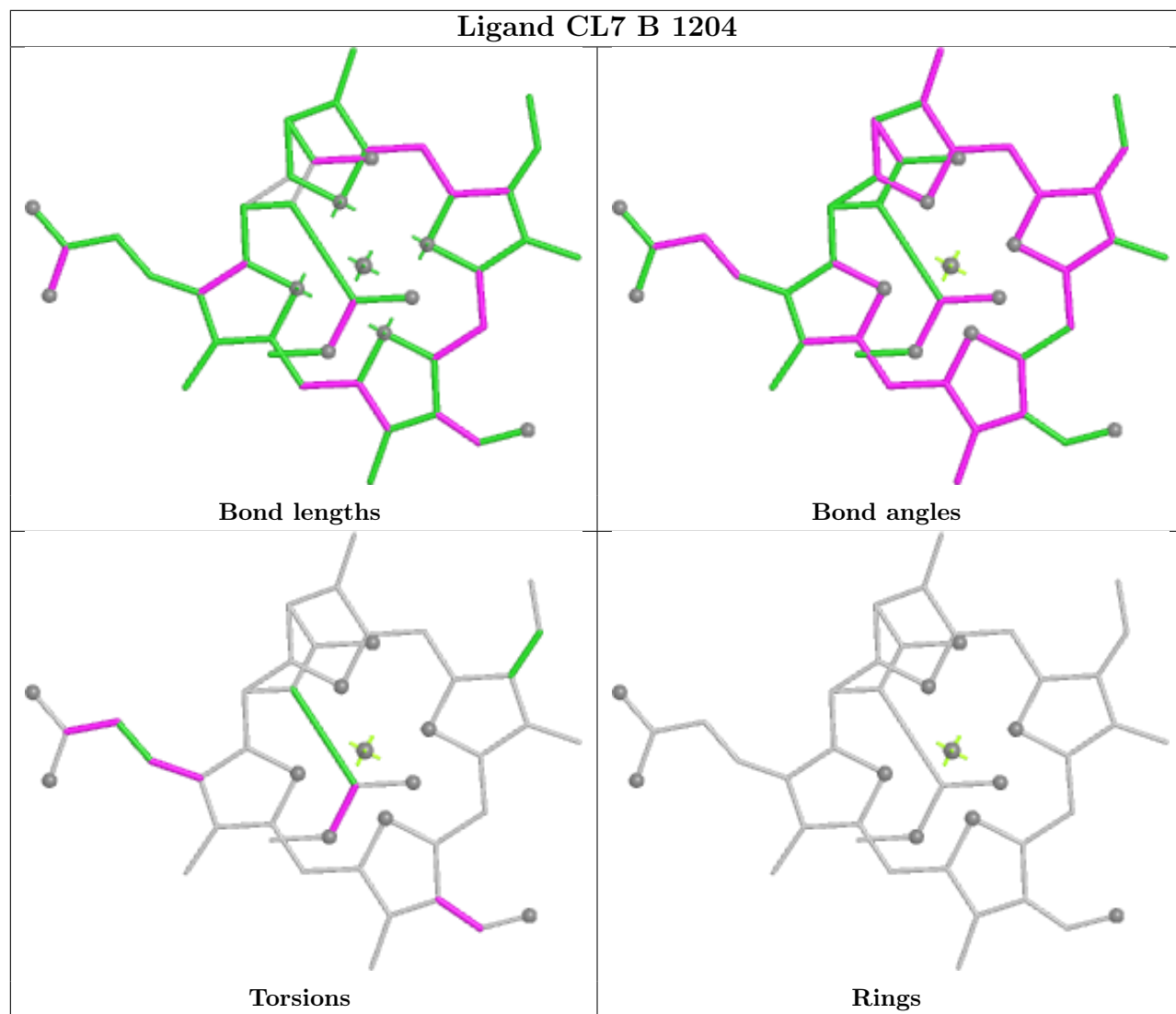


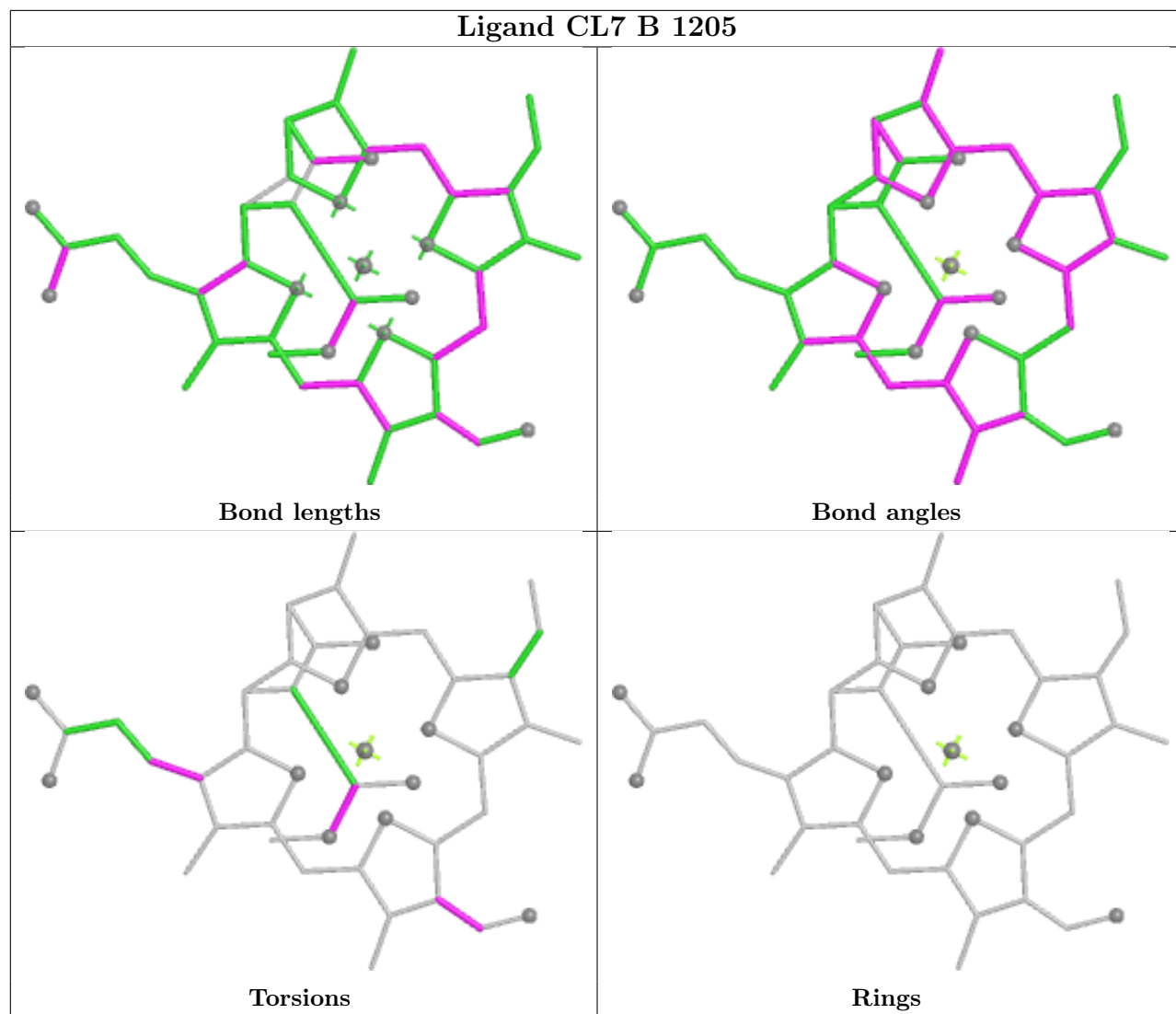


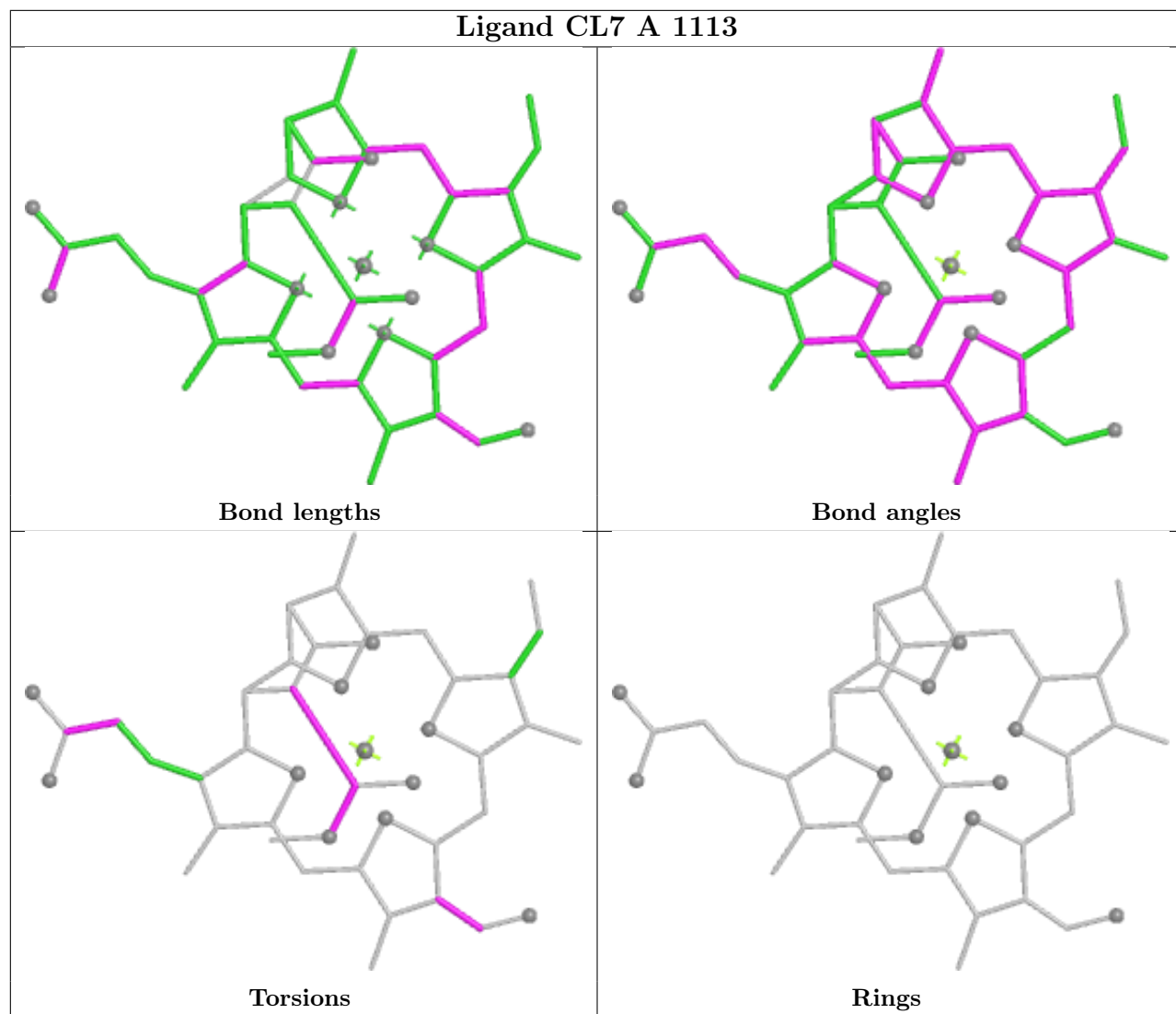


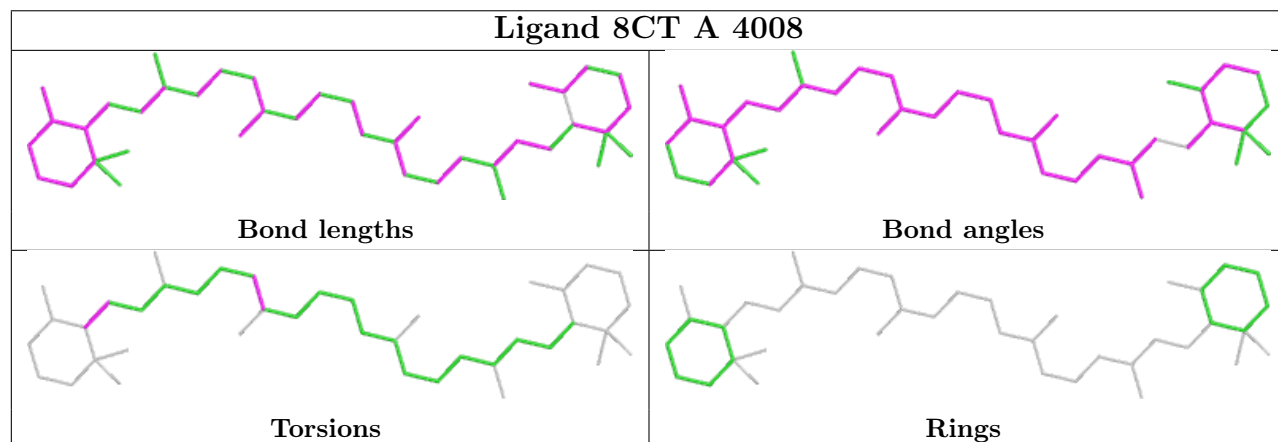
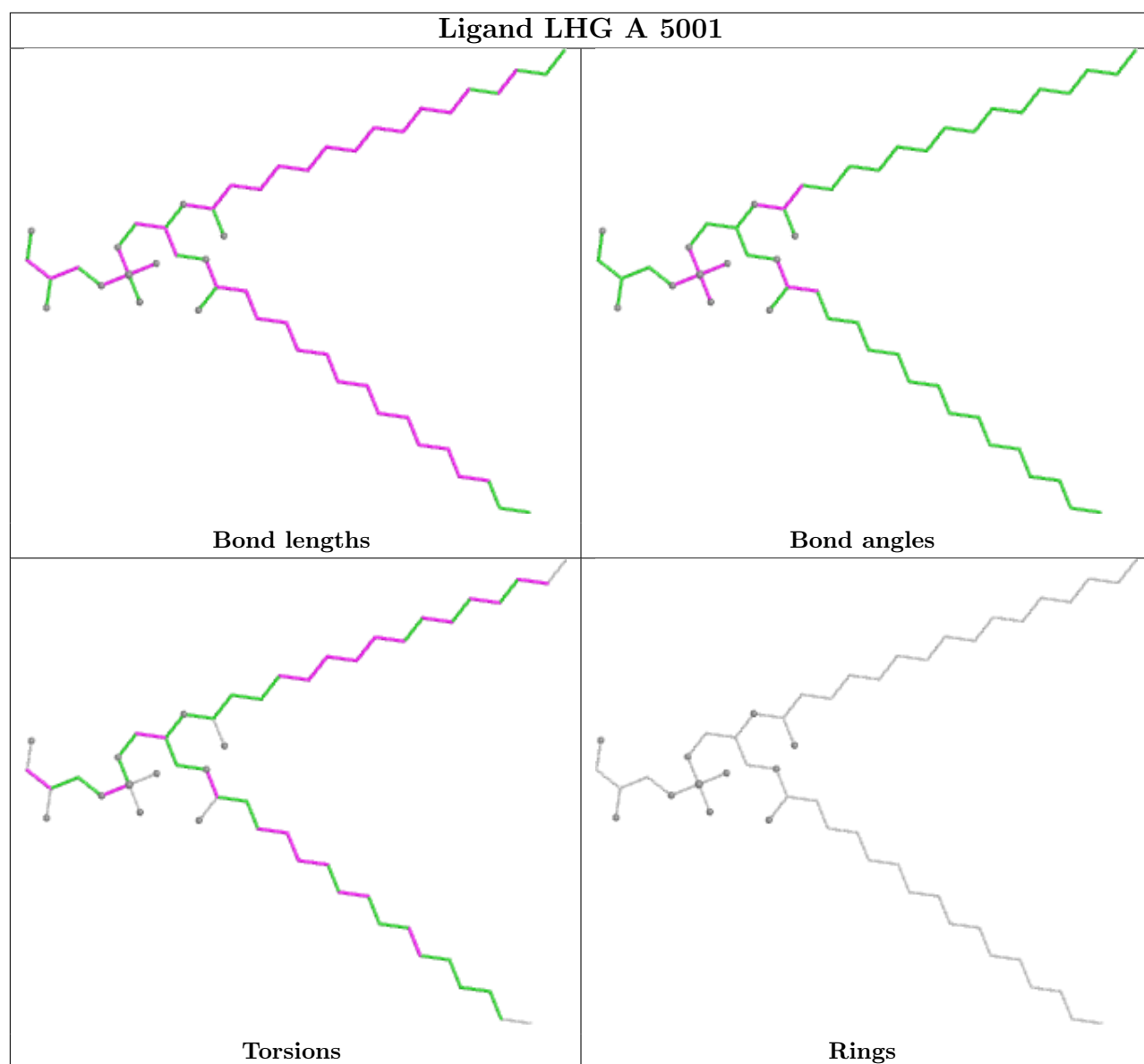


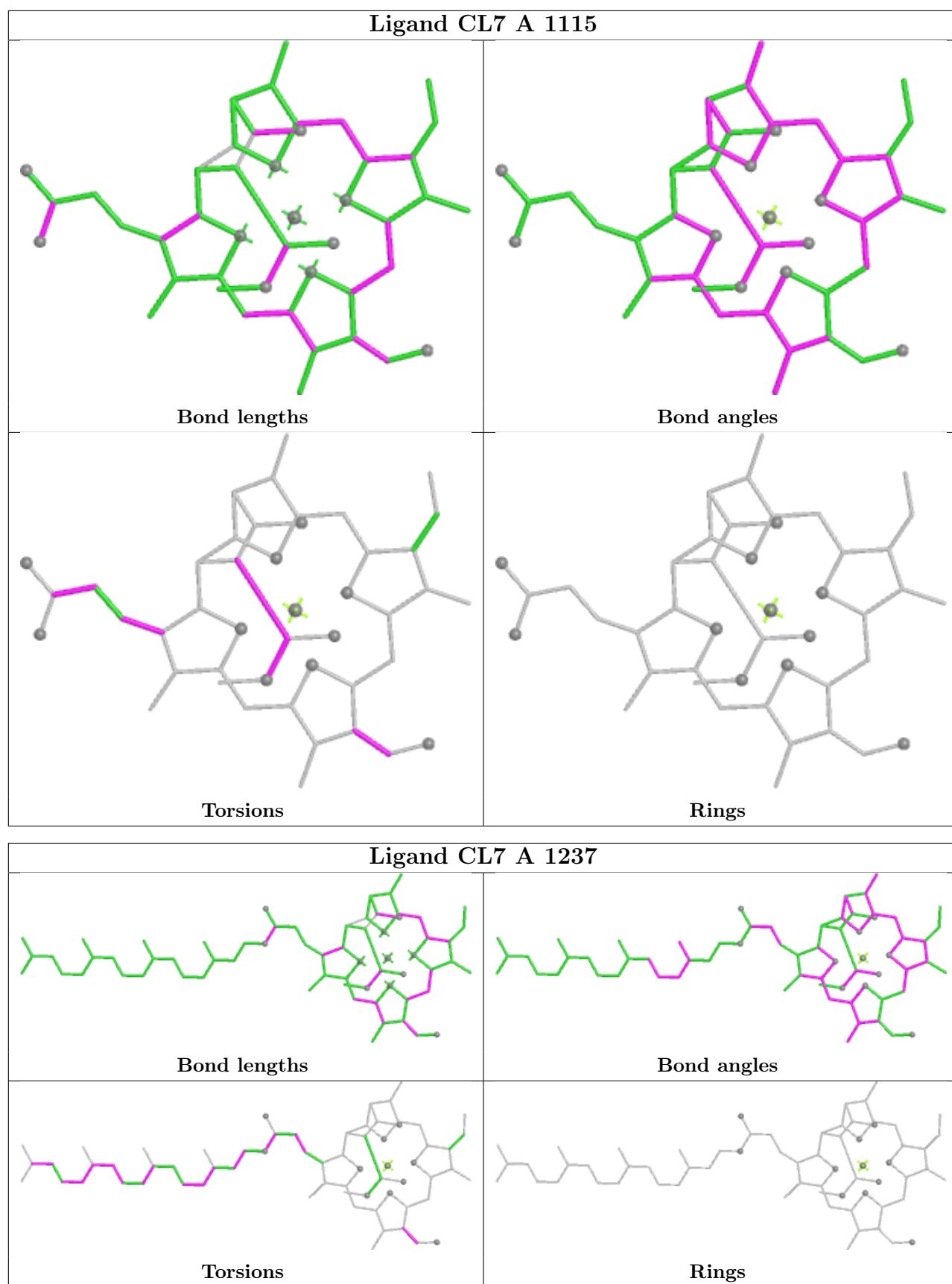


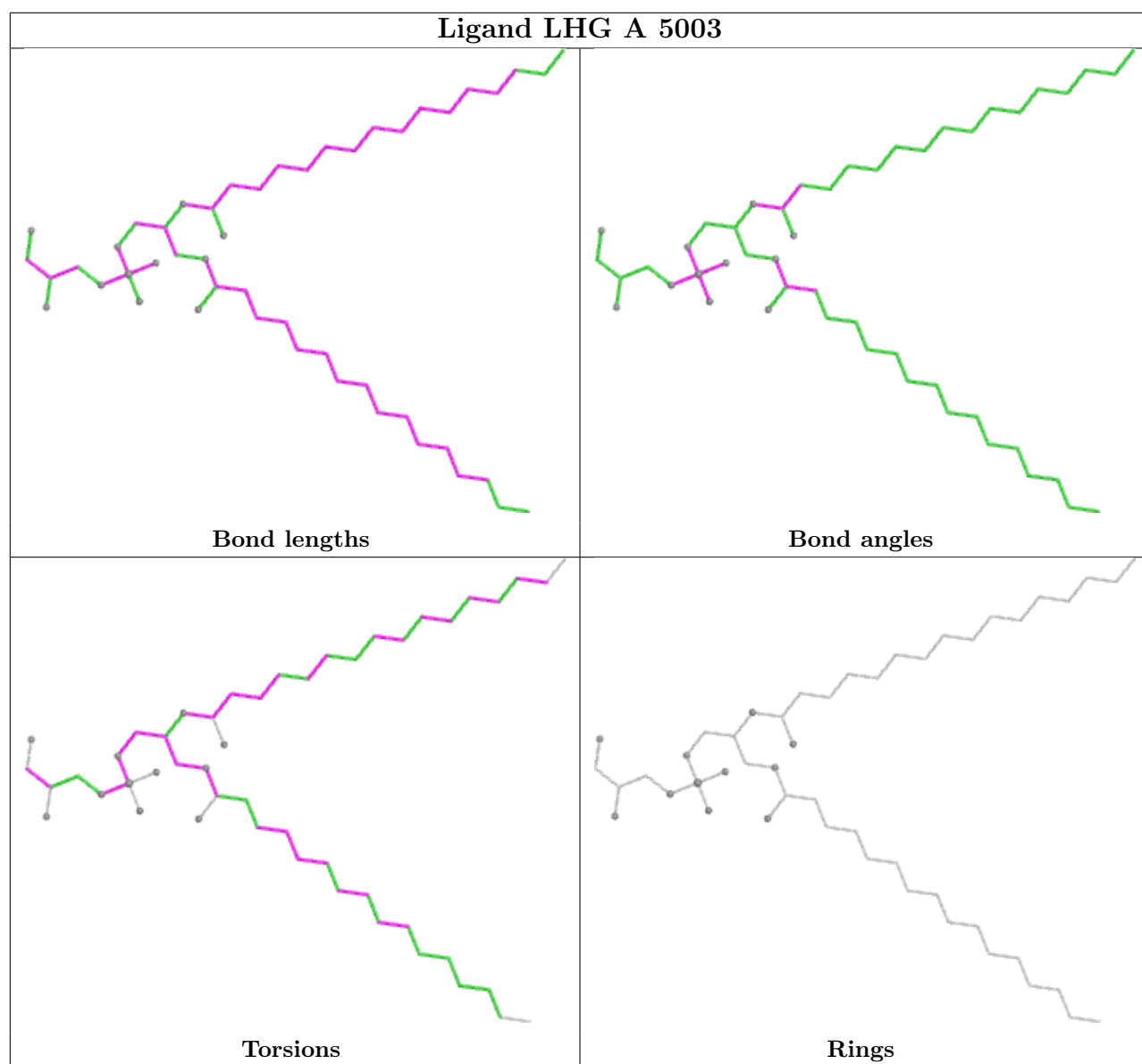


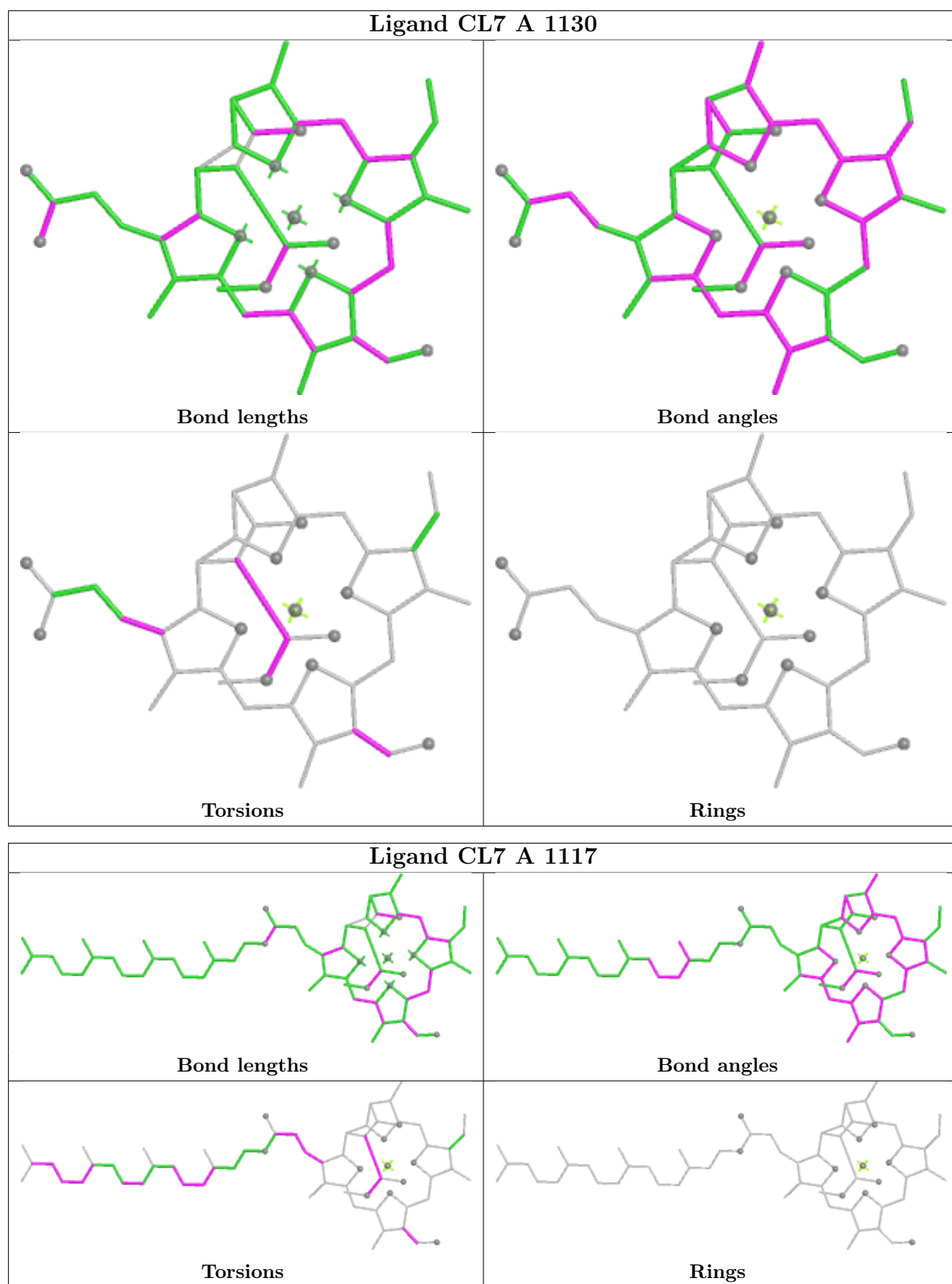


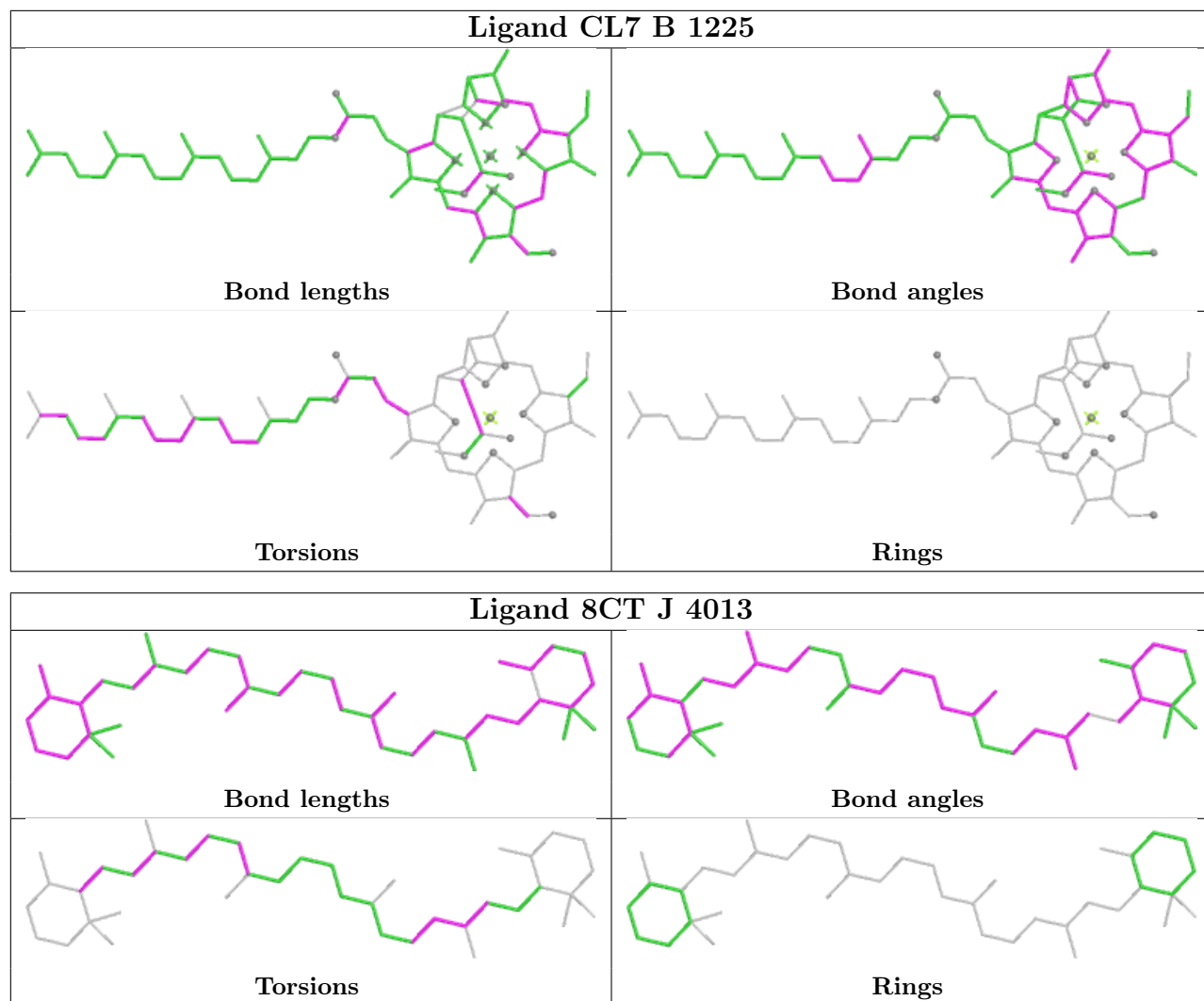


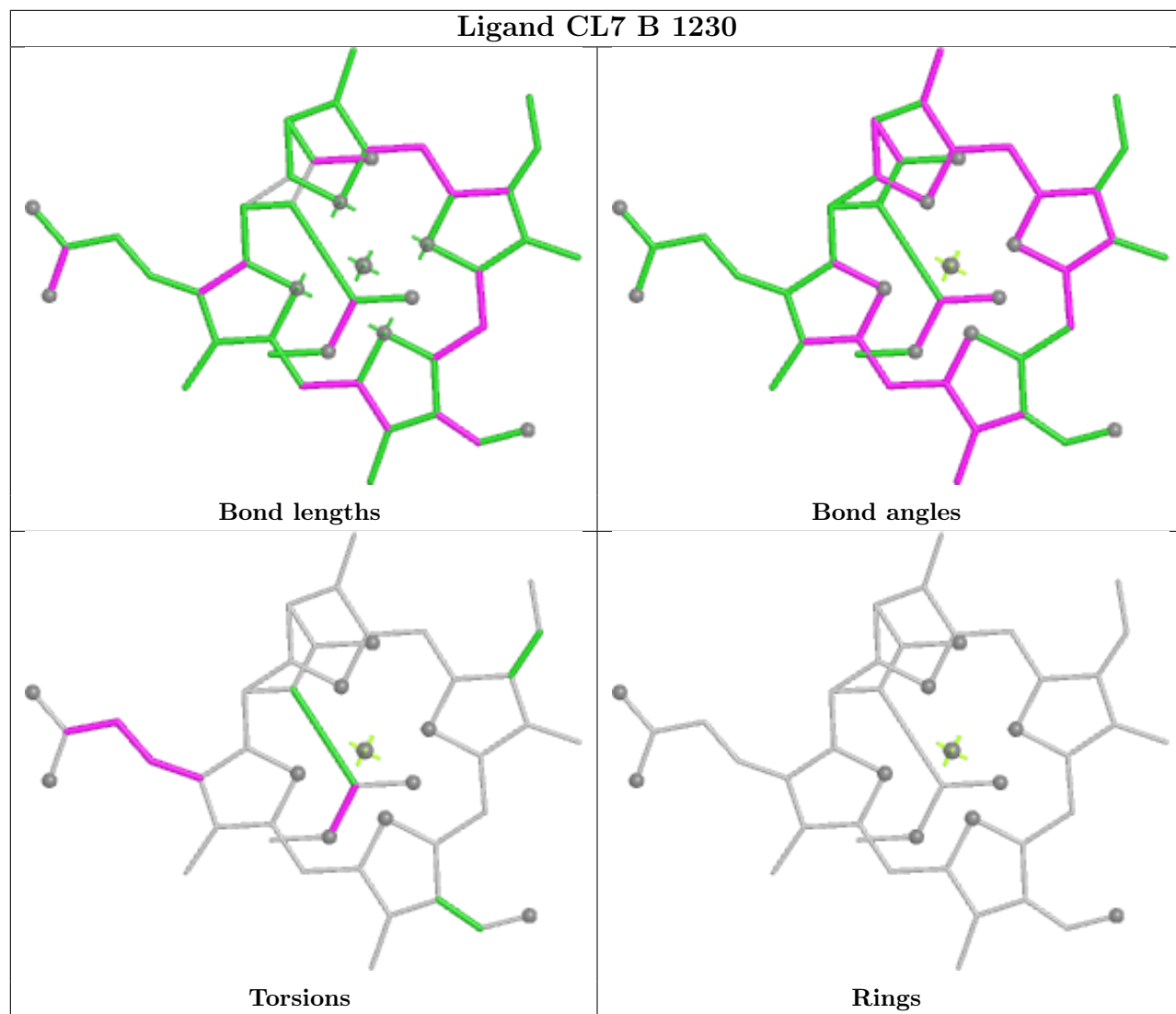


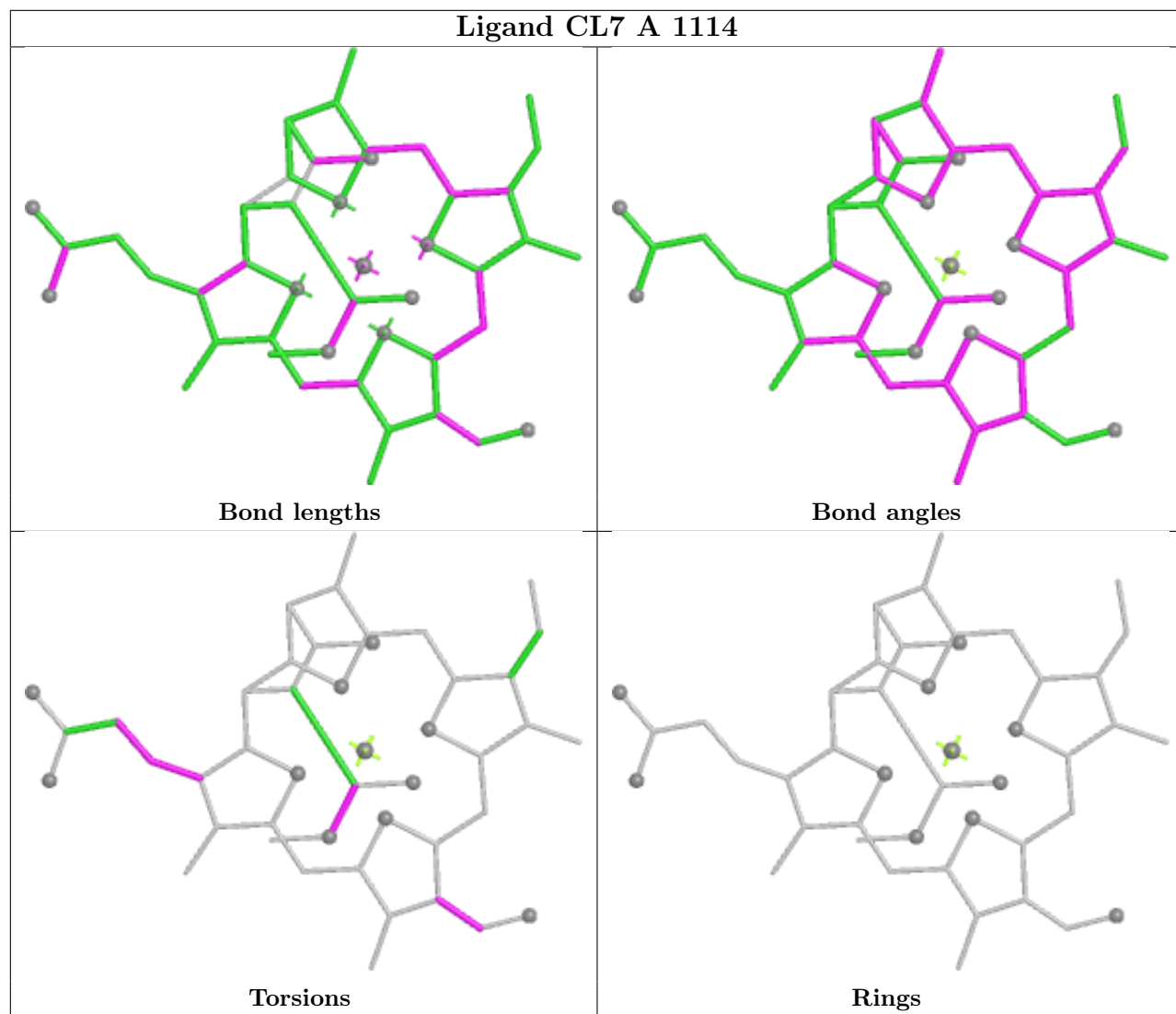


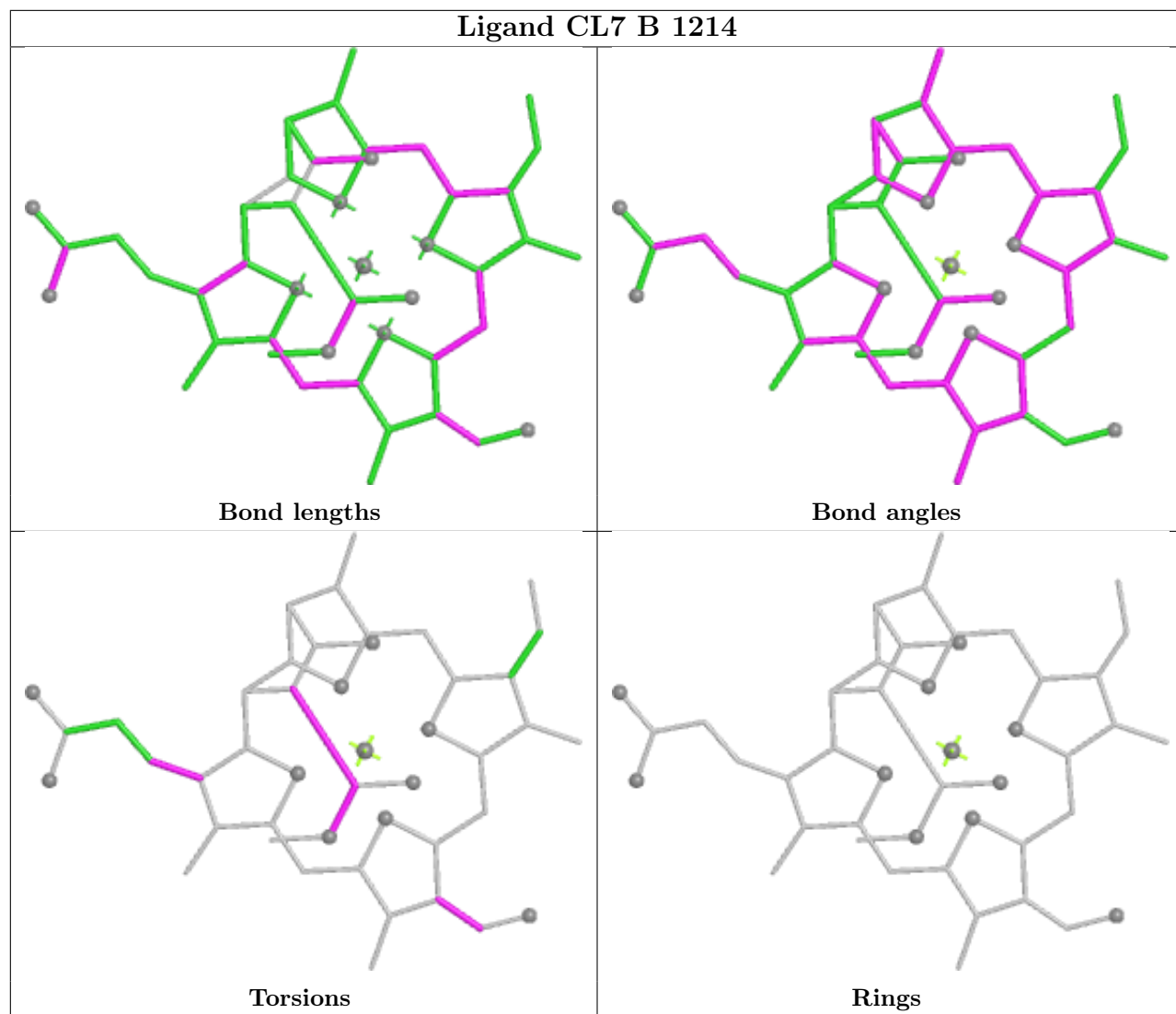


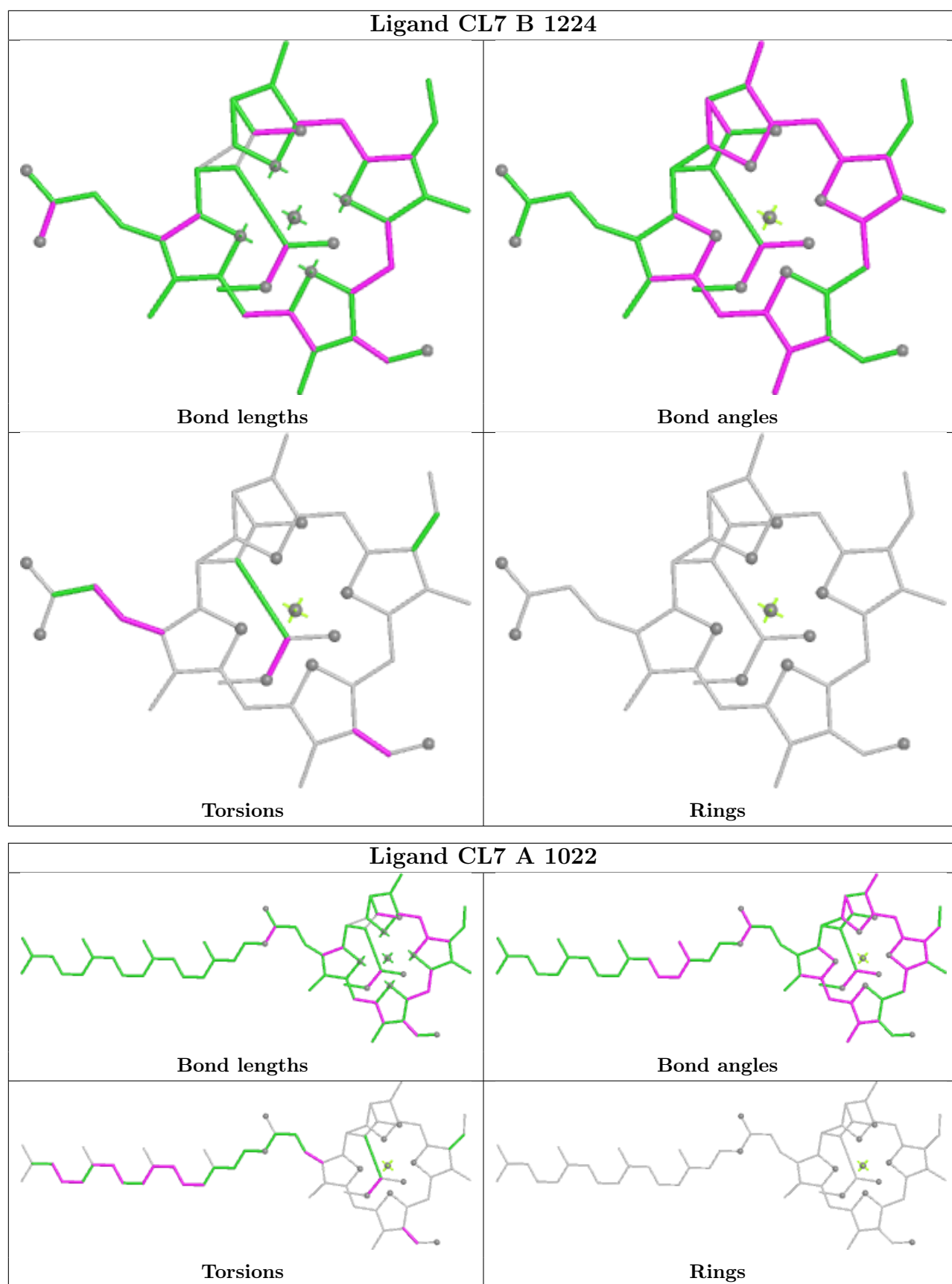


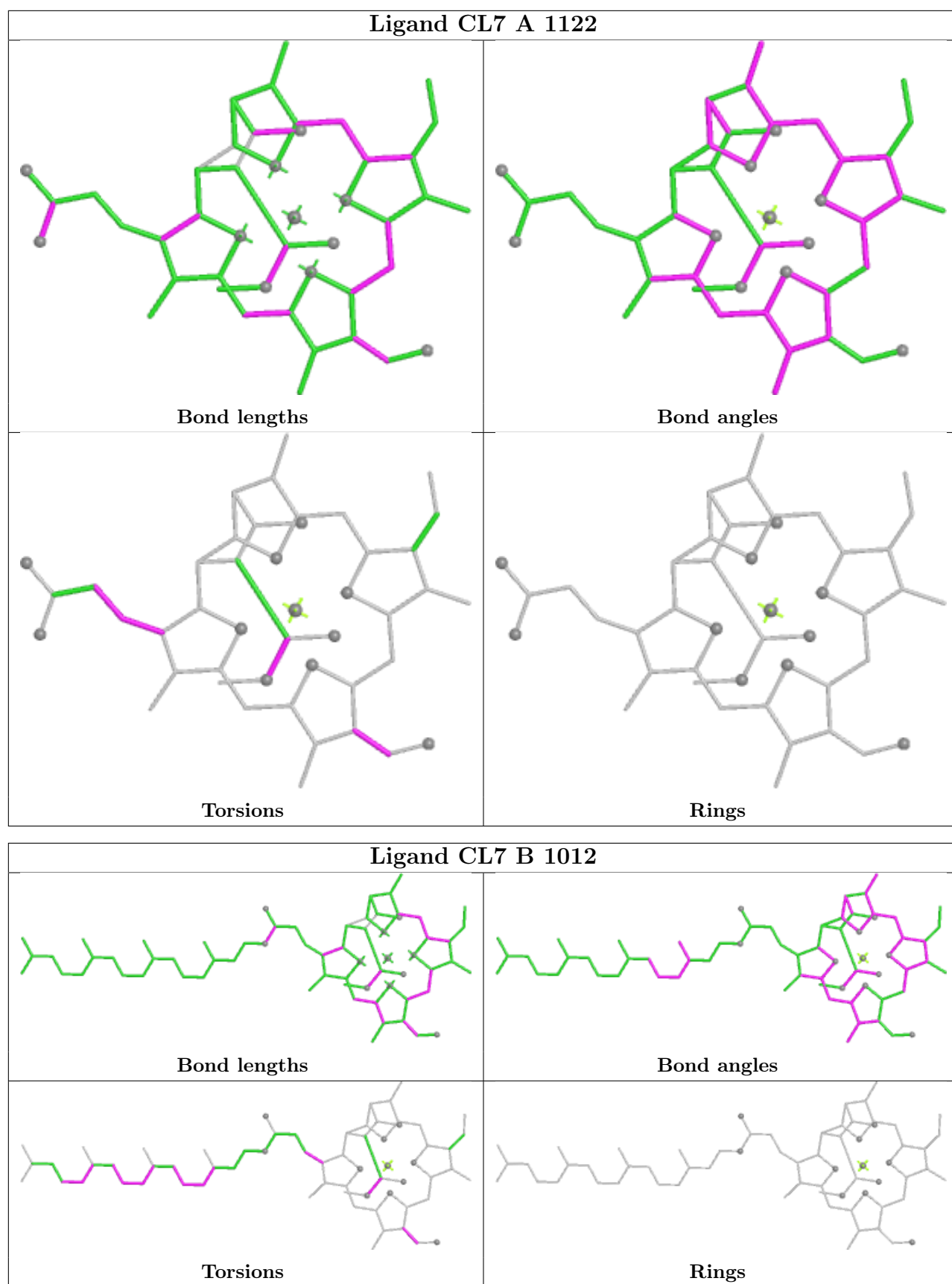


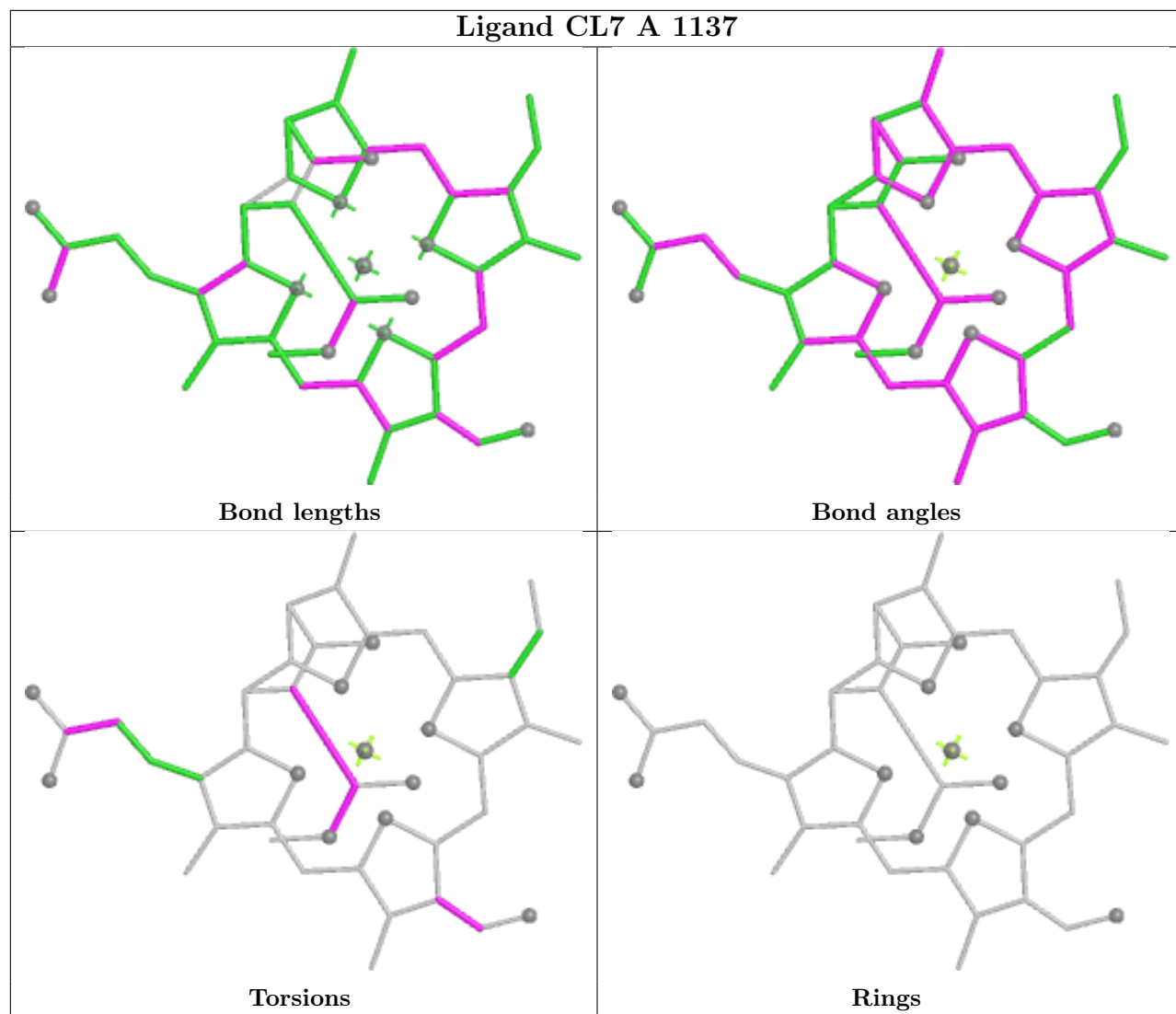


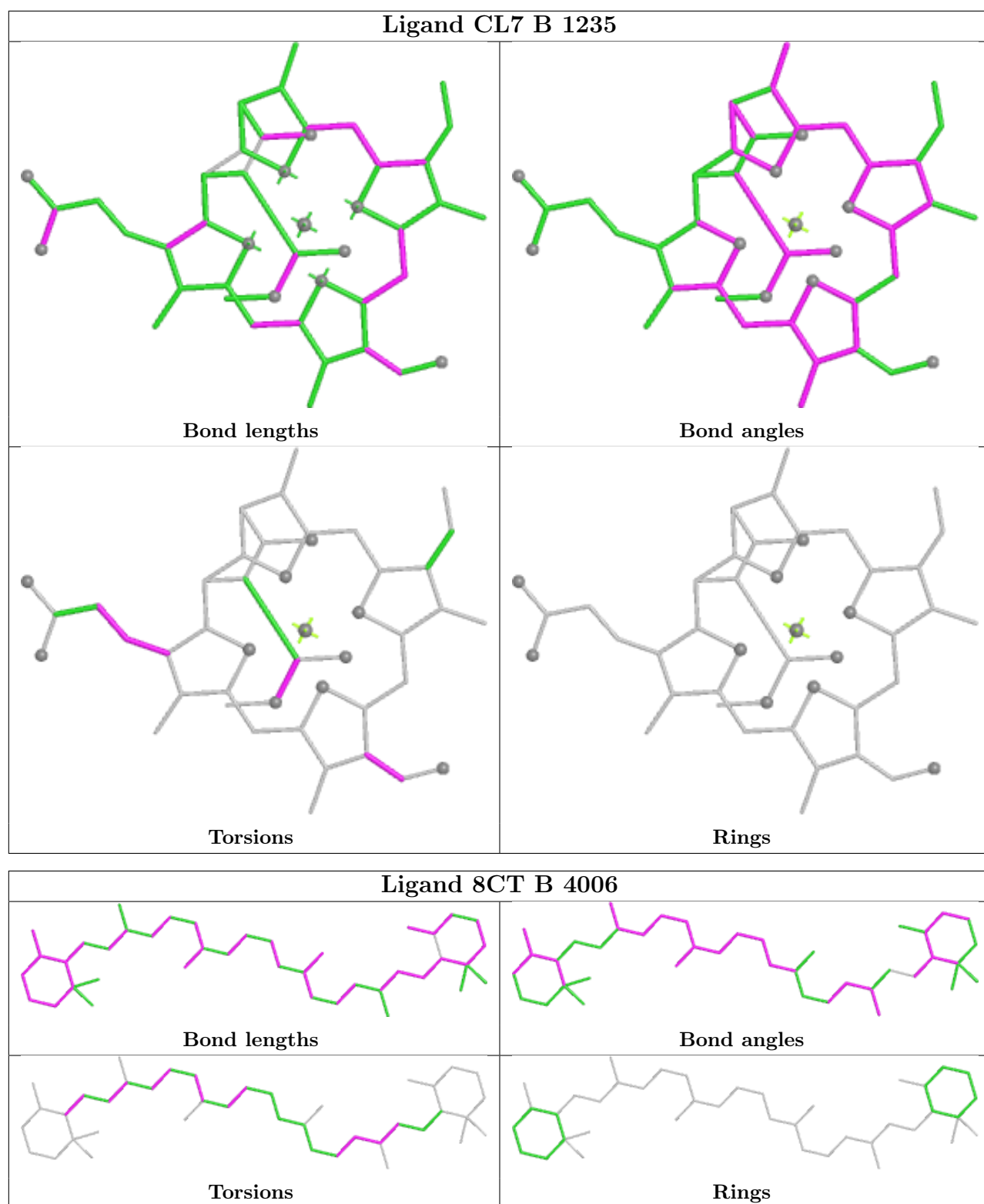


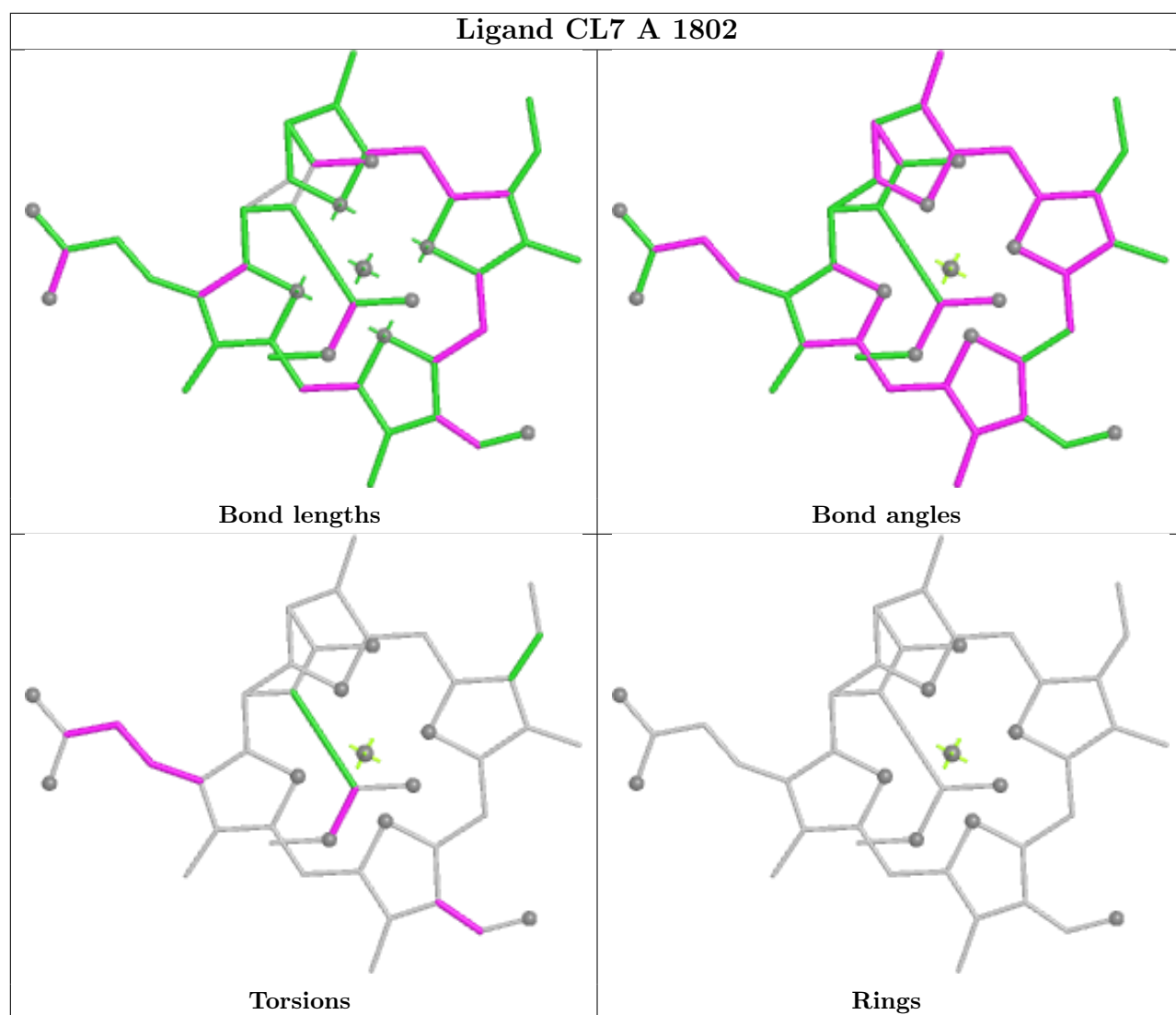


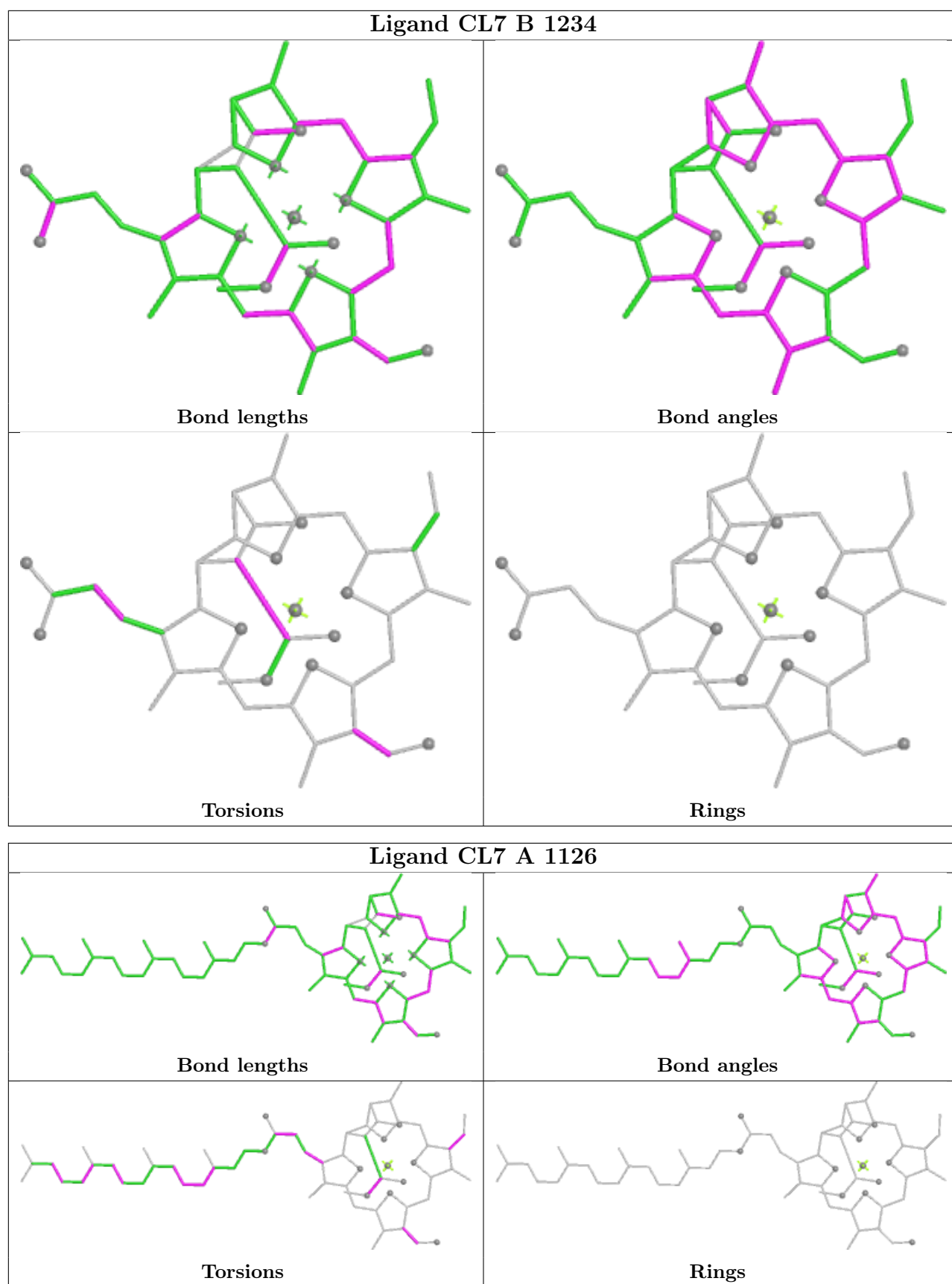


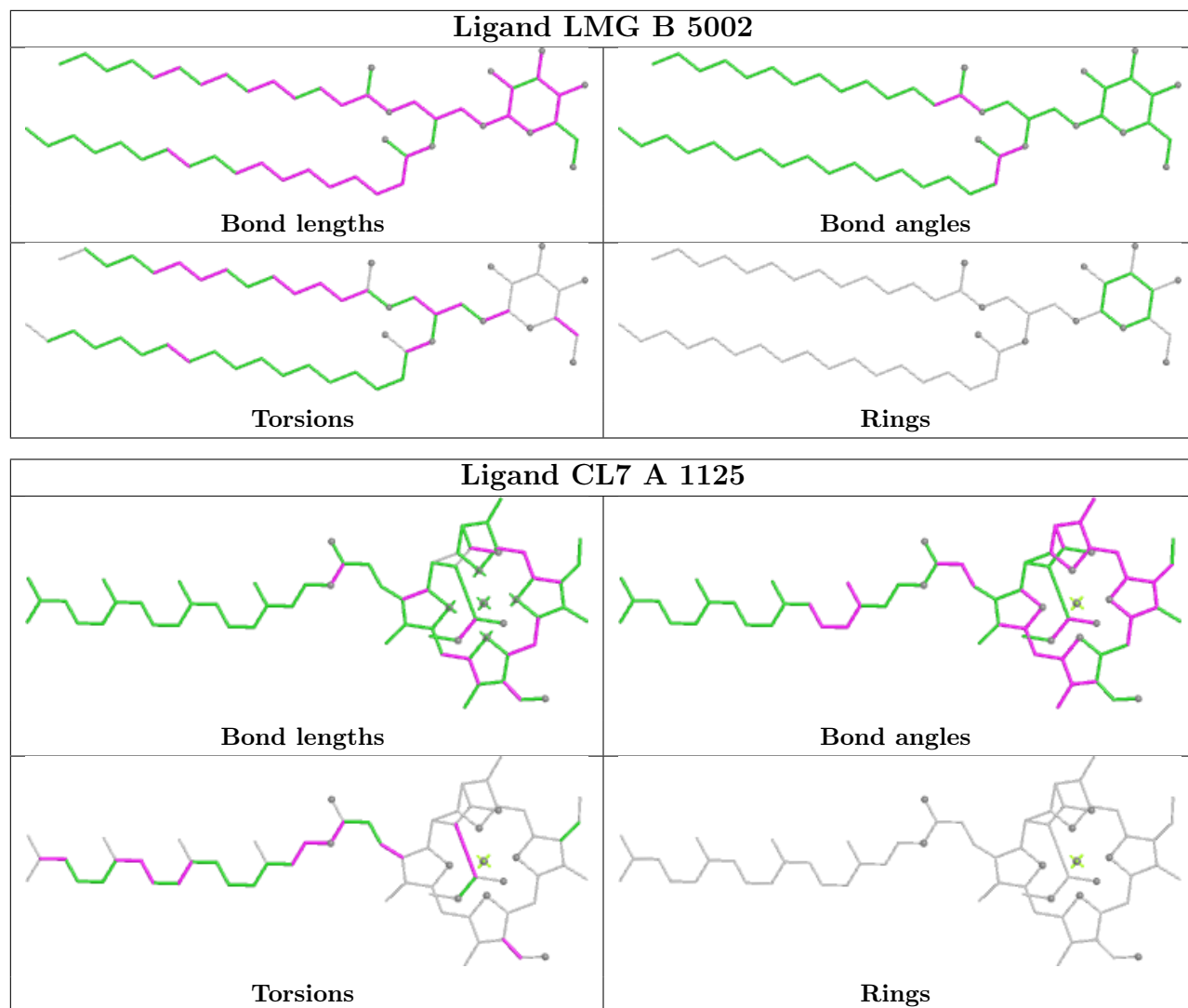


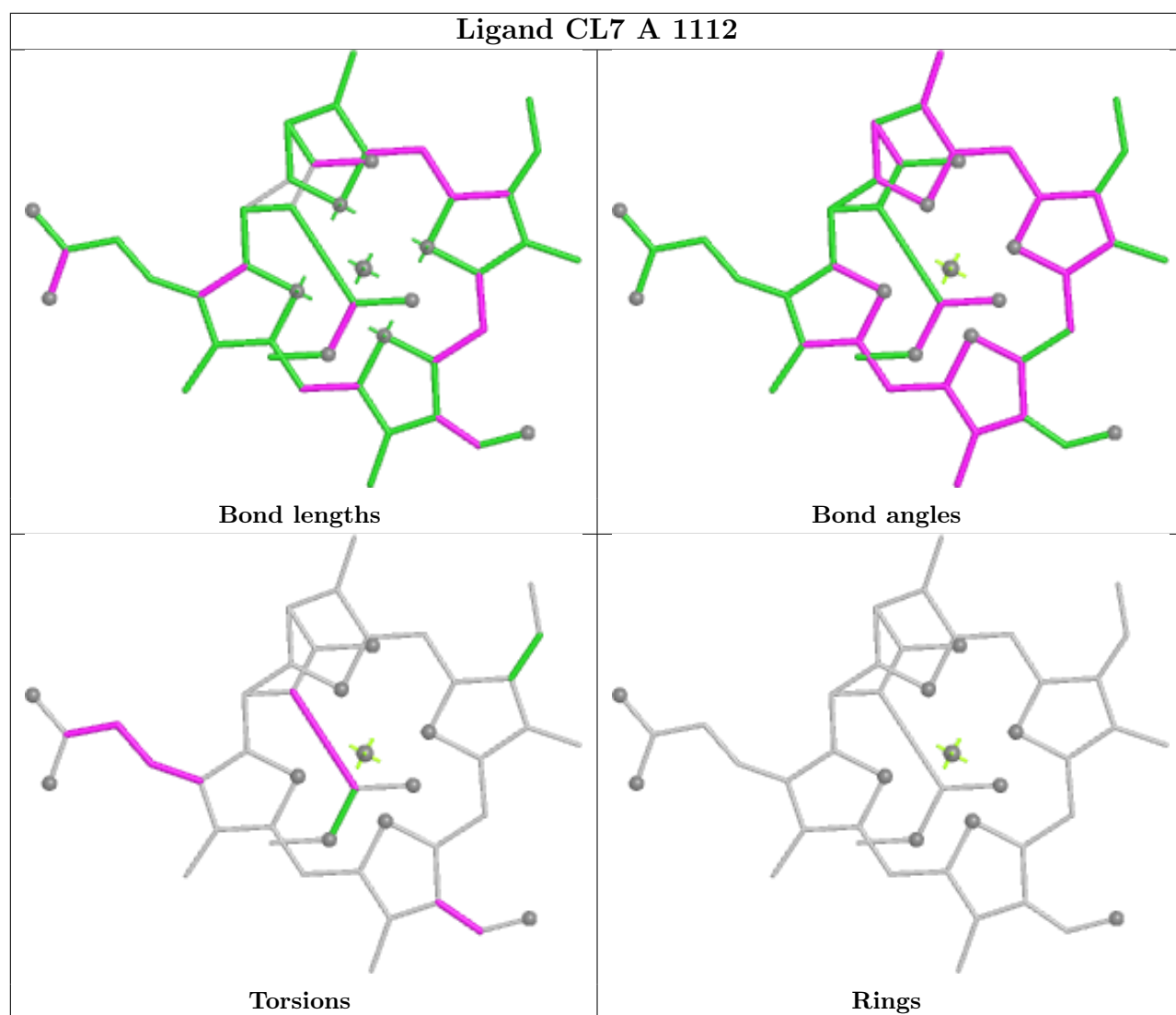












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

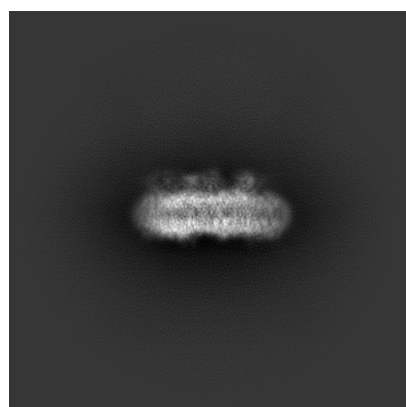
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30882. These allow visual inspection of the internal detail of the map and identification of artifacts.

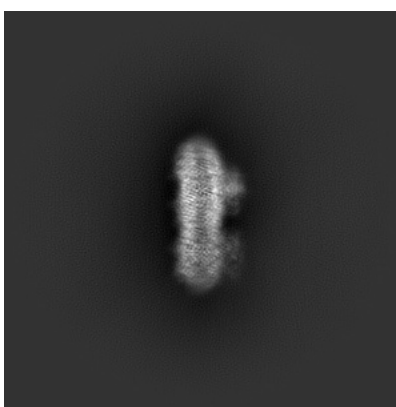
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

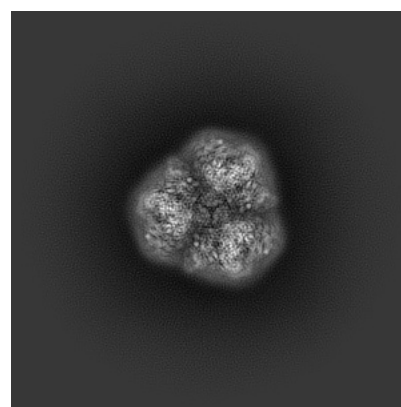
6.1.1 Primary map



X



Y

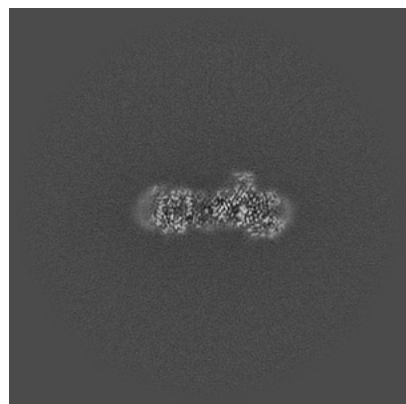


Z

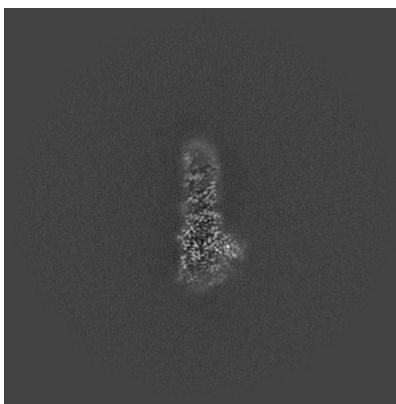
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

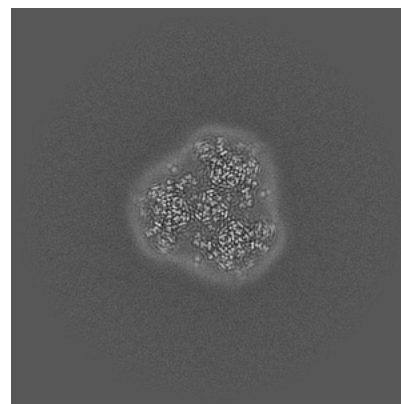
6.2.1 Primary map



X Index: 200



Y Index: 200

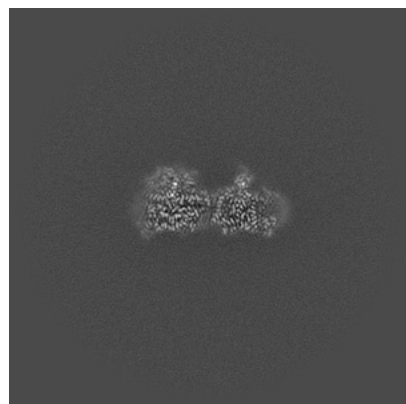


Z Index: 200

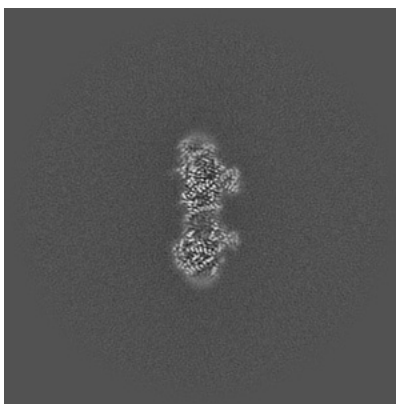
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

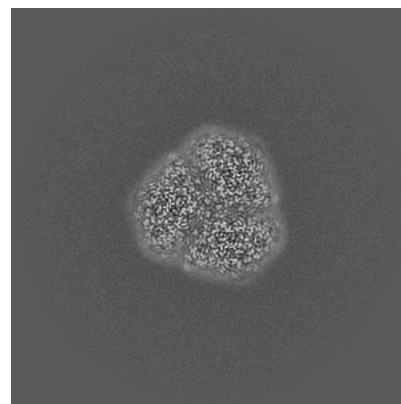
6.3.1 Primary map



X Index: 219



Y Index: 180

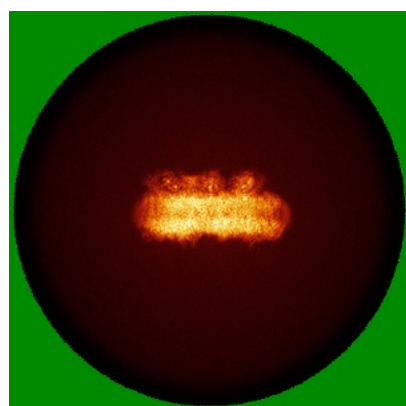


Z Index: 188

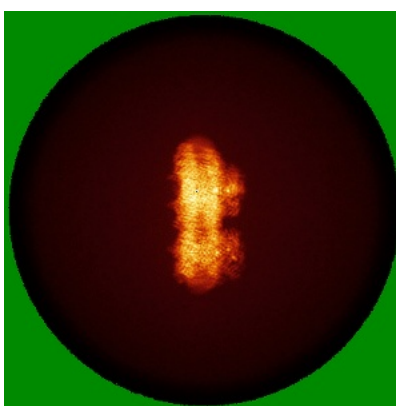
The images above show the largest variance slices of the map in three orthogonal directions.

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

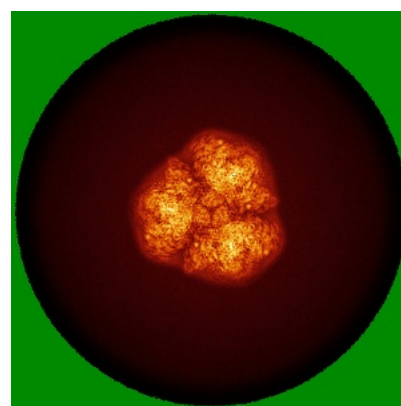
6.4.1 Primary map



X



Y

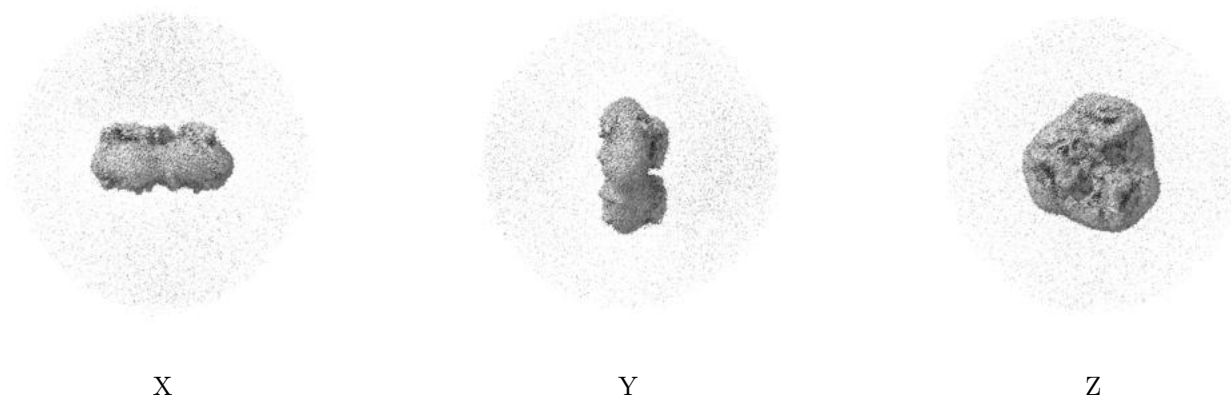


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.171. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

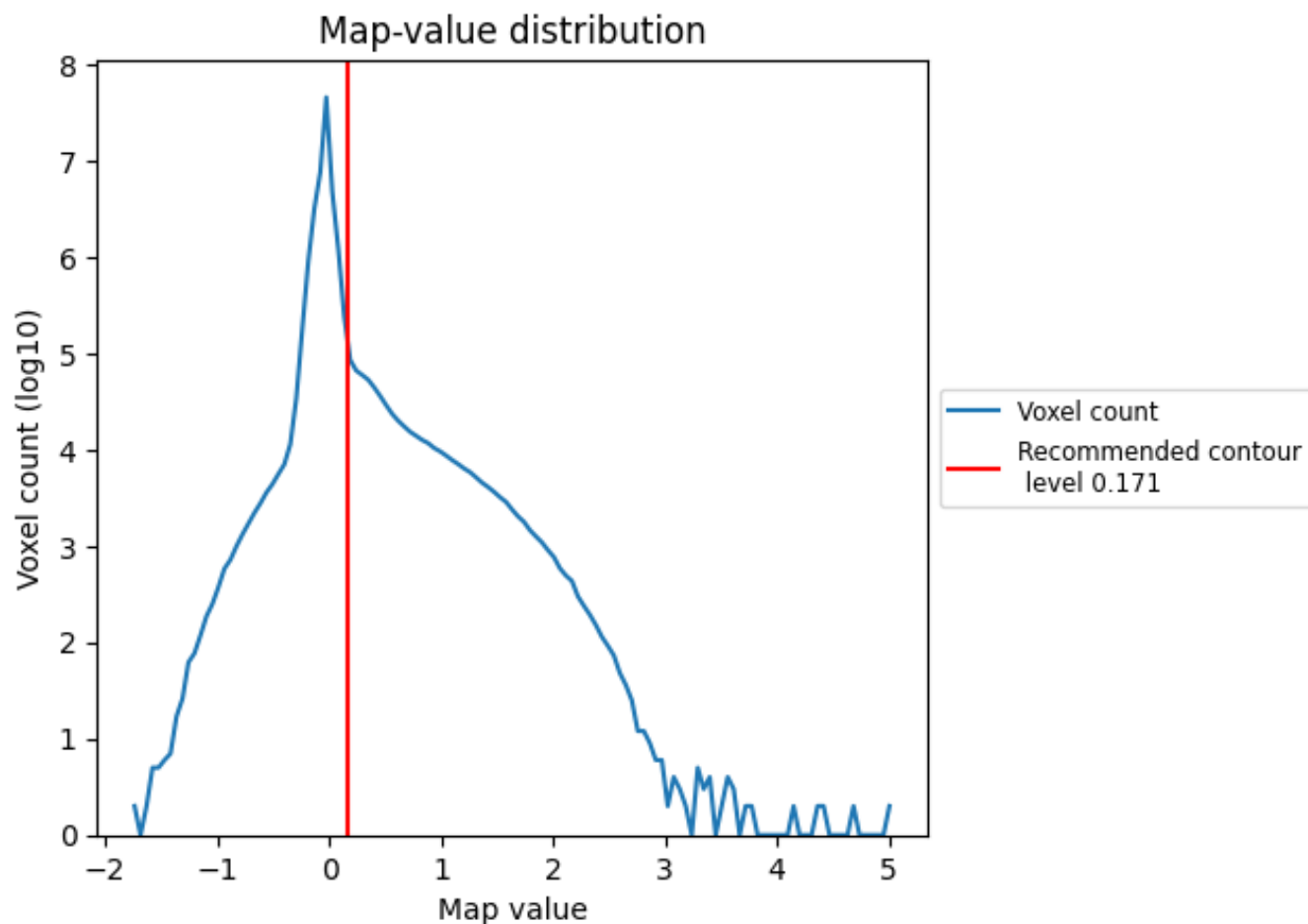
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

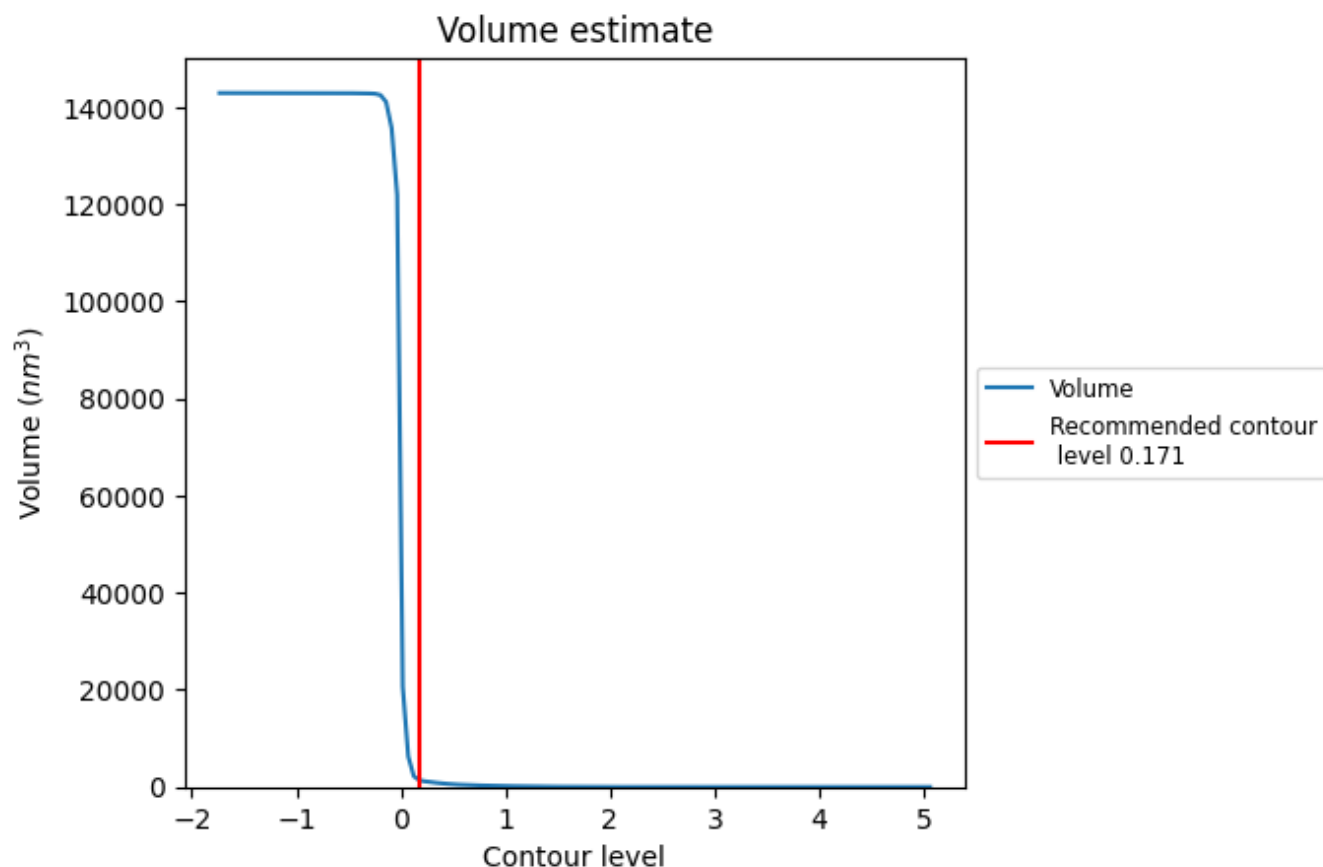
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

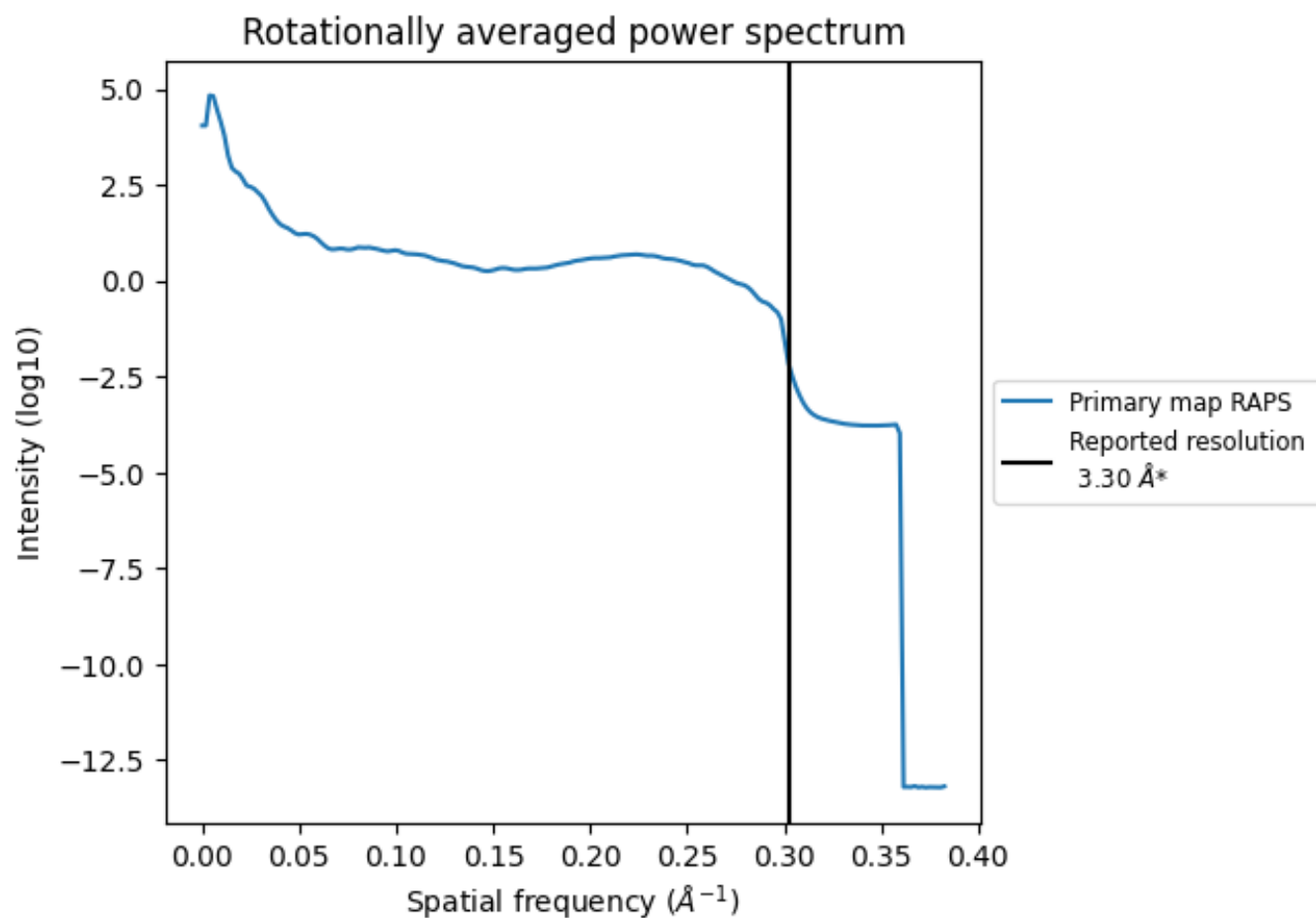
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1462 nm^3 ; this corresponds to an approximate mass of 1320 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

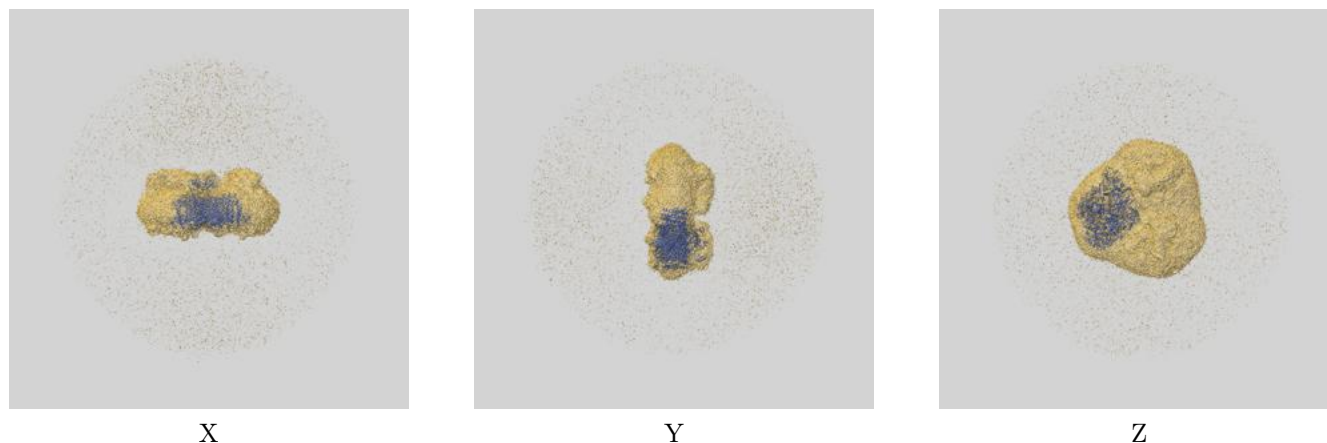
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

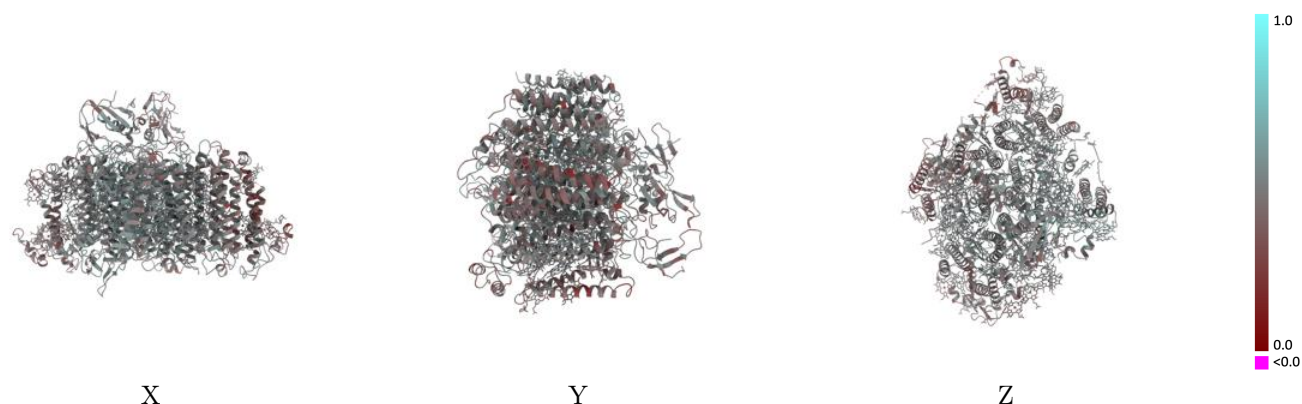
This section contains information regarding the fit between EMDB map EMD-30882 and PDB model 7DWQ. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



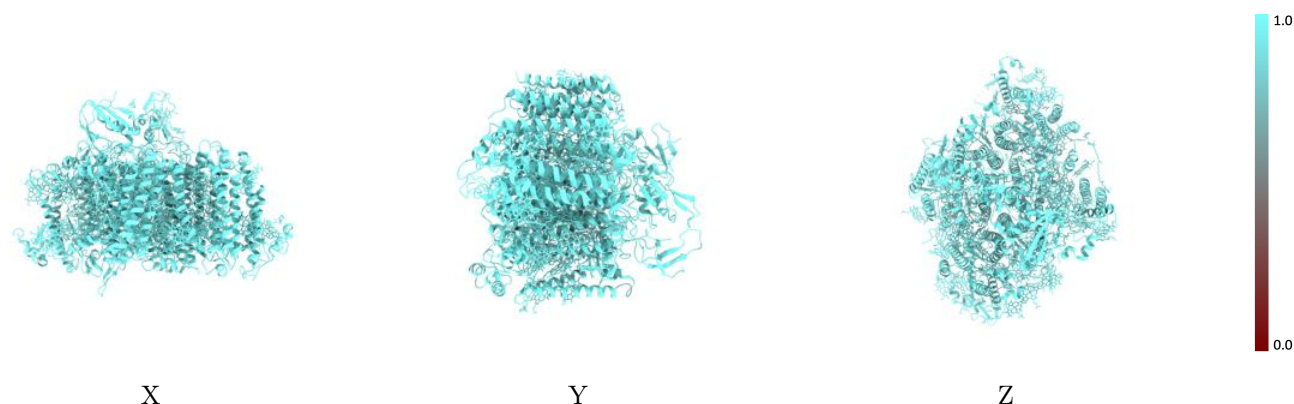
The images above show the 3D surface view of the map at the recommended contour level 0.171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



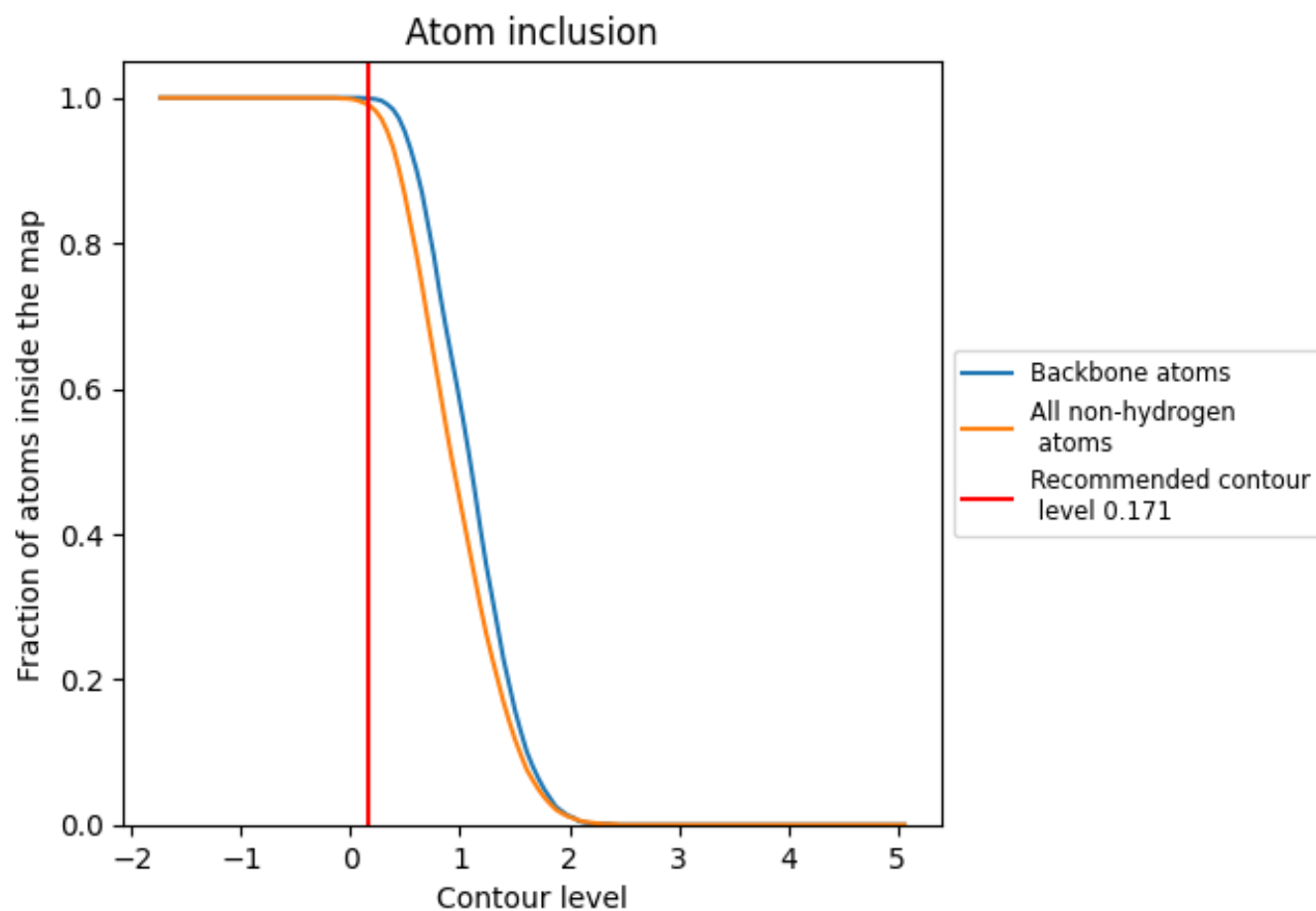
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.171).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9900	0.4690
A	0.9920	0.4790
B	0.9910	0.4710
C	1.0000	0.4540
D	0.9990	0.4810
E	0.9910	0.4300
F	0.9640	0.3750
J	0.9610	0.3970
L	0.9940	0.4920
M	0.9570	0.4250
W	0.9850	0.4930

1.0

0.0

<0.0