



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:15 AM UTC

PDB ID : 6YXR / pdb_00006yxr
EMDB ID : EMD-10995
Title : Dunaliella Minimal Photosystem I
Authors : Nelson, N.; Caspy, I.; Malavath, T.; Klaiman, D.; Shkolinsky, Y.
Deposited on : 2020-05-03
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

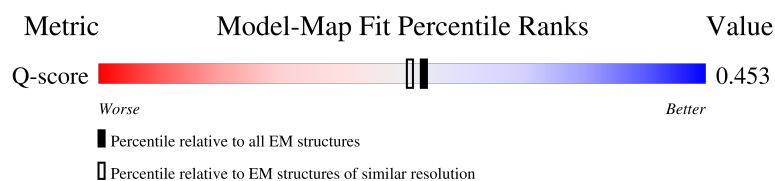
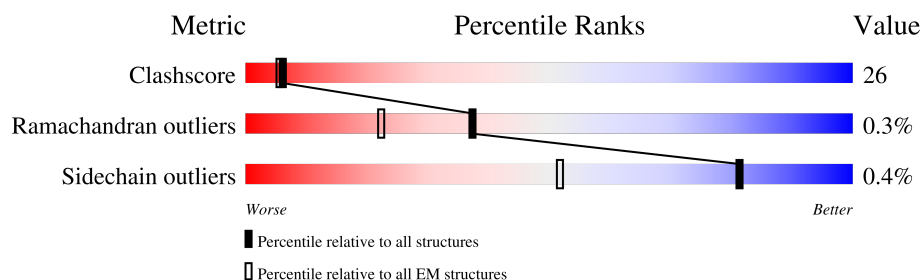
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	1	197	
2	2	208	
3	3	210	
4	4	211	

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Mol	Chain	Length	Quality of chain
5	A	739	
6	B	730	
7	C	80	
8	D	141	
9	E	64	
10	F	163	
11	J	40	

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
12	LUT	1	501	X	-	X	-
12	LUT	2	501	X	-	-	-
12	LUT	3	501	X	-	-	-
12	LUT	4	501	X	X	-	-
14	BCR	A	4003	-	-	X	-
14	BCR	F	4001	-	-	X	-
15	CLA	1	601	X	-	-	-
15	CLA	1	602	X	-	-	-
15	CLA	1	603	X	-	-	-
15	CLA	1	604	X	-	-	-
15	CLA	1	605	X	-	-	-
15	CLA	1	606	X	-	-	-
15	CLA	1	607	X	-	-	-
15	CLA	1	608	X	-	X	-
15	CLA	1	611	X	-	-	-
15	CLA	1	612	X	-	-	-
15	CLA	1	613	X	-	-	-
15	CLA	1	615	X	-	-	-
15	CLA	2	601	X	-	-	-
15	CLA	2	602	X	-	-	-
15	CLA	2	603	X	-	-	-
15	CLA	2	604	X	-	-	-
15	CLA	2	605	X	-	-	-
15	CLA	2	606	X	-	-	-
15	CLA	2	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	2	608	X	-	-	-
15	CLA	2	612	X	-	-	-
15	CLA	3	601	X	-	-	-
15	CLA	3	603	X	-	-	-
15	CLA	3	605	X	-	-	-
15	CLA	3	606	X	-	-	-
15	CLA	3	607	X	-	-	-
15	CLA	3	608	X	-	-	-
15	CLA	3	609	X	-	-	-
15	CLA	3	610	X	-	-	-
15	CLA	3	611	X	-	-	-
15	CLA	3	612	X	-	-	-
15	CLA	3	613	X	-	-	-
15	CLA	3	614	X	-	-	-
15	CLA	3	615	X	-	-	-
15	CLA	4	601	X	-	-	-
15	CLA	4	602	X	-	-	-
15	CLA	4	603	X	-	-	-
15	CLA	4	604	X	-	-	-
15	CLA	4	605	X	-	-	-
15	CLA	4	606	X	-	-	-
15	CLA	4	607	X	-	-	-
15	CLA	4	608	X	-	-	-
15	CLA	4	609	X	-	-	-
15	CLA	4	612	X	-	-	-
15	CLA	4	616	X	-	-	-
15	CLA	A	1012	X	-	X	-
15	CLA	A	1013	X	-	X	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	-	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1108	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1111	X	-	-	-
15	CLA	A	1112	X	-	X	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	-
15	CLA	A	1117	X	-	-	-
15	CLA	A	1118	X	-	-	-
15	CLA	A	1119	X	-	-	-
15	CLA	A	1120	X	-	-	-
15	CLA	A	1121	X	-	-	-
15	CLA	A	1122	X	-	-	-
15	CLA	A	1123	X	-	X	-
15	CLA	A	1124	X	-	-	-
15	CLA	A	1125	X	-	-	-
15	CLA	A	1126	X	-	X	-
15	CLA	A	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-
15	CLA	A	1132	X	-	-	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	X	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1139	X	-	-	-
15	CLA	A	1141	X	-	-	-
15	CLA	B	1021	X	-	-	-
15	CLA	B	1022	X	-	-	-
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	-	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1213	X	-	-	-
15	CLA	B	1214	X	-	-	-
15	CLA	B	1215	X	-	X	-
15	CLA	B	1216	X	-	X	-
15	CLA	B	1217	X	-	-	-
15	CLA	B	1218	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	-
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	-	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	-
15	CLA	B	1228	X	-	-	-
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	X	-
15	CLA	B	1231	X	-	-	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	B	1240	X	-	-	-
15	CLA	F	1301	X	-	-	-
15	CLA	F	1302	X	-	-	-
15	CLA	J	1302	X	-	-	-
16	CHL	1	609	X	-	-	-
16	CHL	1	610	X	-	-	-
16	CHL	2	609	X	-	-	-
16	CHL	2	610	X	-	-	-
16	CHL	2	611	X	-	-	-
16	CHL	2	613	X	-	-	-
16	CHL	3	604	X	-	-	-
16	CHL	4	610	X	-	-	-
16	CHL	4	611	X	-	-	-
16	CHL	4	613	X	-	-	-
20	CL0	A	1011	X	-	-	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 31910 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	197	Total	C	N	O	S	0	0
			1501	963	255	276	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	204	ALA	GLU	conflict	UNP C1K003

- Molecule 2 is a protein called Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	208	Total	C	N	O	S	0	0
			1609	1033	272	297	7		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	210	Total	C	N	O	S	0	0
			1609	1050	263	291	5		

- Molecule 4 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	211	Total	C	N	O	S	0	0
			1637	1058	272	303	4		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	739	Total	C	N	O	S	0	0
			5799	3789	991	1001	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	730	Total	C	N	O	S	0	0
			5784	3799	970	1002	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	141	Total	C	N	O	S	0	0
			1116	714	195	201	6		

- Molecule 9 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	64	Total	C	N	O	0	0
			515	327	89	99		

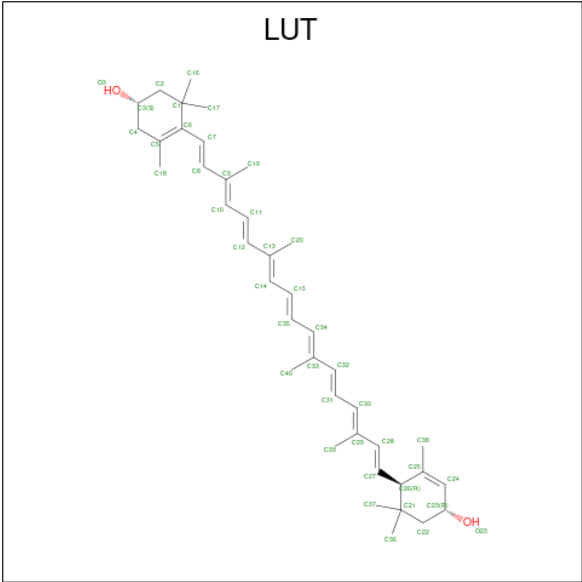
- Molecule 10 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	163	Total	C	N	O	S	0	0
			1285	828	218	237	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit IX.

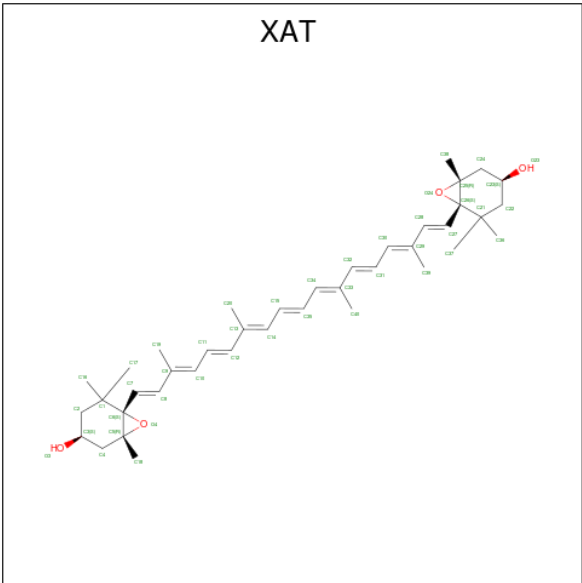
Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	40	Total	C	N	O	S	0	0
			316	214	46	55	1		

- Molecule 12 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



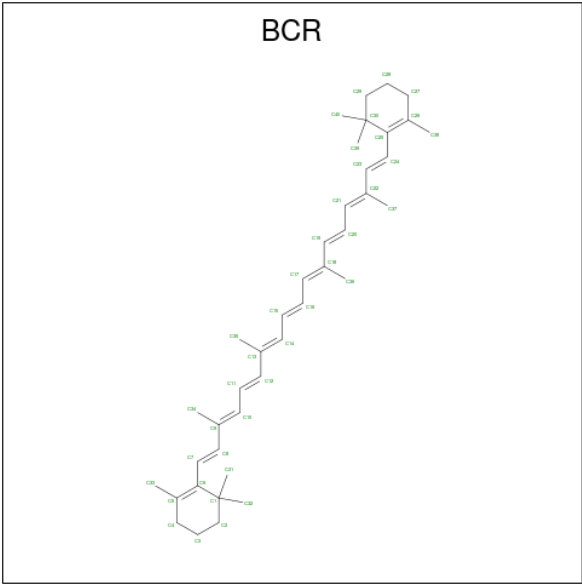
Mol	Chain	Residues	Atoms			AltConf
12	1	1	Total	C	O	0
			42	40	2	
12	2	1	Total	C	O	0
			42	40	2	
12	3	1	Total	C	O	0
			42	40	2	
12	4	1	Total	C	O	0
			42	40	2	

- Molecule 13 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
13	1	1	Total	C	O	0
			44	40	4	
13	2	1	Total	C	O	0
			44	40	4	
13	3	1	Total	C	O	0
			44	40	4	
13	4	1	Total	C	O	0
			44	40	4	

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



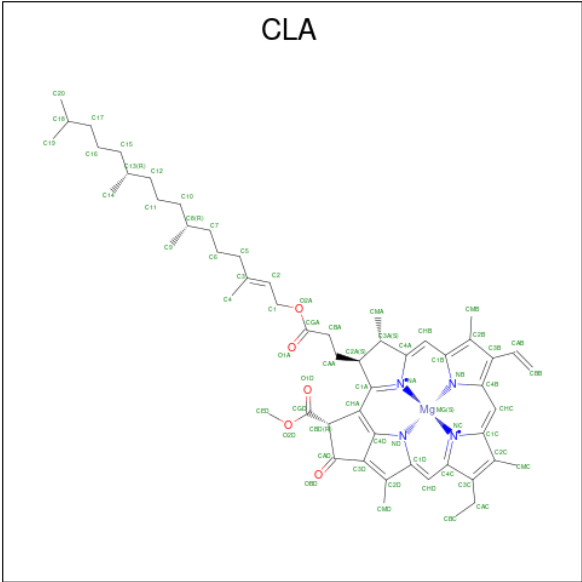
Mol	Chain	Residues	Atoms		AltConf
14	1	1	Total	C	0
			40	40	
14	2	1	Total	C	0
			40	40	
14	3	1	Total	C	0
			40	40	
14	3	1	Total	C	0
			40	40	
14	3	1	Total	C	0
			40	40	
14	4	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	J	1	Total C 40 40	0
14	J	1	Total C 40 40	0

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
15	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
15	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
15	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
15	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
15	3	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
15	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
15	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
15	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
15	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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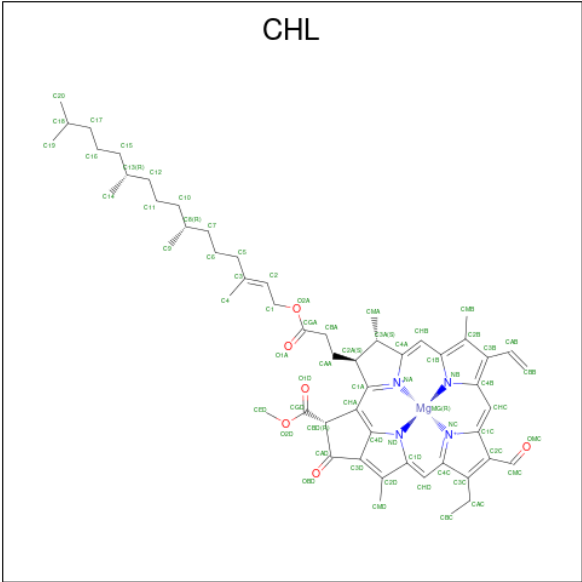
Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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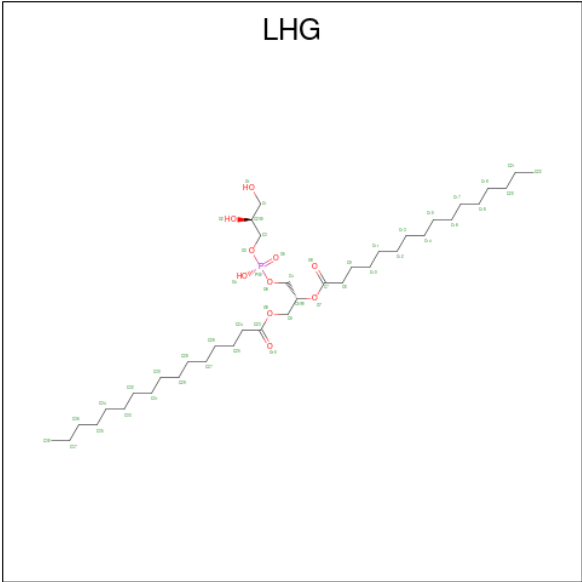
Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			52	44	1	4	3	
15	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
15	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	F	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
15	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 16 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



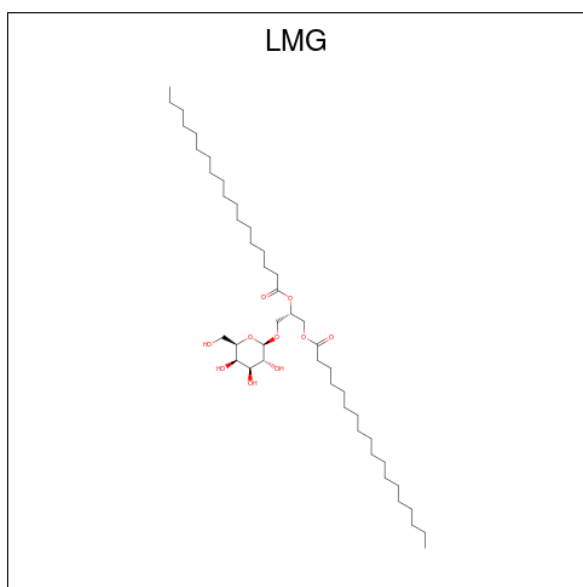
Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	2	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
16	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
16	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
16	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



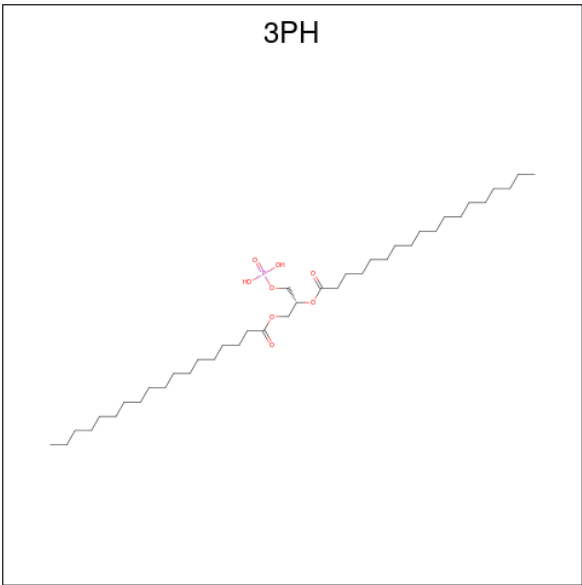
Mol	Chain	Residues	Atoms				AltConf
17	1	1	Total	C	O	P	0
			49	38	10	1	
17	2	1	Total	C	O	P	0
			35	24	10	1	
17	3	1	Total	C	O	P	0
			48	37	10	1	
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	B	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



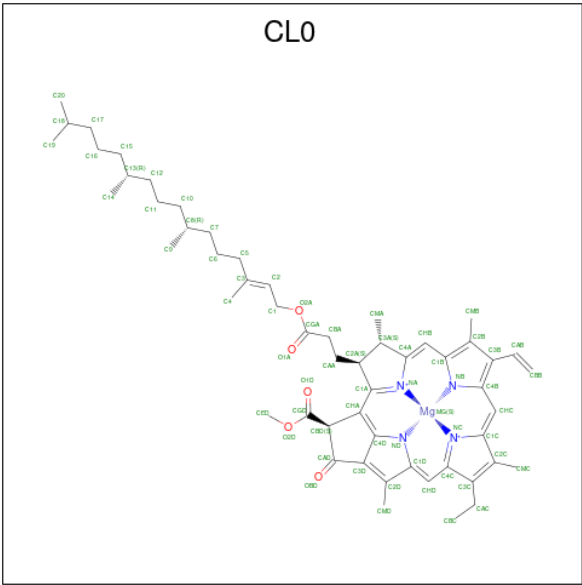
Mol	Chain	Residues	Atoms			AltConf
18	2	1	Total	C	O	0
			50	40	10	
18	2	1	Total	C	O	0
			40	30	10	
18	2	1	Total	C	O	0
			50	40	10	
18	4	1	Total	C	O	0
			37	27	10	
18	B	1	Total	C	O	0
			39	29	10	

- Molecule 19 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



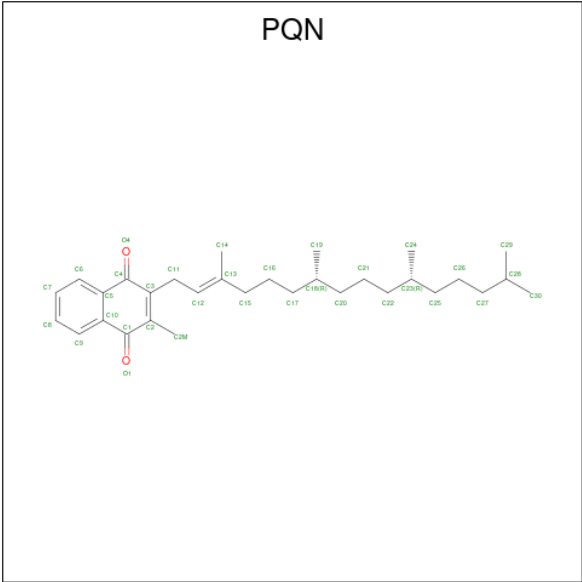
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	3	1	22	13	8	1	0

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



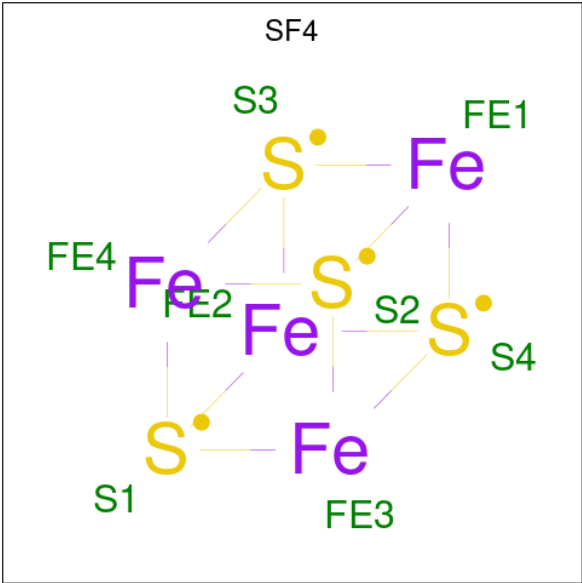
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



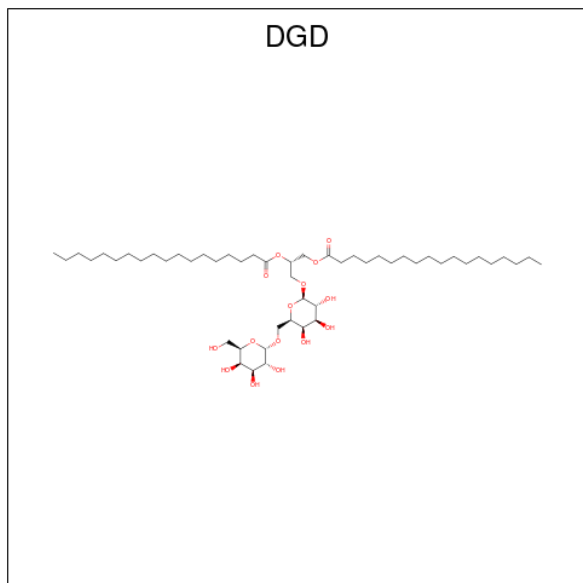
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	B	1	61	46	15	0

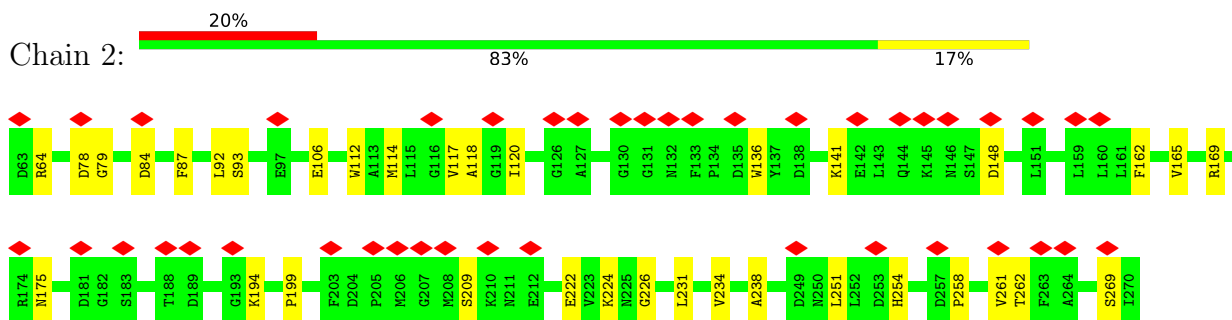
3 Residue-property plots

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.

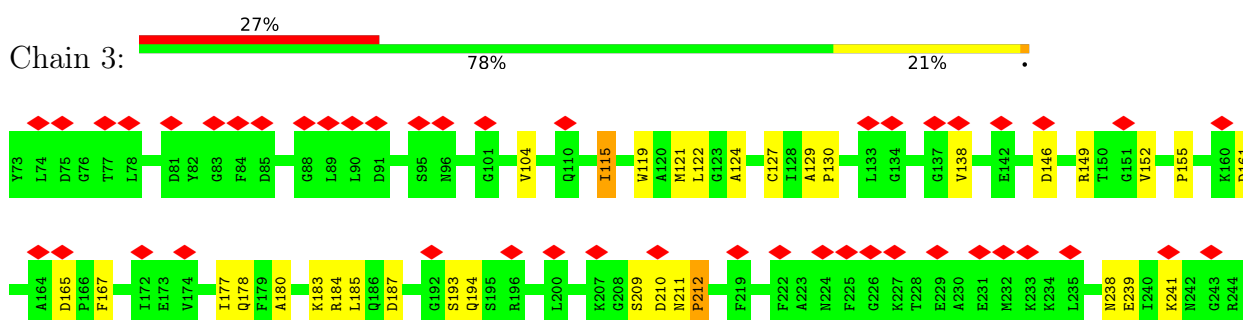
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

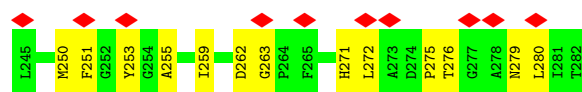


- Molecule 2: Lhca2

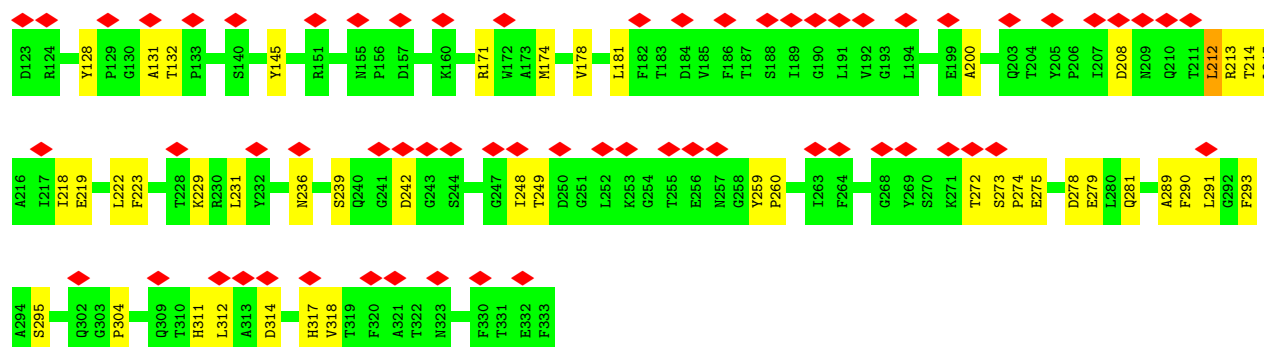
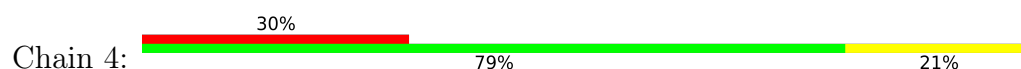


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

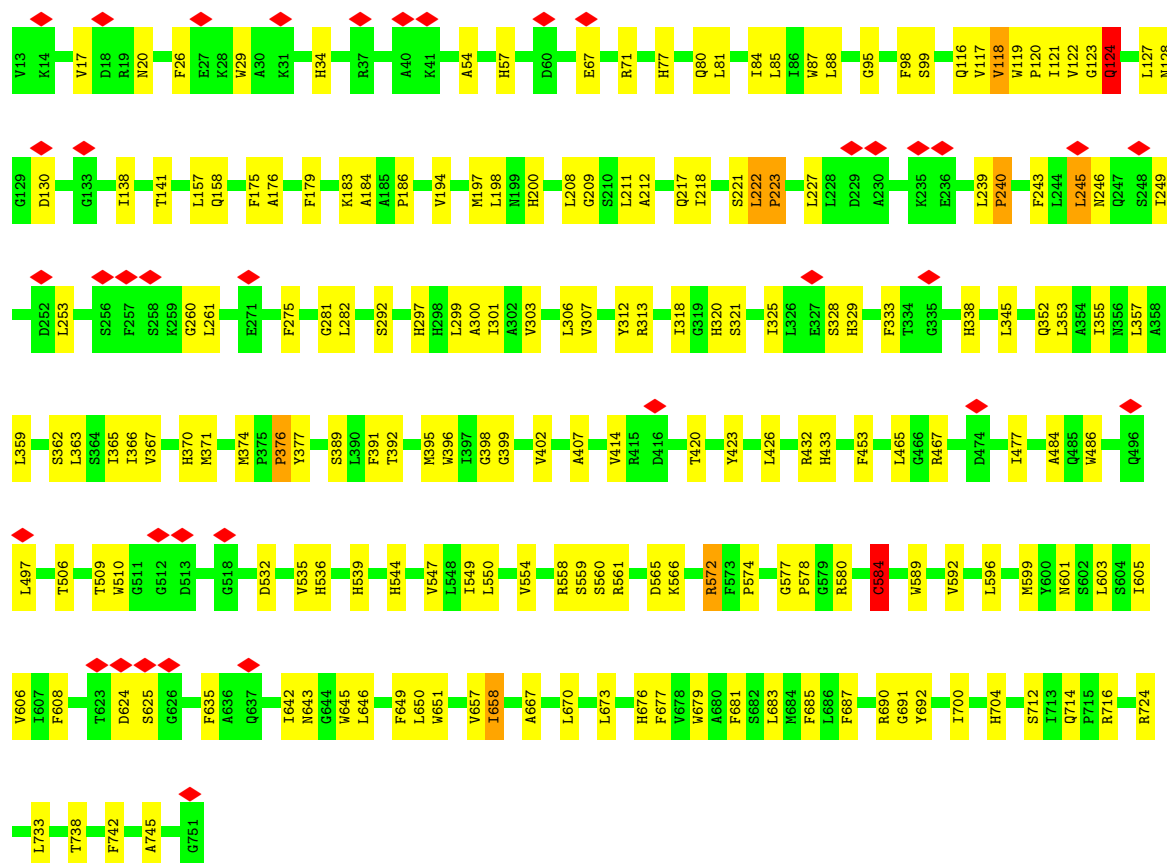
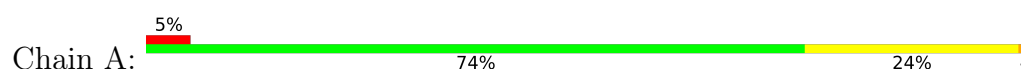




- Molecule 4: Lhca4



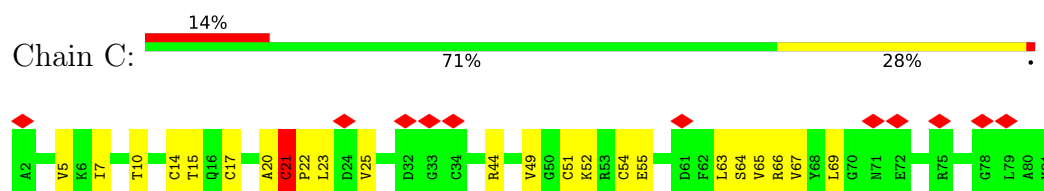
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



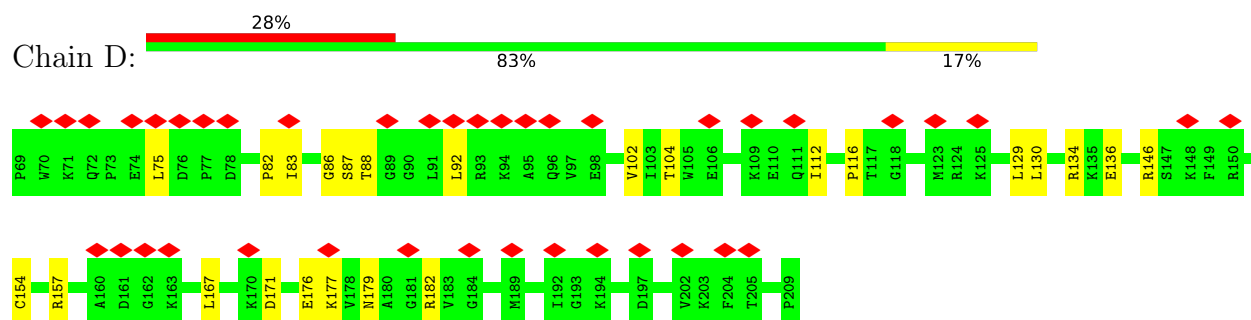
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 7: Photosystem I iron-sulfur center

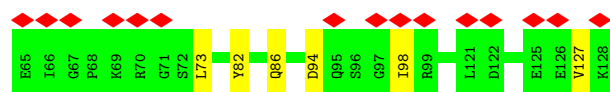


• Molecule 8: Psad

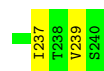
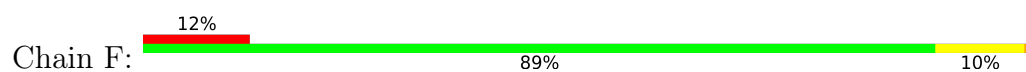


• Molecule 9: Psae





- Molecule 10: PsaF



- Molecule 11: Photosystem I reaction center subunit IX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45969	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 ($e^-/\text{\AA}^2$)	42.68	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.128	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	384.12003, 384.12003, 384.12003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, PQN, SF4, BCR, CLA, 3PH, LHG, XAT, LUT, CL0, CHL, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.25	0/1540	0.42	0/2088
2	2	0.28	0/1656	0.43	0/2243
3	3	0.67	2/1657 (0.1%)	0.90	4/2253 (0.2%)
4	4	0.28	0/1687	0.49	0/2300
5	A	0.71	6/5995 (0.1%)	0.91	15/8179 (0.2%)
6	B	0.50	2/5997 (0.0%)	0.65	4/8198 (0.0%)
7	C	0.79	1/610 (0.2%)	1.04	2/828 (0.2%)
8	D	0.28	0/1145	0.45	0/1546
9	E	0.26	0/525	0.42	0/712
10	F	0.64	2/1313 (0.2%)	0.83	5/1776 (0.3%)
11	J	1.47	3/326 (0.9%)	1.87	6/445 (1.3%)
All	All	0.58	16/22451 (0.1%)	0.76	36/30568 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	4	0	2
5	A	0	1
7	C	0	1
All	All	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	240	PRO	N-CA	18.01	1.70	1.47
6	B	559	PRO	N-CA	17.87	1.70	1.47
5	A	223	PRO	N-CA	17.83	1.70	1.47
10	F	167	PRO	N-CA	17.68	1.70	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	212	PRO	N-CA	17.55	1.70	1.47
11	J	12	PRO	N-CA	17.28	1.70	1.47
11	J	35	ASP	C-N	13.28	1.50	1.33
7	C	21	CYS	C-N	12.69	1.51	1.34
5	A	377	TYR	C-N	12.33	1.49	1.33
5	A	222	LEU	C-N	10.78	1.45	1.34
3	3	211	ASN	C-N	10.68	1.45	1.34
11	J	11	ALA	C-N	7.78	1.45	1.33
5	A	124	GLN	C-O	-6.34	1.16	1.24
10	F	166	ILE	C-N	6.01	1.42	1.33
6	B	558	PHE	C-N	5.09	1.45	1.33
5	A	239	LEU	C-N	5.01	1.45	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	211	ASN	CA-C-N	19.99	139.41	119.82
3	3	211	ASN	C-N-CA	19.99	139.41	119.82
5	A	222	LEU	CA-C-N	19.90	139.32	119.82
5	A	222	LEU	C-N-CA	19.90	139.32	119.82
10	F	166	ILE	CA-C-N	16.35	138.44	119.47
10	F	166	ILE	C-N-CA	16.35	138.44	119.47
11	J	11	ALA	CA-C-N	16.22	137.81	119.32
11	J	11	ALA	C-N-CA	16.22	137.81	119.32
11	J	35	ASP	CA-C-N	15.65	136.90	119.99
11	J	35	ASP	C-N-CA	15.65	136.90	119.99
5	A	239	LEU	CA-C-N	15.47	139.18	119.84
5	A	239	LEU	C-N-CA	15.47	139.18	119.84
6	B	558	PHE	CA-C-N	15.19	138.83	119.84
6	B	558	PHE	C-N-CA	15.19	138.83	119.84
7	C	21	CYS	CA-C-N	13.23	133.74	119.05
7	C	21	CYS	C-N-CA	13.23	133.74	119.05
5	A	377	TYR	CA-C-N	12.21	132.18	119.85
5	A	377	TYR	C-N-CA	12.21	132.18	119.85
5	A	240	PRO	CA-N-CD	-8.85	99.61	112.00
10	F	167	PRO	CA-N-CD	-8.54	100.04	112.00
3	3	212	PRO	CA-N-CD	-8.38	100.27	112.00
5	A	223	PRO	CA-N-CD	-8.30	100.37	112.00
11	J	12	PRO	CA-N-CD	-8.01	100.78	112.00
6	B	559	PRO	CA-N-CD	-7.92	100.92	112.00
5	A	377	TYR	CB-CA-C	-7.01	98.96	109.26
10	F	167	PRO	N-CA-C	-6.96	103.72	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	584	CYS	CA-C-O	-6.31	113.41	120.54
6	B	571	ILE	CB-CA-C	-6.20	105.60	111.06
5	A	584	CYS	CA-C-N	5.75	130.81	122.36
5	A	584	CYS	C-N-CA	5.75	130.81	122.36
5	A	299	LEU	CA-C-N	5.72	127.94	120.28
5	A	299	LEU	C-N-CA	5.72	127.94	120.28
10	F	167	PRO	CB-CA-C	5.65	121.70	112.26
3	3	115	ILE	N-CA-C	-5.23	105.61	110.53
11	J	34	PRO	N-CA-C	5.14	119.28	111.11
5	A	572	ARG	NE-CZ-NH1	-5.03	116.47	121.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	213	ARG	Peptide
4	4	274	PRO	Peptide
5	A	124	GLN	Mainchain
7	C	20	ALA	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1501	0	1469	137	0
2	2	1609	0	1556	48	0
3	3	1609	0	1567	75	0
4	4	1637	0	1579	64	0
5	A	5799	0	5629	268	0
6	B	5784	0	5529	366	0
7	C	600	0	584	20	0
8	D	1116	0	1126	20	0
9	E	515	0	508	4	0
10	F	1285	0	1304	28	0
11	J	316	0	319	28	0
12	1	42	0	56	31	0
12	2	42	0	56	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	3	42	0	56	11	0
12	4	42	0	56	20	0
13	1	44	0	56	2	0
13	2	44	0	56	3	0
13	3	44	0	56	13	0
13	4	44	0	56	3	0
14	1	40	0	56	4	0
14	2	40	0	56	1	0
14	3	120	0	165	6	0
14	4	40	0	56	4	0
14	A	280	0	367	103	0
14	B	240	0	330	30	0
14	F	80	0	105	30	0
14	J	80	0	105	33	0
15	1	633	0	562	99	0
15	2	580	0	573	25	0
15	3	732	0	700	92	0
15	4	632	0	604	25	0
15	A	2487	0	2450	470	0
15	B	2411	0	2350	402	0
15	F	95	0	72	13	0
15	J	42	0	30	6	0
16	1	113	0	101	1	0
16	2	204	0	165	9	0
16	3	61	0	56	11	0
16	4	159	0	125	8	0
17	1	49	0	74	9	0
17	2	35	0	40	1	0
17	3	48	0	68	8	0
17	A	98	0	148	17	0
17	B	42	0	57	0	0
18	2	140	0	196	15	0
18	4	37	0	44	1	0
18	B	39	0	48	2	0
19	3	22	0	17	3	0
20	A	65	0	72	20	0
21	A	33	0	46	8	0
21	B	33	0	46	10	0
22	A	8	0	0	1	0
22	C	16	0	0	0	0
23	B	61	0	83	13	0
All	All	31910	0	31585	1656	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 26.

All (1656) 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)
11:J:12:PRO:N	11:J:12:PRO:CA	1.70	1.48
15:B:1223:CLA:C4B	15:B:1231:CLA:HMA3	1.43	1.47
5:A:240:PRO:CA	5:A:240:PRO:N	1.70	1.46
3:3:212:PRO:N	3:3:212:PRO:CA	1.70	1.43
6:B:559:PRO:N	6:B:559:PRO:CA	1.70	1.43
5:A:223:PRO:N	5:A:223:PRO:CA	1.70	1.35
10:F:167:PRO:N	10:F:167:PRO:CA	1.70	1.35
6:B:518:PHE:CE1	14:F:4001:BCR:H381	1.72	1.23
5:A:158:GLN:OE1	15:A:1112:CLA:HED1	1.33	1.23
5:A:158:GLN:CD	15:A:1112:CLA:HED1	1.65	1.21
15:B:1223:CLA:CHC	15:B:1231:CLA:CMA	2.18	1.21
1:1:127:ILE:HD12	15:1:613:CLA:C3D	1.70	1.21
15:B:1223:CLA:C4B	15:B:1231:CLA:CMA	2.18	1.20
15:B:1223:CLA:CHC	15:B:1231:CLA:HMA3	1.71	1.19
4:4:289:ALA:HB2	12:4:501:LUT:C39	1.74	1.18
5:A:158:GLN:OE1	15:A:1112:CLA:CED	1.93	1.16
15:A:1121:CLA:HHC	15:A:1121:CLA:HBB1	1.25	1.16
15:A:1110:CLA:H41	15:A:1110:CLA:H72	1.18	1.14
6:B:518:PHE:HE1	14:F:4001:BCR:C38	1.59	1.14
15:B:1236:CLA:HHC	15:B:1236:CLA:HBB1	1.26	1.13
15:A:1110:CLA:HHC	15:A:1110:CLA:HBB1	1.28	1.13
1:1:86:ALA:HB1	12:1:501:LUT:H30	1.18	1.12
14:B:4006:BCR:H403	14:B:4006:BCR:H23C	1.31	1.12
15:A:1131:CLA:HHC	15:A:1131:CLA:HBB1	1.29	1.12
15:A:1107:CLA:HBD	15:A:1107:CLA:HBA1	1.32	1.11
15:A:1110:CLA:HBA1	15:A:1110:CLA:HBD	1.24	1.10
6:B:518:PHE:CE1	14:F:4001:BCR:C38	2.32	1.10
5:A:389:SER:HB3	15:A:1126:CLA:HMA3	1.25	1.09
15:A:1103:CLA:H52	14:A:4003:BCR:H282	1.23	1.09
7:C:7:ILE:HG22	7:C:65:VAL:HG22	1.19	1.09
15:3:612:CLA:H2A	15:3:612:CLA:HED2	1.14	1.09
15:A:1114:CLA:HHC	15:A:1114:CLA:HBB1	1.36	1.06
6:B:276:HIS:HB3	15:B:1214:CLA:HMB2	1.35	1.06
4:4:289:ALA:HB2	12:4:501:LUT:H392	1.36	1.04
15:A:1130:CLA:H2A	15:A:1130:CLA:HED2	1.08	1.03
15:A:1103:CLA:H72	14:A:4003:BCR:H373	1.35	1.03
5:A:389:SER:HB3	15:A:1126:CLA:CMA	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:613:CLA:HBB1	15:3:613:CLA:HMB3	1.40	1.02
6:B:51:HIS:CE1	15:B:1202:CLA:ND	2.26	1.02
15:A:1105:CLA:HMB1	15:A:1105:CLA:HBB1	1.42	1.00
6:B:518:PHE:HE1	14:F:4001:BCR:H381	0.87	1.00
15:A:1106:CLA:HMB1	15:A:1106:CLA:HBB1	1.43	1.00
15:A:1012:CLA:H41	6:B:439:VAL:HG13	1.44	1.00
15:A:1105:CLA:HBD	15:A:1105:CLA:HBA1	1.44	1.00
15:A:1135:CLA:HMB1	15:A:1135:CLA:HBB1	1.43	0.99
15:A:1135:CLA:H2A	15:A:1135:CLA:HED2	1.43	0.99
15:B:1225:CLA:HBB1	15:B:1225:CLA:HMB3	1.43	0.99
15:A:1103:CLA:C5	14:A:4003:BCR:H282	1.92	0.99
15:A:1124:CLA:HMB1	15:A:1124:CLA:HBB1	1.42	0.99
14:F:4001:BCR:H23C	14:F:4001:BCR:H403	1.43	0.99
15:A:1102:CLA:HMB1	15:A:1102:CLA:HBB1	1.44	0.98
15:B:1222:CLA:HBB1	15:B:1222:CLA:HMB3	1.43	0.98
15:3:612:CLA:H2A	15:3:612:CLA:CED	1.94	0.98
6:B:494:TRP:CD1	15:B:1231:CLA:HED1	1.99	0.98
1:1:184:ALA:HB2	12:1:501:LUT:H401	1.43	0.98
5:A:667:ALA:HB3	15:A:1106:CLA:CBC	1.93	0.97
6:B:124:TRP:CZ2	15:B:1210:CLA:H191	1.99	0.97
15:A:1110:CLA:HBA1	15:A:1110:CLA:CBD	1.94	0.97
15:B:1229:CLA:CED	15:B:1229:CLA:H2A	1.94	0.97
15:A:1105:CLA:HBA1	15:A:1105:CLA:CBD	1.95	0.97
15:A:1138:CLA:HBB1	15:A:1138:CLA:HMB1	1.47	0.97
1:1:154:PRO:O	15:1:601:CLA:HED2	1.65	0.96
14:A:4002:BCR:H323	14:A:4002:BCR:H342	1.48	0.96
15:B:1229:CLA:HBB1	15:B:1229:CLA:HMB1	1.48	0.96
15:B:1021:CLA:HBB1	15:B:1021:CLA:HMB1	1.47	0.95
1:1:187:ALA:HB1	12:1:501:LUT:H382	1.48	0.95
15:A:1123:CLA:HMB1	15:A:1123:CLA:HBB1	1.44	0.95
15:B:1230:CLA:HBB1	15:B:1230:CLA:HMB3	1.46	0.95
15:A:1130:CLA:O2A	6:B:687:PRO:HD3	1.67	0.94
4:4:178:VAL:HG22	12:4:501:LUT:H15	1.50	0.94
15:A:1130:CLA:HMB3	15:A:1130:CLA:HBB1	1.47	0.94
3:3:104:VAL:HG22	15:A:1108:CLA:CED	1.98	0.93
1:1:127:ILE:CD1	15:1:613:CLA:C3D	2.46	0.93
6:B:180:LEU:HD21	15:B:1216:CLA:C3B	1.99	0.93
15:A:1013:CLA:H51	15:A:1013:CLA:H92	1.50	0.93
15:A:1127:CLA:HBB1	15:A:1127:CLA:HMB1	1.51	0.93
1:1:217:ASN:HD21	15:1:608:CLA:HMA1	1.34	0.93
15:A:1112:CLA:H171	14:A:4003:BCR:H10C	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:86:ALA:CB	12:1:501:LUT:H30	1.98	0.93
15:A:1137:CLA:H2A	15:A:1137:CLA:HED2	1.49	0.92
14:A:4007:BCR:C10	15:B:1022:CLA:H161	1.98	0.92
15:3:605:CLA:HBB1	15:3:605:CLA:HMB3	1.52	0.92
6:B:292:TYR:OH	15:B:1216:CLA:O1D	1.87	0.92
6:B:656:LEU:HD12	15:B:1023:CLA:CBB	2.00	0.92
1:1:209:HIS:HE1	15:1:608:CLA:NA	1.63	0.92
15:A:1112:CLA:HBB1	15:A:1112:CLA:HMB3	1.50	0.92
15:A:1101:CLA:HBB1	14:J:4002:BCR:H271	1.47	0.92
15:A:1106:CLA:H2A	15:A:1106:CLA:HED2	1.49	0.91
6:B:54:GLN:HE22	15:B:1203:CLA:MG	0.69	0.91
3:3:104:VAL:HG22	15:A:1108:CLA:HED2	1.49	0.91
15:A:1115:CLA:HBB1	15:A:1115:CLA:HMB1	1.52	0.91
15:B:1223:CLA:NB	15:B:1231:CLA:HMA3	1.84	0.91
15:A:1137:CLA:HBB1	15:A:1137:CLA:HMB1	1.53	0.91
6:B:656:LEU:HD12	15:B:1023:CLA:HBB2	1.51	0.91
15:A:1130:CLA:HED2	15:A:1130:CLA:C2A	2.00	0.91
1:1:218:PHE:HE2	15:1:608:CLA:O2D	1.54	0.91
17:3:801:LHG:H102	17:3:801:LHG:HC62	1.50	0.91
14:A:4007:BCR:H14C	15:B:1023:CLA:H193	1.50	0.91
6:B:656:LEU:CD1	15:B:1023:CLA:CBB	2.49	0.91
15:3:612:CLA:HBB1	15:3:612:CLA:HMB1	1.53	0.91
7:C:52:LYS:HE2	7:C:69:LEU:CD1	2.01	0.90
15:B:1224:CLA:HBC3	23:B:5002:DGD:HBC3	1.53	0.90
6:B:50:SER:OG	15:B:1202:CLA:CBB	2.18	0.90
6:B:54:GLN:NE2	15:B:1203:CLA:NA	2.19	0.90
6:B:463:TRP:CZ2	15:F:1302:CLA:CBA	2.55	0.90
6:B:464:ILE:HD11	15:B:1234:CLA:H12	1.50	0.90
15:A:1110:CLA:H41	15:A:1110:CLA:C7	2.00	0.90
5:A:681:PHE:HZ	15:A:1140:CLA:HBC2	1.37	0.90
4:4:229:LYS:HD3	16:4:611:CHL:OMC	1.72	0.90
11:J:26:LEU:HD13	14:J:4001:BCR:HC7	1.53	0.90
14:A:4003:BCR:C22	14:A:4003:BCR:H383	2.02	0.89
15:A:1124:CLA:H51	15:A:1135:CLA:H11	1.52	0.89
15:B:1234:CLA:HMB1	15:B:1234:CLA:HBB1	1.53	0.89
3:3:259:ILE:HD12	15:3:603:CLA:CMD	2.02	0.89
6:B:191:TRP:CZ2	15:B:1215:CLA:CAD	2.55	0.89
5:A:118:VAL:HG23	5:A:128:ASN:OD1	1.72	0.89
18:2:804:LMG:H311	15:3:610:CLA:HBB1	1.53	0.88
3:3:184:ARG:HG3	15:3:611:CLA:CHD	2.04	0.88
15:A:1105:CLA:HBA1	15:A:1105:CLA:CHA	2.01	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:431:GLY:HA2	6:B:526:LEU:HD22	1.54	0.88
5:A:389:SER:CB	15:A:1126:CLA:HMA3	2.03	0.88
15:A:1103:CLA:H72	14:A:4003:BCR:C37	2.03	0.88
6:B:139:SER:OG	14:B:4003:BCR:H401	1.74	0.88
3:3:271:HIS:CD2	15:3:608:CLA:NC	2.41	0.88
5:A:158:GLN:CD	15:A:1112:CLA:CED	2.39	0.87
6:B:373:TYR:OH	15:B:1234:CLA:HMC2	1.74	0.87
1:1:191:PHE:CZ	12:1:501:LUT:H27	2.09	0.87
11:J:26:LEU:HD12	14:J:4001:BCR:H343	1.55	0.87
15:A:1108:CLA:HBB1	15:A:1108:CLA:HMB1	1.57	0.86
6:B:300:HIS:CD2	15:B:1219:CLA:OBD	2.27	0.86
15:3:615:CLA:H2A	15:3:615:CLA:HED2	1.57	0.86
15:A:1107:CLA:HBA1	15:A:1107:CLA:CBD	2.05	0.86
20:A:1011:CL0:H8	20:A:1011:CL0:CGD	2.05	0.86
1:1:191:PHE:CZ	12:1:501:LUT:H392	2.11	0.86
15:3:615:CLA:H2A	15:3:615:CLA:CED	2.05	0.86
1:1:179:LYS:NZ	17:1:801:LHG:O5	2.09	0.85
15:A:1120:CLA:HMB1	15:A:1120:CLA:HBB1	1.58	0.85
1:1:131:GLU:OE2	15:1:613:CLA:C3B	2.25	0.85
5:A:532:ASP:OD1	5:A:635:PHE:HE2	1.59	0.85
14:A:4006:BCR:H331	14:A:4006:BCR:C8	2.05	0.85
6:B:288:ALA:HB2	15:B:1216:CLA:C3C	2.07	0.85
5:A:217:GLN:HA	5:A:221:SER:HB3	1.56	0.85
14:A:4003:BCR:H383	14:A:4003:BCR:C37	2.06	0.85
15:A:1111:CLA:HMB1	15:A:1111:CLA:HBB1	1.58	0.84
1:1:191:PHE:HZ	12:1:501:LUT:H27	1.42	0.84
6:B:451:GLU:OE2	10:F:129:ARG:NH1	2.10	0.84
5:A:667:ALA:HB3	15:A:1106:CLA:HBC2	1.59	0.84
15:A:1128:CLA:HBB1	15:A:1128:CLA:HMB3	1.60	0.84
15:J:1302:CLA:HBB1	15:J:1302:CLA:HMB1	1.58	0.84
6:B:90:HIS:CE1	15:B:1205:CLA:NC	2.46	0.84
6:B:94:ASP:OD2	15:B:1206:CLA:NB	2.11	0.84
15:A:1130:CLA:H2A	15:A:1130:CLA:CED	2.02	0.84
15:B:1229:CLA:H2A	15:B:1229:CLA:HED2	1.60	0.84
6:B:721:THR:HB	15:B:1021:CLA:O1D	1.78	0.83
6:B:231:TRP:O	15:B:1213:CLA:H3A	1.77	0.83
16:3:604:CHL:HMB3	16:3:604:CHL:HBB1	1.57	0.83
5:A:352:GLN:HG3	15:A:1123:CLA:H141	1.58	0.83
6:B:124:TRP:HZ2	15:B:1210:CLA:H191	1.40	0.83
1:1:182:ARG:HB2	17:1:801:LHG:H101	1.60	0.83
5:A:497:LEU:HD21	15:A:1134:CLA:HBC2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:320:HIS:HB3	5:A:325:ILE:HD11	1.61	0.83
6:B:721:THR:CG2	15:B:1021:CLA:O1D	2.27	0.82
15:A:1136:CLA:HBB1	15:A:1136:CLA:HHC	1.61	0.82
15:B:1235:CLA:HBC2	14:F:4001:BCR:C39	2.09	0.82
5:A:506:THR:HG22	15:A:1116:CLA:H2	1.61	0.82
6:B:68:HIS:NE2	15:B:1204:CLA:NB	2.26	0.82
6:B:54:GLN:NE2	15:B:1203:CLA:NB	2.28	0.82
18:4:801:LMG:HO4	18:4:801:LMG:HO5	1.23	0.82
15:A:1013:CLA:H203	15:A:1140:CLA:H61	1.61	0.82
5:A:357:LEU:HD23	15:A:1103:CLA:HED1	1.62	0.82
1:1:217:ASN:HD21	15:1:608:CLA:CMA	1.93	0.81
18:2:804:LMG:H311	15:3:610:CLA:CBB	2.09	0.81
15:A:1119:CLA:HMB2	15:A:1123:CLA:HMA2	1.61	0.81
14:J:4001:BCR:H392	14:J:4001:BCR:H23C	1.62	0.81
2:2:254:HIS:CD2	15:2:608:CLA:NC	2.48	0.81
15:A:1137:CLA:H2A	15:A:1137:CLA:CED	2.10	0.81
15:B:1235:CLA:HMB1	15:B:1235:CLA:HBB1	1.63	0.81
15:B:1234:CLA:HBC2	15:B:1234:CLA:HHD	1.60	0.81
6:B:518:PHE:CE1	14:F:4001:BCR:H382	2.15	0.81
4:4:178:VAL:CG2	12:4:501:LUT:H15	2.11	0.81
6:B:188:SER:HB2	15:B:1215:CLA:HMC2	1.61	0.80
5:A:667:ALA:CB	15:A:1106:CLA:HBC2	2.12	0.80
15:A:1108:CLA:H92	15:A:1112:CLA:H193	1.64	0.80
15:A:1124:CLA:C5	15:A:1135:CLA:H11	2.10	0.80
14:B:4005:BCR:H403	14:B:4005:BCR:H23C	1.64	0.80
15:A:1121:CLA:HHC	15:A:1121:CLA:CBB	2.10	0.80
7:C:25:VAL:HG13	7:C:44:ARG:O	1.81	0.80
14:B:4005:BCR:H403	14:B:4005:BCR:C23	2.12	0.80
14:F:4001:BCR:H403	14:F:4001:BCR:C23	2.09	0.80
6:B:451:GLU:OE2	10:F:129:ARG:NH2	2.14	0.80
15:B:1223:CLA:CHC	15:B:1231:CLA:HMA1	2.10	0.80
5:A:486:TRP:HZ3	15:A:1133:CLA:HAC1	1.47	0.80
6:B:89:ALA:HB1	15:B:1205:CLA:CAD	2.12	0.79
15:B:1236:CLA:HHC	15:B:1236:CLA:CBB	2.11	0.79
5:A:29:TRP:HE1	15:A:1109:CLA:CHB	1.95	0.79
1:1:86:ALA:HB1	12:1:501:LUT:C30	2.05	0.79
6:B:68:HIS:CE1	15:B:1204:CLA:NA	2.51	0.79
6:B:277:HIS:HE2	15:B:1215:CLA:HMB1	1.48	0.79
6:B:27:ALA:CB	23:B:5002:DGD:HG2	2.14	0.78
6:B:119:SER:O	6:B:372:LEU:HD21	1.83	0.78
15:B:1214:CLA:H43	15:B:1231:CLA:HED3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:596:LEU:HD21	15:A:1128:CLA:HBC1	1.65	0.78
15:B:1222:CLA:H2A	15:B:1222:CLA:HED2	1.64	0.78
3:3:271:HIS:CD2	15:3:608:CLA:C1C	2.67	0.78
5:A:374:MET:HE1	15:A:1125:CLA:CBB	2.14	0.78
15:A:1131:CLA:HHC	15:A:1131:CLA:CBB	2.12	0.78
14:A:4007:BCR:H14C	15:B:1023:CLA:C19	2.13	0.78
3:3:187:ASP:OD2	15:3:611:CLA:HBC1	1.83	0.78
5:A:572:ARG:NH1	17:A:5002:LHG:O10	2.17	0.78
5:A:681:PHE:HZ	15:A:1140:CLA:CBC	1.97	0.78
15:A:1110:CLA:HHC	15:A:1110:CLA:CBB	2.13	0.78
6:B:191:TRP:CZ2	15:B:1215:CLA:O1D	2.37	0.78
6:B:463:TRP:CZ2	15:F:1302:CLA:HBA1	2.17	0.78
15:A:1106:CLA:H2A	15:A:1106:CLA:CED	2.13	0.78
20:A:1011:CL0:H12	15:A:1012:CLA:OBD	1.84	0.78
1:1:131:GLU:OE2	15:1:613:CLA:C4B	2.32	0.77
4:4:289:ALA:CB	12:4:501:LUT:H392	2.12	0.77
5:A:687:PHE:CD2	6:B:665:LEU:HD23	2.19	0.77
6:B:277:HIS:CE1	15:B:1214:CLA:C1D	2.55	0.77
6:B:435:LEU:O	6:B:439:VAL:HG23	1.84	0.77
1:1:70:ARG:NE	15:1:605:CLA:O1A	2.18	0.77
1:1:131:GLU:OE2	15:1:613:CLA:C2B	2.32	0.77
4:4:171:ARG:O	15:4:601:CLA:HMC1	1.85	0.77
15:B:1230:CLA:HBB1	15:B:1230:CLA:CMB	2.13	0.77
1:1:218:PHE:CE2	15:1:608:CLA:O2D	2.36	0.77
15:3:615:CLA:HBB1	15:3:615:CLA:HMB1	1.64	0.77
5:A:325:ILE:HA	15:A:1120:CLA:HED2	1.67	0.77
5:A:497:LEU:CD2	15:A:1134:CLA:HBC2	2.15	0.77
15:A:1013:CLA:H12	15:A:1013:CLA:CMA	2.14	0.77
6:B:180:LEU:CD2	15:B:1216:CLA:C3B	2.62	0.77
18:2:804:LMG:H291	15:A:1114:CLA:CAD	2.15	0.77
15:A:1128:CLA:HED2	15:A:1128:CLA:H2A	1.67	0.77
6:B:451:GLU:CD	10:F:129:ARG:HH12	1.92	0.77
15:B:1229:CLA:HBB1	15:B:1229:CLA:CMB	2.15	0.77
3:3:259:ILE:HD12	15:3:603:CLA:HMD1	1.67	0.77
6:B:54:GLN:NE2	15:B:1203:CLA:MG	1.41	0.77
6:B:437:LEU:CD1	14:F:4001:BCR:H383	2.15	0.77
5:A:374:MET:HE1	15:A:1125:CLA:CAB	2.14	0.76
15:A:1107:CLA:HBB1	15:A:1107:CLA:HMB3	1.67	0.76
6:B:701:LEU:HG	21:B:2002:PQN:O4	1.84	0.76
5:A:307:VAL:O	15:A:1121:CLA:HBC1	1.85	0.76
15:A:1133:CLA:C3D	15:A:1134:CLA:HMB1	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1013:CLA:HMB1	15:A:1013:CLA:HBB1	1.67	0.76
6:B:518:PHE:CZ	14:F:4001:BCR:H382	2.21	0.76
5:A:359:LEU:HD11	15:A:1123:CLA:HMB2	1.68	0.76
6:B:520:VAL:HG11	6:B:594:TYR:CG	2.20	0.76
15:A:1138:CLA:HBB2	10:F:182:GLY:HA3	1.66	0.76
14:A:4007:BCR:C11	15:B:1022:CLA:H152	2.15	0.76
6:B:51:HIS:CE1	15:B:1202:CLA:C4D	2.69	0.76
7:C:52:LYS:HE2	7:C:69:LEU:HD11	1.67	0.76
15:A:1124:CLA:HBB1	15:A:1124:CLA:CMB	2.15	0.76
17:3:801:LHG:O5	17:3:801:LHG:O2	2.04	0.75
5:A:71:ARG:NH1	5:A:186:PRO:O	2.19	0.75
1:1:221:ASN:ND2	15:1:603:CLA:OBD	2.19	0.75
1:1:127:ILE:HD12	15:1:613:CLA:CAD	2.15	0.75
1:1:183:LEU:HD21	15:1:607:CLA:HAC1	1.68	0.75
2:2:254:HIS:CE1	15:2:608:CLA:NA	2.55	0.75
15:A:1114:CLA:HHC	15:A:1114:CLA:CBB	2.15	0.75
11:J:23:SER:HA	14:J:4001:BCR:H341	1.68	0.75
5:A:667:ALA:HB3	15:A:1106:CLA:HBC1	1.68	0.75
15:A:1112:CLA:H41	15:A:1114:CLA:H72	1.67	0.75
5:A:396:TRP:CD1	15:A:1126:CLA:HAB	2.20	0.75
5:A:223:PRO:HB2	5:A:243:PHE:CE1	2.22	0.74
3:3:241:LYS:HE2	15:3:607:CLA:O1D	1.87	0.74
5:A:158:GLN:OE1	15:A:1112:CLA:HED3	1.85	0.74
15:A:1133:CLA:C4D	15:A:1134:CLA:HMB1	2.17	0.74
13:3:502:XAT:H403	15:3:605:CLA:CBB	2.17	0.74
15:3:605:CLA:H93	15:A:1111:CLA:C20	2.17	0.74
15:3:605:CLA:H152	15:A:1108:CLA:HBC1	1.69	0.74
1:1:154:PRO:O	15:1:601:CLA:CED	2.35	0.74
6:B:464:ILE:CD1	15:B:1234:CLA:H12	2.17	0.74
4:4:289:ALA:HB2	12:4:501:LUT:H391	1.68	0.74
5:A:157:LEU:HD13	15:A:1114:CLA:HED1	1.70	0.74
6:B:276:HIS:HB3	15:B:1214:CLA:CMB	2.18	0.74
6:B:701:LEU:HB2	21:B:2002:PQN:C6	2.18	0.74
15:B:1235:CLA:HBC2	14:F:4001:BCR:H393	1.70	0.74
7:C:22:PRO:HG2	7:C:23:LEU:HD12	1.69	0.74
6:B:518:PHE:CZ	14:F:4001:BCR:C38	2.71	0.73
15:3:605:CLA:H93	15:A:1111:CLA:H202	1.68	0.73
5:A:376:PRO:HB3	15:A:1117:CLA:HMA2	1.69	0.73
6:B:374:THR:HG22	6:B:592:THR:CG2	2.18	0.73
1:1:218:PHE:CE2	15:1:608:CLA:CED	2.72	0.73
6:B:437:LEU:HD11	14:F:4001:BCR:H383	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:254:HIS:NE2	15:2:608:CLA:MG	1.46	0.73
14:B:4006:BCR:H23C	14:B:4006:BCR:C40	2.15	0.73
15:A:1105:CLA:HBD	15:A:1105:CLA:CBA	2.19	0.73
6:B:32:PHE:CE2	15:B:1202:CLA:HMC1	2.23	0.73
6:B:92:ILE:HD13	15:B:1206:CLA:HMD2	1.71	0.73
17:A:5002:LHG:O2	17:A:5002:LHG:O4	2.06	0.73
15:A:1137:CLA:HBC3	17:A:5001:LHG:H322	1.68	0.73
18:2:804:LMG:H392	17:3:801:LHG:H342	1.71	0.72
6:B:30:HIS:HB2	15:B:1226:CLA:O1A	1.89	0.72
6:B:300:HIS:HD2	15:B:1219:CLA:OBD	1.70	0.72
6:B:27:ALA:HB1	23:B:5002:DGD:HG2	1.71	0.72
5:A:363:LEU:HD21	15:A:1117:CLA:H71	1.71	0.72
15:A:1103:CLA:C3	14:A:4003:BCR:H282	2.19	0.72
15:A:1130:CLA:HBB1	15:A:1130:CLA:CMB	2.20	0.72
3:3:124:ALA:HB3	12:3:501:LUT:H32	1.70	0.72
7:C:7:ILE:CG2	7:C:65:VAL:HG22	2.10	0.72
1:1:209:HIS:CD2	15:1:608:CLA:C4B	2.73	0.72
1:1:191:PHE:HE1	12:1:501:LUT:C24	2.03	0.72
15:B:1021:CLA:HBB1	15:B:1021:CLA:CMB	2.20	0.72
15:B:1222:CLA:HBB1	15:B:1222:CLA:CMB	2.20	0.72
14:B:4006:BCR:H403	14:B:4006:BCR:C23	2.16	0.72
5:A:497:LEU:CD2	15:A:1134:CLA:CBC	2.68	0.72
14:A:4002:BCR:H383	14:A:4008:BCR:C31	2.20	0.72
3:3:272:LEU:HD22	15:3:608:CLA:CAB	2.20	0.72
6:B:96:HIS:CE1	15:B:1206:CLA:CMB	2.73	0.72
10:F:217:TRP:CD1	10:F:218:PRO:HD3	2.24	0.72
6:B:721:THR:CB	15:B:1021:CLA:O1D	2.38	0.71
6:B:463:TRP:CZ2	15:F:1302:CLA:HBA2	2.25	0.71
11:J:26:LEU:CD1	14:J:4001:BCR:H343	2.19	0.71
6:B:355:SER:CB	15:B:1223:CLA:HAC2	2.20	0.71
7:C:10:THR:OG1	7:C:64:SER:HB3	1.90	0.71
6:B:451:GLU:CG	10:F:129:ARG:HH12	2.04	0.71
15:A:1130:CLA:O2A	6:B:687:PRO:CD	2.38	0.71
6:B:57:ILE:HG13	15:B:1201:CLA:HBB2	1.73	0.71
1:1:127:ILE:HD12	15:1:613:CLA:C4D	2.20	0.71
19:3:802:3PH:H322	5:A:179:PHE:HE1	1.56	0.71
4:4:222:LEU:HD22	14:4:503:BCR:C16	2.20	0.71
1:1:90:LEU:HD21	12:1:501:LUT:H363	1.71	0.71
5:A:95:GLY:O	5:A:99:SER:OG	2.06	0.71
15:A:1138:CLA:HBB1	15:A:1138:CLA:CMB	2.20	0.71
6:B:96:HIS:CE1	15:B:1206:CLA:HMB3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:4006:BCR:H331	14:B:4006:BCR:C8	2.21	0.70
1:1:209:HIS:CD2	15:1:608:CLA:C1C	2.74	0.70
1:1:86:ALA:HB1	12:1:501:LUT:H391	1.74	0.70
15:B:1235:CLA:HMC1	14:F:4001:BCR:C39	2.21	0.70
14:A:4007:BCR:C16	14:A:4007:BCR:H351	2.21	0.70
15:3:612:CLA:HBB1	15:3:612:CLA:CMB	2.21	0.70
15:A:1123:CLA:H2	15:A:1123:CLA:H71	1.72	0.70
6:B:191:TRP:CZ2	15:B:1215:CLA:OBD	2.45	0.70
6:B:616:TYR:OH	6:B:622:ARG:NH2	2.25	0.70
1:1:139:GLU:OE2	1:1:142:ARG:NH2	2.24	0.69
4:4:178:VAL:HG22	12:4:501:LUT:C15	2.22	0.69
20:A:1011:CL0:H13	20:A:1011:CL0:H15	1.74	0.69
15:A:1137:CLA:CHD	17:A:5001:LHG:H342	2.22	0.69
6:B:191:TRP:HZ2	15:B:1215:CLA:O1D	1.74	0.69
15:B:1222:CLA:H71	15:B:1240:CLA:H191	1.73	0.69
15:3:615:CLA:HED2	15:3:615:CLA:CBA	2.22	0.69
15:A:1108:CLA:HBB1	15:A:1108:CLA:CMB	2.22	0.69
15:A:1111:CLA:HBB1	15:A:1111:CLA:CMB	2.21	0.69
14:F:4001:BCR:H23C	14:F:4001:BCR:C40	2.19	0.69
1:1:127:ILE:CD1	15:1:613:CLA:CAD	2.71	0.69
3:3:104:VAL:CG2	15:A:1108:CLA:CED	2.68	0.69
6:B:50:SER:OG	15:B:1202:CLA:CAB	2.39	0.69
14:J:4002:BCR:H331	14:J:4002:BCR:HC8	1.74	0.69
1:1:209:HIS:CD2	15:1:608:CLA:NC	2.60	0.69
15:A:1115:CLA:HBB1	15:A:1115:CLA:CMB	2.21	0.69
14:A:4002:BCR:H323	14:A:4002:BCR:C34	2.23	0.69
15:B:1236:CLA:HED2	15:B:1236:CLA:H2A	1.74	0.69
4:4:312:LEU:HD21	15:4:608:CLA:HMC3	1.73	0.69
15:A:1013:CLA:H12	15:A:1013:CLA:HMA3	1.74	0.69
14:A:4002:BCR:H342	14:A:4002:BCR:C32	2.23	0.69
6:B:139:SER:HB2	14:B:4003:BCR:H391	1.73	0.69
1:1:131:GLU:HG3	15:1:613:CLA:CHB	2.23	0.69
5:A:399:GLY:HA3	5:A:603:LEU:HD11	1.74	0.69
15:A:1116:CLA:H92	15:A:1133:CLA:O1A	1.92	0.69
15:B:1228:CLA:HBB1	15:B:1228:CLA:HMB1	1.75	0.69
15:3:605:CLA:HBB1	15:3:605:CLA:CMB	2.21	0.69
15:A:1138:CLA:H51	14:B:4006:BCR:H14C	1.75	0.69
18:2:804:LMG:C31	15:3:610:CLA:HBB1	2.23	0.69
13:3:502:XAT:H383	16:3:604:CHL:H102	1.73	0.69
4:4:279:GLU:OE2	15:4:601:CLA:NB	2.25	0.69
5:A:245:LEU:HD23	5:A:245:LEU:N	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:116:ILE:O	15:B:1205:CLA:HMD2	1.93	0.69
6:B:722:TYR:HB2	15:B:1021:CLA:HED3	1.74	0.69
14:J:4002:BCR:H331	14:J:4002:BCR:C8	2.23	0.69
1:1:141:LEU:HD13	15:1:611:CLA:HAB	1.73	0.69
15:A:1137:CLA:HBB1	15:A:1137:CLA:CMB	2.22	0.69
6:B:30:HIS:N	15:B:1226:CLA:O1A	2.25	0.69
16:2:609:CHL:HHB	15:3:615:CLA:O1D	1.93	0.69
2:2:136:TRP:O	13:2:502:XAT:O3	2.11	0.68
15:A:1128:CLA:HBB1	15:A:1128:CLA:CMB	2.22	0.68
15:A:1137:CLA:C5	14:A:4005:BCR:H352	2.23	0.68
14:A:4005:BCR:H331	14:A:4005:BCR:C8	2.22	0.68
6:B:58:ILE:HG12	15:B:1203:CLA:CMC	2.23	0.68
6:B:701:LEU:HB2	21:B:2002:PQN:H6	1.74	0.68
15:B:1235:CLA:HBC2	14:F:4001:BCR:H392	1.74	0.68
1:1:198:THR:HG21	15:1:603:CLA:HED1	1.76	0.68
15:3:613:CLA:HBB1	15:3:613:CLA:CMB	2.21	0.68
15:B:1229:CLA:HMB1	15:B:1229:CLA:CBB	2.24	0.68
5:A:130:ASP:OD1	10:F:109:TYR:OH	2.08	0.68
14:A:4007:BCR:H10C	15:B:1022:CLA:H161	1.74	0.68
14:A:4007:BCR:H331	14:A:4007:BCR:C8	2.24	0.68
6:B:92:ILE:CD1	15:B:1206:CLA:HMD2	2.24	0.68
12:3:501:LUT:H192	15:3:601:CLA:H71	1.76	0.68
15:3:612:CLA:HED2	15:3:612:CLA:C2A	2.09	0.68
4:4:223:PHE:CE1	14:4:503:BCR:H361	2.29	0.68
14:A:4002:BCR:H383	14:A:4008:BCR:H311	1.76	0.68
15:A:1120:CLA:HBB1	15:A:1120:CLA:CMB	2.23	0.67
14:A:4003:BCR:H383	14:A:4003:BCR:H372	1.75	0.67
6:B:232:ALA:HA	15:B:1213:CLA:HAA2	1.76	0.67
15:B:1210:CLA:H193	15:B:1225:CLA:H52	1.76	0.67
1:1:213:PRO:HG2	15:1:608:CLA:CMB	2.23	0.67
15:3:615:CLA:HBB1	15:3:615:CLA:CMB	2.24	0.67
15:A:1106:CLA:HBB1	15:A:1106:CLA:CMB	2.22	0.67
15:B:1230:CLA:HMB3	15:B:1230:CLA:CBB	2.24	0.67
15:A:1107:CLA:CMA	11:J:27:ILE:HD13	2.25	0.67
15:B:1223:CLA:C3B	15:B:1231:CLA:CMA	2.73	0.67
5:A:374:MET:SD	15:A:1116:CLA:HBD	2.35	0.67
6:B:61:TRP:CG	15:B:1203:CLA:HBC1	2.30	0.67
3:3:275:PRO:CG	15:3:608:CLA:HMA1	2.24	0.67
6:B:187:SER:HB2	15:B:1215:CLA:HAC1	1.75	0.67
4:4:229:LYS:CD	16:4:611:CHL:OMC	2.43	0.67
15:A:1012:CLA:C4	6:B:439:VAL:HG22	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1122:CLA:H41	15:A:1122:CLA:H71	1.75	0.67
6:B:309:HIS:HB3	15:B:1240:CLA:OBD	1.95	0.67
6:B:656:LEU:HB2	15:B:1022:CLA:O1A	1.94	0.67
3:3:271:HIS:HE1	15:3:608:CLA:C4D	2.08	0.67
15:A:1123:CLA:H2A	15:A:1123:CLA:HED2	1.76	0.67
15:B:1235:CLA:HBB1	15:B:1235:CLA:CMB	2.25	0.67
3:3:155:PRO:HG2	15:A:1114:CLA:HBC2	1.76	0.67
10:F:217:TRP:CG	10:F:218:PRO:HD3	2.30	0.67
6:B:191:TRP:CE3	15:B:1215:CLA:HMD1	2.29	0.66
6:B:377:GLN:OE1	6:B:377:GLN:HA	1.94	0.66
1:1:213:PRO:HB3	15:1:608:CLA:C1B	2.25	0.66
6:B:559:PRO:HB3	6:B:703:ILE:HD12	1.76	0.66
15:B:1236:CLA:H43	14:B:4005:BCR:H10C	1.76	0.66
7:C:17:CYS:O	7:C:21:CYS:SG	2.52	0.66
5:A:80:GLN:HG2	15:A:1103:CLA:CMA	2.25	0.66
15:A:1136:CLA:C5	15:A:1136:CLA:H92	2.25	0.66
4:4:218:ILE:HD13	16:4:613:CHL:HED2	1.77	0.66
6:B:90:HIS:CD2	15:B:1205:CLA:C4D	2.76	0.66
6:B:721:THR:HG22	15:B:1021:CLA:O1D	1.95	0.66
15:A:1138:CLA:H92	14:B:4006:BCR:H16C	1.78	0.66
14:A:4002:BCR:C21	14:A:4003:BCR:HC31	2.26	0.66
3:3:124:ALA:CB	12:3:501:LUT:H32	2.25	0.66
6:B:89:ALA:CB	15:B:1205:CLA:CAD	2.74	0.66
5:A:667:ALA:CB	15:A:1106:CLA:CBC	2.72	0.66
15:A:1136:CLA:HHC	15:A:1136:CLA:CBB	2.26	0.66
6:B:30:HIS:O	15:B:1226:CLA:HAA1	1.96	0.66
1:1:87:ALA:HB2	12:1:501:LUT:H35	1.76	0.66
19:3:802:3PH:C34	5:A:175:PHE:HZ	2.09	0.66
6:B:89:ALA:HB1	15:B:1205:CLA:C3D	2.25	0.66
5:A:303:VAL:HG22	14:A:4008:BCR:H352	1.78	0.65
15:A:1137:CLA:H51	14:A:4005:BCR:H352	1.75	0.65
6:B:51:HIS:CE1	15:B:1202:CLA:C1D	2.78	0.65
6:B:90:HIS:HD2	15:B:1205:CLA:C4D	2.08	0.65
3:3:271:HIS:HE1	15:3:608:CLA:ND	1.81	0.65
3:3:275:PRO:HG2	15:3:608:CLA:CMA	2.26	0.65
6:B:89:ALA:CB	15:B:1205:CLA:C3D	2.73	0.65
6:B:191:TRP:CE2	15:B:1215:CLA:C3D	2.80	0.65
15:B:1205:CLA:O1A	15:B:1224:CLA:HBD	1.96	0.65
15:J:1302:CLA:HBB1	15:J:1302:CLA:CMB	2.23	0.65
6:B:463:TRP:CE2	15:F:1302:CLA:HAA2	2.32	0.65
5:A:687:PHE:CE2	6:B:665:LEU:HD23	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1011:CL0:C3B	15:A:1012:CLA:HED1	2.26	0.65
15:A:1112:CLA:HBB1	15:A:1112:CLA:CMB	2.24	0.65
15:3:605:CLA:HED3	15:3:605:CLA:H62	1.79	0.65
15:A:1105:CLA:H51	15:J:1302:CLA:HBC1	1.79	0.65
5:A:158:GLN:CG	15:A:1112:CLA:HED1	2.26	0.65
5:A:392:THR:OG1	15:A:1126:CLA:CMB	2.45	0.65
15:A:1110:CLA:HBA1	15:A:1110:CLA:CHA	2.26	0.65
15:A:1124:CLA:HMB1	15:A:1124:CLA:CBB	2.23	0.65
6:B:175:ARG:NE	15:B:1221:CLA:HMD3	2.11	0.65
6:B:213:PHE:HB3	15:B:1211:CLA:CMD	2.26	0.65
6:B:139:SER:HG	14:B:4003:BCR:H401	1.60	0.65
15:B:1230:CLA:HAA2	11:J:36:PRO:HG2	1.79	0.65
10:F:164:VAL:C	10:F:167:PRO:HD2	2.22	0.65
14:J:4002:BCR:C23	14:J:4002:BCR:H403	2.26	0.65
1:1:131:GLU:OE2	15:1:613:CLA:C1B	2.45	0.64
6:B:51:HIS:HE1	15:B:1202:CLA:C1D	2.10	0.64
1:1:184:ALA:HB2	12:1:501:LUT:C40	2.23	0.64
1:1:209:HIS:CD2	15:1:608:CLA:NB	2.44	0.64
1:1:81:TRP:NE1	15:1:611:CLA:HED3	2.12	0.64
15:A:1013:CLA:HBB1	15:A:1013:CLA:CMB	2.26	0.64
15:A:1112:CLA:H12	15:A:1114:CLA:HMB1	1.80	0.64
1:1:217:ASN:ND2	15:1:608:CLA:HMA1	2.09	0.64
5:A:313:ARG:HH21	5:A:321:SER:HB3	1.62	0.64
15:B:1228:CLA:HBB1	15:B:1228:CLA:CMB	2.28	0.64
1:1:209:HIS:CD2	15:1:608:CLA:CHC	2.80	0.64
5:A:561:ARG:O	8:D:134:ARG:NH1	2.31	0.64
14:A:4006:BCR:H331	14:A:4006:BCR:HC8	1.79	0.64
14:A:4007:BCR:H351	14:A:4007:BCR:H16C	1.78	0.64
6:B:374:THR:HG22	6:B:592:THR:HG21	1.79	0.64
6:B:451:GLU:OE2	10:F:129:ARG:CZ	2.46	0.64
1:1:91:ALA:HB2	15:1:601:CLA:C20	2.28	0.64
3:3:193:SER:OG	3:3:194:GLN:OE1	2.13	0.64
3:3:275:PRO:HG2	15:3:608:CLA:HMA1	1.79	0.64
14:A:4002:BCR:C38	14:A:4008:BCR:H311	2.28	0.64
5:A:497:LEU:HD21	15:A:1134:CLA:CBC	2.28	0.64
1:1:213:PRO:HB3	15:1:608:CLA:CHB	2.27	0.64
5:A:580:ARG:HG2	7:C:49:VAL:CG2	2.28	0.64
21:A:2001:PQN:H241	21:A:2001:PQN:H271	1.80	0.64
6:B:180:LEU:HD21	15:B:1216:CLA:C2B	2.27	0.64
8:D:134:ARG:NH2	8:D:136:GLU:OE1	2.31	0.64
1:1:91:ALA:CB	15:1:601:CLA:H201	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1118:CLA:HBB1	15:A:1118:CLA:HMB1	1.80	0.63
6:B:94:ASP:OD2	15:B:1206:CLA:MG	1.41	0.63
1:1:91:ALA:HB2	15:1:601:CLA:H18	1.80	0.63
1:1:209:HIS:HD2	15:1:608:CLA:C1C	2.11	0.63
4:4:304:PRO:O	12:4:501:LUT:O23	2.15	0.63
15:A:1012:CLA:H112	15:A:1126:CLA:C20	2.28	0.63
5:A:646:LEU:HD22	6:B:652:LEU:HD21	1.79	0.63
14:A:4005:BCR:C23	14:A:4005:BCR:H382	2.29	0.63
5:A:208:LEU:HD21	15:A:1118:CLA:HMC1	1.81	0.63
2:2:169:ARG:NH2	15:2:612:CLA:O1D	2.31	0.63
4:4:219:GLU:OE2	16:4:613:CHL:C2B	2.47	0.63
6:B:50:SER:OG	15:B:1202:CLA:HBB1	1.97	0.63
6:B:656:LEU:CD1	15:B:1023:CLA:HBB2	2.22	0.63
5:A:402:VAL:HG13	14:A:4005:BCR:H371	1.80	0.63
6:B:115:ASN:ND2	15:B:1205:CLA:HAC2	2.13	0.63
6:B:187:SER:HB2	15:B:1215:CLA:CAC	2.29	0.63
15:A:1116:CLA:C4	15:A:1133:CLA:HAA1	2.29	0.62
6:B:51:HIS:HD2	15:B:1202:CLA:NB	1.89	0.62
1:1:158:PHE:CD1	15:1:601:CLA:HMD2	2.34	0.62
5:A:141:THR:O	15:A:1126:CLA:HMA1	2.00	0.62
15:A:1013:CLA:HMA3	15:A:1013:CLA:C2	2.29	0.62
1:1:209:HIS:HD2	15:1:608:CLA:CHC	2.12	0.62
6:B:277:HIS:HE2	15:B:1215:CLA:CMB	2.13	0.62
1:1:191:PHE:CE2	12:1:501:LUT:H392	2.35	0.62
6:B:302:LEU:HD13	15:B:1221:CLA:HAC2	1.82	0.62
1:1:127:ILE:CD1	15:1:613:CLA:C2D	2.78	0.62
15:A:1013:CLA:H12	15:A:1013:CLA:HMA1	1.81	0.62
15:A:1105:CLA:HBB1	15:A:1105:CLA:CMB	2.24	0.62
6:B:347:SER:HB3	15:B:1222:CLA:OBD	1.98	0.62
1:1:87:ALA:HB2	12:1:501:LUT:C35	2.28	0.62
13:3:502:XAT:C31	15:3:605:CLA:HMB3	2.29	0.62
15:A:1013:CLA:H41	6:B:435:LEU:HD22	1.81	0.62
15:B:1205:CLA:C4	15:B:1224:CLA:H11	2.29	0.62
15:B:1223:CLA:C4B	15:B:1231:CLA:HMA1	2.23	0.62
16:3:604:CHL:H12	16:3:604:CHL:CHB	2.30	0.62
15:A:1112:CLA:C5	15:A:1112:CLA:H92	2.30	0.62
6:B:210:TRP:N	15:B:1211:CLA:OBD	2.33	0.62
6:B:274:MET:SD	15:B:1215:CLA:CMA	2.88	0.62
15:B:1235:CLA:CMC	14:F:4001:BCR:H393	2.30	0.62
1:1:47:LEU:O	1:1:53:ASN:ND2	2.33	0.61
1:1:87:ALA:HB1	15:1:601:CLA:H172	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:188:SER:HB2	15:B:1215:CLA:CMC	2.29	0.61
1:1:81:TRP:CE2	15:1:611:CLA:HED3	2.34	0.61
3:3:279:ASN:OD1	3:3:280:LEU:N	2.34	0.61
6:B:277:HIS:CE1	15:B:1214:CLA:C4C	2.81	0.61
15:B:1227:CLA:HAB	15:B:1236:CLA:HBB2	1.81	0.61
2:2:64:ARG:NH1	2:2:84:ASP:OD2	2.34	0.61
20:A:1011:CL0:CMB	15:A:1012:CLA:OBD	2.48	0.61
10:F:164:VAL:O	10:F:167:PRO:HD2	2.00	0.61
10:F:167:PRO:N	10:F:167:PRO:C	2.57	0.61
15:A:1127:CLA:HBB1	15:A:1127:CLA:CMB	2.25	0.61
15:A:1135:CLA:HBB1	15:A:1135:CLA:CMB	2.25	0.61
15:A:1131:CLA:CAB	15:A:1132:CLA:HMB1	2.30	0.61
15:B:1222:CLA:HMB3	15:B:1222:CLA:CBB	2.27	0.61
5:A:453:PHE:HE1	15:B:1022:CLA:HMA3	1.65	0.61
15:A:1123:CLA:HBB1	15:A:1123:CLA:CMB	2.24	0.61
6:B:213:PHE:CB	15:B:1211:CLA:HMD3	2.30	0.61
15:B:1235:CLA:CMC	14:F:4001:BCR:C39	2.79	0.61
15:A:1107:CLA:HBB1	15:A:1107:CLA:CMB	2.30	0.61
6:B:58:ILE:HG12	15:B:1203:CLA:C2C	2.30	0.61
15:B:1023:CLA:H3A	15:B:1023:CLA:CGA	2.31	0.61
12:3:501:LUT:H391	15:3:614:CLA:HMC2	1.83	0.61
15:2:616:CLA:H192	15:2:616:CLA:H141	1.82	0.61
3:3:272:LEU:HD22	15:3:608:CLA:HAB	1.83	0.61
5:A:389:SER:CB	15:A:1126:CLA:CMA	2.71	0.61
15:A:1122:CLA:H43	14:A:4005:BCR:H351	1.81	0.61
1:1:213:PRO:HG2	15:1:608:CLA:HMB3	1.82	0.60
2:2:194:LYS:NZ	2:2:209:SER:O	2.33	0.60
15:A:1135:CLA:H2A	15:A:1135:CLA:CED	2.24	0.60
1:1:71:TYR:CD2	15:1:604:CLA:O1A	2.54	0.60
15:3:606:CLA:O1A	15:3:613:CLA:HMD3	2.01	0.60
5:A:54:ALA:O	15:A:1128:CLA:O1A	2.20	0.60
15:A:1102:CLA:HBB1	15:A:1102:CLA:CMB	2.27	0.60
14:J:4002:BCR:H271	14:J:4002:BCR:H393	1.82	0.60
15:A:1012:CLA:C4	6:B:439:VAL:HG13	2.27	0.60
15:A:1012:CLA:HBB1	15:A:1012:CLA:HMB1	1.83	0.60
6:B:65:ASN:ND2	15:B:1224:CLA:HED1	2.15	0.60
6:B:381:GLY:HA2	15:B:1222:CLA:HAC2	1.82	0.60
6:B:706:ALA:HB2	21:B:2002:PQN:C7	2.32	0.60
2:2:269:SER:HB2	15:2:616:CLA:ND	2.15	0.60
4:4:279:GLU:OE2	15:4:601:CLA:C1B	2.49	0.60
15:A:1133:CLA:ND	14:A:4005:BCR:HC31	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:704:HIS:CE1	15:A:1139:CLA:HAC1	2.37	0.60
6:B:373:TYR:OH	15:B:1234:CLA:CMC	2.47	0.60
1:1:131:GLU:HA	15:1:613:CLA:HMA1	1.83	0.60
6:B:47:ILE:HG12	15:B:1202:CLA:C2C	2.31	0.60
6:B:209:GLY:C	15:B:1211:CLA:HMD1	2.25	0.60
6:B:463:TRP:NE1	15:F:1302:CLA:HAA2	2.16	0.60
15:B:1231:CLA:C4C	15:B:1232:CLA:CBB	2.79	0.60
5:A:77:HIS:HB3	15:A:1111:CLA:HED2	1.84	0.60
15:B:1222:CLA:H71	15:B:1240:CLA:C19	2.31	0.60
5:A:561:ARG:NH1	8:D:92:LEU:HD11	2.17	0.60
6:B:213:PHE:CE2	15:B:1211:CLA:CBC	2.85	0.60
15:B:1225:CLA:HBB1	15:B:1225:CLA:CMB	2.25	0.60
15:3:606:CLA:O1A	15:3:613:CLA:CMD	2.50	0.60
5:A:313:ARG:HG2	5:A:313:ARG:O	2.01	0.60
15:A:1012:CLA:HBB1	15:A:1012:CLA:CMB	2.31	0.60
15:A:1012:CLA:H162	14:A:4006:BCR:H14C	1.82	0.60
14:F:4001:BCR:C13	11:J:39:PHE:HB2	2.32	0.60
14:F:4001:BCR:H353	11:J:39:PHE:HB2	1.83	0.60
5:A:486:TRP:HZ3	15:A:1133:CLA:CAC	2.13	0.60
2:2:254:HIS:NE2	15:2:608:CLA:NB	2.49	0.59
6:B:30:HIS:CB	15:B:1226:CLA:O1A	2.49	0.59
15:A:1103:CLA:H162	14:A:4002:BCR:H341	1.83	0.59
6:B:54:GLN:HG2	15:B:1202:CLA:CMA	2.31	0.59
6:B:281:ILE:HD11	15:B:1214:CLA:C3C	2.32	0.59
4:4:278:ASP:OD1	15:4:607:CLA:CED	2.51	0.59
15:B:1229:CLA:HAC2	10:F:168:THR:HA	1.84	0.59
3:3:104:VAL:CG2	15:A:1108:CLA:HED1	2.32	0.59
6:B:274:MET:SD	15:B:1215:CLA:HMA3	2.43	0.59
15:B:1021:CLA:HMB1	15:B:1021:CLA:CBB	2.28	0.59
11:J:33:PHE:N	11:J:34:PRO:HD3	2.17	0.59
2:2:148:ASP:O	4:4:317:HIS:NE2	2.35	0.59
5:A:121:ILE:HD11	5:A:124:GLN:NE2	2.17	0.59
5:A:506:THR:HA	15:A:1116:CLA:O1A	2.02	0.59
5:A:690:ARG:HG2	5:A:690:ARG:O	2.02	0.59
15:A:1107:CLA:HMA1	11:J:27:ILE:HD13	1.84	0.59
15:B:1234:CLA:HBB1	15:B:1234:CLA:CMB	2.28	0.59
1:1:83:MET:HB3	12:1:501:LUT:H14	1.84	0.59
5:A:222:LEU:N	5:A:223:PRO:HD2	2.16	0.59
5:A:577:GLY:HA3	7:C:51:CYS:O	2.03	0.59
6:B:458:PRO:HB2	15:B:1235:CLA:OBD	2.02	0.59
6:B:27:ALA:HB2	23:B:5002:DGD:HA21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:676:HIS:HB3	15:A:1012:CLA:HBD	1.84	0.59
15:B:1223:CLA:HHC	15:B:1231:CLA:CMA	2.30	0.59
1:1:91:ALA:HB2	15:1:601:CLA:C18	2.33	0.59
5:A:376:PRO:HG3	15:A:1117:CLA:HAA2	1.84	0.59
6:B:191:TRP:CE2	15:B:1215:CLA:CAD	2.86	0.59
6:B:463:TRP:CH2	15:F:1302:CLA:HBA2	2.38	0.59
5:A:194:VAL:HG13	15:A:1123:CLA:HMD1	1.85	0.59
15:3:605:CLA:H71	15:A:1111:CLA:H201	1.83	0.58
15:A:1102:CLA:HBC1	17:A:5002:LHG:H132	1.84	0.58
15:A:1124:CLA:H51	15:A:1135:CLA:H42	1.85	0.58
15:A:1131:CLA:H2A	15:A:1131:CLA:O1D	2.02	0.58
6:B:278:HIS:CE1	15:B:1215:CLA:C4A	2.86	0.58
5:A:123:GLY:HA3	6:B:447:PHE:CD2	2.39	0.58
5:A:275:PHE:O	5:A:292:SER:OG	2.16	0.58
5:A:691:GLY:HA3	6:B:571:ILE:HG23	1.84	0.58
15:B:1223:CLA:HHC	15:B:1231:CLA:HMA1	1.83	0.58
15:B:1224:CLA:H92	15:B:1224:CLA:ND	2.18	0.58
5:A:57:HIS:CE1	15:A:1103:CLA:HBB2	2.37	0.58
5:A:685:PHE:HA	21:A:2001:PQN:H9	1.84	0.58
20:A:1011:CL0:H66	15:B:1022:CLA:HMB1	1.85	0.58
15:A:1124:CLA:O1D	15:A:1124:CLA:H2A	2.02	0.58
15:A:1133:CLA:C3D	15:A:1134:CLA:CMB	2.81	0.58
3:3:104:VAL:HG23	3:3:104:VAL:O	2.03	0.58
5:A:506:THR:HG22	15:A:1116:CLA:C2	2.33	0.58
5:A:550:LEU:HD23	14:A:4005:BCR:H402	1.86	0.58
6:B:175:ARG:HG2	15:B:1221:CLA:OBD	2.02	0.58
6:B:522:HIS:CD2	14:F:4001:BCR:H271	2.37	0.58
6:B:559:PRO:N	6:B:559:PRO:C	2.58	0.58
15:3:613:CLA:HMB3	15:3:613:CLA:CBB	2.25	0.58
15:A:1136:CLA:C9	15:A:1136:CLA:H51	2.32	0.58
5:A:687:PHE:CG	6:B:665:LEU:HD23	2.38	0.58
6:B:184:PHE:CE2	15:B:1216:CLA:HBB2	2.38	0.58
6:B:191:TRP:NE1	15:B:1215:CLA:O1D	2.36	0.58
6:B:309:HIS:NE2	15:B:1219:CLA:NB	2.51	0.58
20:A:1011:CL0:H15	20:A:1011:CL0:CMB	2.33	0.58
15:A:1117:CLA:H143	15:A:1125:CLA:C9	2.33	0.58
14:A:4007:BCR:C10	15:B:1022:CLA:C16	2.78	0.58
15:B:1228:CLA:HMC2	15:B:1236:CLA:HAC2	1.84	0.58
6:B:374:THR:CG2	6:B:592:THR:HG23	2.34	0.58
11:J:12:PRO:HB2	14:J:4002:BCR:H291	1.86	0.58
1:1:218:PHE:HE2	15:1:608:CLA:CED	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:367:VAL:HG12	5:A:371:MET:HE2	1.86	0.58
6:B:168:TRP:CZ2	15:B:1210:CLA:HAC2	2.39	0.58
1:1:91:ALA:N	15:1:601:CLA:H191	2.19	0.58
16:4:610:CHL:HBC3	16:4:610:CHL:HHD	1.86	0.58
5:A:376:PRO:CG	15:A:1117:CLA:HAA2	2.34	0.58
5:A:667:ALA:HB1	15:A:1106:CLA:HMC3	1.85	0.58
6:B:50:SER:CB	15:B:1202:CLA:HBB1	2.34	0.58
1:1:90:LEU:HB2	15:1:601:CLA:H193	1.86	0.57
1:1:91:ALA:HB2	15:1:601:CLA:H201	1.86	0.57
1:1:202:ILE:HG23	12:1:501:LUT:O23	2.04	0.57
2:2:254:HIS:NE2	15:2:608:CLA:NC	2.51	0.57
5:A:301:ILE:HD11	15:A:1116:CLA:HBC2	1.86	0.57
15:A:1115:CLA:HMB1	15:A:1115:CLA:CBB	2.30	0.57
15:A:1102:CLA:HMB1	15:A:1102:CLA:CBB	2.28	0.57
6:B:27:ALA:HB3	23:B:5002:DGD:HG2	1.85	0.57
6:B:701:LEU:HD22	6:B:705:GLN:NE2	2.20	0.57
15:F:1301:CLA:HHC	15:F:1301:CLA:HBB1	1.84	0.57
2:2:254:HIS:NE2	15:2:608:CLA:ND	2.53	0.57
5:A:176:ALA:HB2	15:A:1108:CLA:C2C	2.34	0.57
5:A:374:MET:HE2	15:A:1116:CLA:CAA	2.35	0.57
5:A:392:THR:OG1	15:A:1126:CLA:HMB1	2.04	0.57
15:A:1013:CLA:HMA3	15:A:1013:CLA:C1	2.34	0.57
15:A:1110:CLA:HED2	15:A:1111:CLA:HBC1	1.86	0.57
15:A:1135:CLA:HMB1	15:A:1135:CLA:CBB	2.27	0.57
6:B:287:VAL:HG11	15:B:1219:CLA:H172	1.86	0.57
15:3:605:CLA:O1D	15:3:605:CLA:H2A	2.04	0.57
15:A:1104:CLA:H192	15:A:1104:CLA:C15	2.35	0.57
15:A:1107:CLA:O1D	15:A:1107:CLA:H2A	2.04	0.57
6:B:374:THR:HG22	6:B:592:THR:HG23	1.85	0.57
6:B:479:LEU:HD22	15:B:1231:CLA:HMD2	1.85	0.57
5:A:222:LEU:H	5:A:223:PRO:HD2	1.68	0.57
15:A:1108:CLA:HMB1	15:A:1108:CLA:CBB	2.32	0.57
14:A:4002:BCR:H342	14:A:4002:BCR:C6	2.34	0.57
6:B:465:GLN:NE2	15:B:1234:CLA:OBD	2.34	0.57
4:4:260:PRO:HG2	15:4:601:CLA:OBD	2.04	0.57
15:A:1101:CLA:H202	15:A:1106:CLA:H193	1.87	0.57
1:1:179:LYS:CE	17:1:801:LHG:O5	2.53	0.57
5:A:681:PHE:CZ	15:A:1140:CLA:HBC2	2.29	0.57
6:B:292:TYR:CZ	15:B:1216:CLA:O1D	2.57	0.57
3:3:152:VAL:HG21	13:3:502:XAT:H41	1.85	0.57
4:4:290:PHE:CE1	13:4:502:XAT:H192	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1105:CLA:HMB1	15:A:1105:CLA:CBB	2.27	0.57
15:A:1130:CLA:HMB3	15:A:1130:CLA:CBB	2.28	0.57
1:1:190:GLY:HA2	15:1:603:CLA:C1C	2.34	0.57
2:2:234:VAL:HG21	13:2:502:XAT:H401	1.86	0.57
5:A:486:TRP:CZ3	15:A:1133:CLA:HAC1	2.35	0.57
15:A:1126:CLA:C20	15:A:1126:CLA:H151	2.35	0.57
15:A:1128:CLA:HMB3	15:A:1128:CLA:CBB	2.34	0.57
6:B:187:SER:CB	15:B:1215:CLA:HBC1	2.34	0.57
3:3:124:ALA:HB1	12:3:501:LUT:H31	1.87	0.56
5:A:227:LEU:CD1	5:A:253:LEU:HD21	2.35	0.56
5:A:306:LEU:HD13	14:A:4008:BCR:C14	2.34	0.56
5:A:365:ILE:HG22	15:A:1124:CLA:HED2	1.87	0.56
8:D:146:ARG:NH2	8:D:176:GLU:OE2	2.38	0.56
5:A:197:MET:HE1	15:A:1123:CLA:H122	1.87	0.56
15:A:1137:CLA:C4C	17:A:5001:LHG:H331	2.35	0.56
6:B:30:HIS:C	15:B:1226:CLA:HAA1	2.30	0.56
6:B:68:HIS:NE2	15:B:1204:CLA:C1B	2.68	0.56
6:B:288:ALA:HB2	15:B:1216:CLA:C2C	2.34	0.56
6:B:291:MET:HE1	15:B:1216:CLA:C3D	2.36	0.56
12:1:501:LUT:H383	15:1:603:CLA:HMB2	1.87	0.56
15:3:605:CLA:HMB3	15:3:605:CLA:CBB	2.31	0.56
15:3:615:CLA:HMB1	15:3:615:CLA:CBB	2.35	0.56
4:4:295:SER:OG	15:4:616:CLA:OBD	2.24	0.56
5:A:359:LEU:HD13	15:A:1123:CLA:HHB	1.88	0.56
5:A:389:SER:HB3	15:A:1126:CLA:HMA2	1.84	0.56
15:A:1101:CLA:HBB1	14:J:4002:BCR:C27	2.28	0.56
6:B:191:TRP:HZ2	15:B:1215:CLA:CGD	2.18	0.56
1:1:131:GLU:HA	15:1:613:CLA:CMA	2.35	0.56
6:B:187:SER:HB3	15:B:1215:CLA:HBC1	1.87	0.56
6:B:213:PHE:HB3	15:B:1211:CLA:HMD3	1.87	0.56
15:A:1127:CLA:HMB1	15:A:1127:CLA:CBB	2.30	0.56
6:B:373:TYR:CZ	15:B:1234:CLA:HMC2	2.41	0.56
6:B:425:TRP:HZ3	15:B:1236:CLA:HBC2	1.70	0.56
14:F:4001:BCR:H10C	11:J:39:PHE:HA	1.87	0.56
5:A:223:PRO:HB2	5:A:243:PHE:CD1	2.41	0.56
5:A:353:LEU:HB2	15:A:1103:CLA:HMD3	1.88	0.56
1:1:205:ALA:HB1	15:1:603:CLA:O1D	2.06	0.56
3:3:239:GLU:OE1	15:3:601:CLA:C4A	2.54	0.56
6:B:277:HIS:NE2	15:B:1215:CLA:HMB1	2.20	0.56
6:B:292:TYR:CE1	15:B:1216:CLA:O1D	2.59	0.56
6:B:657:VAL:HG12	6:B:713:HIS:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1122:CLA:H71	15:A:1137:CLA:H12	1.86	0.56
4:4:311:HIS:HE1	15:4:608:CLA:NA	2.01	0.56
5:A:497:LEU:HD23	15:A:1134:CLA:CBC	2.35	0.56
5:A:535:VAL:HG12	5:A:539:HIS:NE2	2.21	0.56
15:B:1230:CLA:CMB	15:B:1230:CLA:CBB	2.84	0.56
15:B:1235:CLA:HMB1	15:B:1235:CLA:CBB	2.36	0.56
3:3:155:PRO:HG2	15:A:1114:CLA:CBC	2.36	0.56
5:A:484:ALA:HB2	15:A:1136:CLA:HED2	1.88	0.56
15:A:1103:CLA:H52	14:A:4003:BCR:C28	2.16	0.56
15:A:1106:CLA:HMB1	15:A:1106:CLA:CBB	2.27	0.56
15:A:1112:CLA:HMB3	15:A:1112:CLA:CBB	2.32	0.56
6:B:658:TYR:CE1	6:B:662:PHE:CZ	2.94	0.56
15:B:1224:CLA:H92	15:B:1224:CLA:C4D	2.35	0.56
15:B:1224:CLA:HBB1	15:B:1224:CLA:CMB	2.35	0.56
15:B:1225:CLA:H151	15:B:1225:CLA:H193	1.87	0.56
15:B:1240:CLA:H2A	15:B:1240:CLA:HED3	1.87	0.56
2:2:258:PRO:HB3	15:2:608:CLA:CHB	2.36	0.55
5:A:453:PHE:CE1	15:B:1022:CLA:HMA3	2.41	0.55
6:B:30:HIS:CA	15:B:1226:CLA:O1A	2.54	0.55
2:2:234:VAL:CG2	13:2:502:XAT:H401	2.36	0.55
5:A:122:VAL:HG21	15:B:1230:CLA:CMD	2.37	0.55
5:A:561:ARG:HH12	8:D:92:LEU:HD11	1.72	0.55
15:A:1012:CLA:O1D	15:A:1012:CLA:H2A	2.07	0.55
15:A:1121:CLA:HBB1	15:A:1121:CLA:CHC	2.16	0.55
15:B:1235:CLA:HMC1	14:F:4001:BCR:H393	1.88	0.55
8:D:171:ASP:OD2	8:D:179:ASN:ND2	2.40	0.55
1:1:109:THR:OG1	1:1:111:ASP:OD1	2.21	0.55
16:3:604:CHL:HMB3	16:3:604:CHL:CBB	2.33	0.55
6:B:191:TRP:CH2	15:B:1215:CLA:OBD	2.59	0.55
6:B:291:MET:HE1	15:B:1216:CLA:CAD	2.37	0.55
4:4:145:TYR:OH	4:4:281:GLN:NE2	2.40	0.55
5:A:352:GLN:HG3	15:A:1123:CLA:C14	2.33	0.55
5:A:357:LEU:HD23	15:A:1103:CLA:CED	2.35	0.55
5:A:486:TRP:CZ3	15:A:1133:CLA:CAC	2.90	0.55
15:A:1136:CLA:H92	15:A:1136:CLA:H51	1.87	0.55
6:B:175:ARG:HB3	15:B:1221:CLA:HMD2	1.89	0.55
15:B:1210:CLA:H192	15:B:1225:CLA:H2	1.87	0.55
4:4:279:GLU:OE2	15:4:601:CLA:C4A	2.54	0.55
5:A:80:GLN:HG2	15:A:1103:CLA:HMA2	1.87	0.55
15:A:1013:CLA:HMD2	6:B:534:ILE:HD13	1.88	0.55
15:A:1119:CLA:CMB	15:A:1123:CLA:HMA2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1137:CLA:HMB1	15:A:1137:CLA:CBB	2.31	0.55
14:A:4006:BCR:H372	6:B:439:VAL:HG21	1.88	0.55
6:B:121:VAL:HG21	15:B:1205:CLA:HED1	1.89	0.55
15:B:1230:CLA:C5	15:B:1230:CLA:H92	2.37	0.55
15:B:1235:CLA:C2C	14:F:4001:BCR:H393	2.37	0.55
3:3:253:TYR:HE1	12:3:501:LUT:C25	2.19	0.55
15:3:612:CLA:HMB1	15:3:612:CLA:CBB	2.31	0.55
5:A:363:LEU:HD22	15:A:1127:CLA:HBC1	1.89	0.55
15:A:1133:CLA:C4D	15:A:1134:CLA:CMB	2.85	0.55
15:B:1236:CLA:HBA2	15:B:1240:CLA:H201	1.89	0.55
6:B:128:ILE:HG22	15:B:1215:CLA:HED2	1.88	0.55
6:B:277:HIS:HE1	15:B:1214:CLA:C4C	2.19	0.55
6:B:528:LEU:HD12	15:B:1236:CLA:HED3	1.88	0.55
15:B:1205:CLA:H43	15:B:1224:CLA:H11	1.89	0.55
18:2:804:LMG:H291	15:A:1114:CLA:C3D	2.37	0.55
3:3:280:LEU:HD12	15:3:603:CLA:H2	1.89	0.55
5:A:683:LEU:HB2	15:A:1013:CLA:HMC2	1.88	0.55
15:A:1121:CLA:C3D	14:A:4008:BCR:H393	2.37	0.55
16:3:604:CHL:C3A	16:3:604:CHL:CGA	2.85	0.55
4:4:222:LEU:HD22	14:4:503:BCR:H16C	1.89	0.55
14:A:4007:BCR:H362	15:B:1023:CLA:H122	1.89	0.55
6:B:191:TRP:CE2	15:B:1215:CLA:O1D	2.59	0.55
6:B:374:THR:CG2	6:B:592:THR:CG2	2.83	0.55
15:A:1103:CLA:C3	14:A:4003:BCR:C28	2.84	0.54
14:A:4002:BCR:C34	14:A:4002:BCR:C6	2.85	0.54
6:B:280:ALA:HB1	15:B:1213:CLA:HBC2	1.89	0.54
5:A:657:VAL:HG22	5:A:745:ALA:HB3	1.88	0.54
15:A:1110:CLA:C1A	15:A:1110:CLA:CGA	2.85	0.54
15:A:1120:CLA:O1D	15:A:1120:CLA:H2A	2.07	0.54
15:A:1137:CLA:H52	14:A:4005:BCR:H352	1.89	0.54
15:B:1234:CLA:HBC2	15:B:1234:CLA:CHD	2.36	0.54
1:1:86:ALA:CB	12:1:501:LUT:H391	2.37	0.54
15:A:1013:CLA:CGA	15:A:1013:CLA:H3A	2.37	0.54
15:A:1105:CLA:CAB	14:J:4001:BCR:H402	2.38	0.54
15:A:1110:CLA:CHA	15:A:1110:CLA:CBA	2.85	0.54
15:A:1140:CLA:H152	14:J:4001:BCR:H10C	1.89	0.54
1:1:190:GLY:CA	15:1:603:CLA:C1C	2.86	0.54
5:A:506:THR:CG2	15:A:1116:CLA:H2	2.37	0.54
15:A:1122:CLA:CBB	15:A:1122:CLA:H191	2.36	0.54
15:A:1126:CLA:O1D	15:A:1127:CLA:HHB	2.08	0.54
6:B:285:PHE:CE2	15:B:1216:CLA:HAB	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:458:PRO:CB	15:B:1235:CLA:OBD	2.56	0.54
15:B:1222:CLA:C3B	15:B:1236:CLA:HMA3	2.38	0.54
15:J:1302:CLA:HMB1	15:J:1302:CLA:CBB	2.34	0.54
3:3:275:PRO:CG	15:3:608:CLA:CMA	2.85	0.54
4:4:223:PHE:HE1	14:4:503:BCR:H20C	1.72	0.54
15:A:1141:CLA:NB	17:A:5001:LHG:O5	2.41	0.54
6:B:278:HIS:HE1	15:B:1215:CLA:C4A	2.20	0.54
15:B:1225:CLA:HMB3	15:B:1225:CLA:CBB	2.28	0.54
1:1:187:ALA:CB	12:1:501:LUT:H382	2.32	0.54
5:A:608:PHE:CD1	5:A:649:PHE:HE2	2.25	0.54
6:B:59:PHE:HD2	6:B:143:LEU:HD22	1.71	0.54
6:B:191:TRP:CZ2	15:B:1215:CLA:CGD	2.90	0.54
16:3:604:CHL:CHB	16:3:604:CHL:C1	2.86	0.54
5:A:118:VAL:HA	15:A:1107:CLA:HED2	1.90	0.54
5:A:211:LEU:HD21	14:A:4008:BCR:H10C	1.90	0.54
15:A:1111:CLA:C2	15:A:1111:CLA:HBA2	2.37	0.54
14:A:4002:BCR:C20	14:A:4003:BCR:HC31	2.38	0.54
6:B:494:TRP:NE1	15:B:1231:CLA:HED1	2.23	0.54
15:B:1224:CLA:CGA	15:B:1224:CLA:C3A	2.85	0.54
15:B:1230:CLA:C5	15:B:1230:CLA:C9	2.85	0.54
15:B:1230:CLA:C9	15:B:1230:CLA:H52	2.38	0.54
4:4:293:PHE:HE1	12:4:501:LUT:C25	2.21	0.54
15:A:1112:CLA:C5	15:A:1112:CLA:C9	2.86	0.54
14:A:4002:BCR:H393	14:A:4002:BCR:H271	1.89	0.54
6:B:213:PHE:CE2	15:B:1211:CLA:HBC2	2.43	0.54
1:1:87:ALA:O	15:1:601:CLA:H18	2.08	0.53
4:4:178:VAL:CG2	12:4:501:LUT:C15	2.85	0.53
4:4:181:LEU:HD22	12:4:501:LUT:H31	1.90	0.53
4:4:279:GLU:OE2	15:4:601:CLA:CHB	2.55	0.53
15:A:1113:CLA:NB	14:A:4008:BCR:HC21	2.23	0.53
15:A:1123:CLA:HMB1	15:A:1123:CLA:CBB	2.28	0.53
6:B:188:SER:HB2	15:B:1215:CLA:C2C	2.37	0.53
6:B:524:ILE:HD13	6:B:591:VAL:HG22	1.90	0.53
1:1:71:TYR:C	15:1:604:CLA:HMA1	2.33	0.53
5:A:687:PHE:CD1	6:B:665:LEU:HB3	2.42	0.53
15:A:1013:CLA:HMB1	15:A:1013:CLA:CBB	2.37	0.53
14:A:4005:BCR:C23	14:A:4005:BCR:C38	2.87	0.53
5:A:127:LEU:HB3	5:A:138:ILE:HD11	1.89	0.53
20:A:1011:CL0:CAB	15:A:1012:CLA:HED1	2.37	0.53
14:A:4006:BCR:H382	14:A:4006:BCR:C23	2.38	0.53
2:2:112:TRP:CE2	16:2:611:CHL:HED3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4003:BCR:C25	14:A:4003:BCR:H371	2.38	0.53
1:1:182:ARG:HB3	17:1:801:LHG:H112	1.89	0.53
15:A:1118:CLA:HBB1	15:A:1118:CLA:CMB	2.39	0.53
15:A:1136:CLA:C5	15:A:1136:CLA:C9	2.87	0.53
14:A:4007:BCR:C14	15:B:1023:CLA:H193	2.31	0.53
6:B:58:ILE:HG21	14:B:4002:BCR:H392	1.91	0.53
15:A:1112:CLA:C9	15:A:1112:CLA:H52	2.39	0.53
15:A:1123:CLA:H2	15:A:1123:CLA:C7	2.39	0.53
6:B:51:HIS:HD2	15:B:1202:CLA:C1B	2.22	0.53
12:4:501:LUT:H30	12:4:501:LUT:H402	1.90	0.53
15:A:1119:CLA:CMD	15:A:1121:CLA:CBB	2.86	0.53
6:B:47:ILE:HD13	15:B:1202:CLA:HAC1	1.90	0.53
6:B:50:SER:OG	15:B:1202:CLA:C3B	2.56	0.53
6:B:217:LEU:HD22	15:B:1212:CLA:OBD	2.09	0.53
15:B:1227:CLA:HBB2	15:B:1236:CLA:CBB	2.39	0.53
15:A:1111:CLA:CMC	15:A:1111:CLA:HBC3	2.38	0.53
15:A:1119:CLA:H8	14:A:4004:BCR:H10C	1.91	0.53
6:B:274:MET:SD	15:B:1215:CLA:HMA2	2.49	0.53
5:A:212:ALA:HB2	14:A:4002:BCR:H363	1.90	0.53
15:A:1139:CLA:H172	11:J:17:GLY:O	2.09	0.53
2:2:117:VAL:HG11	12:2:501:LUT:C31	2.39	0.53
4:4:128:TYR:CD2	4:4:132:THR:HG21	2.44	0.53
5:A:374:MET:HE2	15:A:1116:CLA:HAA2	1.90	0.53
15:A:1120:CLA:HMB1	15:A:1120:CLA:CBB	2.34	0.53
6:B:180:LEU:HD21	15:B:1216:CLA:C4B	2.38	0.53
6:B:180:LEU:CD2	15:B:1216:CLA:CAB	2.87	0.53
15:B:1220:CLA:O1A	14:B:4004:BCR:H12C	2.09	0.53
18:2:803:LMG:HC91	5:A:26:PHE:CE1	2.43	0.52
5:A:121:ILE:HD11	5:A:124:GLN:HE22	1.73	0.52
15:A:1122:CLA:H51	15:A:1137:CLA:H52	1.91	0.52
6:B:175:ARG:HB3	15:B:1221:CLA:CMD	2.38	0.52
16:2:609:CHL:HMA1	15:3:615:CLA:OBD	2.10	0.52
6:B:493:LEU:HD12	15:B:1232:CLA:HED2	1.91	0.52
4:4:174:MET:HB3	12:4:501:LUT:C14	2.40	0.52
15:A:1107:CLA:O1A	14:J:4002:BCR:H353	2.09	0.52
6:B:347:SER:HB3	15:B:1222:CLA:CAD	2.39	0.52
3:3:187:ASP:OD2	15:3:611:CLA:CBC	2.57	0.52
17:3:801:LHG:H252	15:A:1114:CLA:HBC1	1.90	0.52
5:A:359:LEU:HD11	15:A:1123:CLA:CMB	2.36	0.52
15:A:1107:CLA:CBD	15:A:1107:CLA:CBA	2.85	0.52
6:B:288:ALA:CB	15:B:1216:CLA:C3C	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1112:CLA:C1	15:A:1114:CLA:HMB1	2.39	0.52
15:A:1138:CLA:HMB1	15:A:1138:CLA:CBB	2.28	0.52
6:B:341:SER:HA	15:B:1223:CLA:H51	1.90	0.52
6:B:68:HIS:HE1	15:B:1204:CLA:NA	2.03	0.52
6:B:528:LEU:HD12	15:B:1236:CLA:CED	2.40	0.52
15:B:1223:CLA:HBC3	15:B:1223:CLA:HHD	1.90	0.52
11:J:26:LEU:HB2	14:J:4001:BCR:H342	1.91	0.52
3:3:115:ILE:HG22	15:3:612:CLA:HMD2	1.92	0.52
15:B:1224:CLA:HBB1	15:B:1224:CLA:HMB1	1.92	0.52
1:1:193:GLY:O	15:1:603:CLA:HMD3	2.10	0.52
16:3:604:CHL:HBB1	16:3:604:CHL:CMB	2.34	0.52
17:3:801:LHG:HC32	5:A:246:ASN:HD21	1.74	0.52
2:2:199:PRO:O	15:2:601:CLA:HED2	2.09	0.52
16:3:604:CHL:CGA	16:3:604:CHL:C4A	2.87	0.52
4:4:314:ASP:O	4:4:318:VAL:HG22	2.10	0.52
15:A:1013:CLA:CMA	15:A:1013:CLA:C1	2.85	0.52
6:B:28:THR:CG2	23:B:5002:DGD:HG31	2.39	0.52
7:C:52:LYS:HE2	7:C:69:LEU:HD13	1.91	0.52
1:1:209:HIS:CE1	15:1:608:CLA:C4A	2.83	0.52
2:2:162:PHE:CE1	14:2:503:BCR:H361	2.45	0.52
3:3:259:ILE:HD11	14:3:504:BCR:H281	1.91	0.52
6:B:231:TRP:O	15:B:1213:CLA:C3A	2.54	0.52
6:B:430:LEU:HD11	15:B:1235:CLA:HMB1	1.90	0.52
15:A:1107:CLA:O1A	15:A:1107:CLA:H2	2.10	0.51
15:A:1111:CLA:HMB1	15:A:1111:CLA:CBB	2.33	0.51
15:A:1131:CLA:HBB1	15:A:1131:CLA:CHC	2.18	0.51
5:A:589:TRP:NE1	15:A:1128:CLA:OBD	2.43	0.51
15:A:1113:CLA:CHA	15:A:1113:CLA:HBA2	2.40	0.51
6:B:464:ILE:HD11	15:B:1234:CLA:C1	2.32	0.51
15:B:1229:CLA:CGA	14:B:4006:BCR:H362	2.39	0.51
3:3:119:TRP:CE2	15:3:611:CLA:HED2	2.45	0.51
5:A:20:ASN:N	5:A:183:LYS:O	2.43	0.51
5:A:81:LEU:CD1	15:A:1111:CLA:HED1	2.40	0.51
5:A:605:ILE:CD1	20:A:1011:CL0:H64	2.41	0.51
15:A:1107:CLA:HMA2	11:J:27:ILE:HD13	1.92	0.51
15:B:1228:CLA:HMB1	15:B:1228:CLA:CBB	2.40	0.51
15:B:1229:CLA:C2B	14:B:4006:BCR:H21C	2.40	0.51
1:1:182:ARG:HB2	17:1:801:LHG:C10	2.34	0.51
4:4:311:HIS:CD2	15:4:608:CLA:C1C	2.93	0.51
5:A:209:GLY:HA2	14:A:4003:BCR:C14	2.40	0.51
5:A:599:MET:C	5:A:599:MET:SD	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:714:GLN:OE1	5:A:716:ARG:NH2	2.43	0.51
5:A:396:TRP:HA	5:A:603:LEU:HD13	1.93	0.51
5:A:605:ILE:HD11	20:A:1011:CL0:C20	2.39	0.51
14:B:4006:BCR:C8	14:B:4006:BCR:C33	2.89	0.51
2:2:251:LEU:HD12	12:2:501:LUT:H373	1.92	0.51
5:A:329:HIS:NE2	15:A:1120:CLA:NA	2.59	0.51
14:A:4003:BCR:C37	14:A:4003:BCR:C38	2.85	0.51
6:B:232:ALA:CA	15:B:1213:CLA:HAA2	2.41	0.51
14:B:4005:BCR:C23	14:B:4005:BCR:C40	2.85	0.51
7:C:25:VAL:HG12	7:C:25:VAL:O	2.10	0.51
1:1:70:ARG:NH2	15:1:605:CLA:O1A	2.44	0.51
3:3:122:LEU:HG	15:3:601:CLA:HMC3	1.92	0.51
5:A:420:THR:HA	8:D:112:ILE:HG21	1.93	0.51
5:A:549:ILE:HG12	6:B:671:TYR:OH	2.11	0.51
6:B:277:HIS:CE1	15:B:1214:CLA:CHD	2.91	0.51
2:2:117:VAL:HG11	12:2:501:LUT:H31	1.92	0.51
4:4:311:HIS:HD2	15:4:608:CLA:C1C	2.24	0.51
15:A:1124:CLA:H52	15:A:1135:CLA:H11	1.93	0.51
15:A:1128:CLA:H2A	15:A:1128:CLA:CED	2.38	0.51
1:1:176:LYS:HG2	15:1:607:CLA:O2D	2.11	0.51
1:1:179:LYS:HD2	15:1:607:CLA:CGD	2.40	0.51
3:3:152:VAL:HG21	13:3:502:XAT:C4	2.40	0.51
5:A:677:PHE:CG	14:A:4006:BCR:H363	2.46	0.51
6:B:115:ASN:ND2	15:B:1205:CLA:CAC	2.74	0.51
5:A:547:VAL:HG11	15:A:1137:CLA:HMB3	1.93	0.51
6:B:10:SER:CB	23:B:5002:DGD:HE61	2.41	0.51
15:B:1222:CLA:C2B	15:B:1236:CLA:HMA3	2.41	0.51
2:2:254:HIS:HE1	15:2:608:CLA:NA	2.05	0.50
5:A:608:PHE:HB3	5:A:645:TRP:HZ3	1.76	0.50
14:A:4007:BCR:H311	15:B:1022:CLA:C20	2.42	0.50
1:1:213:PRO:CB	15:1:608:CLA:CHB	2.89	0.50
4:4:291:LEU:HD22	13:4:502:XAT:H403	1.93	0.50
14:A:4005:BCR:H382	14:A:4005:BCR:H23C	1.92	0.50
6:B:96:HIS:CE1	15:B:1206:CLA:HMB1	2.45	0.50
6:B:213:PHE:CE2	15:B:1211:CLA:HBC1	2.46	0.50
6:B:288:ALA:CB	15:B:1216:CLA:C2C	2.90	0.50
2:2:165:VAL:HG13	16:2:611:CHL:NB	2.27	0.50
4:4:289:ALA:HB2	12:4:501:LUT:C29	2.39	0.50
5:A:578:PRO:HG3	6:B:560:CYS:SG	2.51	0.50
5:A:608:PHE:CD1	5:A:649:PHE:CE2	2.99	0.50
5:A:712:SER:N	10:F:199:GLU:OE2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1119:CLA:HMB2	15:A:1123:CLA:CMA	2.37	0.50
14:B:4006:BCR:C40	14:B:4006:BCR:C23	2.85	0.50
15:3:606:CLA:HMA3	15:3:613:CLA:C3C	2.42	0.50
15:A:1116:CLA:C4	15:A:1133:CLA:CAA	2.90	0.50
15:A:1122:CLA:H202	15:A:1122:CLA:H152	1.92	0.50
14:A:4002:BCR:C21	14:A:4003:BCR:C3	2.90	0.50
11:J:31:ARG:HD2	14:J:4002:BCR:HC31	1.94	0.50
5:A:396:TRP:NE1	15:A:1126:CLA:HAB	2.26	0.50
14:J:4002:BCR:H393	14:J:4002:BCR:C27	2.41	0.50
3:3:271:HIS:HD2	15:3:608:CLA:CHC	2.24	0.50
15:A:1117:CLA:CGA	15:A:1117:CLA:C3A	2.88	0.50
14:A:4003:BCR:C22	14:A:4003:BCR:C38	2.86	0.50
6:B:187:SER:C	15:B:1215:CLA:HAC2	2.37	0.50
6:B:231:TRP:O	15:B:1213:CLA:CMA	2.60	0.50
6:B:274:MET:HG2	15:B:1214:CLA:HMA3	1.92	0.50
1:1:44:LYS:N	1:1:55:ASN:OD1	2.43	0.50
3:3:209:SER:OG	3:3:210:ASP:N	2.45	0.50
12:4:501:LUT:H202	15:4:601:CLA:HAB	1.93	0.50
15:A:1126:CLA:H8	14:A:4006:BCR:H343	1.93	0.50
15:A:1136:CLA:C1A	15:A:1136:CLA:CGA	2.90	0.50
6:B:180:LEU:CD2	15:B:1216:CLA:C4B	2.90	0.50
15:3:605:CLA:H93	15:A:1111:CLA:H201	1.92	0.50
1:1:81:TRP:CZ3	15:1:606:CLA:HBB2	2.47	0.50
3:3:255:ALA:CB	15:3:603:CLA:HAC2	2.42	0.50
5:A:211:LEU:CD2	14:A:4008:BCR:H10C	2.42	0.50
15:A:1126:CLA:H192	14:J:4001:BCR:H14C	1.94	0.50
15:A:1133:CLA:H11	14:A:4005:BCR:H332	1.93	0.50
6:B:278:HIS:HE1	15:B:1215:CLA:NA	2.00	0.50
12:2:501:LUT:H10	12:2:501:LUT:H203	1.94	0.49
4:4:273:SER:O	4:4:275:GLU:N	2.43	0.49
5:A:681:PHE:CZ	15:A:1140:CLA:CBC	2.86	0.49
1:1:81:TRP:HZ3	15:1:606:CLA:HBB2	1.77	0.49
5:A:84:ILE:HG21	15:A:1103:CLA:H8	1.93	0.49
15:A:1105:CLA:O1D	15:A:1105:CLA:H2A	2.11	0.49
6:B:68:HIS:CE1	15:B:1204:CLA:C4A	2.94	0.49
6:B:298:ILE:HB	15:B:1218:CLA:OBD	2.11	0.49
15:B:1234:CLA:HMB1	15:B:1234:CLA:CBB	2.33	0.49
10:F:217:TRP:N	10:F:218:PRO:CD	2.76	0.49
4:4:278:ASP:OD1	15:4:607:CLA:O2D	2.31	0.49
13:4:502:XAT:H31	15:4:604:CLA:HMC2	1.94	0.49
5:A:646:LEU:HD23	6:B:633:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:90:HIS:CE1	15:B:1205:CLA:C1C	2.94	0.49
2:2:222:GLU:OE1	15:2:601:CLA:HMA3	2.12	0.49
17:3:801:LHG:H162	17:3:801:LHG:H271	1.94	0.49
7:C:55:GLU:HB3	7:C:63:LEU:HD13	1.95	0.49
14:F:4001:BCR:C35	11:J:39:PHE:HB2	2.42	0.49
1:1:70:ARG:CZ	15:1:605:CLA:O1A	2.61	0.49
5:A:365:ILE:HG22	15:A:1124:CLA:CED	2.42	0.49
5:A:532:ASP:OD1	5:A:635:PHE:CE2	2.51	0.49
5:A:560:SER:OG	5:A:561:ARG:N	2.45	0.49
15:A:1125:CLA:H122	15:A:1125:CLA:H91	1.95	0.49
6:B:431:GLY:CA	6:B:526:LEU:HD22	2.36	0.49
1:1:159:ASP:OD1	1:1:159:ASP:N	2.46	0.49
4:4:242:ASP:O	4:4:249:THR:HG21	2.12	0.49
5:A:300:ALA:HA	15:A:1115:CLA:HMC3	1.94	0.49
6:B:214:LEU:O	15:B:1212:CLA:CED	2.60	0.49
15:B:1227:CLA:HBB2	15:B:1236:CLA:HBB1	1.94	0.49
1:1:180:ASN:N	15:1:607:CLA:HMD1	2.27	0.49
4:4:219:GLU:HG3	16:4:613:CHL:HMB3	1.93	0.49
5:A:218:ILE:HD12	5:A:275:PHE:HD2	1.77	0.49
15:A:1124:CLA:H51	15:A:1135:CLA:C4	2.43	0.49
14:J:4002:BCR:H403	14:J:4002:BCR:H23C	1.94	0.49
6:B:302:LEU:HD13	15:B:1221:CLA:CAC	2.42	0.49
6:B:633:ILE:HG13	15:B:1021:CLA:HBC1	1.95	0.49
10:F:163:GLU:O	10:F:167:PRO:HG2	2.13	0.49
3:3:121:MET:SD	15:3:601:CLA:CAB	3.01	0.49
3:3:271:HIS:CD2	15:3:608:CLA:CHC	2.96	0.49
15:A:1114:CLA:HBB1	15:A:1114:CLA:CHC	2.23	0.49
6:B:68:HIS:NE2	15:B:1204:CLA:NA	2.60	0.49
6:B:231:TRP:C	15:B:1213:CLA:H3A	2.38	0.49
15:B:1222:CLA:H2A	15:B:1222:CLA:CED	2.39	0.49
15:A:1121:CLA:CHA	15:A:1121:CLA:HBA2	2.41	0.48
15:A:1122:CLA:HMD2	14:A:4004:BCR:H343	1.94	0.48
15:A:1116:CLA:H43	15:A:1133:CLA:HAA1	1.95	0.48
6:B:96:HIS:HE1	15:B:1206:CLA:HMB3	1.75	0.48
15:F:1301:CLA:HHC	15:F:1301:CLA:CBB	2.43	0.48
18:2:804:LMG:H112	18:2:804:LMG:HC71	1.93	0.48
5:A:432:ARG:NE	8:D:86:GLY:O	2.45	0.48
15:A:1012:CLA:HMB1	15:A:1012:CLA:CBB	2.43	0.48
15:A:1104:CLA:H192	15:A:1104:CLA:H151	1.94	0.48
15:A:1128:CLA:H18	15:A:1140:CLA:H3A	1.94	0.48
15:A:1136:CLA:HBB1	15:A:1136:CLA:CHC	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:187:SER:CB	15:B:1215:CLA:CAC	2.91	0.48
6:B:276:HIS:CB	15:B:1214:CLA:HMB2	2.24	0.48
6:B:706:ALA:CB	21:B:2002:PQN:C8	2.92	0.48
15:B:1224:CLA:H92	15:B:1224:CLA:C1D	2.43	0.48
1:1:127:ILE:HD12	15:1:613:CLA:C2D	2.30	0.48
5:A:536:HIS:HA	5:A:539:HIS:HD2	1.78	0.48
15:A:1101:CLA:HMA1	17:A:5002:LHG:H221	1.96	0.48
6:B:139:SER:CB	14:B:4003:BCR:H391	2.42	0.48
6:B:416:LYS:CE	10:F:239:VAL:HG11	2.44	0.48
8:D:177:LYS:O	8:D:182:ARG:NH2	2.44	0.48
1:1:137:VAL:HG11	14:1:503:BCR:C11	2.43	0.48
18:2:804:LMG:O9	18:2:804:LMG:H132	2.13	0.48
18:2:804:LMG:H241	15:3:610:CLA:C2	2.43	0.48
18:2:804:LMG:H241	15:3:610:CLA:H2	1.96	0.48
12:3:501:LUT:H401	15:3:614:CLA:CBB	2.43	0.48
5:A:643:ASN:HB2	6:B:636:TYR:OH	2.14	0.48
20:A:1011:CL0:H21	6:B:626:TRP:HD1	1.78	0.48
6:B:213:PHE:CD1	15:B:1211:CLA:HMD2	2.48	0.48
6:B:463:TRP:HZ2	15:F:1302:CLA:HBA1	1.73	0.48
1:1:187:ALA:HB3	12:1:501:LUT:H393	1.95	0.48
5:A:85:LEU:HG	15:A:1103:CLA:H91	1.96	0.48
20:A:1011:CL0:CBB	15:B:1021:CLA:HAA1	2.44	0.48
15:A:1112:CLA:CBB	14:A:4003:BCR:H16C	2.44	0.48
15:A:1128:CLA:H162	15:A:1140:CLA:HMA2	1.96	0.48
14:A:4007:BCR:H10C	15:B:1022:CLA:C16	2.41	0.48
1:1:143:ASN:OD1	1:1:151:ARG:NH1	2.44	0.48
5:A:158:GLN:HB3	15:A:1112:CLA:HED1	1.94	0.48
15:A:1102:CLA:HBA1	15:A:1109:CLA:ND	2.29	0.48
6:B:432:PHE:HD2	15:B:1229:CLA:HED1	1.79	0.48
11:J:26:LEU:HB2	14:J:4001:BCR:C34	2.42	0.48
15:A:1012:CLA:H111	15:A:1126:CLA:H143	1.95	0.48
15:A:1102:CLA:H192	11:J:16:LEU:HD11	1.96	0.48
1:1:182:ARG:CB	17:1:801:LHG:H112	2.43	0.48
3:3:280:LEU:N	15:3:603:CLA:O1A	2.44	0.48
17:3:801:LHG:O10	17:3:801:LHG:H142	2.14	0.48
5:A:88:LEU:HD22	14:A:4002:BCR:HC31	1.95	0.48
6:B:438:TYR:CD1	6:B:617:LEU:HG	2.49	0.48
15:A:1102:CLA:H143	15:A:1102:CLA:H172	1.96	0.48
14:A:4003:BCR:H371	14:A:4003:BCR:C26	2.44	0.48
14:A:4003:BCR:H15C	14:A:4003:BCR:H351	1.69	0.48
16:3:604:CHL:H12	16:3:604:CHL:C1B	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:355:ILE:HG12	14:A:4004:BCR:HC7	1.96	0.47
15:A:1122:CLA:C7	15:A:1137:CLA:H12	2.43	0.47
6:B:664:PHE:HA	21:B:2002:PQN:H9	1.96	0.47
16:3:604:CHL:HBD	16:3:604:CHL:HAA1	1.96	0.47
5:A:67:GLU:OE2	5:A:71:ARG:NH2	2.47	0.47
5:A:657:VAL:HG21	5:A:742:PHE:HA	1.96	0.47
6:B:658:TYR:CE1	6:B:662:PHE:CE1	3.01	0.47
5:A:658:ILE:HD11	20:A:1011:CL0:H23	1.97	0.47
15:A:1113:CLA:C4B	14:A:4008:BCR:HC21	2.44	0.47
6:B:277:HIS:NE2	15:B:1215:CLA:CMB	2.74	0.47
3:3:180:ALA:HB1	15:3:611:CLA:C1B	2.44	0.47
4:4:259:TYR:HA	15:4:601:CLA:O1D	2.14	0.47
4:4:279:GLU:OE2	15:4:601:CLA:NA	2.47	0.47
12:4:501:LUT:H383	15:4:603:CLA:C2B	2.45	0.47
5:A:467:ARG:HH22	15:A:1132:CLA:HMD2	1.80	0.47
5:A:497:LEU:HD23	15:A:1134:CLA:HBC3	1.96	0.47
15:A:1012:CLA:H42	6:B:439:VAL:HG22	1.94	0.47
15:A:1137:CLA:NC	17:A:5001:LHG:H331	2.30	0.47
14:A:4002:BCR:C22	14:A:4003:BCR:HC31	2.43	0.47
8:D:157:ARG:HB2	8:D:167:LEU:HD11	1.96	0.47
1:1:213:PRO:CG	15:1:608:CLA:CMB	2.92	0.47
1:1:176:LYS:HG2	15:1:607:CLA:CED	2.45	0.47
12:1:501:LUT:H383	15:1:603:CLA:CMB	2.44	0.47
16:2:609:CHL:CHB	15:3:615:CLA:O1D	2.60	0.47
15:A:1107:CLA:HBB2	15:B:1230:CLA:CHD	2.44	0.47
15:A:1117:CLA:H151	15:A:1125:CLA:H92	1.97	0.47
15:A:1124:CLA:HHB	15:A:1137:CLA:HBA1	1.96	0.47
6:B:356:LEU:HG	15:B:1223:CLA:HMC2	1.97	0.47
6:B:356:LEU:CD1	15:B:1223:CLA:HMC2	2.45	0.47
1:1:131:GLU:OE2	15:1:613:CLA:NB	2.46	0.47
2:2:254:HIS:NE2	15:2:608:CLA:NA	2.62	0.47
5:A:81:LEU:HD11	15:A:1111:CLA:HED1	1.97	0.47
5:A:301:ILE:CD1	15:A:1116:CLA:HBC2	2.44	0.47
5:A:465:LEU:O	6:B:98:GLY:N	2.47	0.47
5:A:580:ARG:HG2	7:C:49:VAL:HG22	1.95	0.47
5:A:677:PHE:HB2	15:A:1012:CLA:O1A	2.14	0.47
15:A:1107:CLA:HMB3	15:A:1107:CLA:CBB	2.40	0.47
15:A:1119:CLA:CMB	15:A:1123:CLA:HED1	2.45	0.47
6:B:55:LEU:CD1	15:B:1210:CLA:HED1	2.45	0.47
6:B:653:PHE:CZ	15:B:1239:CLA:CMB	2.98	0.47
7:C:21:CYS:SG	7:C:54:CYS:HB3	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:189:LEU:HB3	15:1:603:CLA:HMC2	1.97	0.47
5:A:670:LEU:HD12	15:A:1107:CLA:HAC1	1.96	0.47
15:A:1111:CLA:CMB	15:A:1111:CLA:CBB	2.93	0.47
14:A:4007:BCR:H10C	15:B:1022:CLA:C15	2.45	0.47
6:B:94:ASP:OD2	15:B:1206:CLA:NA	2.47	0.47
15:B:1229:CLA:HED2	15:B:1229:CLA:C2A	2.39	0.47
2:2:114:MET:HE3	2:2:226:GLY:CA	2.45	0.47
15:3:608:CLA:HBC3	15:3:608:CLA:HMC1	1.96	0.47
4:4:200:ALA:HB1	15:4:606:CLA:CED	2.44	0.47
4:4:236:ASN:O	4:4:239:SER:OG	2.14	0.47
5:A:158:GLN:CB	15:A:1112:CLA:HED1	2.45	0.47
5:A:535:VAL:O	5:A:539:HIS:CD2	2.68	0.47
15:A:1133:CLA:CBD	15:A:1134:CLA:HMB3	2.45	0.47
15:A:1136:CLA:H92	15:A:1136:CLA:H52	1.96	0.47
6:B:285:PHE:HE2	15:B:1216:CLA:HBB2	1.80	0.47
6:B:701:LEU:HG	21:B:2002:PQN:C4	2.45	0.47
15:B:1205:CLA:H43	15:B:1224:CLA:C1	2.45	0.47
5:A:98:PHE:HB3	5:A:117:VAL:HG12	1.97	0.47
5:A:392:THR:OG1	15:A:1126:CLA:HMB3	2.14	0.47
15:A:1013:CLA:C14	21:A:2001:PQN:H293	2.45	0.47
15:A:1112:CLA:H142	15:A:1112:CLA:H111	1.62	0.47
6:B:213:PHE:HE2	15:B:1211:CLA:HBC1	1.79	0.47
15:B:1222:CLA:HAA2	15:B:1223:CLA:OBD	2.14	0.47
15:B:1225:CLA:H18	14:B:4002:BCR:H352	1.97	0.47
15:B:1230:CLA:NC	14:J:4001:BCR:HC21	2.30	0.47
3:3:161:ASP:OD1	3:3:161:ASP:N	2.47	0.46
15:A:1102:CLA:H61	15:A:1102:CLA:H41	1.58	0.46
6:B:288:ALA:HB2	15:B:1216:CLA:CAC	2.44	0.46
15:A:1119:CLA:CMB	15:A:1119:CLA:HBB1	2.45	0.46
6:B:475:PHE:HB3	6:B:477:LEU:HD23	1.97	0.46
6:B:722:TYR:HB2	15:B:1021:CLA:CED	2.43	0.46
15:B:1205:CLA:HBA1	15:B:1224:CLA:OBD	2.15	0.46
14:F:4001:BCR:H331	14:F:4001:BCR:C8	2.46	0.46
2:2:106:GLU:OE2	15:2:604:CLA:NA	2.47	0.46
4:4:248:ILE:HG22	4:4:248:ILE:O	2.16	0.46
20:A:1011:CL0:H12	15:A:1012:CLA:CAD	2.45	0.46
15:A:1126:CLA:H151	15:A:1126:CLA:H202	1.96	0.46
6:B:590:TRP:CD1	15:B:1021:CLA:H122	2.50	0.46
15:B:1023:CLA:HBC2	15:B:1023:CLA:HHD	1.97	0.46
15:B:1228:CLA:O1A	10:F:231:LEU:HD21	2.14	0.46
1:1:87:ALA:HB2	12:1:501:LUT:C15	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:238:ASN:ND2	15:3:614:CLA:O1A	2.49	0.46
5:A:357:LEU:CD2	15:A:1103:CLA:HED1	2.40	0.46
5:A:624:ASP:OD1	5:A:625:SER:N	2.48	0.46
15:A:1126:CLA:HBC3	17:A:5002:LHG:H383	1.97	0.46
6:B:28:THR:HG23	23:B:5002:DGD:HG31	1.96	0.46
5:A:554:VAL:HG11	15:A:1119:CLA:H201	1.98	0.46
15:A:1103:CLA:CMB	15:A:1103:CLA:HBB1	2.46	0.46
6:B:27:ALA:HB1	23:B:5002:DGD:HB21	1.97	0.46
6:B:58:ILE:HG21	14:B:4002:BCR:C39	2.45	0.46
6:B:493:LEU:CD1	15:B:1232:CLA:HED2	2.46	0.46
5:A:362:SER:CB	14:A:4005:BCR:H361	2.45	0.46
5:A:432:ARG:HG2	8:D:87:SER:HB3	1.98	0.46
5:A:606:VAL:HG12	5:A:606:VAL:O	2.14	0.46
20:A:1011:CL0:H8	20:A:1011:CL0:O1D	2.15	0.46
15:A:1013:CLA:C19	17:A:5002:LHG:H201	2.45	0.46
15:A:1108:CLA:H62	15:A:1108:CLA:H41	1.69	0.46
15:A:1112:CLA:HBA2	15:A:1114:CLA:HMB2	1.97	0.46
15:A:1119:CLA:H52	15:A:1122:CLA:H42	1.96	0.46
15:A:1124:CLA:H3A	15:A:1124:CLA:HBA2	1.49	0.46
6:B:456:ILE:HD13	14:F:4001:BCR:H24C	1.97	0.46
2:2:141:LYS:HB2	16:2:610:CHL:O1D	2.16	0.46
3:3:138:VAL:O	15:3:609:CLA:CBC	2.64	0.46
5:A:116:GLN:O	5:A:116:GLN:HG2	2.15	0.46
5:A:122:VAL:CG2	15:B:1230:CLA:CMD	2.94	0.46
5:A:497:LEU:CD2	15:A:1134:CLA:HBC3	2.45	0.46
5:A:679:TRP:CD2	20:A:1011:CL0:H4	2.51	0.46
15:A:1127:CLA:H12	14:A:4003:BCR:H24C	1.98	0.46
14:A:4006:BCR:H382	14:A:4006:BCR:H23C	1.96	0.46
15:B:1227:CLA:HAB	15:B:1236:CLA:CBB	2.45	0.46
5:A:281:GLY:C	5:A:282:LEU:HD12	2.41	0.46
5:A:625:SER:O	5:A:625:SER:OG	2.28	0.46
15:A:1101:CLA:H62	15:A:1101:CLA:H2	1.68	0.46
15:A:1138:CLA:CMB	15:A:1138:CLA:CBB	2.92	0.46
6:B:231:TRP:O	15:B:1213:CLA:HMA3	2.15	0.46
6:B:658:TYR:CD1	6:B:658:TYR:C	2.93	0.46
5:A:200:HIS:CE1	15:A:1118:CLA:HMD2	2.51	0.46
15:A:1110:CLA:CBB	15:A:1110:CLA:H91	2.46	0.46
15:A:1125:CLA:H11	14:A:4005:BCR:H16C	1.97	0.46
14:A:4002:BCR:H351	14:A:4002:BCR:H15C	1.74	0.46
15:B:1222:CLA:CMB	15:B:1222:CLA:CBB	2.92	0.46
15:B:1230:CLA:HBA2	14:B:4006:BCR:H272	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1236:CLA:CBA	15:B:1240:CLA:C20	2.93	0.46
8:D:129:LEU:C	8:D:130:LEU:HD12	2.41	0.46
13:3:502:XAT:H381	13:3:502:XAT:C28	2.46	0.46
4:4:174:MET:HB3	12:4:501:LUT:H14	1.98	0.46
15:A:1109:CLA:C4A	15:A:1109:CLA:HBA1	2.44	0.46
15:A:1115:CLA:CMB	15:A:1115:CLA:CBB	2.93	0.46
6:B:61:TRP:CD1	15:B:1203:CLA:HBC1	2.51	0.46
6:B:432:PHE:CD2	15:B:1229:CLA:HED1	2.51	0.46
7:C:5:VAL:HG22	7:C:67:VAL:HG22	1.97	0.46
14:A:4007:BCR:C12	15:B:1022:CLA:H152	2.44	0.45
6:B:10:SER:HB2	23:B:5002:DGD:HE61	1.98	0.45
15:B:1231:CLA:H61	15:B:1231:CLA:H41	1.58	0.45
15:B:1236:CLA:HBB1	15:B:1236:CLA:CHC	2.16	0.45
2:2:269:SER:HA	15:2:616:CLA:NA	2.31	0.45
15:A:1137:CLA:CMB	15:A:1137:CLA:CBB	2.94	0.45
14:A:4007:BCR:H17C	21:B:2002:PQN:H243	1.98	0.45
6:B:377:GLN:OE1	15:B:1222:CLA:HMD2	2.16	0.45
11:J:11:ALA:N	11:J:12:PRO:HD2	2.31	0.45
14:3:504:BCR:H351	14:3:504:BCR:H15C	1.50	0.45
5:A:208:LEU:HD11	15:A:1118:CLA:HBC3	1.99	0.45
15:A:1124:CLA:CMB	15:A:1124:CLA:CBB	2.88	0.45
6:B:57:ILE:HG13	15:B:1201:CLA:CBB	2.44	0.45
15:B:1223:CLA:C3B	15:B:1231:CLA:HMA1	2.44	0.45
1:1:52:GLY:HA3	1:1:178:LEU:HD23	1.99	0.45
5:A:367:VAL:HA	15:A:1117:CLA:H42	1.99	0.45
5:A:407:ALA:HB2	5:A:592:VAL:HG21	1.97	0.45
15:A:1106:CLA:H61	15:A:1106:CLA:H93	1.72	0.45
15:A:1110:CLA:HED2	15:A:1111:CLA:CBC	2.45	0.45
15:A:1141:CLA:HMB2	14:A:4004:BCR:H21C	1.98	0.45
14:A:4002:BCR:H393	14:A:4002:BCR:C27	2.46	0.45
15:B:1230:CLA:ND	14:J:4001:BCR:HC41	2.31	0.45
11:J:12:PRO:N	11:J:12:PRO:C	2.64	0.45
5:A:733:LEU:HD22	15:A:1140:CLA:HMA1	1.98	0.45
15:A:1112:CLA:H12	15:A:1114:CLA:CMB	2.45	0.45
21:A:2001:PQN:H271	21:A:2001:PQN:C24	2.47	0.45
6:B:266:THR:O	6:B:268:SER:N	2.50	0.45
6:B:456:ILE:HA	10:F:148:LEU:HB2	1.97	0.45
6:B:479:LEU:HD11	6:B:495:LEU:HD21	1.99	0.45
4:4:218:ILE:HD13	16:4:613:CHL:CED	2.44	0.45
5:A:218:ILE:HD12	5:A:275:PHE:CD2	2.51	0.45
15:A:1122:CLA:H41	15:A:1122:CLA:C7	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:124:TRP:CH2	15:B:1210:CLA:H191	2.46	0.45
15:3:615:CLA:CMB	15:3:615:CLA:CBB	2.94	0.45
6:B:213:PHE:CG	15:B:1211:CLA:CMD	2.99	0.45
6:B:305:ILE:HG21	15:B:1220:CLA:HED2	1.99	0.45
1:1:134:ALA:HB1	14:1:503:BCR:C16	2.47	0.45
12:1:501:LUT:H383	15:1:603:CLA:C2B	2.47	0.45
3:3:183:LYS:HB3	15:3:611:CLA:HMC3	1.99	0.45
3:3:275:PRO:HG2	15:3:608:CLA:HMA3	1.97	0.45
13:3:502:XAT:H31	13:3:502:XAT:H391	1.72	0.45
5:A:34:HIS:HE1	15:A:1109:CLA:CED	2.28	0.45
5:A:157:LEU:HD23	5:A:157:LEU:O	2.17	0.45
20:A:1011:CL0:H15	15:B:1021:CLA:HAA1	1.99	0.45
15:A:1104:CLA:H91	17:A:5002:LHG:H362	1.99	0.45
6:B:668:TRP:O	6:B:672:TRP:HD1	1.99	0.45
15:B:1021:CLA:H111	15:B:1021:CLA:C16	2.47	0.45
15:B:1230:CLA:CBA	14:B:4006:BCR:H272	2.47	0.45
15:3:612:CLA:CMB	15:3:612:CLA:CBB	2.93	0.45
5:A:122:VAL:HG21	15:B:1230:CLA:HMD2	1.97	0.45
1:1:221:ASN:HD21	15:1:603:CLA:CAD	2.25	0.44
2:2:261:VAL:HG23	2:2:261:VAL:O	2.17	0.44
3:3:262:ASP:OD1	3:3:263:GLY:N	2.48	0.44
4:4:231:LEU:HD12	15:4:612:CLA:CMA	2.46	0.44
5:A:510:TRP:HZ3	15:A:1135:CLA:O1D	1.99	0.44
15:A:1012:CLA:H43	6:B:439:VAL:HG22	1.96	0.44
1:1:179:LYS:HE2	17:1:801:LHG:O5	2.17	0.44
5:A:345:LEU:HB3	5:A:352:GLN:HE21	1.81	0.44
5:A:645:TRP:O	5:A:650:LEU:HD13	2.17	0.44
5:A:724:ARG:HE	6:B:668:TRP:HZ3	1.65	0.44
15:A:1013:CLA:H143	21:A:2001:PQN:H261	1.98	0.44
15:A:1102:CLA:C9	14:J:4002:BCR:H383	2.47	0.44
15:A:1135:CLA:HMA2	15:A:1135:CLA:HBA1	2.00	0.44
6:B:527:GLY:HA2	6:B:583:TRP:CZ3	2.52	0.44
15:B:1208:CLA:HBC3	18:B:5003:LMG:H362	1.99	0.44
15:B:1229:CLA:CMB	15:B:1229:CLA:CBB	2.85	0.44
9:E:86:GLN:CD	10:F:237:ILE:HD11	2.41	0.44
1:1:209:HIS:HE1	15:1:608:CLA:C1A	2.28	0.44
15:1:603:CLA:H143	16:1:609:CHL:H92	1.98	0.44
2:2:117:VAL:CG1	12:2:501:LUT:H31	2.47	0.44
2:2:120:ILE:HG23	2:2:136:TRP:HB3	2.00	0.44
2:2:254:HIS:HD2	15:2:608:CLA:NC	2.07	0.44
3:3:146:ASP:OD2	3:3:149:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4:605:CLA:C4	10:F:222:ILE:HG13	2.46	0.44
5:A:467:ARG:NH2	15:A:1132:CLA:HMD2	2.32	0.44
6:B:10:SER:CB	23:B:5002:DGD:C6E	2.95	0.44
6:B:90:HIS:HD2	15:B:1205:CLA:CHA	2.30	0.44
6:B:213:PHE:CB	15:B:1211:CLA:CMD	2.91	0.44
14:B:4006:BCR:H351	14:B:4006:BCR:H15C	1.71	0.44
15:4:608:CLA:HHD	15:4:608:CLA:HBC2	1.99	0.44
5:A:687:PHE:HB2	15:A:1013:CLA:CBC	2.48	0.44
5:A:700:ILE:CG2	15:A:1139:CLA:HAC2	2.47	0.44
15:A:1013:CLA:H92	15:A:1013:CLA:C5	2.35	0.44
15:A:1013:CLA:C4	6:B:435:LEU:HD22	2.47	0.44
15:A:1113:CLA:CMB	15:A:1113:CLA:HBB1	2.47	0.44
15:A:1123:CLA:H61	15:A:1123:CLA:O1D	2.17	0.44
15:A:1124:CLA:C3B	15:A:1137:CLA:HMA3	2.46	0.44
17:A:5002:LHG:H02	17:A:5002:LHG:P	2.37	0.44
6:B:416:LYS:HE2	10:F:239:VAL:HG11	2.00	0.44
15:B:1021:CLA:HBA2	15:B:1021:CLA:H3A	1.62	0.44
5:A:651:TRP:O	5:A:651:TRP:CD2	2.70	0.44
15:A:1138:CLA:HED3	6:B:421:SER:HB2	1.99	0.44
6:B:316:LEU:CD2	15:B:1240:CLA:H43	2.47	0.44
1:1:81:TRP:CE2	15:1:611:CLA:CED	2.99	0.44
1:1:190:GLY:HA2	15:1:603:CLA:C2C	2.46	0.44
14:3:504:BCR:H14C	15:3:612:CLA:H142	2.00	0.44
5:A:433:HIS:NE2	15:A:1129:CLA:ND	2.66	0.44
15:A:1109:CLA:H61	15:A:1109:CLA:H41	1.58	0.44
15:A:1123:CLA:H61	15:A:1123:CLA:HBD	2.00	0.44
6:B:44:TYR:CZ	6:B:331:LEU:HD21	2.52	0.44
6:B:560:CYS:SG	6:B:562:GLY:N	2.88	0.44
15:B:1021:CLA:CMB	15:B:1021:CLA:CBB	2.92	0.44
1:1:91:ALA:HA	15:1:601:CLA:H201	1.99	0.44
1:1:141:LEU:CD1	15:1:611:CLA:HAB	2.43	0.44
12:3:501:LUT:C17	15:3:601:CLA:H72	2.47	0.44
5:A:338:HIS:HE1	15:A:1122:CLA:ND	2.16	0.44
5:A:345:LEU:HB3	5:A:352:GLN:NE2	2.32	0.44
5:A:547:VAL:HG13	14:A:4005:BCR:H391	2.00	0.44
15:A:1138:CLA:H102	15:A:1138:CLA:H61	1.51	0.44
6:B:184:PHE:CE2	15:B:1216:CLA:CBB	3.01	0.44
15:B:1240:CLA:CED	14:B:4004:BCR:H353	2.48	0.44
1:1:131:GLU:HG3	15:1:613:CLA:C1B	2.46	0.44
1:1:137:VAL:HG11	14:1:503:BCR:H12C	1.99	0.44
5:A:414:VAL:O	5:A:558:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1013:CLA:H143	21:A:2001:PQN:H293	2.00	0.44
15:A:1119:CLA:CMB	15:A:1123:CLA:CED	2.96	0.44
6:B:118:THR:HG22	6:B:371:SER:OG	2.17	0.44
6:B:374:THR:CG2	6:B:592:THR:HG21	2.48	0.44
15:B:1225:CLA:HBA2	15:B:1225:CLA:H3A	1.52	0.44
18:B:5003:LMG:O5	18:B:5003:LMG:O4	2.20	0.44
14:J:4002:BCR:H351	14:J:4002:BCR:H16C	2.00	0.44
1:1:83:MET:HB3	12:1:501:LUT:C14	2.47	0.43
13:1:502:XAT:H402	15:1:605:CLA:C3B	2.48	0.43
2:2:112:TRP:CE2	16:2:611:CHL:CED	3.01	0.43
2:2:238:ALA:CB	15:2:603:CLA:HAC2	2.48	0.43
3:3:276:THR:HG23	15:3:608:CLA:HMA3	2.00	0.43
13:3:502:XAT:H403	15:3:605:CLA:HBB2	1.95	0.43
5:A:601:ASN:HD22	5:A:601:ASN:C	2.24	0.43
15:A:1112:CLA:HMC1	15:A:1113:CLA:HMB1	1.99	0.43
14:A:4008:BCR:H15C	14:A:4008:BCR:H351	1.86	0.43
6:B:278:HIS:CD2	15:B:1215:CLA:C1C	3.00	0.43
2:2:118:ALA:HB2	12:2:501:LUT:H15	1.99	0.43
2:2:224:LYS:HD2	15:2:607:CLA:O1D	2.18	0.43
3:3:180:ALA:CB	15:3:611:CLA:C1B	2.96	0.43
5:A:198:LEU:HD13	5:A:312:TYR:CZ	2.53	0.43
5:A:398:GLY:O	5:A:402:VAL:HG23	2.17	0.43
15:A:1013:CLA:H143	15:A:1013:CLA:H161	1.85	0.43
14:A:4007:BCR:H352	15:B:1022:CLA:H121	1.99	0.43
6:B:463:TRP:CZ2	15:F:1302:CLA:HAA2	2.53	0.43
6:B:530:THR:HG21	6:B:583:TRP:CZ2	2.53	0.43
15:B:1227:CLA:CAB	15:B:1236:CLA:HBB2	2.46	0.43
15:B:1230:CLA:H52	15:B:1230:CLA:H93	2.00	0.43
15:B:1235:CLA:H41	15:B:1235:CLA:H61	1.31	0.43
1:1:122:PHE:HD2	1:1:126:THR:HG21	1.83	0.43
15:B:1224:CLA:HMB1	15:B:1224:CLA:CBB	2.48	0.43
1:1:194:GLN:HA	15:1:603:CLA:C2D	2.49	0.43
1:1:210:LEU:HD11	15:1:608:CLA:HMC3	2.00	0.43
2:2:262:THR:HA	15:2:603:CLA:O1A	2.19	0.43
5:A:88:LEU:HD13	15:A:1103:CLA:H102	2.00	0.43
5:A:673:LEU:HD21	6:B:621:LEU:HD22	2.01	0.43
15:A:1140:CLA:C15	14:J:4001:BCR:H10C	2.48	0.43
6:B:278:HIS:HD2	15:B:1215:CLA:C1C	2.30	0.43
6:B:309:HIS:CB	15:B:1240:CLA:OBD	2.66	0.43
2:2:165:VAL:HG22	16:2:611:CHL:C2B	2.49	0.43
3:3:259:ILE:CD1	15:3:603:CLA:HMD1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:68:HIS:NE2	15:B:1204:CLA:C4A	2.82	0.43
6:B:302:LEU:HD23	15:B:1216:CLA:HED2	2.00	0.43
6:B:718:TYR:O	6:B:718:TYR:CD1	2.71	0.43
8:D:75:LEU:HD11	8:D:102:VAL:HG21	2.00	0.43
2:2:251:LEU:CD1	12:2:501:LUT:H373	2.49	0.43
2:2:258:PRO:CB	15:2:608:CLA:CHB	2.97	0.43
12:3:501:LUT:C20	14:3:506:BCR:H373	2.48	0.43
4:4:259:TYR:HB3	15:4:601:CLA:HED2	2.00	0.43
15:A:1012:CLA:H112	15:A:1126:CLA:H201	1.98	0.43
6:B:57:ILE:HG21	15:B:1203:CLA:HMD2	2.00	0.43
6:B:213:PHE:CG	15:B:1211:CLA:HMD3	2.53	0.43
15:B:1235:CLA:HAC1	10:F:150:SER:OG	2.19	0.43
13:1:502:XAT:H401	13:1:502:XAT:C15	2.49	0.43
15:1:603:CLA:H51	15:1:603:CLA:H93	2.01	0.43
15:A:1138:CLA:CBB	10:F:182:GLY:HA3	2.43	0.43
6:B:90:HIS:HE1	15:B:1205:CLA:C1C	2.31	0.43
6:B:633:ILE:HG13	15:B:1021:CLA:CBC	2.48	0.43
1:1:182:ARG:CB	17:1:801:LHG:C11	2.97	0.43
3:3:250:MET:HB3	13:3:502:XAT:H203	2.01	0.43
13:3:502:XAT:C28	13:3:502:XAT:C38	2.97	0.43
5:A:642:ILE:HD12	15:B:1022:CLA:H12	2.01	0.43
5:A:714:GLN:OE1	9:E:82:TYR:OH	2.31	0.43
15:A:1012:CLA:CMB	15:A:1012:CLA:CBB	2.97	0.43
15:A:1104:CLA:H42	17:A:5002:LHG:H261	2.00	0.43
15:A:1104:CLA:H41	17:A:5002:LHG:H281	2.00	0.43
15:A:1122:CLA:H202	15:A:1122:CLA:C15	2.48	0.43
15:A:1128:CLA:CMB	15:A:1128:CLA:CBB	2.93	0.43
15:A:1135:CLA:HBA1	15:A:1135:CLA:CMA	2.47	0.43
15:A:1140:CLA:C4A	15:A:1140:CLA:HBA1	2.49	0.43
6:B:47:ILE:CD1	15:B:1202:CLA:CAC	2.97	0.43
6:B:287:VAL:CG1	15:B:1219:CLA:H172	2.48	0.43
6:B:390:HIS:NE2	15:B:1226:CLA:ND	2.67	0.43
1:1:127:ILE:HG21	15:1:613:CLA:C1D	2.48	0.43
3:3:271:HIS:CD2	15:3:608:CLA:NB	2.86	0.43
3:3:271:HIS:HD2	15:3:608:CLA:C1C	2.24	0.43
5:A:355:ILE:HD13	14:A:4004:BCR:H342	2.01	0.43
15:A:1125:CLA:H91	15:A:1125:CLA:C12	2.49	0.43
14:A:4007:BCR:H17C	21:B:2002:PQN:C24	2.49	0.43
6:B:438:TYR:HD1	6:B:617:LEU:HG	1.83	0.43
6:B:494:TRP:CH2	15:B:1232:CLA:HMA3	2.54	0.43
14:J:4002:BCR:C23	14:J:4002:BCR:C40	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:129:ALA:HB3	3:3:130:PRO:HD3	2.00	0.43
5:A:559:SER:CB	8:D:116:PRO:O	2.67	0.43
5:A:589:TRP:CD1	15:A:1128:CLA:OBD	2.72	0.43
15:A:1104:CLA:H161	15:A:1104:CLA:H141	1.64	0.43
15:A:1125:CLA:H142	15:A:1125:CLA:H111	1.69	0.43
1:1:90:LEU:HB2	15:1:601:CLA:C19	2.49	0.42
1:1:193:GLY:O	15:1:603:CLA:CMD	2.67	0.42
1:1:213:PRO:HG2	15:1:608:CLA:HMB1	2.01	0.42
12:1:501:LUT:H10	12:1:501:LUT:H202	2.01	0.42
18:2:803:LMG:H322	11:J:4:PHE:CZ	2.54	0.42
5:A:338:HIS:CE1	15:A:1122:CLA:ND	2.87	0.42
15:A:1116:CLA:CGA	15:A:1116:CLA:H3A	2.47	0.42
15:A:1116:CLA:HBC3	15:A:1116:CLA:HHD	2.01	0.42
15:A:1122:CLA:H191	15:A:1122:CLA:HBB1	2.00	0.42
15:A:1130:CLA:HMA3	6:B:686:THR:HA	2.00	0.42
6:B:10:SER:HB3	23:B:5002:DGD:HE62	2.01	0.42
6:B:44:TYR:CE1	6:B:331:LEU:HD21	2.54	0.42
6:B:157:HIS:NE2	15:B:1208:CLA:NB	2.67	0.42
15:B:1229:CLA:H2A	15:B:1229:CLA:O2D	2.18	0.42
2:2:92:LEU:O	2:2:93:SER:OG	2.33	0.42
5:A:34:HIS:CE1	15:A:1109:CLA:HED1	2.54	0.42
5:A:318:ILE:O	5:A:318:ILE:HG13	2.19	0.42
6:B:344:THR:CG2	15:B:1222:CLA:HED1	2.48	0.42
15:B:1235:CLA:CMC	14:F:4001:BCR:H391	2.48	0.42
18:2:804:LMG:C7	18:2:804:LMG:C11	2.95	0.42
5:A:544:HIS:NE2	15:A:1137:CLA:NB	2.67	0.42
6:B:10:SER:HB3	23:B:5002:DGD:C6E	2.50	0.42
14:F:4002:BCR:H351	14:F:4002:BCR:H15C	1.82	0.42
4:4:304:PRO:C	12:4:501:LUT:O23	2.61	0.42
5:A:423:TYR:OH	8:D:83:ILE:HG22	2.19	0.42
15:A:1127:CLA:H122	14:A:4003:BCR:H381	2.01	0.42
15:A:1137:CLA:H91	15:A:1137:CLA:H112	1.65	0.42
6:B:276:HIS:ND1	15:B:1214:CLA:HMB3	2.35	0.42
15:J:1302:CLA:CMB	15:J:1302:CLA:CBB	2.95	0.42
3:3:185:LEU:HD22	15:3:612:CLA:CMA	2.49	0.42
3:3:187:ASP:OD2	15:3:611:CLA:CAC	2.67	0.42
5:A:328:SER:OG	15:A:1120:CLA:HED3	2.20	0.42
5:A:584:CYS:HB3	22:A:3001:SF4:S2	2.60	0.42
6:B:451:GLU:CG	10:F:129:ARG:NH1	2.79	0.42
15:B:1228:CLA:H62	15:B:1228:CLA:H41	1.71	0.42
7:C:7:ILE:HA	7:C:64:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:181:LEU:HD13	12:4:501:LUT:C36	2.49	0.42
4:4:260:PRO:O	15:4:601:CLA:O2D	2.38	0.42
4:4:272:THR:HG23	4:4:272:THR:O	2.20	0.42
5:A:208:LEU:HD11	15:A:1118:CLA:CBC	2.49	0.42
5:A:565:ASP:N	5:A:565:ASP:OD1	2.52	0.42
5:A:574:PRO:HA	5:A:724:ARG:HH12	1.85	0.42
6:B:47:ILE:HG12	15:B:1202:CLA:C3C	2.50	0.42
6:B:231:TRP:HZ3	15:B:1213:CLA:H71	1.84	0.42
15:B:1208:CLA:HBC2	15:B:1208:CLA:HHD	2.02	0.42
11:J:26:LEU:CB	14:J:4001:BCR:H342	2.50	0.42
14:J:4001:BCR:C23	14:J:4001:BCR:H403	2.50	0.42
14:J:4002:BCR:H351	14:J:4002:BCR:C16	2.50	0.42
5:A:119:TRP:CE3	14:J:4002:BCR:H333	2.54	0.42
5:A:223:PRO:N	5:A:223:PRO:C	2.66	0.42
5:A:559:SER:HB2	8:D:116:PRO:O	2.20	0.42
5:A:738:THR:HG21	20:A:1011:CL0:H28	2.01	0.42
6:B:90:HIS:HD2	15:B:1205:CLA:C1A	2.33	0.42
6:B:214:LEU:O	15:B:1212:CLA:HED2	2.19	0.42
6:B:348:LEU:HD21	15:B:1223:CLA:HAA2	2.01	0.42
6:B:651:PHE:HZ	15:B:1021:CLA:CHD	2.32	0.42
15:B:1224:CLA:O1D	15:B:1224:CLA:H2A	2.19	0.42
11:J:33:PHE:N	11:J:34:PRO:CD	2.82	0.42
1:1:71:TYR:HD2	15:1:604:CLA:O1A	2.00	0.42
2:2:78:ASP:OD2	2:2:79:GLY:N	2.52	0.42
5:A:212:ALA:HA	15:A:1113:CLA:HBB2	2.01	0.42
5:A:561:ARG:NH2	8:D:88:THR:O	2.52	0.42
6:B:309:HIS:HA	15:B:1240:CLA:HMD3	2.02	0.42
15:B:1216:CLA:HBC2	15:B:1221:CLA:H172	2.01	0.42
7:C:63:LEU:HB2	7:C:66:ARG:HD3	2.02	0.42
1:1:191:PHE:CE1	12:1:501:LUT:H27	2.50	0.42
12:1:501:LUT:H203	15:1:601:CLA:CMC	2.50	0.42
15:B:1231:CLA:CHD	15:B:1232:CLA:HBB1	2.49	0.42
15:B:1238:CLA:HBC2	15:B:1238:CLA:HHD	2.02	0.42
14:B:4005:BCR:H15C	14:B:4005:BCR:H351	1.49	0.42
10:F:171:PHE:CD2	10:F:171:PHE:C	2.97	0.42
2:2:254:HIS:CD2	15:2:608:CLA:C1C	3.03	0.42
4:4:215:LEU:HA	4:4:218:ILE:HG22	2.01	0.42
5:A:122:VAL:CG2	15:B:1230:CLA:HMD1	2.50	0.42
15:A:1133:CLA:CHA	15:A:1133:CLA:HBA1	2.48	0.42
6:B:287:VAL:O	15:B:1218:CLA:HAC1	2.20	0.42
6:B:300:HIS:NE2	15:B:1219:CLA:OBD	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1202:CLA:HBC2	15:B:1226:CLA:HMA1	2.02	0.42
14:B:4006:BCR:H24C	15:F:1301:CLA:HMB2	2.02	0.42
15:2:608:CLA:HBC2	15:2:608:CLA:HHD	2.03	0.41
5:A:601:ASN:C	5:A:601:ASN:ND2	2.78	0.41
15:A:1103:CLA:H52	14:A:4003:BCR:H371	2.01	0.41
15:A:1105:CLA:H111	15:J:1302:CLA:CBC	2.49	0.41
15:A:1107:CLA:CBA	15:A:1107:CLA:CGD	2.98	0.41
15:A:1111:CLA:HBA2	15:A:1111:CLA:H2	2.02	0.41
15:A:1139:CLA:H52	15:A:1139:CLA:H11	1.85	0.41
17:A:5002:LHG:C21	17:A:5002:LHG:H172	2.50	0.41
2:2:254:HIS:HD2	15:2:608:CLA:C1C	2.32	0.41
3:3:241:LYS:HE2	15:3:607:CLA:CGD	2.48	0.41
3:3:251:PHE:HB2	13:3:502:XAT:H401	2.02	0.41
3:3:280:LEU:CD1	15:3:603:CLA:H2	2.48	0.41
13:3:502:XAT:C38	16:3:604:CHL:H102	2.47	0.41
4:4:174:MET:HB3	12:4:501:LUT:C20	2.50	0.41
15:B:1224:CLA:C1D	15:B:1224:CLA:C9	2.98	0.41
5:A:338:HIS:H	5:A:426:LEU:HD12	1.85	0.41
6:B:54:GLN:HE21	15:B:1203:CLA:C1B	2.33	0.41
15:B:1022:CLA:O1A	15:B:1022:CLA:H2	2.20	0.41
3:3:177:ILE:CD1	14:3:503:BCR:H361	2.50	0.41
15:3:603:CLA:HMB2	15:3:608:CLA:HBC1	2.02	0.41
5:A:370:HIS:HB3	15:A:1116:CLA:OBD	2.20	0.41
5:A:467:ARG:HH22	15:A:1132:CLA:CMD	2.32	0.41
15:A:1012:CLA:H92	15:A:1012:CLA:H62	1.82	0.41
15:A:1133:CLA:H11	15:A:1133:CLA:H52	1.80	0.41
6:B:281:ILE:HG21	15:B:1215:CLA:HAB	2.03	0.41
6:B:706:ALA:HB2	21:B:2002:PQN:C8	2.50	0.41
1:1:81:TRP:HZ3	15:1:606:CLA:CBB	2.33	0.41
1:1:115:TRP:CD1	15:1:606:CLA:C3D	3.03	0.41
12:1:501:LUT:H202	12:1:501:LUT:C10	2.50	0.41
12:1:501:LUT:H203	15:1:601:CLA:HMC3	2.02	0.41
3:3:259:ILE:CD1	15:3:603:CLA:CMD	2.89	0.41
5:A:87:TRP:HZ3	14:A:4003:BCR:H401	1.86	0.41
15:A:1102:CLA:H3A	15:A:1102:CLA:HBA2	1.23	0.41
15:A:1122:CLA:H112	15:A:1122:CLA:H143	1.53	0.41
6:B:54:GLN:NE2	15:B:1203:CLA:ND	2.63	0.41
7:C:22:PRO:HG2	7:C:23:LEU:CD1	2.44	0.41
2:2:175:ASN:CB	4:4:131:ALA:HB2	2.50	0.41
3:3:127:CYS:SG	13:3:502:XAT:H162	2.61	0.41
4:4:208:ASP:OD1	4:4:208:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:355:ILE:CD1	14:A:4004:BCR:HC7	2.50	0.41
5:A:509:THR:HG21	15:A:1125:CLA:HBC1	2.03	0.41
15:A:1119:CLA:H142	15:A:1124:CLA:HBB2	2.02	0.41
15:A:1121:CLA:C2D	14:A:4008:BCR:H393	2.50	0.41
15:B:1228:CLA:CMB	15:B:1228:CLA:CBB	2.96	0.41
2:2:231:LEU:HD11	17:2:801:LHG:H282	2.02	0.41
15:3:603:CLA:H61	15:3:603:CLA:H41	1.96	0.41
5:A:208:LEU:HD22	14:A:4002:BCR:C37	2.51	0.41
15:A:1113:CLA:HBB1	15:A:1113:CLA:HMB1	2.01	0.41
15:A:1122:CLA:H71	15:A:1137:CLA:C1	2.50	0.41
1:1:153:TYR:HA	15:1:601:CLA:O1D	2.20	0.41
1:1:182:ARG:HB3	17:1:801:LHG:C11	2.50	0.41
3:3:239:GLU:OE1	15:3:601:CLA:C1B	2.68	0.41
19:3:802:3PH:C34	5:A:175:PHE:CZ	2.97	0.41
15:A:1126:CLA:H92	15:A:1126:CLA:H61	1.69	0.41
6:B:463:TRP:CZ2	15:F:1302:CLA:CAA	3.03	0.41
15:B:1225:CLA:H142	15:B:1225:CLA:H111	1.58	0.41
14:F:4001:BCR:C11	11:J:39:PHE:HA	2.51	0.41
1:1:90:LEU:CD2	12:1:501:LUT:H363	2.45	0.41
1:1:179:LYS:HD2	15:1:607:CLA:O1D	2.21	0.41
2:2:87:PHE:HB3	15:2:604:CLA:CAD	2.51	0.41
3:3:121:MET:O	12:3:501:LUT:C15	2.69	0.41
4:4:181:LEU:HD23	15:4:602:CLA:HBB2	2.03	0.41
5:A:29:TRP:HE1	15:A:1109:CLA:HBB	1.80	0.41
5:A:116:GLN:HB3	5:A:138:ILE:HB	2.02	0.41
5:A:333:PHE:HD1	17:A:5001:LHG:O4	2.03	0.41
5:A:366:ILE:HG21	15:A:1117:CLA:H201	2.02	0.41
5:A:486:TRP:CZ3	15:A:1133:CLA:HAC2	2.56	0.41
14:A:4007:BCR:C11	15:B:1022:CLA:C15	2.92	0.41
6:B:54:GLN:HG2	15:B:1202:CLA:HMA2	2.03	0.41
6:B:97:PHE:CE1	15:B:1206:CLA:HBC3	2.55	0.41
6:B:458:PRO:HA	15:B:1235:CLA:CMD	2.51	0.41
6:B:572:SER:OG	6:B:575:ASP:OD2	2.36	0.41
8:D:82:PRO:HG2	8:D:130:LEU:HD11	2.02	0.41
1:1:127:ILE:HD11	15:1:613:CLA:C3D	2.46	0.41
18:2:804:LMG:H391	17:3:801:LHG:C31	2.51	0.41
5:A:122:VAL:HG11	15:B:1230:CLA:OBD	2.21	0.41
5:A:345:LEU:HB3	15:A:1123:CLA:HBC3	2.03	0.41
5:A:566:LYS:NZ	6:B:674:GLU:OE2	2.38	0.41
20:A:1011:CL0:H69	20:A:1011:CL0:H58	2.02	0.41
15:A:1116:CLA:H41	15:A:1133:CLA:HAA1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1141:CLA:CMB	14:A:4004:BCR:H21C	2.50	0.41
21:A:2001:PQN:H111	21:A:2001:PQN:H2M1	1.85	0.41
14:A:4003:BCR:HC42	14:A:4003:BCR:H312	2.02	0.41
6:B:430:LEU:HB3	6:B:526:LEU:HB2	2.03	0.41
6:B:439:VAL:HB	15:B:1230:CLA:HMC2	2.03	0.41
11:J:29:ILE:O	11:J:29:ILE:CG2	2.69	0.41
14:J:4001:BCR:H15C	14:J:4001:BCR:H351	1.67	0.41
18:2:804:LMG:C12	3:3:167:PHE:HZ	2.34	0.40
4:4:212:LEU:O	4:4:214:THR:N	2.43	0.40
4:4:219:GLU:OE2	16:4:613:CHL:C3B	2.69	0.40
5:A:297:HIS:HE2	15:A:1117:CLA:C3B	2.34	0.40
5:A:374:MET:CE	15:A:1116:CLA:HBD	2.50	0.40
5:A:391:PHE:O	5:A:395:MET:HG2	2.21	0.40
5:A:432:ARG:O	8:D:87:SER:HA	2.21	0.40
15:A:1110:CLA:H2A	15:A:1110:CLA:O1D	2.22	0.40
15:A:1111:CLA:HBC3	15:A:1111:CLA:HMC1	2.02	0.40
15:A:1126:CLA:H202	15:A:1126:CLA:C15	2.52	0.40
6:B:231:TRP:CZ3	15:B:1213:CLA:H51	2.56	0.40
15:B:1223:CLA:HAA2	15:B:1223:CLA:HBD	2.02	0.40
9:E:73:LEU:HB2	9:E:127:VAL:HG11	2.02	0.40
14:3:506:BCR:H361	14:3:506:BCR:H20C	1.75	0.40
5:A:246:ASN:HD22	5:A:249:ILE:HD11	1.86	0.40
5:A:692:TYR:N	6:B:570:ASP:O	2.54	0.40
15:A:1112:CLA:HBB2	14:A:4003:BCR:H16C	2.02	0.40
15:A:1136:CLA:H51	15:A:1136:CLA:H8	1.63	0.40
8:D:104:THR:HG1	8:D:154:CYS:HG	1.64	0.40
11:J:16:LEU:C	11:J:16:LEU:HD23	2.46	0.40
1:1:88:GLY:O	1:1:92:VAL:HG23	2.21	0.40
1:1:91:ALA:CA	15:1:601:CLA:H201	2.51	0.40
1:1:137:VAL:CG1	14:1:503:BCR:H12C	2.50	0.40
16:2:609:CHL:CBA	3:3:178:GLN:HE21	2.35	0.40
3:3:165:ASP:OD1	3:3:165:ASP:N	2.54	0.40
5:A:17:VAL:HG11	5:A:184:ALA:HB1	2.04	0.40
5:A:122:VAL:CG2	15:B:1230:CLA:HMD2	2.52	0.40
15:A:1013:CLA:H162	15:A:1013:CLA:H193	1.77	0.40
15:A:1104:CLA:H162	15:A:1104:CLA:H203	1.82	0.40
15:A:1122:CLA:C4	14:A:4005:BCR:H351	2.48	0.40
6:B:176:LEU:HD11	15:B:1216:CLA:HMA2	2.03	0.40
15:B:1227:CLA:CBB	15:B:1236:CLA:CBB	2.99	0.40
4:4:318:VAL:O	4:4:318:VAL:HG23	2.21	0.40
5:A:246:ASN:HB2	5:A:249:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1105:CLA:CMB	15:A:1105:CLA:CBB	2.95	0.40
15:A:1112:CLA:CMB	15:A:1112:CLA:CBB	2.96	0.40
15:A:1113:CLA:C3B	14:A:4008:BCR:H323	2.52	0.40
6:B:142:PHE:HE2	14:B:4003:BCR:C21	2.34	0.40
6:B:187:SER:HB2	15:B:1215:CLA:CBC	2.51	0.40
6:B:191:TRP:CD2	15:B:1215:CLA:C2D	3.04	0.40
6:B:449:THR:HG22	10:F:129:ARG:NH2	2.37	0.40
15:B:1225:CLA:C2	14:B:4002:BCR:H291	2.52	0.40
15:B:1235:CLA:CGA	15:B:1235:CLA:C1A	3.00	0.40
3:3:124:ALA:HB1	12:3:501:LUT:C31	2.48	0.40
3:3:212:PRO:N	3:3:212:PRO:C	2.65	0.40
3:3:275:PRO:HG3	15:3:608:CLA:HMA1	2.02	0.40
5:A:658:ILE:HD11	20:A:1011:CL0:CBC	2.52	0.40
15:A:1102:CLA:H122	15:A:1102:CLA:H161	1.67	0.40
15:A:1117:CLA:C3A	15:A:1117:CLA:O1A	2.70	0.40
21:A:2001:PQN:H301	15:F:1301:CLA:HMC3	2.03	0.40
6:B:344:THR:HG23	15:B:1222:CLA:HED1	2.03	0.40
7:C:14:CYS:O	7:C:15:THR:OG1	2.30	0.40
9:E:94:ASP:OD2	9:E:98:ILE:HD12	2.22	0.40
14:J:4001:BCR:H321	14:J:4001:BCR:HC8	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	195/197 (99%)	188 (96%)	7 (4%)	0	100	100
2	2	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
3	3	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
4	4	209/211 (99%)	192 (92%)	16 (8%)	1 (0%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	737/739 (100%)	698 (95%)	34 (5%)	5 (1%)	18	47
6	B	728/730 (100%)	709 (97%)	18 (2%)	1 (0%)	48	78
7	C	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
8	D	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
9	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
10	F	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
11	J	38/40 (95%)	34 (90%)	4 (10%)	0	100	100
All	All	2761/2783 (99%)	2642 (96%)	112 (4%)	7 (0%)	37	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	261	LEU
5	A	120	PRO
4	4	212	LEU
5	A	477	ILE
5	A	260	GLY
6	B	559	PRO
5	A	376	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	152/152 (100%)	152 (100%)	0	100	100
2	2	167/167 (100%)	167 (100%)	0	100	100
3	3	160/160 (100%)	160 (100%)	0	100	100
4	4	169/169 (100%)	169 (100%)	0	100	100
5	A	598/598 (100%)	594 (99%)	4 (1%)	76	78
6	B	590/590 (100%)	587 (100%)	3 (0%)	81	81
7	C	68/68 (100%)	67 (98%)	1 (2%)	57	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	D	121/121 (100%)	121 (100%)	0	100	100
9	E	57/57 (100%)	57 (100%)	0	100	100
10	F	136/136 (100%)	136 (100%)	0	100	100
11	J	35/35 (100%)	33 (94%)	2 (6%)	18	45
All	All	2253/2253 (100%)	2243 (100%)	10 (0%)	81	83

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

Mol	Chain	Res	Type
5	A	118	VAL
5	A	245	LEU
5	A	584	CYS
5	A	658	ILE
6	B	374	THR
6	B	526	LEU
6	B	569	CYS
7	C	21	CYS
11	J	23	SER
11	J	35	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	209	HIS
1	1	217	ASN
2	2	109	HIS
2	2	225	ASN
3	3	224	ASN
3	3	242	ASN
3	3	271	HIS
4	4	155	ASN
4	4	300	ASN
4	4	302	GLN
5	A	124	GLN
5	A	193	ASN
5	A	241	HIS
5	A	246	ASN
5	A	393	HIS
5	A	536	HIS
5	A	722	GLN

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Mol	Chain	Res	Type
6	B	30	HIS
6	B	54	GLN
6	B	300	HIS
6	B	376	HIS
6	B	522	HIS
9	E	86	GLN
10	F	223	GLN
10	F	236	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

194 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	$\# Z > 2$
15	CLA	4	616	4	55,59,73	1.29	9 (16%)	64,96,113	1.35	5 (7%)
15	CLA	B	1201	-	47,51,73	1.39	9 (19%)	55,86,113	1.38	4 (7%)
15	CLA	A	1116	-	60,64,73	1.51	9 (15%)	71,102,113	1.90	17 (23%)
15	CLA	2	608	-	54,58,73	1.30	8 (14%)	64,95,113	1.41	5 (7%)
15	CLA	A	1114	-	59,63,73	1.44	7 (11%)	70,101,113	2.12	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	3	610	-	54,58,73	1.30	9 (16%)	64,95,113	1.40	7 (10%)
14	BCR	2	503	-	41,41,41	1.20	3 (7%)	56,56,56	1.22	8 (14%)
14	BCR	J	4001	-	41,41,41	1.61	4 (9%)	56,56,56	4.49	15 (26%)
15	CLA	B	1229	-	64,68,73	1.41	6 (9%)	76,107,113	2.08	22 (28%)
14	BCR	A	4005	-	41,41,41	1.68	6 (14%)	56,56,56	4.24	19 (33%)
15	CLA	1	603	-	64,68,73	1.18	9 (14%)	76,107,113	1.44	11 (14%)
15	CLA	4	603	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	7 (8%)
18	LMG	B	5003	-	39,39,55	0.86	1 (2%)	47,47,63	1.25	5 (10%)
15	CLA	A	1123	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	18 (21%)
15	CLA	A	1103	-	69,73,73	1.34	6 (8%)	82,113,113	2.00	20 (24%)
15	CLA	B	1022	-	69,73,73	1.47	10 (14%)	82,113,113	1.79	21 (25%)
15	CLA	A	1136	-	69,73,73	1.35	7 (10%)	82,113,113	1.93	18 (21%)
15	CLA	B	1207	-	50,54,73	1.33	7 (14%)	59,90,113	1.38	4 (6%)
13	XAT	4	502	-	41,47,47	2.67	20 (48%)	54,74,74	9.42	30 (55%)
14	BCR	F	4001	-	41,41,41	1.81	7 (17%)	56,56,56	4.43	22 (39%)
15	CLA	B	1214	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	8 (9%)
15	CLA	3	611	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
15	CLA	B	1223	-	69,73,73	1.38	6 (8%)	82,113,113	2.05	15 (18%)
15	CLA	2	603	2	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
15	CLA	4	602	-	54,58,73	1.32	9 (16%)	64,95,113	1.40	5 (7%)
15	CLA	4	605	-	69,73,73	1.16	8 (11%)	82,113,113	1.33	6 (7%)
14	BCR	B	4005	-	41,41,41	1.61	4 (9%)	56,56,56	4.62	14 (25%)
15	CLA	A	1104	-	69,73,73	1.35	8 (11%)	82,113,113	1.85	20 (24%)
15	CLA	4	609	4	64,68,73	1.19	7 (10%)	76,107,113	1.39	6 (7%)
15	CLA	1	608	-	59,63,73	1.25	8 (13%)	70,101,113	1.36	6 (8%)
15	CLA	4	601	4	64,68,73	1.19	9 (14%)	76,107,113	1.36	8 (10%)
22	SF4	A	3001	6,5	0,12,12	-	-	-	-	-
12	LUT	4	501	-	42,43,43	6.31	29 (69%)	51,60,60	2.80	21 (41%)
15	CLA	B	1230	-	59,63,73	1.45	6 (10%)	70,101,113	2.07	19 (27%)
15	CLA	4	604	-	64,68,73	1.19	9 (14%)	76,107,113	1.39	7 (9%)
15	CLA	J	1302	-	46,50,73	1.65	6 (13%)	53,85,113	2.12	15 (28%)
15	CLA	A	1112	-	69,73,73	1.34	6 (8%)	82,113,113	1.90	19 (23%)
21	PQN	A	2001	-	34,34,34	0.90	2 (5%)	43,45,45	1.53	7 (16%)
15	CLA	A	1121	-	49,53,73	1.61	6 (12%)	58,89,113	2.09	15 (25%)
14	BCR	B	4002	-	41,41,41	1.19	2 (4%)	56,56,56	1.43	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	A	4007	-	41,41,41	1.65	5 (12%)	56,56,56	4.62	19 (33%)
18	LMG	2	804	-	50,50,55	1.17	5 (10%)	58,58,63	1.12	4 (6%)
15	CLA	B	1224	-	65,69,73	1.40	5 (7%)	77,108,113	1.94	19 (24%)
14	BCR	J	4002	-	41,41,41	1.60	4 (9%)	56,56,56	4.61	16 (28%)
15	CLA	B	1226	-	69,73,73	1.14	7 (10%)	82,113,113	1.46	6 (7%)
15	CLA	B	1231	-	64,68,73	1.34	6 (9%)	76,107,113	2.03	21 (27%)
15	CLA	3	607	-	64,68,73	1.21	8 (12%)	76,107,113	1.33	5 (6%)
23	DGD	B	5002	-	62,62,67	0.85	2 (3%)	76,76,81	1.39	12 (15%)
16	CHL	4	613	-	55,69,74	1.60	8 (14%)	52,108,114	1.94	10 (19%)
14	BCR	3	506	-	41,41,41	1.27	3 (7%)	56,56,56	1.27	7 (12%)
15	CLA	3	613	-	50,54,73	1.58	7 (14%)	59,90,113	2.09	16 (27%)
15	CLA	A	1126	-	69,73,73	1.35	5 (7%)	82,113,113	1.90	17 (20%)
17	LHG	2	801	15	34,34,48	0.81	1 (2%)	37,40,54	1.26	3 (8%)
15	CLA	B	1202	-	69,73,73	1.18	9 (13%)	82,113,113	1.28	6 (7%)
14	BCR	A	4004	-	41,41,41	1.61	4 (9%)	56,56,56	4.70	19 (33%)
15	CLA	B	1212	-	59,63,73	1.25	8 (13%)	70,101,113	1.35	5 (7%)
15	CLA	A	1106	5	69,73,73	1.35	6 (8%)	82,113,113	1.89	20 (24%)
15	CLA	A	1141	17	45,49,73	1.40	9 (20%)	54,84,113	1.43	6 (11%)
15	CLA	B	1216	-	63,67,73	1.22	9 (14%)	74,105,113	1.34	7 (9%)
15	CLA	B	1221	-	69,73,73	1.17	10 (14%)	82,113,113	1.36	6 (7%)
15	CLA	B	1234	-	59,63,73	1.47	7 (11%)	70,101,113	2.00	17 (24%)
15	CLA	A	1138	-	69,73,73	1.35	7 (10%)	82,113,113	1.87	18 (21%)
17	LHG	B	5001	15	41,41,48	0.74	1 (2%)	44,47,54	1.27	3 (6%)
15	CLA	A	1132	-	49,53,73	1.36	9 (18%)	58,89,113	1.67	9 (15%)
15	CLA	1	615	1	51,55,73	1.44	9 (17%)	59,90,113	1.50	6 (10%)
15	CLA	2	605	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	6 (7%)
15	CLA	B	1236	-	53,57,73	1.53	6 (11%)	61,93,113	2.16	18 (29%)
14	BCR	4	503	-	41,41,41	1.27	4 (9%)	56,56,56	1.36	9 (16%)
15	CLA	4	607	-	64,68,73	1.22	9 (14%)	76,107,113	1.34	7 (9%)
14	BCR	A	4003	-	41,41,41	1.61	4 (9%)	56,56,56	4.42	21 (37%)
15	CLA	2	616	2	69,73,73	1.17	9 (13%)	82,113,113	1.47	11 (13%)
15	CLA	A	1127	-	69,73,73	1.40	7 (10%)	82,113,113	1.92	19 (23%)
15	CLA	3	601	3	64,68,73	1.19	9 (14%)	76,107,113	1.36	5 (6%)
17	LHG	1	801	15	48,48,48	0.62	0	51,54,54	1.21	4 (7%)
16	CHL	4	610	-	41,55,74	2.11	9 (21%)	35,91,114	2.08	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	LMG	2	802	-	50,50,55	0.69	0	58,58,63	1.26	5 (8%)
15	CLA	3	609	-	46,50,73	1.39	7 (15%)	53,85,113	1.49	5 (9%)
14	BCR	B	4006	-	41,41,41	1.61	4 (9%)	56,56,56	4.68	19 (33%)
15	CLA	B	1209	-	50,54,73	1.33	8 (16%)	59,90,113	1.41	4 (6%)
15	CLA	1	613	-	49,53,73	1.36	8 (16%)	58,89,113	1.41	4 (6%)
15	CLA	1	611	-	52,56,73	1.33	9 (17%)	61,92,113	1.36	4 (6%)
15	CLA	B	1218	-	49,53,73	1.39	7 (14%)	58,89,113	1.46	5 (8%)
15	CLA	F	1301	-	50,54,73	1.56	6 (12%)	59,90,113	2.07	15 (25%)
15	CLA	2	607	17	64,68,73	1.20	10 (15%)	76,107,113	1.32	6 (7%)
17	LHG	A	5001	15	48,48,48	0.37	0	51,54,54	1.11	3 (5%)
15	CLA	3	603	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	7 (8%)
15	CLA	A	1122	-	69,73,73	1.35	6 (8%)	82,113,113	1.95	20 (24%)
13	XAT	3	502	-	41,47,47	0.71	2 (4%)	54,74,74	2.29	13 (24%)
15	CLA	3	606	-	59,63,73	1.23	8 (13%)	70,101,113	1.35	5 (7%)
15	CLA	A	1105	-	64,68,73	1.41	7 (10%)	76,107,113	1.99	19 (25%)
16	CHL	1	610	-	41,55,74	1.94	9 (21%)	35,91,114	2.18	10 (28%)
16	CHL	4	611	-	45,59,74	1.99	8 (17%)	40,96,114	2.04	10 (25%)
15	CLA	B	1237	-	49,53,73	1.37	8 (16%)	58,89,113	1.46	4 (6%)
15	CLA	A	1012	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	18 (21%)
16	CHL	2	609	2	60,74,74	1.85	8 (13%)	58,114,114	1.77	10 (17%)
22	SF4	C	3003	7	0,12,12	-	-	-	-	-
15	CLA	B	1225	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
15	CLA	A	1120	-	46,50,73	1.64	6 (13%)	53,85,113	2.13	15 (28%)
15	CLA	B	1222	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	18 (21%)
14	BCR	A	4002	-	41,41,41	1.60	4 (9%)	56,56,56	4.69	18 (32%)
15	CLA	A	1113	-	49,53,73	1.59	5 (10%)	58,89,113	2.10	16 (27%)
15	CLA	A	1119	-	69,73,73	1.34	6 (8%)	82,113,113	1.84	18 (21%)
15	CLA	A	1130	-	49,53,73	1.59	6 (12%)	58,89,113	2.09	16 (27%)
15	CLA	3	605	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	18 (21%)
15	CLA	A	1115	-	49,53,73	1.58	6 (12%)	58,89,113	2.06	16 (27%)
15	CLA	3	608	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
15	CLA	B	1023	-	69,73,73	1.41	9 (13%)	82,113,113	1.82	12 (14%)
14	BCR	1	503	-	41,41,41	1.16	2 (4%)	56,56,56	1.38	11 (19%)
15	CLA	B	1211	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	8 (9%)
15	CLA	B	1235	-	64,68,73	1.40	7 (10%)	76,107,113	1.97	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	SF4	C	3002	7	0,12,12	-	-	-		
15	CLA	B	1208	-	64,68,73	1.21	6 (9%)	76,107,113	1.23	4 (5%)
17	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.17	4 (7%)
16	CHL	2	611	-	42,56,74	2.09	8 (19%)	36,92,114	2.10	9 (25%)
15	CLA	B	1021	-	69,73,73	1.34	6 (8%)	82,113,113	1.88	18 (21%)
15	CLA	A	1013	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	19 (23%)
15	CLA	1	607	17	50,54,73	1.33	9 (18%)	59,90,113	1.37	5 (8%)
15	CLA	1	601	-	69,73,73	1.14	9 (13%)	82,113,113	1.23	6 (7%)
15	CLA	A	1125	-	69,73,73	1.46	7 (10%)	82,113,113	2.37	21 (25%)
15	CLA	4	606	-	54,58,73	1.31	9 (16%)	64,95,113	1.44	6 (9%)
15	CLA	A	1140	-	65,69,73	1.59	9 (13%)	77,108,113	2.99	15 (19%)
15	CLA	A	1111	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	19 (23%)
16	CHL	3	604	-	55,69,74	1.25	9 (16%)	52,108,114	1.77	11 (21%)
14	BCR	3	503	-	41,41,41	1.21	3 (7%)	56,56,56	1.23	9 (16%)
15	CLA	B	1204	-	49,53,73	1.36	9 (18%)	58,89,113	1.50	6 (10%)
14	BCR	A	4006	-	41,41,41	1.62	4 (9%)	56,56,56	4.50	16 (28%)
15	CLA	4	608	-	50,54,73	1.35	9 (18%)	59,90,113	1.59	8 (13%)
15	CLA	3	612	3	69,73,73	1.35	6 (8%)	82,113,113	1.88	18 (21%)
14	BCR	F	4002	-	41,41,41	1.63	4 (9%)	56,56,56	4.51	17 (30%)
15	CLA	B	1203	6	69,73,73	1.17	10 (14%)	82,113,113	1.30	4 (4%)
15	CLA	2	604	2	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
13	XAT	1	502	-	41,47,47	2.68	20 (48%)	54,74,74	9.50	23 (42%)
15	CLA	2	606	-	49,53,73	1.38	9 (18%)	58,89,113	1.43	5 (8%)
16	CHL	2	613	-	40,54,74	1.70	8 (20%)	34,90,114	2.11	9 (26%)
15	CLA	B	1210	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	9 (10%)
18	LMG	2	803	-	40,40,55	0.88	2 (5%)	48,48,63	1.20	6 (12%)
15	CLA	B	1228	-	64,68,73	1.40	7 (10%)	76,107,113	1.93	20 (26%)
20	CL0	A	1011	-	58,73,73	3.22	17 (29%)	60,113,113	2.89	19 (31%)
15	CLA	A	1137	-	65,69,73	1.39	6 (9%)	77,108,113	1.94	18 (23%)
15	CLA	1	605	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	3 (3%)
14	BCR	3	504	-	41,41,41	1.62	4 (9%)	56,56,56	4.55	13 (23%)
15	CLA	1	612	1	44,48,73	1.43	7 (15%)	51,82,113	1.42	5 (9%)
15	CLA	4	612	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	5 (6%)
12	LUT	1	501	-	42,43,43	6.26	27 (64%)	51,60,60	2.25	16 (31%)
13	XAT	2	502	-	41,47,47	2.72	19 (46%)	54,74,74	9.14	29 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1102	-	69,73,73	1.34	6 (8%)	82,113,113	2.00	18 (21%)
15	CLA	A	1107	5	55,59,73	1.50	6 (10%)	64,96,113	2.10	19 (29%)
16	CHL	2	610	-	38,52,74	2.07	9 (23%)	31,87,114	2.24	8 (25%)
19	3PH	3	802	-	21,21,47	1.27	4 (19%)	24,26,52	1.34	2 (8%)
14	BCR	B	4004	-	41,41,41	1.18	2 (4%)	56,56,56	1.35	8 (14%)
15	CLA	A	1108	-	59,63,73	1.45	6 (10%)	70,101,113	2.03	19 (27%)
15	CLA	A	1128	-	69,73,73	1.35	7 (10%)	82,113,113	1.98	21 (25%)
15	CLA	B	1240	17	69,73,73	1.17	9 (13%)	82,113,113	1.36	8 (9%)
16	CHL	1	609	-	60,74,74	1.85	8 (13%)	58,114,114	1.69	9 (15%)
18	LMG	4	801	-	37,37,55	1.01	3 (8%)	45,45,63	1.31	3 (6%)
15	CLA	A	1118	-	46,50,73	1.72	8 (17%)	53,85,113	2.39	14 (26%)
15	CLA	1	604	1	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
15	CLA	2	602	-	49,53,73	1.38	7 (14%)	58,89,113	1.42	5 (8%)
15	CLA	1	606	-	54,58,73	1.31	8 (14%)	64,95,113	1.41	6 (9%)
15	CLA	A	1133	-	69,73,73	1.46	9 (13%)	82,113,113	1.90	25 (30%)
15	CLA	A	1135	-	55,59,73	1.51	6 (10%)	64,96,113	2.11	19 (29%)
15	CLA	B	1232	-	50,54,73	1.35	9 (18%)	59,90,113	1.41	5 (8%)
15	CLA	B	1215	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)
15	CLA	2	612	2	59,63,73	1.24	8 (13%)	70,101,113	1.31	5 (7%)
15	CLA	B	1220	-	55,59,73	1.31	9 (16%)	64,96,113	1.40	6 (9%)
15	CLA	A	1101	-	69,73,73	1.33	6 (8%)	82,113,113	1.91	17 (20%)
12	LUT	2	501	-	42,43,43	6.41	30 (71%)	51,60,60	2.41	17 (33%)
15	CLA	B	1227	-	69,73,73	1.37	8 (11%)	82,113,113	1.83	17 (20%)
15	CLA	B	1205	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	6 (7%)
15	CLA	A	1117	-	69,73,73	1.34	7 (10%)	82,113,113	1.97	21 (25%)
14	BCR	B	4003	-	41,41,41	1.17	2 (4%)	56,56,56	1.46	10 (17%)
15	CLA	B	1239	-	46,50,73	1.40	7 (15%)	53,85,113	1.59	6 (11%)
15	CLA	A	1109	-	69,73,73	1.36	6 (8%)	82,113,113	1.86	19 (23%)
15	CLA	F	1302	10	53,57,73	1.31	8 (15%)	61,93,113	1.43	6 (9%)
15	CLA	2	601	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	6 (7%)
15	CLA	B	1206	-	49,53,73	1.35	9 (18%)	58,89,113	1.41	5 (8%)
15	CLA	A	1124	-	64,68,73	1.44	6 (9%)	76,107,113	1.90	19 (25%)
15	CLA	A	1129	-	59,63,73	1.26	9 (15%)	70,101,113	1.37	6 (8%)
15	CLA	B	1213	-	59,63,73	1.24	9 (15%)	70,101,113	1.37	5 (7%)
14	BCR	B	4001	-	41,41,41	1.20	3 (7%)	56,56,56	1.40	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	3	615	3	46,50,73	1.64	6 (13%)	53,85,113	2.17	15 (28%)
14	BCR	A	4008	-	41,41,41	1.66	6 (14%)	56,56,56	4.24	19 (33%)
15	CLA	1	602	-	50,54,73	1.36	9 (18%)	59,90,113	1.36	4 (6%)
15	CLA	A	1110	-	59,63,73	1.45	7 (11%)	70,101,113	2.01	19 (27%)
12	LUT	3	501	-	42,43,43	6.41	29 (69%)	51,60,60	3.06	21 (41%)
15	CLA	A	1139	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	18 (21%)
15	CLA	B	1238	-	55,59,73	1.54	10 (18%)	62,95,113	1.82	11 (17%)
15	CLA	A	1131	-	49,53,73	1.59	7 (14%)	58,89,113	2.08	16 (27%)
15	CLA	3	614	-	56,60,73	1.31	9 (16%)	65,97,113	1.45	5 (7%)
17	LHG	3	801	-	46,46,48	0.44	0	48,51,54	1.18	5 (10%)
15	CLA	B	1217	-	50,54,73	1.35	8 (16%)	59,90,113	1.38	4 (6%)
21	PQN	B	2002	-	34,34,34	0.70	0	43,45,45	0.92	1 (2%)
15	CLA	B	1219	-	69,73,73	1.17	8 (11%)	82,113,113	1.17	5 (6%)
15	CLA	A	1134	5	46,50,73	2.20	13 (28%)	53,85,113	3.75	26 (49%)

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
15	CLA	4	616	4	1/1/12/20	7/23/99/115	-
15	CLA	B	1201	-	1/1/10/20	1/13/89/115	-
15	CLA	A	1116	-	1/1/13/20	9/29/105/115	-
15	CLA	2	608	-	1/1/12/20	3/21/97/115	-
15	CLA	A	1114	-	1/1/13/20	8/27/103/115	-
15	CLA	3	610	-	1/1/12/20	6/21/97/115	-
14	BCR	2	503	-	-	20/29/63/63	0/2/2/2
14	BCR	J	4001	-	-	13/29/63/63	0/2/2/2
15	CLA	B	1229	-	1/1/14/20	19/33/109/115	-
15	CLA	1	603	-	1/1/14/20	13/33/109/115	-
14	BCR	A	4005	-	-	11/29/63/63	0/2/2/2
15	CLA	4	603	-	1/1/15/20	13/39/115/115	-
18	LMG	B	5003	-	-	14/34/54/70	0/1/1/1
15	CLA	A	1123	-	1/1/15/20	18/39/115/115	-
15	CLA	A	1103	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1022	-	1/1/15/20	20/39/115/115	-
15	CLA	A	1136	-	1/1/15/20	14/39/115/115	-
15	CLA	B	1207	-	-	11/17/93/115	-
13	XAT	4	502	-	-	15/31/93/93	0/4/4/4
15	CLA	B	1214	-	1/1/15/20	8/39/115/115	-
14	BCR	F	4001	-	-	16/29/63/63	0/2/2/2
15	CLA	3	611	-	1/1/15/20	8/39/115/115	-
15	CLA	B	1223	-	1/1/15/20	4/39/115/115	-
15	CLA	2	603	2	1/1/15/20	7/39/115/115	-
15	CLA	4	602	-	1/1/12/20	9/21/97/115	-
15	CLA	4	605	-	1/1/15/20	11/39/115/115	-
14	BCR	B	4005	-	-	14/29/63/63	0/2/2/2
15	CLA	A	1104	-	1/1/15/20	12/39/115/115	-
15	CLA	4	609	4	1/1/14/20	10/33/109/115	-
15	CLA	1	608	-	1/1/13/20	11/27/103/115	-
15	CLA	4	601	4	1/1/14/20	9/33/109/115	-
22	SF4	A	3001	6,5	-	-	0/6/5/5
12	LUT	4	501	-	1/1/12/27	20/29/67/67	0/2/2/2
15	CLA	B	1230	-	1/1/13/20	14/27/103/115	-
15	CLA	4	604	-	1/1/14/20	15/33/109/115	-
15	CLA	J	1302	-	1/1/10/20	4/12/88/115	-
15	CLA	A	1112	-	1/1/15/20	18/39/115/115	-
21	PQN	A	2001	-	-	3/23/43/43	0/2/2/2
15	CLA	A	1121	-	1/1/11/20	5/15/91/115	-
14	BCR	B	4002	-	-	14/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	8/29/63/63	0/2/2/2
18	LMG	2	804	-	-	26/45/65/70	0/1/1/1
15	CLA	B	1224	-	1/1/14/20	11/35/111/115	-
14	BCR	J	4002	-	-	16/29/63/63	0/2/2/2
15	CLA	B	1226	-	1/1/15/20	10/39/115/115	-
15	CLA	B	1231	-	1/1/14/20	8/33/109/115	-
15	CLA	3	607	-	1/1/14/20	10/33/109/115	-
23	DGD	B	5002	-	-	17/50/90/95	0/2/2/2
16	CHL	4	613	-	4/4/19/26	2/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	3	506	-	-	14/29/63/63	0/2/2/2
15	CLA	3	613	-	1/1/11/20	7/17/93/115	-
15	CLA	A	1126	-	1/1/15/20	23/39/115/115	-
17	LHG	2	801	15	-	19/39/39/53	-
15	CLA	B	1202	-	1/1/15/20	14/39/115/115	-
15	CLA	B	1212	-	1/1/13/20	5/27/103/115	-
15	CLA	B	1234	-	1/1/13/20	11/27/103/115	-
15	CLA	A	1106	5	1/1/15/20	12/39/115/115	-
15	CLA	A	1141	17	1/1/10/20	4/10/86/115	-
15	CLA	B	1216	-	1/1/13/20	10/32/108/115	-
15	CLA	B	1221	-	1/1/15/20	16/39/115/115	-
14	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1138	-	1/1/15/20	15/39/115/115	-
17	LHG	B	5001	15	-	25/46/46/53	-
15	CLA	A	1132	-	1/1/11/20	9/15/91/115	-
15	CLA	1	615	1	1/1/11/20	13/15/91/115	-
15	CLA	2	605	-	1/1/15/20	13/39/115/115	-
15	CLA	B	1236	-	1/1/11/20	10/20/96/115	-
14	BCR	4	503	-	-	16/29/63/63	0/2/2/2
15	CLA	4	607	-	1/1/14/20	11/33/109/115	-
15	CLA	A	1127	-	1/1/15/20	17/39/115/115	-
14	BCR	A	4003	-	-	11/29/63/63	0/2/2/2
15	CLA	2	616	2	-	16/39/115/115	-
15	CLA	3	601	3	1/1/14/20	11/33/109/115	-
17	LHG	1	801	15	-	22/53/53/53	-
16	CHL	4	610	-	3/3/16/26	4/17/115/137	-
18	LMG	2	802	-	-	20/45/65/70	0/1/1/1
15	CLA	3	609	-	1/1/10/20	4/12/88/115	-
14	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
15	CLA	B	1209	-	1/1/11/20	5/17/93/115	-
15	CLA	1	613	-	1/1/11/20	6/15/91/115	-
15	CLA	1	611	-	1/1/11/20	5/19/95/115	-
15	CLA	B	1218	-	1/1/11/20	5/15/91/115	-
15	CLA	F	1301	-	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	2	607	17	1/1/14/20	9/33/109/115	-
17	LHG	A	5001	15	-	19/53/53/53	-
15	CLA	3	603	-	1/1/15/20	12/39/115/115	-
15	CLA	A	1122	-	1/1/15/20	15/39/115/115	-
13	XAT	3	502	-	-	15/31/93/93	0/4/4/4
15	CLA	3	606	-	1/1/13/20	6/27/103/115	-
15	CLA	A	1105	-	1/1/14/20	16/33/109/115	-
16	CHL	1	610	-	3/3/16/26	2/17/115/137	-
16	CHL	4	611	-	3/3/17/26	0/21/119/137	-
15	CLA	B	1237	-	1/1/11/20	6/15/91/115	-
15	CLA	A	1012	-	1/1/15/20	16/39/115/115	-
16	CHL	2	609	2	4/4/20/26	11/39/137/137	-
22	SF4	C	3003	7	-	-	0/6/5/5
15	CLA	B	1225	-	1/1/15/20	19/39/115/115	-
15	CLA	A	1120	-	1/1/10/20	8/12/88/115	-
15	CLA	B	1222	-	1/1/15/20	13/39/115/115	-
14	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1113	-	1/1/11/20	5/15/91/115	-
15	CLA	A	1119	-	1/1/15/20	12/39/115/115	-
15	CLA	A	1130	-	1/1/11/20	9/15/91/115	-
15	CLA	3	605	-	1/1/15/20	15/39/115/115	-
15	CLA	A	1115	-	1/1/11/20	3/15/91/115	-
15	CLA	3	608	-	1/1/15/20	17/39/115/115	-
15	CLA	B	1211	-	1/1/15/20	13/39/115/115	-
15	CLA	B	1235	-	1/1/14/20	14/33/109/115	-
14	BCR	1	503	-	-	19/29/63/63	0/2/2/2
15	CLA	B	1023	-	-	17/39/115/115	-
22	SF4	C	3002	7	-	-	0/6/5/5
15	CLA	B	1208	-	1/1/14/20	11/33/109/115	-
17	LHG	A	5002	-	-	29/53/53/53	-
16	CHL	2	611	-	3/3/16/26	2/18/116/137	-
15	CLA	B	1021	-	1/1/15/20	20/39/115/115	-
15	CLA	A	1013	-	1/1/15/20	13/39/115/115	-
15	CLA	1	607	17	1/1/11/20	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	1	601	-	1/1/15/20	7/39/115/115	-
15	CLA	A	1125	-	1/1/15/20	12/39/115/115	-
15	CLA	4	606	-	1/1/12/20	7/21/97/115	-
15	CLA	A	1140	-	-	6/35/111/115	-
15	CLA	A	1111	-	1/1/15/20	20/39/115/115	-
16	CHL	3	604	-	4/4/19/26	8/33/131/137	-
14	BCR	3	503	-	-	17/29/63/63	0/2/2/2
15	CLA	B	1204	-	1/1/11/20	6/15/91/115	-
14	BCR	A	4006	-	-	11/29/63/63	0/2/2/2
15	CLA	4	608	-	1/1/11/20	6/17/93/115	-
15	CLA	3	612	3	1/1/15/20	15/39/115/115	-
14	BCR	F	4002	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1203	6	1/1/15/20	10/39/115/115	-
15	CLA	2	604	2	1/1/15/20	15/39/115/115	-
13	XAT	1	502	-	-	12/31/93/93	0/4/4/4
15	CLA	2	606	-	1/1/11/20	6/15/91/115	-
16	CHL	2	613	-	3/3/16/26	6/15/113/137	-
15	CLA	B	1210	-	-	5/39/115/115	-
18	LMG	2	803	-	-	20/35/55/70	0/1/1/1
15	CLA	B	1228	-	1/1/14/20	12/33/109/115	-
20	CL0	A	1011	-	3/3/20/25	22/37/135/135	-
15	CLA	A	1137	-	1/1/14/20	14/35/111/115	-
15	CLA	1	605	-	1/1/15/20	14/39/115/115	-
14	BCR	3	504	-	-	13/29/63/63	0/2/2/2
15	CLA	1	612	1	1/1/9/20	4/10/82/115	-
15	CLA	4	612	-	1/1/15/20	8/39/115/115	-
12	LUT	1	501	-	1/1/12/27	22/29/67/67	0/2/2/2
15	CLA	A	1102	-	1/1/15/20	21/39/115/115	-
15	CLA	A	1107	5	1/1/12/20	9/23/99/115	-
13	XAT	2	502	-	-	12/31/93/93	0/4/4/4
16	CHL	2	610	-	3/3/15/26	3/13/111/137	-
19	3PH	3	802	-	-	14/23/23/49	-
15	CLA	A	1108	-	1/1/13/20	12/27/103/115	-
14	BCR	B	4004	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1128	-	1/1/15/20	12/39/115/115	-
15	CLA	B	1240	17	1/1/15/20	11/39/115/115	-
16	CHL	1	609	-	4/4/20/26	12/39/137/137	-
18	LMG	4	801	-	-	10/32/52/70	0/1/1/1
15	CLA	A	1118	-	1/1/10/20	0/12/88/115	-
15	CLA	1	604	1	1/1/15/20	6/39/115/115	-
15	CLA	2	602	-	1/1/11/20	7/15/91/115	-
15	CLA	1	606	-	1/1/12/20	4/21/97/115	-
15	CLA	A	1135	-	1/1/12/20	11/23/99/115	-
15	CLA	A	1133	-	-	22/39/115/115	-
15	CLA	B	1232	-	1/1/11/20	6/17/93/115	-
15	CLA	B	1215	-	1/1/15/20	10/39/115/115	-
15	CLA	2	612	2	1/1/13/20	3/27/103/115	-
15	CLA	B	1220	-	1/1/12/20	7/23/99/115	-
15	CLA	A	1101	-	1/1/15/20	17/39/115/115	-
12	LUT	2	501	-	1/1/12/27	18/29/67/67	0/2/2/2
15	CLA	B	1227	-	1/1/15/20	15/39/115/115	-
15	CLA	B	1205	-	1/1/15/20	9/39/115/115	-
15	CLA	A	1117	-	1/1/15/20	10/39/115/115	-
14	BCR	B	4003	-	-	22/29/63/63	0/2/2/2
15	CLA	B	1239	-	1/1/10/20	5/12/88/115	-
15	CLA	A	1109	-	1/1/15/20	13/39/115/115	-
15	CLA	F	1302	10	1/1/11/20	7/20/96/115	-
15	CLA	2	601	-	1/1/15/20	13/39/115/115	-
15	CLA	B	1206	-	1/1/11/20	4/15/91/115	-
15	CLA	A	1124	-	1/1/14/20	12/33/109/115	-
15	CLA	A	1129	-	1/1/13/20	8/27/103/115	-
15	CLA	B	1213	-	1/1/13/20	3/27/103/115	-
14	BCR	B	4001	-	-	17/29/63/63	0/2/2/2
15	CLA	3	615	3	1/1/10/20	6/12/88/115	-
14	BCR	A	4008	-	-	16/29/63/63	0/2/2/2
15	CLA	1	602	-	1/1/11/20	6/17/93/115	-
15	CLA	A	1110	-	1/1/13/20	7/27/103/115	-
12	LUT	3	501	-	1/1/12/27	18/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1139	-	1/1/15/20	15/39/115/115	-
15	CLA	B	1238	-	2/2/12/20	9/20/96/115	-
15	CLA	A	1131	-	1/1/11/20	8/15/91/115	-
15	CLA	3	614	-	1/1/12/20	6/24/100/115	-
17	LHG	3	801	-	-	26/49/49/53	-
15	CLA	B	1217	-	1/1/11/20	8/17/93/115	-
21	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
15	CLA	B	1219	-	-	12/39/115/115	-
15	CLA	A	1134	5	-	6/12/88/115	-

All (1419) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	2	501	LUT	C24-C25	22.39	1.59	1.33
12	3	501	LUT	C24-C25	22.08	1.59	1.33
12	1	501	LUT	C24-C25	21.99	1.59	1.33
12	4	501	LUT	C24-C25	21.78	1.59	1.33
12	3	501	LUT	C22-C21	-16.33	1.34	1.54
12	2	501	LUT	C22-C21	-16.18	1.34	1.54
12	1	501	LUT	C5-C6	15.64	1.60	1.34
12	4	501	LUT	C5-C6	15.55	1.60	1.34
12	4	501	LUT	C22-C21	-15.50	1.35	1.54
12	2	501	LUT	C5-C6	15.34	1.60	1.34
12	1	501	LUT	C22-C21	-15.32	1.36	1.54
12	3	501	LUT	C5-C6	15.30	1.60	1.34
12	3	501	LUT	C2-C3	-12.49	1.34	1.52
12	4	501	LUT	C2-C3	-12.10	1.35	1.52
12	1	501	LUT	C2-C3	-11.85	1.35	1.52
12	2	501	LUT	C2-C3	-11.79	1.35	1.52
12	1	501	LUT	C22-C23	11.66	1.66	1.52
12	4	501	LUT	C22-C23	11.17	1.65	1.52
12	2	501	LUT	C22-C23	10.99	1.65	1.52
12	3	501	LUT	C22-C23	10.52	1.64	1.52
20	A	1011	CL0	C1D-C2D	9.49	1.50	1.39
20	A	1011	CL0	C1A-CHA	9.26	1.50	1.40
20	A	1011	CL0	C1B-C2B	8.94	1.49	1.39
15	A	1134	CLA	MG-NA	8.86	2.27	2.06
16	1	609	CHL	C3A-C2A	-8.58	1.47	1.54
15	A	1140	CLA	MG-NA	8.49	2.26	2.06
16	2	611	CHL	C3A-C2A	-8.21	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	609	CHL	C3A-C2A	-8.10	1.47	1.54
16	2	610	CHL	C3A-C2A	-7.93	1.47	1.54
16	4	611	CHL	C3A-C2A	-7.80	1.48	1.54
16	4	610	CHL	C3A-C2A	-7.74	1.48	1.54
15	A	1125	CLA	MG-NA	7.64	2.24	2.06
20	A	1011	CL0	C3B-C4B	7.53	1.48	1.41
12	4	501	LUT	C4-C3	7.41	1.65	1.52
12	1	501	LUT	C4-C3	7.32	1.65	1.52
12	2	501	LUT	C4-C3	7.30	1.65	1.52
12	3	501	LUT	C8-C9	7.15	1.61	1.46
12	3	501	LUT	C4-C3	7.08	1.64	1.52
16	1	609	CHL	C3B-C4B	6.97	1.48	1.41
15	B	1223	CLA	MG-NA	6.96	2.22	2.06
15	A	1118	CLA	MG-NA	6.89	2.22	2.06
16	4	611	CHL	C3B-C4B	6.85	1.48	1.41
15	A	1133	CLA	MG-NA	6.84	2.22	2.06
15	B	1023	CLA	MG-NA	6.76	2.22	2.06
16	4	613	CHL	C3B-C4B	6.75	1.48	1.41
15	B	1022	CLA	MG-NA	6.63	2.22	2.06
16	2	611	CHL	C3B-C4B	6.62	1.47	1.41
16	1	610	CHL	C3A-C2A	-6.50	1.49	1.54
16	2	609	CHL	C3B-C4B	6.48	1.47	1.41
15	A	1124	CLA	MG-NA	6.47	2.21	2.06
16	1	610	CHL	C3B-C4B	6.43	1.47	1.41
15	B	1234	CLA	MG-NA	6.43	2.21	2.06
15	A	1121	CLA	MG-NA	6.43	2.21	2.06
15	A	1127	CLA	MG-NA	6.42	2.21	2.06
15	A	1128	CLA	MG-NA	6.41	2.21	2.06
15	A	1130	CLA	MG-NA	6.40	2.21	2.06
15	B	1224	CLA	MG-NA	6.40	2.21	2.06
15	A	1111	CLA	MG-NA	6.37	2.21	2.06
15	A	1105	CLA	MG-NA	6.37	2.21	2.06
15	3	605	CLA	MG-NA	6.37	2.21	2.06
15	A	1131	CLA	MG-NA	6.36	2.21	2.06
15	3	613	CLA	MG-NA	6.36	2.21	2.06
15	A	1126	CLA	MG-NA	6.35	2.21	2.06
16	4	610	CHL	C3B-C4B	6.35	1.47	1.41
15	A	1135	CLA	MG-NA	6.34	2.21	2.06
15	B	1227	CLA	MG-NA	6.34	2.21	2.06
15	A	1012	CLA	MG-NA	6.33	2.21	2.06
15	A	1106	CLA	MG-NA	6.33	2.21	2.06
15	B	1222	CLA	MG-NA	6.33	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1013	CLA	MG-NA	6.33	2.21	2.06
15	J	1302	CLA	MG-NA	6.33	2.21	2.06
15	A	1120	CLA	MG-NA	6.32	2.21	2.06
15	A	1137	CLA	MG-NA	6.32	2.21	2.06
15	A	1112	CLA	MG-NA	6.32	2.21	2.06
15	3	615	CLA	MG-NA	6.31	2.21	2.06
15	A	1116	CLA	MG-NA	6.31	2.21	2.06
15	A	1136	CLA	MG-NA	6.30	2.21	2.06
15	3	612	CLA	MG-NA	6.30	2.21	2.06
15	A	1108	CLA	MG-NA	6.30	2.21	2.06
15	A	1109	CLA	MG-NA	6.30	2.21	2.06
15	B	1228	CLA	MG-NA	6.30	2.21	2.06
15	A	1123	CLA	MG-NA	6.29	2.21	2.06
15	B	1238	CLA	C2-C3	6.29	1.53	1.33
15	A	1115	CLA	MG-NA	6.29	2.21	2.06
15	B	1236	CLA	MG-NA	6.28	2.21	2.06
15	B	1229	CLA	MG-NA	6.28	2.21	2.06
15	A	1138	CLA	MG-NA	6.28	2.21	2.06
15	B	1231	CLA	MG-NA	6.27	2.21	2.06
15	B	1235	CLA	MG-NA	6.27	2.21	2.06
15	A	1113	CLA	MG-NA	6.27	2.21	2.06
15	B	1225	CLA	MG-NA	6.26	2.21	2.06
15	A	1122	CLA	MG-NA	6.26	2.21	2.06
15	A	1110	CLA	MG-NA	6.25	2.21	2.06
15	A	1107	CLA	MG-NA	6.24	2.21	2.06
15	A	1104	CLA	MG-NA	6.24	2.21	2.06
15	F	1301	CLA	MG-NA	6.22	2.21	2.06
15	B	1021	CLA	MG-NA	6.22	2.21	2.06
15	A	1103	CLA	MG-NA	6.21	2.21	2.06
15	A	1101	CLA	MG-NA	6.18	2.21	2.06
15	B	1230	CLA	MG-NA	6.18	2.21	2.06
15	A	1117	CLA	MG-NA	6.18	2.21	2.06
15	A	1139	CLA	MG-NA	6.18	2.21	2.06
15	A	1114	CLA	MG-NA	6.16	2.20	2.06
15	A	1119	CLA	MG-NA	6.15	2.20	2.06
16	2	613	CHL	C3B-C4B	6.14	1.47	1.41
15	A	1102	CLA	MG-NA	6.13	2.20	2.06
16	2	610	CHL	C3B-C4B	6.01	1.47	1.41
12	3	501	LUT	C28-C29	5.94	1.58	1.46
14	A	4003	BCR	C24-C23	5.90	1.50	1.33
14	3	504	BCR	C24-C23	5.86	1.50	1.33
14	B	4005	BCR	C24-C23	5.83	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	4001	BCR	C24-C23	5.83	1.50	1.33
14	J	4002	BCR	C24-C23	5.82	1.50	1.33
14	A	4008	BCR	C24-C23	5.81	1.50	1.33
14	B	4006	BCR	C24-C23	5.80	1.50	1.33
14	A	4006	BCR	C24-C23	5.77	1.50	1.33
14	A	4005	BCR	C11-C12	-5.77	1.19	1.34
14	A	4004	BCR	C24-C23	5.76	1.50	1.33
12	2	501	LUT	C28-C29	5.76	1.58	1.46
14	A	4002	BCR	C24-C23	5.74	1.50	1.33
12	2	501	LUT	C8-C9	5.72	1.58	1.46
14	F	4002	BCR	C24-C23	5.72	1.50	1.33
12	2	501	LUT	C1-C6	-5.71	1.46	1.53
12	4	501	LUT	C1-C6	-5.70	1.46	1.53
12	4	501	LUT	C8-C9	5.69	1.58	1.46
14	F	4001	BCR	C24-C23	5.65	1.49	1.33
12	1	501	LUT	C8-C9	5.64	1.58	1.46
14	A	4007	BCR	C24-C23	5.56	1.49	1.33
12	1	501	LUT	C1-C6	-5.55	1.46	1.53
20	A	1011	CL0	CHC-C4B	5.55	1.48	1.39
14	F	4001	BCR	C11-C12	-5.50	1.20	1.34
14	A	4005	BCR	C24-C23	5.50	1.49	1.33
12	2	501	LUT	C32-C33	5.44	1.57	1.46
14	A	4008	BCR	C11-C12	-5.41	1.20	1.34
16	2	609	CHL	C1A-CHA	-5.39	1.33	1.40
20	A	1011	CL0	CHB-C1B	5.38	1.48	1.39
13	4	502	XAT	C22-C23	-5.35	1.44	1.52
14	F	4002	BCR	C11-C12	-5.31	1.20	1.34
14	A	4007	BCR	C11-C12	-5.30	1.20	1.34
12	4	501	LUT	C23-C24	-5.26	1.43	1.50
20	A	1011	CL0	O2A-C1	5.24	1.60	1.46
13	4	502	XAT	C8-C9	5.24	1.57	1.46
12	4	501	LUT	C32-C33	5.20	1.57	1.46
12	3	501	LUT	C15-C14	5.19	1.59	1.43
16	4	613	CHL	C3A-C2A	-5.17	1.50	1.54
12	2	501	LUT	C15-C14	5.17	1.59	1.43
14	B	4006	BCR	C11-C12	-5.16	1.21	1.34
14	A	4006	BCR	C11-C12	-5.14	1.21	1.34
12	4	501	LUT	C15-C14	5.06	1.58	1.43
14	3	504	BCR	C11-C12	-5.05	1.21	1.34
14	B	4005	BCR	C11-C12	-5.03	1.21	1.34
20	A	1011	CL0	O2D-CGD	5.03	1.45	1.33
12	3	501	LUT	C4-C5	-5.02	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	4002	BCR	C11-C12	-5.00	1.21	1.34
14	A	4004	BCR	C11-C12	-4.99	1.21	1.34
14	J	4001	BCR	C11-C12	-4.99	1.21	1.34
20	A	1011	CL0	CHD-C1D	4.99	1.47	1.39
12	1	501	LUT	C15-C14	4.97	1.58	1.43
13	2	502	XAT	C22-C23	-4.96	1.45	1.52
13	1	502	XAT	C32-C33	4.96	1.56	1.46
20	A	1011	CL0	OBD-CAD	4.95	1.28	1.22
13	1	502	XAT	C22-C23	-4.94	1.45	1.52
14	A	4003	BCR	C11-C12	-4.94	1.21	1.34
12	2	501	LUT	C4-C5	-4.94	1.43	1.51
12	3	501	LUT	C23-C24	-4.93	1.43	1.50
13	1	502	XAT	C8-C9	4.92	1.56	1.46
14	A	4002	BCR	C11-C12	-4.89	1.21	1.34
13	2	502	XAT	C28-C29	4.87	1.56	1.46
13	2	502	XAT	C8-C9	4.85	1.56	1.46
12	4	501	LUT	C28-C29	4.83	1.56	1.46
20	A	1011	CL0	CHC-C1C	4.79	1.48	1.39
12	1	501	LUT	C28-C29	4.78	1.56	1.46
13	1	502	XAT	C28-C29	4.77	1.56	1.46
20	A	1011	CL0	CHD-C4C	4.77	1.48	1.39
20	A	1011	CL0	C3B-C2B	4.76	1.46	1.40
13	1	502	XAT	C12-C13	4.74	1.56	1.46
13	2	502	XAT	C32-C33	4.72	1.56	1.46
13	4	502	XAT	C12-C13	4.72	1.56	1.46
16	1	609	CHL	C1A-CHA	-4.71	1.34	1.40
13	2	502	XAT	C12-C13	4.70	1.56	1.46
12	3	501	LUT	C40-C33	4.69	1.60	1.50
15	B	1230	CLA	CBB-CAB	4.67	1.52	1.30
13	1	502	XAT	C4-C5	4.64	1.58	1.52
14	A	4007	BCR	C16-C17	-4.62	1.28	1.43
12	1	501	LUT	C4-C5	-4.60	1.43	1.51
14	A	4005	BCR	C16-C17	-4.60	1.28	1.43
12	4	501	LUT	C11-C10	4.59	1.57	1.43
13	4	502	XAT	C32-C33	4.58	1.55	1.46
12	2	501	LUT	C40-C33	4.56	1.60	1.50
15	B	1223	CLA	CBB-CAB	4.53	1.52	1.30
15	A	1134	CLA	CHD-C1D	4.53	1.47	1.38
15	B	1023	CLA	CBB-CAB	4.52	1.52	1.30
15	B	1229	CLA	CBB-CAB	4.52	1.52	1.30
12	1	501	LUT	C11-C10	4.52	1.57	1.43
15	A	1133	CLA	CBB-CAB	4.51	1.52	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	2	501	LUT	C11-C10	4.51	1.57	1.43
20	A	1011	CL0	C3D-C4D	-4.51	1.34	1.41
12	3	501	LUT	C19-C9	4.50	1.59	1.50
15	A	1140	CLA	CBB-CAB	4.49	1.52	1.30
14	F	4001	BCR	C16-C17	-4.48	1.29	1.43
12	2	501	LUT	C23-C24	-4.47	1.44	1.50
20	A	1011	CL0	C3D-C2D	4.46	1.47	1.39
12	4	501	LUT	C4-C5	-4.46	1.44	1.51
14	A	4002	BCR	C10-C9	4.45	1.46	1.35
15	B	1022	CLA	CBB-CAB	4.43	1.51	1.30
12	4	501	LUT	C40-C33	4.42	1.59	1.50
15	B	1224	CLA	CBB-CAB	4.41	1.51	1.30
15	B	1227	CLA	CBB-CAB	4.41	1.51	1.30
15	A	1013	CLA	CBB-CAB	4.39	1.51	1.30
15	A	1124	CLA	CBB-CAB	4.39	1.51	1.30
15	A	1121	CLA	CBB-CAB	4.39	1.51	1.30
15	A	1137	CLA	CBB-CAB	4.39	1.51	1.30
15	J	1302	CLA	CBB-CAB	4.39	1.51	1.30
15	A	1103	CLA	CBB-CAB	4.39	1.51	1.30
14	B	4001	BCR	C1-C6	-4.38	1.48	1.53
15	3	613	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1122	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1130	CLA	CBB-CAB	4.38	1.51	1.30
15	B	1225	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1131	CLA	CBB-CAB	4.38	1.51	1.30
13	2	502	XAT	C4-C5	4.38	1.58	1.52
15	A	1123	CLA	CBB-CAB	4.38	1.51	1.30
15	B	1231	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1114	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1110	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1118	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1117	CLA	CBB-CAB	4.38	1.51	1.30
15	3	615	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1115	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1106	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1138	CLA	CBB-CAB	4.38	1.51	1.30
15	A	1119	CLA	CBB-CAB	4.37	1.51	1.30
15	A	1136	CLA	CBB-CAB	4.37	1.51	1.30
15	B	1021	CLA	CBB-CAB	4.37	1.51	1.30
15	3	612	CLA	CBB-CAB	4.37	1.51	1.30
12	3	501	LUT	C1-C6	-4.37	1.48	1.53
15	A	1120	CLA	CBB-CAB	4.37	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	4002	BCR	C16-C17	-4.37	1.29	1.43
15	A	1126	CLA	CBB-CAB	4.37	1.51	1.30
15	A	1128	CLA	CBB-CAB	4.37	1.51	1.30
15	3	605	CLA	CBB-CAB	4.37	1.51	1.30
15	A	1127	CLA	CBB-CAB	4.37	1.51	1.30
15	A	1102	CLA	CBB-CAB	4.37	1.51	1.30
15	A	1139	CLA	CBB-CAB	4.37	1.51	1.30
15	B	1235	CLA	CBB-CAB	4.37	1.51	1.30
12	3	501	LUT	C32-C33	4.36	1.55	1.46
15	B	1228	CLA	CBB-CAB	4.36	1.51	1.30
15	A	1108	CLA	CBB-CAB	4.36	1.51	1.30
15	B	1234	CLA	CBB-CAB	4.36	1.51	1.30
15	B	1236	CLA	CBB-CAB	4.36	1.51	1.30
15	B	1222	CLA	CBB-CAB	4.36	1.51	1.30
15	A	1135	CLA	CBB-CAB	4.36	1.51	1.30
15	A	1111	CLA	CBB-CAB	4.36	1.51	1.30
15	A	1109	CLA	CBB-CAB	4.36	1.51	1.30
15	A	1012	CLA	CBB-CAB	4.36	1.51	1.30
15	A	1105	CLA	CBB-CAB	4.34	1.51	1.30
15	A	1107	CLA	CBB-CAB	4.34	1.51	1.30
15	A	1101	CLA	CBB-CAB	4.34	1.51	1.30
15	A	1112	CLA	CBB-CAB	4.34	1.51	1.30
15	A	1116	CLA	CBB-CAB	4.33	1.51	1.30
12	1	501	LUT	C23-C24	-4.32	1.44	1.50
15	A	1104	CLA	CBB-CAB	4.30	1.51	1.30
14	A	4004	BCR	C10-C9	4.30	1.45	1.35
14	3	506	BCR	C1-C6	-4.30	1.48	1.53
15	A	1113	CLA	CBB-CAB	4.30	1.51	1.30
15	F	1301	CLA	CBB-CAB	4.29	1.51	1.30
12	4	501	LUT	C21-C26	4.29	1.68	1.56
13	4	502	XAT	C11-C10	4.27	1.56	1.43
14	A	4003	BCR	C10-C9	4.27	1.45	1.35
15	A	1125	CLA	CBB-CAB	4.25	1.50	1.30
14	A	4008	BCR	C16-C17	-4.24	1.30	1.43
13	4	502	XAT	C28-C29	4.24	1.55	1.46
12	3	501	LUT	C21-C26	4.24	1.68	1.56
13	1	502	XAT	C35-C34	4.22	1.56	1.43
13	4	502	XAT	C15-C14	4.22	1.56	1.43
13	2	502	XAT	C35-C34	4.21	1.56	1.43
12	3	501	LUT	C11-C10	4.21	1.56	1.43
14	J	4001	BCR	C10-C9	4.20	1.45	1.35
14	3	504	BCR	C10-C9	4.20	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4005	BCR	C10-C9	4.19	1.45	1.35
12	1	501	LUT	C40-C33	4.19	1.59	1.50
14	A	4006	BCR	C10-C9	4.19	1.45	1.35
13	4	502	XAT	C4-C5	4.18	1.58	1.52
12	2	501	LUT	C21-C26	4.15	1.68	1.56
14	B	4006	BCR	C16-C17	-4.15	1.30	1.43
13	2	502	XAT	C15-C14	4.15	1.56	1.43
13	4	502	XAT	C35-C34	4.13	1.56	1.43
16	3	604	CHL	C3B-C4B	4.12	1.45	1.41
15	A	1134	CLA	CBB-CAB	4.12	1.50	1.30
14	A	4004	BCR	C16-C17	-4.12	1.30	1.43
14	A	4006	BCR	C16-C17	-4.11	1.30	1.43
14	B	4005	BCR	C16-C17	-4.10	1.30	1.43
12	3	501	LUT	C28-C27	4.09	1.41	1.32
15	B	1022	CLA	MG-ND	-4.09	1.97	2.05
14	J	4002	BCR	C10-C9	4.09	1.45	1.35
14	J	4001	BCR	C16-C17	-4.08	1.30	1.43
13	2	502	XAT	C11-C10	4.06	1.55	1.43
12	1	501	LUT	C32-C33	4.06	1.54	1.46
14	3	504	BCR	C16-C17	-4.05	1.30	1.43
13	1	502	XAT	C31-C30	4.05	1.55	1.43
12	2	501	LUT	C19-C9	4.03	1.59	1.50
15	A	1133	CLA	C1C-NC	-4.03	1.31	1.37
14	J	4002	BCR	C16-C17	-4.02	1.30	1.43
14	A	4003	BCR	C16-C17	-4.02	1.30	1.43
12	3	501	LUT	C35-C34	4.02	1.55	1.43
12	2	501	LUT	C2-C1	4.02	1.66	1.54
14	B	4002	BCR	C30-C25	-4.02	1.48	1.53
12	4	501	LUT	C19-C9	4.02	1.59	1.50
12	1	501	LUT	C2-C1	4.01	1.66	1.54
14	4	503	BCR	C1-C6	-3.99	1.48	1.53
12	1	501	LUT	C35-C34	3.97	1.55	1.43
13	1	502	XAT	C15-C14	3.97	1.55	1.43
13	1	502	XAT	C11-C10	3.96	1.55	1.43
14	A	4002	BCR	C16-C17	-3.94	1.31	1.43
12	4	501	LUT	C35-C34	3.94	1.55	1.43
14	F	4002	BCR	C10-C9	3.93	1.44	1.35
14	B	4006	BCR	C10-C9	3.92	1.44	1.35
16	2	609	CHL	C2C-C3C	3.90	1.40	1.36
15	A	1124	CLA	MG-ND	-3.90	1.98	2.05
12	3	501	LUT	C2-C1	3.89	1.66	1.54
12	1	501	LUT	C19-C9	3.89	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	503	BCR	C1-C6	-3.89	1.48	1.53
12	2	501	LUT	C35-C34	3.88	1.55	1.43
12	1	501	LUT	C21-C26	3.88	1.67	1.56
12	4	501	LUT	C12-C13	3.88	1.54	1.46
15	A	1116	CLA	MG-ND	-3.85	1.98	2.05
14	1	503	BCR	C30-C25	-3.84	1.48	1.53
13	2	502	XAT	C26-C27	3.84	1.57	1.50
13	4	502	XAT	C31-C30	3.83	1.55	1.43
13	4	502	XAT	C6-C7	3.83	1.57	1.50
14	F	4001	BCR	C10-C9	3.82	1.44	1.35
12	2	501	LUT	C28-C27	3.82	1.41	1.32
14	3	506	BCR	C30-C25	-3.81	1.48	1.53
13	2	502	XAT	C24-C23	3.80	1.57	1.52
12	4	501	LUT	C2-C1	3.80	1.66	1.54
13	2	502	XAT	C31-C30	3.80	1.55	1.43
12	1	501	LUT	C12-C13	3.77	1.54	1.46
14	A	4008	BCR	C10-C9	3.77	1.44	1.35
16	4	610	CHL	C2C-C3C	3.76	1.40	1.36
12	2	501	LUT	C12-C13	3.75	1.54	1.46
13	2	502	XAT	C6-C7	3.74	1.57	1.50
16	1	610	CHL	C1A-CHA	-3.73	1.35	1.40
14	F	4001	BCR	C40-C30	-3.73	1.46	1.53
18	2	804	LMG	C37-C36	-3.71	1.33	1.51
14	3	503	BCR	C30-C25	-3.70	1.49	1.53
16	4	611	CHL	C1A-CHA	-3.70	1.35	1.40
14	4	503	BCR	C30-C25	-3.70	1.49	1.53
18	2	804	LMG	C25-C24	-3.69	1.33	1.51
18	2	804	LMG	C22-C21	-3.68	1.33	1.51
18	2	804	LMG	C19-C18	-3.66	1.33	1.51
12	3	501	LUT	C8-C7	3.66	1.44	1.33
16	2	611	CHL	C1A-CHA	-3.66	1.35	1.40
15	B	1229	CLA	MG-ND	-3.64	1.98	2.05
12	3	501	LUT	C12-C13	3.63	1.53	1.46
14	3	503	BCR	C1-C6	-3.61	1.49	1.53
13	1	502	XAT	C6-C7	3.61	1.56	1.50
12	2	501	LUT	C31-C30	3.61	1.54	1.43
16	4	610	CHL	CBB-CAB	3.60	1.51	1.29
16	1	610	CHL	CBB-CAB	3.59	1.51	1.29
13	1	502	XAT	C2-C1	-3.59	1.49	1.54
15	A	1013	CLA	MG-ND	-3.56	1.98	2.05
15	A	1105	CLA	MG-ND	-3.56	1.98	2.05
15	B	1224	CLA	MG-ND	-3.56	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1126	CLA	MG-ND	-3.54	1.98	2.05
15	A	1127	CLA	MG-ND	-3.53	1.98	2.05
21	A	2001	PQN	C10-C5	-3.53	1.35	1.40
15	1	615	CLA	C2-C3	3.53	1.51	1.29
16	4	611	CHL	CBB-CAB	3.53	1.51	1.29
14	B	4004	BCR	C30-C25	-3.52	1.49	1.53
16	4	610	CHL	C1A-CHA	-3.52	1.36	1.40
14	A	4005	BCR	C10-C9	3.51	1.43	1.35
15	A	1109	CLA	MG-ND	-3.50	1.98	2.05
13	4	502	XAT	C26-C27	3.49	1.56	1.50
15	A	1113	CLA	MG-ND	-3.49	1.98	2.05
15	A	1112	CLA	MG-ND	-3.49	1.98	2.05
15	A	1118	CLA	MG-ND	-3.49	1.98	2.05
15	A	1012	CLA	MG-ND	-3.48	1.98	2.05
13	4	502	XAT	C2-C1	-3.48	1.49	1.54
16	2	613	CHL	CBB-CAB	3.48	1.51	1.29
16	2	611	CHL	CBB-CAB	3.48	1.51	1.29
15	B	1021	CLA	MG-ND	-3.48	1.98	2.05
13	2	502	XAT	C2-C1	-3.48	1.49	1.54
15	A	1122	CLA	MG-ND	-3.48	1.98	2.05
15	B	1235	CLA	MG-ND	-3.47	1.98	2.05
16	4	613	CHL	CBB-CAB	3.47	1.51	1.29
15	A	1106	CLA	MG-ND	-3.47	1.98	2.05
15	B	1222	CLA	MG-ND	-3.47	1.98	2.05
16	3	604	CHL	CBB-CAB	3.47	1.51	1.29
15	A	1107	CLA	MG-ND	-3.47	1.98	2.05
15	3	612	CLA	MG-ND	-3.47	1.98	2.05
15	B	1225	CLA	MG-ND	-3.46	1.98	2.05
15	A	1108	CLA	MG-ND	-3.46	1.98	2.05
15	B	1236	CLA	MG-ND	-3.46	1.98	2.05
15	A	1121	CLA	MG-ND	-3.46	1.98	2.05
15	A	1103	CLA	MG-ND	-3.46	1.98	2.05
15	A	1102	CLA	MG-ND	-3.45	1.98	2.05
15	J	1302	CLA	MG-ND	-3.45	1.98	2.05
15	A	1137	CLA	MG-ND	-3.45	1.98	2.05
15	1	615	CLA	C1D-ND	3.45	1.42	1.37
15	A	1104	CLA	MG-ND	-3.45	1.98	2.05
14	B	4003	BCR	C30-C25	-3.45	1.49	1.53
15	3	613	CLA	MG-ND	-3.44	1.99	2.05
15	A	1115	CLA	MG-ND	-3.44	1.99	2.05
15	A	1123	CLA	MG-ND	-3.43	1.99	2.05
15	A	1117	CLA	MG-ND	-3.43	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1138	CLA	MG-ND	-3.43	1.99	2.05
15	3	615	CLA	MG-ND	-3.43	1.99	2.05
16	2	613	CHL	C1A-CHA	-3.43	1.36	1.40
15	A	1111	CLA	MG-ND	-3.43	1.99	2.05
15	A	1128	CLA	MG-ND	-3.42	1.99	2.05
15	A	1135	CLA	MG-ND	-3.42	1.99	2.05
15	A	1120	CLA	MG-ND	-3.42	1.99	2.05
15	B	1228	CLA	MG-ND	-3.42	1.99	2.05
15	A	1101	CLA	MG-ND	-3.41	1.99	2.05
14	A	4007	BCR	C10-C9	3.41	1.43	1.35
15	A	1125	CLA	MG-ND	-3.40	1.99	2.05
15	A	1136	CLA	MG-ND	-3.40	1.99	2.05
15	A	1139	CLA	MG-ND	-3.40	1.99	2.05
15	B	1218	CLA	C4B-NB	3.40	1.42	1.37
16	3	604	CHL	C1A-CHA	-3.40	1.36	1.40
16	1	609	CHL	CBB-CAB	3.39	1.50	1.29
15	A	1110	CLA	MG-ND	-3.38	1.99	2.05
12	3	501	LUT	C7-C6	3.38	1.56	1.45
15	F	1301	CLA	MG-ND	-3.37	1.99	2.05
15	A	1131	CLA	MG-ND	-3.37	1.99	2.05
15	3	605	CLA	MG-ND	-3.35	1.99	2.05
16	2	609	CHL	CBB-CAB	3.34	1.50	1.29
15	B	1226	CLA	C1B-C2B	3.34	1.51	1.43
15	1	611	CLA	C1D-ND	3.32	1.42	1.37
13	1	502	XAT	C26-C27	3.32	1.56	1.50
14	2	503	BCR	C30-C25	-3.31	1.49	1.53
15	A	1114	CLA	MG-ND	-3.31	1.99	2.05
15	3	607	CLA	C1D-ND	3.31	1.42	1.37
14	B	4004	BCR	C1-C6	-3.28	1.49	1.53
15	A	1119	CLA	MG-ND	-3.28	1.99	2.05
15	A	1130	CLA	MG-ND	-3.28	1.99	2.05
15	3	614	CLA	C4B-NB	3.26	1.42	1.37
14	B	4002	BCR	C1-C6	-3.25	1.49	1.53
15	1	602	CLA	C1D-ND	3.25	1.42	1.37
12	4	501	LUT	C31-C30	3.25	1.53	1.43
15	2	616	CLA	C1D-ND	3.25	1.42	1.37
12	3	501	LUT	C31-C30	3.24	1.53	1.43
16	2	610	CHL	CBB-CAB	3.24	1.49	1.29
15	B	1214	CLA	C1D-ND	3.23	1.42	1.37
15	A	1116	CLA	C4B-NB	-3.23	1.33	1.37
15	B	1234	CLA	MG-ND	-3.23	1.99	2.05
15	1	613	CLA	C1D-ND	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1210	CLA	C1D-ND	3.23	1.42	1.37
15	B	1239	CLA	C1D-ND	3.22	1.42	1.37
15	B	1219	CLA	C4B-NB	3.21	1.42	1.37
15	A	1140	CLA	MG-NC	3.21	2.13	2.06
15	1	606	CLA	C1D-ND	3.21	1.42	1.37
15	F	1302	CLA	C1D-ND	3.20	1.42	1.37
15	3	609	CLA	C1D-ND	3.20	1.42	1.37
15	B	1232	CLA	C4B-NB	3.20	1.42	1.37
15	4	603	CLA	C1D-ND	3.20	1.42	1.37
15	A	1127	CLA	C1C-NC	-3.19	1.32	1.37
15	3	614	CLA	C1D-ND	3.19	1.42	1.37
15	4	607	CLA	C1D-ND	3.18	1.42	1.37
15	1	612	CLA	C1D-ND	3.18	1.42	1.37
15	B	1232	CLA	C1D-ND	3.17	1.42	1.37
14	1	503	BCR	C1-C6	-3.16	1.49	1.53
15	3	610	CLA	C1D-ND	3.16	1.42	1.37
15	B	1223	CLA	C3D-C4D	-3.16	1.37	1.44
15	B	1227	CLA	MG-ND	-3.16	1.99	2.05
15	2	602	CLA	C1D-ND	3.16	1.42	1.37
15	B	1202	CLA	C1D-ND	3.15	1.42	1.37
16	2	610	CHL	C1A-CHA	-3.15	1.36	1.40
15	A	1119	CLA	C1C-NC	-3.15	1.32	1.37
15	A	1141	CLA	C1D-ND	3.15	1.42	1.37
15	4	606	CLA	C1D-ND	3.15	1.42	1.37
15	B	1230	CLA	MG-ND	-3.14	1.99	2.05
15	B	1217	CLA	C1D-ND	3.14	1.42	1.37
16	2	613	CHL	C3A-C2A	-3.14	1.52	1.54
15	B	1218	CLA	C1D-ND	3.13	1.42	1.37
16	4	613	CHL	C1A-CHA	-3.13	1.36	1.40
15	1	605	CLA	C1D-ND	3.13	1.42	1.37
15	B	1207	CLA	C1D-ND	3.13	1.42	1.37
15	1	607	CLA	C1D-ND	3.13	1.42	1.37
15	2	606	CLA	C1D-ND	3.13	1.42	1.37
15	A	1134	CLA	MG-NC	3.12	2.13	2.06
15	4	616	CLA	C1D-ND	3.11	1.41	1.37
15	B	1212	CLA	C1D-ND	3.11	1.41	1.37
15	1	608	CLA	C1D-ND	3.10	1.41	1.37
15	3	608	CLA	C1D-ND	3.10	1.41	1.37
12	4	501	LUT	C8-C7	3.10	1.42	1.33
15	B	1234	CLA	C4B-NB	-3.10	1.33	1.37
15	3	611	CLA	C1D-ND	3.09	1.41	1.37
15	B	1215	CLA	C1D-ND	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	2	501	LUT	C8-C7	3.08	1.42	1.33
12	4	501	LUT	C7-C6	3.08	1.55	1.45
15	4	605	CLA	C1D-ND	3.08	1.41	1.37
15	4	602	CLA	C1D-ND	3.08	1.41	1.37
15	2	612	CLA	C1D-ND	3.08	1.41	1.37
12	2	501	LUT	O23-C23	-3.08	1.38	1.43
15	B	1227	CLA	C1C-NC	-3.07	1.33	1.37
15	2	602	CLA	C4B-NB	3.07	1.41	1.37
15	B	1202	CLA	C4B-NB	3.07	1.41	1.37
16	2	609	CHL	CHB-C4A	-3.07	1.34	1.38
12	4	501	LUT	C28-C27	3.07	1.39	1.32
15	4	609	CLA	C1D-ND	3.07	1.41	1.37
12	2	501	LUT	C7-C6	3.06	1.55	1.45
15	A	1113	CLA	C1C-NC	-3.05	1.33	1.37
15	2	603	CLA	C1D-ND	3.05	1.41	1.37
15	A	1013	CLA	C1C-NC	-3.05	1.33	1.37
15	4	612	CLA	C1D-ND	3.05	1.41	1.37
15	B	1201	CLA	C1D-ND	3.05	1.41	1.37
15	4	603	CLA	C4B-NB	3.04	1.41	1.37
15	A	1102	CLA	C1C-NC	-3.04	1.33	1.37
15	B	1219	CLA	C1D-ND	3.04	1.41	1.37
15	A	1139	CLA	C1C-NC	-3.03	1.33	1.37
15	B	1239	CLA	C1B-C2B	3.03	1.50	1.43
16	2	610	CHL	CHB-C4A	-3.03	1.35	1.38
15	A	1124	CLA	C4B-NB	-3.03	1.33	1.37
15	B	1227	CLA	C4B-NB	-3.03	1.33	1.37
15	4	602	CLA	C4B-NB	3.02	1.41	1.37
15	A	1113	CLA	C4B-NB	-3.02	1.33	1.37
15	B	1023	CLA	CHD-C1D	3.02	1.44	1.38
15	2	608	CLA	C1D-ND	3.02	1.41	1.37
15	A	1105	CLA	C1C-NC	-3.02	1.33	1.37
14	B	4003	BCR	C1-C6	-3.02	1.49	1.53
15	2	603	CLA	C4B-NB	3.01	1.41	1.37
12	3	501	LUT	O23-C23	-3.01	1.38	1.43
15	A	1134	CLA	CHD-C4C	3.01	1.46	1.39
15	A	1122	CLA	C1C-NC	-3.01	1.33	1.37
15	2	601	CLA	C1D-ND	3.01	1.41	1.37
16	1	609	CHL	CHB-C4A	-3.01	1.35	1.38
15	A	1102	CLA	C4B-NB	-3.01	1.33	1.37
12	1	501	LUT	C7-C6	3.00	1.55	1.45
15	2	605	CLA	C1D-ND	3.00	1.41	1.37
15	B	1226	CLA	C1D-ND	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1013	CLA	C4B-NB	-3.00	1.33	1.37
15	A	1114	CLA	C1C-NC	-3.00	1.33	1.37
15	A	1106	CLA	C1C-NC	-3.00	1.33	1.37
15	3	603	CLA	C1B-C2B	3.00	1.50	1.43
12	1	501	LUT	C28-C27	3.00	1.39	1.32
15	B	1225	CLA	C1C-NC	-2.99	1.33	1.37
15	B	1205	CLA	C1D-ND	2.99	1.41	1.37
15	A	1136	CLA	C1C-NC	-2.99	1.33	1.37
15	A	1103	CLA	C1C-NC	-2.99	1.33	1.37
16	4	613	CHL	CHB-C4A	-2.99	1.35	1.38
15	B	1228	CLA	C1C-NC	-2.99	1.33	1.37
15	B	1221	CLA	C1D-ND	2.99	1.41	1.37
15	1	605	CLA	C1B-C2B	2.98	1.50	1.43
15	3	605	CLA	C1C-NC	-2.98	1.33	1.37
15	1	601	CLA	C1D-ND	2.98	1.41	1.37
15	3	603	CLA	C1D-ND	2.98	1.41	1.37
15	B	1237	CLA	C1D-ND	2.97	1.41	1.37
13	2	502	XAT	C38-C25	2.97	1.56	1.51
15	A	1107	CLA	C1C-NC	-2.97	1.33	1.37
15	F	1301	CLA	C1C-NC	-2.97	1.33	1.37
15	A	1137	CLA	C1C-NC	-2.97	1.33	1.37
15	B	1213	CLA	C1D-ND	2.97	1.41	1.37
15	A	1138	CLA	C1C-NC	-2.97	1.33	1.37
15	A	1128	CLA	C1C-NC	-2.97	1.33	1.37
15	A	1121	CLA	C1C-NC	-2.97	1.33	1.37
16	2	613	CHL	CHB-C4A	-2.96	1.35	1.38
15	A	1122	CLA	C4B-NB	-2.96	1.34	1.37
15	4	601	CLA	C1D-ND	2.96	1.41	1.37
15	B	1230	CLA	C1C-NC	-2.96	1.33	1.37
15	A	1109	CLA	C1C-NC	-2.96	1.33	1.37
15	A	1116	CLA	C1C-NC	-2.95	1.33	1.37
15	B	1203	CLA	C1D-ND	2.95	1.41	1.37
15	A	1123	CLA	C1C-NC	-2.95	1.33	1.37
15	J	1302	CLA	C1C-NC	-2.95	1.33	1.37
15	A	1124	CLA	C1C-NC	-2.95	1.33	1.37
15	2	607	CLA	C1D-ND	2.95	1.41	1.37
15	A	1108	CLA	C1C-NC	-2.95	1.33	1.37
15	A	1112	CLA	C1C-NC	-2.95	1.33	1.37
15	A	1110	CLA	C1C-NC	-2.95	1.33	1.37
15	A	1126	CLA	C1C-NC	-2.95	1.33	1.37
15	B	1218	CLA	C3B-C4B	2.94	1.51	1.42
15	B	1204	CLA	C1D-ND	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1224	CLA	C1C-NC	-2.94	1.33	1.37
12	1	501	LUT	C8-C7	2.94	1.41	1.33
15	A	1120	CLA	C1C-NC	-2.94	1.33	1.37
15	A	1117	CLA	C1C-NC	-2.94	1.33	1.37
15	B	1206	CLA	C1D-ND	2.94	1.41	1.37
15	B	1236	CLA	C1C-NC	-2.94	1.33	1.37
15	A	1105	CLA	C4B-NB	-2.94	1.34	1.37
15	B	1235	CLA	C1C-NC	-2.94	1.33	1.37
15	A	1130	CLA	C1C-NC	-2.93	1.33	1.37
15	3	615	CLA	C1C-NC	-2.93	1.33	1.37
15	A	1135	CLA	C1C-NC	-2.93	1.33	1.37
15	A	1132	CLA	C1D-ND	2.93	1.41	1.37
20	A	1011	CL0	CHB-C4A	-2.93	1.35	1.38
15	3	607	CLA	C4B-NB	2.93	1.41	1.37
16	1	609	CHL	C2C-C3C	2.93	1.39	1.36
15	B	1021	CLA	C1C-NC	-2.93	1.33	1.37
15	B	1229	CLA	C4B-NB	-2.93	1.34	1.37
15	A	1111	CLA	C1C-NC	-2.92	1.33	1.37
12	1	501	LUT	O23-C23	-2.92	1.38	1.43
15	A	1118	CLA	C1C-NC	-2.92	1.33	1.37
16	2	611	CHL	CHB-C4A	-2.92	1.35	1.38
15	A	1127	CLA	C4B-NB	-2.92	1.34	1.37
15	B	1220	CLA	C1D-ND	2.92	1.41	1.37
15	1	603	CLA	C1D-ND	2.92	1.41	1.37
15	A	1012	CLA	C1C-NC	-2.91	1.33	1.37
15	A	1115	CLA	C1C-NC	-2.91	1.33	1.37
12	1	501	LUT	C31-C30	2.91	1.52	1.43
16	4	611	CHL	CHB-C4A	-2.91	1.35	1.38
15	B	1209	CLA	C1D-ND	2.91	1.41	1.37
15	B	1229	CLA	C1C-NC	-2.91	1.33	1.37
15	B	1234	CLA	C1C-NC	-2.91	1.33	1.37
12	4	501	LUT	O23-C23	-2.91	1.38	1.43
15	B	1222	CLA	C1C-NC	-2.90	1.33	1.37
15	1	605	CLA	C4B-NB	2.90	1.41	1.37
15	B	1022	CLA	C1C-NC	-2.90	1.33	1.37
15	B	1207	CLA	C4B-NB	2.90	1.41	1.37
15	A	1131	CLA	C1C-NC	-2.89	1.33	1.37
15	4	604	CLA	C1D-ND	2.89	1.41	1.37
15	B	1208	CLA	C1D-ND	2.88	1.41	1.37
15	A	1103	CLA	C4B-NB	-2.88	1.34	1.37
15	A	1109	CLA	C4B-NB	-2.88	1.34	1.37
15	A	1117	CLA	C4B-NB	-2.88	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	608	CLA	C4B-NB	2.88	1.41	1.37
15	1	612	CLA	C1B-C2B	2.88	1.49	1.43
15	4	607	CLA	C4B-NB	2.88	1.41	1.37
15	3	612	CLA	C1C-NC	-2.88	1.33	1.37
15	A	1133	CLA	CHD-C1D	2.88	1.44	1.38
15	B	1223	CLA	C4B-NB	-2.87	1.34	1.37
15	3	613	CLA	C1C-NC	-2.87	1.33	1.37
15	1	606	CLA	C4B-NB	2.87	1.41	1.37
15	A	1101	CLA	C1C-NC	-2.87	1.33	1.37
15	A	1125	CLA	C4B-NB	-2.87	1.34	1.37
15	B	1216	CLA	CMD-C2D	-2.87	1.44	1.50
15	F	1302	CLA	C4B-NB	2.86	1.41	1.37
15	A	1119	CLA	C4B-NB	-2.86	1.34	1.37
15	A	1139	CLA	C4B-NB	-2.86	1.34	1.37
16	4	610	CHL	CHB-C4A	-2.86	1.35	1.38
15	1	612	CLA	C4B-NB	2.86	1.41	1.37
15	1	613	CLA	C4B-NB	2.86	1.41	1.37
15	B	1218	CLA	C1B-C2B	2.85	1.49	1.43
15	3	606	CLA	C1D-ND	2.85	1.41	1.37
15	2	604	CLA	C1D-ND	2.85	1.41	1.37
15	B	1240	CLA	C1D-ND	2.85	1.41	1.37
15	A	1125	CLA	C1C-NC	-2.84	1.33	1.37
15	A	1126	CLA	C4B-NB	-2.84	1.34	1.37
15	2	608	CLA	C4B-NB	2.84	1.41	1.37
15	A	1129	CLA	C1D-ND	2.84	1.41	1.37
15	J	1302	CLA	C4B-NB	-2.84	1.34	1.37
16	1	610	CHL	C1D-C2D	2.84	1.42	1.39
15	B	1211	CLA	C1D-ND	2.84	1.41	1.37
15	A	1114	CLA	C4B-NB	-2.84	1.34	1.37
15	B	1225	CLA	C4B-NB	-2.84	1.34	1.37
15	A	1118	CLA	C4B-NB	-2.83	1.34	1.37
14	B	4001	BCR	C30-C25	-2.83	1.50	1.53
15	1	602	CLA	C4B-NB	2.83	1.41	1.37
15	B	1235	CLA	C4B-NB	-2.83	1.34	1.37
16	2	613	CHL	C1D-C2D	2.83	1.42	1.39
16	3	604	CHL	C1D-C2D	2.83	1.42	1.39
15	A	1133	CLA	CMB-C2B	-2.82	1.45	1.50
15	A	1104	CLA	C1C-NC	-2.82	1.33	1.37
15	B	1239	CLA	C4B-NB	2.82	1.41	1.37
15	3	609	CLA	C1B-C2B	2.81	1.49	1.43
15	A	1132	CLA	C1B-C2B	2.81	1.49	1.43
15	3	601	CLA	C1D-ND	2.81	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1238	CLA	C4B-NB	2.81	1.41	1.37
15	4	607	CLA	C1B-C2B	2.81	1.49	1.43
17	2	801	LHG	O7-C5	-2.80	1.40	1.46
15	A	1112	CLA	C4B-NB	-2.80	1.34	1.37
15	A	1130	CLA	C4B-NB	-2.80	1.34	1.37
15	4	606	CLA	C4B-NB	2.79	1.41	1.37
15	A	1141	CLA	C4B-NB	2.79	1.41	1.37
15	B	1209	CLA	C1B-C2B	2.79	1.49	1.43
15	A	1123	CLA	C4B-NB	-2.79	1.34	1.37
15	B	1208	CLA	C4B-NB	2.79	1.41	1.37
15	1	603	CLA	C4B-NB	2.79	1.41	1.37
16	4	613	CHL	C1D-C2D	2.79	1.42	1.39
15	A	1106	CLA	C4B-NB	-2.79	1.34	1.37
16	4	613	CHL	C1B-C2B	2.79	1.42	1.39
13	4	502	XAT	C8-C7	2.78	1.38	1.32
15	A	1136	CLA	C4B-NB	-2.78	1.34	1.37
15	A	1135	CLA	C4B-NB	-2.78	1.34	1.37
15	A	1115	CLA	C4B-NB	-2.78	1.34	1.37
15	A	1121	CLA	C4B-NB	-2.78	1.34	1.37
15	B	1212	CLA	C4B-NB	2.78	1.41	1.37
15	A	1137	CLA	C4B-NB	-2.78	1.34	1.37
15	B	1216	CLA	C1D-ND	2.78	1.41	1.37
15	1	606	CLA	C1B-C2B	2.78	1.49	1.43
15	4	616	CLA	C4B-NB	2.77	1.41	1.37
15	2	616	CLA	C4B-NB	2.77	1.41	1.37
15	2	602	CLA	C1B-C2B	2.77	1.49	1.43
15	2	606	CLA	C1B-C2B	2.77	1.49	1.43
15	A	1138	CLA	C4B-NB	-2.77	1.34	1.37
15	A	1120	CLA	C4B-NB	-2.77	1.34	1.37
15	B	1224	CLA	C4B-NB	-2.77	1.34	1.37
15	3	605	CLA	C4B-NB	-2.76	1.34	1.37
15	A	1012	CLA	C4B-NB	-2.76	1.34	1.37
15	B	1201	CLA	C4B-NB	2.76	1.41	1.37
15	B	1204	CLA	C1B-C2B	2.76	1.49	1.43
15	A	1128	CLA	C4B-NB	-2.76	1.34	1.37
15	B	1212	CLA	C1B-C2B	2.75	1.49	1.43
15	4	606	CLA	C1B-C2B	2.75	1.49	1.43
15	B	1022	CLA	C4B-NB	-2.75	1.34	1.37
15	4	609	CLA	C1B-C2B	2.75	1.49	1.43
15	B	1222	CLA	C4B-NB	-2.75	1.34	1.37
15	B	1231	CLA	C1C-NC	-2.75	1.33	1.37
15	A	1108	CLA	C4B-NB	-2.74	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	613	CLA	C1B-C2B	2.74	1.49	1.43
15	3	610	CLA	C4B-NB	2.74	1.41	1.37
15	3	611	CLA	C1B-C2B	2.74	1.49	1.43
15	B	1236	CLA	C4B-NB	-2.74	1.34	1.37
15	3	607	CLA	C1B-C2B	2.74	1.49	1.43
15	B	1220	CLA	C4B-NB	2.74	1.41	1.37
15	3	612	CLA	C4B-NB	-2.74	1.34	1.37
15	B	1205	CLA	C4B-NB	2.74	1.41	1.37
15	A	1134	CLA	C1C-C2C	2.73	1.50	1.44
15	B	1214	CLA	C4B-NB	2.73	1.41	1.37
15	3	608	CLA	C1B-C2B	2.72	1.49	1.43
15	A	1131	CLA	C4B-NB	-2.72	1.34	1.37
15	A	1140	CLA	MG-ND	-2.72	2.00	2.05
15	A	1129	CLA	CMD-C2D	-2.72	1.45	1.50
16	1	610	CHL	CHB-C4A	-2.72	1.35	1.38
12	3	501	LUT	C26-C27	2.71	1.54	1.50
15	B	1226	CLA	CMD-C2D	-2.71	1.45	1.50
15	A	1110	CLA	C4B-NB	-2.71	1.34	1.37
15	1	611	CLA	C4B-NB	2.71	1.41	1.37
15	3	615	CLA	C4B-NB	-2.71	1.34	1.37
15	B	1023	CLA	MG-NC	2.71	2.12	2.06
19	3	802	3PH	O21-C2	-2.71	1.40	1.46
15	B	1021	CLA	C4B-NB	-2.71	1.34	1.37
15	B	1022	CLA	C1C-C2C	2.70	1.50	1.44
15	A	1141	CLA	C1B-C2B	2.70	1.49	1.43
15	1	604	CLA	C1D-ND	2.70	1.41	1.37
15	B	1217	CLA	C4B-NB	2.70	1.41	1.37
15	A	1107	CLA	C4B-NB	-2.70	1.34	1.37
15	2	605	CLA	C1B-C2B	2.70	1.49	1.43
15	B	1228	CLA	C4B-NB	-2.70	1.34	1.37
15	F	1302	CLA	C1B-C2B	2.69	1.49	1.43
16	4	610	CHL	C1B-C2B	2.69	1.42	1.39
16	4	610	CHL	C1D-C2D	2.69	1.42	1.39
15	A	1111	CLA	C4B-NB	-2.69	1.34	1.37
15	3	603	CLA	C4B-NB	2.69	1.41	1.37
15	B	1237	CLA	C1B-C2B	2.68	1.49	1.43
17	B	5001	LHG	O7-C5	-2.68	1.40	1.46
15	B	1210	CLA	C4B-NB	2.68	1.41	1.37
16	3	604	CHL	C1B-C2B	2.68	1.42	1.39
12	3	501	LUT	C10-C9	2.68	1.42	1.35
16	2	611	CHL	C1B-C2B	2.68	1.42	1.39
15	4	608	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	502	XAT	C8-C7	2.68	1.38	1.32
15	3	609	CLA	C4B-NB	2.68	1.41	1.37
15	A	1129	CLA	C4B-NB	2.67	1.41	1.37
15	3	613	CLA	C4B-NB	-2.67	1.34	1.37
15	1	603	CLA	C3B-C4B	2.67	1.50	1.42
15	A	1104	CLA	C4B-NB	-2.67	1.34	1.37
15	B	1206	CLA	C4B-NB	2.66	1.41	1.37
15	B	1206	CLA	C1B-C2B	2.66	1.49	1.43
15	2	612	CLA	CMD-C2D	-2.66	1.45	1.50
15	2	601	CLA	C4B-NB	2.66	1.41	1.37
23	B	5002	DGD	O2G-C2G	-2.66	1.40	1.46
16	2	609	CHL	C1D-C2D	2.66	1.42	1.39
15	B	1238	CLA	C1D-ND	2.66	1.41	1.37
15	3	608	CLA	C4B-NB	2.65	1.41	1.37
15	B	1211	CLA	C4B-NB	2.65	1.41	1.37
12	1	501	LUT	C17-C1	2.65	1.58	1.53
15	3	610	CLA	C1B-C2B	2.64	1.49	1.43
16	4	611	CHL	C1B-C2B	2.64	1.42	1.39
15	F	1301	CLA	C4B-NB	-2.64	1.34	1.37
15	B	1213	CLA	C1B-C2B	2.64	1.49	1.43
15	A	1134	CLA	C4C-C3C	2.63	1.49	1.45
15	1	611	CLA	C1B-C2B	2.63	1.49	1.43
16	4	611	CHL	C1D-C2D	2.63	1.42	1.39
15	4	608	CLA	C1D-ND	2.63	1.41	1.37
15	B	1231	CLA	MG-ND	-2.63	2.00	2.05
15	B	1203	CLA	C1B-C2B	2.63	1.49	1.43
16	2	611	CHL	C1D-C2D	2.63	1.42	1.39
15	B	1237	CLA	C4B-NB	2.63	1.41	1.37
15	B	1217	CLA	C1B-C2B	2.63	1.49	1.43
15	A	1133	CLA	C4B-NB	-2.63	1.34	1.37
15	B	1221	CLA	CMD-C2D	-2.63	1.45	1.50
15	2	605	CLA	C4B-NB	2.63	1.41	1.37
15	B	1209	CLA	C4B-NB	2.63	1.41	1.37
15	1	607	CLA	C4B-NB	2.62	1.41	1.37
15	B	1240	CLA	C4B-NB	2.62	1.41	1.37
15	B	1215	CLA	C4B-NB	2.62	1.41	1.37
15	B	1216	CLA	MG-NB	-2.62	2.00	2.05
15	3	611	CLA	C4B-NB	2.62	1.41	1.37
15	1	604	CLA	C4B-NB	2.62	1.41	1.37
15	2	606	CLA	C4B-NB	2.62	1.41	1.37
15	2	608	CLA	C1B-C2B	2.62	1.49	1.43
15	3	606	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1208	CLA	C1B-C2B	2.61	1.49	1.43
15	B	1231	CLA	C4B-NB	-2.61	1.34	1.37
15	4	616	CLA	C1B-C2B	2.61	1.49	1.43
15	1	604	CLA	C1B-C2B	2.60	1.49	1.43
15	B	1215	CLA	C1B-C2B	2.60	1.49	1.43
15	B	1240	CLA	C1B-C2B	2.60	1.49	1.43
15	1	608	CLA	C1B-C2B	2.60	1.49	1.43
12	2	501	LUT	C17-C1	2.60	1.58	1.53
15	2	607	CLA	C4B-NB	2.59	1.41	1.37
15	1	602	CLA	C3B-C4B	2.59	1.50	1.42
15	3	606	CLA	C4B-NB	2.59	1.41	1.37
15	A	1134	CLA	CHC-C1C	2.59	1.43	1.38
15	B	1204	CLA	C4B-NB	2.59	1.41	1.37
15	4	608	CLA	CMD-C2D	-2.59	1.45	1.50
13	1	502	XAT	C24-C23	2.59	1.56	1.52
16	2	610	CHL	C1D-C2D	2.58	1.42	1.39
15	4	608	CLA	C4B-NB	2.58	1.41	1.37
16	3	604	CHL	CHB-C4A	-2.58	1.35	1.38
15	4	612	CLA	C1B-C2B	2.57	1.49	1.43
16	3	604	CHL	C3A-C2A	-2.57	1.52	1.54
15	4	605	CLA	C1B-C2B	2.57	1.49	1.43
15	3	614	CLA	C3B-C4B	2.56	1.50	1.42
16	1	610	CHL	C2C-C3C	2.55	1.38	1.36
15	B	1023	CLA	C4B-NB	-2.55	1.34	1.37
13	1	502	XAT	C18-C5	2.55	1.55	1.51
15	2	604	CLA	C4B-NB	2.55	1.41	1.37
15	B	1230	CLA	C4B-NB	-2.55	1.34	1.37
16	1	610	CHL	C1B-C2B	2.55	1.42	1.39
15	A	1101	CLA	C4B-NB	-2.55	1.34	1.37
15	1	615	CLA	C4B-NB	2.54	1.41	1.37
15	B	1240	CLA	MG-NB	-2.54	2.00	2.05
15	2	603	CLA	C1B-C2B	2.54	1.49	1.43
15	B	1221	CLA	C4B-NB	2.54	1.41	1.37
15	2	616	CLA	C1B-C2B	2.54	1.49	1.43
15	B	1214	CLA	CMB-C2B	-2.54	1.45	1.50
15	B	1232	CLA	C1B-C2B	2.54	1.49	1.43
15	B	1237	CLA	CMD-C2D	-2.53	1.45	1.50
15	1	615	CLA	C1B-C2B	2.53	1.49	1.43
15	B	1213	CLA	C4B-NB	2.53	1.41	1.37
15	4	604	CLA	C4B-NB	2.53	1.41	1.37
15	B	1239	CLA	CMD-C2D	-2.53	1.45	1.50
15	1	607	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	601	CLA	CMB-C2B	-2.52	1.45	1.50
15	1	601	CLA	C1B-C2B	2.52	1.49	1.43
21	A	2001	PQN	C3-C2	-2.52	1.30	1.35
15	2	612	CLA	C1B-C2B	2.52	1.49	1.43
15	B	1207	CLA	C1B-C2B	2.52	1.49	1.43
15	A	1134	CLA	C4B-NB	-2.52	1.34	1.37
15	2	607	CLA	C1B-C2B	2.51	1.49	1.43
15	B	1205	CLA	CMD-C2D	-2.51	1.45	1.50
15	B	1210	CLA	C1B-C2B	2.51	1.49	1.43
15	4	612	CLA	C4B-NB	2.51	1.41	1.37
15	B	1226	CLA	C4B-NB	2.51	1.41	1.37
15	2	604	CLA	C1B-C2B	2.51	1.49	1.43
15	4	602	CLA	C3B-C4B	2.50	1.50	1.42
16	1	609	CHL	C1B-C2B	2.50	1.42	1.39
15	2	612	CLA	C4B-NB	2.50	1.41	1.37
15	1	603	CLA	C1B-C2B	2.49	1.49	1.43
15	B	1202	CLA	CMD-C2D	-2.49	1.45	1.50
15	4	601	CLA	C4B-NB	2.49	1.41	1.37
15	4	607	CLA	CMD-C2D	-2.49	1.45	1.50
15	4	605	CLA	C4B-NB	2.49	1.41	1.37
15	A	1125	CLA	MG-NC	2.49	2.12	2.06
15	B	1211	CLA	CMD-C2D	-2.49	1.45	1.50
15	A	1140	CLA	C1C-C2C	2.49	1.49	1.44
15	2	604	CLA	CMD-C2D	-2.48	1.45	1.50
15	1	602	CLA	CMD-C2D	-2.48	1.45	1.50
15	B	1232	CLA	C3B-C4B	2.48	1.50	1.42
12	4	501	LUT	C17-C1	2.48	1.58	1.53
15	B	1205	CLA	C3B-C4B	2.48	1.49	1.42
16	1	609	CHL	C1D-C2D	2.47	1.42	1.39
15	4	605	CLA	CMD-C2D	-2.47	1.45	1.50
15	B	1219	CLA	C1B-C2B	2.47	1.48	1.43
15	2	603	CLA	CMD-C2D	-2.47	1.45	1.50
15	B	1202	CLA	C1B-C2B	2.47	1.48	1.43
15	A	1134	CLA	C1A-CHA	2.47	1.53	1.43
15	B	1223	CLA	C1C-NC	-2.46	1.34	1.37
16	2	610	CHL	C1B-C2B	2.46	1.42	1.39
15	B	1216	CLA	C4B-NB	2.46	1.41	1.37
15	2	616	CLA	MG-NB	-2.46	2.00	2.05
15	B	1215	CLA	CMD-C2D	-2.46	1.45	1.50
15	B	1238	CLA	C3B-C4B	2.46	1.49	1.42
15	2	605	CLA	CMB-C2B	-2.46	1.45	1.50
15	B	1220	CLA	C1B-C2B	2.46	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1022	CLA	CHC-C1C	2.45	1.43	1.38
18	2	803	LMG	O7-C8	-2.45	1.40	1.46
15	1	608	CLA	CMD-C2D	-2.45	1.45	1.50
15	B	1203	CLA	C4B-NB	2.45	1.41	1.37
15	4	601	CLA	CMD-C2D	-2.45	1.45	1.50
18	4	801	LMG	O8-C9	-2.45	1.39	1.45
15	4	604	CLA	CMD-C2D	-2.45	1.45	1.50
15	2	603	CLA	C3B-C4B	2.45	1.49	1.42
15	2	607	CLA	CMB-C2B	-2.44	1.45	1.50
15	3	603	CLA	CMD-C2D	-2.44	1.45	1.50
15	4	608	CLA	MG-NB	-2.44	2.00	2.05
16	2	613	CHL	C1B-C2B	2.44	1.42	1.39
15	3	611	CLA	CMD-C2D	-2.44	1.45	1.50
15	1	604	CLA	CMD-C2D	-2.44	1.45	1.50
15	4	616	CLA	CMD-C2D	-2.44	1.45	1.50
15	4	606	CLA	MG-NB	-2.44	2.01	2.05
15	B	1238	CLA	CMD-C2D	-2.43	1.45	1.50
15	B	1201	CLA	CMD-C2D	-2.43	1.45	1.50
15	B	1240	CLA	CMD-C2D	-2.43	1.45	1.50
16	2	609	CHL	C1B-C2B	2.43	1.42	1.39
15	1	602	CLA	C1B-C2B	2.43	1.48	1.43
15	3	608	CLA	CMD-C2D	-2.43	1.45	1.50
18	4	801	LMG	O7-C8	-2.43	1.40	1.46
15	2	602	CLA	CMD-C2D	-2.42	1.45	1.50
15	3	603	CLA	CMB-C2B	-2.42	1.45	1.50
15	B	1216	CLA	CMC-C2C	-2.42	1.45	1.50
15	3	601	CLA	C3B-C4B	2.42	1.49	1.42
15	4	605	CLA	MG-NB	-2.42	2.01	2.05
13	4	502	XAT	C19-C9	2.42	1.55	1.50
15	B	1215	CLA	C3B-C4B	2.42	1.49	1.42
15	4	602	CLA	CMD-C2D	-2.42	1.45	1.50
13	4	502	XAT	C24-C23	2.42	1.55	1.52
15	A	1133	CLA	MG-NC	2.42	2.12	2.06
15	4	612	CLA	CMD-C2D	-2.42	1.45	1.50
15	B	1205	CLA	C1B-C2B	2.42	1.48	1.43
15	2	603	CLA	CMB-C2B	-2.42	1.45	1.50
15	A	1129	CLA	C1B-C2B	2.41	1.48	1.43
15	2	601	CLA	C3B-C4B	2.41	1.49	1.42
15	4	604	CLA	C1B-C2B	2.41	1.48	1.43
15	B	1216	CLA	CMB-C2B	-2.41	1.45	1.50
15	B	1023	CLA	C3D-C4D	-2.41	1.38	1.44
15	4	603	CLA	CMB-C2B	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1209	CLA	CMD-C2D	-2.41	1.45	1.50
15	B	1238	CLA	C1B-C2B	2.41	1.48	1.43
15	4	605	CLA	CMB-C2B	-2.41	1.45	1.50
15	3	601	CLA	C4B-NB	2.41	1.41	1.37
12	2	501	LUT	C20-C13	2.40	1.55	1.50
15	B	1211	CLA	C1B-C2B	2.40	1.48	1.43
15	2	604	CLA	MG-NB	-2.40	2.01	2.05
19	3	802	3PH	O31-C31	2.40	1.40	1.33
15	2	601	CLA	C1B-C2B	2.40	1.48	1.43
15	3	610	CLA	CMD-C2D	-2.40	1.45	1.50
15	B	1217	CLA	CMD-C2D	-2.40	1.45	1.50
15	B	1201	CLA	CMB-C2B	-2.40	1.45	1.50
15	B	1203	CLA	CMD-C2D	-2.40	1.45	1.50
13	1	502	XAT	C19-C9	2.40	1.55	1.50
15	2	607	CLA	CMD-C2D	-2.40	1.45	1.50
15	4	602	CLA	C1B-C2B	2.40	1.48	1.43
15	4	603	CLA	C3B-C4B	2.40	1.49	1.42
15	A	1134	CLA	C1C-NC	-2.40	1.34	1.37
15	B	1210	CLA	CMD-C2D	-2.39	1.45	1.50
15	3	609	CLA	CMB-C2B	-2.39	1.45	1.50
15	4	609	CLA	CMD-C2D	-2.39	1.45	1.50
15	2	602	CLA	C3B-C4B	2.39	1.49	1.42
15	B	1202	CLA	CHC-C1C	2.39	1.43	1.38
15	3	614	CLA	CMB-C2B	-2.39	1.45	1.50
15	3	601	CLA	CHC-C1C	2.39	1.43	1.38
15	B	1211	CLA	CMB-C2B	-2.39	1.45	1.50
15	B	1219	CLA	CMB-C2B	-2.39	1.45	1.50
15	3	601	CLA	C1B-C2B	2.39	1.48	1.43
15	3	601	CLA	CMD-C2D	-2.39	1.45	1.50
15	A	1132	CLA	CMD-C2D	-2.39	1.45	1.50
18	2	804	LMG	C40-C39	-2.38	1.33	1.50
15	1	604	CLA	MG-NB	-2.38	2.01	2.05
15	A	1132	CLA	C4B-NB	2.38	1.41	1.37
15	B	1208	CLA	CMB-C2B	-2.38	1.45	1.50
15	B	1201	CLA	CHC-C1C	2.38	1.43	1.38
15	B	1210	CLA	MG-NB	-2.38	2.01	2.05
15	1	612	CLA	C3B-C4B	2.38	1.49	1.42
15	A	1125	CLA	C1C-C2C	2.37	1.49	1.44
15	2	606	CLA	CMD-C2D	-2.37	1.45	1.50
15	B	1208	CLA	CMD-C2D	-2.37	1.45	1.50
15	B	1221	CLA	C1B-C2B	2.37	1.48	1.43
15	B	1212	CLA	CMB-C2B	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	605	CLA	MG-NB	-2.37	2.01	2.05
15	B	1232	CLA	CMD-C2D	-2.37	1.45	1.50
15	B	1204	CLA	CMD-C2D	-2.36	1.45	1.50
15	3	614	CLA	CMC-C2C	-2.36	1.45	1.50
15	1	608	CLA	MG-NB	-2.36	2.01	2.05
15	2	608	CLA	CMD-C2D	-2.36	1.45	1.50
15	B	1220	CLA	CMD-C2D	-2.36	1.45	1.50
15	B	1216	CLA	C1B-C2B	2.36	1.48	1.43
15	B	1218	CLA	CMD-C2D	-2.36	1.45	1.50
16	4	613	CHL	C2C-C3C	2.36	1.38	1.36
15	1	601	CLA	MG-NB	-2.35	2.01	2.05
13	4	502	XAT	C38-C25	2.35	1.55	1.51
16	2	613	CHL	C2C-C3C	2.35	1.38	1.36
15	2	607	CLA	MG-NB	-2.35	2.01	2.05
15	B	1220	CLA	CMB-C2B	-2.35	1.46	1.50
12	2	501	LUT	C31-C32	2.34	1.40	1.34
15	1	615	CLA	MG-NB	-2.34	2.01	2.05
15	F	1302	CLA	CMD-C2D	-2.34	1.46	1.50
15	4	603	CLA	C1B-C2B	2.34	1.48	1.43
14	A	4007	BCR	C1-C6	-2.34	1.50	1.53
15	3	611	CLA	CMB-C2B	-2.34	1.46	1.50
15	B	1202	CLA	CMB-C2B	-2.34	1.46	1.50
15	1	606	CLA	CMD-C2D	-2.33	1.46	1.50
15	4	604	CLA	CMC-C2C	-2.33	1.46	1.50
15	B	1214	CLA	CMD-C2D	-2.33	1.46	1.50
15	A	1116	CLA	CHD-C1D	2.33	1.42	1.38
14	A	4005	BCR	C12-C13	-2.33	1.41	1.46
15	B	1237	CLA	MG-NB	-2.33	2.01	2.05
15	B	1208	CLA	MG-NB	-2.33	2.01	2.05
14	A	4008	BCR	C1-C6	-2.33	1.50	1.53
15	B	1217	CLA	CMB-C2B	-2.33	1.46	1.50
15	B	1022	CLA	C3D-C4D	-2.33	1.39	1.44
15	1	611	CLA	C3B-C4B	2.33	1.49	1.42
15	1	601	CLA	CMD-C2D	-2.32	1.46	1.50
15	A	1127	CLA	C3D-C4D	-2.32	1.39	1.44
16	2	610	CHL	C2C-C3C	2.32	1.38	1.36
15	A	1129	CLA	CMB-C2B	-2.32	1.46	1.50
15	B	1213	CLA	MG-NB	-2.32	2.01	2.05
15	4	609	CLA	MG-NB	-2.32	2.01	2.05
15	A	1141	CLA	CMD-C2D	-2.32	1.46	1.50
15	B	1207	CLA	C3B-C4B	2.32	1.49	1.42
15	1	601	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	601	CLA	C3B-C4B	2.31	1.49	1.42
15	B	1202	CLA	C3B-C4B	2.31	1.49	1.42
15	A	1129	CLA	MG-NB	-2.31	2.01	2.05
15	3	607	CLA	CMD-C2D	-2.31	1.46	1.50
15	B	1237	CLA	CMB-C2B	-2.31	1.46	1.50
15	3	608	CLA	MG-NB	-2.31	2.01	2.05
15	B	1219	CLA	CMD-C2D	-2.31	1.46	1.50
15	B	1201	CLA	C1B-C2B	2.31	1.48	1.43
15	4	607	CLA	CMC-C2C	-2.31	1.46	1.50
15	2	601	CLA	CHC-C1C	2.30	1.43	1.38
15	B	1217	CLA	MG-NB	-2.30	2.01	2.05
14	F	4001	BCR	C12-C13	-2.30	1.41	1.46
15	4	603	CLA	CMC-C2C	-2.30	1.46	1.50
15	A	1129	CLA	CMC-C2C	-2.30	1.46	1.50
15	1	601	CLA	C3B-C4B	2.30	1.49	1.42
15	B	1226	CLA	CMC-C2C	-2.30	1.46	1.50
15	B	1221	CLA	MG-NB	-2.30	2.01	2.05
15	3	601	CLA	CMB-C2B	-2.30	1.46	1.50
15	3	606	CLA	MG-NB	-2.30	2.01	2.05
15	A	1141	CLA	CMB-C2B	-2.30	1.46	1.50
15	B	1212	CLA	CMD-C2D	-2.30	1.46	1.50
15	A	1141	CLA	MG-NB	-2.30	2.01	2.05
15	3	606	CLA	CMD-C2D	-2.29	1.46	1.50
15	4	604	CLA	CHC-C1C	2.29	1.43	1.38
15	1	607	CLA	C3B-C4B	2.29	1.49	1.42
15	B	1219	CLA	C3B-C4B	2.29	1.49	1.42
15	3	601	CLA	MG-NB	-2.29	2.01	2.05
15	B	1211	CLA	MG-NB	-2.29	2.01	2.05
15	1	604	CLA	CMB-C2B	-2.29	1.46	1.50
15	B	1238	CLA	CMB-C2B	-2.29	1.46	1.50
12	4	501	LUT	C11-C12	2.29	1.40	1.34
15	4	606	CLA	CMC-C2C	-2.29	1.46	1.50
15	B	1239	CLA	CMB-C2B	-2.28	1.46	1.50
15	B	1206	CLA	MG-NB	-2.28	2.01	2.05
15	4	602	CLA	CMB-C2B	-2.28	1.46	1.50
15	2	605	CLA	CMD-C2D	-2.28	1.46	1.50
15	B	1023	CLA	C1C-NC	-2.28	1.34	1.37
15	1	605	CLA	CMD-C2D	-2.28	1.46	1.50
15	A	1116	CLA	MG-NC	2.28	2.11	2.06
15	4	601	CLA	MG-NB	-2.28	2.01	2.05
15	3	606	CLA	CHC-C1C	2.28	1.43	1.38
15	B	1204	CLA	CMB-C2B	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1203	CLA	CMB-C2B	-2.28	1.46	1.50
15	B	1201	CLA	MG-NB	-2.28	2.01	2.05
15	B	1221	CLA	C3B-C4B	2.28	1.49	1.42
15	B	1232	CLA	CMB-C2B	-2.27	1.46	1.50
13	1	502	XAT	C38-C25	2.27	1.55	1.51
15	B	1210	CLA	CMB-C2B	-2.27	1.46	1.50
15	3	606	CLA	C3B-C4B	2.27	1.49	1.42
15	B	1215	CLA	CMC-C2C	-2.27	1.46	1.50
15	A	1141	CLA	CMC-C2C	-2.27	1.46	1.50
15	A	1132	CLA	CHC-C1C	2.27	1.43	1.38
14	F	4001	BCR	C1-C6	-2.26	1.50	1.53
15	1	613	CLA	CHC-C1C	2.26	1.43	1.38
18	B	5003	LMG	O1-C1	2.26	1.44	1.40
15	1	607	CLA	CMD-C2D	-2.26	1.46	1.50
15	B	1203	CLA	CMC-C2C	-2.26	1.46	1.50
15	2	601	CLA	CMB-C2B	-2.26	1.46	1.50
15	B	1209	CLA	MG-NB	-2.26	2.01	2.05
15	B	1216	CLA	MG-ND	-2.26	2.01	2.05
15	1	606	CLA	C3B-C4B	2.26	1.49	1.42
12	3	501	LUT	C20-C13	2.26	1.55	1.50
15	B	1205	CLA	CMB-C2B	-2.26	1.46	1.50
15	B	1219	CLA	MG-NB	-2.26	2.01	2.05
15	4	609	CLA	C4B-NB	2.26	1.40	1.37
15	B	1201	CLA	C3B-C4B	2.26	1.49	1.42
15	2	601	CLA	MG-NB	-2.26	2.01	2.05
15	4	606	CLA	CMD-C2D	-2.25	1.46	1.50
15	4	609	CLA	CMC-C2C	-2.25	1.46	1.50
15	B	1220	CLA	CHC-C1C	2.25	1.43	1.38
15	2	604	CLA	CMB-C2B	-2.25	1.46	1.50
15	4	612	CLA	C3B-C4B	2.25	1.49	1.42
15	2	612	CLA	MG-NB	-2.25	2.01	2.05
15	B	1220	CLA	CMC-C2C	-2.25	1.46	1.50
15	3	614	CLA	CMD-C2D	-2.25	1.46	1.50
15	1	605	CLA	CMB-C2B	-2.25	1.46	1.50
16	4	610	CHL	CHA-CBD	2.25	1.54	1.51
15	A	1133	CLA	C3B-C2B	-2.25	1.33	1.41
15	2	616	CLA	CMB-C2B	-2.25	1.46	1.50
15	B	1220	CLA	MG-NB	-2.25	2.01	2.05
15	1	603	CLA	CHC-C1C	2.25	1.43	1.38
15	B	1210	CLA	CMC-C2C	-2.24	1.46	1.50
15	B	1213	CLA	CMD-C2D	-2.24	1.46	1.50
13	1	502	XAT	C8-C7	2.24	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1104	CLA	C1C-C2C	2.24	1.49	1.44
15	A	1140	CLA	CHB-C4A	2.24	1.43	1.37
15	2	606	CLA	CMB-C2B	-2.24	1.46	1.50
15	1	603	CLA	CMD-C2D	-2.24	1.46	1.50
12	1	501	LUT	C11-C12	2.23	1.40	1.34
15	A	1118	CLA	MG-NC	2.23	2.11	2.06
15	3	608	CLA	C3B-C4B	2.23	1.49	1.42
15	B	1210	CLA	C3B-C4B	2.23	1.49	1.42
15	B	1022	CLA	MG-NC	2.23	2.11	2.06
15	2	606	CLA	MG-NB	-2.23	2.01	2.05
15	2	616	CLA	CMD-C2D	-2.23	1.46	1.50
15	B	1214	CLA	C1B-C2B	2.23	1.48	1.43
15	3	610	CLA	MG-NB	-2.23	2.01	2.05
15	B	1240	CLA	CMB-C2B	-2.23	1.46	1.50
15	B	1211	CLA	CHC-C1C	2.23	1.43	1.38
15	B	1217	CLA	CMC-C2C	-2.23	1.46	1.50
15	1	606	CLA	CHC-C1C	2.22	1.42	1.38
15	1	613	CLA	C3B-C4B	2.22	1.49	1.42
15	2	608	CLA	C3B-C4B	2.22	1.49	1.42
14	A	4005	BCR	C1-C6	-2.22	1.50	1.53
15	1	607	CLA	MG-NB	-2.22	2.01	2.05
15	2	612	CLA	CHC-C1C	2.22	1.42	1.38
15	A	1132	CLA	MG-NB	-2.22	2.01	2.05
15	3	614	CLA	C1B-C2B	2.22	1.48	1.43
15	3	609	CLA	CMD-C2D	-2.22	1.46	1.50
15	F	1302	CLA	C3B-C4B	2.22	1.49	1.42
15	B	1212	CLA	MG-NB	-2.21	2.01	2.05
15	3	611	CLA	CMC-C2C	-2.21	1.46	1.50
15	A	1140	CLA	C1A-CHA	2.21	1.52	1.43
15	1	607	CLA	CMB-C2B	-2.21	1.46	1.50
15	1	601	CLA	C4B-NB	2.21	1.40	1.37
15	4	616	CLA	MG-NB	-2.21	2.01	2.05
15	B	1220	CLA	C3B-C4B	2.21	1.49	1.42
15	B	1232	CLA	CMC-C2C	-2.20	1.46	1.50
15	4	608	CLA	CMB-C2B	-2.20	1.46	1.50
15	B	1206	CLA	CMC-C2C	-2.20	1.46	1.50
15	1	611	CLA	CMD-C2D	-2.20	1.46	1.50
15	2	602	CLA	CMB-C2B	-2.20	1.46	1.50
15	1	606	CLA	MG-NB	-2.20	2.01	2.05
15	B	1238	CLA	MG-NB	-2.20	2.01	2.05
15	A	1116	CLA	C3D-C4D	-2.20	1.39	1.44
15	B	1221	CLA	CMC-C2C	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1209	CLA	CMB-C2B	-2.19	1.46	1.50
15	B	1207	CLA	CMB-C2B	-2.19	1.46	1.50
15	2	606	CLA	C3B-C4B	2.19	1.49	1.42
15	4	612	CLA	MG-NB	-2.19	2.01	2.05
15	2	601	CLA	CMC-C2C	-2.19	1.46	1.50
15	B	1206	CLA	CMB-C2B	-2.19	1.46	1.50
15	B	1214	CLA	CMC-C2C	-2.19	1.46	1.50
15	4	603	CLA	CMD-C2D	-2.19	1.46	1.50
15	A	1119	CLA	C1C-C2C	2.19	1.49	1.44
16	2	610	CHL	CHA-CBD	2.19	1.54	1.51
13	2	502	XAT	C39-C29	2.18	1.55	1.50
15	B	1215	CLA	MG-NB	-2.18	2.01	2.05
15	4	609	CLA	CMB-C2B	-2.18	1.46	1.50
15	B	1206	CLA	CMD-C2D	-2.18	1.46	1.50
15	B	1211	CLA	C3B-C4B	2.18	1.49	1.42
14	3	506	BCR	C33-C5	-2.18	1.47	1.50
15	3	607	CLA	C3B-C4B	2.18	1.49	1.42
15	4	604	CLA	CMB-C2B	-2.18	1.46	1.50
15	B	1213	CLA	CMB-C2B	-2.18	1.46	1.50
15	4	601	CLA	CMC-C2C	-2.18	1.46	1.50
15	B	1201	CLA	CMC-C2C	-2.18	1.46	1.50
15	B	1203	CLA	MG-NB	-2.18	2.01	2.05
19	3	802	3PH	O31-C3	-2.18	1.40	1.45
15	4	616	CLA	CMB-C2B	-2.18	1.46	1.50
15	B	1207	CLA	CHC-C1C	2.18	1.42	1.38
15	B	1204	CLA	MG-NB	-2.18	2.01	2.05
15	F	1302	CLA	CMC-C2C	-2.17	1.46	1.50
15	4	604	CLA	C3B-C4B	2.17	1.49	1.42
15	2	608	CLA	CMB-C2B	-2.17	1.46	1.50
15	4	601	CLA	C1B-C2B	2.17	1.48	1.43
15	F	1302	CLA	MG-NB	-2.17	2.01	2.05
15	4	606	CLA	CMB-C2B	-2.17	1.46	1.50
14	2	503	BCR	C33-C5	-2.17	1.47	1.50
15	2	616	CLA	C3B-C4B	2.17	1.49	1.42
15	2	601	CLA	CMD-C2D	-2.17	1.46	1.50
15	3	603	CLA	CMC-C2C	-2.17	1.46	1.50
15	B	1203	CLA	C3B-C4B	2.17	1.49	1.42
15	4	604	CLA	MG-NB	-2.17	2.01	2.05
15	B	1226	CLA	C3B-C4B	2.17	1.49	1.42
15	4	612	CLA	CHC-C1C	2.17	1.42	1.38
15	B	1204	CLA	CMC-C2C	-2.17	1.46	1.50
15	2	608	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1218	CLA	CMC-C2C	-2.16	1.46	1.50
15	3	610	CLA	CMC-C2C	-2.16	1.46	1.50
15	A	1124	CLA	C1C-C2C	2.16	1.48	1.44
15	4	602	CLA	MG-NB	-2.16	2.01	2.05
15	2	612	CLA	CMB-C2B	-2.16	1.46	1.50
15	B	1237	CLA	C3B-C4B	2.16	1.49	1.42
12	4	501	LUT	C26-C27	2.16	1.53	1.50
15	A	1118	CLA	C1A-CHA	2.16	1.52	1.43
15	2	603	CLA	CMC-C2C	-2.16	1.46	1.50
15	3	610	CLA	CMB-C2B	-2.16	1.46	1.50
15	B	1228	CLA	C1C-C2C	2.16	1.48	1.44
15	F	1302	CLA	CMB-C2B	-2.16	1.46	1.50
12	2	501	LUT	C10-C9	2.16	1.40	1.35
15	4	601	CLA	CHC-C1C	2.16	1.42	1.38
15	3	611	CLA	MG-NB	-2.16	2.01	2.05
15	2	607	CLA	C3B-C4B	2.16	1.49	1.42
15	4	607	CLA	C3B-C4B	2.16	1.49	1.42
15	1	605	CLA	MG-NB	-2.15	2.01	2.05
15	4	608	CLA	CHC-C1C	2.15	1.42	1.38
15	4	607	CLA	CMB-C2B	-2.15	1.46	1.50
15	A	1140	CLA	C1C-NC	-2.15	1.34	1.37
15	3	603	CLA	MG-NB	-2.15	2.01	2.05
16	3	604	CHL	C3B-C2B	-2.15	1.37	1.40
15	2	616	CLA	CHC-C1C	2.15	1.42	1.38
15	1	606	CLA	CMB-C2B	-2.15	1.46	1.50
15	B	1205	CLA	CMC-C2C	-2.15	1.46	1.50
15	B	1206	CLA	C3B-C4B	2.15	1.49	1.42
15	B	1214	CLA	C3B-C4B	2.15	1.49	1.42
15	2	604	CLA	CHC-C1C	2.15	1.42	1.38
15	3	613	CLA	C1C-C2C	2.15	1.48	1.44
15	3	609	CLA	MG-NB	-2.15	2.01	2.05
15	B	1215	CLA	CMB-C2B	-2.15	1.46	1.50
15	B	1221	CLA	C1B-NB	-2.15	1.35	1.37
15	1	611	CLA	CMB-C2B	-2.15	1.46	1.50
15	B	1227	CLA	C3D-C4D	-2.14	1.39	1.44
15	B	1221	CLA	CMB-C2B	-2.14	1.46	1.50
15	B	1202	CLA	CMC-C2C	-2.14	1.46	1.50
15	1	611	CLA	MG-NB	-2.14	2.01	2.05
15	1	605	CLA	CMC-C2C	-2.14	1.46	1.50
15	B	1210	CLA	CHC-C1C	2.14	1.42	1.38
15	1	601	CLA	CMB-C2B	-2.14	1.46	1.50
15	2	604	CLA	C3B-C4B	2.14	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	608	CLA	CHC-C1C	2.14	1.42	1.38
15	1	611	CLA	CHC-C1C	2.14	1.42	1.38
15	B	1240	CLA	C3B-C4B	2.14	1.49	1.42
15	B	1239	CLA	CMC-C2C	-2.14	1.46	1.50
15	1	602	CLA	MG-NB	-2.14	2.01	2.05
15	A	1137	CLA	C1C-C2C	2.13	1.48	1.44
15	B	1211	CLA	CMC-C2C	-2.13	1.46	1.50
15	B	1237	CLA	CHC-C1C	2.13	1.42	1.38
15	4	616	CLA	CHC-C1C	2.13	1.42	1.38
15	B	1023	CLA	C1A-CHA	2.13	1.51	1.43
15	A	1130	CLA	C1C-C2C	2.13	1.48	1.44
19	3	802	3PH	O21-C21	2.13	1.40	1.34
16	4	611	CHL	CHA-CBD	2.13	1.54	1.51
15	B	1217	CLA	C3B-C4B	2.13	1.48	1.42
15	B	1214	CLA	MG-NB	-2.13	2.01	2.05
14	A	4008	BCR	C12-C13	-2.13	1.41	1.46
15	1	608	CLA	CMB-C2B	-2.13	1.46	1.50
15	B	1212	CLA	CMC-C2C	-2.13	1.46	1.50
15	4	607	CLA	MG-NB	-2.13	2.01	2.05
15	1	602	CLA	CMB-C2B	-2.12	1.46	1.50
13	1	502	XAT	C39-C29	2.12	1.55	1.50
15	A	1012	CLA	C1C-C2C	2.12	1.48	1.44
15	B	1219	CLA	CHC-C1C	2.12	1.42	1.38
15	3	607	CLA	CMB-C2B	-2.12	1.46	1.50
15	B	1022	CLA	CHD-C1D	2.12	1.42	1.38
14	3	503	BCR	C33-C5	-2.12	1.47	1.50
15	1	613	CLA	CMB-C2B	-2.12	1.46	1.50
15	1	613	CLA	MG-NB	-2.12	2.01	2.05
15	2	608	CLA	MG-NB	-2.12	2.01	2.05
15	A	1121	CLA	C1C-C2C	2.12	1.48	1.44
15	B	1236	CLA	C1C-C2C	2.12	1.48	1.44
15	3	615	CLA	C1C-C2C	2.12	1.48	1.44
15	1	603	CLA	CMB-C2B	-2.12	1.46	1.50
15	B	1234	CLA	CHD-C1D	2.12	1.42	1.38
15	B	1209	CLA	C3B-C4B	2.11	1.48	1.42
15	3	614	CLA	MG-NB	-2.11	2.01	2.05
13	3	502	XAT	C2-C1	-2.11	1.51	1.54
15	B	1240	CLA	CHC-C1C	2.11	1.42	1.38
15	B	1234	CLA	C3D-C4D	-2.11	1.39	1.44
15	A	1129	CLA	MG-ND	-2.11	2.01	2.05
15	B	1213	CLA	C3B-C4B	2.11	1.48	1.42
15	1	615	CLA	C3B-C4B	2.11	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1228	CLA	C3D-C4D	-2.11	1.39	1.44
15	4	616	CLA	C3B-C4B	2.11	1.48	1.42
15	A	1141	CLA	C3B-C4B	2.11	1.48	1.42
15	1	615	CLA	CHC-C1C	2.11	1.42	1.38
15	1	612	CLA	CMB-C2B	-2.11	1.46	1.50
15	4	603	CLA	MG-NB	-2.11	2.01	2.05
15	J	1302	CLA	C1C-C2C	2.11	1.48	1.44
15	1	604	CLA	CHC-C1C	2.11	1.42	1.38
14	4	503	BCR	C38-C26	-2.11	1.47	1.50
15	3	611	CLA	C3B-C4B	2.10	1.48	1.42
15	4	612	CLA	CMB-C2B	-2.10	1.46	1.50
15	3	607	CLA	MG-NB	-2.10	2.01	2.05
15	A	1106	CLA	C1C-C2C	2.10	1.48	1.44
15	3	610	CLA	C3B-C4B	2.10	1.48	1.42
15	B	1207	CLA	CMD-C2D	-2.10	1.46	1.50
15	3	601	CLA	CMC-C2C	-2.10	1.46	1.50
13	1	502	XAT	C40-C33	2.10	1.55	1.50
15	B	1214	CLA	CHC-C1C	2.10	1.42	1.38
15	A	1104	CLA	CHC-C1C	2.10	1.42	1.38
15	2	606	CLA	CMC-C2C	-2.09	1.46	1.50
15	A	1120	CLA	C1C-C2C	2.09	1.48	1.44
16	2	611	CHL	C2C-C3C	2.09	1.38	1.36
15	B	1209	CLA	CMC-C2C	-2.09	1.46	1.50
15	4	606	CLA	CHC-C1C	2.09	1.42	1.38
18	4	801	LMG	C7-C8	2.09	1.57	1.50
15	B	1204	CLA	CHC-C1C	2.09	1.42	1.38
15	1	607	CLA	CHC-C1C	2.09	1.42	1.38
15	A	1132	CLA	C3C-C2C	2.09	1.41	1.36
15	2	607	CLA	CMC-C2C	-2.09	1.46	1.50
15	1	613	CLA	CMD-C2D	-2.09	1.46	1.50
15	A	1118	CLA	C1C-C2C	2.09	1.48	1.44
15	1	608	CLA	C3B-C4B	2.09	1.48	1.42
16	3	604	CHL	CHA-CBD	2.09	1.54	1.51
15	4	612	CLA	CMC-C2C	-2.09	1.46	1.50
15	3	612	CLA	C1C-C2C	2.09	1.48	1.44
15	B	1213	CLA	CMC-C2C	-2.08	1.46	1.50
15	2	605	CLA	CMC-C2C	-2.08	1.46	1.50
15	A	1134	CLA	CMC-C2C	2.08	1.55	1.50
15	1	612	CLA	MG-NB	-2.08	2.01	2.05
15	B	1211	CLA	MG-ND	-2.08	2.01	2.05
15	A	1129	CLA	C3B-C4B	2.08	1.48	1.42
15	2	606	CLA	CHC-C1C	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1204	CLA	C3B-C4B	2.08	1.48	1.42
15	4	616	CLA	CMC-C2C	-2.08	1.46	1.50
15	B	1212	CLA	C3B-C4B	2.08	1.48	1.42
15	4	605	CLA	C3B-C4B	2.08	1.48	1.42
15	3	605	CLA	C1C-C2C	2.07	1.48	1.44
15	A	1140	CLA	C3D-C4D	-2.07	1.39	1.44
15	3	609	CLA	C3B-C4B	2.07	1.48	1.42
16	1	610	CHL	CHA-CBD	2.07	1.54	1.51
15	A	1136	CLA	C1C-C2C	2.07	1.48	1.44
18	2	803	LMG	O8-C9	-2.07	1.40	1.45
15	1	605	CLA	C3B-C4B	2.07	1.48	1.42
13	3	502	XAT	O24-C25	-2.07	1.43	1.46
15	1	608	CLA	CHC-C1C	2.07	1.42	1.38
15	A	1013	CLA	C3D-C4D	-2.07	1.39	1.44
15	B	1230	CLA	C3D-C4D	-2.07	1.39	1.44
15	1	604	CLA	C3B-C4B	2.07	1.48	1.42
14	B	4001	BCR	C33-C5	-2.07	1.47	1.50
15	A	1128	CLA	C1A-CHA	2.07	1.51	1.43
15	A	1127	CLA	C1C-C2C	2.06	1.48	1.44
15	B	1222	CLA	C1C-C2C	2.06	1.48	1.44
15	A	1105	CLA	C1A-CHA	2.06	1.51	1.43
15	2	604	CLA	CMC-C2C	-2.06	1.46	1.50
15	A	1139	CLA	C1C-C2C	2.06	1.48	1.44
15	1	607	CLA	CMC-C2C	-2.06	1.46	1.50
15	A	1132	CLA	MG-ND	-2.06	2.01	2.05
15	2	607	CLA	CHC-C1C	2.06	1.42	1.38
15	3	607	CLA	CHC-C1C	2.06	1.42	1.38
15	B	1225	CLA	C1C-C2C	2.06	1.48	1.44
15	1	615	CLA	CMC-C2C	-2.06	1.46	1.50
15	B	1215	CLA	CHC-C1C	2.06	1.42	1.38
15	B	1240	CLA	CMC-C2C	-2.06	1.46	1.50
15	A	1122	CLA	C3D-C4D	-2.06	1.39	1.44
15	A	1128	CLA	C1C-C2C	2.06	1.48	1.44
15	1	612	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	1138	CLA	C1C-C2C	2.06	1.48	1.44
15	1	603	CLA	MG-NB	-2.06	2.01	2.05
12	2	501	LUT	C11-C12	2.06	1.40	1.34
15	4	608	CLA	MG-ND	-2.06	2.01	2.05
15	A	1135	CLA	C1C-C2C	2.05	1.48	1.44
15	2	602	CLA	CMC-C2C	-2.05	1.46	1.50
15	2	612	CLA	C3B-C4B	2.05	1.48	1.42
15	A	1131	CLA	C1C-C2C	2.05	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	5002	DGD	O6D-C5D	-2.05	1.39	1.44
15	A	1103	CLA	C1C-C2C	2.05	1.48	1.44
15	1	604	CLA	CMC-C2C	-2.05	1.46	1.50
15	A	1132	CLA	CMB-C2B	-2.05	1.46	1.50
13	4	502	XAT	C40-C33	2.05	1.55	1.50
15	B	1235	CLA	C1C-C2C	2.05	1.48	1.44
15	1	602	CLA	CHC-C1C	2.05	1.42	1.38
13	2	502	XAT	C18-C5	2.05	1.54	1.51
15	B	1227	CLA	C1C-C2C	2.05	1.48	1.44
15	1	601	CLA	CMC-C2C	-2.05	1.46	1.50
15	A	1109	CLA	C1C-C2C	2.04	1.48	1.44
15	A	1112	CLA	C1C-C2C	2.04	1.48	1.44
14	4	503	BCR	C33-C5	-2.04	1.47	1.50
12	3	501	LUT	C11-C12	2.04	1.40	1.34
15	B	1232	CLA	CHC-C1C	2.04	1.42	1.38
15	A	1107	CLA	C3D-C4D	-2.04	1.39	1.44
15	4	607	CLA	CHC-C1C	2.04	1.42	1.38
15	3	610	CLA	CHC-C1C	2.04	1.42	1.38
15	2	605	CLA	C3B-C4B	2.04	1.48	1.42
15	A	1110	CLA	C1C-C2C	2.04	1.48	1.44
15	B	1213	CLA	CHC-C1C	2.04	1.42	1.38
15	3	608	CLA	CMB-C2B	-2.04	1.46	1.50
15	B	1205	CLA	CHC-C1C	2.04	1.42	1.38
15	2	616	CLA	CMC-C2C	-2.04	1.46	1.50
15	A	1123	CLA	C1C-C2C	2.04	1.48	1.44
15	4	608	CLA	C3B-C4B	2.04	1.48	1.42
15	A	1105	CLA	C1C-C2C	2.04	1.48	1.44
15	A	1141	CLA	CHC-C1C	2.04	1.42	1.38
15	A	1117	CLA	C1A-CHA	2.03	1.51	1.43
15	B	1205	CLA	MG-NB	-2.03	2.01	2.05
15	B	1221	CLA	CHC-C1C	2.03	1.42	1.38
15	B	1202	CLA	MG-NB	-2.03	2.01	2.05
15	B	1218	CLA	CHC-C1C	2.03	1.42	1.38
12	4	501	LUT	C10-C9	2.03	1.40	1.35
15	B	1239	CLA	C3B-C4B	2.03	1.48	1.42
15	A	1111	CLA	MG-NC	2.03	2.11	2.06
15	B	1238	CLA	CHC-C1C	2.03	1.42	1.38
15	4	606	CLA	C3B-C4B	2.03	1.48	1.42
15	2	607	CLA	MG-ND	-2.03	2.01	2.05
15	B	1238	CLA	MG-ND	-2.03	2.01	2.05
15	1	603	CLA	CMC-C2C	-2.03	1.46	1.50
15	1	615	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1108	CLA	C1C-C2C	2.03	1.48	1.44
15	A	1117	CLA	C1C-C2C	2.03	1.48	1.44
15	B	1232	CLA	MG-NB	-2.03	2.01	2.05
15	3	611	CLA	CHC-C1C	2.02	1.42	1.38
15	A	1116	CLA	C1C-C2C	2.02	1.48	1.44
15	B	1229	CLA	C3D-C4D	-2.02	1.39	1.44
15	A	1114	CLA	C3D-C4D	-2.02	1.39	1.44
15	B	1231	CLA	C1A-CHA	2.02	1.51	1.43
15	4	602	CLA	CHC-C1C	2.02	1.42	1.38
15	3	605	CLA	C3D-C4D	-2.02	1.39	1.44
15	B	1216	CLA	C3B-C4B	2.02	1.48	1.42
15	3	613	CLA	C3D-C4D	-2.02	1.39	1.44
15	B	1235	CLA	C3D-C4D	-2.02	1.39	1.44
15	B	1225	CLA	C3D-C4D	-2.02	1.39	1.44
13	2	502	XAT	C40-C33	2.02	1.54	1.50
13	4	502	XAT	C20-C13	2.02	1.54	1.50
15	1	611	CLA	CMC-C2C	-2.02	1.46	1.50
15	A	1102	CLA	C1C-C2C	2.02	1.48	1.44
15	4	602	CLA	MG-ND	-2.02	2.01	2.05
15	A	1133	CLA	C1A-CHA	2.01	1.51	1.43
15	A	1110	CLA	C3D-C4D	-2.01	1.39	1.44
15	A	1101	CLA	CHC-C1C	2.01	1.42	1.38
15	B	1223	CLA	MG-NC	2.01	2.11	2.06
15	3	606	CLA	CMC-C2C	-2.01	1.46	1.50
15	A	1114	CLA	C1C-C2C	2.01	1.48	1.44
15	A	1111	CLA	C1C-C2C	2.01	1.48	1.44
15	1	602	CLA	CMC-C2C	-2.01	1.46	1.50
15	A	1115	CLA	C3D-C4D	-2.01	1.39	1.44
15	B	1227	CLA	CHD-C1D	2.01	1.42	1.38
15	B	1021	CLA	C3D-C4D	-2.01	1.39	1.44
15	A	1134	CLA	CHB-C4A	2.01	1.42	1.37
15	B	1206	CLA	MG-ND	-2.01	2.01	2.05
15	F	1301	CLA	C1C-C2C	2.01	1.48	1.44
20	A	1011	CL0	C3A-C2A	-2.01	1.53	1.54
15	A	1138	CLA	C3D-C4D	-2.01	1.39	1.44
15	3	614	CLA	CHC-C1C	2.01	1.42	1.38
15	B	1023	CLA	C1D-ND	-2.01	1.35	1.37
15	B	1222	CLA	C3D-C4D	-2.01	1.39	1.44
15	4	605	CLA	CMC-C2C	-2.01	1.46	1.50
15	3	603	CLA	C3B-C4B	2.01	1.48	1.42
15	B	1203	CLA	MG-ND	-2.00	2.01	2.05
15	A	1139	CLA	C3D-C4D	-2.00	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1131	CLA	C3D-C4D	-2.00	1.39	1.44
15	B	1203	CLA	CHC-C1C	2.00	1.42	1.38
13	4	502	XAT	C39-C29	2.00	1.54	1.50
15	A	1104	CLA	C3D-C4D	-2.00	1.39	1.44
15	A	1136	CLA	C3D-C4D	-2.00	1.39	1.44
15	B	1226	CLA	CHC-C1C	2.00	1.42	1.38

All (2223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	502	XAT	O4-C5-C4	45.80	156.42	113.49
13	1	502	XAT	O24-C25-C24	44.09	154.81	113.49
13	2	502	XAT	O4-C5-C4	43.41	154.17	113.49
13	4	502	XAT	O4-C5-C4	43.33	154.10	113.49
13	4	502	XAT	O24-C25-C24	42.55	153.37	113.49
13	2	502	XAT	O24-C25-C24	40.07	151.04	113.49
15	A	1140	CLA	C4A-NA-C1A	20.48	116.02	106.68
14	A	4006	BCR	C10-C11-C12	19.23	178.91	123.20
14	A	4002	BCR	C10-C11-C12	19.17	178.76	123.20
14	A	4004	BCR	C10-C11-C12	19.16	178.72	123.20
14	B	4006	BCR	C10-C11-C12	19.09	178.50	123.20
14	F	4002	BCR	C10-C11-C12	18.90	177.96	123.20
14	B	4005	BCR	C10-C11-C12	18.77	177.59	123.20
14	A	4008	BCR	C10-C11-C12	18.60	177.09	123.20
14	A	4005	BCR	C10-C11-C12	18.52	176.85	123.20
14	3	504	BCR	C10-C11-C12	18.40	176.52	123.20
14	A	4003	BCR	C10-C11-C12	18.35	176.37	123.20
14	J	4001	BCR	C10-C11-C12	18.23	176.03	123.20
14	F	4001	BCR	C10-C11-C12	18.18	175.89	123.20
14	J	4002	BCR	C10-C11-C12	17.36	173.50	123.20
14	A	4007	BCR	C16-C15-C14	16.98	158.27	123.52
14	J	4002	BCR	C16-C15-C14	15.92	156.10	123.52
15	A	1134	CLA	C4A-NA-C1A	15.73	113.86	106.68
14	A	4004	BCR	C16-C15-C14	15.64	155.52	123.52
14	A	4007	BCR	C10-C11-C12	15.37	167.73	123.20
14	A	4002	BCR	C21-C20-C19	14.74	165.92	123.20
14	B	4005	BCR	C16-C15-C14	14.50	153.20	123.52
14	B	4006	BCR	C11-C10-C9	14.48	147.59	127.28
14	3	504	BCR	C16-C15-C14	14.45	153.09	123.52
14	F	4002	BCR	C21-C20-C19	14.30	164.64	123.20
20	A	1011	CL0	C1B-CHB-C4A	14.30	130.52	121.32
14	F	4001	BCR	C21-C20-C19	14.05	163.90	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4003	BCR	C11-C10-C9	14.02	146.94	127.28
14	J	4001	BCR	C11-C10-C9	13.84	146.69	127.28
13	2	502	XAT	O24-C25-C38	-13.78	99.65	115.05
14	F	4001	BCR	C16-C15-C14	13.67	151.49	123.52
14	A	4006	BCR	C16-C15-C14	13.61	151.36	123.52
13	1	502	XAT	O24-C25-C38	-13.51	99.95	115.05
15	A	1125	CLA	C4A-NA-C1A	13.39	112.79	106.68
14	3	504	BCR	C11-C10-C9	13.28	145.91	127.28
14	J	4001	BCR	C21-C20-C19	13.28	161.68	123.20
14	B	4006	BCR	C21-C20-C19	13.27	161.65	123.20
14	B	4006	BCR	C16-C15-C14	13.23	150.59	123.52
14	A	4007	BCR	C21-C20-C19	13.14	161.26	123.20
14	A	4002	BCR	C16-C15-C14	13.08	150.29	123.52
14	A	4008	BCR	C21-C20-C19	13.08	161.10	123.20
14	B	4005	BCR	C21-C20-C19	13.00	160.87	123.20
14	J	4001	BCR	C16-C15-C14	13.00	150.11	123.52
14	A	4002	BCR	C11-C10-C9	12.96	145.45	127.28
14	J	4002	BCR	C11-C10-C9	12.73	145.13	127.28
14	3	504	BCR	C21-C20-C19	12.67	159.91	123.20
14	A	4003	BCR	C16-C15-C14	12.61	149.32	123.52
14	B	4005	BCR	C11-C10-C9	12.36	144.61	127.28
13	1	502	XAT	O4-C5-C18	-12.32	101.28	115.05
14	A	4004	BCR	C21-C20-C19	12.28	158.79	123.20
15	A	1134	CLA	O2D-CGD-CBD	12.27	132.69	111.23
14	J	4002	BCR	C21-C20-C19	12.23	158.65	123.20
14	A	4004	BCR	C11-C10-C9	12.17	144.35	127.28
13	4	502	XAT	C18-C5-C4	-12.06	100.69	114.24
14	A	4007	BCR	C11-C10-C9	12.03	144.15	127.28
15	A	1118	CLA	C4A-NA-C1A	12.02	112.16	106.68
13	2	502	XAT	C18-C5-C4	-11.82	100.97	114.24
15	B	1223	CLA	C4A-NA-C1A	11.79	112.06	106.68
14	A	4005	BCR	C21-C20-C19	11.53	156.61	123.20
14	A	4006	BCR	C21-C20-C19	11.51	156.54	123.20
13	4	502	XAT	O24-C25-C38	-11.32	102.40	115.05
14	A	4006	BCR	C11-C10-C9	11.28	143.10	127.28
13	1	502	XAT	C38-C25-C24	-11.08	101.79	114.24
14	A	4008	BCR	C16-C15-C14	11.06	146.16	123.52
14	F	4002	BCR	C20-C19-C18	10.83	156.06	126.36
14	A	4003	BCR	C21-C20-C19	10.76	154.37	123.20
14	A	4005	BCR	C16-C15-C14	10.73	145.48	123.52
13	1	502	XAT	C18-C5-C4	-10.67	102.25	114.24
14	A	4006	BCR	C11-C12-C13	10.52	155.20	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	4002	BCR	C11-C12-C13	10.38	154.83	126.36
14	B	4006	BCR	C11-C12-C13	10.37	154.80	126.36
13	4	502	XAT	C38-C25-C24	-10.25	102.72	114.24
14	J	4002	BCR	C11-C12-C13	10.23	154.40	126.36
14	A	4004	BCR	C11-C12-C13	10.14	154.18	126.36
14	A	4002	BCR	C11-C12-C13	10.14	154.18	126.36
14	A	4008	BCR	C11-C12-C13	10.14	154.17	126.36
14	F	4002	BCR	C16-C15-C14	10.04	144.06	123.52
14	A	4005	BCR	C11-C12-C13	9.82	153.30	126.36
14	F	4002	BCR	C11-C10-C9	9.82	141.04	127.28
13	2	502	XAT	O4-C5-C18	-9.65	104.27	115.05
14	F	4001	BCR	C11-C12-C13	9.58	152.62	126.36
14	B	4005	BCR	C11-C12-C13	9.56	152.59	126.36
14	A	4006	BCR	C20-C19-C18	9.46	152.29	126.36
14	A	4003	BCR	C11-C12-C13	9.43	152.21	126.36
14	A	4008	BCR	C11-C10-C9	9.39	140.45	127.28
14	J	4001	BCR	C11-C12-C13	9.32	151.93	126.36
16	4	613	CHL	C1B-CHB-C4A	9.30	127.31	121.32
13	4	502	XAT	O4-C5-C18	-9.30	104.65	115.05
13	4	502	XAT	C11-C10-C9	-9.24	114.32	127.28
14	J	4002	BCR	C20-C19-C18	9.15	151.44	126.36
14	3	504	BCR	C11-C12-C13	9.11	151.34	126.36
15	B	1230	CLA	C4A-NA-C1A	9.03	110.80	106.68
15	B	1229	CLA	C4A-NA-C1A	8.96	110.77	106.68
15	A	1130	CLA	C4A-NA-C1A	8.93	110.75	106.68
14	A	4007	BCR	C15-C14-C13	-8.87	114.84	127.28
14	A	4007	BCR	C20-C19-C18	8.86	150.65	126.36
20	A	1011	CL0	O2D-CGD-CBD	8.84	120.66	110.95
15	A	1117	CLA	C4A-NA-C1A	8.82	110.70	106.68
15	A	1105	CLA	C4A-NA-C1A	8.78	110.69	106.68
15	A	1103	CLA	C4A-NA-C1A	8.73	110.66	106.68
15	A	1114	CLA	C4A-NA-C1A	8.73	110.66	106.68
15	3	605	CLA	C4A-NA-C1A	8.72	110.66	106.68
15	A	1128	CLA	C4A-NA-C1A	8.71	110.65	106.68
15	A	1113	CLA	C4A-NA-C1A	8.70	110.65	106.68
15	A	1102	CLA	C4A-NA-C1A	8.70	110.65	106.68
15	B	1231	CLA	C4A-NA-C1A	8.69	110.64	106.68
15	A	1121	CLA	C4A-NA-C1A	8.68	110.64	106.68
15	A	1119	CLA	C4A-NA-C1A	8.68	110.64	106.68
14	B	4005	BCR	C20-C19-C18	8.67	150.13	126.36
15	A	1135	CLA	C4A-NA-C1A	8.67	110.63	106.68
15	A	1127	CLA	C4A-NA-C1A	8.66	110.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1126	CLA	C4A-NA-C1A	8.65	110.63	106.68
15	B	1226	CLA	C4A-NA-C1A	8.64	110.62	106.68
15	A	1112	CLA	C4A-NA-C1A	8.63	110.62	106.68
15	A	1107	CLA	C4A-NA-C1A	8.62	110.61	106.68
15	B	1222	CLA	C4A-NA-C1A	8.62	110.61	106.68
15	B	1236	CLA	C4A-NA-C1A	8.59	110.60	106.68
15	A	1108	CLA	C4A-NA-C1A	8.58	110.59	106.68
15	A	1139	CLA	C4A-NA-C1A	8.57	110.59	106.68
15	A	1131	CLA	C4A-NA-C1A	8.55	110.58	106.68
15	A	1110	CLA	C4A-NA-C1A	8.54	110.58	106.68
14	3	504	BCR	C20-C19-C18	8.54	149.77	126.36
15	3	615	CLA	C4A-NA-C1A	8.50	110.56	106.68
15	B	1021	CLA	C4A-NA-C1A	8.47	110.54	106.68
15	A	1111	CLA	C4A-NA-C1A	8.45	110.53	106.68
15	A	1012	CLA	C4A-NA-C1A	8.44	110.53	106.68
15	B	1225	CLA	C4A-NA-C1A	8.42	110.52	106.68
15	A	1106	CLA	C4A-NA-C1A	8.40	110.51	106.68
15	J	1302	CLA	C4A-NA-C1A	8.39	110.51	106.68
15	A	1137	CLA	C4A-NA-C1A	8.38	110.50	106.68
15	F	1301	CLA	C4A-NA-C1A	8.38	110.50	106.68
15	A	1013	CLA	C4A-NA-C1A	8.34	110.48	106.68
15	A	1115	CLA	C4A-NA-C1A	8.32	110.47	106.68
15	3	612	CLA	C4A-NA-C1A	8.31	110.47	106.68
15	A	1123	CLA	C4A-NA-C1A	8.31	110.47	106.68
15	3	613	CLA	C4A-NA-C1A	8.27	110.45	106.68
15	A	1136	CLA	C4A-NA-C1A	8.25	110.44	106.68
15	A	1120	CLA	C4A-NA-C1A	8.25	110.44	106.68
14	A	4005	BCR	C20-C19-C18	8.24	148.95	126.36
12	4	501	LUT	C20-C13-C14	-8.23	109.48	122.82
15	B	1235	CLA	C4A-NA-C1A	8.22	110.43	106.68
15	A	1138	CLA	C4A-NA-C1A	8.20	110.42	106.68
16	2	609	CHL	C1B-CHB-C4A	8.19	126.59	121.32
15	B	1228	CLA	C4A-NA-C1A	8.18	110.41	106.68
13	4	502	XAT	C15-C14-C13	-8.17	115.82	127.28
15	A	1122	CLA	C4A-NA-C1A	8.11	110.38	106.68
13	2	502	XAT	C11-C10-C9	-8.09	115.94	127.28
15	A	1101	CLA	C4A-NA-C1A	8.01	110.33	106.68
14	A	4004	BCR	C20-C19-C18	7.93	148.12	126.36
16	1	610	CHL	C1B-CHB-C4A	7.93	126.42	121.32
15	A	1109	CLA	C4A-NA-C1A	7.91	110.29	106.68
15	A	1104	CLA	C4A-NA-C1A	7.90	110.28	106.68
16	4	611	CHL	C1B-CHB-C4A	7.89	126.40	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	502	XAT	C7-C8-C9	-7.88	113.30	125.53
15	B	1239	CLA	C4A-NA-C1A	7.85	110.26	106.68
14	A	4005	BCR	C11-C10-C9	7.84	138.27	127.28
15	3	611	CLA	C4A-NA-C1A	7.83	110.25	106.68
15	A	1132	CLA	C4A-NA-C1A	7.79	110.23	106.68
14	J	4001	BCR	C20-C19-C18	7.78	147.69	126.36
15	B	1224	CLA	C4A-NA-C1A	7.76	110.22	106.68
13	2	502	XAT	C38-C25-C24	-7.76	105.53	114.24
15	B	1234	CLA	C4A-NA-C1A	7.72	110.20	106.68
15	A	1133	CLA	C4A-NA-C1A	7.56	110.13	106.68
15	A	1116	CLA	C4A-NA-C1A	7.56	110.13	106.68
14	F	4001	BCR	C20-C19-C18	7.50	146.93	126.36
15	4	603	CLA	C4A-NA-C1A	7.47	110.09	106.68
12	3	501	LUT	C1-C6-C5	-7.43	112.48	122.64
15	B	1237	CLA	C4A-NA-C1A	7.40	110.06	106.68
15	B	1212	CLA	C4A-NA-C1A	7.39	110.05	106.68
16	2	611	CHL	C1B-CHB-C4A	7.36	126.06	121.32
14	B	4006	BCR	C20-C19-C18	7.34	146.50	126.36
15	1	603	CLA	C4A-NA-C1A	7.34	110.03	106.68
12	3	501	LUT	C12-C13-C14	7.33	130.54	119.01
15	3	603	CLA	C4A-NA-C1A	7.31	110.02	106.68
15	2	605	CLA	C4A-NA-C1A	7.26	109.99	106.68
16	2	610	CHL	C1B-CHB-C4A	7.22	125.97	121.32
12	4	501	LUT	C28-C29-C30	7.20	130.34	119.01
14	F	4001	BCR	C11-C10-C9	7.18	137.35	127.28
15	3	609	CLA	C4A-NA-C1A	7.18	109.96	106.68
15	4	609	CLA	C4A-NA-C1A	7.18	109.95	106.68
12	3	501	LUT	C8-C9-C10	7.17	130.28	119.01
12	3	501	LUT	C19-C9-C10	-7.16	111.21	122.82
15	F	1302	CLA	C4A-NA-C1A	7.15	109.94	106.68
14	A	4007	BCR	C11-C12-C13	7.11	145.86	126.36
14	A	4008	BCR	C20-C19-C18	7.10	145.84	126.36
15	B	1221	CLA	C4A-NA-C1A	7.10	109.92	106.68
16	2	613	CHL	C1B-CHB-C4A	7.09	125.88	121.32
13	3	502	XAT	C31-C30-C29	-7.09	117.33	127.28
15	B	1213	CLA	C4A-NA-C1A	7.09	109.91	106.68
15	B	1203	CLA	C4A-NA-C1A	7.01	109.88	106.68
15	B	1023	CLA	C4A-NA-C1A	6.99	109.87	106.68
15	B	1204	CLA	C4A-NA-C1A	6.98	109.86	106.68
15	4	605	CLA	C4A-NA-C1A	6.93	109.84	106.68
15	1	605	CLA	C4A-NA-C1A	6.92	109.84	106.68
15	2	603	CLA	C4A-NA-C1A	6.91	109.83	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	602	CLA	C4A-NA-C1A	6.90	109.83	106.68
15	B	1209	CLA	C4A-NA-C1A	6.88	109.82	106.68
15	1	608	CLA	C4A-NA-C1A	6.87	109.81	106.68
15	4	606	CLA	C4A-NA-C1A	6.86	109.81	106.68
15	4	602	CLA	C4A-NA-C1A	6.85	109.80	106.68
15	3	607	CLA	C4A-NA-C1A	6.85	109.80	106.68
15	3	614	CLA	C4A-NA-C1A	6.82	109.79	106.68
15	B	1202	CLA	C4A-NA-C1A	6.82	109.79	106.68
15	3	606	CLA	C4A-NA-C1A	6.81	109.79	106.68
13	4	502	XAT	C12-C13-C14	6.78	129.67	119.01
15	B	1217	CLA	C4A-NA-C1A	6.77	109.77	106.68
15	B	1023	CLA	C1-C2-C3	-6.76	115.12	126.20
15	4	612	CLA	C4A-NA-C1A	6.74	109.75	106.68
15	B	1231	CLA	CMD-C2D-C1D	6.73	136.58	124.73
15	B	1220	CLA	C4A-NA-C1A	6.73	109.75	106.68
15	A	1124	CLA	C4A-NA-C1A	6.72	109.74	106.68
15	B	1240	CLA	C4A-NA-C1A	6.71	109.74	106.68
15	2	607	CLA	C4A-NA-C1A	6.70	109.73	106.68
13	2	502	XAT	C18-C5-C6	-6.68	111.31	122.30
15	A	1102	CLA	O2D-CGD-CBD	6.67	122.90	111.23
16	1	609	CHL	C1B-CHB-C4A	6.64	125.59	121.32
15	4	604	CLA	C4A-NA-C1A	6.63	109.70	106.68
15	B	1211	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	B	1232	CLA	C4A-NA-C1A	6.59	109.69	106.68
15	1	606	CLA	C4A-NA-C1A	6.53	109.66	106.68
13	2	502	XAT	C15-C14-C13	-6.53	118.12	127.28
15	1	604	CLA	C4A-NA-C1A	6.53	109.66	106.68
15	A	1134	CLA	O2D-CGD-O1D	-6.51	111.17	123.85
15	B	1215	CLA	C4A-NA-C1A	6.50	109.65	106.68
14	A	4002	BCR	C20-C19-C18	6.50	144.17	126.36
14	A	4003	BCR	C20-C19-C18	6.48	144.14	126.36
15	2	606	CLA	C4A-NA-C1A	6.48	109.63	106.68
15	2	616	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	2	604	CLA	C4A-NA-C1A	6.44	109.62	106.68
15	3	601	CLA	C4A-NA-C1A	6.44	109.62	106.68
13	2	502	XAT	C7-C8-C9	-6.43	115.55	125.53
15	4	607	CLA	C4A-NA-C1A	6.42	109.61	106.68
13	4	502	XAT	O24-C26-C27	-6.41	98.51	116.88
15	A	1125	CLA	C1-C2-C3	-6.39	115.72	126.20
15	2	612	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	B	1205	CLA	C4A-NA-C1A	6.37	109.59	106.68
15	A	1129	CLA	C4A-NA-C1A	6.35	109.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	610	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	B	1214	CLA	C4A-NA-C1A	6.33	109.56	106.68
13	2	502	XAT	C11-C12-C13	-6.31	109.05	126.36
15	B	1227	CLA	C4A-NA-C1A	6.27	109.54	106.68
12	2	501	LUT	C28-C29-C30	6.26	128.86	119.01
15	B	1206	CLA	C4A-NA-C1A	6.26	109.54	106.68
15	B	1218	CLA	C4A-NA-C1A	6.23	109.52	106.68
12	1	501	LUT	C20-C13-C14	-6.22	112.73	122.82
15	B	1207	CLA	C4A-NA-C1A	6.19	109.50	106.68
13	4	502	XAT	C18-C5-C6	-6.19	112.12	122.30
15	A	1141	CLA	C4A-NA-C1A	6.19	109.50	106.68
13	4	502	XAT	C40-C33-C34	-6.16	112.83	122.82
14	A	4004	BCR	C15-C14-C13	-6.16	118.64	127.28
15	B	1227	CLA	CMD-C2D-C1D	6.15	135.56	124.73
15	1	611	CLA	C4A-NA-C1A	6.15	109.48	106.68
15	B	1216	CLA	C4A-NA-C1A	6.14	109.48	106.68
15	1	602	CLA	C4A-NA-C1A	6.13	109.48	106.68
15	1	615	CLA	C4A-NA-C1A	6.13	109.47	106.68
15	1	607	CLA	C4A-NA-C1A	6.12	109.47	106.68
15	1	613	CLA	C4A-NA-C1A	6.12	109.47	106.68
12	4	501	LUT	C40-C33-C34	-6.10	112.93	122.82
15	A	1101	CLA	O2D-CGD-CBD	6.05	121.81	111.23
15	B	1234	CLA	CMD-C2D-C1D	6.05	135.38	124.73
13	3	502	XAT	C15-C14-C13	-6.04	118.81	127.28
15	4	616	CLA	C4A-NA-C1A	6.04	109.43	106.68
16	4	610	CHL	C1B-CHB-C4A	6.01	125.19	121.32
15	B	1208	CLA	C4A-NA-C1A	5.98	109.41	106.68
12	3	501	LUT	C28-C29-C30	5.95	128.36	119.01
15	2	608	CLA	C4A-NA-C1A	5.94	109.39	106.68
15	B	1219	CLA	C4A-NA-C1A	5.94	109.39	106.68
15	A	1140	CLA	O2D-CGD-CBD	5.93	121.60	111.23
15	2	601	CLA	C4A-NA-C1A	5.92	109.38	106.68
15	3	608	CLA	C4A-NA-C1A	5.92	109.38	106.68
13	4	502	XAT	C11-C12-C13	-5.91	110.16	126.36
13	4	502	XAT	C32-C33-C34	5.91	128.30	119.01
15	1	601	CLA	C4A-NA-C1A	5.85	109.35	106.68
15	A	1134	CLA	CHD-C1D-ND	-5.83	116.60	124.80
15	B	1210	CLA	C4A-NA-C1A	5.81	109.33	106.68
15	4	601	CLA	C4A-NA-C1A	5.79	109.32	106.68
16	4	610	CHL	C1C-CHC-C4B	5.79	136.79	116.07
13	1	502	XAT	C18-C5-C6	-5.78	112.79	122.30
15	1	612	CLA	C4A-NA-C1A	5.78	109.31	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1122	CLA	CMD-C2D-C1D	5.73	134.82	124.73
15	A	1104	CLA	CMD-C2D-C1D	5.73	134.82	124.73
15	B	1238	CLA	C1-C2-C3	-5.73	113.39	126.44
15	B	1201	CLA	C4A-NA-C1A	5.72	109.29	106.68
15	B	1238	CLA	CAC-C3C-C4C	5.71	132.21	124.79
15	4	608	CLA	C4A-NA-C1A	5.69	109.28	106.68
15	A	1101	CLA	CMD-C2D-C1D	5.67	134.72	124.73
15	4	608	CLA	CAC-C3C-C4C	5.66	132.15	124.79
15	A	1117	CLA	O2D-CGD-CBD	5.65	121.11	111.23
13	2	502	XAT	C32-C33-C34	5.63	127.86	119.01
15	F	1301	CLA	CMD-C2D-C1D	5.62	134.62	124.73
15	A	1102	CLA	CMD-C2D-C1D	5.58	134.56	124.73
15	A	1139	CLA	CMD-C2D-C1D	5.58	134.55	124.73
15	A	1130	CLA	CMD-C2D-C1D	5.57	134.54	124.73
15	A	1114	CLA	CMD-C2D-C1D	5.57	134.53	124.73
15	A	1120	CLA	CMD-C2D-C1D	5.56	134.52	124.73
15	A	1013	CLA	CMD-C2D-C1D	5.56	134.52	124.73
15	B	1225	CLA	CMD-C2D-C1D	5.54	134.48	124.73
15	A	1123	CLA	CMD-C2D-C1D	5.53	134.47	124.73
15	3	615	CLA	CMD-C2D-C1D	5.52	134.46	124.73
15	A	1013	CLA	O2D-CGD-CBD	5.52	120.89	111.23
15	A	1105	CLA	CMD-C2D-C1D	5.52	134.45	124.73
15	A	1103	CLA	C1-C2-C3	-5.52	117.16	126.20
15	A	1107	CLA	CMD-C2D-C1D	5.51	134.44	124.73
13	1	502	XAT	C11-C10-C9	-5.51	119.55	127.28
15	A	1109	CLA	CMD-C2D-C1D	5.51	134.43	124.73
15	A	1137	CLA	CMD-C2D-C1D	5.51	134.43	124.73
15	A	1108	CLA	CMD-C2D-C1D	5.50	134.42	124.73
13	4	502	XAT	C15-C35-C34	-5.50	112.27	123.52
15	A	1112	CLA	CMD-C2D-C1D	5.50	134.41	124.73
15	A	1121	CLA	CMD-C2D-C1D	5.49	134.40	124.73
15	A	1106	CLA	CMD-C2D-C1D	5.49	134.40	124.73
12	1	501	LUT	C1-C6-C5	-5.49	115.13	122.64
12	3	501	LUT	C38-C25-C24	-5.48	110.38	123.36
15	B	1236	CLA	CMD-C2D-C1D	5.48	134.38	124.73
15	B	1229	CLA	CMD-C2D-C1D	5.48	134.38	124.73
15	A	1131	CLA	CMD-C2D-C1D	5.48	134.37	124.73
15	B	1238	CLA	C4A-NA-C1A	5.47	109.18	106.68
15	3	613	CLA	O2D-CGD-CBD	5.47	120.79	111.23
15	B	1230	CLA	CMD-C2D-C1D	5.47	134.36	124.73
15	A	1117	CLA	CMD-C2D-C1D	5.47	134.35	124.73
15	B	1235	CLA	CMD-C2D-C1D	5.47	134.35	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1227	CLA	O2D-CGD-CBD	5.46	120.78	111.23
15	A	1113	CLA	CMD-C2D-C1D	5.46	134.35	124.73
15	A	1138	CLA	CMD-C2D-C1D	5.46	134.35	124.73
15	B	1228	CLA	CMD-C2D-C1D	5.46	134.35	124.73
15	A	1115	CLA	CMD-C2D-C1D	5.46	134.34	124.73
15	J	1302	CLA	CMD-C2D-C1D	5.45	134.32	124.73
15	3	605	CLA	CMD-C2D-C1D	5.45	134.32	124.73
15	A	1111	CLA	CMD-C2D-C1D	5.44	134.31	124.73
15	A	1106	CLA	O2D-CGD-CBD	5.44	120.74	111.23
15	3	612	CLA	CMD-C2D-C1D	5.44	134.30	124.73
15	A	1125	CLA	CMD-C2D-C1D	5.44	134.30	124.73
15	A	1135	CLA	CMD-C2D-C1D	5.43	134.30	124.73
15	A	1110	CLA	CMD-C2D-C1D	5.43	134.29	124.73
15	A	1126	CLA	CMD-C2D-C1D	5.43	134.29	124.73
15	A	1119	CLA	CMD-C2D-C1D	5.43	134.29	124.73
15	A	1103	CLA	O2D-CGD-CBD	5.43	120.72	111.23
12	2	501	LUT	C40-C33-C34	-5.42	114.04	122.82
15	A	1103	CLA	CMD-C2D-C1D	5.41	134.26	124.73
15	B	1021	CLA	CMD-C2D-C1D	5.41	134.26	124.73
13	2	502	XAT	C40-C33-C34	-5.41	114.06	122.82
15	3	613	CLA	CMD-C2D-C1D	5.39	134.23	124.73
15	B	1023	CLA	CMD-C2D-C1D	5.39	134.22	124.73
15	A	1128	CLA	CMD-C2D-C1D	5.39	134.22	124.73
15	A	1012	CLA	CMD-C2D-C1D	5.38	134.21	124.73
15	A	1136	CLA	CMD-C2D-C1D	5.38	134.20	124.73
15	B	1222	CLA	CMD-C2D-C1D	5.37	134.19	124.73
16	1	609	CHL	C1C-CHC-C4B	5.37	135.28	116.07
15	A	1140	CLA	C1-C2-C3	-5.36	117.41	126.20
15	B	1224	CLA	O2D-CGD-CBD	5.36	120.60	111.23
15	B	1022	CLA	O2D-CGD-CBD	5.36	120.60	111.23
15	A	1128	CLA	O2D-CGD-CBD	5.35	120.59	111.23
20	A	1011	CL0	O2A-CGA-O1A	-5.33	110.30	123.63
12	2	501	LUT	C1-C6-C5	-5.33	115.36	122.64
15	B	1022	CLA	CMD-C2D-C1D	5.31	134.08	124.73
12	4	501	LUT	C12-C13-C14	5.30	127.35	119.01
15	B	1229	CLA	O2D-CGD-CBD	5.30	120.50	111.23
14	A	4005	BCR	C23-C24-C25	-5.30	112.84	127.00
15	3	615	CLA	O2D-CGD-CBD	5.28	120.47	111.23
15	A	1128	CLA	C1-C2-C3	-5.27	117.56	126.20
15	B	1222	CLA	O2D-CGD-CBD	5.27	120.45	111.23
15	A	1111	CLA	O2D-CGD-CBD	5.26	120.42	111.23
15	B	1235	CLA	O2D-CGD-CBD	5.24	120.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	611	CHL	C1C-CHC-C4B	5.23	134.79	116.07
15	A	1116	CLA	CMD-C2D-C1D	5.23	133.93	124.73
14	A	4005	BCR	C33-C5-C6	-5.22	118.79	124.48
15	B	1224	CLA	CMD-C2D-C1D	5.22	133.92	124.73
15	A	1123	CLA	O2D-CGD-CBD	5.21	120.34	111.23
15	B	1236	CLA	O2A-C1-C2	5.21	121.39	108.99
12	4	501	LUT	C27-C28-C29	-5.20	115.13	126.32
15	A	1136	CLA	O2D-CGD-CBD	5.20	120.33	111.23
15	A	1113	CLA	O2D-CGD-CBD	5.19	120.30	111.23
15	A	1124	CLA	CMD-C2D-C1D	5.18	133.85	124.73
15	A	1137	CLA	O2D-CGD-CBD	5.17	120.27	111.23
15	F	1301	CLA	O2D-CGD-CBD	5.17	120.26	111.23
15	A	1012	CLA	O2D-CGD-CBD	5.16	120.25	111.23
15	A	1135	CLA	O2D-CGD-CBD	5.14	120.22	111.23
16	2	613	CHL	C1C-CHC-C4B	5.14	134.45	116.07
16	2	610	CHL	C1C-CHC-C4B	5.14	134.45	116.07
15	B	1230	CLA	O2D-CGD-CBD	5.14	120.21	111.23
16	1	610	CHL	C1C-CHC-C4B	5.13	134.44	116.07
16	4	611	CHL	C1C-CHC-C4B	5.13	134.42	116.07
15	3	605	CLA	O2D-CGD-CBD	5.12	120.17	111.23
16	4	613	CHL	C1C-CHC-C4B	5.11	134.36	116.07
15	A	1108	CLA	O2D-CGD-CBD	5.11	120.16	111.23
15	A	1114	CLA	O2D-CGD-CBD	5.10	120.15	111.23
15	A	1105	CLA	O2D-CGD-CBD	5.10	120.14	111.23
15	B	1236	CLA	O2D-CGD-CBD	5.10	120.14	111.23
12	4	501	LUT	C18-C5-C6	-5.08	118.94	124.48
14	A	4008	BCR	C33-C5-C6	-5.08	118.94	124.48
15	A	1115	CLA	O2D-CGD-CBD	5.07	120.10	111.23
13	2	502	XAT	C15-C35-C34	-5.07	113.15	123.52
15	A	1121	CLA	O2D-CGD-CBD	5.07	120.09	111.23
13	2	502	XAT	O24-C26-C27	-5.05	102.42	116.88
15	A	1131	CLA	O2D-CGD-CBD	5.03	120.02	111.23
15	A	1104	CLA	O2D-CGD-CBD	5.02	120.01	111.23
15	A	1120	CLA	O2D-CGD-CBD	5.01	119.99	111.23
13	2	502	XAT	C31-C30-C29	-5.01	120.25	127.28
12	3	501	LUT	C39-C29-C30	-5.01	114.70	122.82
15	A	1112	CLA	O2D-CGD-CBD	5.01	119.98	111.23
15	A	1107	CLA	O2D-CGD-CBD	5.00	119.98	111.23
14	B	4005	BCR	C15-C14-C13	-5.00	120.26	127.28
13	4	502	XAT	C20-C13-C12	-5.00	110.45	118.09
15	A	1140	CLA	CMD-C2D-C1D	4.99	133.52	124.73
16	2	609	CHL	C1C-CHC-C4B	4.99	133.91	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	612	CLA	O2D-CGD-CBD	4.98	119.93	111.23
15	A	1127	CLA	O2D-CGD-CBD	4.97	119.93	111.23
13	4	502	XAT	C8-C9-C10	4.97	126.83	119.01
15	B	1225	CLA	O2D-CGD-CBD	4.97	119.91	111.23
13	1	502	XAT	O24-C26-C27	-4.95	102.69	116.88
12	1	501	LUT	C18-C5-C6	-4.94	119.09	124.48
15	A	1138	CLA	O2D-CGD-CBD	4.93	119.86	111.23
15	J	1302	CLA	O2D-CGD-CBD	4.93	119.84	111.23
13	4	502	XAT	C7-C8-C9	-4.92	117.90	125.53
14	B	4006	BCR	C33-C5-C6	-4.89	119.15	124.48
15	A	1130	CLA	O2D-CGD-CBD	4.89	119.77	111.23
12	2	501	LUT	C38-C25-C24	-4.87	111.83	123.36
14	A	4002	BCR	C33-C5-C6	-4.87	119.17	124.48
14	3	504	BCR	C15-C14-C13	-4.83	120.51	127.28
15	A	1134	CLA	C3A-C2A-C1A	4.82	108.56	101.34
12	2	501	LUT	C20-C13-C14	-4.81	115.02	122.82
12	1	501	LUT	C28-C29-C30	4.81	126.58	119.01
15	B	1228	CLA	O2D-CGD-CBD	4.81	119.64	111.23
15	A	1109	CLA	O2D-CGD-CBD	4.81	119.63	111.23
15	A	1122	CLA	O2D-CGD-CBD	4.79	119.61	111.23
15	A	1118	CLA	CMD-C2D-C1D	4.76	133.11	124.73
16	3	604	CHL	C1C-CHC-C4B	4.76	133.10	116.07
16	3	604	CHL	C1B-CHB-C4A	4.76	124.38	121.32
14	A	4007	BCR	C33-C5-C6	-4.76	119.30	124.48
15	A	1139	CLA	O2D-CGD-CBD	4.74	119.51	111.23
14	F	4002	BCR	C33-C5-C6	-4.72	119.33	124.48
15	B	1231	CLA	O2D-CGD-CBD	4.72	119.49	111.23
15	B	1229	CLA	C3B-C4B-NB	-4.71	106.32	110.53
12	3	501	LUT	C18-C5-C6	-4.71	119.34	124.48
15	A	1126	CLA	O2D-CGD-CBD	4.71	119.46	111.23
15	A	1119	CLA	O2D-CGD-CBD	4.70	119.45	111.23
13	2	502	XAT	C12-C13-C14	4.69	126.39	119.01
15	B	1022	CLA	C3B-C4B-NB	-4.66	106.37	110.53
15	B	1223	CLA	C1D-ND-C4D	-4.65	103.05	106.31
15	A	1134	CLA	C2C-C1C-NC	4.65	114.87	109.98
14	A	4004	BCR	C33-C5-C6	-4.64	119.42	124.48
15	B	1021	CLA	O2D-CGD-CBD	4.64	119.34	111.23
15	A	1133	CLA	C1-C2-C3	-4.63	118.61	126.20
15	A	1118	CLA	O2D-CGD-CBD	4.63	119.32	111.23
15	A	1134	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
15	B	1223	CLA	CMD-C2D-C1D	4.58	132.78	124.73
13	4	502	XAT	C31-C30-C29	-4.55	120.89	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1110	CLA	O2D-CGD-CBD	4.55	119.18	111.23
15	B	1234	CLA	O2D-CGD-CBD	4.52	119.14	111.23
15	A	1116	CLA	O2D-CGD-CBD	4.52	119.13	111.23
15	A	1139	CLA	C1-C2-C3	-4.52	118.80	126.20
15	A	1127	CLA	CMD-C2D-C1D	4.51	132.67	124.73
17	B	5001	LHG	O4-P-O5	4.49	133.31	112.44
12	2	501	LUT	C39-C29-C30	-4.48	115.56	122.82
15	A	1134	CLA	CAA-C2A-C1A	-4.47	102.25	112.14
17	1	801	LHG	O4-P-O5	4.47	133.23	112.44
13	1	502	XAT	C15-C14-C13	-4.45	121.04	127.28
15	A	1124	CLA	O2D-CGD-CBD	4.45	119.01	111.23
15	A	1125	CLA	O2D-CGD-CBD	4.44	118.99	111.23
15	B	1223	CLA	O2D-CGD-CBD	4.43	118.97	111.23
14	A	4006	BCR	C33-C5-C6	-4.42	119.66	124.48
13	4	502	XAT	C26-C27-C28	-4.42	116.64	125.99
12	1	501	LUT	C12-C13-C14	4.41	125.95	119.01
15	A	1140	CLA	CBA-CAA-C2A	-4.39	100.72	113.79
17	2	801	LHG	O4-P-O5	4.39	132.88	112.44
15	A	1122	CLA	O2A-C1-C2	4.38	124.97	108.11
15	A	1124	CLA	C1-C2-C3	-4.38	119.02	126.20
17	A	5002	LHG	O7-C7-C8	4.36	120.91	111.48
14	B	4005	BCR	C33-C5-C6	-4.33	119.76	124.48
20	A	1011	CL0	O2A-CGA-CBA	4.32	125.01	111.83
14	F	4001	BCR	C38-C26-C25	-4.32	119.77	124.48
14	3	504	BCR	C33-C5-C6	-4.31	119.78	124.48
14	A	4005	BCR	C8-C7-C6	-4.29	115.53	127.00
16	3	604	CHL	CHA-C1A-C2A	-4.28	123.25	133.31
15	A	1133	CLA	C2B-C1B-NB	-4.28	105.89	110.33
20	A	1011	CL0	CHA-C1A-C2A	-4.27	123.27	133.31
15	A	1125	CLA	CMA-C3A-C4A	4.27	123.26	111.77
15	A	1102	CLA	O1D-CGD-CBD	-4.26	116.12	124.52
15	A	1134	CLA	O1D-CGD-CBD	-4.25	116.13	124.52
13	3	502	XAT	C11-C10-C9	-4.25	121.32	127.28
14	F	4001	BCR	C33-C5-C6	-4.22	119.88	124.48
13	1	502	XAT	C31-C30-C29	-4.20	121.39	127.28
17	A	5001	LHG	O7-C7-C8	4.19	120.56	111.48
14	J	4001	BCR	C33-C5-C6	-4.19	119.91	124.48
13	2	502	XAT	C38-C25-C26	-4.19	115.41	122.30
18	2	804	LMG	O7-C10-C11	4.17	120.51	111.48
14	B	4006	BCR	C28-C27-C26	-4.15	106.65	114.06
15	A	1136	CLA	C1-C2-C3	-4.14	119.42	126.20
13	2	502	XAT	C35-C15-C14	4.13	131.97	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	4002	BCR	C33-C5-C6	-4.13	119.98	124.48
15	A	1114	CLA	C1-C2-C3	-4.13	119.44	126.20
12	2	501	LUT	C19-C9-C10	-4.13	116.13	122.82
13	3	502	XAT	C38-C25-C24	4.11	118.86	114.24
15	A	1140	CLA	O2D-CGD-O1D	-4.10	115.87	123.85
15	A	1105	CLA	C1-C2-C3	-4.08	119.51	126.20
16	2	610	CHL	C3D-C4D-CHA	4.07	114.72	108.54
17	3	801	LHG	O7-C7-C8	4.07	120.28	111.48
20	A	1011	CL0	C1C-CHC-C4B	4.06	130.59	116.07
15	A	1126	CLA	C1-C2-C3	-4.06	119.55	126.20
15	B	1222	CLA	C1-C2-C3	-4.05	119.57	126.20
12	1	501	LUT	C27-C28-C29	-4.03	117.67	126.32
14	A	4002	BCR	C27-C26-C25	-4.02	117.27	122.70
14	F	4001	BCR	C29-C30-C25	4.01	116.27	110.44
14	B	4005	BCR	C28-C27-C26	-4.01	106.91	114.06
16	4	611	CHL	C3D-C4D-CHA	4.00	114.63	108.54
12	4	501	LUT	C39-C29-C28	-3.99	111.99	118.09
16	4	613	CHL	C3D-C4D-CHA	3.97	114.58	108.54
15	A	1110	CLA	O2A-C1-C2	3.96	123.34	108.11
19	3	802	3PH	O21-C21-C22	3.96	120.04	111.48
15	A	1134	CLA	CMD-C2D-C1D	3.95	131.68	124.73
12	3	501	LUT	C7-C8-C9	-3.95	120.39	126.23
12	3	501	LUT	C32-C33-C34	3.95	125.22	119.01
14	F	4002	BCR	C28-C27-C26	-3.95	107.02	114.06
16	3	604	CHL	C3D-C4D-CHA	3.94	114.53	108.54
15	4	607	CLA	CAA-C2A-C3A	-3.92	102.40	113.00
16	3	604	CHL	C1A-CHA-C4D	3.92	125.52	118.98
15	A	1127	CLA	O2A-C1-C2	3.92	123.18	108.11
15	A	1135	CLA	C1-C2-C3	-3.91	119.79	126.20
14	B	4003	BCR	C3-C4-C5	-3.91	107.09	114.06
12	4	501	LUT	C1-C6-C5	-3.90	117.31	122.64
16	1	609	CHL	C3D-C4D-CHA	3.90	114.46	108.54
16	1	610	CHL	C3D-C4D-CHA	3.89	114.45	108.54
16	4	610	CHL	C3D-C4D-CHA	3.88	114.44	108.54
16	2	613	CHL	C3D-C4D-CHA	3.88	114.43	108.54
15	B	1227	CLA	O2A-C1-C2	3.87	123.02	108.11
13	1	502	XAT	C38-C25-C26	-3.87	115.93	122.30
16	2	609	CHL	C3D-C4D-CHA	3.86	114.41	108.54
13	4	502	XAT	C38-C25-C26	-3.85	115.97	122.30
15	A	1124	CLA	O2A-C1-C2	3.85	122.91	108.11
12	4	501	LUT	C19-C9-C10	-3.84	116.59	122.82
15	A	1104	CLA	C3B-C4B-NB	-3.83	107.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1235	CLA	C1-C2-C3	-3.82	119.93	126.20
15	B	1021	CLA	C1-C2-C3	-3.82	119.94	126.20
12	1	501	LUT	C39-C29-C30	-3.82	116.63	122.82
15	A	1116	CLA	C2C-C1C-NC	3.82	113.99	109.98
13	2	502	XAT	C8-C9-C10	3.81	125.01	119.01
15	A	1139	CLA	O2A-C1-C2	3.81	122.76	108.11
14	A	4002	BCR	C19-C18-C17	3.78	124.96	119.01
12	1	501	LUT	C19-C9-C10	-3.78	116.69	122.82
15	A	1140	CLA	C2C-C1C-NC	3.78	113.95	109.98
15	B	1218	CLA	CAA-C2A-C3A	-3.77	102.81	113.00
15	B	1231	CLA	O2A-C1-C2	3.76	122.59	108.11
16	2	611	CHL	C3D-C4D-CHA	3.75	114.25	108.54
14	A	4006	BCR	C15-C14-C13	-3.73	122.04	127.28
15	A	1101	CLA	C1-C2-C3	-3.73	120.08	126.20
14	B	4002	BCR	C30-C25-C26	-3.72	117.55	122.64
15	A	1123	CLA	C1-C2-C3	-3.71	120.11	126.20
13	4	502	XAT	C35-C15-C14	3.71	131.12	123.52
15	B	1231	CLA	C1D-ND-C4D	-3.71	103.71	106.31
15	A	1122	CLA	C1-O2A-CGA	3.71	125.64	116.65
15	A	1125	CLA	C1D-ND-C4D	-3.71	103.71	106.31
21	A	2001	PQN	C11-C3-C2	-3.68	118.59	124.89
15	A	1125	CLA	C3B-C4B-NB	-3.68	107.25	110.53
13	3	502	XAT	O24-C25-C38	-3.67	110.95	115.05
12	4	501	LUT	C38-C25-C24	-3.67	114.67	123.36
15	A	1114	CLA	O2A-C1-C2	3.67	122.22	108.11
15	B	1229	CLA	C1-C2-C3	-3.66	120.20	126.20
12	3	501	LUT	C20-C13-C12	-3.66	112.50	118.09
14	A	4002	BCR	C23-C22-C21	3.65	124.75	119.01
15	A	1134	CLA	CHD-C4C-NC	-3.64	118.59	124.23
15	A	1117	CLA	O2A-C1-C2	3.64	122.11	108.11
12	3	501	LUT	C20-C13-C14	-3.63	116.93	122.82
15	B	1232	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
15	B	1230	CLA	C1-C2-C3	-3.63	120.25	126.20
14	A	4007	BCR	C8-C7-C6	-3.62	117.32	127.00
15	B	1201	CLA	C3B-C4B-NB	-3.62	107.30	110.53
16	3	604	CHL	C1-C2-C3	-3.62	120.27	126.20
15	A	1134	CLA	CHD-C4C-C3C	3.60	130.03	124.77
14	J	4002	BCR	C27-C26-C25	-3.60	117.84	122.70
14	F	4002	BCR	C19-C18-C17	-3.60	113.35	119.01
14	A	4005	BCR	C12-C13-C14	-3.59	113.36	119.01
15	A	1101	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
13	3	502	XAT	C8-C9-C10	3.59	124.66	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	5002	LHG	O8-C23-C24	3.59	122.78	111.83
16	1	609	CHL	C1-O2A-CGA	3.59	125.34	116.65
15	4	601	CLA	C3B-C4B-NB	-3.59	107.33	110.53
14	A	4003	BCR	C28-C27-C26	-3.58	107.67	114.06
15	A	1112	CLA	C1-C2-C3	-3.58	120.33	126.20
15	B	1224	CLA	C1-C2-C3	-3.58	120.33	126.20
15	A	1117	CLA	C1-C2-C3	-3.58	120.33	126.20
16	4	610	CHL	CHA-C1A-C2A	-3.57	124.92	133.31
16	2	613	CHL	CHA-C1A-C2A	-3.57	124.92	133.31
14	B	4004	BCR	C2-C1-C6	3.57	115.62	110.44
15	A	1136	CLA	O2A-C1-C2	3.56	121.82	108.11
15	A	1140	CLA	C1D-ND-C4D	-3.56	103.81	106.31
15	B	1023	CLA	O2D-CGD-CBD	3.55	117.44	111.23
21	A	2001	PQN	C14-C13-C15	3.55	121.39	115.23
14	A	4003	BCR	C4-C5-C6	-3.55	117.91	122.70
15	B	1235	CLA	O2A-C1-C2	3.54	121.75	108.11
12	2	501	LUT	C27-C28-C29	-3.53	118.72	126.32
15	A	1111	CLA	O2A-C1-C2	3.53	121.69	108.11
15	3	612	CLA	C1-C2-C3	-3.53	120.42	126.20
15	A	1114	CLA	CMA-C3A-C4A	3.52	121.23	111.77
15	3	605	CLA	C1-C2-C3	-3.52	120.44	126.20
15	4	601	CLA	CAA-C2A-C1A	-3.52	100.45	111.97
15	2	608	CLA	CAA-C2A-C3A	-3.51	103.50	113.00
15	2	616	CLA	C1-O2A-CGA	3.51	125.15	116.65
20	A	1011	CL0	O2A-C1-C2	3.51	121.62	108.11
15	A	1135	CLA	O2A-C1-C2	3.50	121.58	108.11
15	A	1123	CLA	O2A-C1-C2	3.50	121.56	108.11
14	A	4003	BCR	C33-C5-C4	3.49	121.04	113.60
14	A	4002	BCR	C37-C22-C21	-3.49	117.16	122.82
15	B	1225	CLA	O2A-C1-C2	3.48	121.50	108.11
15	B	1022	CLA	C1-C2-C3	-3.48	120.50	126.20
15	4	603	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
15	A	1114	CLA	C1D-ND-C4D	-3.46	103.89	106.31
21	A	2001	PQN	C12-C11-C3	-3.46	103.57	112.08
15	A	1138	CLA	C1-C2-C3	-3.46	120.54	126.20
15	A	1108	CLA	O2A-C1-C2	3.46	121.40	108.11
15	A	1133	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
15	A	1108	CLA	C1-C2-C3	-3.45	120.55	126.20
20	A	1011	CL0	C1-C2-C3	-3.45	120.55	126.20
15	A	1127	CLA	C1-C2-C3	-3.45	120.55	126.20
15	B	1224	CLA	O2A-C1-C2	3.44	121.34	108.11
14	B	4003	BCR	C2-C1-C6	3.44	115.44	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1228	CLA	C1-C2-C3	-3.43	120.57	126.20
15	B	1222	CLA	O2A-C1-C2	3.43	121.32	108.11
16	2	611	CHL	CHA-C1A-C2A	-3.43	125.25	133.31
15	B	1238	CLA	C5-C3-C2	-3.43	112.77	120.36
15	B	1228	CLA	O2A-C1-C2	3.43	121.30	108.11
14	B	4004	BCR	C3-C4-C5	-3.42	107.95	114.06
15	B	1227	CLA	C1-C2-C3	-3.42	120.60	126.20
15	A	1124	CLA	O1D-CGD-CBD	-3.42	117.78	124.52
15	A	1106	CLA	O2A-C1-C2	3.42	121.25	108.11
14	F	4001	BCR	C8-C9-C10	3.41	124.38	119.01
15	3	609	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
15	B	1234	CLA	CMA-C3A-C4A	3.41	120.94	111.77
14	F	4001	BCR	C8-C7-C6	-3.41	117.89	127.00
15	A	1012	CLA	C3B-C4B-NB	-3.40	107.49	110.53
12	4	501	LUT	C37-C21-C26	-3.40	104.39	109.55
14	A	4005	BCR	C38-C26-C25	-3.39	120.78	124.48
16	1	610	CHL	CHA-C1A-C2A	-3.39	125.34	133.31
15	A	1111	CLA	C1-C2-C3	-3.39	120.64	126.20
15	A	1101	CLA	O2A-C1-C2	3.39	121.15	108.11
15	A	1112	CLA	O2A-C1-C2	3.39	121.14	108.11
12	2	501	LUT	C21-C26-C27	-3.39	108.93	112.83
15	A	1102	CLA	O2A-C1-C2	3.39	121.14	108.11
14	F	4001	BCR	C34-C9-C10	-3.38	117.33	122.82
13	1	502	XAT	C36-C21-C26	3.38	119.18	110.05
15	B	1240	CLA	C5-C3-C2	3.38	128.76	121.17
18	4	801	LMG	C1-C2-C3	-3.38	102.90	110.01
14	F	4002	BCR	C27-C26-C25	-3.38	118.14	122.70
14	3	506	BCR	C35-C13-C14	-3.37	117.35	122.82
15	2	601	CLA	C3B-C4B-NB	-3.37	107.52	110.53
15	A	1116	CLA	O2A-C1-C2	3.36	121.05	108.11
15	B	1022	CLA	O2A-C1-C2	3.36	121.05	108.11
15	3	612	CLA	O2A-C1-C2	3.36	121.05	108.11
15	A	1102	CLA	C1-C2-C3	-3.36	120.69	126.20
15	4	605	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
15	B	1223	CLA	O2A-C1-C2	3.36	121.02	108.11
15	B	1202	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
14	J	4002	BCR	C15-C14-C13	-3.35	122.57	127.28
15	B	1021	CLA	O2A-C1-C2	3.35	121.01	108.11
14	A	4003	BCR	C19-C18-C17	3.35	124.28	119.01
15	3	605	CLA	O2A-C1-C2	3.35	121.00	108.11
15	A	1013	CLA	C1D-ND-C4D	-3.35	103.96	106.31
15	B	1234	CLA	O2A-C1-C2	3.35	120.99	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1124	CLA	C3B-C4B-NB	-3.34	107.54	110.53
16	4	613	CHL	C1-O2A-CGA	3.34	124.74	116.65
15	A	1109	CLA	CAA-C2A-C3A	-3.33	104.01	113.00
15	B	1228	CLA	C3B-C4B-NB	-3.32	107.56	110.53
12	4	501	LUT	C20-C13-C12	3.32	123.16	118.09
13	3	502	XAT	C19-C9-C10	-3.32	117.44	122.82
15	A	1105	CLA	O2A-C1-C2	3.32	120.88	108.11
15	B	1225	CLA	C1-C2-C3	-3.32	120.76	126.20
23	B	5002	DGD	O6D-C1D-O3G	-3.32	102.21	110.04
16	4	611	CHL	CHA-C1A-C2A	-3.31	125.53	133.31
14	F	4002	BCR	C36-C18-C19	3.31	123.14	118.09
15	A	1013	CLA	C1-C2-C3	-3.31	120.78	126.20
15	B	1220	CLA	C3B-C4B-NB	-3.30	107.58	110.53
15	B	1204	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
15	1	601	CLA	C3B-C4B-NB	-3.30	107.58	110.53
14	B	4002	BCR	C1-C6-C5	-3.30	118.13	122.64
18	4	801	LMG	O6-C1-O1	-3.30	102.26	110.04
15	B	1239	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
15	B	1226	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
15	A	1118	CLA	C2C-C1C-NC	3.29	113.43	109.98
14	F	4001	BCR	C15-C14-C13	-3.28	122.67	127.28
15	A	1137	CLA	C1-C2-C3	-3.28	120.82	126.20
15	A	1102	CLA	C3B-C4B-NB	-3.28	107.60	110.53
15	B	1229	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
15	A	1139	CLA	C1D-ND-C4D	-3.27	104.02	106.31
15	A	1107	CLA	O2A-C1-C2	3.27	120.70	108.11
15	1	613	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
13	2	502	XAT	C10-C11-C12	3.26	132.64	123.20
14	A	4002	BCR	C36-C18-C17	-3.26	117.54	122.82
15	A	1107	CLA	C1D-ND-C4D	-3.25	104.03	106.31
15	A	1103	CLA	O2A-C1-C2	3.25	120.62	108.11
15	A	1125	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
14	B	4005	BCR	C27-C26-C25	-3.24	118.33	122.70
14	J	4001	BCR	C38-C26-C25	-3.24	120.95	124.48
23	B	5002	DGD	O3G-C3G-C2G	-3.24	102.94	110.82
15	A	1101	CLA	C3B-C4B-NB	-3.24	107.64	110.53
15	B	1022	CLA	C4B-CHC-C1C	3.23	133.85	126.25
14	J	4002	BCR	C30-C25-C26	-3.23	118.22	122.64
15	A	1132	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
14	4	503	BCR	C27-C26-C25	3.23	127.07	122.70
13	1	502	XAT	C6-C7-C8	-3.23	119.16	125.99
15	B	1232	CLA	C3B-C4B-NB	-3.23	107.65	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1132	CLA	CHB-C4A-NA	3.22	129.05	124.40
15	A	1137	CLA	O2A-C1-C2	3.22	120.49	108.11
15	A	1119	CLA	C1D-ND-C4D	-3.22	104.05	106.31
15	4	608	CLA	CAC-C3C-C2C	-3.22	121.65	127.56
15	A	1106	CLA	C1-C2-C3	-3.22	120.93	126.20
12	3	501	LUT	C11-C10-C9	3.22	131.79	127.28
12	4	501	LUT	C40-C33-C32	3.22	123.00	118.09
15	A	1125	CLA	C2D-C1D-ND	3.22	113.31	110.13
12	4	501	LUT	C32-C33-C34	3.21	124.06	119.01
15	A	1133	CLA	CMD-C2D-C1D	3.21	130.38	124.73
15	F	1301	CLA	C3B-C4B-NB	-3.20	107.67	110.53
15	3	613	CLA	C3B-C4B-NB	-3.19	107.68	110.53
14	A	4008	BCR	C34-C9-C10	-3.19	117.65	122.82
15	B	1203	CLA	CHB-C4A-NA	3.19	129.00	124.40
15	A	1136	CLA	C3B-C4B-NB	-3.19	107.69	110.53
17	3	801	LHG	C5-O7-C7	-3.18	110.18	117.80
14	3	504	BCR	C38-C26-C25	-3.18	121.01	124.48
15	B	1214	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
15	1	612	CLA	C3B-C4B-NB	-3.18	107.69	110.53
14	1	503	BCR	C15-C14-C13	-3.18	122.82	127.28
15	A	1127	CLA	C3B-C4B-NB	-3.17	107.70	110.53
15	B	1216	CLA	C3B-C4B-NB	-3.17	107.70	110.53
15	A	1107	CLA	C1-C2-C3	-3.17	121.00	126.20
12	4	501	LUT	C39-C29-C30	-3.17	117.68	122.82
12	3	501	LUT	C4-C5-C6	-3.17	114.25	120.76
15	B	1238	CLA	CAC-C3C-C2C	-3.17	121.74	127.56
16	4	610	CHL	C3C-C4C-NC	-3.16	106.92	114.65
21	A	2001	PQN	C11-C12-C13	-3.16	121.38	126.83
15	A	1126	CLA	CMA-C3A-C4A	3.16	120.27	111.77
15	A	1012	CLA	O2A-C1-C2	3.16	120.26	108.11
15	A	1013	CLA	O2A-C1-C2	3.16	120.26	108.11
16	3	604	CHL	C3C-C4C-NC	-3.16	106.94	114.65
14	A	4003	BCR	C33-C5-C6	-3.16	121.04	124.48
15	A	1122	CLA	CMA-C3A-C4A	3.15	120.25	111.77
16	2	609	CHL	CHA-C1A-C2A	-3.15	125.91	133.31
15	A	1013	CLA	C3B-C4B-NB	-3.15	107.72	110.53
14	J	4002	BCR	C33-C5-C4	3.15	120.30	113.60
15	A	1128	CLA	C3B-C4B-NB	-3.14	107.73	110.53
15	B	1023	CLA	CMD-C2D-C3D	-3.14	120.49	127.69
15	B	1235	CLA	C3B-C4B-NB	-3.14	107.73	110.53
15	A	1138	CLA	C3B-C4B-NB	-3.13	107.73	110.53
13	4	502	XAT	C35-C34-C33	3.13	131.67	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1103	CLA	C1D-ND-C4D	-3.13	104.11	106.31
15	1	606	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
15	B	1202	CLA	C3B-C4B-NB	-3.13	107.73	110.53
15	A	1130	CLA	C3B-C4B-NB	-3.13	107.74	110.53
15	B	1224	CLA	CMA-C3A-C4A	3.13	120.18	111.77
16	2	610	CHL	C3C-C4C-NC	-3.13	107.01	114.65
14	F	4001	BCR	C35-C13-C12	3.13	122.86	118.09
14	B	4003	BCR	C15-C14-C13	-3.12	122.90	127.28
15	3	607	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
15	A	1126	CLA	O2A-C1-C2	3.12	120.12	108.11
15	B	1225	CLA	C3B-C4B-NB	-3.12	107.75	110.53
14	A	4007	BCR	C36-C18-C19	3.12	122.85	118.09
15	B	1215	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
15	A	1106	CLA	C3B-C4B-NB	-3.11	107.75	110.53
15	4	609	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
15	3	613	CLA	CMA-C3A-C4A	3.11	120.12	111.77
20	A	1011	CL0	C4-C3-C5	3.10	120.62	115.23
14	F	4002	BCR	C37-C22-C23	3.10	122.83	118.09
14	B	4002	BCR	C3-C4-C5	-3.10	108.53	114.06
15	A	1126	CLA	C3B-C4B-NB	-3.10	107.76	110.53
15	A	1124	CLA	CHA-C1A-NA	-3.10	119.37	126.39
16	4	611	CHL	C3C-C4C-NC	-3.10	107.08	114.65
15	A	1134	CLA	CAC-C3C-C4C	3.10	128.82	124.79
15	A	1012	CLA	C1-C2-C3	-3.09	121.13	126.20
15	J	1302	CLA	C3B-C4B-NB	-3.09	107.77	110.53
14	4	503	BCR	C15-C16-C17	-3.09	117.19	123.52
15	B	1224	CLA	C3B-C4B-NB	-3.09	107.77	110.53
15	A	1128	CLA	CMA-C3A-C4A	3.09	120.08	111.77
15	2	608	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
15	4	606	CLA	C3B-C4B-NB	-3.09	107.77	110.53
15	A	1111	CLA	C3B-C4B-NB	-3.09	107.77	110.53
15	1	612	CLA	C3A-C2A-C1A	-3.09	103.14	106.30
15	A	1114	CLA	C3B-C4B-NB	-3.09	107.78	110.53
15	1	603	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
15	B	1218	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
15	B	1222	CLA	C3B-C4B-NB	-3.08	107.78	110.53
15	F	1301	CLA	C1D-ND-C4D	-3.08	104.15	106.31
16	2	613	CHL	C3C-C4C-NC	-3.08	107.13	114.65
15	A	1110	CLA	C3B-C4B-NB	-3.08	107.78	110.53
15	A	1108	CLA	C3B-C4B-NB	-3.07	107.79	110.53
15	B	1231	CLA	CMD-C2D-C3D	-3.07	120.64	127.69
15	A	1110	CLA	C1-C2-C3	-3.07	121.16	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	801	LHG	O8-C23-C24	3.07	121.20	111.83
15	3	615	CLA	C3B-C4B-NB	-3.07	107.79	110.53
16	2	611	CHL	C3C-C4C-NC	-3.07	107.15	114.65
15	A	1136	CLA	C1D-ND-C4D	-3.07	104.16	106.31
15	B	1206	CLA	CHB-C4A-NA	3.07	128.82	124.40
15	B	1205	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
15	3	615	CLA	CMA-C3A-C4A	3.06	120.00	111.77
15	A	1101	CLA	C1D-ND-C4D	-3.06	104.17	106.31
15	A	1120	CLA	C1D-ND-C4D	-3.06	104.17	106.31
15	3	612	CLA	C3B-C4B-NB	-3.06	107.80	110.53
15	A	1135	CLA	C3B-C4B-NB	-3.05	107.81	110.53
15	B	1021	CLA	C3B-C4B-NB	-3.05	107.81	110.53
16	2	613	CHL	C1A-CHA-C4D	3.05	124.07	118.98
15	A	1105	CLA	C3B-C4B-NB	-3.05	107.81	110.53
12	3	501	LUT	C21-C26-C27	-3.05	109.32	112.83
15	A	1123	CLA	C3B-C4B-NB	-3.05	107.81	110.53
15	2	616	CLA	O2A-CGA-O1A	-3.05	116.01	123.63
15	A	1123	CLA	C1D-ND-C4D	-3.05	104.17	106.31
15	A	1137	CLA	C3B-C4B-NB	-3.04	107.81	110.53
13	2	502	XAT	C20-C13-C12	-3.04	113.44	118.09
12	2	501	LUT	C26-C27-C28	3.04	129.31	124.58
13	3	502	XAT	C18-C5-C4	3.04	117.65	114.24
15	A	1105	CLA	CMA-C3A-C4A	3.04	119.94	111.77
15	B	1207	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
15	B	1221	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
15	B	1206	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
15	1	602	CLA	C3B-C4B-NB	-3.03	107.82	110.53
16	2	610	CHL	CHA-C1A-C2A	-3.03	126.19	133.31
16	1	610	CHL	C3C-C4C-NC	-3.03	107.24	114.65
23	B	5002	DGD	C1E-O6E-C5E	3.03	119.64	113.72
15	1	615	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
15	A	1103	CLA	C3B-C4B-NB	-3.03	107.83	110.53
15	A	1109	CLA	C3B-C4B-NB	-3.03	107.83	110.53
16	4	613	CHL	CHA-C1A-C2A	-3.03	126.20	133.31
13	2	502	XAT	C26-C27-C28	-3.03	119.59	125.99
15	A	1109	CLA	O2A-C1-C2	3.03	119.75	108.11
15	4	604	CLA	CHB-C4A-NA	3.02	128.76	124.40
15	A	1112	CLA	C3B-C4B-NB	-3.02	107.83	110.53
15	A	1116	CLA	C1C-C2C-C3C	-3.02	103.80	106.98
15	B	1235	CLA	CMA-C3A-C4A	3.02	119.89	111.77
15	B	1239	CLA	CHB-C4A-NA	3.02	128.76	124.40
14	A	4004	BCR	C27-C26-C25	-3.02	118.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1102	CLA	C1D-ND-C4D	-3.02	104.19	106.31
15	A	1120	CLA	C3B-C4B-NB	-3.02	107.83	110.53
15	A	1141	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
15	A	1113	CLA	CMA-C3A-C4A	3.02	119.89	111.77
15	3	605	CLA	C3B-C4B-NB	-3.02	107.83	110.53
15	B	1230	CLA	C3B-C4B-NB	-3.02	107.84	110.53
15	B	1236	CLA	C1D-ND-C4D	-3.02	104.19	106.31
15	A	1131	CLA	C3B-C4B-NB	-3.02	107.84	110.53
15	B	1210	CLA	C3B-C4B-NB	-3.01	107.84	110.53
15	1	603	CLA	CHB-C4A-NA	3.01	128.75	124.40
15	A	1122	CLA	C1-C2-C3	-3.01	121.26	126.20
15	A	1131	CLA	CMA-C3A-C4A	3.01	119.86	111.77
15	A	1113	CLA	C2C-C1C-NC	3.01	113.14	109.98
15	4	602	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
15	B	1225	CLA	C1D-ND-C4D	-3.00	104.20	106.31
15	4	604	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
15	2	602	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	A	4002	BCR	C30-C25-C26	-3.00	118.53	122.64
15	3	605	CLA	C1D-ND-C4D	-3.00	104.21	106.31
14	A	4005	BCR	C37-C22-C23	3.00	122.67	118.09
14	A	4005	BCR	C33-C5-C4	3.00	119.99	113.60
15	A	1122	CLA	C3B-C4B-NB	-3.00	107.86	110.53
16	1	609	CHL	C3C-C4C-NC	-2.99	107.33	114.65
15	A	1135	CLA	CMA-C3A-C4A	2.99	119.82	111.77
15	2	607	CLA	C3B-C4B-NB	-2.99	107.86	110.53
15	2	616	CLA	C3B-C4B-NB	-2.99	107.86	110.53
15	B	1236	CLA	C3B-C4B-NB	-2.99	107.86	110.53
15	A	1137	CLA	CMA-C3A-C4A	2.99	119.81	111.77
15	4	603	CLA	CHB-C4A-NA	2.99	128.71	124.40
15	B	1209	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
15	4	603	CLA	O2D-CGD-CBD	2.98	116.45	111.23
15	B	1230	CLA	O2A-C1-C2	2.98	119.59	108.11
15	3	614	CLA	CHB-C4A-NA	2.98	128.70	124.40
15	B	1221	CLA	C3B-C4B-NB	-2.98	107.87	110.53
15	B	1228	CLA	CMA-C3A-C4A	2.98	119.79	111.77
15	B	1216	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
15	A	1134	CLA	CED-O2D-CGD	2.98	122.67	115.92
16	2	609	CHL	C1-O2A-CGA	2.98	123.86	116.65
15	B	1229	CLA	CMA-C3A-C4A	2.98	119.78	111.77
15	A	1119	CLA	C1-C2-C3	-2.98	121.32	126.20
15	B	1023	CLA	CHD-C1D-ND	-2.98	120.61	124.80
15	B	1240	CLA	C3B-C4B-NB	-2.98	107.87	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1223	CLA	C1-C2-C3	-2.98	121.32	126.20
15	A	1120	CLA	CMA-C3A-C4A	2.98	119.77	111.77
15	2	607	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
15	B	1222	CLA	CMA-C3A-C4A	2.98	119.77	111.77
13	1	502	XAT	C27-C28-C29	-2.97	120.92	125.53
15	A	1110	CLA	C1D-ND-C4D	-2.97	104.23	106.31
15	B	1214	CLA	CHB-C4A-NA	2.97	128.69	124.40
15	B	1227	CLA	CMD-C2D-C3D	-2.97	120.88	127.69
15	A	1108	CLA	C1D-ND-C4D	-2.97	104.23	106.31
15	B	1228	CLA	C1D-ND-C4D	-2.97	104.23	106.31
15	A	1133	CLA	C3B-C2B-C1B	2.97	110.67	107.17
16	1	609	CHL	CHA-C1A-C2A	-2.97	126.34	133.31
15	A	1127	CLA	C2C-C1C-NC	2.97	113.10	109.98
15	B	1238	CLA	C3B-C4B-NB	-2.97	107.88	110.53
15	B	1210	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
15	B	1234	CLA	C3B-C4B-NB	-2.97	107.88	110.53
16	2	609	CHL	C3C-C4C-NC	-2.97	107.40	114.65
15	A	1123	CLA	CMA-C3A-C4A	2.96	119.74	111.77
14	3	506	BCR	C1-C6-C5	-2.96	118.58	122.64
15	A	1121	CLA	C3B-C4B-NB	-2.96	107.89	110.53
13	4	502	XAT	C31-C32-C33	-2.96	118.25	126.36
20	A	1011	CL0	O1D-CGD-CBD	-2.96	120.24	124.72
16	4	613	CHL	C3C-C4C-NC	-2.96	107.42	114.65
15	A	1127	CLA	OBD-CAD-C3D	-2.96	121.51	128.42
15	B	1235	CLA	C1D-ND-C4D	-2.96	104.24	106.31
14	3	504	BCR	C33-C5-C4	2.96	119.90	113.60
15	A	1136	CLA	CMA-C3A-C4A	2.95	119.71	111.77
15	4	608	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
15	A	1137	CLA	C1D-ND-C4D	-2.95	104.24	106.31
15	A	1130	CLA	CMA-C3A-C4A	2.95	119.70	111.77
12	3	501	LUT	C40-C33-C34	-2.95	118.04	122.82
15	1	605	CLA	CHB-C4A-NA	2.95	128.66	124.40
15	A	1111	CLA	CMA-C3A-C4A	2.95	119.70	111.77
15	3	611	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	B	1226	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	A	1108	CLA	CMA-C3A-C4A	2.95	119.69	111.77
15	J	1302	CLA	CMA-C3A-C4A	2.95	119.69	111.77
15	1	608	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	4	616	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	2	502	XAT	C31-C32-C33	-2.94	118.30	126.36
15	A	1131	CLA	C1D-ND-C4D	-2.94	104.25	106.31
15	1	604	CLA	C3B-C4B-NB	-2.94	107.90	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1138	CLA	O2A-C1-C2	2.94	119.43	108.11
15	B	1211	CLA	C3B-C4B-NB	-2.94	107.91	110.53
14	A	4008	BCR	C38-C26-C25	-2.94	121.28	124.48
15	A	1110	CLA	CMA-C3A-C4A	2.94	119.67	111.77
15	A	1111	CLA	C1D-ND-C4D	-2.94	104.25	106.31
15	3	603	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
15	A	1012	CLA	C1D-ND-C4D	-2.93	104.25	106.31
15	2	612	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
15	2	604	CLA	CHB-C4A-NA	2.93	128.63	124.40
15	A	1129	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
15	2	605	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
15	A	1134	CLA	C1D-ND-C4D	-2.93	104.25	106.31
15	A	1106	CLA	C1D-ND-C4D	-2.93	104.25	106.31
14	A	4003	BCR	C29-C30-C25	2.93	114.70	110.44
15	1	611	CLA	C3B-C4B-NB	-2.93	107.91	110.53
15	B	1023	CLA	C1C-C2C-C3C	-2.93	103.90	106.98
15	1	607	CLA	C3B-C4B-NB	-2.93	107.92	110.53
15	A	1106	CLA	CMA-C3A-C4A	2.93	119.64	111.77
15	3	601	CLA	C3B-C4B-NB	-2.93	107.92	110.53
15	A	1140	CLA	C7-C6-C5	-2.93	105.46	113.26
15	3	610	CLA	C3B-C4B-NB	-2.92	107.92	110.53
15	3	615	CLA	C1D-ND-C4D	-2.92	104.26	106.31
15	B	1236	CLA	CMA-C3A-C4A	2.92	119.62	111.77
15	B	1226	CLA	CHB-C4A-NA	2.92	128.61	124.40
15	3	613	CLA	C1D-ND-C4D	-2.92	104.27	106.31
14	A	4005	BCR	C34-C9-C10	-2.92	118.09	122.82
15	4	612	CLA	C3B-C4B-NB	-2.92	107.93	110.53
15	A	1138	CLA	C1D-ND-C4D	-2.92	104.27	106.31
15	A	1112	CLA	CMA-C3A-C4A	2.92	119.61	111.77
18	2	803	LMG	O6-C1-O1	-2.91	103.16	110.04
15	A	1133	CLA	CHA-C4D-ND	2.91	138.56	132.55
15	A	1118	CLA	C1C-C2C-C3C	-2.91	103.92	106.98
15	A	1130	CLA	C1D-ND-C4D	-2.91	104.27	106.31
15	B	1022	CLA	C4A-NA-C1A	2.91	108.01	106.68
15	A	1115	CLA	C3B-C4B-NB	-2.91	107.93	110.53
15	A	1104	CLA	O2A-C1-C2	2.91	119.31	108.11
14	B	4001	BCR	C15-C14-C13	-2.91	123.19	127.28
14	A	4006	BCR	C23-C24-C25	-2.91	119.22	127.00
15	A	1128	CLA	O2A-C1-C2	2.91	119.31	108.11
15	1	615	CLA	C4-C3-C2	-2.91	110.10	125.12
15	1	606	CLA	C3B-C4B-NB	-2.91	107.93	110.53
15	B	1227	CLA	C3B-C4B-NB	-2.91	107.93	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1021	CLA	C1D-ND-C4D	-2.90	104.27	106.31
15	A	1012	CLA	CMA-C3A-C4A	2.90	119.58	111.77
15	2	603	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
14	A	4003	BCR	C8-C9-C10	2.90	123.58	119.01
15	B	1211	CLA	CHB-C4A-NA	2.90	128.59	124.40
15	B	1207	CLA	C3B-C4B-NB	-2.90	107.94	110.53
15	1	604	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	1	503	BCR	C24-C23-C22	-2.90	121.94	126.23
15	J	1302	CLA	C1D-ND-C4D	-2.90	104.28	106.31
15	A	1121	CLA	CMA-C3A-C4A	2.90	119.57	111.77
15	B	1218	CLA	CHB-C4A-NA	2.90	128.58	124.40
15	A	1133	CLA	CHA-C1A-NA	-2.90	119.83	126.39
15	B	1225	CLA	CMA-C3A-C4A	2.90	119.56	111.77
12	3	501	LUT	C26-C27-C28	2.90	129.09	124.58
15	3	605	CLA	CMA-C3A-C4A	2.90	119.56	111.77
15	B	1229	CLA	O2A-C1-C2	2.89	119.25	108.11
15	2	606	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
13	4	502	XAT	C10-C11-C12	2.89	131.58	123.20
15	1	603	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
15	B	1218	CLA	C3B-C4B-NB	-2.89	107.95	110.53
14	F	4001	BCR	C40-C30-C25	-2.89	105.72	110.24
15	B	1231	CLA	CMC-C2C-C1C	2.89	129.54	125.03
15	3	612	CLA	CMA-C3A-C4A	2.89	119.53	111.77
15	A	1110	CLA	C1-O2A-CGA	2.89	123.64	116.65
16	2	610	CHL	C4D-CHA-CBD	-2.88	106.06	108.97
15	B	1223	CLA	CMA-C3A-C4A	2.88	119.52	111.77
15	4	603	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	B	1231	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	3	609	CLA	O2D-CGD-CBD	2.88	116.26	111.23
15	B	1230	CLA	CMB-C2B-C1B	2.88	129.80	125.42
15	B	1222	CLA	C1D-ND-C4D	-2.87	104.30	106.31
15	A	1112	CLA	C1D-ND-C4D	-2.87	104.30	106.31
15	A	1135	CLA	C1D-ND-C4D	-2.87	104.30	106.31
15	A	1127	CLA	CHA-C4D-ND	2.87	138.47	132.55
12	2	501	LUT	C40-C33-C32	2.87	122.47	118.09
14	A	4007	BCR	C34-C9-C8	2.87	122.47	118.09
15	A	1107	CLA	C1C-C2C-C3C	-2.87	103.97	106.98
15	A	1141	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	A	1104	CLA	C1D-ND-C4D	-2.87	104.30	106.31
15	B	1201	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
15	2	602	CLA	CHB-C4A-NA	2.86	128.53	124.40
15	A	1119	CLA	O2A-C1-C2	2.86	119.12	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1139	CLA	C3B-C4B-NB	-2.86	107.98	110.53
15	A	1013	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
15	A	1117	CLA	C3B-C4B-NB	-2.85	107.98	110.53
15	B	1229	CLA	C1D-ND-C4D	-2.85	104.31	106.31
15	A	1103	CLA	CMA-C3A-C4A	2.85	119.43	111.77
12	1	501	LUT	C32-C33-C34	2.85	123.49	119.01
12	2	501	LUT	C32-C33-C34	2.85	123.49	119.01
15	4	606	CLA	C1-C2-C3	-2.85	122.16	126.76
15	1	607	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
15	B	1237	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
15	A	1101	CLA	O2A-CGA-CBA	2.84	120.49	111.83
18	2	802	LMG	O6-C1-O1	-2.84	103.34	110.04
12	3	501	LUT	C27-C28-C29	-2.84	120.22	126.32
15	4	602	CLA	CHB-C4A-NA	2.84	128.50	124.40
15	B	1219	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
15	B	1224	CLA	C1D-ND-C4D	-2.83	104.32	106.31
15	A	1119	CLA	C3B-C4B-NB	-2.83	108.00	110.53
15	A	1116	CLA	CHD-C1D-ND	-2.83	120.81	124.80
15	A	1138	CLA	CMA-C3A-C4A	2.83	119.38	111.77
16	1	610	CHL	C1A-CHA-C4D	2.83	123.70	118.98
14	A	4003	BCR	C36-C18-C17	-2.83	118.23	122.82
15	B	1223	CLA	CAA-C2A-C3A	-2.83	105.36	113.00
12	4	501	LUT	C21-C26-C27	2.83	116.08	112.83
15	B	1212	CLA	CHB-C4A-NA	2.83	128.48	124.40
15	B	1203	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
15	B	1022	CLA	CHA-C4D-ND	2.83	138.38	132.55
15	3	610	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	2	616	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	3	601	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	A	1113	CLA	C1D-ND-C4D	-2.82	104.34	106.31
15	A	1109	CLA	C2C-C1C-NC	2.81	112.94	109.98
14	A	4002	BCR	C15-C14-C13	-2.81	123.33	127.28
14	J	4001	BCR	C8-C9-C10	2.81	123.43	119.01
15	A	1122	CLA	C1D-ND-C4D	-2.81	104.34	106.31
14	B	4002	BCR	C2-C1-C6	2.81	114.52	110.44
15	A	1109	CLA	CMA-C3A-C4A	2.81	119.32	111.77
15	A	1134	CLA	CMA-C3A-C4A	2.81	119.32	111.77
14	B	4001	BCR	C33-C5-C6	-2.81	121.42	124.48
15	B	1226	CLA	C3B-C4B-NB	-2.81	108.03	110.53
14	A	4003	BCR	C34-C9-C10	-2.81	118.27	122.82
15	4	607	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	2	610	CHL	C1A-CHA-C4D	2.80	123.66	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	502	XAT	C11-C12-C13	-2.80	118.68	126.36
16	4	611	CHL	C1A-CHA-C4D	2.80	123.66	118.98
15	4	612	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
15	B	1201	CLA	CHB-C4A-NA	2.80	128.44	124.40
14	B	4005	BCR	C33-C5-C4	2.80	119.56	113.60
15	B	1215	CLA	CHB-C4A-NA	2.80	128.44	124.40
15	B	1229	CLA	C2C-C1C-NC	2.80	112.92	109.98
15	B	1234	CLA	CMD-C2D-C3D	-2.79	121.28	127.69
20	A	1011	CL0	CBC-CAC-C3C	-2.79	108.87	112.87
15	2	616	CLA	C1-C2-C3	-2.79	121.62	126.20
15	A	1113	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
15	A	1132	CLA	CAC-C3C-C2C	2.79	132.69	127.56
15	B	1238	CLA	CBC-CAC-C3C	2.79	119.99	112.42
15	A	1116	CLA	C1-O2A-CGA	2.79	123.40	116.65
16	2	611	CHL	C1-O2A-CGA	2.79	124.59	116.67
15	A	1117	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
15	4	609	CLA	CHB-C4A-NA	2.79	128.42	124.40
15	B	1217	CLA	C3B-C4B-NB	-2.79	108.04	110.53
15	A	1134	CLA	C3D-C2D-C1D	-2.79	102.03	105.83
14	B	4006	BCR	C30-C25-C24	2.78	123.20	115.65
15	1	605	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
15	B	1208	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
21	A	2001	PQN	C7-C8-C9	-2.78	116.81	120.24
15	A	1121	CLA	C2C-C1C-NC	2.78	112.90	109.98
15	B	1238	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
16	4	611	CHL	C4D-CHA-CBD	-2.78	106.17	108.97
12	2	501	LUT	C12-C13-C14	2.77	123.37	119.01
13	1	502	XAT	C37-C21-C36	-2.77	103.34	107.37
15	A	1129	CLA	C3B-C4B-NB	-2.77	108.06	110.53
15	A	1128	CLA	C1D-ND-C4D	-2.77	104.37	106.31
15	B	1211	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
15	3	606	CLA	C3B-C4B-NB	-2.77	108.06	110.53
14	A	4007	BCR	C31-C1-C6	-2.77	105.90	110.24
15	B	1230	CLA	CMA-C3A-C4A	2.77	119.21	111.77
15	A	1133	CLA	OBD-CAD-C3D	-2.77	121.95	128.42
15	B	1227	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
14	J	4001	BCR	C33-C5-C4	2.77	119.49	113.60
15	A	1013	CLA	CMA-C3A-C4A	2.76	119.20	111.77
15	A	1107	CLA	O2A-CGA-CBA	2.76	120.26	111.83
15	3	611	CLA	C3B-C4B-NB	-2.76	108.06	110.53
15	A	1128	CLA	C2C-C1C-NC	2.76	112.88	109.98
15	A	1134	CLA	C2A-C3A-C4A	-2.76	97.41	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1115	CLA	C1D-ND-C4D	-2.76	104.38	106.31
15	A	1114	CLA	CAA-CBA-CGA	-2.76	105.37	113.21
15	A	1139	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
16	3	604	CHL	C1-O2A-CGA	2.76	123.33	116.65
15	2	612	CLA	CHB-C4A-NA	2.76	128.38	124.40
15	B	1231	CLA	CHA-C4D-ND	2.76	138.24	132.55
15	A	1119	CLA	C4B-CHC-C1C	2.76	132.73	126.25
15	2	603	CLA	C3B-C4B-NB	-2.76	108.07	110.53
14	A	4005	BCR	C36-C18-C17	-2.76	118.35	122.82
17	B	5001	LHG	O8-C23-C24	2.76	120.24	111.83
15	3	608	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
14	J	4002	BCR	C35-C13-C12	2.75	122.29	118.09
15	B	1237	CLA	CHB-C4A-NA	2.75	128.37	124.40
14	F	4001	BCR	C28-C29-C30	-2.75	104.70	114.43
15	B	1223	CLA	O1D-CGD-CBD	-2.75	119.10	124.52
14	3	506	BCR	C15-C16-C17	-2.75	117.90	123.52
15	3	605	CLA	C2C-C1C-NC	2.75	112.87	109.98
15	A	1107	CLA	C3B-C4B-NB	-2.75	108.08	110.53
14	J	4001	BCR	C23-C24-C25	-2.74	119.67	127.00
15	3	601	CLA	CHB-C4A-NA	2.74	128.36	124.40
15	A	1013	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
14	A	4004	BCR	C30-C25-C26	-2.74	118.89	122.64
15	F	1302	CLA	CHB-C4A-NA	2.74	128.36	124.40
14	A	4008	BCR	C36-C18-C17	-2.74	118.37	122.82
15	1	602	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
15	F	1301	CLA	CMA-C3A-C4A	2.74	119.14	111.77
15	A	1117	CLA	CMA-C3A-C4A	2.74	119.13	111.77
15	A	1107	CLA	C2C-C1C-NC	2.74	112.86	109.98
15	B	1234	CLA	C2C-C1C-NC	2.74	112.86	109.98
16	2	611	CHL	C1A-CHA-C4D	2.74	123.55	118.98
15	A	1114	CLA	O2A-CGA-CBA	2.74	120.18	111.83
15	3	612	CLA	C1D-ND-C4D	-2.74	104.39	106.31
14	B	4001	BCR	C30-C25-C26	-2.73	118.90	122.64
14	1	503	BCR	C33-C5-C6	-2.73	121.50	124.48
15	A	1109	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
14	F	4001	BCR	C12-C13-C14	-2.73	114.71	119.01
15	A	1127	CLA	C4B-CHC-C1C	2.73	132.66	126.25
15	A	1112	CLA	C2C-C1C-NC	2.73	112.85	109.98
15	A	1117	CLA	C1D-ND-C4D	-2.73	104.40	106.31
15	2	605	CLA	CHB-C4A-NA	2.73	128.33	124.40
15	A	1132	CLA	CAC-C3C-C4C	-2.72	121.24	124.79
15	4	612	CLA	CHB-C4A-NA	2.72	128.33	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1114	CLA	C4B-CHC-C1C	2.72	132.65	126.25
15	A	1140	CLA	C1-O2A-CGA	2.72	123.24	116.65
15	A	1121	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
14	J	4001	BCR	C34-C9-C10	-2.72	118.41	122.82
14	A	4007	BCR	C35-C13-C14	-2.72	118.41	122.82
14	A	4003	BCR	C15-C14-C13	-2.72	123.46	127.28
15	B	1227	CLA	CHA-C4D-ND	2.72	138.16	132.55
15	1	615	CLA	C3B-C4B-NB	-2.72	108.10	110.53
15	3	607	CLA	C3B-C4B-NB	-2.72	108.10	110.53
13	2	502	XAT	C36-C21-C22	-2.72	104.19	108.97
14	B	4006	BCR	C33-C5-C4	2.72	119.39	113.60
15	1	608	CLA	C3B-C4B-NB	-2.72	108.10	110.53
15	4	606	CLA	CHB-C4A-NA	2.72	128.32	124.40
15	A	1114	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
15	A	1140	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
15	B	1240	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
15	A	1105	CLA	C2C-C1C-NC	2.72	112.83	109.98
16	4	610	CHL	C1A-CHA-C4D	2.71	123.51	118.98
14	A	4007	BCR	C40-C30-C25	-2.71	105.99	110.24
15	B	1238	CLA	C4-C3-C5	-2.71	110.52	115.23
15	2	606	CLA	C3B-C4B-NB	-2.71	108.11	110.53
15	A	1127	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
15	A	1121	CLA	C1D-ND-C4D	-2.71	104.41	106.31
14	2	503	BCR	C33-C5-C6	-2.71	121.53	124.48
14	B	4003	BCR	C7-C8-C9	-2.71	122.23	126.23
15	4	607	CLA	CHB-C4A-NA	2.70	128.30	124.40
12	1	501	LUT	C35-C34-C33	-2.70	123.49	127.28
15	1	601	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
15	3	606	CLA	CHB-C4A-NA	2.70	128.30	124.40
15	A	1117	CLA	C2C-C1C-NC	2.70	112.82	109.98
15	B	1224	CLA	C2C-C1C-NC	2.70	112.82	109.98
15	B	1217	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
15	B	1230	CLA	C1D-ND-C4D	-2.70	104.42	106.31
15	A	1117	CLA	CAA-C2A-C3A	-2.70	105.71	113.00
15	2	608	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	3	611	CLA	CHB-C4A-NA	2.69	128.29	124.40
15	B	1234	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
15	A	1134	CLA	CHC-C1C-NC	-2.69	120.25	124.31
19	3	802	3PH	O31-C31-C32	2.69	120.05	111.83
15	3	606	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
15	B	1237	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	B	1209	CLA	CHB-C4A-NA	2.69	128.28	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	5002	LHG	C5-O7-C7	-2.68	111.37	117.80
15	2	616	CLA	CHB-C4A-NA	2.68	128.27	124.40
14	A	4008	BCR	C19-C18-C17	2.68	123.23	119.01
15	A	1140	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	A	1115	CLA	C2C-C1C-NC	2.68	112.80	109.98
15	B	1022	CLA	CBB-CAB-C3B	-2.68	114.14	127.53
15	B	1022	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
13	4	502	XAT	C36-C21-C22	-2.68	104.26	108.97
15	2	612	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	A	1120	CLA	C2C-C1C-NC	2.67	112.79	109.98
15	A	1113	CLA	C3B-C4B-NB	-2.67	108.14	110.53
15	A	1124	CLA	CHA-C4D-ND	2.67	138.06	132.55
15	B	1228	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
15	B	1215	CLA	C1-C2-C3	-2.67	121.82	126.20
15	3	612	CLA	C2C-C1C-NC	2.67	112.79	109.98
16	4	610	CHL	C4C-CHD-C1D	2.67	125.62	116.07
15	1	602	CLA	CHB-C4A-NA	2.67	128.25	124.40
15	A	1116	CLA	C4B-CHC-C1C	2.67	132.52	126.25
17	2	801	LHG	O8-C23-C24	2.67	119.97	111.83
15	3	615	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
15	A	1131	CLA	C2C-C1C-NC	2.67	112.78	109.98
15	B	1224	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
15	A	1102	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
15	A	1120	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
15	A	1107	CLA	CMA-C3A-C4A	2.66	118.93	111.77
15	A	1112	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
15	3	612	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
15	B	1021	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
15	A	1105	CLA	C1D-ND-C4D	-2.66	104.45	106.31
15	A	1134	CLA	C4D-CHA-C1A	2.66	124.41	121.24
15	A	1133	CLA	CGD-CBD-CAD	-2.65	102.25	110.85
15	A	1105	CLA	C4B-CHC-C1C	2.65	132.49	126.25
15	A	1103	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
15	A	1117	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
15	A	1126	CLA	C2C-C1C-NC	2.65	112.76	109.98
15	B	1022	CLA	CMC-C2C-C1C	2.65	129.17	125.03
15	A	1135	CLA	C2C-C1C-NC	2.65	112.76	109.98
15	B	1222	CLA	C2C-C1C-NC	2.65	112.76	109.98
16	2	611	CHL	C4D-CHA-CBD	-2.65	106.30	108.97
15	F	1301	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
15	A	1134	CLA	CAC-C3C-C2C	-2.64	122.70	127.56
15	A	1012	CLA	O2A-CGA-CBA	2.64	119.90	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1126	CLA	C1D-ND-C4D	-2.64	104.46	106.31
15	B	1021	CLA	C2C-C1C-NC	2.64	112.76	109.98
15	3	614	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
15	A	1109	CLA	C1D-ND-C4D	-2.64	104.46	106.31
15	A	1102	CLA	C1-O2A-CGA	2.64	123.04	116.65
15	4	604	CLA	C3B-C4B-NB	-2.64	108.17	110.53
15	A	1122	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
15	B	1222	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
15	A	1125	CLA	C2C-C1C-NC	2.64	112.75	109.98
15	B	1230	CLA	CAA-CBA-CGA	-2.64	105.72	113.21
15	1	601	CLA	CHB-C4A-NA	2.64	128.21	124.40
15	A	1137	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
15	A	1139	CLA	C2C-C1C-NC	2.64	112.75	109.98
15	A	1132	CLA	O2D-CGD-CBD	2.64	115.84	111.23
15	4	606	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
15	2	607	CLA	CHB-C4A-NA	2.64	128.20	124.40
15	A	1133	CLA	O2A-C1-C2	2.63	118.25	108.11
14	A	4007	BCR	C38-C26-C25	-2.63	121.61	124.48
15	3	605	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
15	A	1106	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
15	3	615	CLA	C2C-C1C-NC	2.63	112.75	109.98
15	A	1108	CLA	C2C-C1C-NC	2.63	112.75	109.98
15	2	602	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	B	1213	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	A	1128	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
15	B	1209	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	B	1214	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	J	1302	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
15	B	1205	CLA	O2A-CGA-O1A	-2.63	117.06	123.63
15	A	1124	CLA	C4B-CHC-C1C	2.63	132.42	126.25
15	A	1136	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
15	A	1132	CLA	C3B-C4B-NB	-2.62	108.19	110.53
15	2	604	CLA	C3B-C4B-NB	-2.62	108.19	110.53
15	J	1302	CLA	C2C-C1C-NC	2.62	112.74	109.98
14	B	4004	BCR	C15-C16-C17	-2.62	118.15	123.52
15	A	1122	CLA	C2C-C1C-NC	2.62	112.73	109.98
15	A	1115	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
15	B	1236	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
15	4	601	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
15	4	608	CLA	CBC-CAC-C3C	2.62	119.51	112.42
15	A	1133	CLA	CHD-C1D-ND	-2.62	121.12	124.80
15	A	1131	CLA	C1C-C2C-C3C	-2.62	104.23	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1137	CLA	C2C-C1C-NC	2.62	112.73	109.98
12	4	501	LUT	C7-C6-C5	-2.61	115.53	121.56
15	A	1130	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
15	B	1205	CLA	C3B-C4B-NB	-2.61	108.20	110.53
15	A	1125	CLA	C4D-CHA-C1A	2.61	124.36	121.24
15	A	1134	CLA	C2D-C1D-ND	2.61	112.71	110.13
15	B	1213	CLA	CHB-C4A-NA	2.61	128.17	124.40
14	A	4007	BCR	C37-C22-C23	2.61	122.08	118.09
15	1	612	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
15	B	1235	CLA	C2C-C1C-NC	2.61	112.72	109.98
14	A	4006	BCR	C33-C5-C4	2.61	119.16	113.60
15	A	1125	CLA	O2A-C1-C2	2.61	118.15	108.11
13	4	502	XAT	C36-C21-C26	2.61	117.09	110.05
15	A	1108	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
14	A	4003	BCR	C3-C4-C5	-2.61	109.41	114.06
15	B	1022	CLA	CHA-C1A-NA	-2.61	120.49	126.39
14	A	4005	BCR	C35-C13-C12	2.61	122.07	118.09
15	A	1103	CLA	C4B-CHC-C1C	2.60	132.37	126.25
15	3	613	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
12	1	501	LUT	C40-C33-C34	-2.60	118.60	122.82
15	3	610	CLA	CHB-C4A-NA	2.60	128.16	124.40
15	A	1117	CLA	O2A-CGA-CBA	2.60	119.77	111.83
15	B	1225	CLA	C4B-CHC-C1C	2.60	132.37	126.25
15	A	1115	CLA	CMA-C3A-C4A	2.60	118.77	111.77
15	B	1240	CLA	C4-C3-C2	-2.60	116.95	123.63
15	A	1012	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
15	A	1123	CLA	C2C-C1C-NC	2.60	112.71	109.98
15	A	1134	CLA	C4D-C3D-CAD	-2.60	105.28	108.11
15	B	1240	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
15	A	1106	CLA	C2C-C1C-NC	2.60	112.71	109.98
15	A	1133	CLA	C2A-C3A-C4A	2.60	106.07	101.87
15	A	1136	CLA	C2C-C1C-NC	2.60	112.71	109.98
15	A	1135	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
14	4	503	BCR	C8-C7-C6	-2.60	120.06	127.00
15	A	1127	CLA	CAA-CBA-CGA	-2.60	105.84	113.21
15	B	1235	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
15	A	1012	CLA	C2C-C1C-NC	2.59	112.71	109.98
15	B	1225	CLA	C2C-C1C-NC	2.59	112.71	109.98
15	A	1105	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
15	A	1111	CLA	C2C-C1C-NC	2.59	112.70	109.98
15	B	1228	CLA	C2C-C1C-NC	2.59	112.70	109.98
15	B	1234	CLA	CHA-C4D-ND	2.59	137.90	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1103	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
15	1	604	CLA	CHB-C4A-NA	2.59	128.14	124.40
15	A	1110	CLA	C4B-CHC-C1C	2.59	132.34	126.25
15	A	1130	CLA	C2C-C1C-NC	2.59	112.70	109.98
14	3	503	BCR	C33-C5-C6	-2.59	121.66	124.48
15	1	611	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
15	A	1136	CLA	C4B-CHC-C1C	2.58	132.32	126.25
15	2	604	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
15	4	608	CLA	C3B-C4B-NB	-2.58	108.23	110.53
15	B	1240	CLA	CHB-C4A-NA	2.58	128.12	124.40
15	A	1110	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
15	A	1125	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
15	F	1301	CLA	C4B-CHC-C1C	2.58	132.31	126.25
15	B	1202	CLA	CHB-C4A-NA	2.57	128.12	124.40
14	F	4002	BCR	C23-C22-C21	-2.57	114.96	119.01
15	F	1302	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
15	B	1219	CLA	C3B-C4B-NB	-2.57	108.23	110.53
15	4	605	CLA	C5-C3-C2	2.57	126.94	121.17
15	A	1123	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
15	B	1225	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
16	4	613	CHL	C4C-CHD-C1D	2.57	125.27	116.07
16	4	613	CHL	C4D-CHA-CBD	-2.57	106.38	108.97
15	A	1123	CLA	C4B-CHC-C1C	2.57	132.29	126.25
15	J	1302	CLA	C4B-CHC-C1C	2.57	132.29	126.25
15	A	1137	CLA	O2A-CGA-CBA	2.57	119.67	111.83
15	B	1022	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
15	A	1138	CLA	C4B-CHC-C1C	2.57	132.29	126.25
16	2	609	CHL	C4C-CHD-C1D	2.57	125.26	116.07
15	B	1213	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
12	2	501	LUT	C37-C21-C26	-2.57	105.66	109.55
15	A	1103	CLA	C2C-C1C-NC	2.57	112.68	109.98
14	A	4002	BCR	C34-C9-C10	-2.57	118.66	122.82
15	A	1104	CLA	C4B-CHC-C1C	2.57	132.28	126.25
13	1	502	XAT	C39-C29-C28	2.56	122.00	118.09
15	A	1129	CLA	CHB-C4A-NA	2.56	128.10	124.40
15	B	1214	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
20	A	1011	CL0	C4D-ND-C1D	-2.56	103.28	105.22
15	B	1223	CLA	CHA-C4D-ND	2.56	137.83	132.55
14	J	4002	BCR	C38-C26-C27	2.56	119.06	113.60
15	B	1203	CLA	C3B-C4B-NB	-2.56	108.24	110.53
15	B	1212	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
15	B	1234	CLA	C4B-CHC-C1C	2.56	132.27	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	502	XAT	C18-C5-C6	-2.56	118.09	122.30
15	B	1224	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
15	B	1236	CLA	C2C-C1C-NC	2.56	112.67	109.98
18	2	803	LMG	O1-C7-C8	-2.56	104.59	110.82
15	A	1124	CLA	CMA-C3A-C4A	2.56	118.65	111.77
13	2	502	XAT	C35-C34-C33	2.56	130.87	127.28
15	B	1228	CLA	C4B-CHC-C1C	2.56	132.26	126.25
15	B	1204	CLA	CHB-C4A-NA	2.56	128.09	124.40
14	F	4002	BCR	C33-C5-C4	2.56	119.05	113.60
15	3	605	CLA	C4B-CHC-C1C	2.55	132.25	126.25
15	A	1108	CLA	C4B-CHC-C1C	2.55	132.25	126.25
15	A	1110	CLA	C2C-C1C-NC	2.55	112.66	109.98
15	A	1104	CLA	CHA-C4D-ND	2.55	137.82	132.55
15	A	1115	CLA	C4B-CHC-C1C	2.55	132.25	126.25
15	A	1135	CLA	C4B-CHC-C1C	2.55	132.25	126.25
15	A	1111	CLA	C4B-CHC-C1C	2.55	132.25	126.25
15	A	1137	CLA	C4B-CHC-C1C	2.55	132.25	126.25
15	4	601	CLA	CHB-C4A-NA	2.55	128.08	124.40
13	1	502	XAT	C37-C21-C26	-2.55	103.16	110.05
16	4	610	CHL	C4D-CHA-CBD	-2.55	106.39	108.97
15	A	1111	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
15	4	607	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
15	A	1133	CLA	CMA-C3A-C4A	-2.55	104.92	111.77
15	3	609	CLA	CHB-C4A-NA	2.55	128.08	124.40
14	A	4005	BCR	C23-C22-C21	-2.55	115.00	119.01
15	3	613	CLA	C4B-CHC-C1C	2.55	132.24	126.25
15	3	615	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
15	4	605	CLA	CHB-C4A-NA	2.55	128.08	124.40
15	B	1231	CLA	CHD-C1D-ND	-2.55	121.22	124.80
15	B	1217	CLA	CHB-C4A-NA	2.55	128.07	124.40
15	A	1139	CLA	C4B-CHC-C1C	2.55	132.24	126.25
15	A	1138	CLA	C2C-C1C-NC	2.55	112.66	109.98
15	B	1224	CLA	C4B-CHC-C1C	2.55	132.23	126.25
15	B	1231	CLA	C2D-C1D-ND	2.55	112.64	110.13
15	A	1121	CLA	C4B-CHC-C1C	2.55	132.23	126.25
15	B	1222	CLA	C4B-CHC-C1C	2.55	132.23	126.25
15	B	1230	CLA	C2C-C1C-NC	2.54	112.65	109.98
15	B	1235	CLA	C4B-CHC-C1C	2.54	132.23	126.25
14	3	506	BCR	C27-C26-C25	2.54	126.14	122.70
14	3	506	BCR	C33-C5-C6	-2.54	121.71	124.48
15	A	1013	CLA	C4B-CHC-C1C	2.54	132.22	126.25
15	4	605	CLA	C3B-C4B-NB	-2.54	108.26	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1206	CLA	C3B-C4B-NB	-2.54	108.26	110.53
23	B	5002	DGD	C6D-O5D-C1E	2.54	119.24	113.80
15	A	1103	CLA	CAA-C2A-C1A	-2.54	103.65	111.97
15	A	1120	CLA	C4B-CHC-C1C	2.54	132.22	126.25
15	A	1013	CLA	C2C-C1C-NC	2.54	112.65	109.98
15	B	1207	CLA	CHB-C4A-NA	2.54	128.06	124.40
15	2	606	CLA	CHB-C4A-NA	2.54	128.06	124.40
15	A	1124	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
12	4	501	LUT	C18-C5-C4	2.54	119.08	114.42
15	A	1130	CLA	C4B-CHC-C1C	2.54	132.21	126.25
15	A	1102	CLA	C2C-C1C-NC	2.53	112.64	109.98
15	1	608	CLA	CHB-C4A-NA	2.53	128.06	124.40
16	3	604	CHL	CMA-C3A-C4A	2.53	120.07	114.61
15	3	612	CLA	C4B-CHC-C1C	2.53	132.20	126.25
15	2	601	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
15	B	1224	CLA	OBD-CAD-C3D	-2.53	122.50	128.42
15	A	1136	CLA	O2A-CGA-CBA	2.53	119.55	111.83
15	3	613	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
15	A	1126	CLA	CHA-C4D-ND	2.53	137.76	132.55
15	1	613	CLA	C3B-C4B-NB	-2.53	108.27	110.53
15	2	607	CLA	C1-O2A-CGA	2.53	122.77	116.65
15	2	603	CLA	CHB-C4A-NA	2.53	128.04	124.40
15	B	1230	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
14	1	503	BCR	C27-C26-C25	2.52	126.12	122.70
15	B	1021	CLA	C4B-CHC-C1C	2.52	132.18	126.25
15	A	1116	CLA	C3B-C4B-NB	-2.52	108.28	110.53
15	2	601	CLA	CHB-C4A-NA	2.52	128.04	124.40
14	F	4002	BCR	C34-C9-C10	-2.52	118.73	122.82
15	A	1126	CLA	C4B-CHC-C1C	2.52	132.18	126.25
15	B	1236	CLA	C4B-CHC-C1C	2.52	132.18	126.25
15	A	1138	CLA	O2A-CGA-CBA	2.52	119.53	111.83
15	A	1131	CLA	C4B-CHC-C1C	2.52	132.18	126.25
14	A	4008	BCR	C33-C5-C4	2.52	118.97	113.60
18	2	804	LMG	C8-O7-C10	-2.52	111.76	117.80
13	4	502	XAT	C19-C9-C10	-2.52	118.73	122.82
15	B	1235	CLA	O2A-CGA-CBA	2.52	119.52	111.83
15	1	606	CLA	C1-C2-C3	-2.52	122.69	126.76
15	3	615	CLA	C4B-CHC-C1C	2.52	132.17	126.25
15	A	1012	CLA	C4B-CHC-C1C	2.52	132.17	126.25
14	A	4003	BCR	C27-C26-C25	-2.52	119.30	122.70
14	F	4002	BCR	C38-C26-C27	2.52	118.96	113.60
15	A	1117	CLA	C4B-CHC-C1C	2.52	132.16	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	614	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
15	B	1229	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
18	2	804	LMG	O8-C28-C29	2.51	119.49	111.83
15	A	1112	CLA	C4B-CHC-C1C	2.51	132.15	126.25
13	2	502	XAT	C39-C29-C28	2.51	121.92	118.09
15	B	1221	CLA	CHB-C4A-NA	2.51	128.02	124.40
15	A	1133	CLA	CAA-CBA-CGA	-2.51	106.08	113.21
15	B	1238	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	J	4001	BCR	C15-C14-C13	-2.51	123.76	127.28
15	B	1222	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
14	A	4004	BCR	C33-C5-C4	2.51	118.94	113.60
15	A	1102	CLA	C4B-CHC-C1C	2.51	132.14	126.25
15	B	1021	CLA	O2A-CGA-CBA	2.51	119.47	111.83
15	B	1227	CLA	C4B-CHC-C1C	2.50	132.14	126.25
15	1	606	CLA	CHB-C4A-NA	2.50	128.01	124.40
15	A	1109	CLA	C4B-CHC-C1C	2.50	132.13	126.25
14	A	4007	BCR	C33-C5-C4	2.50	118.93	113.60
16	4	613	CHL	C1A-CHA-C4D	2.50	123.16	118.98
15	A	1128	CLA	C4B-CHC-C1C	2.50	132.13	126.25
15	F	1301	CLA	C2C-C1C-NC	2.50	112.61	109.98
15	B	1236	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
14	B	4001	BCR	C8-C7-C6	-2.50	120.32	127.00
15	A	1138	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
15	A	1121	CLA	CHA-C4D-ND	2.50	137.70	132.55
15	B	1204	CLA	C3B-C4B-NB	-2.50	108.30	110.53
15	A	1106	CLA	C4B-CHC-C1C	2.50	132.12	126.25
14	B	4001	BCR	C15-C16-C17	-2.50	118.41	123.52
14	A	4004	BCR	C38-C26-C27	2.50	118.92	113.60
15	A	1133	CLA	CBB-CAB-C3B	-2.50	115.05	127.53
15	A	1123	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
14	A	4006	BCR	C36-C18-C19	2.50	121.90	118.09
15	A	1137	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
15	A	1112	CLA	CHA-C4D-ND	2.50	137.70	132.55
14	B	4001	BCR	C35-C13-C14	-2.50	118.77	122.82
15	3	613	CLA	C2C-C1C-NC	2.50	112.60	109.98
15	A	1127	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
15	A	1113	CLA	C4B-CHC-C1C	2.49	132.10	126.25
15	1	613	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	B	5002	DGD	O5D-C6D-C5D	-2.49	103.81	109.42
15	A	1134	CLA	CHD-C1D-C2D	2.49	130.66	125.49
15	A	1106	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
15	4	609	CLA	C3B-C4B-NB	-2.48	108.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1204	CLA	O2D-CGD-CBD	2.48	115.57	111.23
15	B	1227	CLA	C1-O2A-CGA	2.48	122.66	116.65
15	A	1118	CLA	CHA-C4D-ND	2.48	137.67	132.55
15	B	1223	CLA	C1D-CHD-C4C	-2.48	120.75	126.02
15	A	1116	CLA	CHD-C4C-NC	-2.48	120.39	124.23
15	A	1133	CLA	O2D-CGD-CBD	2.48	115.56	111.23
15	B	1021	CLA	CHA-C4D-ND	2.48	137.66	132.55
15	3	612	CLA	CHA-C4D-ND	2.48	137.66	132.55
14	4	503	BCR	C11-C10-C9	-2.47	123.81	127.28
15	A	1140	CLA	C2A-C1A-CHA	2.47	128.16	123.87
15	B	1205	CLA	CHB-C4A-NA	2.47	127.97	124.40
15	A	1114	CLA	C2C-C1C-NC	2.47	112.58	109.98
15	2	601	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
17	1	801	LHG	O8-C23-C24	2.47	119.37	111.83
15	A	1105	CLA	CHA-C4D-ND	2.47	137.65	132.55
15	B	1216	CLA	C1-C2-C3	-2.47	122.15	126.20
15	4	616	CLA	C3B-C4B-NB	-2.47	108.33	110.53
15	3	615	CLA	CHA-C4D-ND	2.47	137.64	132.55
15	A	1109	CLA	CHA-C4D-ND	2.47	137.64	132.55
14	A	4006	BCR	C27-C26-C25	-2.47	119.37	122.70
15	A	1104	CLA	C1C-C2C-C3C	-2.47	104.39	106.98
15	4	612	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
15	B	1220	CLA	CHB-C4A-NA	2.46	127.96	124.40
15	A	1114	CLA	CHD-C1D-ND	-2.46	121.34	124.80
15	B	1210	CLA	C1-C2-C3	-2.46	122.16	126.20
15	B	1232	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	A	1135	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
15	A	1106	CLA	CHA-C4D-ND	2.46	137.63	132.55
15	B	1022	CLA	CMA-C3A-C4A	2.46	118.39	111.77
15	B	1223	CLA	CHD-C1D-ND	-2.46	121.34	124.80
15	A	1109	CLA	C1-O2A-CGA	2.46	122.61	116.65
15	A	1107	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
15	3	607	CLA	CHB-C4A-NA	2.46	127.95	124.40
18	2	802	LMG	O1-C7-C8	-2.46	104.83	110.82
15	A	1130	CLA	CHA-C4D-ND	2.46	137.62	132.55
15	A	1101	CLA	CHA-C4D-ND	2.46	137.62	132.55
15	A	1136	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
14	B	4005	BCR	C38-C26-C27	2.46	118.84	113.60
15	A	1137	CLA	CHA-C4D-ND	2.46	137.62	132.55
14	B	4006	BCR	C36-C18-C17	-2.46	118.83	122.82
15	A	1135	CLA	CHA-C4D-ND	2.46	137.62	132.55
14	F	4001	BCR	C40-C30-C39	-2.46	101.60	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	503	BCR	C38-C26-C25	-2.46	121.80	124.48
15	B	1235	CLA	CHA-C4D-ND	2.45	137.61	132.55
15	3	613	CLA	CHA-C4D-ND	2.45	137.61	132.55
12	3	501	LUT	C37-C21-C26	-2.45	105.83	109.55
15	B	1228	CLA	CHA-C4D-ND	2.45	137.61	132.55
16	2	611	CHL	C4C-CHD-C1D	2.45	124.85	116.07
12	3	501	LUT	C7-C6-C5	-2.45	115.91	121.56
16	1	610	CHL	C4C-CHD-C1D	2.45	124.84	116.07
20	A	1011	CL0	CMC-C2C-C1C	2.45	129.15	124.73
15	A	1126	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
15	A	1101	CLA	CHD-C1D-ND	-2.45	121.35	124.80
15	A	1123	CLA	CHA-C4D-ND	2.45	137.61	132.55
15	A	1125	CLA	C4B-CHC-C1C	2.45	132.01	126.25
14	A	4004	BCR	C34-C9-C10	-2.45	118.85	122.82
15	1	615	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	J	1302	CLA	CHA-C4D-ND	2.45	137.60	132.55
15	A	1113	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
15	B	1227	CLA	CAC-C3C-C4C	2.45	127.97	124.79
15	2	616	CLA	C4-C3-C5	2.45	119.48	115.23
16	2	610	CHL	C4C-CHD-C1D	2.45	124.82	116.07
15	A	1122	CLA	C4B-CHC-C1C	2.45	132.00	126.25
15	3	608	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
15	A	1107	CLA	CHA-C4D-ND	2.45	137.60	132.55
15	A	1115	CLA	CHA-C4D-ND	2.45	137.60	132.55
15	B	1236	CLA	CHA-C4D-ND	2.44	137.59	132.55
14	4	503	BCR	C2-C1-C6	2.44	113.99	110.44
20	A	1011	CL0	O2D-CGD-O1D	-2.44	119.10	123.85
15	B	1215	CLA	C3B-C4B-NB	-2.44	108.35	110.53
15	B	1222	CLA	CHA-C4D-ND	2.44	137.59	132.55
15	B	1229	CLA	CMB-C2B-C1B	2.44	129.13	125.42
15	A	1108	CLA	CHA-C4D-ND	2.44	137.58	132.55
15	A	1110	CLA	CHA-C4D-ND	2.44	137.58	132.55
15	B	1230	CLA	C1C-C2C-C3C	-2.44	104.42	106.98
15	A	1012	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
15	A	1105	CLA	CHA-C1A-NA	-2.44	120.87	126.39
15	A	1104	CLA	C1-O2A-CGA	2.44	122.55	116.65
15	A	1138	CLA	CHA-C4D-ND	2.44	137.58	132.55
14	A	4003	BCR	C1-C6-C5	-2.44	119.31	122.64
15	A	1117	CLA	CHA-C4D-ND	2.44	137.58	132.55
15	A	1120	CLA	CHA-C4D-ND	2.44	137.57	132.55
15	B	1235	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
15	B	1023	CLA	CHA-C4D-ND	2.44	137.57	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1021	CLA	CMA-C3A-C4A	2.44	118.32	111.77
14	4	503	BCR	C33-C5-C6	-2.44	121.83	124.48
14	B	4003	BCR	C15-C16-C17	-2.43	118.54	123.52
15	B	1227	CLA	C1D-ND-C4D	-2.43	104.61	106.31
15	A	1140	CLA	C2D-C1D-ND	2.43	112.53	110.13
15	F	1301	CLA	CHD-C1D-ND	-2.43	121.38	124.80
15	3	605	CLA	O2A-CGA-CBA	2.43	119.24	111.83
14	B	4006	BCR	C27-C26-C25	-2.43	119.42	122.70
15	A	1103	CLA	C2D-C1D-ND	2.43	112.53	110.13
15	A	1012	CLA	CHA-C4D-ND	2.43	137.56	132.55
15	B	1230	CLA	CHA-C4D-ND	2.43	137.56	132.55
15	B	1225	CLA	CHA-C4D-ND	2.43	137.56	132.55
13	1	502	XAT	C35-C34-C33	-2.43	123.88	127.28
15	A	1102	CLA	CHA-C4D-ND	2.42	137.55	132.55
15	A	1113	CLA	CHA-C4D-ND	2.42	137.55	132.55
15	A	1128	CLA	CHA-C4D-ND	2.42	137.55	132.55
15	B	1227	CLA	O2A-CGA-CBA	2.42	119.22	111.83
15	B	1023	CLA	O2A-CGA-CBA	2.42	119.22	111.83
15	B	1208	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
15	B	1224	CLA	CHA-C4D-ND	2.42	137.54	132.55
15	A	1107	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
16	1	609	CHL	C1A-CHA-C4D	2.42	123.02	118.98
15	A	1104	CLA	C1-C2-C3	-2.42	122.23	126.20
15	F	1301	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
15	B	1225	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
15	A	1101	CLA	CMD-C2D-C3D	-2.42	122.15	127.69
15	B	1227	CLA	CHD-C1D-ND	-2.42	121.40	124.80
15	A	1013	CLA	C2D-C1D-ND	2.42	112.52	110.13
15	3	608	CLA	C3B-C4B-NB	-2.42	108.37	110.53
15	A	1111	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
12	2	501	LUT	C18-C5-C6	-2.42	121.85	124.48
15	A	1111	CLA	CHA-C4D-ND	2.42	137.53	132.55
15	1	601	CLA	C1-C2-C3	-2.42	122.24	126.20
15	A	1139	CLA	O2A-CGA-CBA	2.41	119.19	111.83
15	B	1229	CLA	CHA-C4D-ND	2.41	137.52	132.55
15	4	607	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
16	2	613	CHL	C4C-CHD-C1D	2.40	124.67	116.07
15	A	1103	CLA	CHA-C4D-ND	2.40	137.51	132.55
15	A	1134	CLA	CMA-C3A-C2A	2.40	123.28	113.98
15	4	602	CLA	O2D-CGD-CBD	2.40	115.43	111.23
16	4	611	CHL	C1-O2A-CGA	2.40	122.47	116.65
15	B	1229	CLA	C4B-CHC-C1C	2.40	131.90	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	1302	CLA	C3B-C4B-NB	-2.40	108.39	110.53
15	F	1301	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
15	A	1136	CLA	CHA-C4D-ND	2.40	137.50	132.55
15	A	1114	CLA	C2D-C1D-ND	2.40	112.50	110.13
13	4	502	XAT	C19-C9-C8	-2.40	114.43	118.09
15	A	1121	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
15	A	1101	CLA	C1C-C2C-C3C	-2.40	104.46	106.98
15	A	1124	CLA	C2C-C1C-NC	2.39	112.50	109.98
15	2	608	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	A	1122	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
15	A	1116	CLA	CHA-C4D-ND	2.39	137.48	132.55
15	A	1105	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
15	4	616	CLA	CHB-C4A-NA	2.39	127.85	124.40
16	1	610	CHL	C4D-CHA-CBD	-2.39	106.56	108.97
15	A	1139	CLA	C2D-C1D-ND	2.39	112.49	110.13
14	3	503	BCR	C27-C26-C25	2.39	125.93	122.70
15	A	1104	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
14	A	4002	BCR	C33-C5-C4	2.39	118.68	113.60
15	A	1101	CLA	C4B-CHC-C1C	2.38	131.85	126.25
13	2	502	XAT	C36-C21-C26	2.38	116.48	110.05
15	A	1104	CLA	CMD-C2D-C3D	-2.38	122.22	127.69
15	A	1101	CLA	C2D-C1D-ND	2.38	112.48	110.13
15	A	1106	CLA	C2D-C1D-ND	2.38	112.48	110.13
15	B	1236	CLA	C2D-C1D-ND	2.38	112.48	110.13
15	3	605	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
16	2	613	CHL	C4D-CHA-CBD	-2.38	106.57	108.97
15	B	1225	CLA	O2A-CGA-CBA	2.38	119.09	111.83
15	F	1301	CLA	CHA-C4D-ND	2.38	137.46	132.55
12	2	501	LUT	C19-C9-C8	2.38	121.72	118.09
15	4	609	CLA	C4-C3-C2	-2.38	117.52	123.63
15	A	1128	CLA	C2D-C1D-ND	2.38	112.48	110.13
20	A	1011	CL0	CMB-C2B-C3B	2.38	129.43	124.68
17	A	5001	LHG	C9-C8-C7	-2.38	104.99	113.69
14	1	503	BCR	C15-C16-C17	-2.38	118.66	123.52
14	A	4008	BCR	C7-C6-C5	-2.37	116.09	121.56
15	A	1116	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
14	A	4007	BCR	C19-C18-C17	-2.37	115.28	119.01
14	F	4001	BCR	C33-C5-C4	2.37	118.65	113.60
15	B	1221	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
15	A	1109	CLA	CBA-CAA-C2A	-2.37	106.75	113.79
12	1	501	LUT	C26-C27-C28	-2.37	120.89	124.58
17	A	5001	LHG	O8-C23-C24	2.37	119.05	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	603	CLA	C4-C3-C5	2.37	119.33	115.23
15	A	1141	CLA	CHB-C4A-NA	2.37	127.81	124.40
15	3	605	CLA	CHA-C4D-ND	2.37	137.43	132.55
16	2	609	CHL	CBA-CAA-C2A	2.37	120.74	113.78
15	A	1013	CLA	CHA-C4D-ND	2.36	137.43	132.55
15	A	1133	CLA	C6-C5-C3	-2.36	107.71	113.47
15	A	1139	CLA	CHD-C1D-ND	-2.36	121.48	124.80
15	B	1236	CLA	O2A-CGA-CBA	2.36	119.04	111.83
15	A	1102	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
14	B	4006	BCR	C24-C25-C26	-2.36	116.11	121.56
14	J	4001	BCR	C36-C18-C17	-2.36	118.99	122.82
15	A	1107	CLA	C4B-CHC-C1C	2.36	131.80	126.25
14	3	503	BCR	C2-C1-C6	2.36	113.87	110.44
15	4	604	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
15	A	1122	CLA	CHA-C4D-ND	2.36	137.41	132.55
14	B	4006	BCR	C34-C9-C10	-2.36	119.00	122.82
15	A	1114	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
15	A	1139	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
15	A	1124	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
15	1	603	CLA	CBA-CAA-C2A	2.35	120.80	113.79
15	B	1208	CLA	CHB-C4A-NA	2.35	127.80	124.40
16	1	609	CHL	C4D-CHA-CBD	-2.35	106.59	108.97
15	A	1108	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
15	A	1139	CLA	CHA-C4D-ND	2.35	137.40	132.55
13	1	502	XAT	C19-C9-C8	2.35	121.68	118.09
15	A	1133	CLA	O2A-CGA-CBA	2.35	119.01	111.83
14	A	4003	BCR	C37-C22-C23	2.35	121.68	118.09
16	4	611	CHL	C4C-CHD-C1D	2.35	124.48	116.07
15	A	1112	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
15	A	1124	CLA	C2D-C1D-ND	2.35	112.45	110.13
15	A	1131	CLA	CHA-C4D-ND	2.35	137.40	132.55
14	A	4006	BCR	C8-C7-C6	-2.35	120.72	127.00
15	A	1118	CLA	C3B-C4B-NB	-2.35	108.43	110.53
15	B	1239	CLA	C3B-C4B-NB	-2.35	108.43	110.53
14	A	4008	BCR	C8-C9-C10	2.35	122.70	119.01
13	1	502	XAT	C26-C27-C28	-2.35	121.03	125.99
15	A	1120	CLA	C2D-C1D-ND	2.35	112.45	110.13
15	4	604	CLA	CBA-CAA-C2A	2.34	120.77	113.79
15	3	601	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
15	A	1124	CLA	C4D-CHA-C1A	2.34	124.04	121.24
14	3	504	BCR	C34-C9-C10	-2.34	119.02	122.82
15	3	615	CLA	C2D-C1D-ND	2.34	112.44	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1136	CLA	C2D-C1D-ND	2.34	112.44	110.13
18	B	5003	LMG	O3-C3-C2	-2.34	104.86	110.38
15	A	1137	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
15	A	1103	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
15	A	1128	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
15	B	1234	CLA	CHD-C1D-ND	-2.34	121.51	124.80
15	2	605	CLA	C3B-C4B-NB	-2.34	108.44	110.53
15	B	1212	CLA	C3B-C4B-NB	-2.34	108.44	110.53
15	A	1118	CLA	CMA-C3A-C4A	2.34	118.05	111.77
15	A	1114	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
15	B	1215	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
15	4	601	CLA	CBA-CAA-C2A	2.33	120.73	113.79
15	A	1132	CLA	CBC-CAC-C3C	2.33	118.74	112.42
14	1	503	BCR	C7-C8-C9	-2.33	122.79	126.23
14	A	4004	BCR	C35-C13-C14	-2.33	119.04	122.82
15	A	1130	CLA	C2D-C1D-ND	2.33	112.43	110.13
14	B	4001	BCR	C1-C6-C5	-2.33	119.45	122.64
15	A	1105	CLA	C2D-C1D-ND	2.33	112.43	110.13
15	A	1115	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
15	1	611	CLA	CHB-C4A-NA	2.33	127.76	124.40
15	A	1119	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
15	B	1022	CLA	C2C-C1C-NC	2.33	112.42	109.98
15	A	1120	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
15	B	1239	CLA	CAC-C3C-C4C	2.32	127.81	124.79
15	A	1112	CLA	C2D-C1D-ND	2.32	112.42	110.13
15	A	1118	CLA	C4B-CHC-C1C	2.32	131.71	126.25
14	F	4001	BCR	C31-C1-C6	-2.32	106.60	110.24
15	4	605	CLA	C4-C3-C2	-2.32	117.67	123.63
15	B	1230	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
15	4	602	CLA	C3B-C4B-NB	-2.32	108.46	110.53
15	1	603	CLA	C3B-C4B-NB	-2.32	108.46	110.53
15	A	1125	CLA	C1-O2A-CGA	2.32	122.26	116.65
15	A	1117	CLA	C2D-C1D-ND	2.32	112.42	110.13
15	A	1123	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
14	B	4004	BCR	C8-C7-C6	-2.32	120.81	127.00
14	B	4005	BCR	C34-C9-C10	-2.31	119.07	122.82
14	B	4004	BCR	C27-C26-C25	2.31	125.83	122.70
16	2	609	CHL	C4D-CHA-CBD	-2.31	106.64	108.97
15	A	1101	CLA	C2C-C1C-NC	2.31	112.41	109.98
15	A	1130	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
15	A	1112	CLA	O2A-CGA-CBA	2.31	118.88	111.83
15	A	1111	CLA	C2D-C1D-ND	2.31	112.41	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1113	CLA	C2D-C1D-ND	2.31	112.41	110.13
15	A	1104	CLA	C2D-C1D-ND	2.31	112.41	110.13
15	B	1228	CLA	C2D-C1D-ND	2.31	112.41	110.13
15	A	1125	CLA	C1C-C2C-C3C	-2.31	104.55	106.98
15	4	606	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
15	A	1013	CLA	CHD-C1D-ND	-2.31	121.55	124.80
15	A	1119	CLA	C2C-C1C-NC	2.31	112.41	109.98
15	B	1212	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
17	B	5001	LHG	C11-C10-C9	-2.31	102.70	114.37
15	F	1302	CLA	CBA-CAA-C2A	2.31	120.66	113.79
14	3	503	BCR	C37-C22-C21	-2.31	119.08	122.82
15	A	1135	CLA	C2D-C1D-ND	2.30	112.41	110.13
15	A	1102	CLA	CHD-C1D-ND	-2.30	121.56	124.80
14	B	4003	BCR	C1-C6-C5	-2.30	119.49	122.64
15	A	1012	CLA	C2D-C1D-ND	2.30	112.40	110.13
14	1	503	BCR	C38-C26-C25	-2.30	121.97	124.48
15	3	612	CLA	O2A-CGA-CBA	2.30	118.85	111.83
15	B	1235	CLA	C2D-C1D-ND	2.30	112.40	110.13
15	4	608	CLA	CHD-C4C-C3C	2.30	128.13	124.77
15	3	613	CLA	C2D-C1D-ND	2.30	112.40	110.13
12	2	501	LUT	C20-C13-C12	2.30	121.60	118.09
15	B	1234	CLA	C6-C5-C3	-2.30	107.87	113.47
15	A	1130	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
15	B	1225	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
14	J	4002	BCR	C23-C24-C25	-2.29	120.87	127.00
15	B	1238	CLA	CHD-C4C-C3C	2.29	128.12	124.77
15	A	1109	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
15	B	1022	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
15	B	1022	CLA	O2A-CGA-CBA	2.29	118.82	111.83
16	1	609	CHL	C4C-CHD-C1D	2.29	124.27	116.07
15	B	1228	CLA	O2A-CGA-CBA	2.29	118.82	111.83
15	A	1108	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
15	2	601	CLA	CBA-CAA-C2A	2.29	120.61	113.79
15	B	1223	CLA	CHA-C1A-NA	-2.29	121.21	126.39
15	3	605	CLA	C2D-C1D-ND	2.29	112.39	110.13
15	B	1225	CLA	C2D-C1D-ND	2.29	112.39	110.13
15	3	615	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
15	A	1126	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
15	B	1223	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
15	J	1302	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
15	A	1129	CLA	CAC-C3C-C4C	2.28	127.76	124.79
15	A	1131	CLA	O2D-CGD-O1D	-2.28	119.40	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	1301	CLA	C2D-C1D-ND	2.28	112.39	110.13
15	A	1013	CLA	O2A-CGA-CBA	2.28	118.80	111.83
15	A	1114	CLA	CHA-C4D-ND	2.28	137.26	132.55
15	A	1123	CLA	C2D-C1D-ND	2.28	112.38	110.13
20	A	1011	CL0	C4C-CHD-C1D	2.28	124.23	116.07
15	A	1127	CLA	CMA-C3A-C4A	2.28	117.90	111.77
14	F	4001	BCR	C38-C26-C27	2.28	118.46	113.60
14	B	4006	BCR	C38-C26-C27	2.28	118.45	113.60
14	1	503	BCR	C11-C10-C9	-2.28	124.08	127.28
15	B	1021	CLA	CHA-C1A-NA	-2.28	121.24	126.39
15	A	1131	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
15	A	1104	CLA	C2C-C1C-NC	2.28	112.37	109.98
15	A	1115	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
15	A	1108	CLA	C2D-C1D-ND	2.28	112.38	110.13
15	A	1138	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
15	3	612	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
15	A	1013	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
15	A	1116	CLA	CAA-C2A-C1A	-2.27	104.53	111.97
15	A	1120	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
15	A	1107	CLA	CHD-C1D-ND	-2.27	121.60	124.80
15	B	1023	CLA	C4B-CHC-C1C	2.27	131.59	126.25
14	A	4005	BCR	C34-C9-C8	2.27	121.56	118.09
15	A	1110	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
14	1	503	BCR	C16-C15-C14	-2.27	118.88	123.52
15	A	1102	CLA	C2D-C1D-ND	2.27	112.37	110.13
15	A	1136	CLA	CHD-C1D-ND	-2.27	121.61	124.80
15	B	1021	CLA	CHD-C1D-ND	-2.27	121.61	124.80
15	B	1202	CLA	O2D-CGD-CBD	2.27	115.20	111.23
15	J	1302	CLA	C2D-C1D-ND	2.27	112.37	110.13
15	A	1121	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
15	A	1127	CLA	C1D-ND-C4D	-2.27	104.72	106.31
15	B	1216	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
15	A	1112	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
15	1	612	CLA	CHB-C4A-NA	2.27	127.67	124.40
14	F	4002	BCR	C35-C13-C12	2.26	121.55	118.09
15	B	1234	CLA	C1D-ND-C4D	-2.26	104.72	106.31
15	B	1210	CLA	CHB-C4A-NA	2.26	127.67	124.40
14	A	4006	BCR	C38-C26-C27	2.26	118.42	113.60
15	3	603	CLA	CHB-C4A-NA	2.26	127.67	124.40
15	A	1110	CLA	C2D-C1D-ND	2.26	112.36	110.13
15	A	1128	CLA	CHA-C1A-NA	-2.26	121.27	126.39
14	J	4002	BCR	C34-C9-C10	-2.26	119.16	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1138	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
23	B	5002	DGD	CFB-CEB-CDB	-2.26	102.95	114.37
14	B	4006	BCR	C15-C14-C13	-2.26	124.11	127.28
15	A	1122	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
15	A	1122	CLA	CHD-C1D-ND	-2.26	121.62	124.80
15	1	604	CLA	CAC-C3C-C4C	2.26	127.73	124.79
15	B	1229	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
14	3	503	BCR	C15-C16-C17	-2.26	118.90	123.52
14	2	503	BCR	C4-C5-C6	2.26	125.75	122.70
15	A	1119	CLA	C1C-C2C-C3C	-2.26	104.61	106.98
15	A	1106	CLA	O2A-CGA-CBA	2.25	118.71	111.83
15	3	603	CLA	C3B-C4B-NB	-2.25	108.52	110.53
15	1	601	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
15	B	1211	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
15	B	1229	CLA	C2D-C1D-ND	2.25	112.36	110.13
15	A	1109	CLA	CHA-C1A-NA	-2.25	121.29	126.39
14	A	4008	BCR	C31-C1-C6	-2.25	106.71	110.24
15	A	1119	CLA	CHD-C1D-ND	-2.25	121.63	124.80
15	3	605	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
15	A	1104	CLA	CHD-C1D-ND	-2.25	121.64	124.80
15	4	616	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
15	A	1109	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
15	A	1131	CLA	C2D-C1D-ND	2.25	112.35	110.13
15	A	1127	CLA	O2A-CGA-CBA	2.25	118.69	111.83
15	A	1126	CLA	CHA-C1A-NA	-2.25	121.30	126.39
15	A	1123	CLA	O2A-CGA-CBA	2.25	118.69	111.83
15	B	1222	CLA	C2D-C1D-ND	2.25	112.35	110.13
15	B	1021	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
15	B	1219	CLA	CHB-C4A-NA	2.25	127.64	124.40
15	J	1302	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
15	A	1119	CLA	C2D-C1D-ND	2.25	112.35	110.13
15	B	1224	CLA	CHA-C1A-NA	-2.24	121.31	126.39
15	A	1106	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
23	B	5002	DGD	O6E-C5E-C4E	2.24	113.74	109.70
15	A	1116	CLA	CHC-C1C-NC	-2.24	120.93	124.31
15	A	1120	CLA	CHD-C1D-ND	-2.24	121.65	124.80
15	A	1115	CLA	CHD-C1D-ND	-2.24	121.65	124.80
15	B	1231	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
15	B	1235	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
15	1	607	CLA	CHB-C4A-NA	2.24	127.63	124.40
14	B	4004	BCR	C11-C10-C9	-2.24	124.14	127.28
15	B	1021	CLA	O2D-CGD-O1D	-2.24	119.50	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1230	CLA	C4B-CHC-C1C	2.24	131.50	126.25
15	A	1137	CLA	C2D-C1D-ND	2.23	112.34	110.13
15	2	604	CLA	CAC-C3C-C4C	2.23	127.70	124.79
15	A	1126	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
14	B	4001	BCR	C2-C3-C4	2.23	116.19	111.28
14	3	503	BCR	C20-C21-C22	-2.23	124.15	127.28
15	A	1122	CLA	C2D-C1D-ND	2.23	112.34	110.13
13	1	502	XAT	C40-C33-C32	2.23	121.50	118.09
15	A	1128	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
15	1	603	CLA	CMB-C2B-C3B	2.23	131.80	126.55
15	B	1234	CLA	CHA-C1A-NA	-2.23	121.34	126.39
14	B	4003	BCR	C35-C13-C14	-2.23	119.20	122.82
15	B	1224	CLA	CHD-C1D-ND	-2.23	121.67	124.80
15	3	612	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
15	A	1122	CLA	O2A-CGA-CBA	2.23	118.63	111.83
15	A	1127	CLA	C2D-C1D-ND	2.23	112.33	110.13
15	A	1138	CLA	C2D-C1D-ND	2.23	112.33	110.13
15	F	1302	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
15	3	612	CLA	C2D-C1D-ND	2.22	112.33	110.13
15	B	1236	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
15	A	1139	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
15	4	603	CLA	C3A-C2A-C1A	2.22	104.67	101.34
17	1	801	LHG	C20-C19-C18	-2.22	103.13	114.37
14	2	503	BCR	C15-C16-C17	-2.22	118.97	123.52
15	A	1111	CLA	O2A-CGA-CBA	2.22	118.61	111.83
15	A	1123	CLA	CHD-C1D-ND	-2.22	121.68	124.80
14	B	4006	BCR	C19-C18-C17	2.22	122.50	119.01
14	A	4002	BCR	C38-C26-C27	2.22	118.33	113.60
15	A	1108	CLA	O2A-CGA-CBA	2.22	118.61	111.83
18	2	803	LMG	O2-C2-C1	-2.22	104.78	110.08
15	1	603	CLA	CAC-C3C-C4C	2.22	127.68	124.79
23	B	5002	DGD	CDB-CCB-CBB	-2.22	103.16	114.37
14	3	504	BCR	C23-C24-C25	-2.22	121.07	127.00
15	A	1105	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
15	B	1224	CLA	O2A-CGA-CBA	2.21	118.59	111.83
15	A	1104	CLA	CAA-C2A-C3A	-2.21	107.02	113.00
14	B	4002	BCR	C11-C10-C9	-2.21	124.17	127.28
15	B	1231	CLA	CMA-C3A-C4A	2.21	117.72	111.77
15	2	604	CLA	CBA-CAA-C2A	2.21	120.37	113.79
14	3	503	BCR	C7-C8-C9	-2.21	122.96	126.23
15	4	601	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
17	1	801	LHG	O8-C23-O10	-2.21	118.10	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1226	CLA	CBA-CAA-C2A	2.21	120.37	113.79
21	A	2001	PQN	C2M-C2-C3	-2.21	120.82	124.45
15	A	1117	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
17	2	801	LHG	C5-O7-C7	-2.21	112.51	117.80
14	B	4003	BCR	C24-C23-C22	-2.21	122.97	126.23
15	A	1111	CLA	CHA-C1A-NA	-2.21	121.39	126.39
14	J	4002	BCR	C4-C5-C6	-2.21	119.72	122.70
14	4	503	BCR	C16-C15-C14	-2.21	119.00	123.52
20	A	1011	CL0	C4C-C3C-C2C	-2.21	104.65	113.37
15	A	1109	CLA	CHD-C1D-ND	-2.21	121.70	124.80
15	A	1012	CLA	CHD-C1D-ND	-2.21	121.70	124.80
15	A	1111	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
15	3	610	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
15	B	1202	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
15	B	1229	CLA	O2A-CGA-CBA	2.20	118.55	111.83
15	A	1110	CLA	CHD-C1D-ND	-2.20	121.70	124.80
15	A	1117	CLA	CHD-C1D-ND	-2.20	121.70	124.80
15	B	1219	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
15	4	608	CLA	CHB-C4A-NA	2.20	127.58	124.40
12	1	501	LUT	C19-C9-C8	2.20	121.45	118.09
15	A	1119	CLA	C6-C5-C3	-2.20	108.11	113.47
14	4	503	BCR	C15-C14-C13	-2.20	124.19	127.28
15	A	1102	CLA	CMA-C3A-C4A	2.20	117.69	111.77
15	A	1103	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
15	A	1135	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
15	B	1210	CLA	O2D-CGD-CBD	2.20	115.08	111.23
18	B	5003	LMG	C7-O1-C1	2.20	118.51	113.80
15	3	613	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
15	A	1012	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
15	A	1122	CLA	CHA-C1A-NA	-2.20	121.41	126.39
15	A	1138	CLA	CHD-C1D-ND	-2.20	121.71	124.80
15	B	1229	CLA	CHD-C1D-ND	-2.20	121.71	124.80
15	B	1231	CLA	C1-C2-C3	-2.20	122.59	126.20
15	A	1113	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
15	A	1136	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
14	B	4002	BCR	C15-C16-C17	-2.20	119.02	123.52
15	A	1121	CLA	C2D-C1D-ND	2.20	112.30	110.13
15	B	1225	CLA	CHD-C1D-ND	-2.20	121.71	124.80
15	B	1234	CLA	O2A-CGA-CBA	2.19	118.53	111.83
15	B	1021	CLA	C2D-C1D-ND	2.19	112.30	110.13
15	A	1117	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
15	B	1204	CLA	O2A-CGA-O1A	-2.19	117.69	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	2002	PQN	C21-C20-C18	-2.19	108.68	115.97
15	A	1111	CLA	CHD-C1D-ND	-2.19	121.72	124.80
15	B	1231	CLA	CAC-C3C-C4C	2.19	127.64	124.79
15	A	1130	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	2	609	CHL	C1A-CHA-C4D	2.19	122.64	118.98
13	3	502	XAT	C39-C29-C30	-2.19	119.27	122.82
15	A	1115	CLA	CHA-C1A-NA	-2.19	121.44	126.39
15	B	1222	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
15	B	1228	CLA	CMD-C2D-C3D	-2.19	122.68	127.69
15	A	1116	CLA	O2D-CGD-O1D	-2.18	119.59	123.85
15	3	615	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	4	610	CHL	C1-O2A-CGA	2.18	123.06	116.07
15	A	1103	CLA	CHD-C1D-ND	-2.18	121.73	124.80
15	B	1023	CLA	C2C-C1C-NC	2.18	112.27	109.98
14	B	4006	BCR	C29-C30-C25	2.18	113.61	110.44
15	A	1118	CLA	CHA-C1A-NA	-2.18	121.45	126.39
14	A	4008	BCR	C35-C13-C12	2.18	121.42	118.09
15	A	1131	CLA	CHD-C1D-ND	-2.18	121.74	124.80
15	B	1023	CLA	C3B-C2B-C1B	-2.18	104.60	107.17
14	1	503	BCR	C2-C1-C6	2.18	113.60	110.44
15	A	1125	CLA	CHA-C4D-ND	2.18	137.04	132.55
15	B	1211	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
15	B	1224	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
15	A	1108	CLA	CHD-C1D-ND	-2.17	121.74	124.80
15	A	1124	CLA	C1-O2A-CGA	2.17	121.91	116.65
15	A	1141	CLA	CMA-C3A-C2A	-2.17	111.24	116.23
15	A	1110	CLA	O2A-CGA-CBA	2.17	118.46	111.83
15	A	1119	CLA	CHA-C4D-ND	2.17	137.03	132.55
15	3	613	CLA	CHA-C1A-NA	-2.17	121.47	126.39
15	3	605	CLA	CHD-C1D-ND	-2.17	121.75	124.80
17	A	5002	LHG	O7-C7-O9	-2.17	118.63	123.70
15	B	1229	CLA	C3B-C2B-C1B	-2.17	104.61	107.17
15	A	1121	CLA	CHA-C1A-NA	-2.17	121.48	126.39
15	3	612	CLA	CHA-C1A-NA	-2.17	121.48	126.39
15	B	1235	CLA	CHA-C1A-NA	-2.17	121.48	126.39
15	3	608	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	B	4006	BCR	C38-C26-C25	-2.17	122.12	124.48
15	A	1107	CLA	C2D-C1D-ND	2.17	112.27	110.13
15	A	1124	CLA	OBD-CAD-C3D	-2.17	123.35	128.42
15	3	615	CLA	CHA-C1A-NA	-2.17	121.49	126.39
15	2	604	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
15	3	606	CLA	C1-O2A-CGA	2.17	121.89	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1137	CLA	CHD-C1D-ND	-2.17	121.75	124.80
12	1	501	LUT	C7-C6-C5	-2.17	116.57	121.56
15	3	613	CLA	CHD-C1D-ND	-2.16	121.76	124.80
14	B	4003	BCR	C28-C27-C26	-2.16	110.20	114.06
15	B	1235	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	3	604	CHL	C4D-CHA-CBD	-2.16	106.79	108.97
18	B	5003	LMG	C1-C2-C3	-2.16	105.46	110.01
14	3	506	BCR	C16-C15-C14	-2.16	119.09	123.52
15	A	1106	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
17	3	801	LHG	O8-C23-O10	-2.16	118.23	123.63
15	A	1112	CLA	CHA-C1A-NA	-2.16	121.50	126.39
15	A	1118	CLA	C2A-C1A-CHA	2.16	127.61	123.87
15	B	1022	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
15	A	1125	CLA	O2A-CGA-CBA	2.16	118.41	111.83
15	B	1213	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	A	1133	CLA	C4D-CHA-C1A	2.16	123.82	121.24
15	A	1126	CLA	O2A-CGA-CBA	2.16	118.41	111.83
15	B	1214	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	B	1222	CLA	O2A-CGA-CBA	2.15	118.40	111.83
15	A	1128	CLA	C1-O2A-CGA	2.15	121.86	116.65
18	2	802	LMG	O2-C2-C1	-2.15	104.94	110.08
15	B	1234	CLA	C1-O2A-CGA	2.15	121.86	116.65
15	A	1012	CLA	CHA-C1A-NA	-2.15	121.52	126.39
15	1	615	CLA	CAC-C3C-C4C	2.15	127.59	124.79
15	B	1215	CLA	CAA-C2A-C1A	-2.15	104.93	111.97
14	A	4004	BCR	C32-C1-C6	-2.15	106.87	110.24
15	A	1101	CLA	CHA-C1A-NA	-2.15	121.53	126.39
15	A	1104	CLA	CMA-C3A-C4A	2.15	117.55	111.77
15	A	1109	CLA	C2D-C1D-ND	2.15	112.25	110.13
14	A	4008	BCR	C37-C22-C23	2.15	121.37	118.09
15	A	1107	CLA	CAA-C2A-C3A	-2.14	107.20	113.00
15	A	1119	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
14	A	4004	BCR	C36-C18-C17	-2.14	119.34	122.82
15	A	1128	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
13	4	502	XAT	C24-C23-C22	-2.14	106.79	110.79
15	A	1118	CLA	C1D-ND-C4D	-2.14	104.81	106.31
14	B	4001	BCR	C28-C27-C26	-2.14	110.24	114.06
15	A	1112	CLA	CHD-C1D-ND	-2.14	121.80	124.80
15	B	1239	CLA	O1D-CGD-CBD	2.14	128.73	124.52
15	B	1231	CLA	C4B-CHC-C1C	2.14	131.27	126.25
15	A	1120	CLA	CHA-C1A-NA	-2.14	121.56	126.39
15	4	603	CLA	O2A-CGA-O1A	-2.13	118.29	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1236	CLA	CHD-C1D-ND	-2.13	121.80	124.80
15	2	616	CLA	C14-C13-C12	-2.13	103.67	111.27
14	4	503	BCR	C38-C26-C25	-2.13	122.16	124.48
15	A	1117	CLA	CHA-C1A-NA	-2.13	121.56	126.39
15	B	1215	CLA	O2D-CGD-CBD	2.13	114.96	111.23
15	3	607	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	3	502	XAT	C17-C1-C16	2.13	110.47	107.37
12	4	501	LUT	C8-C9-C10	2.13	122.36	119.01
15	B	1222	CLA	CHD-C1D-ND	-2.13	121.80	124.80
15	A	1133	CLA	CHD-C4C-NC	-2.13	120.93	124.23
15	B	1224	CLA	C2D-C1D-ND	2.13	112.23	110.13
18	2	802	LMG	O3-C3-C2	-2.13	105.36	110.38
15	A	1113	CLA	CHA-C1A-NA	-2.13	121.57	126.39
14	2	503	BCR	C16-C15-C14	-2.13	119.17	123.52
15	A	1106	CLA	CHA-C1A-NA	-2.13	121.58	126.39
15	B	1227	CLA	CHA-C1A-NA	-2.13	121.58	126.39
15	J	1302	CLA	CHD-C1D-ND	-2.12	121.81	124.80
15	B	1222	CLA	CHA-C1A-NA	-2.12	121.58	126.39
15	3	605	CLA	CHA-C1A-NA	-2.12	121.58	126.39
15	B	1216	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
14	A	4008	BCR	C1-C6-C7	2.12	121.40	115.65
15	A	1105	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
15	A	1127	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
15	B	1230	CLA	CHD-C1D-ND	-2.12	121.82	124.80
15	A	1135	CLA	CHA-C1A-NA	-2.12	121.60	126.39
15	4	609	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
14	2	503	BCR	C8-C7-C6	-2.12	121.35	127.00
15	A	1125	CLA	CHA-C1A-NA	-2.11	121.60	126.39
15	B	1236	CLA	CHA-C1A-NA	-2.11	121.60	126.39
15	B	1228	CLA	CHA-C1A-NA	-2.11	121.60	126.39
15	B	1229	CLA	CHA-C1A-NA	-2.11	121.60	126.39
15	A	1104	CLA	CHA-C1A-NA	-2.11	121.61	126.39
15	A	1106	CLA	CHD-C1D-ND	-2.11	121.83	124.80
16	1	610	CHL	C1-O2A-CGA	2.11	122.83	116.07
15	3	603	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
14	B	4004	BCR	C1-C6-C5	-2.11	119.75	122.64
15	B	1228	CLA	CHD-C1D-ND	-2.11	121.83	124.80
15	1	603	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
15	B	1231	CLA	O2A-CGA-CBA	2.11	118.27	111.83
12	1	501	LUT	C20-C13-C12	2.11	121.31	118.09
14	A	4007	BCR	C39-C30-C25	-2.11	106.93	110.24
15	1	608	CLA	O2A-CGA-O1A	-2.11	118.35	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1113	CLA	CHD-C1D-ND	-2.11	121.83	124.80
15	A	1131	CLA	CHA-C1A-NA	-2.11	121.62	126.39
15	A	1136	CLA	CHA-C1A-NA	-2.11	121.62	126.39
15	A	1126	CLA	C2D-C1D-ND	2.11	112.21	110.13
15	B	1216	CLA	CHB-C4A-NA	2.11	127.44	124.40
15	A	1104	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
12	4	501	LUT	C36-C21-C26	2.10	112.73	109.55
15	J	1302	CLA	CHA-C1A-NA	-2.10	121.63	126.39
14	A	4002	BCR	C32-C1-C6	-2.10	106.95	110.24
15	2	612	CLA	C1-O2A-CGA	2.10	121.74	116.65
15	B	1225	CLA	CHA-C1A-NA	-2.10	121.63	126.39
15	1	607	CLA	CAC-C3C-C4C	2.10	127.52	124.79
15	B	1230	CLA	O2A-CGA-CBA	2.10	118.24	111.83
18	4	801	LMG	O5-C6-C5	-2.10	104.18	111.33
15	A	1133	CLA	C2C-C1C-NC	2.10	112.19	109.98
15	A	1118	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
14	A	4004	BCR	C23-C24-C25	-2.10	121.39	127.00
15	A	1140	CLA	C4B-CHC-C1C	2.10	131.18	126.25
15	A	1122	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
14	A	4006	BCR	C38-C26-C25	-2.10	122.20	124.48
12	1	501	LUT	C4-C5-C6	-2.09	116.46	120.76
15	A	1119	CLA	CMA-C3A-C4A	2.09	117.40	111.77
15	A	1013	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
14	F	4001	BCR	C23-C24-C25	-2.09	121.41	127.00
15	B	1228	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
15	2	602	CLA	C2A-C1A-CHA	2.09	127.49	123.87
15	B	1211	CLA	C1-C2-C3	-2.09	122.77	126.20
15	B	1221	CLA	C2A-C1A-CHA	2.09	127.49	123.87
15	A	1133	CLA	C1C-C2C-C3C	-2.09	104.78	106.98
15	B	1231	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
15	A	1110	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
21	A	2001	PQN	C11-C3-C4	2.09	120.78	118.58
15	A	1110	CLA	CHA-C1A-NA	-2.09	121.67	126.39
15	B	1231	CLA	C2B-C1B-NB	-2.08	108.16	110.33
20	A	1011	CL0	C1A-CHA-C4D	2.08	122.46	118.98
15	B	1231	CLA	C1C-C2C-C3C	-2.08	104.79	106.98
15	A	1135	CLA	CHD-C1D-ND	-2.08	121.87	124.80
15	B	1223	CLA	C1-O2A-CGA	2.08	121.69	116.65
18	2	803	LMG	C1-C2-C3	-2.08	105.63	110.01
15	A	1134	CLA	C4B-CHC-C1C	2.08	131.14	126.25
15	B	1229	CLA	C4B-C3B-C2B	2.08	109.89	107.30
15	A	1108	CLA	CHA-C1A-NA	-2.08	121.69	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1121	CLA	CHD-C1D-ND	-2.08	121.88	124.80
16	4	613	CHL	CMD-C2D-C3D	2.08	128.84	124.68
15	A	1116	CLA	O2A-CGA-CBA	2.08	118.17	111.83
18	2	803	LMG	O3-C3-C2	-2.08	105.48	110.38
15	B	1220	CLA	O2D-CGD-O1D	-2.08	119.81	123.85
14	B	4005	BCR	C23-C24-C25	-2.08	121.45	127.00
14	B	4001	BCR	C35-C13-C12	2.08	121.26	118.09
15	B	1228	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
15	A	1128	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
15	3	613	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
15	A	1137	CLA	CHA-C1A-NA	-2.07	121.70	126.39
15	A	1113	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
14	2	503	BCR	C20-C21-C22	-2.07	124.38	127.28
15	A	1102	CLA	CHA-C1A-NA	-2.07	121.70	126.39
14	A	4006	BCR	C30-C25-C26	-2.07	119.81	122.64
15	A	1013	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
18	2	803	LMG	O7-C10-O9	-2.07	118.87	123.70
15	A	1135	CLA	O2A-CGA-CBA	2.07	118.14	111.83
15	2	616	CLA	C16-C15-C13	2.07	122.83	115.97
15	A	1130	CLA	CHA-C1A-NA	-2.07	121.71	126.39
15	3	612	CLA	CHD-C1D-ND	-2.07	121.89	124.80
15	A	1105	CLA	O2A-CGA-CBA	2.07	118.13	111.83
15	3	609	CLA	C3B-C4B-NB	-2.07	108.69	110.53
15	3	603	CLA	C6-C5-C3	2.07	118.50	113.47
15	1	606	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
15	A	1127	CLA	CMC-C2C-C1C	2.06	128.26	125.03
18	B	5003	LMG	O7-C10-O9	-2.06	118.89	123.70
15	4	604	CLA	CMC-C2C-C1C	2.06	128.25	125.03
15	3	610	CLA	O2D-CGD-CBD	2.06	114.83	111.23
14	1	503	BCR	C8-C7-C6	-2.06	121.50	127.00
23	B	5002	DGD	C3D-C4D-C5D	-2.06	106.50	110.23
23	B	5002	DGD	O2D-C2D-C1D	-2.06	105.17	110.08
15	A	1138	CLA	CHA-C1A-NA	-2.06	121.73	126.39
15	A	1117	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
15	B	1210	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
16	3	604	CHL	CMD-C2D-C3D	2.05	128.79	124.68
18	2	804	LMG	O7-C10-O9	-2.05	118.91	123.70
15	A	1139	CLA	C6-C5-C3	-2.05	108.47	113.47
14	J	4001	BCR	C19-C18-C17	2.05	122.24	119.01
15	B	1214	CLA	CMB-C2B-C3B	2.05	131.38	126.55
15	2	603	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
15	A	1133	CLA	C6-C7-C8	-2.05	109.15	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	1130	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
15	B	1236	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
15	1	608	CLA	C5-C3-C2	2.05	125.77	121.17
15	A	1123	CLA	CHA-C1A-NA	-2.05	121.75	126.39
15	3	614	CLA	C3B-C4B-NB	-2.05	108.70	110.53
18	2	802	LMG	O1-C1-C2	-2.05	105.16	108.27
15	2	606	CLA	CAC-C3C-C4C	2.05	127.45	124.79
15	B	1210	CLA	C6-C5-C3	2.05	118.45	113.47
15	A	1133	CLA	CHB-C4A-NA	-2.05	121.44	124.40
14	3	506	BCR	C8-C7-C6	-2.05	121.53	127.00
15	B	1214	CLA	C4-C3-C2	-2.05	118.37	123.63
15	A	1115	CLA	O2D-CGD-O1D	-2.05	119.87	123.85
14	A	4008	BCR	C23-C24-C25	-2.04	121.54	127.00
15	A	1129	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
12	4	501	LUT	C1-C6-C7	2.04	121.19	115.65
15	B	1235	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
15	B	1022	CLA	CHC-C1C-NC	-2.04	121.24	124.31
15	A	1103	CLA	O2A-CGA-CBA	2.04	118.05	111.83
17	3	801	LHG	O7-C7-O9	-2.04	118.94	123.70
15	B	1211	CLA	CMB-C2B-C3B	2.04	131.34	126.55
20	A	1011	CL0	C6-C5-C3	-2.04	108.50	113.47
15	F	1301	CLA	CHA-C1A-NA	-2.04	121.78	126.39
14	3	503	BCR	C11-C10-C9	-2.04	124.42	127.28
15	A	1111	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
23	B	5002	DGD	O6E-C1E-O5D	-2.04	105.23	110.04
15	4	607	CLA	C2A-C1A-CHA	2.03	127.40	123.87
15	A	1124	CLA	O2A-CGA-CBA	2.03	118.04	111.83
15	1	603	CLA	C3A-C2A-C1A	2.03	104.39	101.34
15	B	1206	CLA	O1D-CGD-CBD	2.03	128.53	124.52
14	A	4004	BCR	C37-C22-C21	-2.03	119.52	122.82
15	2	603	CLA	C3A-C2A-C1A	2.03	104.39	101.34
15	A	1106	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
15	A	1135	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
18	B	5003	LMG	O2-C2-C1	-2.03	105.24	110.08
15	A	1105	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
15	A	1128	CLA	O2A-CGA-CBA	2.03	118.03	111.83
15	3	610	CLA	CBA-CAA-C2A	2.03	119.83	113.79
15	B	1227	CLA	C2C-C1C-NC	2.03	112.11	109.98
15	A	1141	CLA	CAA-C2A-C3A	-2.03	111.58	116.23
15	B	1220	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
15	A	1132	CLA	C3A-C2A-C1A	2.03	104.38	101.34
15	A	1128	CLA	CHD-C1D-ND	-2.03	121.95	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	501	LUT	C1-C6-C7	2.03	121.15	115.65
13	3	502	XAT	C28-C29-C30	2.03	122.19	119.01
15	A	1139	CLA	CAA-CBA-CGA	-2.03	107.46	113.21
14	B	4003	BCR	C8-C7-C6	-2.02	121.59	127.00
13	2	502	XAT	O23-C23-C22	-2.02	105.61	109.75
16	2	613	CHL	CMD-C2D-C3D	2.02	128.73	124.68
15	B	1210	CLA	CAC-C3C-C4C	2.02	127.42	124.79
15	B	1220	CLA	O1D-CGD-CBD	2.02	128.51	124.52
15	A	1119	CLA	C1-O2A-CGA	2.02	121.55	116.65
15	B	1022	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
15	B	1231	CLA	CBA-CAA-C2A	-2.02	107.78	113.79
14	3	504	BCR	C8-C9-C10	2.02	122.19	119.01
15	B	1205	CLA	O1D-CGD-CBD	2.02	128.50	124.52
15	1	604	CLA	CMC-C2C-C1C	2.02	128.19	125.03
16	4	611	CHL	CMD-C2D-C3D	2.02	128.72	124.68
14	A	4004	BCR	C8-C9-C10	2.02	122.18	119.01
15	B	1229	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
15	B	1232	CLA	O1D-CGD-CBD	2.02	128.50	124.52
15	4	601	CLA	C4-C3-C5	2.02	118.73	115.23
15	B	1228	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
14	B	4004	BCR	C33-C5-C6	-2.02	122.28	124.48
15	A	1115	CLA	C2D-C1D-ND	2.02	112.12	110.13
15	B	1230	CLA	C2D-C1D-ND	2.01	112.12	110.13
15	A	1118	CLA	C2D-C1D-ND	2.01	112.12	110.13
15	A	1114	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
15	3	611	CLA	O2D-CGD-CBD	2.01	114.75	111.23
15	A	1107	CLA	CHA-C1A-NA	-2.01	121.83	126.39
15	1	603	CLA	O1D-CGD-CBD	2.01	128.48	124.52
15	B	1240	CLA	C1-C2-C3	2.01	129.49	126.20
16	1	610	CHL	CMD-C2D-C3D	2.01	128.70	124.68
14	2	503	BCR	C27-C26-C25	2.01	125.42	122.70
15	B	1225	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
23	B	5002	DGD	O3E-C3E-C2E	-2.01	105.64	110.38
15	2	605	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
15	A	1125	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
15	B	1235	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
15	1	604	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
15	2	616	CLA	C17-C16-C15	2.01	122.26	113.28
15	A	1125	CLA	CHD-C1D-ND	-2.00	121.98	124.80
14	3	503	BCR	C8-C7-C6	-2.00	121.64	127.00
14	A	4003	BCR	C38-C26-C27	2.00	117.87	113.60
15	2	605	CLA	C1-C2-C3	-2.00	122.91	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	607	CLA	C1-C2-C3	-2.00	122.92	126.20
15	A	1103	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
15	A	1108	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
15	A	1112	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
15	B	1022	CLA	CBA-CAA-C2A	-2.00	107.84	113.79
15	A	1131	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
14	A	4005	BCR	C32-C1-C6	-2.00	107.11	110.24

All (168) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	1	501	LUT	C26
12	2	501	LUT	C26
12	3	501	LUT	C26
12	4	501	LUT	C26
15	1	601	CLA	ND
15	1	602	CLA	ND
15	1	603	CLA	ND
15	1	604	CLA	ND
15	1	605	CLA	ND
15	1	606	CLA	ND
15	1	607	CLA	ND
15	1	608	CLA	ND
15	1	611	CLA	ND
15	1	612	CLA	ND
15	1	613	CLA	ND
15	1	615	CLA	ND
15	2	601	CLA	ND
15	2	602	CLA	ND
15	2	603	CLA	ND
15	2	604	CLA	ND
15	2	605	CLA	ND
15	2	606	CLA	ND
15	2	607	CLA	ND
15	2	608	CLA	ND
15	2	612	CLA	ND
15	3	601	CLA	ND
15	3	603	CLA	ND
15	3	605	CLA	ND
15	3	606	CLA	ND
15	3	607	CLA	ND
15	3	608	CLA	ND

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Mol	Chain	Res	Type	Atom
15	3	609	CLA	ND
15	3	610	CLA	ND
15	3	611	CLA	ND
15	3	612	CLA	ND
15	3	613	CLA	ND
15	3	614	CLA	ND
15	3	615	CLA	ND
15	4	601	CLA	ND
15	4	602	CLA	ND
15	4	603	CLA	ND
15	4	604	CLA	ND
15	4	605	CLA	ND
15	4	606	CLA	ND
15	4	607	CLA	ND
15	4	608	CLA	ND
15	4	609	CLA	ND
15	4	612	CLA	ND
15	4	616	CLA	ND
15	A	1012	CLA	ND
15	A	1013	CLA	ND
15	A	1101	CLA	ND
15	A	1102	CLA	ND
15	A	1103	CLA	ND
15	A	1104	CLA	ND
15	A	1105	CLA	ND
15	A	1106	CLA	ND
15	A	1107	CLA	ND
15	A	1108	CLA	ND
15	A	1109	CLA	ND
15	A	1110	CLA	ND
15	A	1111	CLA	ND
15	A	1112	CLA	ND
15	A	1113	CLA	ND
15	A	1114	CLA	ND
15	A	1115	CLA	ND
15	A	1116	CLA	ND
15	A	1117	CLA	ND
15	A	1118	CLA	ND
15	A	1119	CLA	ND
15	A	1120	CLA	ND
15	A	1121	CLA	ND
15	A	1122	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A	1123	CLA	ND
15	A	1124	CLA	ND
15	A	1125	CLA	ND
15	A	1126	CLA	ND
15	A	1127	CLA	ND
15	A	1128	CLA	ND
15	A	1129	CLA	ND
15	A	1130	CLA	ND
15	A	1131	CLA	ND
15	A	1132	CLA	ND
15	A	1135	CLA	ND
15	A	1136	CLA	ND
15	A	1137	CLA	ND
15	A	1138	CLA	ND
15	A	1139	CLA	ND
15	A	1141	CLA	ND
15	B	1021	CLA	ND
15	B	1022	CLA	ND
15	B	1201	CLA	ND
15	B	1202	CLA	ND
15	B	1203	CLA	ND
15	B	1204	CLA	ND
15	B	1205	CLA	ND
15	B	1206	CLA	ND
15	B	1208	CLA	ND
15	B	1209	CLA	ND
15	B	1211	CLA	ND
15	B	1212	CLA	ND
15	B	1213	CLA	ND
15	B	1214	CLA	ND
15	B	1215	CLA	ND
15	B	1216	CLA	ND
15	B	1217	CLA	ND
15	B	1218	CLA	ND
15	B	1220	CLA	ND
15	B	1221	CLA	ND
15	B	1222	CLA	ND
15	B	1223	CLA	ND
15	B	1224	CLA	ND
15	B	1225	CLA	ND
15	B	1226	CLA	ND
15	B	1227	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B	1228	CLA	ND
15	B	1229	CLA	ND
15	B	1230	CLA	ND
15	B	1231	CLA	ND
15	B	1232	CLA	ND
15	B	1234	CLA	ND
15	B	1235	CLA	ND
15	B	1236	CLA	ND
15	B	1237	CLA	ND
15	B	1238	CLA	ND
15	B	1238	CLA	C8
15	B	1239	CLA	ND
15	B	1240	CLA	ND
15	F	1301	CLA	ND
15	F	1302	CLA	ND
15	J	1302	CLA	ND
16	1	609	CHL	NA
16	1	609	CHL	ND
16	1	609	CHL	NC
16	1	609	CHL	C8
16	1	610	CHL	NA
16	1	610	CHL	ND
16	1	610	CHL	NC
16	2	609	CHL	NA
16	2	609	CHL	ND
16	2	609	CHL	NC
16	2	609	CHL	C8
16	2	610	CHL	NA
16	2	610	CHL	ND
16	2	610	CHL	NC
16	2	611	CHL	NA
16	2	611	CHL	ND
16	2	611	CHL	NC
16	2	613	CHL	NA
16	2	613	CHL	ND
16	2	613	CHL	NC
16	3	604	CHL	NA
16	3	604	CHL	ND
16	3	604	CHL	NC
16	3	604	CHL	C8
16	4	610	CHL	NA
16	4	610	CHL	ND

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Mol	Chain	Res	Type	Atom
16	4	610	CHL	NC
16	4	611	CHL	NA
16	4	611	CHL	ND
16	4	611	CHL	NC
16	4	613	CHL	NA
16	4	613	CHL	ND
16	4	613	CHL	NC
16	4	613	CHL	C8
20	A	1011	CL0	NA
20	A	1011	CL0	ND
20	A	1011	CL0	NC

All (2168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	1	501	LUT	C11-C12-C13-C14
12	2	501	LUT	C25-C26-C27-C28
12	3	501	LUT	C25-C26-C27-C28
12	4	501	LUT	C11-C12-C13-C14
12	4	501	LUT	C21-C26-C27-C28
12	4	501	LUT	C25-C26-C27-C28
12	4	501	LUT	C31-C32-C33-C34
13	1	502	XAT	O4-C6-C7-C8
13	2	502	XAT	C31-C32-C33-C34
13	3	502	XAT	C10-C11-C12-C13
13	3	502	XAT	C11-C12-C13-C14
13	3	502	XAT	C12-C13-C14-C15
13	3	502	XAT	C20-C13-C14-C15
13	3	502	XAT	C25-C26-C27-C28
13	3	502	XAT	O24-C26-C27-C28
13	3	502	XAT	C27-C28-C29-C30
13	3	502	XAT	C27-C28-C29-C39
13	3	502	XAT	C32-C33-C34-C35
13	3	502	XAT	C40-C33-C34-C35
13	4	502	XAT	C7-C8-C9-C19
13	4	502	XAT	C13-C14-C15-C35
13	4	502	XAT	O24-C26-C27-C28
13	4	502	XAT	C27-C28-C29-C30
13	4	502	XAT	C27-C28-C29-C39
13	4	502	XAT	C31-C32-C33-C34
13	4	502	XAT	C31-C32-C33-C40
14	1	503	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	1	503	BCR	C11-C10-C9-C8
14	1	503	BCR	C11-C10-C9-C34
14	1	503	BCR	C10-C11-C12-C13
14	1	503	BCR	C11-C12-C13-C35
14	1	503	BCR	C16-C17-C18-C19
14	1	503	BCR	C16-C17-C18-C36
14	1	503	BCR	C18-C19-C20-C21
14	1	503	BCR	C21-C22-C23-C24
14	1	503	BCR	C37-C22-C23-C24
14	2	503	BCR	C7-C8-C9-C34
14	2	503	BCR	C11-C10-C9-C8
14	2	503	BCR	C10-C11-C12-C13
14	2	503	BCR	C11-C12-C13-C35
14	2	503	BCR	C36-C18-C19-C20
14	2	503	BCR	C20-C21-C22-C37
14	3	503	BCR	C7-C8-C9-C10
14	3	503	BCR	C7-C8-C9-C34
14	3	503	BCR	C11-C10-C9-C8
14	3	503	BCR	C11-C10-C9-C34
14	3	503	BCR	C11-C12-C13-C14
14	3	504	BCR	C11-C10-C9-C8
14	3	504	BCR	C11-C10-C9-C34
14	3	504	BCR	C17-C18-C19-C20
14	3	504	BCR	C36-C18-C19-C20
14	3	506	BCR	C6-C7-C8-C9
14	3	506	BCR	C10-C11-C12-C13
14	3	506	BCR	C11-C12-C13-C14
14	3	506	BCR	C12-C13-C14-C15
14	3	506	BCR	C15-C16-C17-C18
14	3	506	BCR	C16-C17-C18-C19
14	3	506	BCR	C16-C17-C18-C36
14	3	506	BCR	C20-C21-C22-C37
14	4	503	BCR	C7-C8-C9-C34
14	4	503	BCR	C11-C10-C9-C8
14	4	503	BCR	C11-C10-C9-C34
14	4	503	BCR	C11-C12-C13-C35
14	4	503	BCR	C16-C17-C18-C19
14	4	503	BCR	C16-C17-C18-C36
14	4	503	BCR	C18-C19-C20-C21
14	4	503	BCR	C20-C21-C22-C37
14	4	503	BCR	C37-C22-C23-C24
14	4	503	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	4	503	BCR	C23-C24-C25-C30
14	A	4002	BCR	C11-C10-C9-C8
14	A	4002	BCR	C11-C10-C9-C34
14	A	4003	BCR	C11-C10-C9-C8
14	A	4003	BCR	C11-C10-C9-C34
14	A	4003	BCR	C10-C11-C12-C13
14	A	4003	BCR	C11-C12-C13-C14
14	A	4004	BCR	C11-C10-C9-C8
14	A	4004	BCR	C11-C10-C9-C34
14	A	4004	BCR	C10-C11-C12-C13
14	A	4004	BCR	C11-C12-C13-C14
14	A	4004	BCR	C23-C24-C25-C26
14	A	4005	BCR	C11-C10-C9-C8
14	A	4005	BCR	C11-C10-C9-C34
14	A	4005	BCR	C9-C10-C11-C12
14	A	4005	BCR	C10-C11-C12-C13
14	A	4005	BCR	C11-C12-C13-C14
14	A	4005	BCR	C11-C12-C13-C35
14	A	4006	BCR	C11-C10-C9-C8
14	A	4006	BCR	C11-C10-C9-C34
14	A	4006	BCR	C17-C18-C19-C20
14	A	4006	BCR	C36-C18-C19-C20
14	A	4007	BCR	C7-C8-C9-C10
14	A	4007	BCR	C7-C8-C9-C34
14	A	4007	BCR	C10-C11-C12-C13
14	A	4007	BCR	C13-C14-C15-C16
14	A	4007	BCR	C21-C22-C23-C24
14	A	4007	BCR	C37-C22-C23-C24
14	A	4008	BCR	C11-C10-C9-C8
14	A	4008	BCR	C11-C10-C9-C34
14	A	4008	BCR	C10-C11-C12-C13
14	A	4008	BCR	C21-C22-C23-C24
14	A	4008	BCR	C37-C22-C23-C24
14	B	4001	BCR	C7-C8-C9-C10
14	B	4001	BCR	C16-C17-C18-C19
14	B	4001	BCR	C23-C24-C25-C26
14	B	4001	BCR	C23-C24-C25-C30
14	B	4002	BCR	C1-C6-C7-C8
14	B	4002	BCR	C5-C6-C7-C8
14	B	4002	BCR	C11-C10-C9-C34
14	B	4002	BCR	C10-C11-C12-C13
14	B	4002	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
14	B	4002	BCR	C20-C21-C22-C23
14	B	4002	BCR	C22-C23-C24-C25
14	B	4003	BCR	C6-C7-C8-C9
14	B	4003	BCR	C7-C8-C9-C10
14	B	4003	BCR	C11-C10-C9-C8
14	B	4003	BCR	C11-C10-C9-C34
14	B	4003	BCR	C10-C11-C12-C13
14	B	4003	BCR	C11-C12-C13-C14
14	B	4003	BCR	C11-C12-C13-C35
14	B	4003	BCR	C12-C13-C14-C15
14	B	4003	BCR	C35-C13-C14-C15
14	B	4003	BCR	C14-C15-C16-C17
14	B	4003	BCR	C16-C17-C18-C36
14	B	4004	BCR	C7-C8-C9-C34
14	B	4004	BCR	C11-C10-C9-C34
14	B	4004	BCR	C10-C11-C12-C13
14	B	4004	BCR	C11-C12-C13-C14
14	B	4004	BCR	C20-C21-C22-C37
14	B	4005	BCR	C1-C6-C7-C8
14	B	4005	BCR	C5-C6-C7-C8
14	B	4005	BCR	C11-C10-C9-C8
14	B	4005	BCR	C11-C10-C9-C34
14	B	4006	BCR	C11-C10-C9-C8
14	B	4006	BCR	C11-C10-C9-C34
14	B	4006	BCR	C10-C11-C12-C13
14	B	4006	BCR	C17-C18-C19-C20
14	B	4006	BCR	C36-C18-C19-C20
14	B	4006	BCR	C21-C22-C23-C24
14	B	4006	BCR	C37-C22-C23-C24
14	F	4001	BCR	C11-C10-C9-C8
14	F	4001	BCR	C11-C10-C9-C34
14	F	4001	BCR	C9-C10-C11-C12
14	F	4001	BCR	C10-C11-C12-C13
14	F	4001	BCR	C11-C12-C13-C14
14	F	4001	BCR	C11-C12-C13-C35
14	F	4001	BCR	C19-C20-C21-C22
14	F	4001	BCR	C21-C22-C23-C24
14	F	4001	BCR	C37-C22-C23-C24
14	F	4001	BCR	C23-C24-C25-C26
14	F	4001	BCR	C23-C24-C25-C30
14	F	4002	BCR	C7-C8-C9-C10
14	F	4002	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
14	F	4002	BCR	C11-C10-C9-C8
14	F	4002	BCR	C11-C10-C9-C34
14	F	4002	BCR	C10-C11-C12-C13
14	F	4002	BCR	C19-C20-C21-C22
14	J	4001	BCR	C5-C6-C7-C8
14	J	4001	BCR	C11-C10-C9-C8
14	J	4001	BCR	C11-C10-C9-C34
14	J	4001	BCR	C10-C11-C12-C13
14	J	4001	BCR	C11-C12-C13-C14
14	J	4001	BCR	C11-C12-C13-C35
14	J	4001	BCR	C17-C18-C19-C20
14	J	4001	BCR	C19-C20-C21-C22
14	J	4002	BCR	C11-C10-C9-C8
14	J	4002	BCR	C11-C10-C9-C34
14	J	4002	BCR	C10-C11-C12-C13
14	J	4002	BCR	C19-C20-C21-C22
14	J	4002	BCR	C21-C22-C23-C24
14	J	4002	BCR	C37-C22-C23-C24
14	J	4002	BCR	C23-C24-C25-C26
14	J	4002	BCR	C23-C24-C25-C30
15	1	601	CLA	CBD-CGD-O2D-CED
15	1	602	CLA	CBA-CGA-O2A-C1
15	1	603	CLA	C1A-C2A-CAA-CBA
15	1	603	CLA	CBD-CGD-O2D-CED
15	1	604	CLA	CHA-CBD-CGD-O1D
15	1	604	CLA	CHA-CBD-CGD-O2D
15	1	607	CLA	CBD-CGD-O2D-CED
15	1	612	CLA	CBD-CGD-O2D-CED
15	1	615	CLA	CBD-CGD-O2D-CED
15	2	601	CLA	C1A-C2A-CAA-CBA
15	2	601	CLA	C3A-C2A-CAA-CBA
15	2	601	CLA	CBD-CGD-O2D-CED
15	2	602	CLA	CBD-CGD-O2D-CED
15	2	603	CLA	CBD-CGD-O2D-CED
15	2	604	CLA	C1A-C2A-CAA-CBA
15	2	604	CLA	C3A-C2A-CAA-CBA
15	2	605	CLA	CBD-CGD-O2D-CED
15	2	606	CLA	CBD-CGD-O2D-CED
15	2	616	CLA	C1A-C2A-CAA-CBA
15	2	616	CLA	C3A-C2A-CAA-CBA
15	2	616	CLA	CBD-CGD-O2D-CED
15	3	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	3	605	CLA	C14-C13-C15-C16
15	3	606	CLA	CBD-CGD-O2D-CED
15	3	607	CLA	C2B-C3B-CAB-CBB
15	3	607	CLA	C4B-C3B-CAB-CBB
15	3	608	CLA	C3A-C2A-CAA-CBA
15	3	608	CLA	CBD-CGD-O2D-CED
15	3	609	CLA	CHA-CBD-CGD-O1D
15	3	609	CLA	CHA-CBD-CGD-O2D
15	3	611	CLA	CBD-CGD-O2D-CED
15	3	612	CLA	CHA-CBD-CGD-O1D
15	3	612	CLA	CHA-CBD-CGD-O2D
15	3	613	CLA	C1A-C2A-CAA-CBA
15	3	613	CLA	C3A-C2A-CAA-CBA
15	3	613	CLA	CBD-CGD-O2D-CED
15	3	615	CLA	C1A-C2A-CAA-CBA
15	3	615	CLA	C3A-C2A-CAA-CBA
15	3	615	CLA	CHA-CBD-CGD-O1D
15	3	615	CLA	CHA-CBD-CGD-O2D
15	3	615	CLA	CBD-CGD-O2D-CED
15	4	601	CLA	C1A-C2A-CAA-CBA
15	4	601	CLA	C3A-C2A-CAA-CBA
15	4	602	CLA	CHA-CBD-CGD-O1D
15	4	602	CLA	CHA-CBD-CGD-O2D
15	4	602	CLA	CBD-CGD-O2D-CED
15	4	604	CLA	C3A-C2A-CAA-CBA
15	4	604	CLA	CHA-CBD-CGD-O1D
15	4	604	CLA	CHA-CBD-CGD-O2D
15	4	606	CLA	CBD-CGD-O2D-CED
15	4	608	CLA	C2B-C3B-CAB-CBB
15	4	608	CLA	C4B-C3B-CAB-CBB
15	4	608	CLA	C2C-C3C-CAC-CBC
15	4	608	CLA	C4C-C3C-CAC-CBC
15	4	616	CLA	C1A-C2A-CAA-CBA
15	4	616	CLA	C3A-C2A-CAA-CBA
15	4	616	CLA	CBD-CGD-O2D-CED
15	A	1012	CLA	CBD-CGD-O2D-CED
15	A	1013	CLA	C2-C1-O2A-CGA
15	A	1013	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	CHA-CBD-CGD-O1D
15	A	1101	CLA	CHA-CBD-CGD-O2D
15	A	1102	CLA	C3A-C2A-CAA-CBA
15	A	1102	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	A	1103	CLA	CAD-CBD-CGD-O1D
15	A	1103	CLA	CAD-CBD-CGD-O2D
15	A	1105	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C3A-C2A-CAA-CBA
15	A	1106	CLA	CHA-CBD-CGD-O1D
15	A	1106	CLA	CHA-CBD-CGD-O2D
15	A	1106	CLA	CBD-CGD-O2D-CED
15	A	1107	CLA	C1A-C2A-CAA-CBA
15	A	1107	CLA	C2-C1-O2A-CGA
15	A	1108	CLA	C1A-C2A-CAA-CBA
15	A	1108	CLA	C3A-C2A-CAA-CBA
15	A	1110	CLA	C1A-C2A-CAA-CBA
15	A	1111	CLA	C2-C1-O2A-CGA
15	A	1113	CLA	CBD-CGD-O2D-CED
15	A	1114	CLA	CBD-CGD-O2D-CED
15	A	1116	CLA	C3A-C2A-CAA-CBA
15	A	1117	CLA	CHA-CBD-CGD-O1D
15	A	1117	CLA	CHA-CBD-CGD-O2D
15	A	1120	CLA	C1A-C2A-CAA-CBA
15	A	1122	CLA	C2-C1-O2A-CGA
15	A	1123	CLA	C2-C1-O2A-CGA
15	A	1123	CLA	CHA-CBD-CGD-O1D
15	A	1123	CLA	CHA-CBD-CGD-O2D
15	A	1123	CLA	CBD-CGD-O2D-CED
15	A	1124	CLA	C3A-C2A-CAA-CBA
15	A	1124	CLA	CAD-CBD-CGD-O1D
15	A	1124	CLA	CAD-CBD-CGD-O2D
15	A	1126	CLA	C1A-C2A-CAA-CBA
15	A	1126	CLA	C3A-C2A-CAA-CBA
15	A	1126	CLA	C2-C1-O2A-CGA
15	A	1128	CLA	CHA-CBD-CGD-O1D
15	A	1128	CLA	CHA-CBD-CGD-O2D
15	A	1129	CLA	CBD-CGD-O2D-CED
15	A	1130	CLA	C3A-C2A-CAA-CBA
15	A	1130	CLA	CHA-CBD-CGD-O1D
15	A	1130	CLA	CHA-CBD-CGD-O2D
15	A	1131	CLA	CBD-CGD-O2D-CED
15	A	1132	CLA	C2B-C3B-CAB-CBB
15	A	1132	CLA	C4B-C3B-CAB-CBB
15	A	1132	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	C1A-C2A-CAA-CBA
15	A	1133	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	A	1133	CLA	C4B-C3B-CAB-CBB
15	A	1134	CLA	CHA-CBD-CGD-O1D
15	A	1134	CLA	CHA-CBD-CGD-O2D
15	A	1135	CLA	C1A-C2A-CAA-CBA
15	A	1135	CLA	C3A-C2A-CAA-CBA
15	A	1135	CLA	CHA-CBD-CGD-O1D
15	A	1135	CLA	CHA-CBD-CGD-O2D
15	A	1135	CLA	CBD-CGD-O2D-CED
15	A	1135	CLA	C2-C3-C5-C6
15	A	1135	CLA	C4-C3-C5-C6
15	A	1136	CLA	CBD-CGD-O2D-CED
15	A	1137	CLA	C1A-C2A-CAA-CBA
15	A	1137	CLA	C3A-C2A-CAA-CBA
15	A	1137	CLA	CHA-CBD-CGD-O1D
15	A	1137	CLA	CHA-CBD-CGD-O2D
15	A	1137	CLA	CBD-CGD-O2D-CED
15	A	1138	CLA	CBD-CGD-O2D-CED
15	A	1139	CLA	CBD-CGD-O2D-CED
15	A	1141	CLA	CAD-CBD-CGD-O1D
15	A	1141	CLA	CAD-CBD-CGD-O2D
15	B	1021	CLA	C1A-C2A-CAA-CBA
15	B	1021	CLA	C3A-C2A-CAA-CBA
15	B	1022	CLA	C1A-C2A-CAA-CBA
15	B	1022	CLA	C3A-C2A-CAA-CBA
15	B	1022	CLA	C2-C1-O2A-CGA
15	B	1022	CLA	CBD-CGD-O2D-CED
15	B	1023	CLA	CBD-CGD-O2D-CED
15	B	1202	CLA	C1A-C2A-CAA-CBA
15	B	1202	CLA	C3A-C2A-CAA-CBA
15	B	1203	CLA	CBD-CGD-O2D-CED
15	B	1204	CLA	C1A-C2A-CAA-CBA
15	B	1204	CLA	C3A-C2A-CAA-CBA
15	B	1204	CLA	CHA-CBD-CGD-O1D
15	B	1204	CLA	CHA-CBD-CGD-O2D
15	B	1207	CLA	CBA-CGA-O2A-C1
15	B	1207	CLA	CAD-CBD-CGD-O1D
15	B	1207	CLA	CAD-CBD-CGD-O2D
15	B	1210	CLA	C1A-C2A-CAA-CBA
15	B	1211	CLA	CHA-CBD-CGD-O1D
15	B	1211	CLA	CHA-CBD-CGD-O2D
15	B	1212	CLA	CHA-CBD-CGD-O2D
15	B	1214	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	B	1214	CLA	C4B-C3B-CAB-CBB
15	B	1217	CLA	CBA-CGA-O2A-C1
15	B	1217	CLA	O1A-CGA-O2A-C1
15	B	1217	CLA	C2B-C3B-CAB-CBB
15	B	1217	CLA	C4B-C3B-CAB-CBB
15	B	1218	CLA	CHA-CBD-CGD-O1D
15	B	1218	CLA	CHA-CBD-CGD-O2D
15	B	1220	CLA	C2B-C3B-CAB-CBB
15	B	1220	CLA	C4B-C3B-CAB-CBB
15	B	1221	CLA	CHA-CBD-CGD-O1D
15	B	1221	CLA	CHA-CBD-CGD-O2D
15	B	1222	CLA	C1A-C2A-CAA-CBA
15	B	1222	CLA	C3A-C2A-CAA-CBA
15	B	1222	CLA	CHA-CBD-CGD-O1D
15	B	1222	CLA	CHA-CBD-CGD-O2D
15	B	1222	CLA	CBD-CGD-O2D-CED
15	B	1222	CLA	C11-C10-C8-C9
15	B	1224	CLA	C1A-C2A-CAA-CBA
15	B	1224	CLA	C3A-C2A-CAA-CBA
15	B	1225	CLA	C1A-C2A-CAA-CBA
15	B	1225	CLA	C3A-C2A-CAA-CBA
15	B	1226	CLA	C11-C12-C13-C14
15	B	1227	CLA	CAD-CBD-CGD-O1D
15	B	1227	CLA	CAD-CBD-CGD-O2D
15	B	1227	CLA	CBD-CGD-O2D-CED
15	B	1228	CLA	CBD-CGD-O2D-CED
15	B	1228	CLA	C2-C3-C5-C6
15	B	1228	CLA	C4-C3-C5-C6
15	B	1229	CLA	C1A-C2A-CAA-CBA
15	B	1229	CLA	C3A-C2A-CAA-CBA
15	B	1229	CLA	C2-C1-O2A-CGA
15	B	1229	CLA	CHA-CBD-CGD-O1D
15	B	1229	CLA	CHA-CBD-CGD-O2D
15	B	1230	CLA	C3A-C2A-CAA-CBA
15	B	1232	CLA	CAD-CBD-CGD-O1D
15	B	1232	CLA	CAD-CBD-CGD-O2D
15	B	1234	CLA	C1A-C2A-CAA-CBA
15	B	1234	CLA	CHA-CBD-CGD-O1D
15	B	1234	CLA	CHA-CBD-CGD-O2D
15	B	1235	CLA	CBD-CGD-O2D-CED
15	B	1236	CLA	CHA-CBD-CGD-O1D
15	B	1236	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	B	1236	CLA	CBD-CGD-O2D-CED
15	B	1238	CLA	C1A-C2A-CAA-CBA
15	B	1238	CLA	C2C-C3C-CAC-CBC
15	B	1238	CLA	C4C-C3C-CAC-CBC
15	B	1238	CLA	C1-C2-C3-C5
15	B	1240	CLA	CBD-CGD-O2D-CED
15	J	1302	CLA	C1A-C2A-CAA-CBA
16	2	613	CHL	C1A-C2A-CAA-CBA
16	2	613	CHL	C3A-C2A-CAA-CBA
16	2	613	CHL	CHA-CBD-CGD-O1D
16	2	613	CHL	CHA-CBD-CGD-O2D
16	4	610	CHL	C4C-C3C-CAC-CBC
17	1	801	LHG	C3-O3-P-O4
17	2	801	LHG	C3-O3-P-O6
17	2	801	LHG	C4-O6-P-O3
17	2	801	LHG	C4-O6-P-O4
17	2	801	LHG	C4-O6-P-O5
17	3	801	LHG	C2-C3-O3-P
17	3	801	LHG	C3-O3-P-O4
17	3	801	LHG	C3-O3-P-O6
17	3	801	LHG	O9-C7-O7-C5
17	3	801	LHG	C8-C7-O7-C5
17	A	5001	LHG	O1-C1-C2-C3
17	A	5002	LHG	C4-O6-P-O3
17	A	5002	LHG	C4-O6-P-O5
17	B	5001	LHG	C1-C2-C3-O3
17	B	5001	LHG	O2-C2-C3-O3
17	B	5001	LHG	C3-O3-P-O5
17	B	5001	LHG	C3-O3-P-O6
17	B	5001	LHG	C4-O6-P-O3
17	B	5001	LHG	C4-O6-P-O5
17	B	5001	LHG	C8-C7-O7-C5
18	2	803	LMG	C11-C10-O7-C8
18	2	804	LMG	C2-C1-O1-C7
18	2	804	LMG	O6-C1-O1-C7
18	2	804	LMG	O9-C10-O7-C8
18	2	804	LMG	C11-C10-O7-C8
19	3	802	3PH	C1-O11-P-O13
19	3	802	3PH	C1-O11-P-O14
19	3	802	3PH	C1-O11-P-O12
20	A	1011	CL0	C2-C1-O2A-CGA
20	A	1011	CL0	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	5002	DGD	C2B-C1B-O2G-C2G
15	3	608	CLA	C4C-C3C-CAC-CBC
15	1	612	CLA	O1D-CGD-O2D-CED
15	1	615	CLA	O1D-CGD-O2D-CED
15	A	1109	CLA	O1D-CGD-O2D-CED
15	A	1126	CLA	O1D-CGD-O2D-CED
15	A	1139	CLA	O1D-CGD-O2D-CED
15	B	1021	CLA	O1D-CGD-O2D-CED
15	B	1205	CLA	O1D-CGD-O2D-CED
15	1	613	CLA	O1D-CGD-O2D-CED
15	2	602	CLA	O1D-CGD-O2D-CED
15	2	606	CLA	O1D-CGD-O2D-CED
15	A	1129	CLA	O1D-CGD-O2D-CED
15	B	1023	CLA	O1D-CGD-O2D-CED
15	1	608	CLA	CBD-CGD-O2D-CED
15	1	611	CLA	CBD-CGD-O2D-CED
15	1	613	CLA	CBD-CGD-O2D-CED
15	2	604	CLA	CBD-CGD-O2D-CED
15	3	603	CLA	CBD-CGD-O2D-CED
15	3	605	CLA	CBD-CGD-O2D-CED
15	3	607	CLA	CBD-CGD-O2D-CED
15	3	612	CLA	CBD-CGD-O2D-CED
15	4	603	CLA	CBD-CGD-O2D-CED
15	4	609	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	CBD-CGD-O2D-CED
15	A	1107	CLA	CBD-CGD-O2D-CED
15	A	1108	CLA	CBD-CGD-O2D-CED
15	A	1109	CLA	CBD-CGD-O2D-CED
15	A	1112	CLA	CBD-CGD-O2D-CED
15	A	1117	CLA	CBD-CGD-O2D-CED
15	A	1120	CLA	CBD-CGD-O2D-CED
15	A	1121	CLA	CBD-CGD-O2D-CED
15	A	1126	CLA	CBD-CGD-O2D-CED
15	A	1127	CLA	CBD-CGD-O2D-CED
15	A	1128	CLA	CBD-CGD-O2D-CED
15	A	1130	CLA	CBD-CGD-O2D-CED
15	A	1140	CLA	CBD-CGD-O2D-CED
15	A	1141	CLA	CBD-CGD-O2D-CED
15	B	1021	CLA	CBD-CGD-O2D-CED
15	B	1205	CLA	CBD-CGD-O2D-CED
15	B	1206	CLA	CBD-CGD-O2D-CED
15	B	1216	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1217	CLA	CBD-CGD-O2D-CED
15	B	1225	CLA	CBD-CGD-O2D-CED
15	B	1229	CLA	CBD-CGD-O2D-CED
15	B	1230	CLA	CBD-CGD-O2D-CED
15	J	1302	CLA	CBD-CGD-O2D-CED
15	A	1101	CLA	O1A-CGA-O2A-C1
19	3	802	3PH	O32-C31-O31-C3
15	1	602	CLA	O1A-CGA-O2A-C1
15	B	1207	CLA	O1A-CGA-O2A-C1
16	4	610	CHL	C2C-C3C-CAC-CBC
15	3	608	CLA	C2C-C3C-CAC-CBC
15	A	1132	CLA	C2C-C3C-CAC-CBC
15	1	603	CLA	O1D-CGD-O2D-CED
15	2	605	CLA	O1D-CGD-O2D-CED
15	B	1203	CLA	O1D-CGD-O2D-CED
15	2	616	CLA	C13-C15-C16-C17
15	4	608	CLA	CBA-CGA-O2A-C1
15	F	1301	CLA	CBA-CGA-O2A-C1
18	2	804	LMG	C8-C9-O8-C28
15	A	1132	CLA	C4C-C3C-CAC-CBC
15	3	612	CLA	O1D-CGD-O2D-CED
15	A	1112	CLA	O1D-CGD-O2D-CED
15	A	1121	CLA	O1D-CGD-O2D-CED
15	A	1130	CLA	O1D-CGD-O2D-CED
15	B	1206	CLA	O1D-CGD-O2D-CED
15	B	1216	CLA	O1D-CGD-O2D-CED
15	B	1229	CLA	O1D-CGD-O2D-CED
15	J	1302	CLA	O1D-CGD-O2D-CED
15	B	1219	CLA	CBD-CGD-O2D-CED
15	F	1301	CLA	CBD-CGD-O2D-CED
15	2	605	CLA	O1A-CGA-O2A-C1
15	2	616	CLA	O1A-CGA-O2A-C1
15	3	603	CLA	O1A-CGA-O2A-C1
15	3	612	CLA	O1A-CGA-O2A-C1
15	3	614	CLA	O1A-CGA-O2A-C1
15	4	605	CLA	O1A-CGA-O2A-C1
15	4	606	CLA	O1A-CGA-O2A-C1
15	4	607	CLA	O1A-CGA-O2A-C1
15	4	612	CLA	O1A-CGA-O2A-C1
15	4	616	CLA	O1A-CGA-O2A-C1
15	A	1111	CLA	O1A-CGA-O2A-C1
15	B	1208	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	B	1213	CLA	O1A-CGA-O2A-C1
15	B	1214	CLA	O1A-CGA-O2A-C1
15	B	1222	CLA	O1A-CGA-O2A-C1
15	B	1227	CLA	O1A-CGA-O2A-C1
15	F	1302	CLA	O1A-CGA-O2A-C1
18	2	803	LMG	O10-C28-O8-C9
18	B	5003	LMG	O10-C28-O8-C9
15	4	608	CLA	O1A-CGA-O2A-C1
15	F	1301	CLA	O1A-CGA-O2A-C1
15	1	607	CLA	O1D-CGD-O2D-CED
15	3	603	CLA	O1D-CGD-O2D-CED
15	3	608	CLA	O1D-CGD-O2D-CED
15	3	611	CLA	O1D-CGD-O2D-CED
15	3	613	CLA	O1D-CGD-O2D-CED
15	4	616	CLA	O1D-CGD-O2D-CED
15	A	1108	CLA	O1D-CGD-O2D-CED
15	B	1225	CLA	O1D-CGD-O2D-CED
15	B	1228	CLA	O1D-CGD-O2D-CED
15	B	1235	CLA	O1D-CGD-O2D-CED
15	1	601	CLA	O1D-CGD-O2D-CED
15	3	615	CLA	O1D-CGD-O2D-CED
15	4	602	CLA	O1D-CGD-O2D-CED
15	A	1012	CLA	O1D-CGD-O2D-CED
15	A	1113	CLA	O1D-CGD-O2D-CED
15	A	1114	CLA	O1D-CGD-O2D-CED
15	A	1132	CLA	O1D-CGD-O2D-CED
15	A	1135	CLA	O1D-CGD-O2D-CED
15	A	1137	CLA	O1D-CGD-O2D-CED
15	A	1138	CLA	O1D-CGD-O2D-CED
15	B	1022	CLA	O1D-CGD-O2D-CED
15	B	1227	CLA	O1D-CGD-O2D-CED
15	B	1236	CLA	O1D-CGD-O2D-CED
20	A	1011	CL0	O1D-CGD-O2D-CED
15	A	1136	CLA	C5-C6-C7-C8
15	3	601	CLA	O1A-CGA-O2A-C1
17	B	5001	LHG	O9-C7-O7-C5
18	2	803	LMG	O9-C10-O7-C8
23	B	5002	DGD	O1B-C1B-O2G-C2G
15	A	1123	CLA	O1D-CGD-O2D-CED
15	B	1209	CLA	CBA-CGA-O2A-C1
15	B	1209	CLA	O1A-CGA-O2A-C1
18	B	5003	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
15	2	601	CLA	C3-C5-C6-C7
15	2	605	CLA	C3-C5-C6-C7
15	A	1105	CLA	C3-C5-C6-C7
15	A	1106	CLA	C3-C5-C6-C7
15	A	1112	CLA	C3-C5-C6-C7
15	A	1114	CLA	C3-C5-C6-C7
15	A	1125	CLA	C3-C5-C6-C7
15	A	1128	CLA	C3-C5-C6-C7
15	B	1021	CLA	C3-C5-C6-C7
15	B	1205	CLA	C3-C5-C6-C7
15	B	1227	CLA	C3-C5-C6-C7
15	B	1229	CLA	C3-C5-C6-C7
15	B	1230	CLA	C3-C5-C6-C7
15	B	1235	CLA	C3-C5-C6-C7
15	B	1240	CLA	O1D-CGD-O2D-CED
15	4	606	CLA	CBA-CGA-O2A-C1
15	4	607	CLA	CBA-CGA-O2A-C1
15	4	612	CLA	CBA-CGA-O2A-C1
15	A	1101	CLA	CBA-CGA-O2A-C1
15	A	1111	CLA	CBA-CGA-O2A-C1
15	A	1119	CLA	CBA-CGA-O2A-C1
15	B	1214	CLA	CBA-CGA-O2A-C1
15	B	1222	CLA	CBA-CGA-O2A-C1
15	B	1230	CLA	CBA-CGA-O2A-C1
15	B	1234	CLA	CBA-CGA-O2A-C1
18	2	803	LMG	C29-C28-O8-C9
18	B	5003	LMG	C29-C28-O8-C9
19	3	802	3PH	C32-C31-O31-C3
15	1	602	CLA	CBD-CGD-O2D-CED
15	2	607	CLA	CBD-CGD-O2D-CED
15	3	614	CLA	CBD-CGD-O2D-CED
15	4	604	CLA	CBD-CGD-O2D-CED
15	A	1103	CLA	CBD-CGD-O2D-CED
15	A	1105	CLA	CBD-CGD-O2D-CED
15	A	1111	CLA	CBD-CGD-O2D-CED
15	A	1124	CLA	CBD-CGD-O2D-CED
15	A	1125	CLA	CBD-CGD-O2D-CED
15	B	1221	CLA	CBD-CGD-O2D-CED
15	B	1232	CLA	CBD-CGD-O2D-CED
15	B	1238	CLA	CBD-CGD-O2D-CED
15	F	1302	CLA	CBD-CGD-O2D-CED
15	B	1234	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
15	1	611	CLA	O1D-CGD-O2D-CED
15	2	601	CLA	O1D-CGD-O2D-CED
15	2	603	CLA	O1D-CGD-O2D-CED
15	2	616	CLA	O1D-CGD-O2D-CED
15	3	601	CLA	O1D-CGD-O2D-CED
15	3	606	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	O1D-CGD-O2D-CED
15	4	606	CLA	O1D-CGD-O2D-CED
15	A	1013	CLA	O1D-CGD-O2D-CED
15	A	1106	CLA	O1D-CGD-O2D-CED
15	A	1127	CLA	O1D-CGD-O2D-CED
15	A	1131	CLA	O1D-CGD-O2D-CED
15	A	1136	CLA	O1D-CGD-O2D-CED
15	A	1112	CLA	O1A-CGA-O2A-C1
15	1	612	CLA	C2C-C3C-CAC-CBC
15	B	1222	CLA	O1D-CGD-O2D-CED
15	1	603	CLA	C4-C3-C5-C6
15	3	606	CLA	C4-C3-C5-C6
15	A	1133	CLA	C4-C3-C5-C6
15	A	1139	CLA	C4-C3-C5-C6
15	A	1140	CLA	C4-C3-C5-C6
15	B	1225	CLA	C4-C3-C5-C6
15	3	606	CLA	C2-C3-C5-C6
15	A	1133	CLA	C2-C3-C5-C6
15	A	1139	CLA	C2-C3-C5-C6
15	A	1140	CLA	C2-C3-C5-C6
15	B	1237	CLA	CBD-CGD-O2D-CED
15	2	604	CLA	O1D-CGD-O2D-CED
15	A	1107	CLA	O1D-CGD-O2D-CED
15	A	1122	CLA	C2A-CAA-CBA-CGA
16	3	604	CHL	C2A-CAA-CBA-CGA
15	3	611	CLA	C3-C5-C6-C7
15	4	603	CLA	C3-C5-C6-C7
15	4	609	CLA	C3-C5-C6-C7
15	A	1116	CLA	C3-C5-C6-C7
21	B	2002	PQN	C13-C15-C16-C17
15	1	603	CLA	CBA-CGA-O2A-C1
15	1	606	CLA	CBA-CGA-O2A-C1
15	1	608	CLA	CBA-CGA-O2A-C1
15	2	605	CLA	CBA-CGA-O2A-C1
15	2	616	CLA	CBA-CGA-O2A-C1
15	3	601	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	3	603	CLA	CBA-CGA-O2A-C1
15	3	612	CLA	CBA-CGA-O2A-C1
15	3	614	CLA	CBA-CGA-O2A-C1
15	4	605	CLA	CBA-CGA-O2A-C1
15	4	616	CLA	CBA-CGA-O2A-C1
15	B	1208	CLA	CBA-CGA-O2A-C1
15	B	1213	CLA	CBA-CGA-O2A-C1
15	B	1227	CLA	CBA-CGA-O2A-C1
15	F	1302	CLA	CBA-CGA-O2A-C1
17	1	801	LHG	C24-C23-O8-C6
18	B	5003	LMG	O6-C5-C6-O5
13	1	502	XAT	C9-C10-C11-C12
13	1	502	XAT	C33-C34-C35-C15
13	2	502	XAT	C9-C10-C11-C12
13	3	502	XAT	C13-C14-C15-C35
13	4	502	XAT	C9-C10-C11-C12
14	A	4004	BCR	C19-C20-C21-C22
14	A	4006	BCR	C9-C10-C11-C12
14	B	4001	BCR	C19-C20-C21-C22
14	B	4005	BCR	C9-C10-C11-C12
14	B	4006	BCR	C9-C10-C11-C12
14	B	4006	BCR	C19-C20-C21-C22
14	J	4002	BCR	C13-C14-C15-C16
15	1	603	CLA	O1A-CGA-O2A-C1
15	1	605	CLA	O1A-CGA-O2A-C1
15	1	606	CLA	O1A-CGA-O2A-C1
15	1	608	CLA	O1A-CGA-O2A-C1
15	3	610	CLA	O1A-CGA-O2A-C1
15	4	603	CLA	O1A-CGA-O2A-C1
15	A	1119	CLA	O1A-CGA-O2A-C1
15	B	1211	CLA	O1A-CGA-O2A-C1
15	B	1221	CLA	O1A-CGA-O2A-C1
15	B	1234	CLA	O1A-CGA-O2A-C1
19	3	802	3PH	O22-C21-O21-C2
18	2	804	LMG	C17-C18-C19-C20
18	2	804	LMG	C20-C21-C22-C23
18	2	804	LMG	C23-C24-C25-C26
15	B	1234	CLA	C4C-C3C-CAC-CBC
15	A	1111	CLA	C2C-C3C-CAC-CBC
15	A	1120	CLA	O1D-CGD-O2D-CED
15	A	1128	CLA	O1D-CGD-O2D-CED
15	A	1140	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	1230	CLA	O1D-CGD-O2D-CED
15	3	608	CLA	C3-C5-C6-C7
15	3	609	CLA	CBD-CGD-O2D-CED
15	A	1119	CLA	CBD-CGD-O2D-CED
15	A	1134	CLA	CBD-CGD-O2D-CED
15	B	1209	CLA	CBD-CGD-O2D-CED
17	1	801	LHG	O2-C2-C3-O3
17	A	5002	LHG	O2-C2-C3-O3
15	1	608	CLA	O1D-CGD-O2D-CED
15	1	605	CLA	CBA-CGA-O2A-C1
15	2	601	CLA	CBA-CGA-O2A-C1
15	2	603	CLA	CBA-CGA-O2A-C1
15	2	604	CLA	CBA-CGA-O2A-C1
15	3	610	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	CBA-CGA-O2A-C1
15	A	1112	CLA	CBA-CGA-O2A-C1
15	A	1122	CLA	CBA-CGA-O2A-C1
15	B	1211	CLA	CBA-CGA-O2A-C1
15	B	1219	CLA	CBA-CGA-O2A-C1
15	A	1104	CLA	O1A-CGA-O2A-C1
15	B	1230	CLA	O1A-CGA-O2A-C1
15	B	1207	CLA	C2C-C3C-CAC-CBC
15	3	605	CLA	O1D-CGD-O2D-CED
15	3	607	CLA	O1D-CGD-O2D-CED
15	B	1207	CLA	CBD-CGD-O2D-CED
17	A	5002	LHG	C8-C7-O7-C5
19	3	802	3PH	C22-C21-O21-C2
15	2	603	CLA	O1A-CGA-O2A-C1
15	A	1104	CLA	CBD-CGD-O2D-CED
15	B	1023	CLA	C2C-C3C-CAC-CBC
15	4	609	CLA	O1D-CGD-O2D-CED
15	A	1101	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	CBA-CGA-O2A-C1
15	B	1221	CLA	CBA-CGA-O2A-C1
15	3	603	CLA	C4-C3-C5-C6
15	4	601	CLA	C4-C3-C5-C6
15	A	1102	CLA	C4-C3-C5-C6
15	A	1109	CLA	C4-C3-C5-C6
15	1	605	CLA	C2-C3-C5-C6
15	3	603	CLA	C2-C3-C5-C6
15	4	601	CLA	C2-C3-C5-C6
15	A	1109	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	B	1238	CLA	C2-C3-C5-C6
15	2	601	CLA	O1A-CGA-O2A-C1
17	B	5001	LHG	O10-C23-O8-C6
17	A	5002	LHG	O9-C7-O7-C5
15	A	1132	CLA	C2A-CAA-CBA-CGA
15	B	1022	CLA	C2A-CAA-CBA-CGA
15	A	1117	CLA	O1D-CGD-O2D-CED
15	B	1217	CLA	O1D-CGD-O2D-CED
15	F	1301	CLA	O1D-CGD-O2D-CED
15	2	604	CLA	O1A-CGA-O2A-C1
15	A	1122	CLA	O1A-CGA-O2A-C1
15	B	1219	CLA	O1A-CGA-O2A-C1
17	1	801	LHG	O10-C23-O8-C6
15	A	1109	CLA	CBA-CGA-O2A-C1
15	B	1228	CLA	CBA-CGA-O2A-C1
15	4	601	CLA	CBD-CGD-O2D-CED
15	A	1122	CLA	CBD-CGD-O2D-CED
15	A	1133	CLA	CBD-CGD-O2D-CED
15	B	1211	CLA	CBD-CGD-O2D-CED
15	B	1232	CLA	CBA-CGA-O2A-C1
15	A	1141	CLA	O1D-CGD-O2D-CED
15	1	612	CLA	C4C-C3C-CAC-CBC
14	1	503	BCR	C13-C14-C15-C16
14	4	503	BCR	C9-C10-C11-C12
14	A	4004	BCR	C9-C10-C11-C12
14	A	4007	BCR	C9-C10-C11-C12
14	F	4001	BCR	C13-C14-C15-C16
15	A	1114	CLA	O1A-CGA-O2A-C1
15	A	1135	CLA	O1A-CGA-O2A-C1
15	B	1228	CLA	O1A-CGA-O2A-C1
15	1	615	CLA	C2C-C3C-CAC-CBC
17	1	801	LHG	O9-C7-O7-C5
17	A	5002	LHG	C1-C2-C3-O3
15	3	607	CLA	CBA-CGA-O2A-C1
15	3	608	CLA	CBA-CGA-O2A-C1
15	4	604	CLA	CBA-CGA-O2A-C1
15	A	1013	CLA	CBA-CGA-O2A-C1
15	A	1114	CLA	CBA-CGA-O2A-C1
15	A	1135	CLA	CBA-CGA-O2A-C1
15	B	1215	CLA	CBA-CGA-O2A-C1
15	B	1220	CLA	CBA-CGA-O2A-C1
15	B	1231	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	B	1235	CLA	CBA-CGA-O2A-C1
17	3	801	LHG	C24-C23-O8-C6
17	B	5001	LHG	C24-C23-O8-C6
20	A	1011	CL0	CBA-CGA-O2A-C1
15	1	602	CLA	O1D-CGD-O2D-CED
15	A	1125	CLA	O1D-CGD-O2D-CED
15	B	1219	CLA	O1D-CGD-O2D-CED
15	B	1235	CLA	O1A-CGA-O2A-C1
15	1	605	CLA	C4-C3-C5-C6
15	B	1235	CLA	C4-C3-C5-C6
15	1	603	CLA	C2-C3-C5-C6
15	A	1102	CLA	C2-C3-C5-C6
15	B	1225	CLA	C2-C3-C5-C6
15	B	1235	CLA	C2-C3-C5-C6
15	1	608	CLA	C3-C5-C6-C7
15	3	607	CLA	C3-C5-C6-C7
15	1	603	CLA	C6-C7-C8-C9
15	2	607	CLA	C11-C10-C8-C9
15	A	1012	CLA	C6-C7-C8-C9
15	A	1013	CLA	C11-C10-C8-C9
15	A	1102	CLA	C11-C10-C8-C9
15	A	1104	CLA	C14-C13-C15-C16
15	A	1106	CLA	C11-C12-C13-C14
15	A	1112	CLA	C11-C12-C13-C14
15	A	1125	CLA	C11-C12-C13-C14
15	A	1126	CLA	C6-C7-C8-C9
15	A	1133	CLA	C11-C10-C8-C9
15	A	1137	CLA	C11-C10-C8-C9
15	B	1022	CLA	C11-C12-C13-C14
15	B	1023	CLA	C6-C7-C8-C9
15	B	1225	CLA	C11-C12-C13-C14
16	1	609	CHL	C11-C10-C8-C9
20	A	1011	CL0	C14-C13-C15-C16
17	2	801	LHG	O2-C2-C3-O3
15	A	1124	CLA	O1D-CGD-O2D-CED
12	1	501	LUT	C11-C12-C13-C20
12	1	501	LUT	C27-C28-C29-C39
12	1	501	LUT	C31-C32-C33-C40
12	3	501	LUT	C31-C32-C33-C40
12	4	501	LUT	C11-C12-C13-C20
12	4	501	LUT	C31-C32-C33-C40
13	2	502	XAT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
13	2	502	XAT	C31-C32-C33-C40
13	3	502	XAT	C11-C12-C13-C20
14	1	503	BCR	C7-C8-C9-C34
14	3	503	BCR	C11-C12-C13-C35
14	3	503	BCR	C37-C22-C23-C24
14	3	506	BCR	C7-C8-C9-C34
14	4	503	BCR	C36-C18-C19-C20
14	A	4003	BCR	C11-C12-C13-C35
14	A	4004	BCR	C11-C12-C13-C35
14	A	4006	BCR	C11-C12-C13-C35
14	A	4008	BCR	C7-C8-C9-C34
14	B	4001	BCR	C7-C8-C9-C34
14	B	4001	BCR	C11-C12-C13-C35
14	B	4002	BCR	C7-C8-C9-C34
14	B	4002	BCR	C11-C12-C13-C35
14	B	4003	BCR	C7-C8-C9-C34
14	B	4004	BCR	C11-C12-C13-C35
14	B	4005	BCR	C36-C18-C19-C20
14	B	4005	BCR	C37-C22-C23-C24
14	F	4002	BCR	C11-C12-C13-C35
14	J	4001	BCR	C36-C18-C19-C20
14	J	4002	BCR	C11-C12-C13-C35
14	J	4002	BCR	C36-C18-C19-C20
12	1	501	LUT	C27-C28-C29-C30
12	1	501	LUT	C31-C32-C33-C34
12	3	501	LUT	C31-C32-C33-C34
13	2	502	XAT	C7-C8-C9-C10
13	2	502	XAT	C11-C12-C13-C14
13	4	502	XAT	C7-C8-C9-C10
13	4	502	XAT	C11-C12-C13-C14
14	1	503	BCR	C11-C12-C13-C14
14	4	503	BCR	C11-C12-C13-C14
14	A	4006	BCR	C11-C12-C13-C14
14	A	4008	BCR	C7-C8-C9-C10
14	A	4008	BCR	C11-C12-C13-C14
14	B	4003	BCR	C21-C22-C23-C24
14	B	4005	BCR	C17-C18-C19-C20
14	B	4005	BCR	C21-C22-C23-C24
14	F	4002	BCR	C11-C12-C13-C14
14	J	4002	BCR	C11-C12-C13-C14
14	J	4002	BCR	C17-C18-C19-C20
15	1	608	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	A	1135	CLA	C2A-CAA-CBA-CGA
15	B	1220	CLA	C2A-CAA-CBA-CGA
15	B	1225	CLA	C2A-CAA-CBA-CGA
15	A	1111	CLA	C4C-C3C-CAC-CBC
15	3	608	CLA	O1A-CGA-O2A-C1
15	B	1215	CLA	O1A-CGA-O2A-C1
15	B	1225	CLA	C13-C15-C16-C17
15	2	606	CLA	C2C-C3C-CAC-CBC
23	B	5002	DGD	O2G-C2G-C3G-O3G
15	A	1103	CLA	O1D-CGD-O2D-CED
17	2	801	LHG	C24-C23-O8-C6
15	1	603	CLA	C8-C10-C11-C12
17	3	801	LHG	C23-C24-C25-C26
15	2	616	CLA	C2-C1-O2A-CGA
15	3	605	CLA	C2-C1-O2A-CGA
15	3	612	CLA	C2-C1-O2A-CGA
15	A	1012	CLA	C2-C1-O2A-CGA
15	A	1108	CLA	C2-C1-O2A-CGA
15	A	1110	CLA	C2-C1-O2A-CGA
15	A	1124	CLA	C2-C1-O2A-CGA
15	A	1137	CLA	C2-C1-O2A-CGA
15	A	1139	CLA	C2-C1-O2A-CGA
15	B	1225	CLA	C2-C1-O2A-CGA
15	B	1228	CLA	C2-C1-O2A-CGA
15	B	1230	CLA	C2-C1-O2A-CGA
15	B	1236	CLA	C2-C1-O2A-CGA
15	A	1105	CLA	O1D-CGD-O2D-CED
15	A	1111	CLA	O1D-CGD-O2D-CED
15	B	1221	CLA	O1D-CGD-O2D-CED
15	F	1302	CLA	O1D-CGD-O2D-CED
15	4	603	CLA	C10-C11-C12-C13
15	A	1112	CLA	C8-C10-C11-C12
15	A	1133	CLA	C13-C15-C16-C17
15	A	1138	CLA	C8-C10-C11-C12
15	A	1137	CLA	C3-C5-C6-C7
15	B	1232	CLA	O1D-CGD-O2D-CED
15	B	1202	CLA	CBD-CGD-O2D-CED
15	A	1102	CLA	C12-C13-C15-C16
15	A	1126	CLA	C11-C10-C8-C7
15	B	1021	CLA	C11-C12-C13-C15
15	B	1240	CLA	CBA-CGA-O2A-C1
18	4	801	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
12	4	501	LUT	C9-C10-C11-C12
13	1	502	XAT	C13-C14-C15-C35
13	2	502	XAT	C29-C30-C31-C32
14	A	4005	BCR	C13-C14-C15-C16
14	B	4001	BCR	C13-C14-C15-C16
14	B	4003	BCR	C15-C16-C17-C18
14	B	4005	BCR	C19-C20-C21-C22
14	F	4002	BCR	C9-C10-C11-C12
14	J	4002	BCR	C9-C10-C11-C12
15	2	607	CLA	O1D-CGD-O2D-CED
15	3	614	CLA	O1D-CGD-O2D-CED
15	4	612	CLA	C3-C5-C6-C7
15	B	1201	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C15-C16-C17-C18
15	B	1211	CLA	C13-C15-C16-C17
17	A	5001	LHG	C23-C24-C25-C26
15	3	607	CLA	O1A-CGA-O2A-C1
15	4	604	CLA	O1A-CGA-O2A-C1
20	A	1011	CL0	O1A-CGA-O2A-C1
15	A	1102	CLA	CBD-CGD-O2D-CED
15	B	1238	CLA	O1D-CGD-O2D-CED
15	1	605	CLA	C8-C10-C11-C12
15	3	612	CLA	C8-C10-C11-C12
15	4	607	CLA	C5-C6-C7-C8
15	4	612	CLA	C5-C6-C7-C8
15	A	1123	CLA	C10-C11-C12-C13
16	4	613	CHL	C8-C10-C11-C12
15	1	615	CLA	C2A-CAA-CBA-CGA
15	A	1127	CLA	C2A-CAA-CBA-CGA
15	A	1133	CLA	C2A-CAA-CBA-CGA
15	B	1207	CLA	C2A-CAA-CBA-CGA
16	1	610	CHL	C2A-CAA-CBA-CGA
16	4	610	CHL	C2A-CAA-CBA-CGA
15	A	1102	CLA	C10-C11-C12-C13
15	B	1227	CLA	C15-C16-C17-C18
17	1	801	LHG	C23-C24-C25-C26
17	2	801	LHG	C23-C24-C25-C26
18	B	5003	LMG	C28-C29-C30-C31
15	A	1013	CLA	O1A-CGA-O2A-C1
15	A	1109	CLA	O1A-CGA-O2A-C1
15	B	1220	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
15	3	606	CLA	C5-C6-C7-C8
15	A	1013	CLA	C15-C16-C17-C18
15	A	1101	CLA	C5-C6-C7-C8
15	A	1109	CLA	C15-C16-C17-C18
15	A	1122	CLA	C5-C6-C7-C8
15	A	1126	CLA	C10-C11-C12-C13
15	B	1227	CLA	C10-C11-C12-C13
20	A	1011	CL0	C5-C6-C7-C8
15	A	1125	CLA	CBA-CGA-O2A-C1
17	3	801	LHG	O10-C23-O8-C6
15	B	1207	CLA	C4C-C3C-CAC-CBC
15	3	612	CLA	C5-C6-C7-C8
15	4	605	CLA	C13-C15-C16-C17
15	A	1106	CLA	C5-C6-C7-C8
15	A	1112	CLA	C10-C11-C12-C13
15	A	1119	CLA	O1D-CGD-O2D-CED
15	4	604	CLA	O1D-CGD-O2D-CED
15	B	1209	CLA	O1D-CGD-O2D-CED
15	A	1139	CLA	C8-C10-C11-C12
15	B	1203	CLA	C5-C6-C7-C8
15	B	1225	CLA	C10-C11-C12-C13
15	B	1228	CLA	C8-C10-C11-C12
15	1	607	CLA	C2C-C3C-CAC-CBC
15	B	1231	CLA	O1A-CGA-O2A-C1
15	3	609	CLA	O1D-CGD-O2D-CED
15	B	1237	CLA	O1D-CGD-O2D-CED
15	A	1124	CLA	C10-C11-C12-C13
15	A	1128	CLA	C15-C16-C17-C18
15	B	1238	CLA	C5-C6-C7-C8
16	1	609	CHL	C13-C15-C16-C17
15	3	605	CLA	CBA-CGA-O2A-C1
15	A	1123	CLA	CBA-CGA-O2A-C1
15	1	611	CLA	O2A-C1-C2-C3
15	A	1134	CLA	O1D-CGD-O2D-CED
15	B	1222	CLA	C8-C10-C11-C12
16	1	609	CHL	C5-C6-C7-C8
15	3	601	CLA	C3-C5-C6-C7
12	1	501	LUT	C29-C30-C31-C32
13	1	502	XAT	C29-C30-C31-C32
13	2	502	XAT	C13-C14-C15-C35
14	1	503	BCR	C19-C20-C21-C22
14	3	504	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
14	A	4006	BCR	C19-C20-C21-C22
14	B	4003	BCR	C13-C14-C15-C16
15	4	604	CLA	C10-C11-C12-C13
17	2	801	LHG	O9-C7-O7-C5
17	2	801	LHG	C1-C2-C3-O3
15	2	602	CLA	C2A-CAA-CBA-CGA
15	A	1105	CLA	C2A-CAA-CBA-CGA
15	A	1126	CLA	CBA-CGA-O2A-C1
15	A	1139	CLA	CBA-CGA-O2A-C1
15	B	1216	CLA	CBA-CGA-O2A-C1
15	3	603	CLA	C13-C15-C16-C17
15	A	1101	CLA	C13-C15-C16-C17
15	A	1119	CLA	C5-C6-C7-C8
15	A	1122	CLA	C10-C11-C12-C13
15	A	1136	CLA	C10-C11-C12-C13
15	B	1219	CLA	C8-C10-C11-C12
15	B	1219	CLA	C13-C15-C16-C17
15	B	1222	CLA	C5-C6-C7-C8
15	B	1224	CLA	C8-C10-C11-C12
15	B	1226	CLA	C15-C16-C17-C18
15	B	1229	CLA	C8-C10-C11-C12
16	2	609	CHL	C13-C15-C16-C17
21	B	2002	PQN	C20-C21-C22-C23
15	B	1221	CLA	C3-C5-C6-C7
15	A	1104	CLA	O1D-CGD-O2D-CED
15	2	605	CLA	C10-C11-C12-C13
15	2	607	CLA	C10-C11-C12-C13
15	2	616	CLA	C15-C16-C17-C18
15	4	607	CLA	C8-C10-C11-C12
15	A	1109	CLA	C10-C11-C12-C13
15	A	1117	CLA	C15-C16-C17-C18
15	A	1137	CLA	C8-C10-C11-C12
15	B	1021	CLA	C13-C15-C16-C17
15	B	1227	CLA	C13-C15-C16-C17
16	2	609	CHL	C5-C6-C7-C8
15	A	1109	CLA	C13-C15-C16-C17
15	A	1111	CLA	C10-C11-C12-C13
15	A	1123	CLA	C8-C10-C11-C12
15	A	1129	CLA	C5-C6-C7-C8
15	A	1140	CLA	C10-C11-C12-C13
16	2	609	CHL	C10-C11-C12-C13
15	4	609	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	A	1107	CLA	CBA-CGA-O2A-C1
16	2	610	CHL	C2A-CAA-CBA-CGA
15	A	1133	CLA	O1D-CGD-O2D-CED
15	3	603	CLA	C5-C6-C7-C8
15	3	605	CLA	C3-C5-C6-C7
15	B	1207	CLA	O1D-CGD-O2D-CED
15	B	1240	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	C5-C6-C7-C8
15	A	1125	CLA	O1A-CGA-O2A-C1
14	2	503	BCR	C11-C10-C9-C34
14	3	503	BCR	C35-C13-C14-C15
14	3	503	BCR	C16-C17-C18-C36
14	3	506	BCR	C35-C13-C14-C15
14	B	4001	BCR	C16-C17-C18-C36
14	B	4001	BCR	C20-C21-C22-C37
14	B	4002	BCR	C20-C21-C22-C37
12	1	501	LUT	C7-C8-C9-C19
12	2	501	LUT	C27-C28-C29-C39
12	3	501	LUT	C11-C12-C13-C20
12	4	501	LUT	C27-C28-C29-C39
13	2	502	XAT	C11-C12-C13-C20
13	4	502	XAT	C11-C12-C13-C20
14	2	503	BCR	C37-C22-C23-C24
14	3	504	BCR	C11-C12-C13-C35
14	A	4008	BCR	C11-C12-C13-C35
17	A	5002	LHG	C2-C3-O3-P
12	3	501	LUT	C11-C12-C13-C14
12	4	501	LUT	C27-C28-C29-C30
15	A	1126	CLA	O1A-CGA-O2A-C1
15	3	607	CLA	C2A-CAA-CBA-CGA
15	A	1108	CLA	C2A-CAA-CBA-CGA
15	B	1213	CLA	C2A-CAA-CBA-CGA
15	B	1215	CLA	C2A-CAA-CBA-CGA
17	1	801	LHG	O1-C1-C2-C3
17	B	5001	LHG	O1-C1-C2-C3
15	A	1128	CLA	C16-C17-C18-C20
15	B	1228	CLA	C11-C12-C13-C14
15	2	605	CLA	C5-C6-C7-C8
15	4	605	CLA	C10-C11-C12-C13
14	2	503	BCR	C20-C21-C22-C23
14	3	506	BCR	C11-C10-C9-C8
14	3	506	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
14	B	4002	BCR	C11-C10-C9-C8
14	B	4002	BCR	C16-C17-C18-C19
14	B	4003	BCR	C16-C17-C18-C19
14	B	4004	BCR	C11-C10-C9-C8
14	B	4004	BCR	C20-C21-C22-C23
18	2	803	LMG	O6-C1-O1-C7
15	3	611	CLA	C8-C10-C11-C12
15	A	1138	CLA	C5-C6-C7-C8
15	B	1226	CLA	CBD-CGD-O2D-CED
15	A	1122	CLA	O1D-CGD-O2D-CED
15	A	1103	CLA	C2-C1-O2A-CGA
15	A	1112	CLA	C2-C1-O2A-CGA
15	B	1021	CLA	C2-C1-O2A-CGA
15	1	605	CLA	C16-C17-C18-C19
15	2	601	CLA	C16-C17-C18-C19
15	2	601	CLA	C16-C17-C18-C20
15	4	607	CLA	C11-C12-C13-C15
15	A	1112	CLA	C16-C17-C18-C19
15	B	1022	CLA	C16-C17-C18-C19
15	B	1211	CLA	C16-C17-C18-C19
15	B	1225	CLA	C16-C17-C18-C20
15	B	1228	CLA	C11-C12-C13-C15
15	A	1123	CLA	O1A-CGA-O2A-C1
15	4	603	CLA	C5-C6-C7-C8
15	B	1225	CLA	C5-C6-C7-C8
15	B	1228	CLA	C10-C11-C12-C13
16	1	609	CHL	C10-C11-C12-C13
18	2	803	LMG	C11-C12-C13-C14
13	3	502	XAT	C14-C15-C35-C34
14	3	506	BCR	C14-C15-C16-C17
17	A	5002	LHG	C13-C14-C15-C16
15	A	1139	CLA	C10-C11-C12-C13
17	A	5001	LHG	C29-C30-C31-C32
17	A	5002	LHG	C28-C29-C30-C31
17	A	5002	LHG	C33-C34-C35-C36
15	A	1139	CLA	O1A-CGA-O2A-C1
17	1	801	LHG	O1-C1-C2-O2
17	1	801	LHG	C12-C13-C14-C15
15	4	601	CLA	O1D-CGD-O2D-CED
15	4	601	CLA	C4B-C3B-CAB-CBB
15	1	605	CLA	C16-C17-C18-C20
15	4	607	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	A	1128	CLA	C16-C17-C18-C19
15	B	1023	CLA	C4C-C3C-CAC-CBC
15	2	603	CLA	C5-C6-C7-C8
15	A	1103	CLA	C5-C6-C7-C8
18	2	802	LMG	C11-C10-O7-C8
15	A	1123	CLA	C11-C12-C13-C15
15	B	1225	CLA	C11-C10-C8-C7
15	A	1013	CLA	C10-C11-C12-C13
15	A	1137	CLA	C5-C6-C7-C8
18	2	802	LMG	C38-C39-C40-C41
15	3	605	CLA	O1A-CGA-O2A-C1
15	1	602	CLA	C3A-C2A-CAA-CBA
15	1	613	CLA	C3A-C2A-CAA-CBA
15	1	615	CLA	C3A-C2A-CAA-CBA
15	4	605	CLA	C3A-C2A-CAA-CBA
15	A	1101	CLA	C3A-C2A-CAA-CBA
15	A	1103	CLA	C3A-C2A-CAA-CBA
15	A	1104	CLA	C3A-C2A-CAA-CBA
15	A	1105	CLA	C3A-C2A-CAA-CBA
15	A	1110	CLA	C3A-C2A-CAA-CBA
15	A	1133	CLA	C3A-C2A-CAA-CBA
15	B	1207	CLA	C3A-C2A-CAA-CBA
15	B	1210	CLA	C3A-C2A-CAA-CBA
15	B	1234	CLA	C3A-C2A-CAA-CBA
16	3	604	CHL	C3A-C2A-CAA-CBA
15	A	1123	CLA	C5-C6-C7-C8
15	B	1231	CLA	C5-C6-C7-C8
13	3	502	XAT	C9-C10-C11-C12
15	A	1107	CLA	O1A-CGA-O2A-C1
15	B	1229	CLA	O1A-CGA-O2A-C1
15	B	1232	CLA	O1A-CGA-O2A-C1
17	1	801	LHG	C29-C30-C31-C32
15	1	615	CLA	C4C-C3C-CAC-CBC
15	A	1108	CLA	CBA-CGA-O2A-C1
15	A	1124	CLA	CBA-CGA-O2A-C1
17	B	5001	LHG	C16-C17-C18-C19
18	B	5003	LMG	C30-C31-C32-C33
15	4	609	CLA	O1A-CGA-O2A-C1
18	4	801	LMG	C33-C34-C35-C36
15	A	1133	CLA	C10-C11-C12-C13
17	3	801	LHG	C14-C15-C16-C17
17	B	5001	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
15	B	1225	CLA	C16-C17-C18-C19
17	A	5002	LHG	C7-C8-C9-C10
14	1	503	BCR	C23-C24-C25-C26
14	1	503	BCR	C23-C24-C25-C30
14	2	503	BCR	C1-C6-C7-C8
14	2	503	BCR	C5-C6-C7-C8
14	3	504	BCR	C1-C6-C7-C8
14	3	504	BCR	C5-C6-C7-C8
14	3	504	BCR	C23-C24-C25-C26
14	3	504	BCR	C23-C24-C25-C30
14	A	4002	BCR	C1-C6-C7-C8
14	A	4002	BCR	C5-C6-C7-C8
14	A	4003	BCR	C1-C6-C7-C8
14	A	4003	BCR	C5-C6-C7-C8
14	A	4004	BCR	C23-C24-C25-C30
14	B	4001	BCR	C1-C6-C7-C8
14	B	4001	BCR	C5-C6-C7-C8
14	B	4003	BCR	C23-C24-C25-C26
14	B	4003	BCR	C23-C24-C25-C30
14	J	4001	BCR	C1-C6-C7-C8
14	J	4001	BCR	C23-C24-C25-C26
14	J	4001	BCR	C23-C24-C25-C30
17	2	801	LHG	C8-C7-O7-C5
15	B	1229	CLA	CBA-CGA-O2A-C1
15	2	603	CLA	C2A-CAA-CBA-CGA
15	B	1214	CLA	C2A-CAA-CBA-CGA
18	2	802	LMG	C10-C11-C12-C13
15	B	1216	CLA	O1A-CGA-O2A-C1
14	2	503	BCR	C18-C19-C20-C21
14	3	503	BCR	C10-C11-C12-C13
14	3	503	BCR	C18-C19-C20-C21
14	B	4001	BCR	C10-C11-C12-C13
14	B	4005	BCR	C10-C11-C12-C13
15	1	604	CLA	C16-C17-C18-C19
15	A	1112	CLA	C16-C17-C18-C20
17	3	801	LHG	C11-C12-C13-C14
17	A	5001	LHG	C30-C31-C32-C33
15	3	608	CLA	C6-C7-C8-C9
15	4	601	CLA	C5-C6-C7-C8
23	B	5002	DGD	CAB-CBB-CCB-CDB
17	A	5001	LHG	C32-C33-C34-C35
15	B	1220	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	2	605	CLA	C8-C10-C11-C12
15	3	603	CLA	C15-C16-C17-C18
15	A	1108	CLA	O1A-CGA-O2A-C1
17	B	5001	LHG	C27-C28-C29-C30
15	B	1240	CLA	C13-C15-C16-C17
12	1	501	LUT	C9-C10-C11-C12
12	3	501	LUT	C29-C30-C31-C32
14	A	4006	BCR	C13-C14-C15-C16
16	3	604	CHL	C11-C12-C13-C15
17	1	801	LHG	C8-C7-O7-C5
17	2	801	LHG	C28-C29-C30-C31
17	1	801	LHG	C28-C29-C30-C31
15	B	1223	CLA	C10-C11-C12-C13
17	1	801	LHG	C26-C27-C28-C29
12	2	501	LUT	C11-C12-C13-C20
14	B	4003	BCR	C36-C18-C19-C20
14	F	4002	BCR	C37-C22-C23-C24
17	A	5001	LHG	C14-C15-C16-C17
14	2	503	BCR	C17-C18-C19-C20
14	3	503	BCR	C21-C22-C23-C24
14	F	4002	BCR	C21-C22-C23-C24
15	1	604	CLA	C16-C17-C18-C20
15	2	604	CLA	C16-C17-C18-C19
15	2	604	CLA	C16-C17-C18-C20
15	A	1133	CLA	C16-C17-C18-C20
15	B	1211	CLA	C16-C17-C18-C20
15	B	1208	CLA	C2C-C3C-CAC-CBC
15	B	1211	CLA	O1D-CGD-O2D-CED
17	3	801	LHG	C26-C27-C28-C29
15	A	1101	CLA	C3-C5-C6-C7
15	2	612	CLA	C5-C6-C7-C8
15	4	607	CLA	C10-C11-C12-C13
15	B	1208	CLA	C8-C10-C11-C12
15	B	1212	CLA	C5-C6-C7-C8
15	B	1221	CLA	C15-C16-C17-C18
18	2	804	LMG	C28-C29-C30-C31
18	2	802	LMG	O9-C10-O7-C8
15	3	611	CLA	C10-C11-C12-C13
15	A	1103	CLA	C15-C16-C17-C18
15	A	1136	CLA	C13-C15-C16-C17
15	A	1124	CLA	O1A-CGA-O2A-C1
18	2	803	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	A	5002	LHG	C23-C24-C25-C26
15	3	601	CLA	C5-C6-C7-C8
15	B	1231	CLA	C8-C10-C11-C12
15	B	1212	CLA	C3-C5-C6-C7
15	2	606	CLA	C4C-C3C-CAC-CBC
17	3	801	LHG	C12-C13-C14-C15
15	A	1139	CLA	C16-C17-C18-C20
15	B	1022	CLA	C16-C17-C18-C20
17	A	5002	LHG	C11-C12-C13-C14
15	B	1231	CLA	C4-C3-C5-C6
17	A	5002	LHG	C17-C18-C19-C20
18	2	803	LMG	C29-C30-C31-C32
15	1	601	CLA	C10-C11-C12-C13
15	A	1104	CLA	C13-C15-C16-C17
18	B	5003	LMG	C11-C10-O7-C8
15	A	1133	CLA	C16-C17-C18-C19
17	A	5001	LHG	O1-C1-C2-O2
18	4	801	LMG	O10-C28-O8-C9
15	1	602	CLA	C1A-C2A-CAA-CBA
15	1	613	CLA	C1A-C2A-CAA-CBA
15	1	615	CLA	C1A-C2A-CAA-CBA
15	3	606	CLA	C1A-C2A-CAA-CBA
15	3	608	CLA	C1A-C2A-CAA-CBA
15	4	604	CLA	C1A-C2A-CAA-CBA
15	4	605	CLA	C1A-C2A-CAA-CBA
15	A	1101	CLA	C1A-C2A-CAA-CBA
15	A	1102	CLA	C1A-C2A-CAA-CBA
15	A	1103	CLA	C1A-C2A-CAA-CBA
15	A	1104	CLA	C1A-C2A-CAA-CBA
15	A	1106	CLA	C1A-C2A-CAA-CBA
15	A	1112	CLA	C1A-C2A-CAA-CBA
15	A	1113	CLA	C1A-C2A-CAA-CBA
15	A	1116	CLA	C1A-C2A-CAA-CBA
15	A	1121	CLA	C1A-C2A-CAA-CBA
15	A	1124	CLA	C1A-C2A-CAA-CBA
15	A	1130	CLA	C1A-C2A-CAA-CBA
15	B	1207	CLA	C1A-C2A-CAA-CBA
15	B	1230	CLA	C1A-C2A-CAA-CBA
15	B	1236	CLA	C1A-C2A-CAA-CBA
15	4	605	CLA	C5-C6-C7-C8
15	1	605	CLA	C12-C13-C15-C16
15	3	605	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
15	3	611	CLA	C12-C13-C15-C16
15	A	1111	CLA	C11-C12-C13-C15
15	A	1126	CLA	C11-C12-C13-C15
15	A	1128	CLA	C11-C10-C8-C7
15	A	1133	CLA	C11-C10-C8-C7
15	B	1022	CLA	C11-C10-C8-C7
15	B	1023	CLA	C6-C7-C8-C10
15	B	1203	CLA	C12-C13-C15-C16
15	B	1222	CLA	C11-C10-C8-C7
15	B	1235	CLA	C11-C10-C8-C7
15	A	1110	CLA	C6-C7-C8-C10
15	B	1023	CLA	C16-C17-C18-C19
15	A	1128	CLA	C13-C15-C16-C17
15	A	1120	CLA	C3A-C2A-CAA-CBA
15	B	1238	CLA	C3A-C2A-CAA-CBA
15	J	1302	CLA	C3A-C2A-CAA-CBA
15	A	1127	CLA	C15-C16-C17-C18
15	B	1202	CLA	C15-C16-C17-C18
15	A	1103	CLA	C2-C3-C5-C6
15	B	1210	CLA	C2-C3-C5-C6
15	B	1215	CLA	C5-C6-C7-C8
15	3	603	CLA	C2A-CAA-CBA-CGA
15	A	1115	CLA	C2A-CAA-CBA-CGA
15	2	601	CLA	C11-C12-C13-C14
15	2	605	CLA	C6-C7-C8-C9
15	3	612	CLA	C6-C7-C8-C9
15	3	612	CLA	C14-C13-C15-C16
15	A	1101	CLA	C6-C7-C8-C9
15	A	1116	CLA	C6-C7-C8-C9
15	A	1122	CLA	C11-C12-C13-C14
15	A	1127	CLA	C14-C13-C15-C16
15	A	1128	CLA	C11-C10-C8-C9
15	A	1139	CLA	C6-C7-C8-C9
15	B	1022	CLA	C11-C10-C8-C9
15	B	1225	CLA	C11-C10-C8-C9
15	B	1227	CLA	C11-C10-C8-C9
15	B	1235	CLA	C11-C10-C8-C9
15	A	1117	CLA	CBA-CGA-O2A-C1
15	B	1202	CLA	CBA-CGA-O2A-C1
16	2	609	CHL	CBA-CGA-O2A-C1
15	1	607	CLA	C4C-C3C-CAC-CBC
15	2	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	3	605	CLA	C10-C11-C12-C13
17	2	801	LHG	C4-C5-C6-O8
18	2	803	LMG	C7-C8-C9-O8
23	B	5002	DGD	O1G-C1G-C2G-C3G
18	2	803	LMG	O6-C5-C6-O5
15	A	1112	CLA	C15-C16-C17-C18
15	A	1110	CLA	C6-C7-C8-C9
15	1	605	CLA	C5-C6-C7-C8
14	2	503	BCR	C16-C17-C18-C36
15	B	1222	CLA	C15-C16-C17-C18
18	2	804	LMG	O6-C5-C6-O5
15	A	1117	CLA	O1A-CGA-O2A-C1
15	A	1103	CLA	C4-C3-C5-C6
15	B	1210	CLA	C4-C3-C5-C6
13	1	502	XAT	C7-C8-C9-C19
14	A	4002	BCR	C37-C22-C23-C24
14	F	4001	BCR	C7-C8-C9-C34
18	2	802	LMG	C15-C16-C17-C18
15	A	1124	CLA	C11-C12-C13-C15
14	A	4002	BCR	C11-C12-C13-C14
14	A	4002	BCR	C21-C22-C23-C24
14	F	4001	BCR	C7-C8-C9-C10
15	B	1202	CLA	O1A-CGA-O2A-C1
15	4	609	CLA	C5-C6-C7-C8
15	A	1102	CLA	C8-C10-C11-C12
15	A	1126	CLA	C8-C10-C11-C12
17	1	801	LHG	C11-C10-C9-C8
15	4	605	CLA	C8-C10-C11-C12
15	B	1021	CLA	CBA-CGA-O2A-C1
18	2	804	LMG	C29-C28-O8-C9
19	3	802	3PH	C23-C24-C25-C26
15	4	616	CLA	O2A-C1-C2-C3
17	A	5002	LHG	C31-C32-C33-C34
14	A	4005	BCR	C19-C20-C21-C22
15	A	1139	CLA	C16-C17-C18-C19
15	B	1205	CLA	C16-C17-C18-C19
15	B	1202	CLA	C3-C5-C6-C7
23	B	5002	DGD	C2A-C3A-C4A-C5A
14	B	4001	BCR	C12-C13-C14-C15
23	B	5002	DGD	C5A-C6A-C7A-C8A
17	3	801	LHG	O6-C4-C5-O7
15	4	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	B	1208	CLA	CBD-CGD-O2D-CED
18	2	802	LMG	C29-C30-C31-C32
17	A	5001	LHG	C19-C20-C21-C22
15	A	1126	CLA	CAA-CBA-CGA-O2A
15	2	607	CLA	C2C-C3C-CAC-CBC
17	A	5001	LHG	C27-C28-C29-C30
18	2	802	LMG	C41-C42-C43-C44
15	B	1022	CLA	CBA-CGA-O2A-C1
17	3	801	LHG	C11-C10-C9-C8
18	2	802	LMG	C32-C33-C34-C35
15	A	1102	CLA	O1D-CGD-O2D-CED
15	B	1205	CLA	C16-C17-C18-C20
15	B	1229	CLA	C11-C12-C13-C14
20	A	1011	CL0	C16-C17-C18-C19
15	3	601	CLA	C4-C3-C5-C6
15	3	612	CLA	C4-C3-C5-C6
15	A	1108	CLA	C4-C3-C5-C6
15	B	1211	CLA	C4-C3-C5-C6
15	A	1102	CLA	CBA-CGA-O2A-C1
15	B	1225	CLA	CBA-CGA-O2A-C1
18	2	802	LMG	C18-C19-C20-C21
18	4	801	LMG	C12-C13-C14-C15
17	A	5002	LHG	O1-C1-C2-O2
17	B	5001	LHG	O1-C1-C2-O2
15	1	605	CLA	C14-C13-C15-C16
15	3	605	CLA	C11-C12-C13-C14
15	3	611	CLA	C14-C13-C15-C16
15	A	1111	CLA	C11-C12-C13-C14
15	A	1112	CLA	C11-C10-C8-C9
15	A	1123	CLA	C11-C12-C13-C14
15	A	1126	CLA	C11-C12-C13-C14
15	A	1136	CLA	C14-C13-C15-C16
15	B	1023	CLA	C14-C13-C15-C16
15	B	1216	CLA	C6-C7-C8-C9
15	B	1219	CLA	C11-C12-C13-C14
15	B	1229	CLA	C6-C7-C8-C9
15	B	1210	CLA	C5-C6-C7-C8
15	1	615	CLA	C4B-C3B-CAB-CBB
15	4	607	CLA	C4B-C3B-CAB-CBB
15	A	1122	CLA	C4B-C3B-CAB-CBB
15	B	1022	CLA	C4B-C3B-CAB-CBB
15	B	1208	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	2	802	LMG	C34-C35-C36-C37
15	A	1111	CLA	C13-C15-C16-C17
15	B	1023	CLA	C16-C17-C18-C20
15	3	605	CLA	C2A-CAA-CBA-CGA
18	B	5003	LMG	C2-C1-O1-C7
23	B	5002	DGD	C7B-C8B-C9B-CAB
15	4	604	CLA	C3-C5-C6-C7
15	B	1226	CLA	C3-C5-C6-C7
19	3	802	3PH	O11-C1-C2-C3
17	1	801	LHG	C30-C31-C32-C33
23	B	5002	DGD	C4B-C5B-C6B-C7B
15	1	604	CLA	C11-C12-C13-C15
15	2	601	CLA	C11-C12-C13-C15
15	2	605	CLA	C6-C7-C8-C10
15	3	605	CLA	C6-C7-C8-C10
15	3	605	CLA	C12-C13-C15-C16
15	3	612	CLA	C12-C13-C15-C16
15	A	1101	CLA	C6-C7-C8-C10
15	A	1109	CLA	C6-C7-C8-C10
15	A	1111	CLA	C12-C13-C15-C16
15	A	1112	CLA	C11-C10-C8-C7
15	A	1116	CLA	C6-C7-C8-C10
15	A	1119	CLA	C6-C7-C8-C10
15	A	1127	CLA	C12-C13-C15-C16
15	A	1133	CLA	C6-C7-C8-C10
15	A	1133	CLA	C11-C12-C13-C15
15	A	1136	CLA	C12-C13-C15-C16
15	A	1139	CLA	C6-C7-C8-C10
15	B	1021	CLA	C6-C7-C8-C10
15	B	1023	CLA	C12-C13-C15-C16
15	B	1202	CLA	C11-C10-C8-C7
15	B	1216	CLA	C6-C7-C8-C10
15	B	1219	CLA	C11-C12-C13-C15
15	B	1227	CLA	C11-C10-C8-C7
15	B	1229	CLA	C6-C7-C8-C10
20	A	1011	CL0	C11-C10-C8-C7
15	3	613	CLA	CBA-CGA-O2A-C1
15	A	1123	CLA	C4-C3-C5-C6
15	B	1215	CLA	C3A-C2A-CAA-CBA
15	B	1229	CLA	C4-C3-C5-C6
15	A	1126	CLA	C15-C16-C17-C18
15	B	1223	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	A	2001	PQN	C23-C25-C26-C27
15	B	1240	CLA	CAA-CBA-CGA-O2A
15	A	1134	CLA	C2C-C3C-CAC-CBC
18	B	5003	LMG	C13-C14-C15-C16
15	1	601	CLA	C5-C6-C7-C8
15	1	601	CLA	CBA-CGA-O2A-C1
12	3	501	LUT	C33-C34-C35-C15
14	3	503	BCR	C19-C20-C21-C22
14	A	4002	BCR	C9-C10-C11-C12
14	A	4008	BCR	C9-C10-C11-C12
14	A	4008	BCR	C15-C16-C17-C18
14	A	4002	BCR	C11-C12-C13-C35
14	B	4003	BCR	C37-C22-C23-C24
17	A	5002	LHG	C35-C36-C37-C38
15	B	1021	CLA	O1A-CGA-O2A-C1
18	2	804	LMG	O10-C28-O8-C9
15	B	1205	CLA	C15-C16-C17-C18
15	3	611	CLA	C2A-CAA-CBA-CGA
15	A	1127	CLA	CBA-CGA-O2A-C1
15	A	1136	CLA	CBA-CGA-O2A-C1
18	2	802	LMG	O1-C7-C8-C9
18	2	804	LMG	C7-C8-C9-O8
19	3	802	3PH	C1-C2-C3-O31
23	B	5002	DGD	C1G-C2G-C3G-O3G
17	A	5001	LHG	C25-C26-C27-C28
15	A	1124	CLA	C11-C12-C13-C14
15	B	1229	CLA	C11-C12-C13-C15
16	1	609	CHL	C16-C17-C18-C19
18	2	803	LMG	C15-C16-C17-C18
15	B	1216	CLA	C8-C10-C11-C12
15	3	612	CLA	C2-C3-C5-C6
15	A	1123	CLA	C2-C3-C5-C6
15	B	1211	CLA	C2-C3-C5-C6
15	B	1229	CLA	C2-C3-C5-C6
15	A	1111	CLA	C3-C5-C6-C7
15	B	1202	CLA	O1D-CGD-O2D-CED
17	A	5001	LHG	C34-C35-C36-C37
15	A	1123	CLA	C16-C17-C18-C19
15	3	607	CLA	C10-C11-C12-C13
15	B	1023	CLA	C5-C6-C7-C8
17	A	5002	LHG	O6-C4-C5-O7
19	3	802	3PH	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
14	2	503	BCR	C23-C24-C25-C30
14	3	503	BCR	C1-C6-C7-C8
14	A	4008	BCR	C1-C6-C7-C8
14	A	4008	BCR	C23-C24-C25-C30
14	B	4003	BCR	C1-C6-C7-C8
14	B	4005	BCR	C23-C24-C25-C26
15	4	607	CLA	C2B-C3B-CAB-CBB
15	A	1102	CLA	O1A-CGA-O2A-C1
15	B	1215	CLA	C15-C16-C17-C18
15	4	609	CLA	C2A-CAA-CBA-CGA
15	A	1101	CLA	C2A-CAA-CBA-CGA
15	A	1104	CLA	C10-C11-C12-C13
17	A	5002	LHG	O7-C5-C6-O8
18	2	802	LMG	O1-C7-C8-O7
19	3	802	3PH	O21-C2-C3-O31
15	B	1205	CLA	C4-C3-C5-C6
14	A	4002	BCR	C10-C11-C12-C13
17	B	5001	LHG	C11-C12-C13-C14
18	2	803	LMG	C19-C20-C21-C22
18	2	802	LMG	C13-C14-C15-C16
15	A	1109	CLA	C6-C7-C8-C9
15	A	1117	CLA	C14-C13-C15-C16
15	A	1133	CLA	C11-C12-C13-C14
15	B	1021	CLA	C6-C7-C8-C9
15	B	1202	CLA	C11-C10-C8-C9
15	B	1203	CLA	C14-C13-C15-C16
20	A	1011	CL0	C11-C10-C8-C9
18	B	5003	LMG	C12-C13-C14-C15
14	4	503	BCR	C6-C7-C8-C9
18	2	803	LMG	C17-C18-C19-C20
15	A	1129	CLA	C3-C5-C6-C7
19	3	802	3PH	C22-C23-C24-C25
15	4	602	CLA	O1A-CGA-O2A-C1
17	3	801	LHG	C7-C8-C9-C10
15	A	1105	CLA	C10-C11-C12-C13
15	B	1214	CLA	C8-C10-C11-C12
15	B	1220	CLA	O1D-CGD-O2D-CED
14	A	4002	BCR	C15-C16-C17-C18
14	B	4002	BCR	C19-C20-C21-C22
15	1	601	CLA	C13-C15-C16-C17
17	1	801	LHG	C1-C2-C3-O3
14	B	4002	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
17	3	801	LHG	O6-C4-C5-C6
20	A	1011	CL0	C16-C17-C18-C20
15	4	603	CLA	C13-C15-C16-C17
20	A	1011	CL0	C15-C16-C17-C18
13	1	502	XAT	C11-C12-C13-C20
14	J	4002	BCR	C7-C8-C9-C34
15	2	604	CLA	C11-C10-C8-C7
15	A	1013	CLA	C11-C12-C13-C15
15	A	1112	CLA	C11-C12-C13-C15
15	A	1117	CLA	C12-C13-C15-C16
15	B	1022	CLA	C11-C12-C13-C15
15	B	1224	CLA	C6-C7-C8-C10
15	B	1226	CLA	C11-C12-C13-C15
16	1	609	CHL	C6-C7-C8-C10
18	2	802	LMG	C42-C43-C44-C45
12	1	501	LUT	C7-C8-C9-C10
12	2	501	LUT	C27-C28-C29-C30
13	1	502	XAT	C11-C12-C13-C14
13	1	502	XAT	C27-C28-C29-C30
14	2	503	BCR	C7-C8-C9-C10
14	2	503	BCR	C21-C22-C23-C24
14	3	504	BCR	C11-C12-C13-C14
14	B	4001	BCR	C17-C18-C19-C20
15	1	601	CLA	O1A-CGA-O2A-C1
17	2	801	LHG	O10-C23-O8-C6
15	B	1226	CLA	C10-C11-C12-C13
15	B	1204	CLA	C2A-CAA-CBA-CGA
15	A	1123	CLA	C16-C17-C18-C20
16	1	609	CHL	C16-C17-C18-C20
15	B	1226	CLA	O1D-CGD-O2D-CED
15	A	1127	CLA	O1A-CGA-O2A-C1
15	B	1234	CLA	C3-C5-C6-C7
15	B	1221	CLA	O2A-C1-C2-C3
18	2	802	LMG	C9-C8-O7-C10
15	B	1022	CLA	O1A-CGA-O2A-C1
15	B	1225	CLA	O1A-CGA-O2A-C1
15	B	1219	CLA	C10-C11-C12-C13
15	4	605	CLA	C16-C17-C18-C20
15	A	1108	CLA	C6-C7-C8-C10
15	A	1136	CLA	O1A-CGA-O2A-C1
16	2	609	CHL	O1A-CGA-O2A-C1
15	A	1136	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	2	601	CLA	C5-C6-C7-C8
18	2	802	LMG	C36-C37-C38-C39
14	1	503	BCR	C12-C13-C14-C15
14	3	503	BCR	C16-C17-C18-C19
17	A	5002	LHG	C4-C5-C6-O8
17	B	5001	LHG	C4-C5-C6-O8
15	B	1203	CLA	C13-C15-C16-C17
20	A	1011	CL0	C8-C10-C11-C12
15	3	612	CLA	C3-C5-C6-C7
15	2	612	CLA	C4-C3-C5-C6
15	A	1127	CLA	C4-C3-C5-C6
15	B	1205	CLA	C2-C3-C5-C6
17	B	5001	LHG	O7-C5-C6-O8
15	3	605	CLA	C6-C7-C8-C9
15	A	1138	CLA	C11-C12-C13-C14
15	B	1221	CLA	C6-C7-C8-C9
18	B	5003	LMG	C33-C34-C35-C36
15	A	1106	CLA	C15-C16-C17-C18
15	A	1137	CLA	C10-C11-C12-C13
15	A	1133	CLA	C2-C1-O2A-CGA
15	B	1231	CLA	C2-C1-O2A-CGA
15	A	1111	CLA	C15-C16-C17-C18
16	2	609	CHL	C3-C5-C6-C7
15	A	1108	CLA	C6-C7-C8-C9
14	B	4001	BCR	C14-C15-C16-C17
18	2	804	LMG	C30-C31-C32-C33
18	2	804	LMG	C29-C30-C31-C32
16	3	604	CHL	C11-C12-C13-C14
16	4	613	CHL	C11-C12-C13-C15
18	4	801	LMG	C4-C5-C6-O5
15	B	1023	CLA	O1A-CGA-O2A-C1
15	1	607	CLA	C4B-C3B-CAB-CBB
15	2	602	CLA	C1A-C2A-CAA-CBA
15	3	608	CLA	C4B-C3B-CAB-CBB
15	B	1215	CLA	C1A-C2A-CAA-CBA
15	B	1237	CLA	C4B-C3B-CAB-CBB
15	B	1239	CLA	C4B-C3B-CAB-CBB
15	2	616	CLA	C4-C3-C5-C6
14	2	503	BCR	C11-C12-C13-C14
15	A	1012	CLA	C2A-CAA-CBA-CGA
15	B	1208	CLA	O1D-CGD-O2D-CED
17	A	5002	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
17	A	5002	LHG	C18-C19-C20-C21
15	A	1107	CLA	C2-C3-C5-C6
15	4	603	CLA	C6-C7-C8-C10
15	4	609	CLA	C6-C7-C8-C10
15	A	1104	CLA	C12-C13-C15-C16
15	A	1105	CLA	C11-C10-C8-C7
15	A	1106	CLA	C11-C12-C13-C15
15	A	1125	CLA	C11-C10-C8-C7
15	A	1126	CLA	C6-C7-C8-C10
15	A	1126	CLA	C12-C13-C15-C16
15	A	1138	CLA	C12-C13-C15-C16
15	B	1022	CLA	C12-C13-C15-C16
15	B	1023	CLA	C11-C10-C8-C7
20	A	1011	CL0	C6-C7-C8-C10
20	A	1011	CL0	C12-C13-C15-C16
18	2	804	LMG	C21-C22-C23-C24
15	B	1219	CLA	C16-C17-C18-C20
17	A	5002	LHG	C10-C11-C12-C13
15	A	1134	CLA	C4C-C3C-CAC-CBC
17	A	5001	LHG	C12-C13-C14-C15
15	A	1013	CLA	C11-C12-C13-C14
15	B	1224	CLA	C6-C7-C8-C9
15	A	1116	CLA	O1A-CGA-O2A-C1
13	3	502	XAT	C29-C30-C31-C32
14	3	504	BCR	C9-C10-C11-C12
14	A	4007	BCR	C15-C16-C17-C18
15	B	1236	CLA	C1-C2-C3-C4
18	2	803	LMG	O7-C8-C9-O8
18	2	804	LMG	O7-C8-C9-O8
18	4	801	LMG	O1-C7-C8-O7
23	B	5002	DGD	O1G-C1G-C2G-O2G
15	F	1302	CLA	O2A-C1-C2-C3
18	2	803	LMG	C2-C1-O1-C7
17	A	5002	LHG	O8-C23-C24-C25
15	2	612	CLA	C2-C3-C5-C6
15	3	601	CLA	C2-C3-C5-C6
15	A	1127	CLA	C2-C3-C5-C6
15	1	603	CLA	CAD-CBD-CGD-O2D
15	1	615	CLA	CAD-CBD-CGD-O2D
15	2	602	CLA	CAD-CBD-CGD-O2D
15	4	606	CLA	CAD-CBD-CGD-O2D
15	A	1012	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	A	1105	CLA	CAD-CBD-CGD-O2D
15	A	1131	CLA	CAD-CBD-CGD-O2D
15	B	1217	CLA	CAD-CBD-CGD-O2D
15	B	1239	CLA	CAD-CBD-CGD-O2D
16	1	609	CHL	CAD-CBD-CGD-O2D
16	2	609	CHL	CAD-CBD-CGD-O2D
20	A	1011	CL0	CAD-CBD-CGD-O2D
17	B	5001	LHG	C15-C16-C17-C18
15	B	1023	CLA	CBA-CGA-O2A-C1
15	B	1203	CLA	C3-C5-C6-C7
15	3	614	CLA	C3-C5-C6-C7
12	1	501	LUT	C33-C34-C35-C15
12	2	501	LUT	C9-C10-C11-C12
14	3	503	BCR	C9-C10-C11-C12
14	A	4003	BCR	C9-C10-C11-C12
14	A	4008	BCR	C19-C20-C21-C22
15	1	603	CLA	CAD-CBD-CGD-O1D
15	1	615	CLA	CAD-CBD-CGD-O1D
15	2	602	CLA	CAD-CBD-CGD-O1D
15	2	608	CLA	CHA-CBD-CGD-O1D
15	4	603	CLA	CHA-CBD-CGD-O1D
15	4	603	CLA	CHA-CBD-CGD-O2D
15	4	606	CLA	CAD-CBD-CGD-O1D
15	A	1012	CLA	CAD-CBD-CGD-O1D
15	A	1102	CLA	CHA-CBD-CGD-O1D
15	A	1105	CLA	CAD-CBD-CGD-O1D
15	A	1120	CLA	CAD-CBD-CGD-O1D
15	A	1131	CLA	CAD-CBD-CGD-O1D
15	B	1202	CLA	CHA-CBD-CGD-O1D
15	B	1202	CLA	CHA-CBD-CGD-O2D
15	B	1212	CLA	CHA-CBD-CGD-O1D
15	B	1217	CLA	CAD-CBD-CGD-O1D
15	B	1230	CLA	CHA-CBD-CGD-O1D
15	B	1230	CLA	CHA-CBD-CGD-O2D
15	B	1239	CLA	CAD-CBD-CGD-O1D
16	1	609	CHL	CAD-CBD-CGD-O1D
16	2	609	CHL	CAD-CBD-CGD-O1D
17	2	801	LHG	C3-O3-P-O5
17	A	5002	LHG	C3-O3-P-O5
17	B	5001	LHG	C3-O3-P-O4
17	B	5001	LHG	C4-O6-P-O4
20	A	1011	CL0	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	A	1114	CLA	C5-C6-C7-C8
15	2	608	CLA	C2C-C3C-CAC-CBC
17	3	801	LHG	C28-C29-C30-C31
20	A	1011	CL0	C4-C3-C5-C6
15	1	607	CLA	C2B-C3B-CAB-CBB
15	4	601	CLA	C2B-C3B-CAB-CBB
17	A	5001	LHG	C10-C11-C12-C13
23	B	5002	DGD	C3B-C4B-C5B-C6B
15	B	1231	CLA	C2-C3-C5-C6
14	A	4005	BCR	C36-C18-C19-C20
17	3	801	LHG	C5-C4-O6-P
15	B	1219	CLA	C16-C17-C18-C19
17	3	801	LHG	C27-C28-C29-C30
15	2	607	CLA	C4C-C3C-CAC-CBC
15	4	612	CLA	C16-C17-C18-C19
17	1	801	LHG	C4-C5-O7-C7
18	2	804	LMG	C9-C8-O7-C10
12	1	501	LUT	C10-C11-C12-C13
12	1	501	LUT	C30-C31-C32-C33
12	2	501	LUT	C10-C11-C12-C13
12	2	501	LUT	C30-C31-C32-C33
12	3	501	LUT	C10-C11-C12-C13
12	3	501	LUT	C30-C31-C32-C33
12	4	501	LUT	C10-C11-C12-C13
12	4	501	LUT	C30-C31-C32-C33
14	3	504	BCR	C10-C11-C12-C13
14	A	4003	BCR	C18-C19-C20-C21
14	A	4004	BCR	C18-C19-C20-C21
14	B	4005	BCR	C18-C19-C20-C21
14	F	4002	BCR	C18-C19-C20-C21
15	4	605	CLA	C16-C17-C18-C19
21	B	2002	PQN	C26-C27-C28-C29
15	B	1224	CLA	C10-C11-C12-C13
15	1	604	CLA	C11-C12-C13-C14
15	4	603	CLA	C6-C7-C8-C9
15	A	1105	CLA	C11-C10-C8-C9
15	A	1111	CLA	C11-C10-C8-C9
15	A	1111	CLA	C14-C13-C15-C16
15	A	1119	CLA	C6-C7-C8-C9
15	A	1133	CLA	C6-C7-C8-C9
15	B	1022	CLA	C14-C13-C15-C16
21	A	2001	PQN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	2	802	LMG	C39-C40-C41-C42
15	B	1224	CLA	C11-C10-C8-C7
17	2	801	LHG	C10-C11-C12-C13
15	A	1138	CLA	C2A-CAA-CBA-CGA
15	B	1211	CLA	C15-C16-C17-C18
18	2	804	LMG	C18-C19-C20-C21
15	A	1114	CLA	C4-C3-C5-C6
15	A	1108	CLA	C2-C3-C5-C6
15	1	611	CLA	O1A-CGA-O2A-C1
17	2	801	LHG	O7-C5-C6-O8
23	B	5002	DGD	CAA-CBA-CCA-CDA
14	A	4003	BCR	C19-C20-C21-C22
15	A	1111	CLA	C2A-CAA-CBA-CGA
15	B	1223	CLA	C2-C1-O2A-CGA
21	B	2002	PQN	C26-C27-C28-C30
15	B	1021	CLA	CAA-CBA-CGA-O2A
15	A	1126	CLA	C5-C6-C7-C8
14	B	4004	BCR	C36-C18-C19-C20
15	A	1106	CLA	C2A-CAA-CBA-CGA
15	A	1126	CLA	C2A-CAA-CBA-CGA
14	F	4001	BCR	C15-C16-C17-C18
15	3	601	CLA	C11-C12-C13-C15
15	B	1219	CLA	C5-C6-C7-C8
15	A	1126	CLA	CAA-CBA-CGA-O1A
15	3	613	CLA	O1A-CGA-O2A-C1
15	2	604	CLA	C11-C10-C8-C9
15	4	609	CLA	C6-C7-C8-C9
15	A	1102	CLA	C14-C13-C15-C16
15	A	1126	CLA	C14-C13-C15-C16
15	A	1139	CLA	C14-C13-C15-C16
15	B	1023	CLA	C11-C10-C8-C9
20	A	1011	CL0	C6-C7-C8-C9
15	A	1116	CLA	CBA-CGA-O2A-C1
15	1	608	CLA	C4B-C3B-CAB-CBB
15	A	1109	CLA	C4B-C3B-CAB-CBB
15	B	1202	CLA	C4B-C3B-CAB-CBB
15	B	1214	CLA	C15-C16-C17-C18
15	A	1131	CLA	C2C-C3C-CAC-CBC
23	B	5002	DGD	C7A-C8A-C9A-CAA
15	1	611	CLA	CBA-CGA-O2A-C1
15	A	1012	CLA	CBA-CGA-O2A-C1
15	A	1012	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	A	1012	CLA	O1A-CGA-O2A-C1
15	B	1021	CLA	C4-C3-C5-C6
15	B	1221	CLA	C4-C3-C5-C6
15	B	1234	CLA	C4-C3-C5-C6
15	3	610	CLA	O1D-CGD-O2D-CED
18	2	804	LMG	C22-C23-C24-C25
15	2	616	CLA	C11-C12-C13-C15
15	3	608	CLA	C12-C13-C15-C16
15	A	1127	CLA	C11-C12-C13-C15
15	A	1138	CLA	C13-C15-C16-C17
15	B	1227	CLA	C8-C10-C11-C12
17	2	801	LHG	C9-C10-C11-C12
23	B	5002	DGD	C9B-CAB-CBB-CCB
15	2	602	CLA	C3A-C2A-CAA-CBA
15	A	1112	CLA	C13-C15-C16-C17
12	1	501	LUT	C11-C10-C9-C19
12	1	501	LUT	C20-C13-C14-C15
12	1	501	LUT	C39-C29-C30-C31
12	1	501	LUT	C40-C33-C34-C35
12	2	501	LUT	C11-C10-C9-C19
12	2	501	LUT	C20-C13-C14-C15
12	2	501	LUT	C39-C29-C30-C31
12	2	501	LUT	C40-C33-C34-C35
12	3	501	LUT	C11-C10-C9-C19
12	3	501	LUT	C20-C13-C14-C15
12	3	501	LUT	C39-C29-C30-C31
12	3	501	LUT	C40-C33-C34-C35
12	4	501	LUT	C11-C10-C9-C19
12	4	501	LUT	C20-C13-C14-C15
12	4	501	LUT	C39-C29-C30-C31
12	4	501	LUT	C40-C33-C34-C35
13	2	502	XAT	C40-C33-C34-C35
13	4	502	XAT	C40-C33-C34-C35
14	A	4004	BCR	C16-C17-C18-C36
14	A	4006	BCR	C16-C17-C18-C36
12	2	501	LUT	C13-C14-C15-C35
13	4	502	XAT	C29-C30-C31-C32
13	4	502	XAT	C33-C34-C35-C15
14	3	506	BCR	C9-C10-C11-C12
14	J	4001	BCR	C9-C10-C11-C12
15	B	1208	CLA	C2-C1-O2A-CGA
14	A	4003	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	3	608	CLA	CAA-CBA-CGA-O2A
15	A	1107	CLA	C4-C3-C5-C6
18	2	803	LMG	C30-C31-C32-C33
15	2	616	CLA	C2-C3-C5-C6
20	A	1011	CL0	C2-C3-C5-C6
16	2	613	CHL	CAA-CBA-CGA-O2A
17	3	801	LHG	C15-C16-C17-C18
17	3	801	LHG	C16-C17-C18-C19
15	3	608	CLA	C14-C13-C15-C16
15	A	1125	CLA	C11-C10-C8-C9
15	A	1127	CLA	C11-C12-C13-C14
15	B	1228	CLA	C6-C7-C8-C9
15	B	1240	CLA	C14-C13-C15-C16
17	A	5001	LHG	C28-C29-C30-C31
18	2	804	LMG	C7-C8-O7-C10
18	2	802	LMG	C30-C31-C32-C33
12	2	501	LUT	C33-C34-C35-C15
18	2	804	LMG	C10-C11-C12-C13
15	3	601	CLA	C11-C12-C13-C14
15	B	1234	CLA	C2-C3-C5-C6
12	1	501	LUT	C11-C10-C9-C8
12	1	501	LUT	C12-C13-C14-C15
12	1	501	LUT	C28-C29-C30-C31
12	1	501	LUT	C32-C33-C34-C35
12	2	501	LUT	C11-C10-C9-C8
12	2	501	LUT	C12-C13-C14-C15
12	2	501	LUT	C28-C29-C30-C31
12	2	501	LUT	C32-C33-C34-C35
12	3	501	LUT	C11-C10-C9-C8
12	3	501	LUT	C12-C13-C14-C15
12	3	501	LUT	C28-C29-C30-C31
12	3	501	LUT	C32-C33-C34-C35
12	4	501	LUT	C11-C10-C9-C8
12	4	501	LUT	C12-C13-C14-C15
12	4	501	LUT	C28-C29-C30-C31
12	4	501	LUT	C32-C33-C34-C35
13	2	502	XAT	C32-C33-C34-C35
13	4	502	XAT	C32-C33-C34-C35
14	A	4004	BCR	C16-C17-C18-C19
14	A	4006	BCR	C16-C17-C18-C19
15	1	607	CLA	C1A-C2A-CAA-CBA
15	B	1209	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	B	1216	CLA	C1A-C2A-CAA-CBA
15	B	1240	CLA	C1A-C2A-CAA-CBA
15	B	1240	CLA	C16-C17-C18-C19
15	B	1230	CLA	C5-C6-C7-C8
12	1	501	LUT	C5-C6-C7-C8
12	3	501	LUT	C5-C6-C7-C8
14	1	503	BCR	C1-C6-C7-C8
14	2	503	BCR	C23-C24-C25-C26
14	3	503	BCR	C5-C6-C7-C8
14	A	4008	BCR	C5-C6-C7-C8
14	A	4008	BCR	C23-C24-C25-C26
14	B	4003	BCR	C5-C6-C7-C8
14	B	4005	BCR	C23-C24-C25-C30
15	1	608	CLA	C2B-C3B-CAB-CBB
15	1	615	CLA	C2B-C3B-CAB-CBB
15	3	608	CLA	C2B-C3B-CAB-CBB
15	A	1109	CLA	C2B-C3B-CAB-CBB
15	A	1122	CLA	C2B-C3B-CAB-CBB
15	B	1208	CLA	C2B-C3B-CAB-CBB
15	B	1237	CLA	C2B-C3B-CAB-CBB
15	B	1239	CLA	C2B-C3B-CAB-CBB
15	3	610	CLA	CBD-CGD-O2D-CED
16	2	613	CHL	CAA-CBA-CGA-O1A
15	4	607	CLA	C4-C3-C5-C6
15	A	1126	CLA	C4-C3-C5-C6
15	B	1021	CLA	C2-C3-C5-C6
15	A	1129	CLA	C2C-C3C-CAC-CBC
15	1	603	CLA	C6-C7-C8-C10
15	4	604	CLA	C11-C10-C8-C7
15	4	612	CLA	C11-C12-C13-C15
15	A	1102	CLA	C6-C7-C8-C10
15	A	1102	CLA	C11-C10-C8-C7
15	A	1105	CLA	C6-C7-C8-C10
15	A	1123	CLA	C6-C7-C8-C10
15	A	1139	CLA	C12-C13-C15-C16
15	B	1225	CLA	C11-C12-C13-C15
15	B	1226	CLA	C11-C10-C8-C7
15	2	605	CLA	C16-C17-C18-C19
15	A	1127	CLA	C16-C17-C18-C20
15	3	614	CLA	C2A-CAA-CBA-CGA
15	4	604	CLA	C2A-CAA-CBA-CGA
15	B	1235	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	1	502	XAT	C27-C28-C29-C39
15	A	1127	CLA	C2C-C3C-CAC-CBC
15	B	1229	CLA	C10-C11-C12-C13
15	A	1114	CLA	C2-C3-C5-C6
23	B	5002	DGD	O1A-C1A-O1G-C1G
17	A	5002	LHG	C26-C27-C28-C29
17	3	801	LHG	O2-C2-C3-O3
18	2	803	LMG	C31-C32-C33-C34
15	A	1101	CLA	C15-C16-C17-C18
15	A	1122	CLA	C6-C7-C8-C9
15	2	604	CLA	C15-C16-C17-C18
15	A	1119	CLA	C4-C3-C5-C6
15	B	1224	CLA	C4-C3-C5-C6
15	B	1227	CLA	C4-C3-C5-C6
17	1	801	LHG	C2-C3-O3-P
15	B	1224	CLA	C2-C3-C5-C6
15	A	1013	CLA	C8-C10-C11-C12
15	A	1127	CLA	C8-C10-C11-C12
15	B	1224	CLA	C3-C5-C6-C7
15	B	1022	CLA	C2C-C3C-CAC-CBC
15	A	1130	CLA	CAA-CBA-CGA-O2A
15	A	1138	CLA	O1A-CGA-O2A-C1
18	B	5003	LMG	C14-C15-C16-C17
15	1	613	CLA	CAA-CBA-CGA-O2A
15	B	1215	CLA	C8-C10-C11-C12
23	B	5002	DGD	C2B-C3B-C4B-C5B
17	1	801	LHG	C15-C16-C17-C18
15	B	1203	CLA	C4-C3-C5-C6
15	3	613	CLA	CAA-CBA-CGA-O2A
15	A	1116	CLA	C4B-C3B-CAB-CBB
15	B	1023	CLA	C4B-C3B-CAB-CBB
15	B	1240	CLA	CAA-CBA-CGA-O1A
15	1	607	CLA	CAA-CBA-CGA-O2A
15	1	606	CLA	O1D-CGD-O2D-CED
15	A	1111	CLA	C16-C17-C18-C19
18	4	801	LMG	C30-C31-C32-C33
16	2	610	CHL	CHA-CBD-CGD-O1D
16	2	610	CHL	CHA-CBD-CGD-O2D
16	2	611	CHL	CHA-CBD-CGD-O1D
16	2	611	CHL	CHA-CBD-CGD-O2D
16	3	604	CHL	CHA-CBD-CGD-O1D
16	3	604	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	4	610	CHL	CHA-CBD-CGD-O2D
15	A	1112	CLA	C5-C6-C7-C8
19	3	802	3PH	O21-C21-C22-C23
15	A	1121	CLA	CAA-CBA-CGA-O2A
15	B	1212	CLA	C4-C3-C5-C6
15	A	1113	CLA	CAA-CBA-CGA-O2A
15	2	607	CLA	C11-C10-C8-C7
15	B	1211	CLA	C11-C12-C13-C15
15	1	615	CLA	CAA-CBA-CGA-O1A
15	A	1120	CLA	C2C-C3C-CAC-CBC
18	2	804	LMG	C11-C12-C13-C14
15	A	1119	CLA	C11-C10-C8-C9
18	4	801	LMG	C8-C7-O1-C1
17	A	5002	LHG	C12-C13-C14-C15
15	2	605	CLA	C2A-CAA-CBA-CGA
15	B	1215	CLA	C2-C1-O2A-CGA
15	B	1221	CLA	C2-C1-O2A-CGA
15	1	603	CLA	C3A-C2A-CAA-CBA
15	4	612	CLA	C3A-C2A-CAA-CBA
15	A	1127	CLA	C3A-C2A-CAA-CBA
15	1	615	CLA	CAA-CBA-CGA-O2A
15	B	1216	CLA	C10-C11-C12-C13
15	A	1119	CLA	C2-C3-C5-C6
15	A	1115	CLA	CAA-CBA-CGA-O2A
15	B	1239	CLA	O1D-CGD-O2D-CED
15	A	1138	CLA	CBA-CGA-O2A-C1
17	A	5002	LHG	C11-C10-C9-C8
15	A	1127	CLA	CAA-CBA-CGA-O2A
15	1	613	CLA	CAA-CBA-CGA-O1A
15	B	1237	CLA	CAA-CBA-CGA-O2A
15	B	1240	CLA	C16-C17-C18-C20
15	A	1130	CLA	CAA-CBA-CGA-O1A
15	4	606	CLA	C2A-CAA-CBA-CGA
15	A	1132	CLA	CAA-CBA-CGA-O2A
17	3	801	LHG	C13-C14-C15-C16
15	B	1203	CLA	CBA-CGA-O2A-C1
13	1	502	XAT	O24-C26-C27-C28
13	2	502	XAT	O4-C6-C7-C8
14	4	503	BCR	C20-C21-C22-C23
15	A	1115	CLA	CAA-CBA-CGA-O1A
15	B	1203	CLA	O1A-CGA-O2A-C1
15	B	1202	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	B	1231	CLA	C10-C11-C12-C13
18	B	5003	LMG	O1-C7-C8-C9
15	A	1101	CLA	C8-C10-C11-C12
15	B	1221	CLA	C5-C6-C7-C8
15	A	1126	CLA	C3-C5-C6-C7
17	3	801	LHG	C33-C34-C35-C36
15	2	606	CLA	C2A-CAA-CBA-CGA
15	B	1229	CLA	C2A-CAA-CBA-CGA
14	A	4005	BCR	C15-C16-C17-C18
15	B	1221	CLA	C16-C17-C18-C19
15	A	1113	CLA	CAA-CBA-CGA-O1A
15	A	1121	CLA	CAA-CBA-CGA-O1A
15	A	1105	CLA	CAA-CBA-CGA-O2A
15	A	1138	CLA	CAA-CBA-CGA-O2A
15	A	1104	CLA	C15-C16-C17-C18
15	A	1138	CLA	C14-C13-C15-C16
15	A	1140	CLA	C6-C7-C8-C9
16	3	604	CHL	C11-C10-C8-C9
16	2	609	CHL	CAA-CBA-CGA-O2A
15	A	1132	CLA	CAA-CBA-CGA-O1A
18	2	802	LMG	C28-C29-C30-C31
12	2	501	LUT	C11-C12-C13-C14
15	A	1102	CLA	C13-C15-C16-C17
15	A	1102	CLA	C2A-CAA-CBA-CGA
15	A	1012	CLA	C6-C7-C8-C10
15	A	1013	CLA	C11-C10-C8-C7
15	A	1103	CLA	C6-C7-C8-C10
15	A	1122	CLA	C6-C7-C8-C10
15	A	1122	CLA	C11-C12-C13-C15
15	A	1125	CLA	C11-C12-C13-C15
12	4	501	LUT	C5-C6-C7-C8
14	1	503	BCR	C5-C6-C7-C8
15	2	607	CLA	C2B-C3B-CAB-CBB
15	2	616	CLA	C2B-C3B-CAB-CBB
15	A	1116	CLA	C2B-C3B-CAB-CBB
15	A	1130	CLA	C2B-C3B-CAB-CBB
15	A	1138	CLA	C2B-C3B-CAB-CBB
15	B	1021	CLA	C2B-C3B-CAB-CBB
15	B	1022	CLA	C2B-C3B-CAB-CBB
17	A	5001	LHG	C24-C25-C26-C27
17	3	801	LHG	O7-C7-C8-C9
15	1	605	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	2	601	CLA	C2-C1-O2A-CGA
15	A	1102	CLA	C2-C1-O2A-CGA
15	A	1012	CLA	C10-C11-C12-C13
17	1	801	LHG	C9-C10-C11-C12
15	1	605	CLA	CAA-CBA-CGA-O2A
15	A	1129	CLA	CAA-CBA-CGA-O2A
21	A	2001	PQN	C18-C20-C21-C22
15	B	1221	CLA	C16-C17-C18-C20
17	B	5001	LHG	C23-C24-C25-C26
15	A	1125	CLA	C2-C3-C5-C6
15	A	1131	CLA	C4C-C3C-CAC-CBC
15	B	1023	CLA	C2A-CAA-CBA-CGA
15	A	1131	CLA	CAA-CBA-CGA-O2A
15	B	1235	CLA	CAA-CBA-CGA-O2A
15	F	1301	CLA	CAA-CBA-CGA-O2A
17	2	801	LHG	C11-C12-C13-C14
15	3	608	CLA	C10-C11-C12-C13
15	A	1136	CLA	CAA-CBA-CGA-O2A
15	A	1128	CLA	C10-C11-C12-C13
15	B	1237	CLA	CAA-CBA-CGA-O1A
15	A	1110	CLA	C5-C6-C7-C8
15	A	1111	CLA	CAA-CBA-CGA-O2A
17	A	5001	LHG	O10-C23-O8-C6
15	A	1105	CLA	C6-C7-C8-C9
15	A	1123	CLA	C6-C7-C8-C9
15	B	1021	CLA	C11-C12-C13-C14
15	B	1208	CLA	C6-C7-C8-C9
15	B	1214	CLA	C14-C13-C15-C16
15	B	1226	CLA	C11-C10-C8-C9
18	2	804	LMG	O1-C7-C8-C9
18	B	5003	LMG	C7-C8-C9-O8
15	3	605	CLA	C5-C6-C7-C8
15	2	607	CLA	C4B-C3B-CAB-CBB
15	2	616	CLA	C4B-C3B-CAB-CBB
15	B	1218	CLA	CAA-CBA-CGA-O1A
15	A	1110	CLA	C4-C3-C5-C6
15	2	604	CLA	CAA-CBA-CGA-O2A
15	A	1119	CLA	CAA-CBA-CGA-O2A
15	B	1236	CLA	CAA-CBA-CGA-O2A
15	F	1302	CLA	CAA-CBA-CGA-O2A
16	1	609	CHL	CAA-CBA-CGA-O2A
17	A	5001	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	B	5001	LHG	O7-C7-C8-C9
18	2	802	LMG	C33-C34-C35-C36
13	1	502	XAT	C7-C8-C9-C10
14	A	4005	BCR	C17-C18-C19-C20
14	B	4004	BCR	C7-C8-C9-C10
14	J	4002	BCR	C7-C8-C9-C10
14	2	503	BCR	C19-C20-C21-C22
15	1	606	CLA	CBD-CGD-O2D-CED
15	B	1235	CLA	C11-C12-C13-C14
15	A	1125	CLA	C10-C11-C12-C13
15	B	1218	CLA	CAA-CBA-CGA-O2A
15	1	608	CLA	CAA-CBA-CGA-O2A
15	A	1012	CLA	CAA-CBA-CGA-O2A
15	B	1230	CLA	CAA-CBA-CGA-O2A
15	4	602	CLA	CAA-CBA-CGA-O2A
15	A	1125	CLA	C4-C3-C5-C6
15	A	1136	CLA	C4-C3-C5-C6
15	2	604	CLA	C2-C1-O2A-CGA
15	3	610	CLA	C2-C1-O2A-CGA
15	2	616	CLA	C11-C10-C8-C7
15	A	1012	CLA	C11-C12-C13-C15
15	A	1101	CLA	C11-C10-C8-C7
15	A	1137	CLA	C11-C10-C8-C7
15	A	1137	CLA	C11-C12-C13-C15
15	B	1215	CLA	C11-C10-C8-C7
15	B	1235	CLA	C6-C7-C8-C10
15	A	1136	CLA	C2-C3-C5-C6
15	B	1208	CLA	C4C-C3C-CAC-CBC
15	4	609	CLA	C11-C12-C13-C15
15	2	616	CLA	C8-C10-C11-C12
18	2	803	LMG	O7-C10-C11-C12
15	3	601	CLA	C2A-CAA-CBA-CGA
15	4	603	CLA	C2A-CAA-CBA-CGA
15	B	1021	CLA	C8-C10-C11-C12
15	B	1206	CLA	CAA-CBA-CGA-O2A
15	2	608	CLA	C3A-C2A-CAA-CBA
15	4	607	CLA	C3A-C2A-CAA-CBA
15	B	1218	CLA	C3A-C2A-CAA-CBA
15	B	1226	CLA	C3A-C2A-CAA-CBA
20	A	1011	CL0	C3A-C2A-CAA-CBA
15	1	608	CLA	C5-C6-C7-C8
15	3	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	B	1221	CLA	C2-C3-C5-C6
14	B	4001	BCR	C11-C10-C9-C8
15	A	1131	CLA	CAA-CBA-CGA-O1A
15	A	1105	CLA	C5-C6-C7-C8
15	A	1105	CLA	CAA-CBA-CGA-O1A
15	F	1301	CLA	CAA-CBA-CGA-O1A
17	B	5001	LHG	O9-C7-C8-C9
18	2	804	LMG	C12-C13-C14-C15
17	A	5001	LHG	C24-C23-O8-C6
18	2	803	LMG	C16-C17-C18-C19
15	4	602	CLA	C2A-CAA-CBA-CGA
15	4	604	CLA	C11-C10-C8-C9
15	4	612	CLA	C11-C12-C13-C14
15	A	1012	CLA	C11-C12-C13-C14
15	A	1102	CLA	C6-C7-C8-C9
15	A	1103	CLA	C6-C7-C8-C9
15	A	1104	CLA	C6-C7-C8-C9
15	A	1138	CLA	C11-C10-C8-C9
15	B	1224	CLA	C11-C10-C8-C9
15	4	604	CLA	CAA-CBA-CGA-O2A
15	B	1236	CLA	CAA-CBA-CGA-O1A
17	B	5001	LHG	O10-C23-C24-C25
15	B	1205	CLA	C10-C11-C12-C13
14	A	4002	BCR	C13-C14-C15-C16
14	B	4004	BCR	C9-C10-C11-C12
15	2	606	CLA	CAA-CBA-CGA-O2A
15	A	1117	CLA	C16-C17-C18-C20
15	4	602	CLA	CAA-CBA-CGA-O1A
16	1	609	CHL	CAA-CBA-CGA-O1A
17	3	801	LHG	O9-C7-C8-C9
18	4	801	LMG	O10-C28-C29-C30
15	3	603	CLA	C8-C10-C11-C12
15	A	1120	CLA	C4C-C3C-CAC-CBC
14	B	4006	BCR	C7-C8-C9-C10
14	F	4001	BCR	C17-C18-C19-C20
15	1	605	CLA	CAA-CBA-CGA-O1A
16	2	609	CHL	CAA-CBA-CGA-O1A
15	B	1236	CLA	O1A-CGA-O2A-C1
18	2	803	LMG	O1-C7-C8-O7
18	2	804	LMG	O1-C7-C8-O7
15	A	1136	CLA	CAA-CBA-CGA-O1A
15	A	1138	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	4	801	LMG	C14-C15-C16-C17
16	2	609	CHL	C8-C10-C11-C12
15	2	604	CLA	CAA-CBA-CGA-O1A
15	A	1111	CLA	CAA-CBA-CGA-O1A
15	A	1119	CLA	CAA-CBA-CGA-O1A
15	B	1227	CLA	C2-C3-C5-C6
15	A	1129	CLA	CAA-CBA-CGA-O1A
15	B	1235	CLA	CAA-CBA-CGA-O1A
15	2	605	CLA	C16-C17-C18-C20
15	1	605	CLA	CAD-CBD-CGD-O2D
15	3	607	CLA	CAD-CBD-CGD-O2D
15	3	608	CLA	CAD-CBD-CGD-O2D
15	4	605	CLA	CAD-CBD-CGD-O2D
15	A	1120	CLA	CAD-CBD-CGD-O2D
15	A	1133	CLA	CAD-CBD-CGD-O2D
15	B	1216	CLA	CAD-CBD-CGD-O2D
15	B	1230	CLA	CAD-CBD-CGD-O2D
16	1	610	CHL	CAA-CBA-CGA-O2A
15	B	1223	CLA	C2C-C3C-CAC-CBC
17	1	801	LHG	O9-C7-C8-C9
15	A	1129	CLA	C4C-C3C-CAC-CBC
16	1	609	CHL	C2-C1-O2A-CGA
15	B	1204	CLA	CAA-CBA-CGA-O1A
15	1	608	CLA	CAA-CBA-CGA-O1A
20	A	1011	CL0	CAA-CBA-CGA-O2A
16	3	604	CHL	C1A-C2A-CAA-CBA
17	1	801	LHG	C13-C14-C15-C16
15	B	1230	CLA	CAA-CBA-CGA-O1A
15	A	1013	CLA	C13-C15-C16-C17
15	3	610	CLA	CAA-CBA-CGA-O2A
15	A	1107	CLA	CAA-CBA-CGA-O2A
15	A	1122	CLA	C16-C17-C18-C20
17	A	5001	LHG	O9-C7-C8-C9
15	B	1022	CLA	C4C-C3C-CAC-CBC
15	A	1133	CLA	CAA-CBA-CGA-O2A
17	2	801	LHG	O8-C23-C24-C25
15	2	603	CLA	C15-C16-C17-C18
15	B	1206	CLA	CAA-CBA-CGA-O1A
15	4	604	CLA	CAA-CBA-CGA-O1A
15	A	1012	CLA	CAA-CBA-CGA-O1A
15	F	1302	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

176 monomers are involved in 1422 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4	616	CLA	1	0
15	B	1201	CLA	2	0
15	A	1116	CLA	18	0
15	2	608	CLA	14	0
15	A	1114	CLA	14	0
15	3	610	CLA	5	0
14	2	503	BCR	1	0
14	J	4001	BCR	17	0
15	B	1229	CLA	13	0
14	A	4005	BCR	16	0
15	1	603	CLA	16	0
15	4	603	CLA	1	0
18	B	5003	LMG	2	0
15	A	1123	CLA	21	0
15	A	1103	CLA	20	0
15	B	1022	CLA	16	0
15	A	1136	CLA	11	0
13	4	502	XAT	3	0
14	F	4001	BCR	29	0
15	B	1214	CLA	11	0
15	3	611	CLA	8	0
15	B	1223	CLA	19	0
15	2	603	CLA	2	0
15	4	602	CLA	1	0
15	4	605	CLA	1	0
14	B	4005	BCR	5	0
15	A	1104	CLA	7	0
15	1	608	CLA	25	0
15	4	601	CLA	11	0
22	A	3001	SF4	1	0
12	4	501	LUT	20	0
15	B	1230	CLA	21	0
15	4	604	CLA	1	0
15	J	1302	CLA	6	0
15	A	1112	CLA	26	0
21	A	2001	PQN	8	0
15	A	1121	CLA	8	0
14	B	4002	BCR	4	0
14	A	4007	BCR	19	0
18	2	804	LMG	13	0
15	B	1224	CLA	16	0
14	J	4002	BCR	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1226	CLA	8	0
15	B	1231	CLA	18	0
15	3	607	CLA	2	0
23	B	5002	DGD	13	0
16	4	613	CHL	5	0
14	3	506	BCR	2	0
15	3	613	CLA	6	0
15	A	1126	CLA	22	0
17	2	801	LHG	1	0
15	B	1202	CLA	19	0
14	A	4004	BCR	7	0
15	B	1212	CLA	3	0
15	A	1106	CLA	13	0
15	A	1141	CLA	3	0
15	B	1216	CLA	23	0
15	B	1221	CLA	7	0
15	B	1234	CLA	12	0
15	A	1138	CLA	10	0
15	A	1132	CLA	4	0
15	B	1236	CLA	19	0
14	4	503	BCR	4	0
15	4	607	CLA	2	0
14	A	4003	BCR	28	0
15	2	616	CLA	3	0
15	A	1127	CLA	7	0
15	3	601	CLA	6	0
17	1	801	LHG	9	0
16	4	610	CHL	1	0
15	3	609	CLA	1	0
14	B	4006	BCR	14	0
15	1	613	CLA	18	0
15	1	611	CLA	5	0
15	B	1218	CLA	2	0
15	F	1301	CLA	4	0
15	2	607	CLA	1	0
17	A	5001	LHG	6	0
15	3	603	CLA	10	0
15	A	1122	CLA	17	0
13	3	502	XAT	13	0
15	3	606	CLA	3	0
15	A	1105	CLA	12	0
16	4	611	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1012	CLA	22	0
16	2	609	CHL	4	0
15	B	1225	CLA	10	0
15	A	1120	CLA	7	0
15	B	1222	CLA	17	0
14	A	4002	BCR	19	0
15	A	1113	CLA	8	0
15	A	1119	CLA	11	0
15	A	1130	CLA	9	0
15	3	605	CLA	13	0
15	A	1115	CLA	5	0
15	3	608	CLA	19	0
15	B	1023	CLA	10	0
14	1	503	BCR	4	0
15	B	1211	CLA	13	0
15	B	1235	CLA	19	0
15	B	1208	CLA	3	0
17	A	5002	LHG	11	0
16	2	611	CHL	4	0
15	B	1021	CLA	18	0
15	A	1013	CLA	24	0
15	1	607	CLA	6	0
15	1	601	CLA	18	0
15	A	1125	CLA	9	0
15	4	606	CLA	1	0
15	A	1140	CLA	11	0
15	A	1111	CLA	17	0
16	3	604	CHL	11	0
14	3	503	BCR	1	0
15	B	1204	CLA	7	0
14	A	4006	BCR	8	0
15	4	608	CLA	5	0
15	3	612	CLA	10	0
14	F	4002	BCR	1	0
15	B	1203	CLA	11	0
15	2	604	CLA	2	0
13	1	502	XAT	2	0
15	B	1210	CLA	7	0
18	2	803	LMG	2	0
15	B	1228	CLA	7	0
20	A	1011	CL0	20	0
15	A	1137	CLA	22	0

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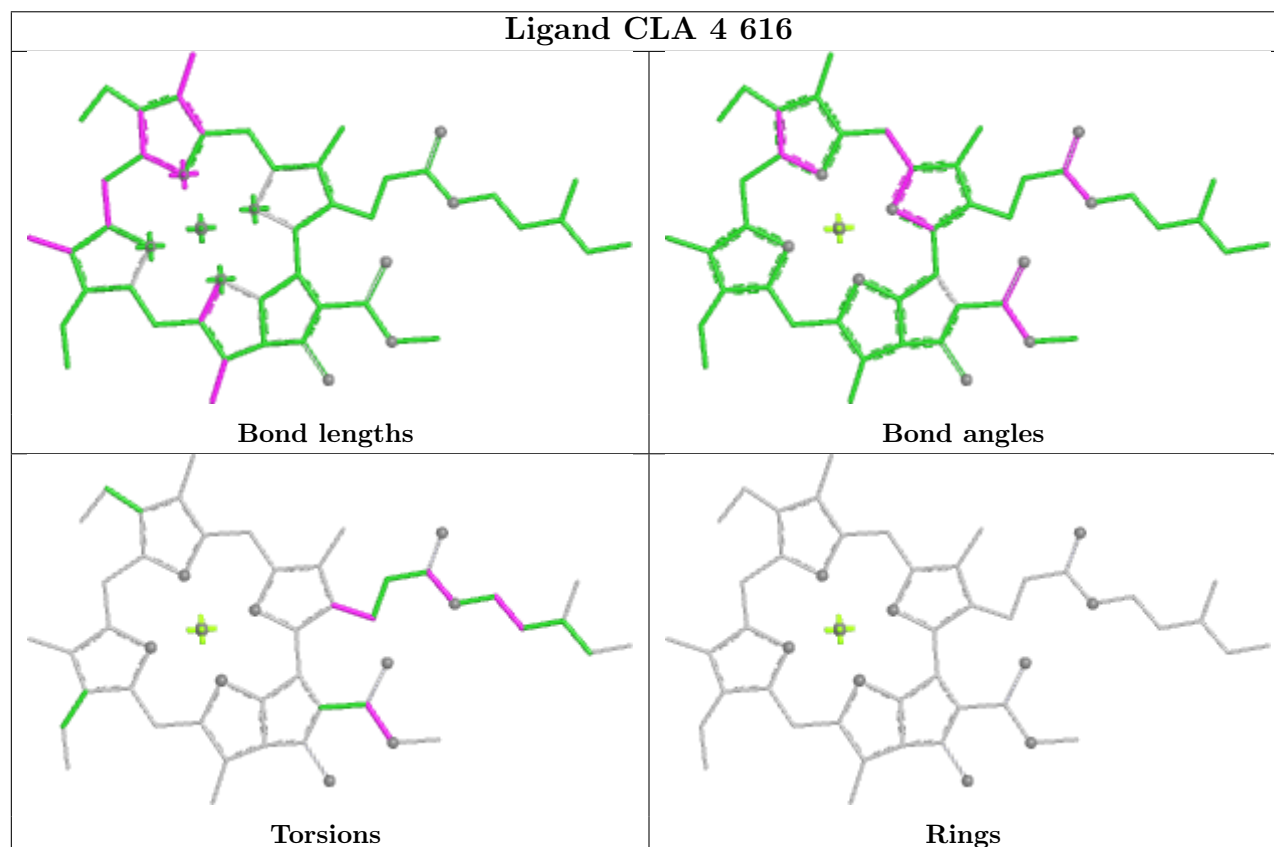
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	1	605	CLA	4	0
14	3	504	BCR	3	0
15	4	612	CLA	1	0
12	1	501	LUT	31	0
13	2	502	XAT	3	0
15	A	1102	CLA	11	0
15	A	1107	CLA	16	0
16	2	610	CHL	1	0
19	3	802	3PH	3	0
14	B	4004	BCR	2	0
15	A	1108	CLA	11	0
15	A	1128	CLA	12	0
15	B	1240	CLA	10	0
16	1	609	CHL	1	0
18	4	801	LMG	1	0
15	A	1118	CLA	6	0
15	1	604	CLA	3	0
15	1	606	CLA	4	0
15	A	1133	CLA	19	0
15	A	1135	CLA	13	0
15	B	1232	CLA	5	0
15	B	1215	CLA	37	0
15	2	612	CLA	1	0
15	B	1220	CLA	2	0
15	A	1101	CLA	5	0
12	2	501	LUT	7	0
15	B	1227	CLA	6	0
15	B	1205	CLA	20	0
15	A	1117	CLA	11	0
14	B	4003	BCR	5	0
15	B	1239	CLA	1	0
15	A	1109	CLA	7	0
15	F	1302	CLA	9	0
15	2	601	CLA	2	0
15	B	1206	CLA	10	0
15	A	1124	CLA	16	0
15	A	1129	CLA	1	0
15	B	1213	CLA	10	0
15	3	615	CLA	10	0
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15	A	1110	CLA	13	0
12	3	501	LUT	11	0

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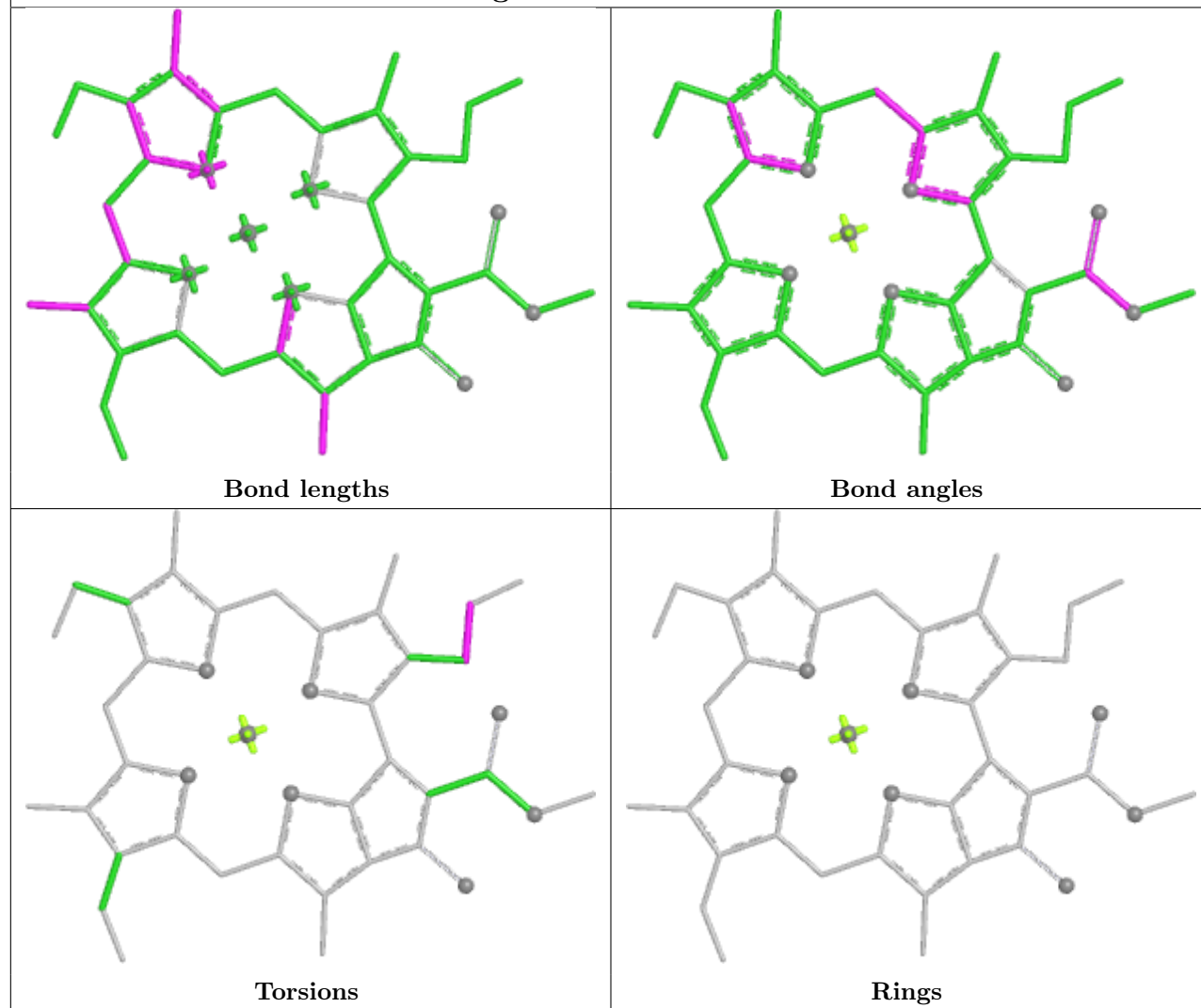
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1139	CLA	4	0
15	B	1238	CLA	1	0
15	A	1131	CLA	5	0
15	3	614	CLA	3	0
17	3	801	LHG	8	0
21	B	2002	PQN	10	0
15	B	1219	CLA	6	0
15	A	1134	CLA	12	0

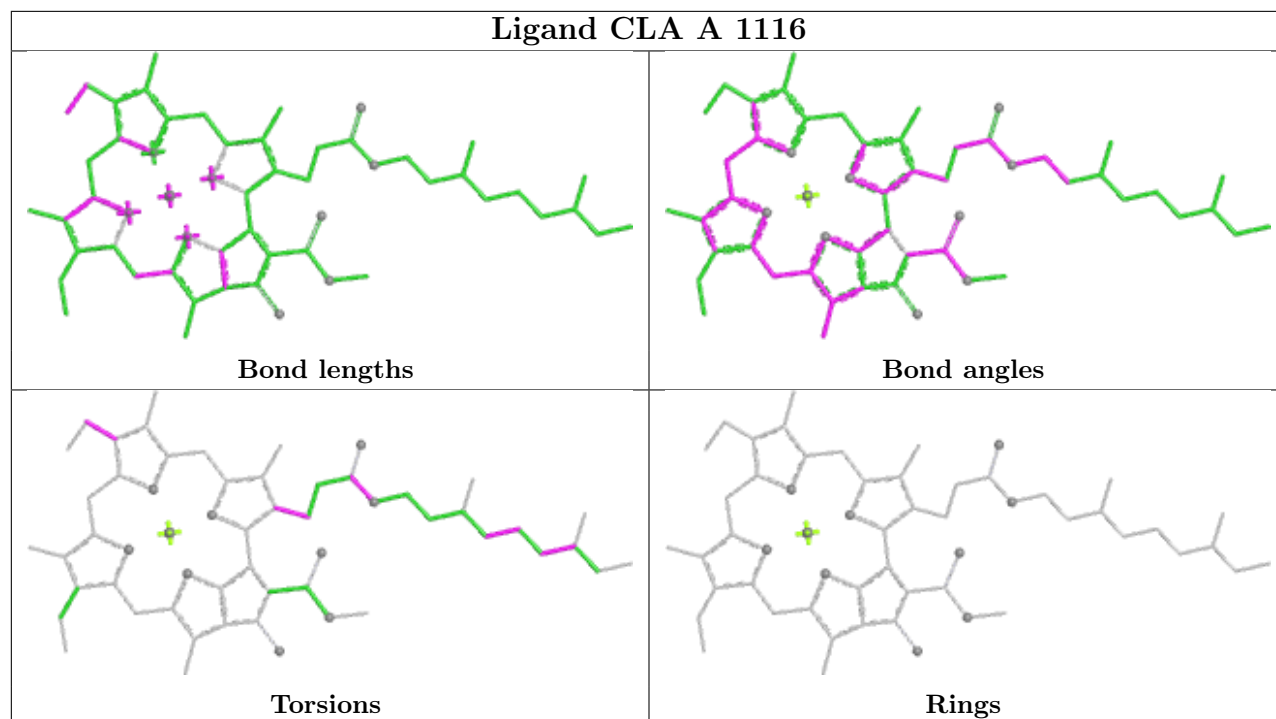
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



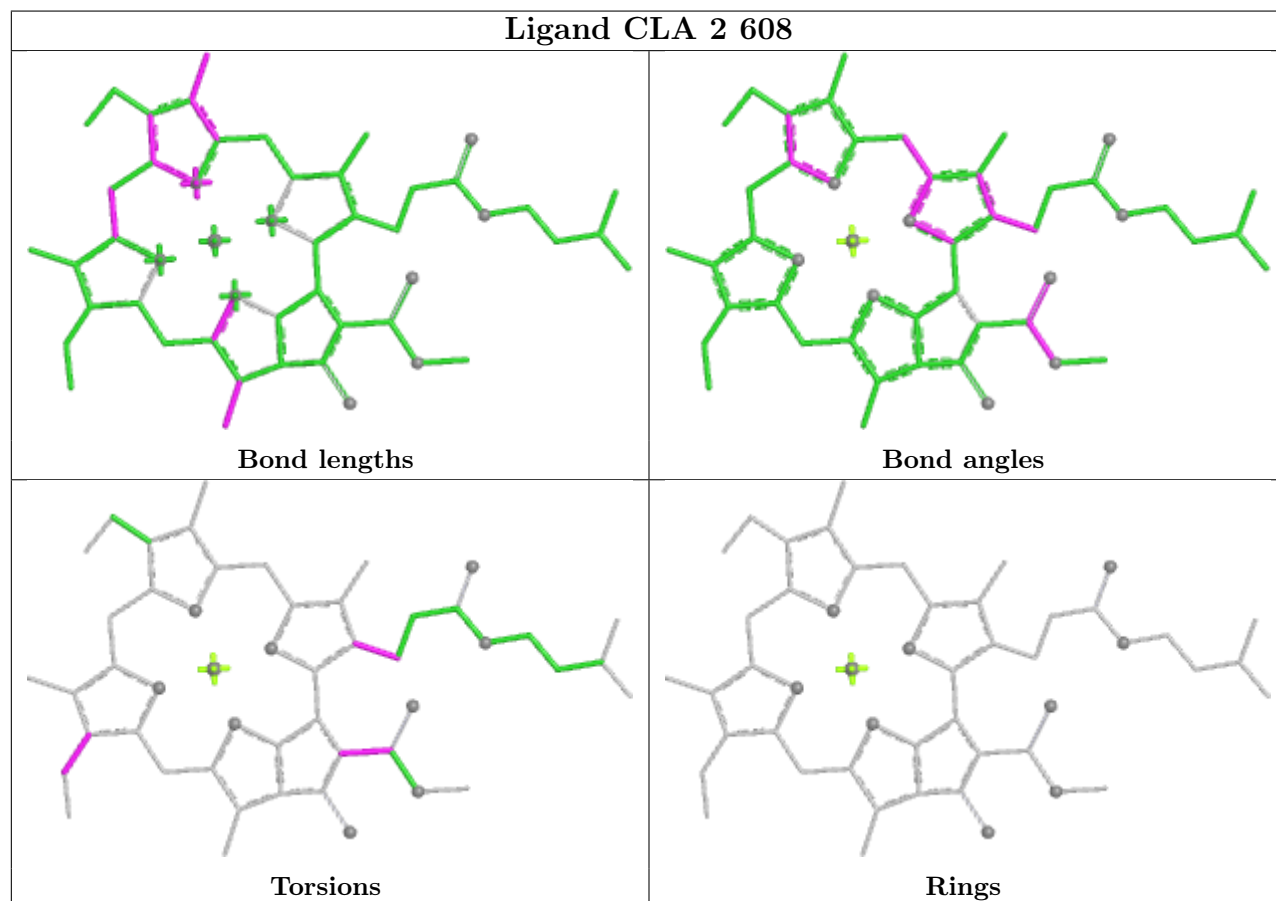
Ligand CLA B 1201



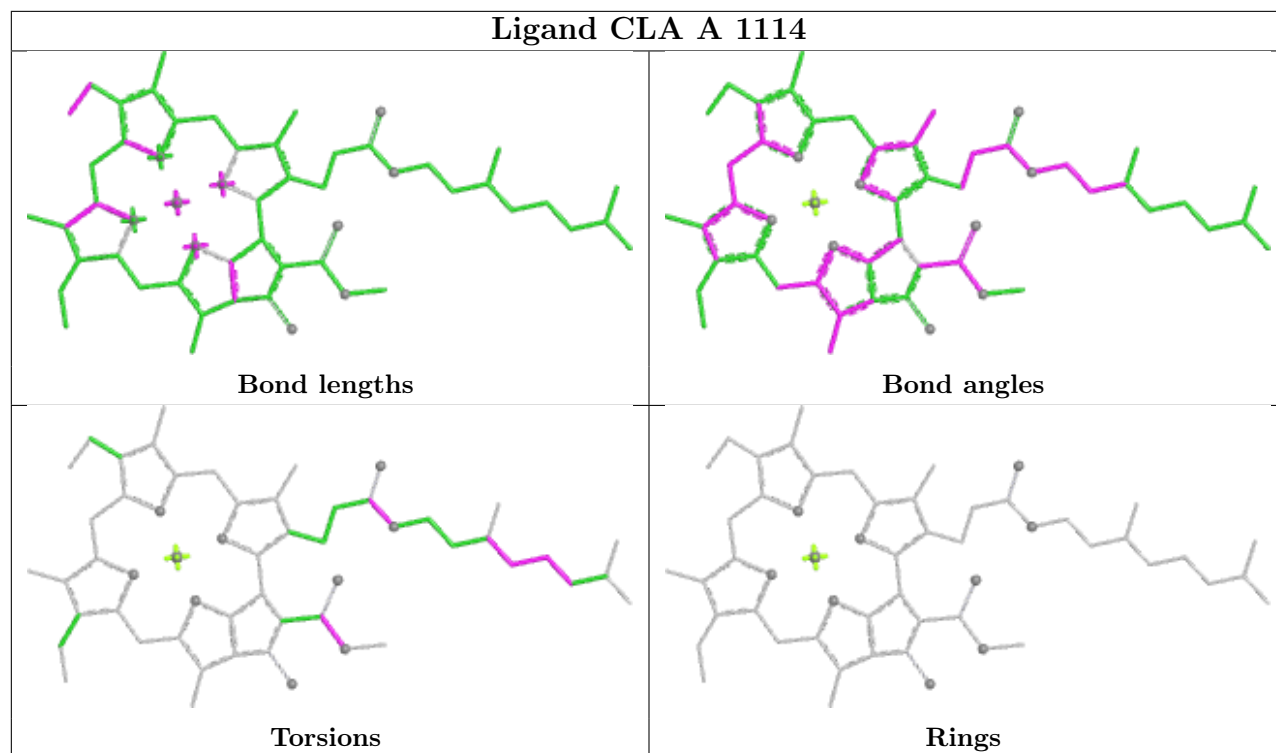
Ligand CLA A 1116



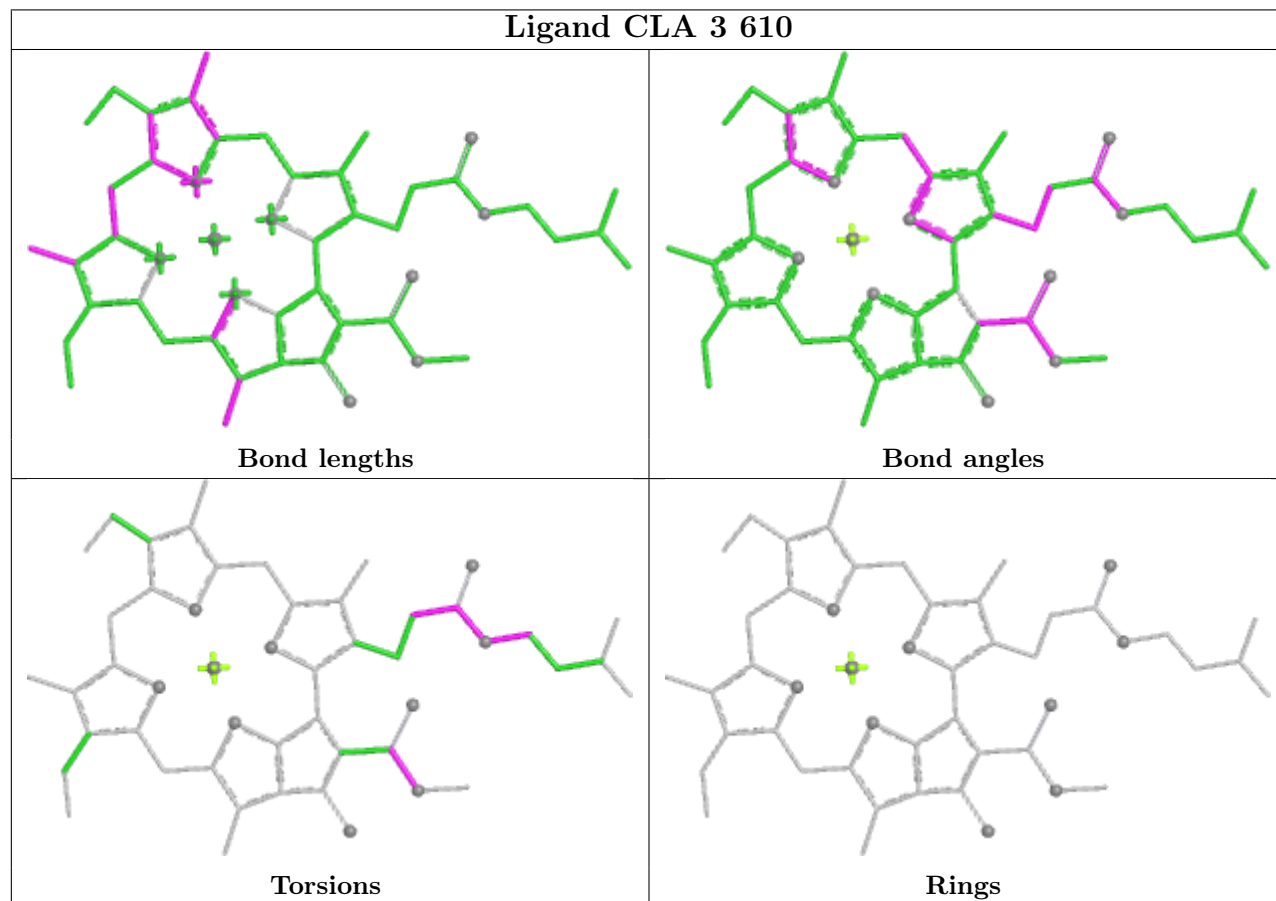
Ligand CLA 2 608

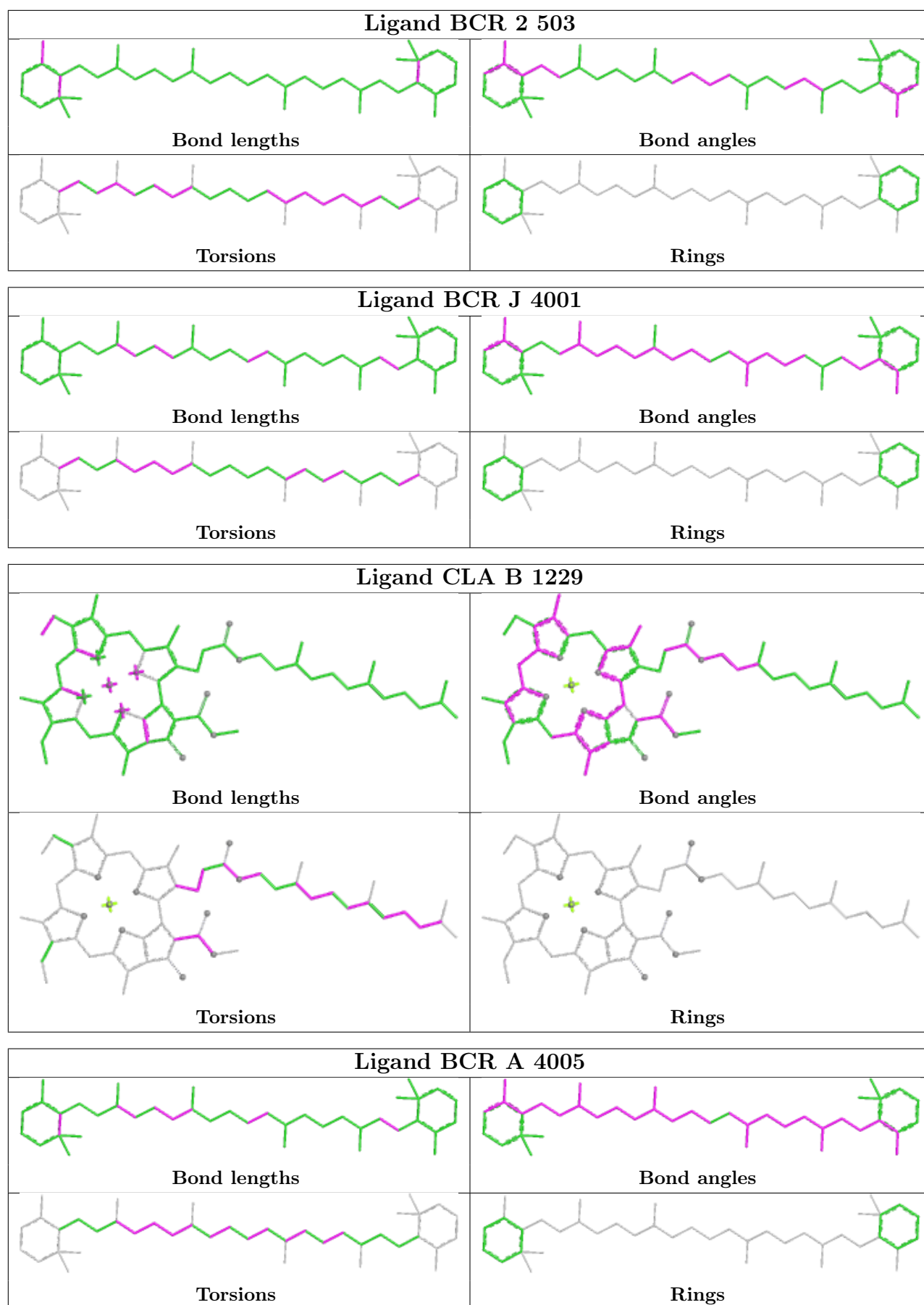


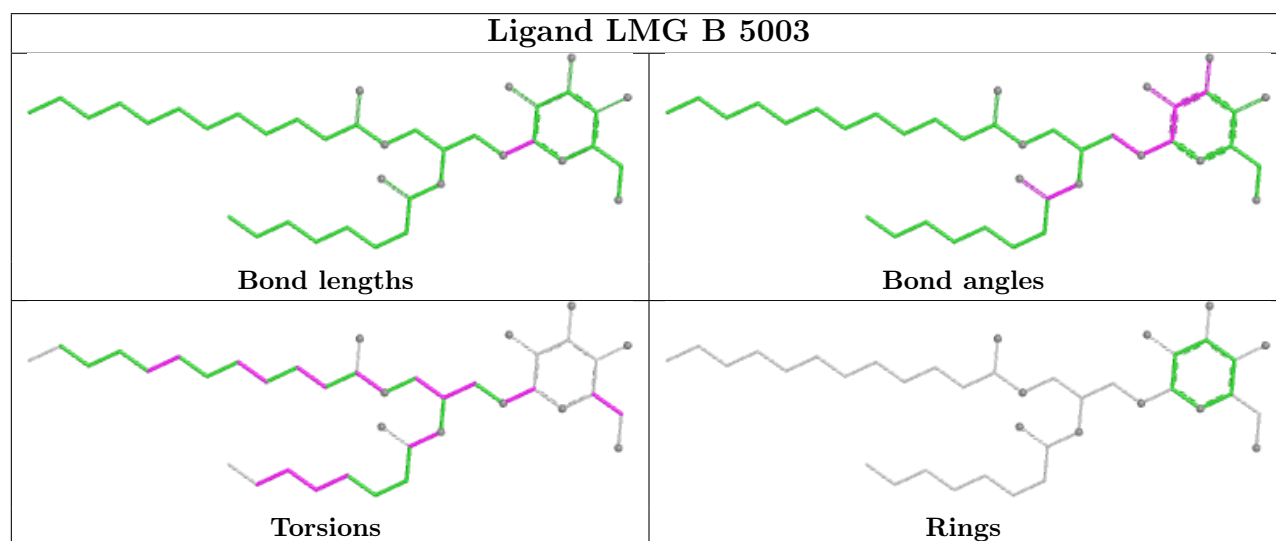
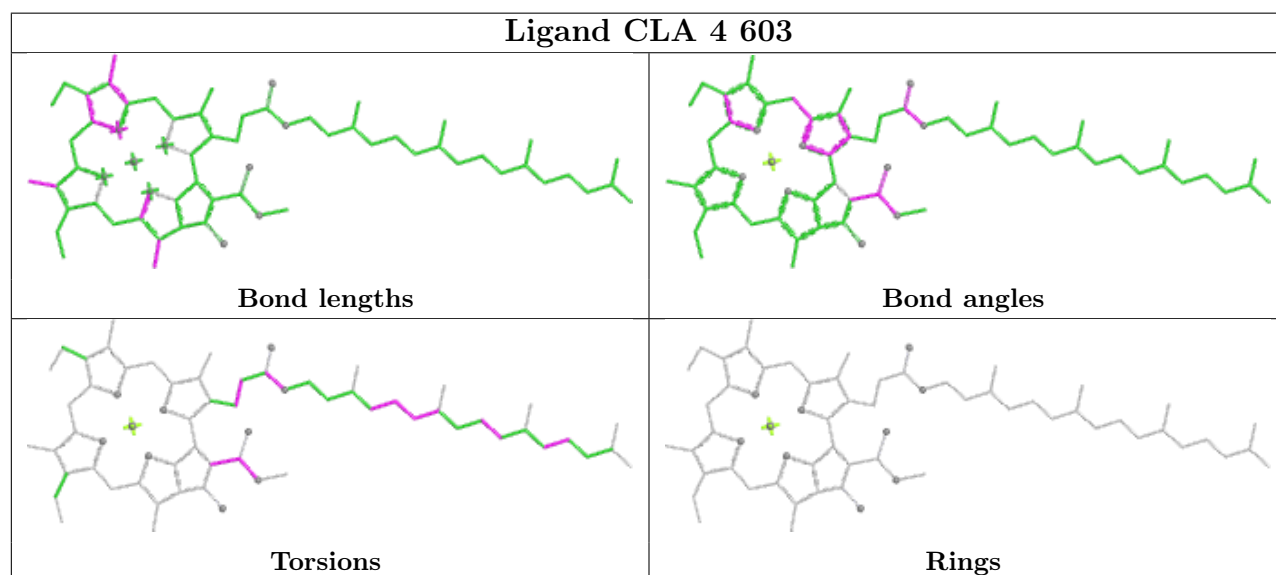
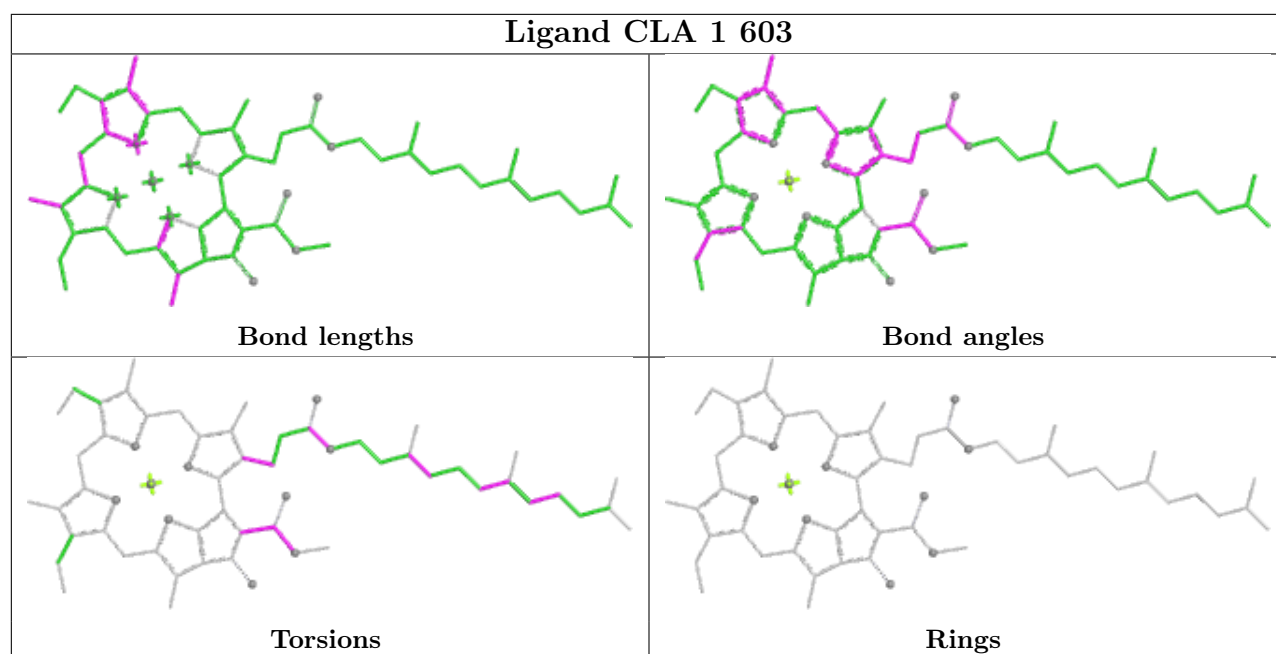
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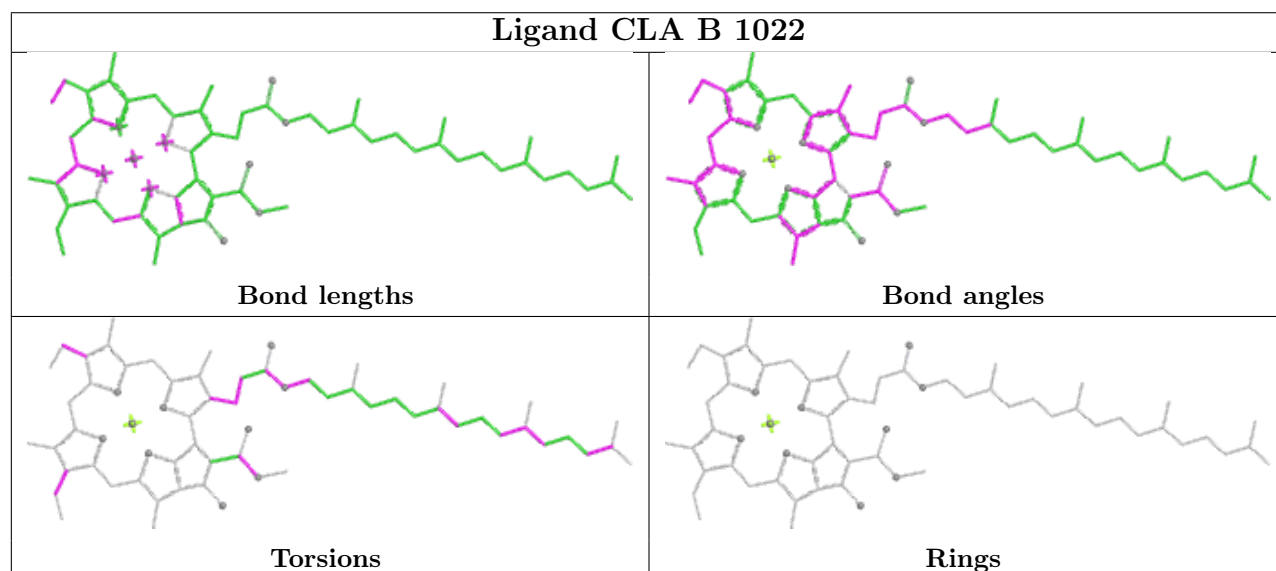
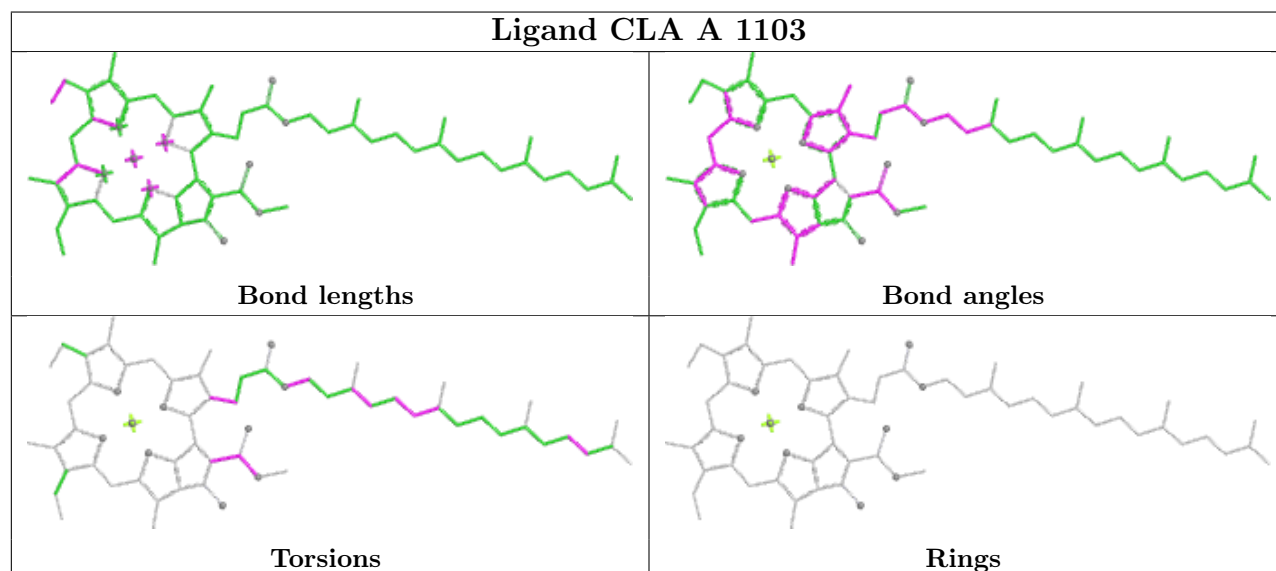
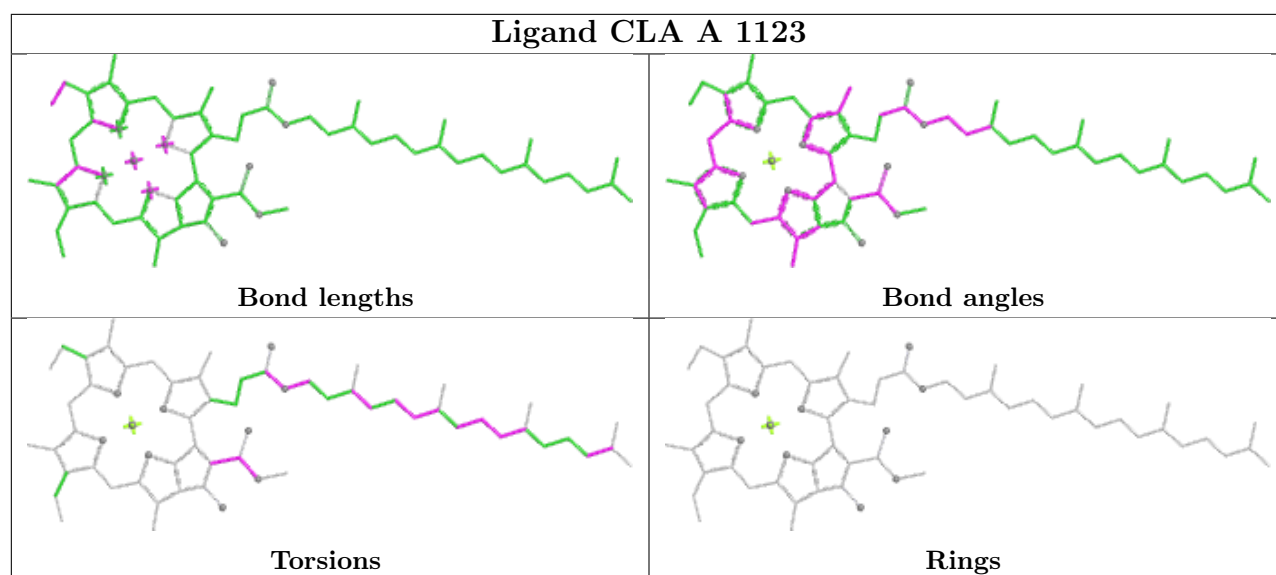


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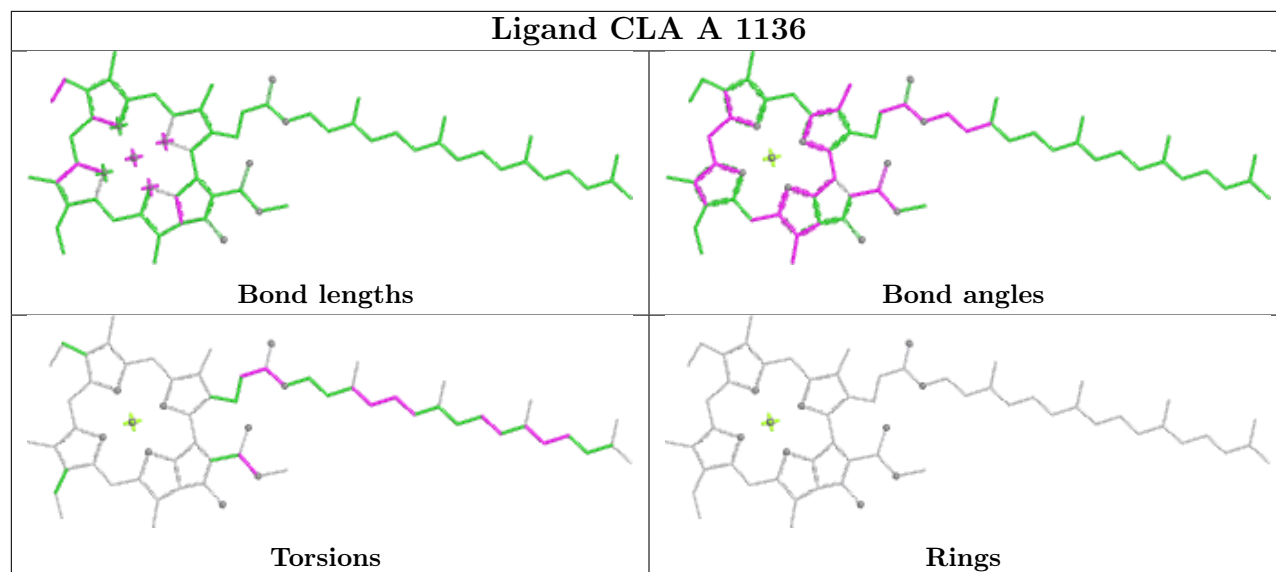




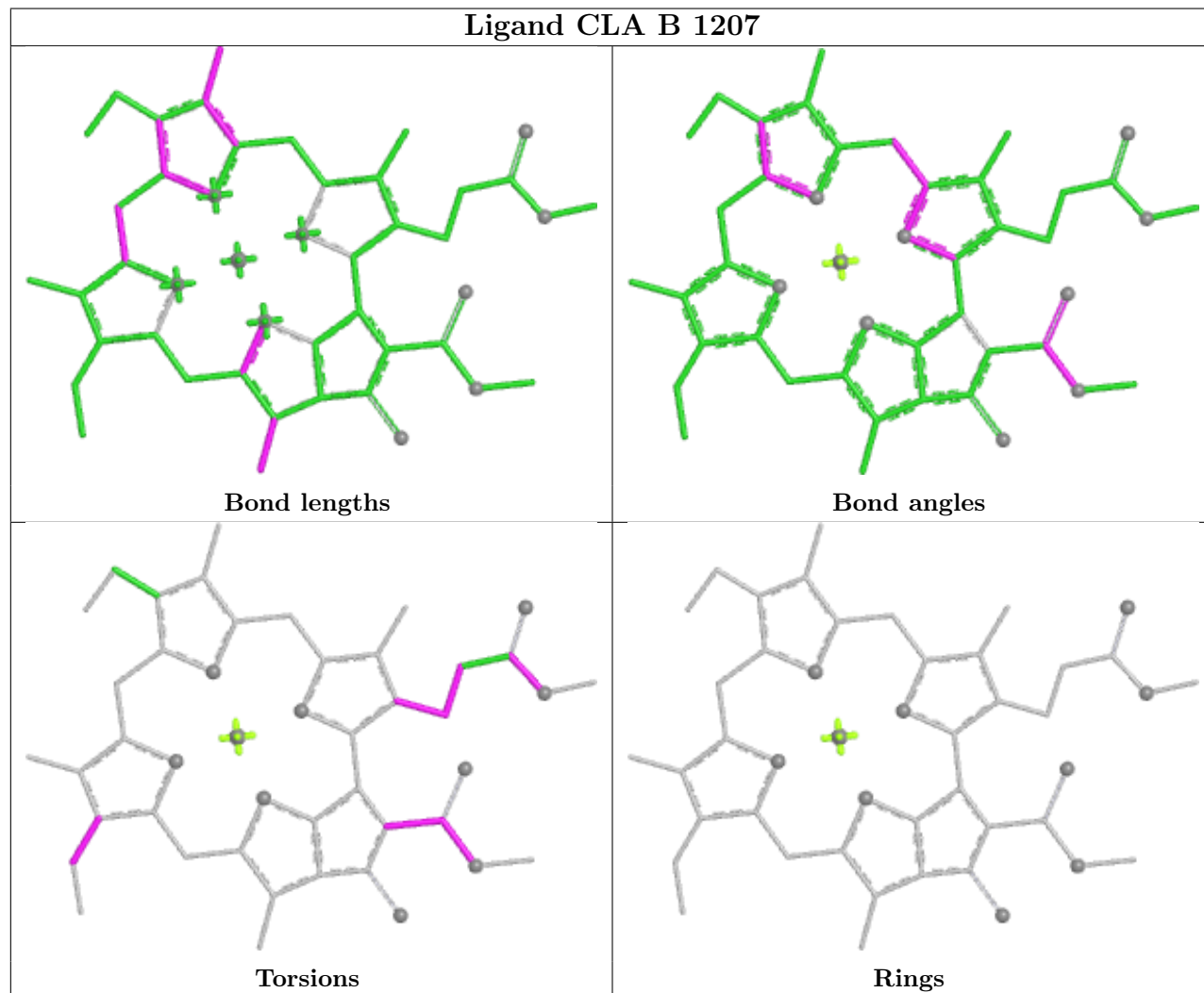


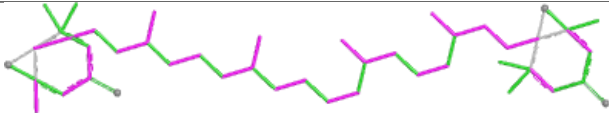
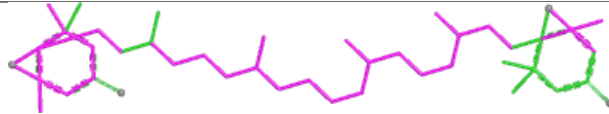
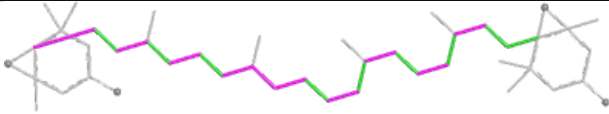
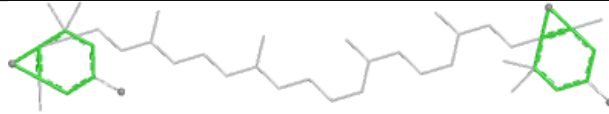


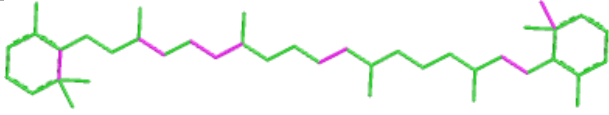
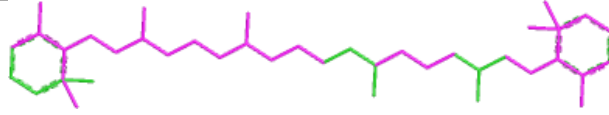
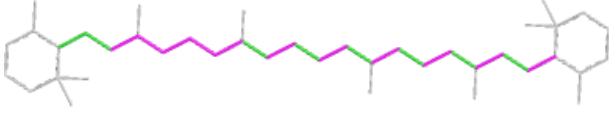
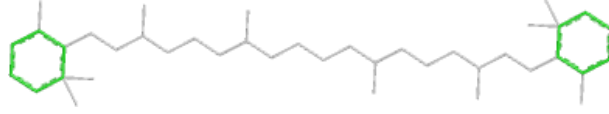
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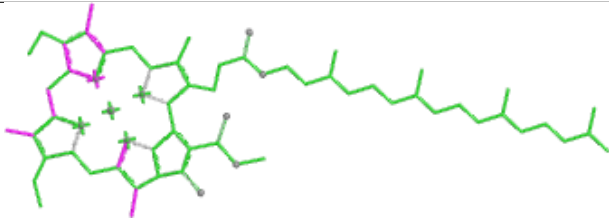
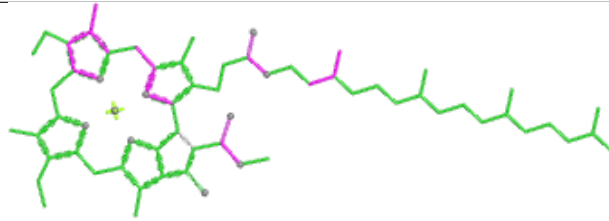
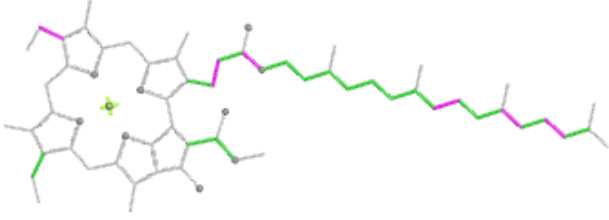
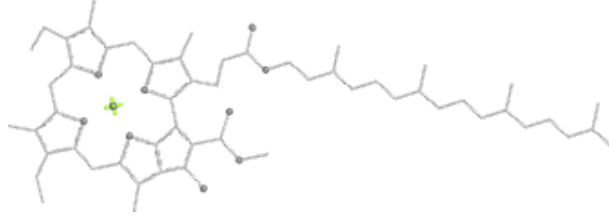


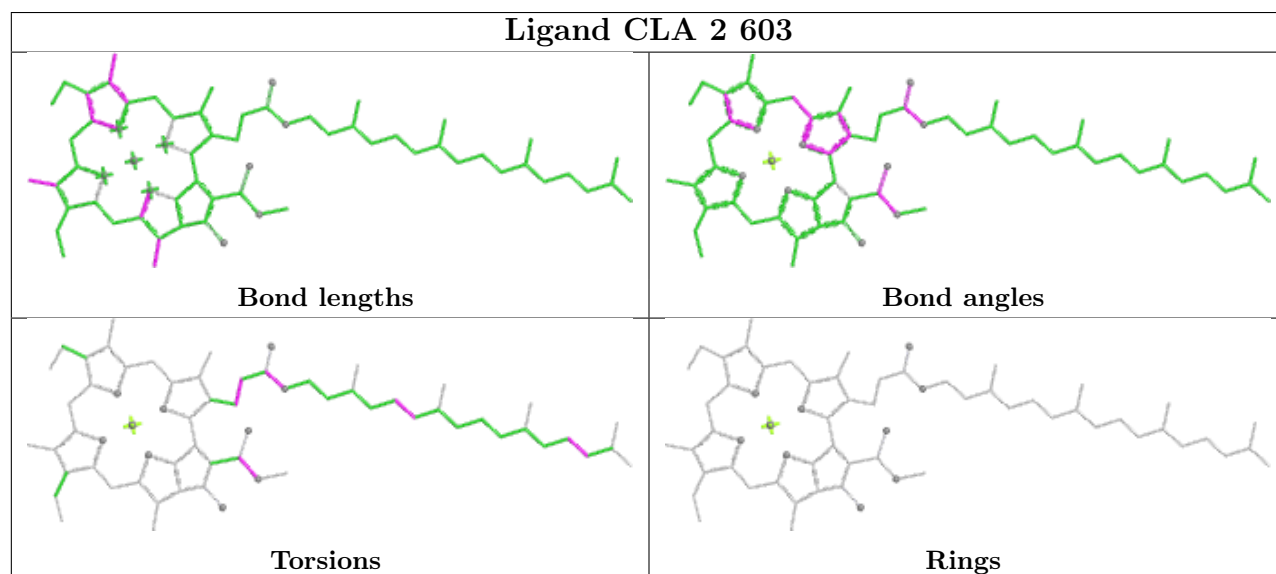
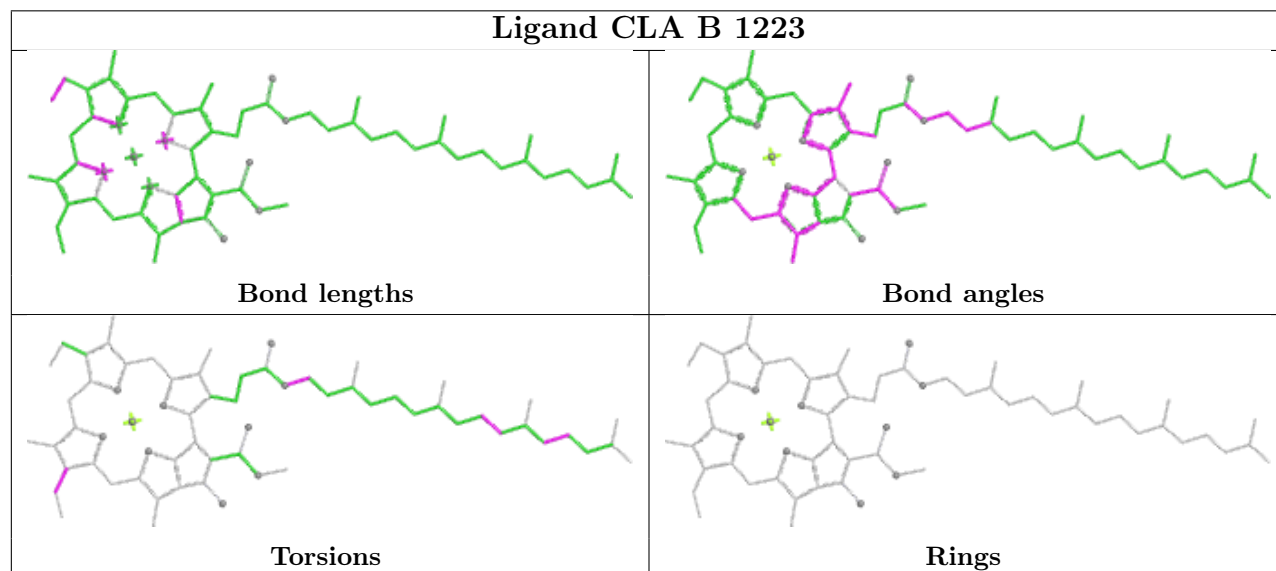
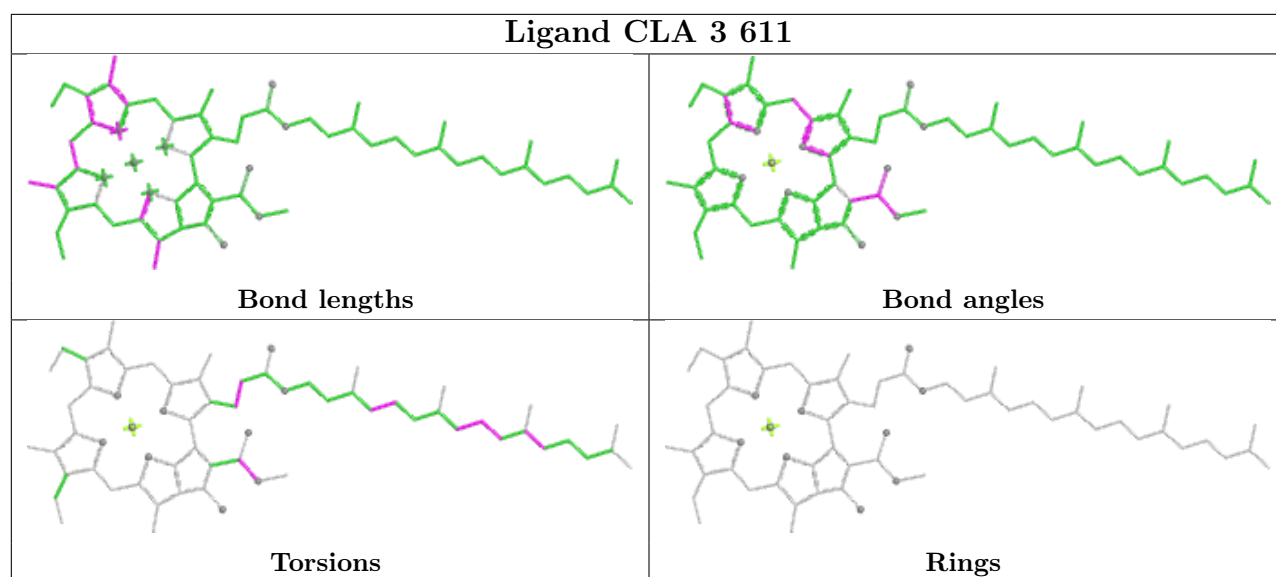
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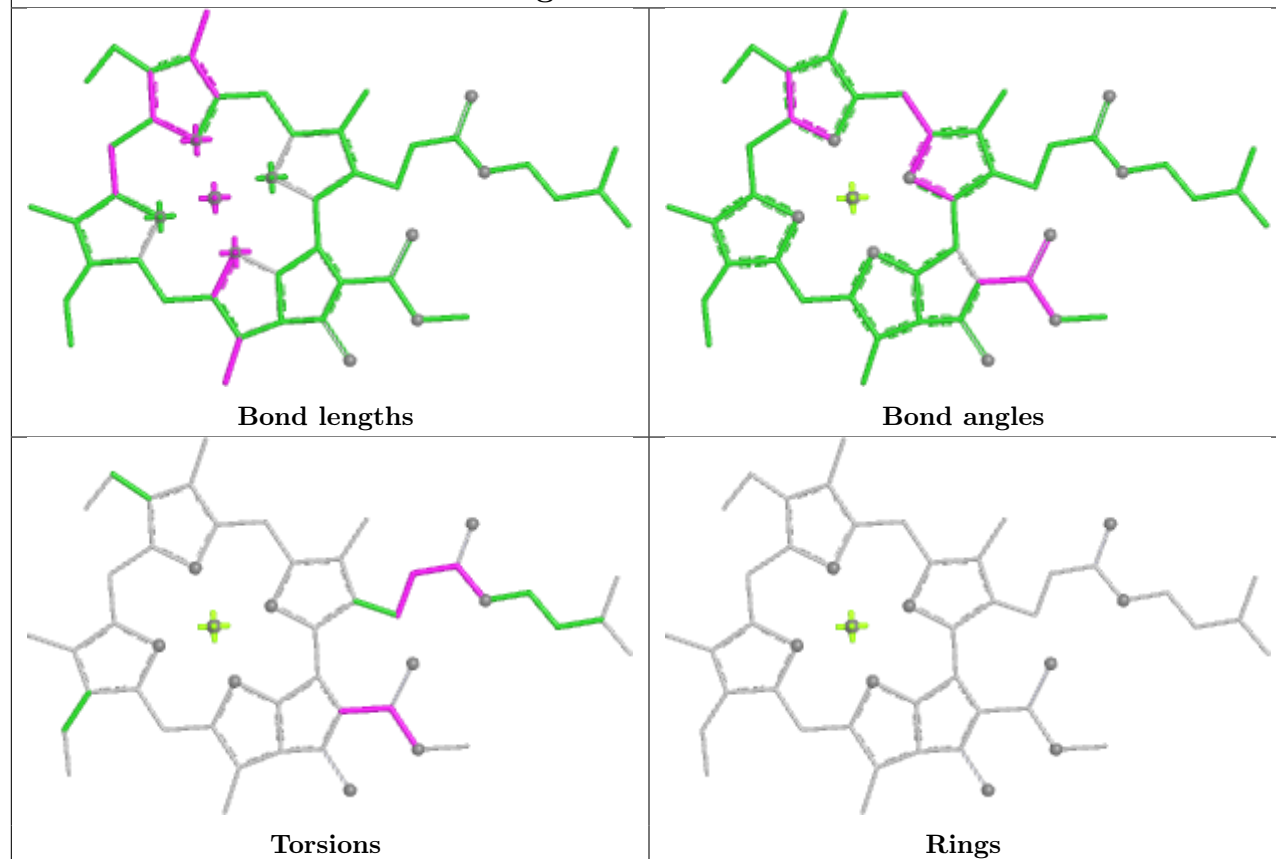
Ligand XAT 4 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

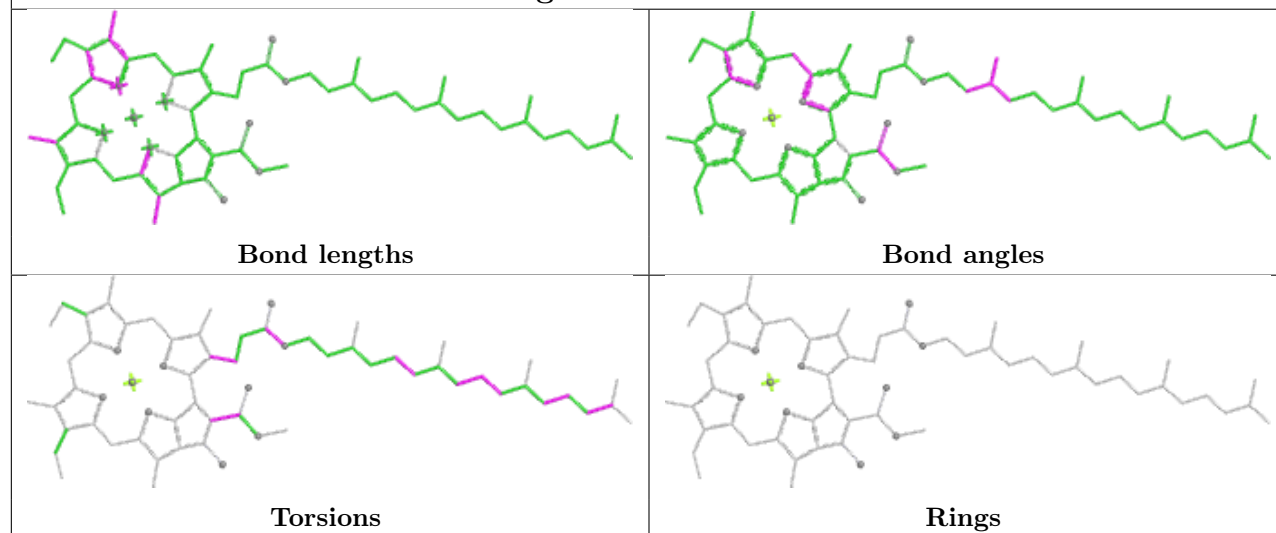
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Bond lengths	Bond angles
	
Torsions	Rings

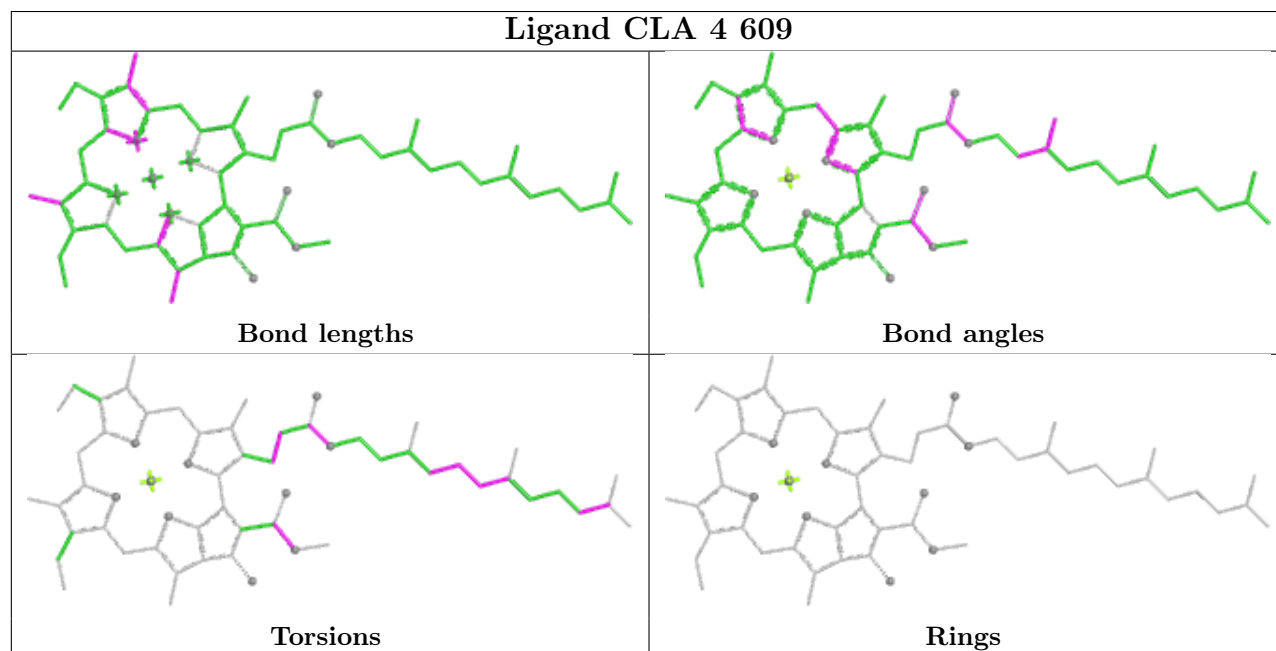
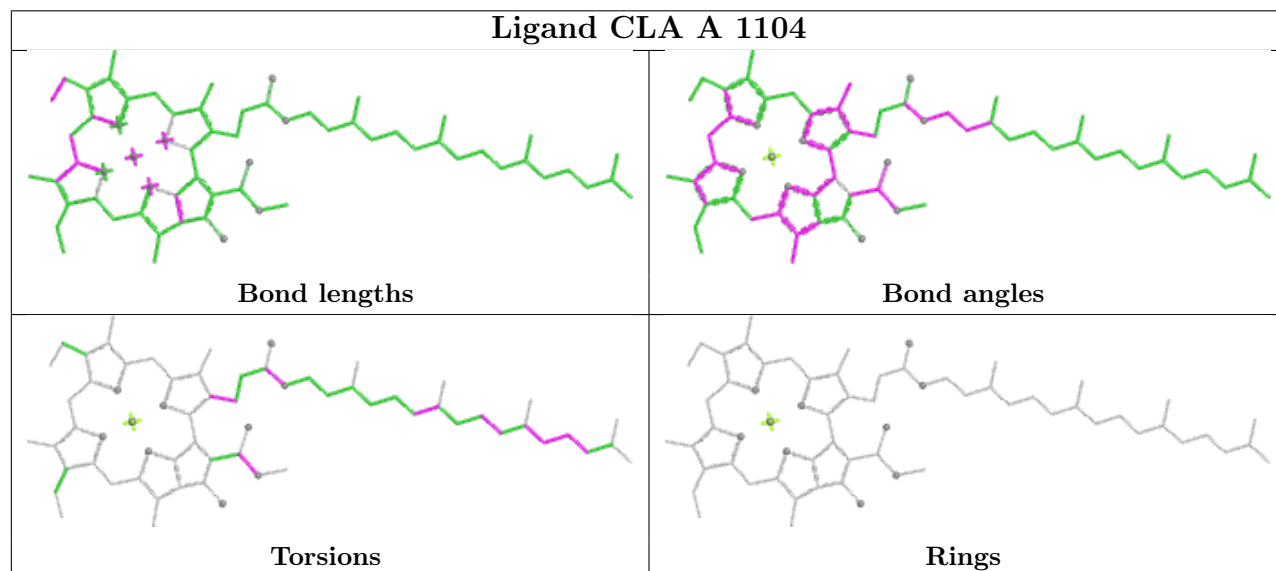
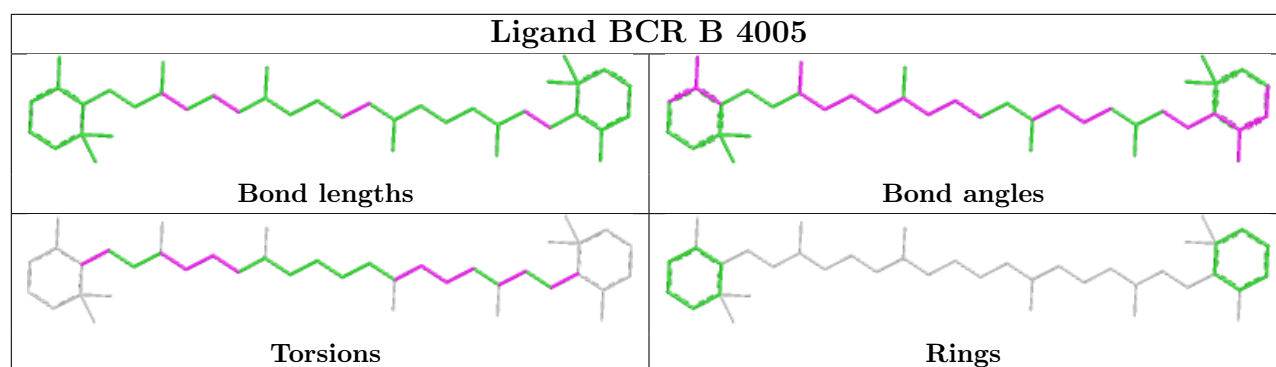


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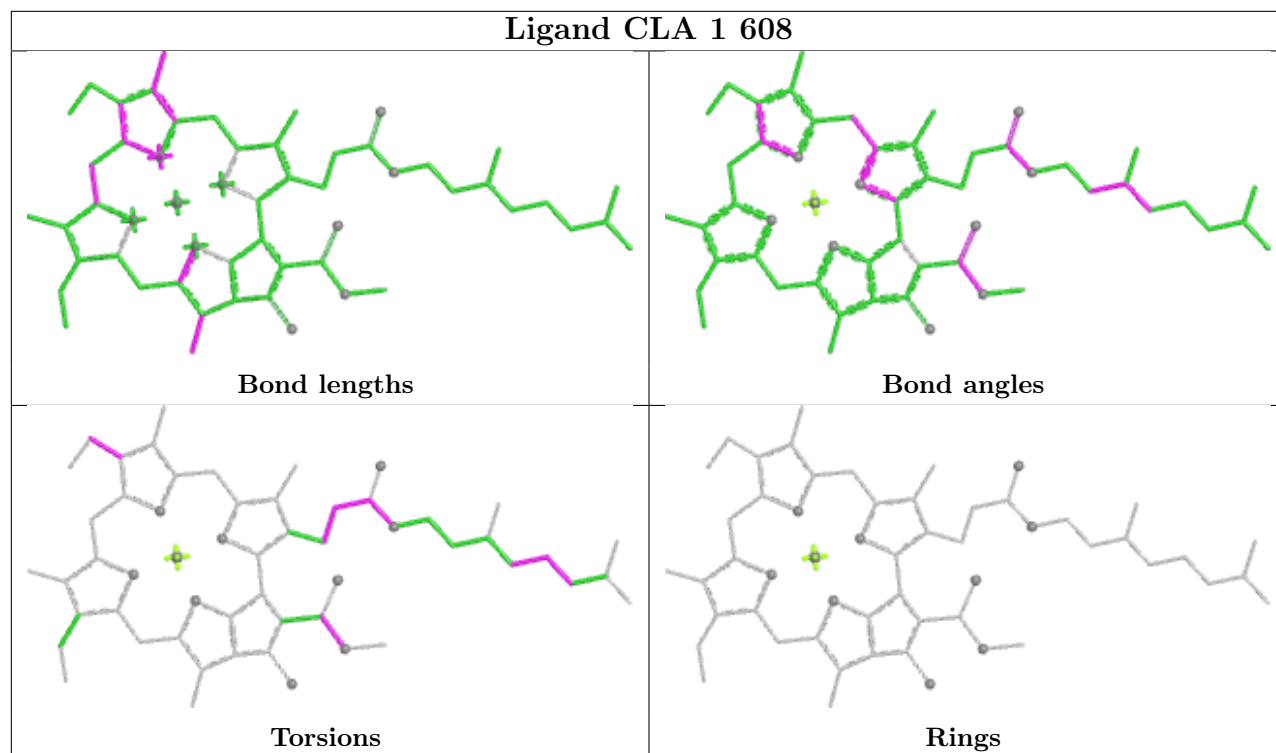


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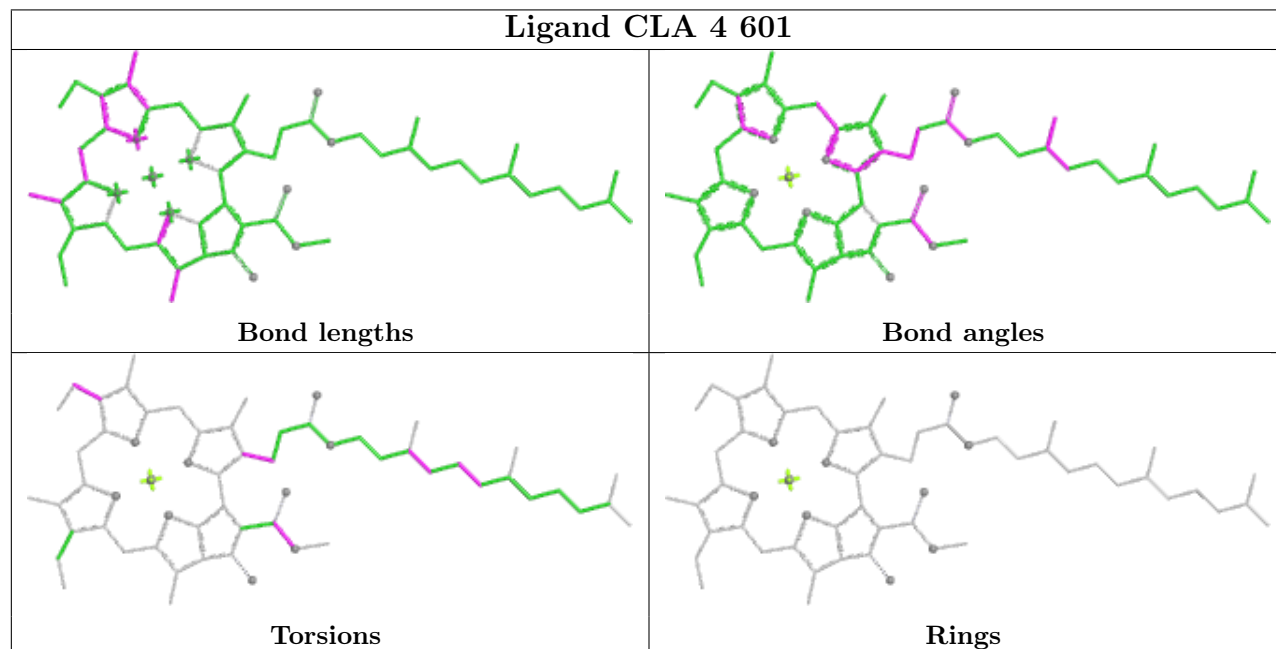




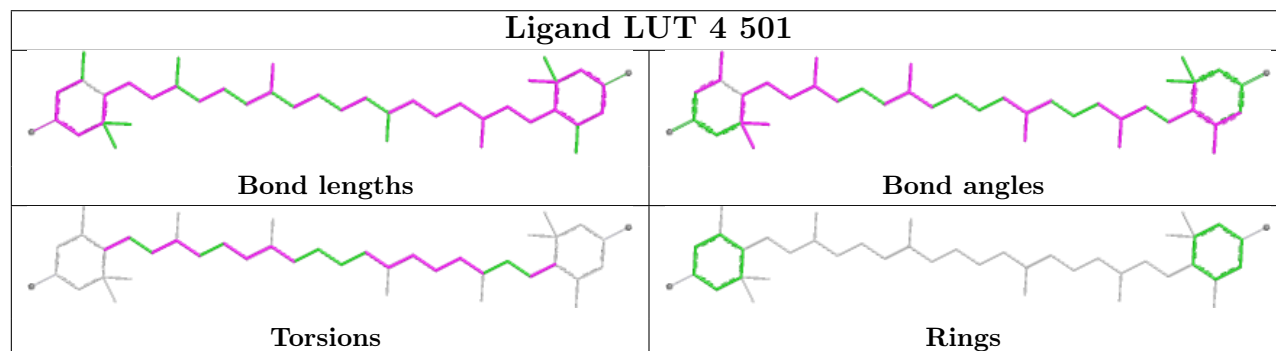
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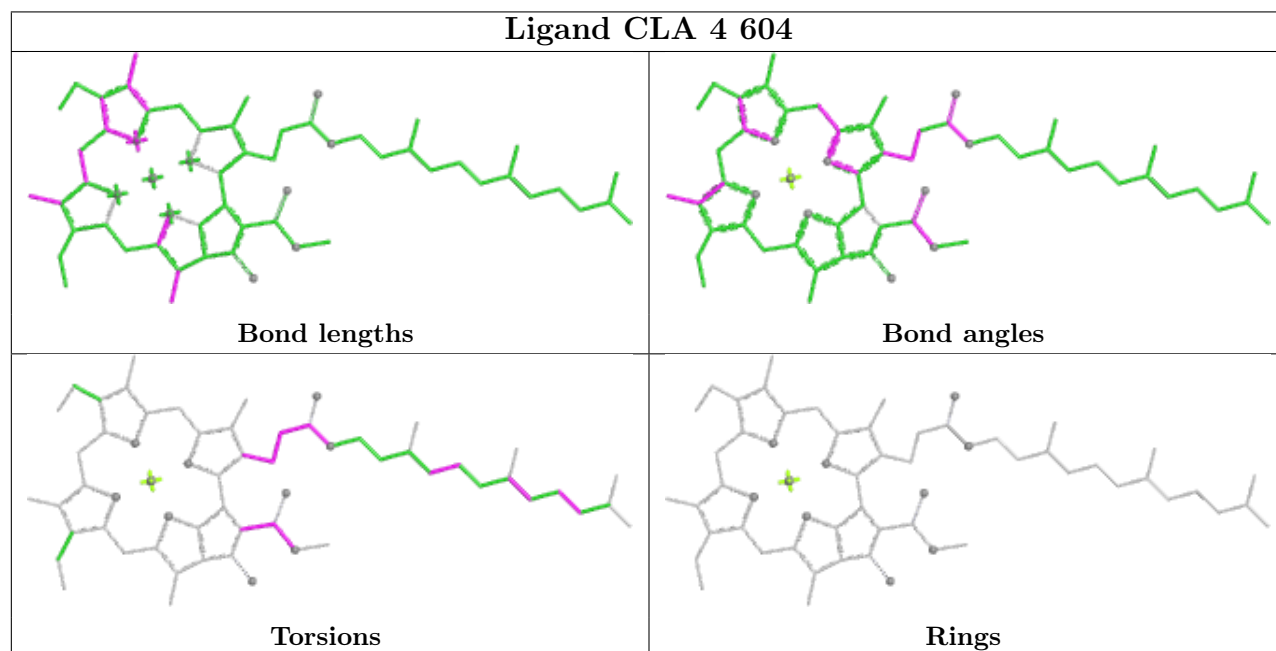
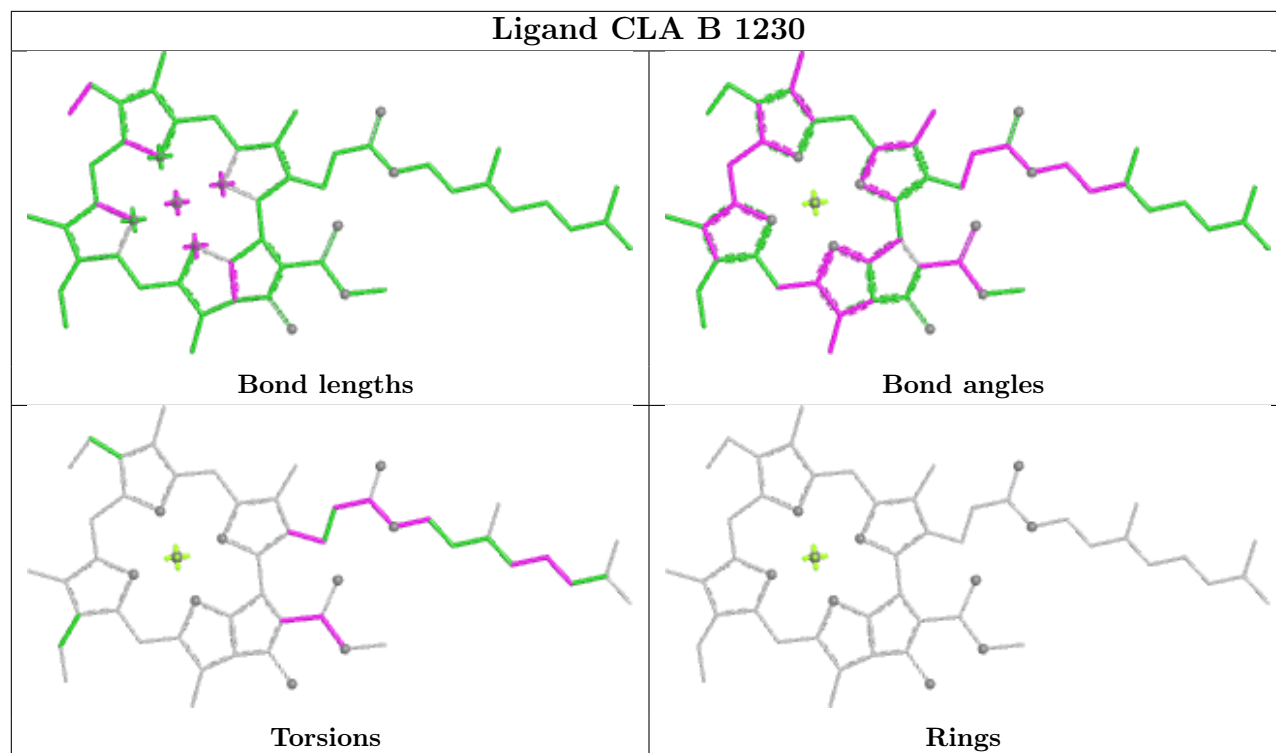


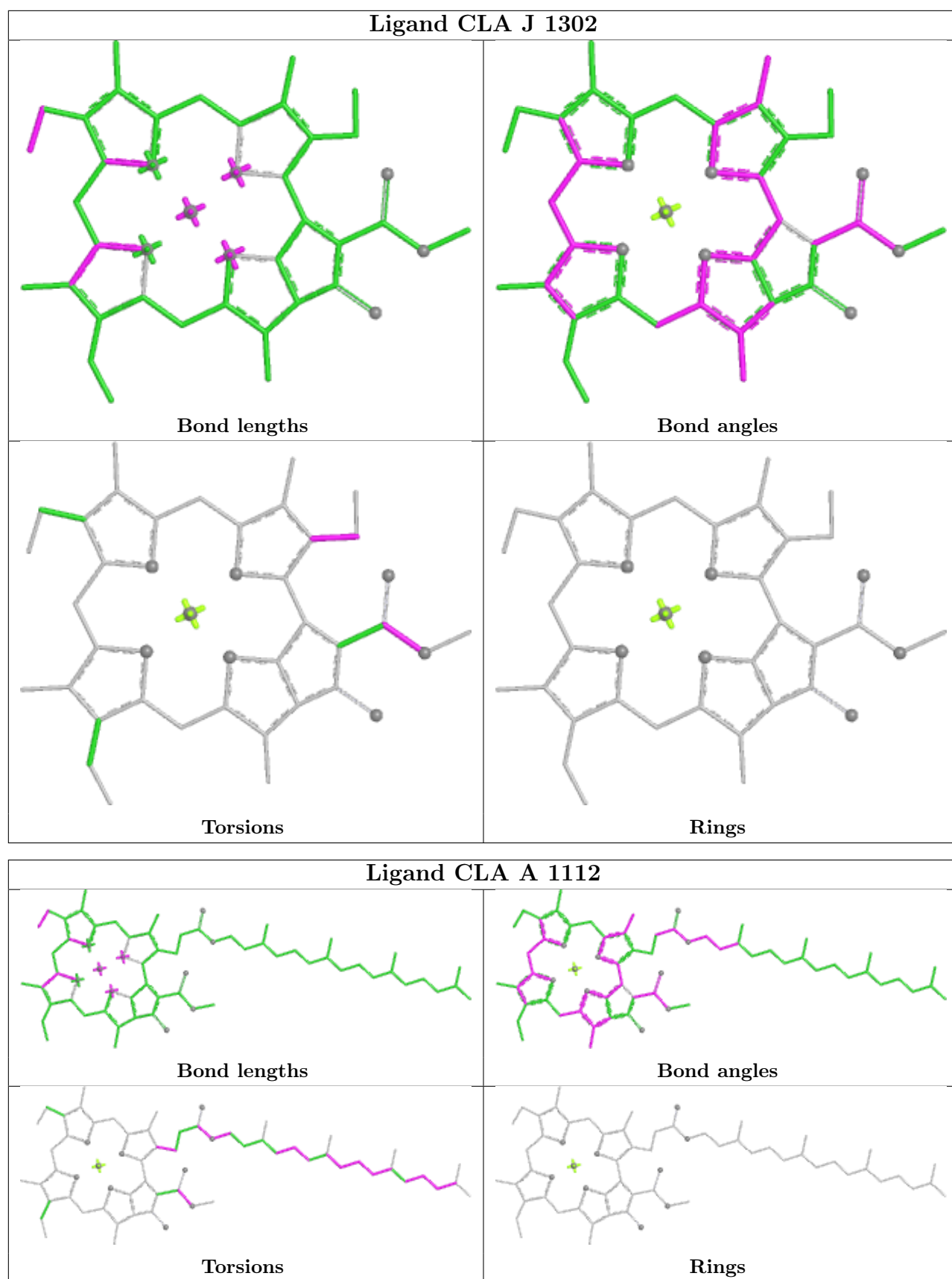
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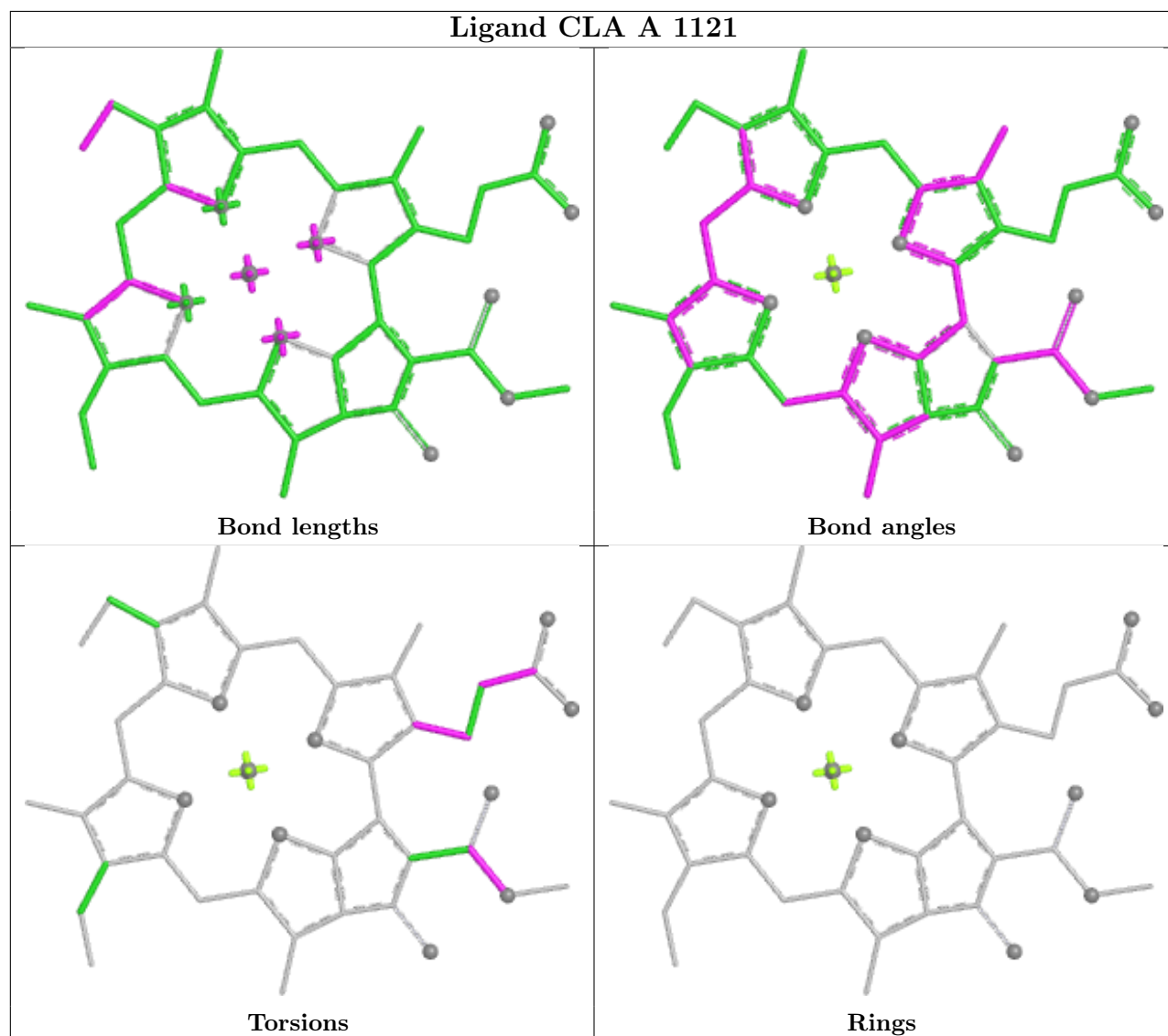
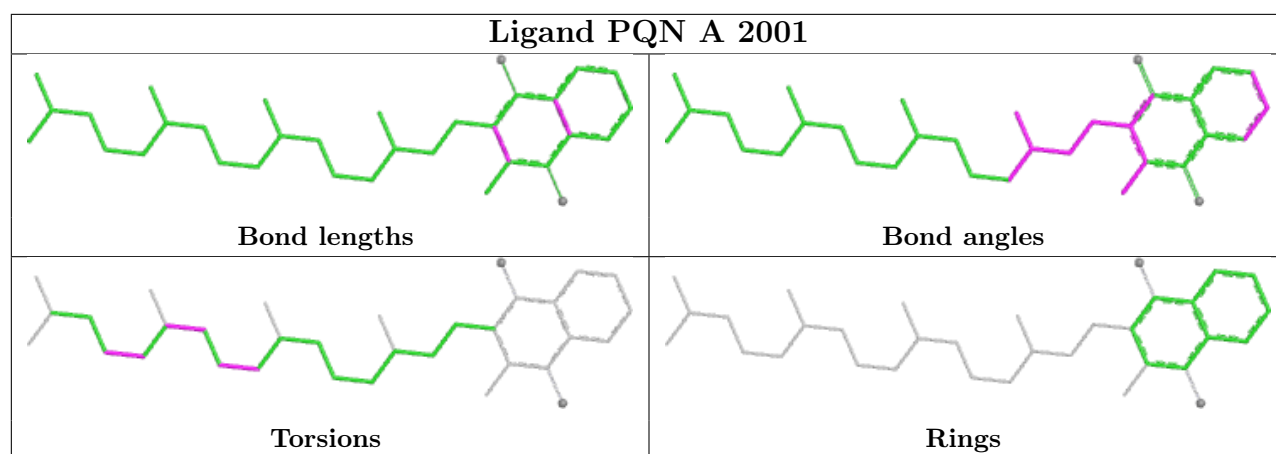


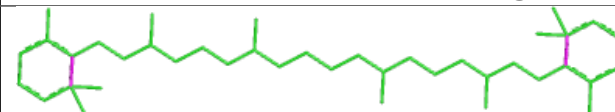
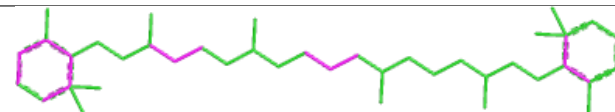
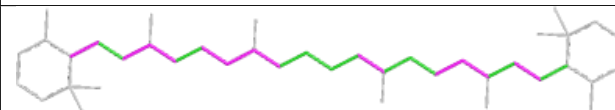
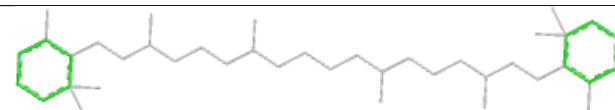
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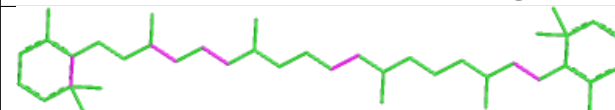
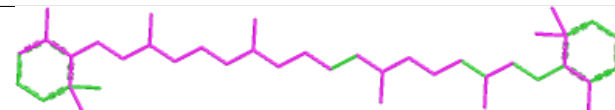
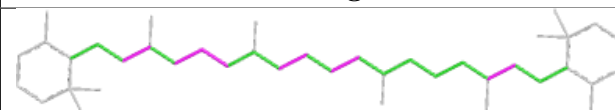
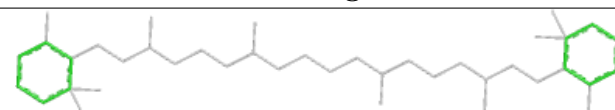


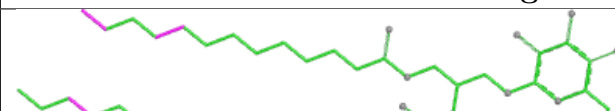
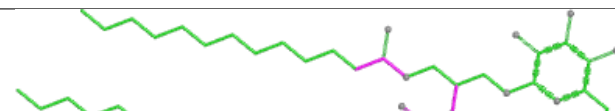
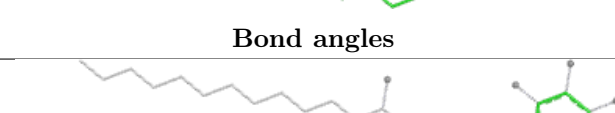


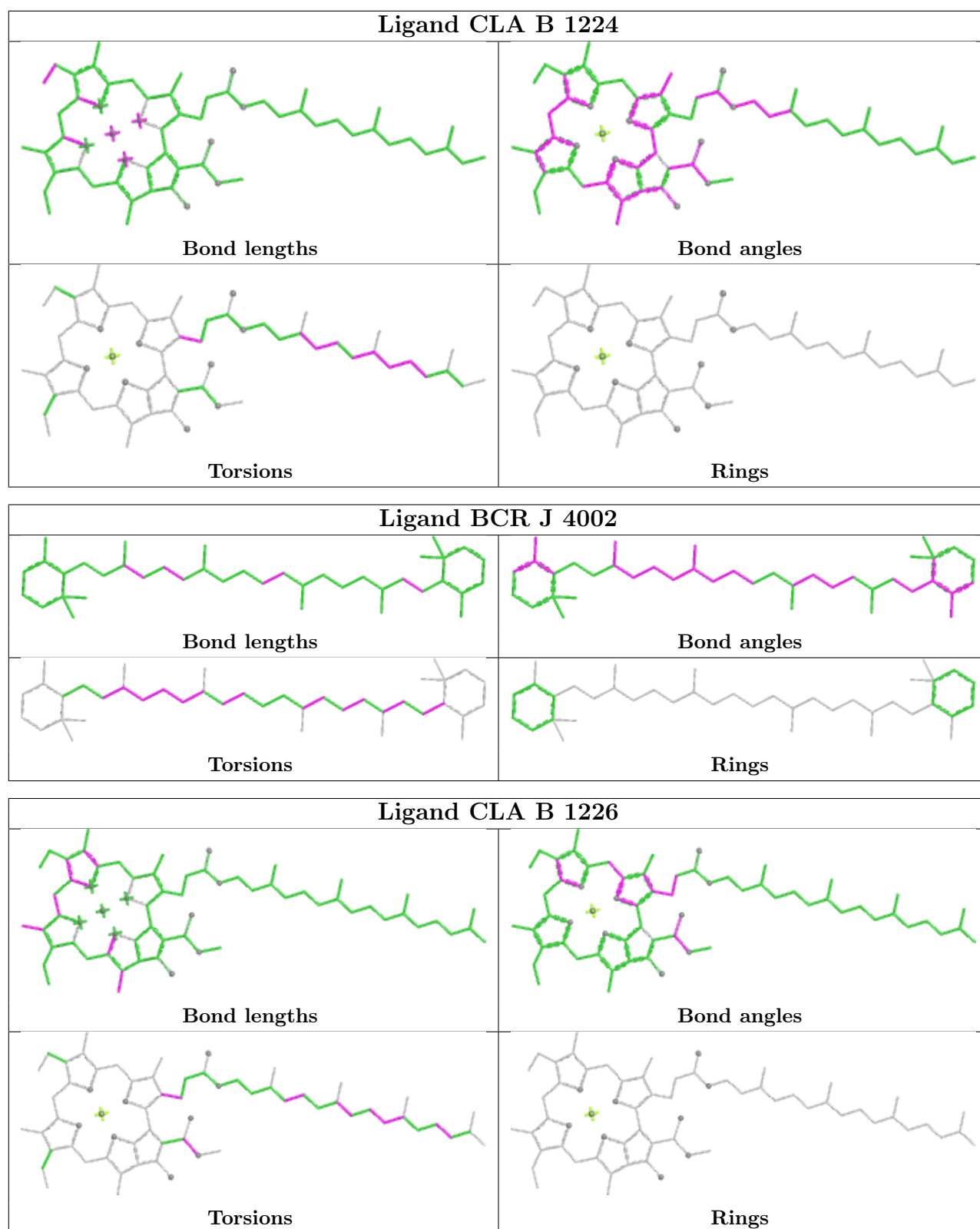


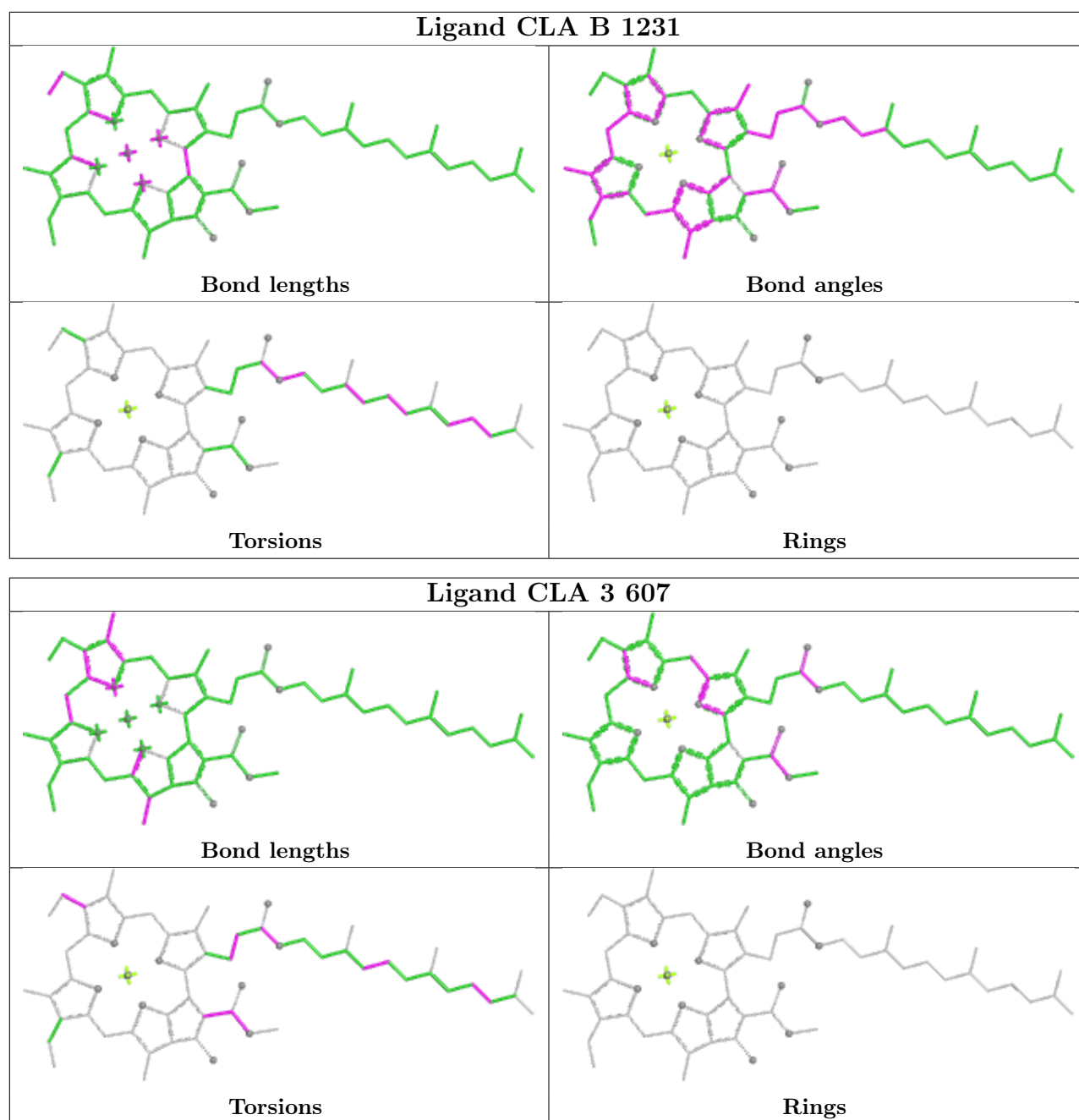


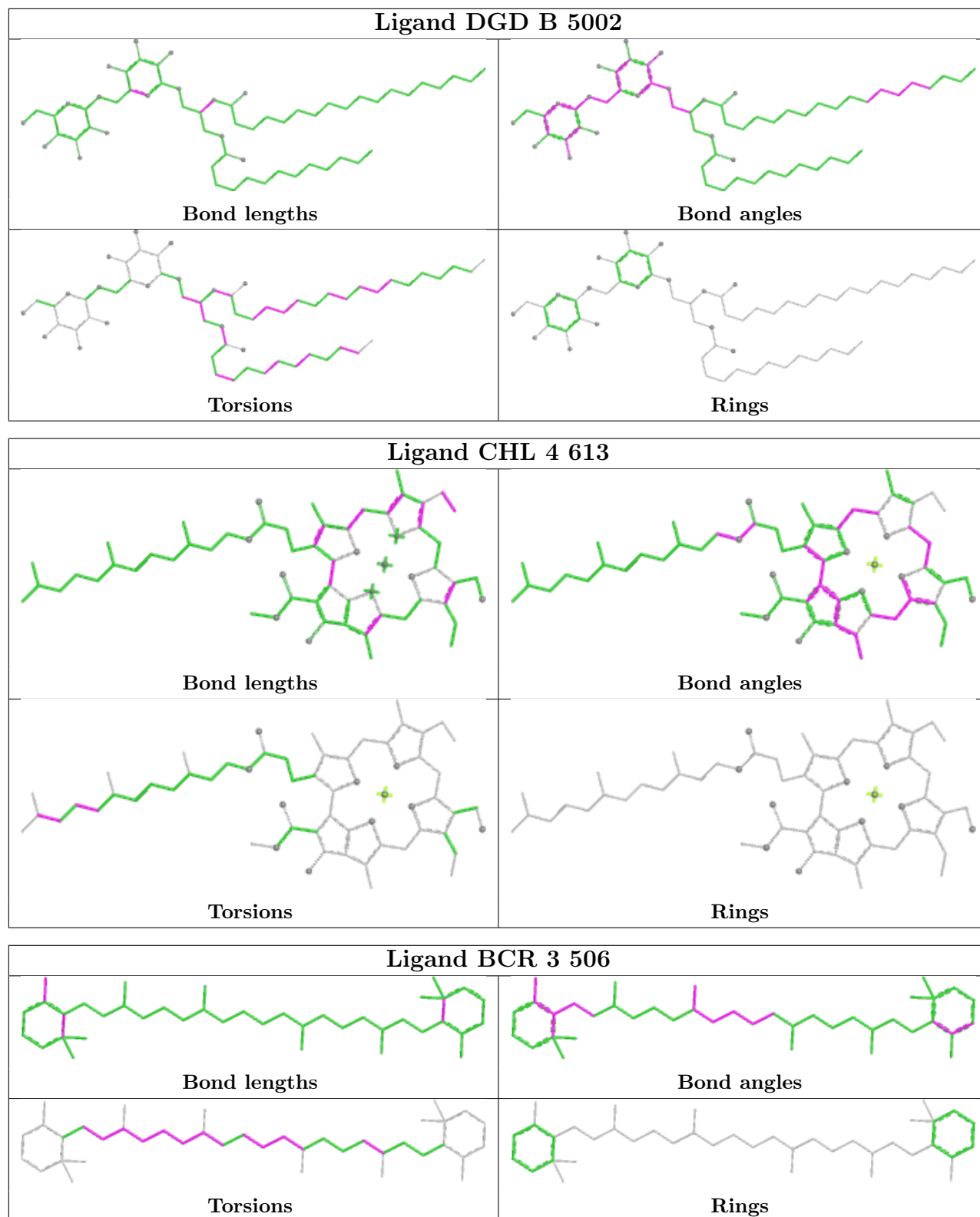
Ligand BCR B 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 4007	
	
Bond lengths	Bond angles
	
Torsions	Rings

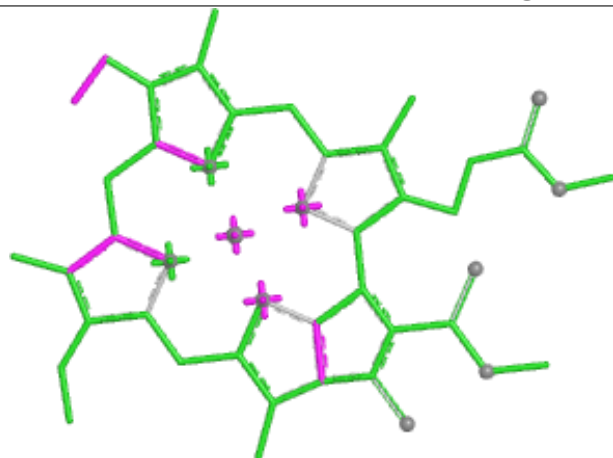
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Bond lengths	Bond angles
	
Torsions	Rings



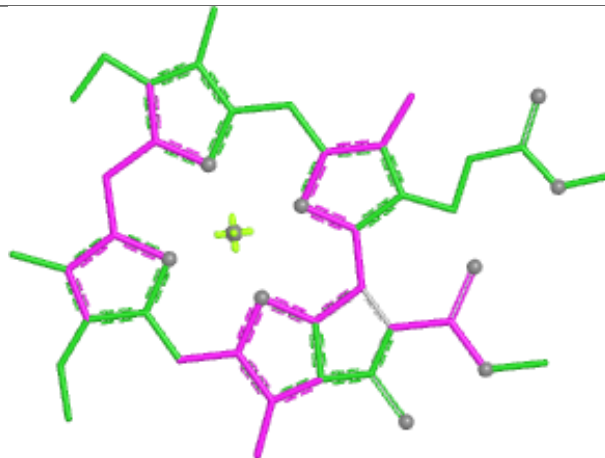




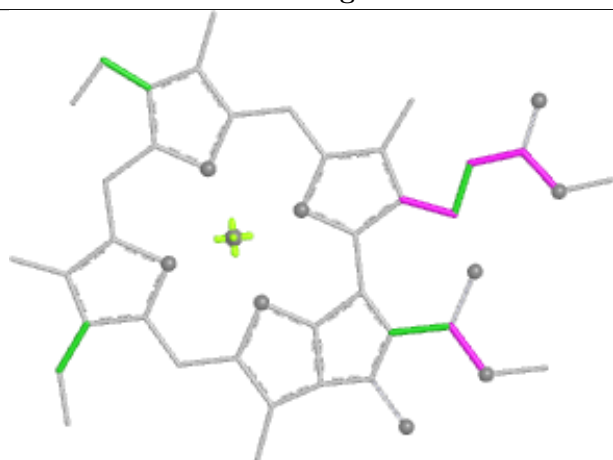
Ligand CLA 3 613



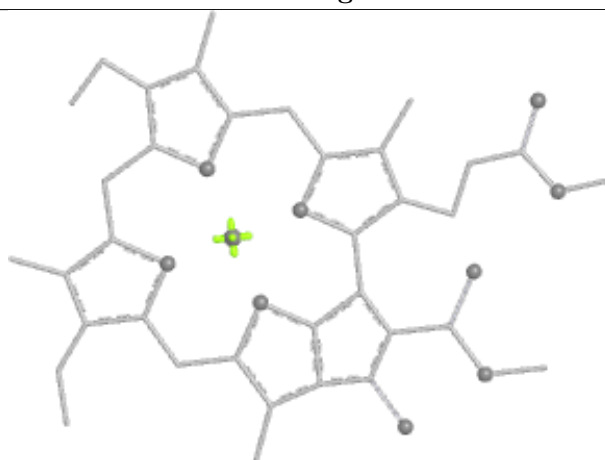
Bond lengths



Bond angles

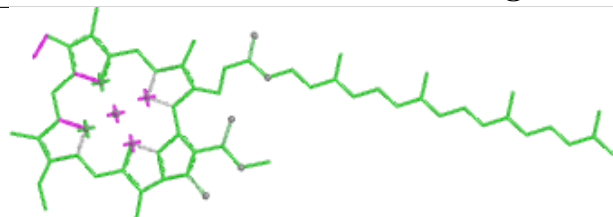


Torsions

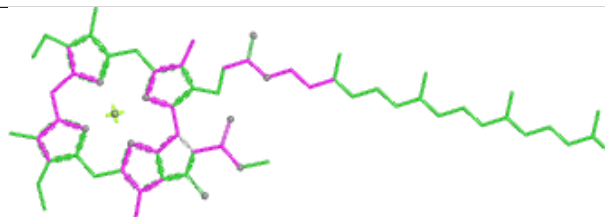


Rings

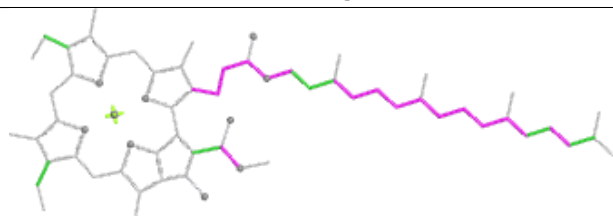
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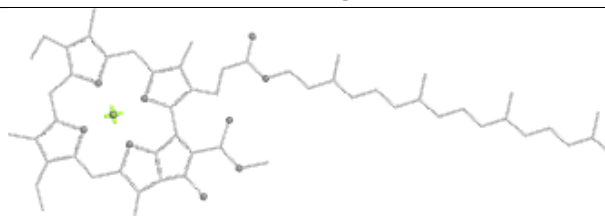
Bond lengths



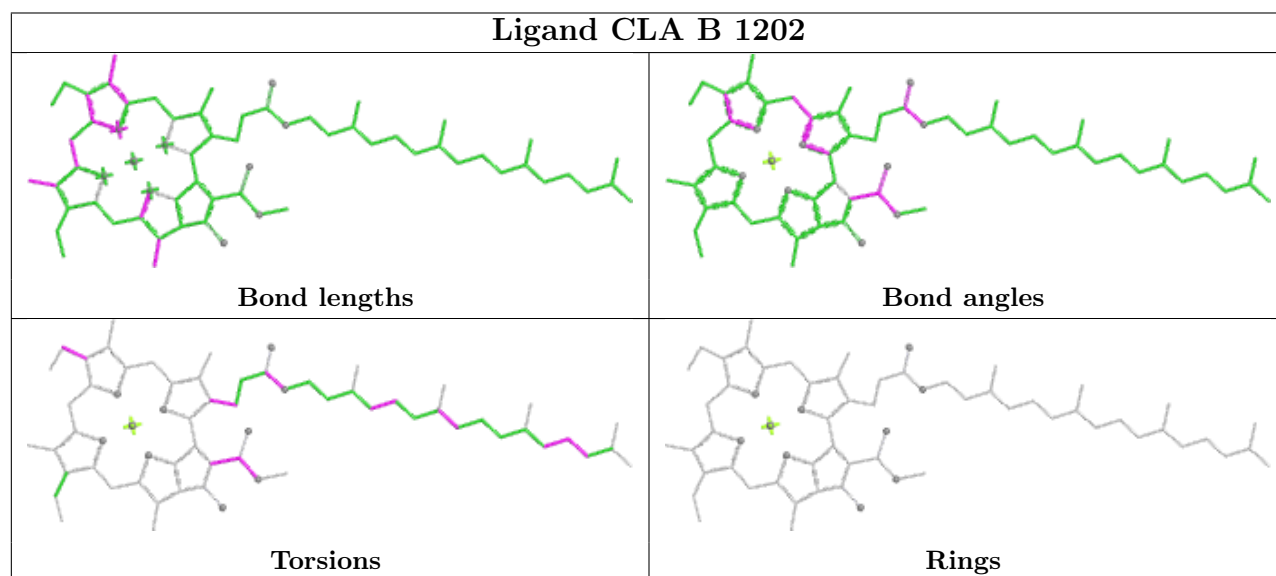
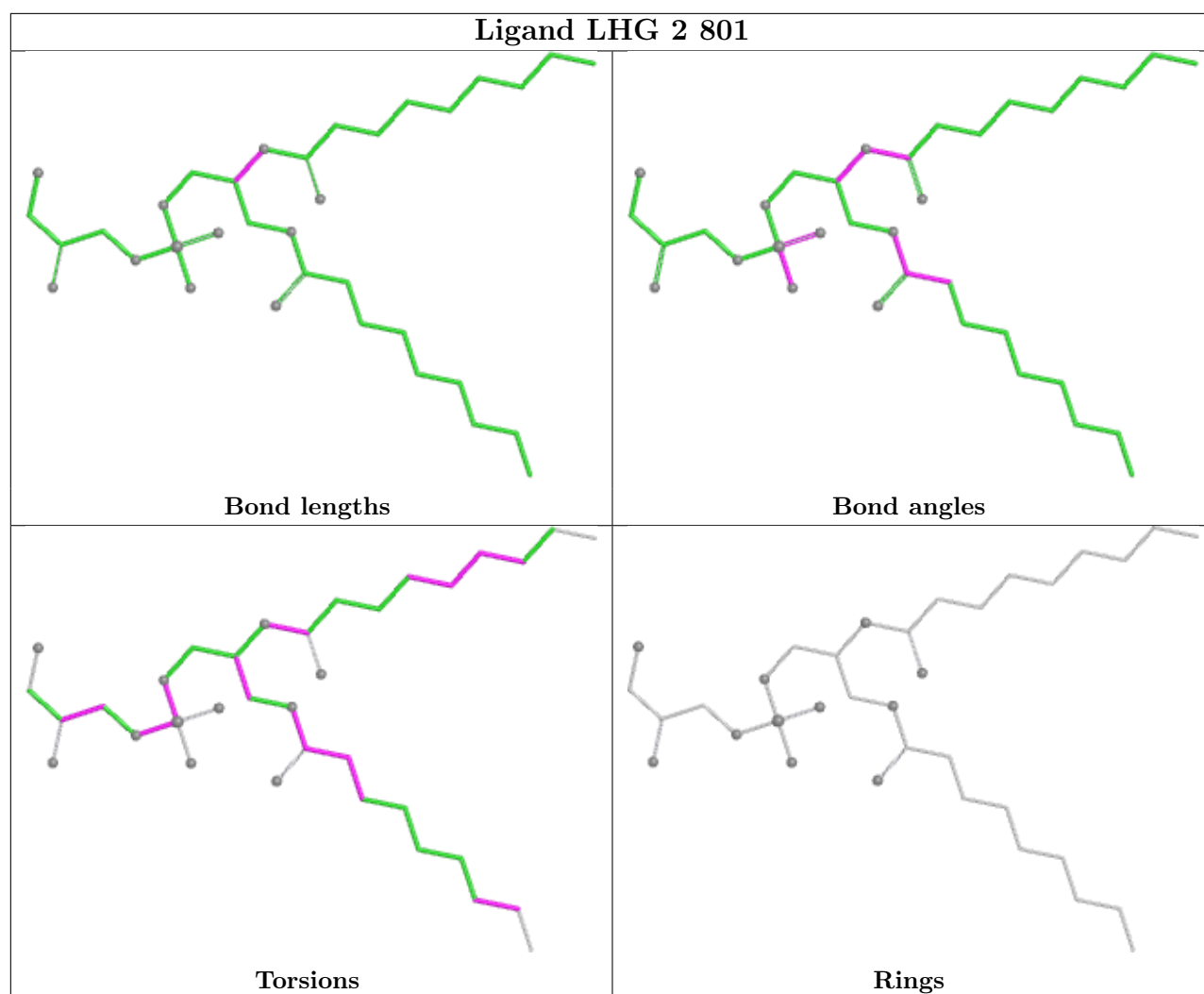
Bond angles

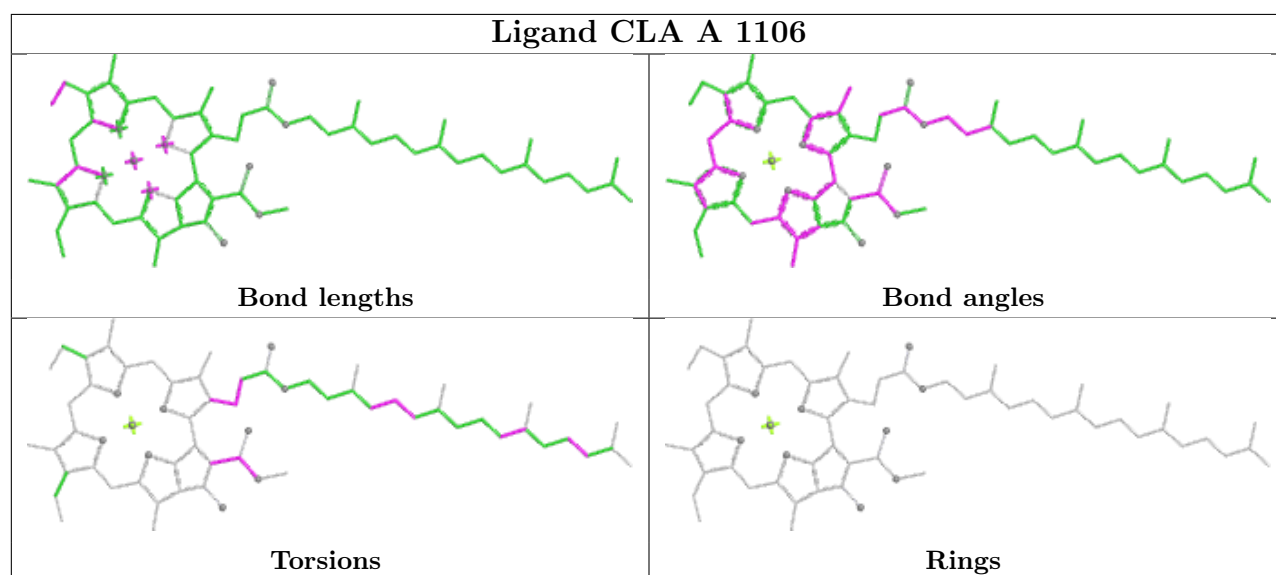
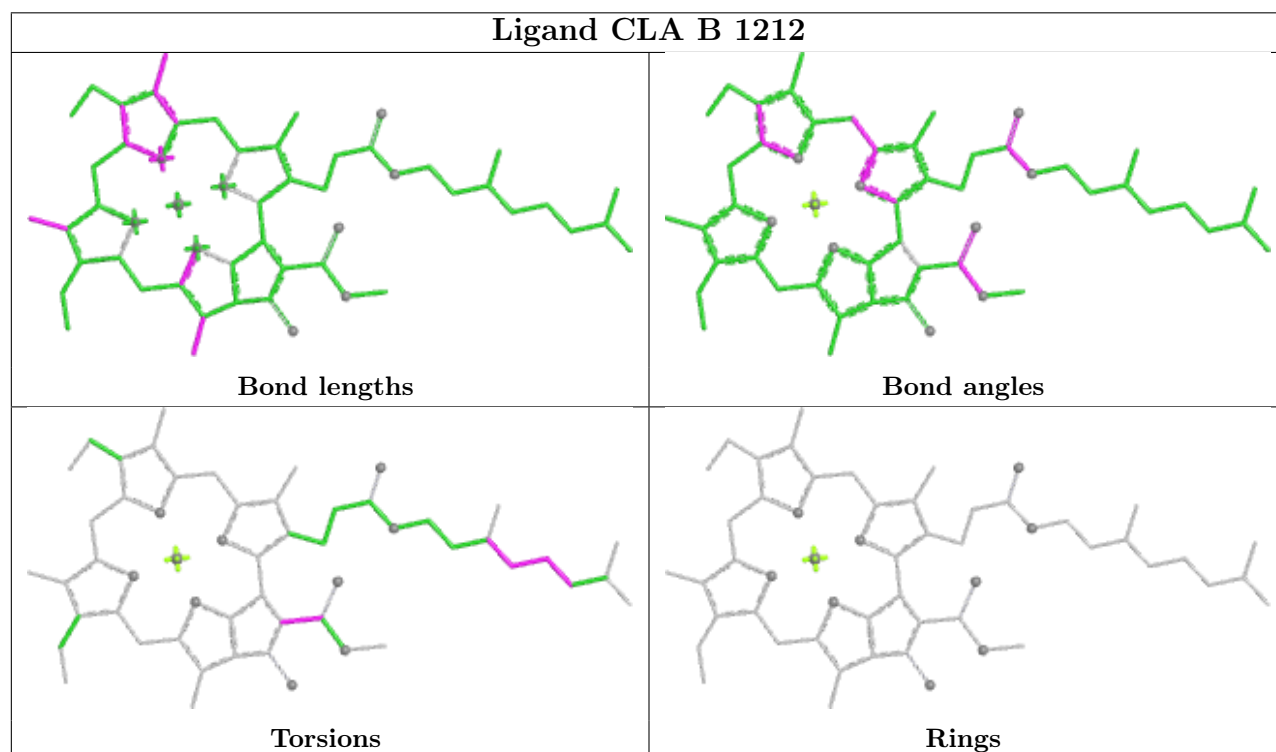
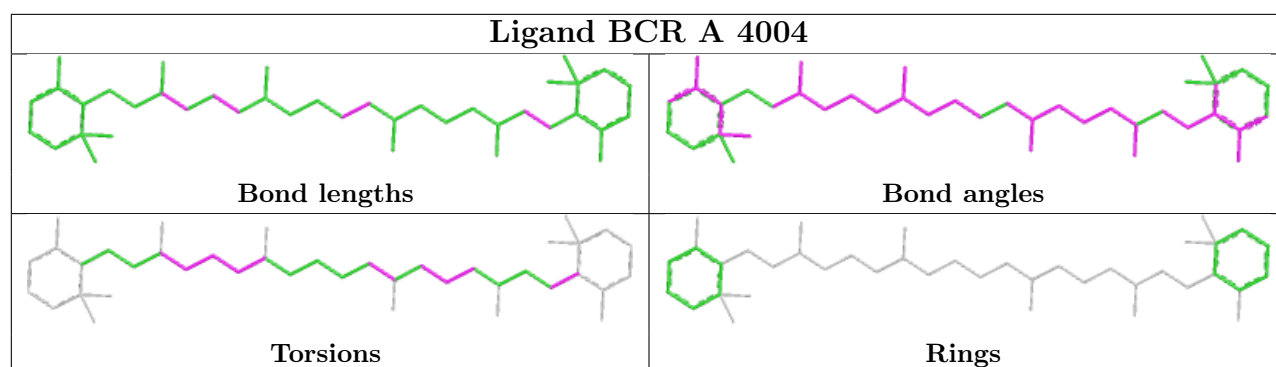


Torsions

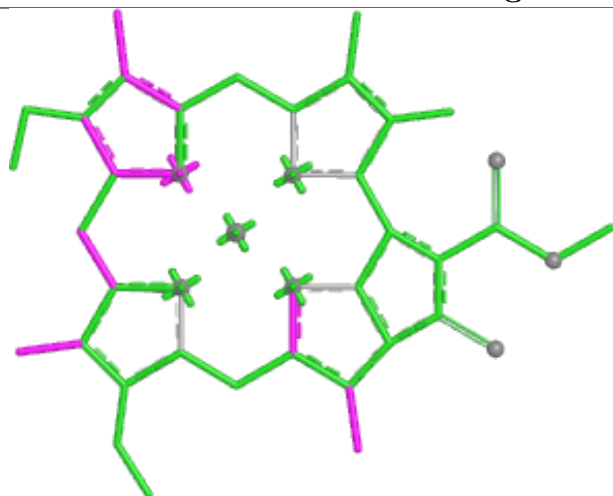


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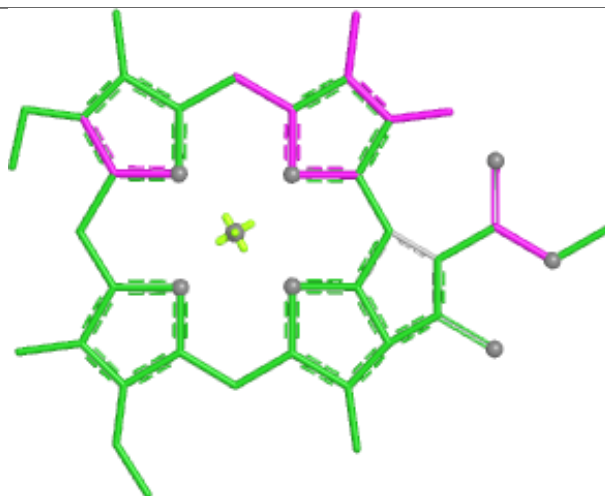




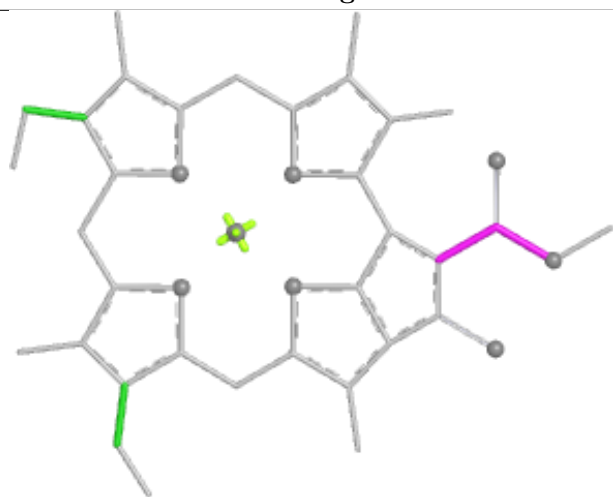
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Bond lengths



Bond angles

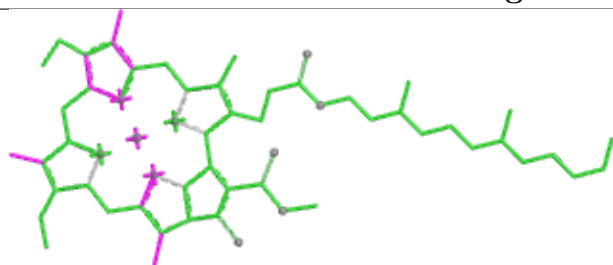


Torsions

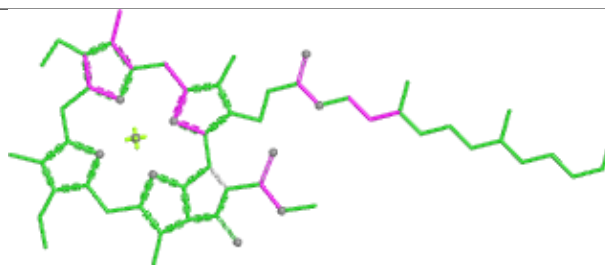


Rings

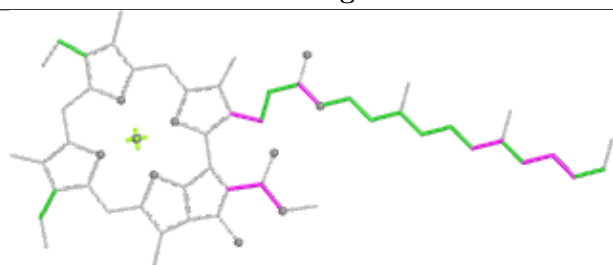
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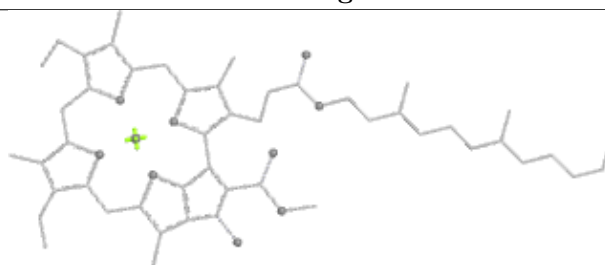
Bond lengths



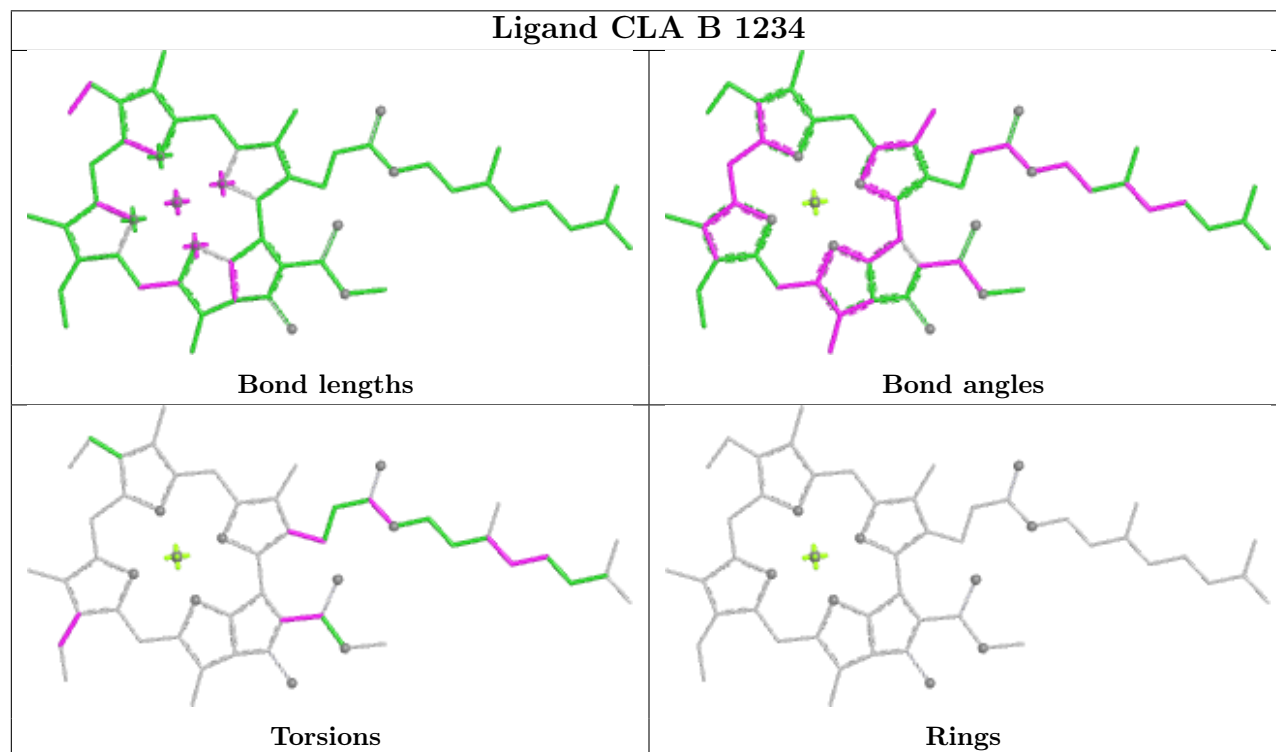
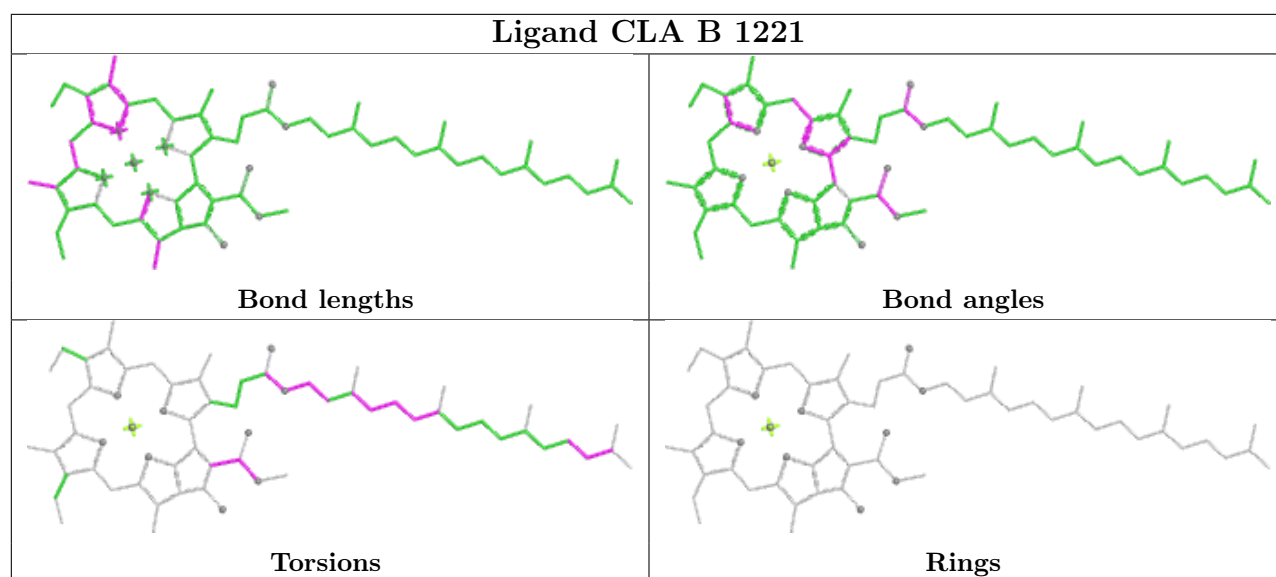
Bond angles

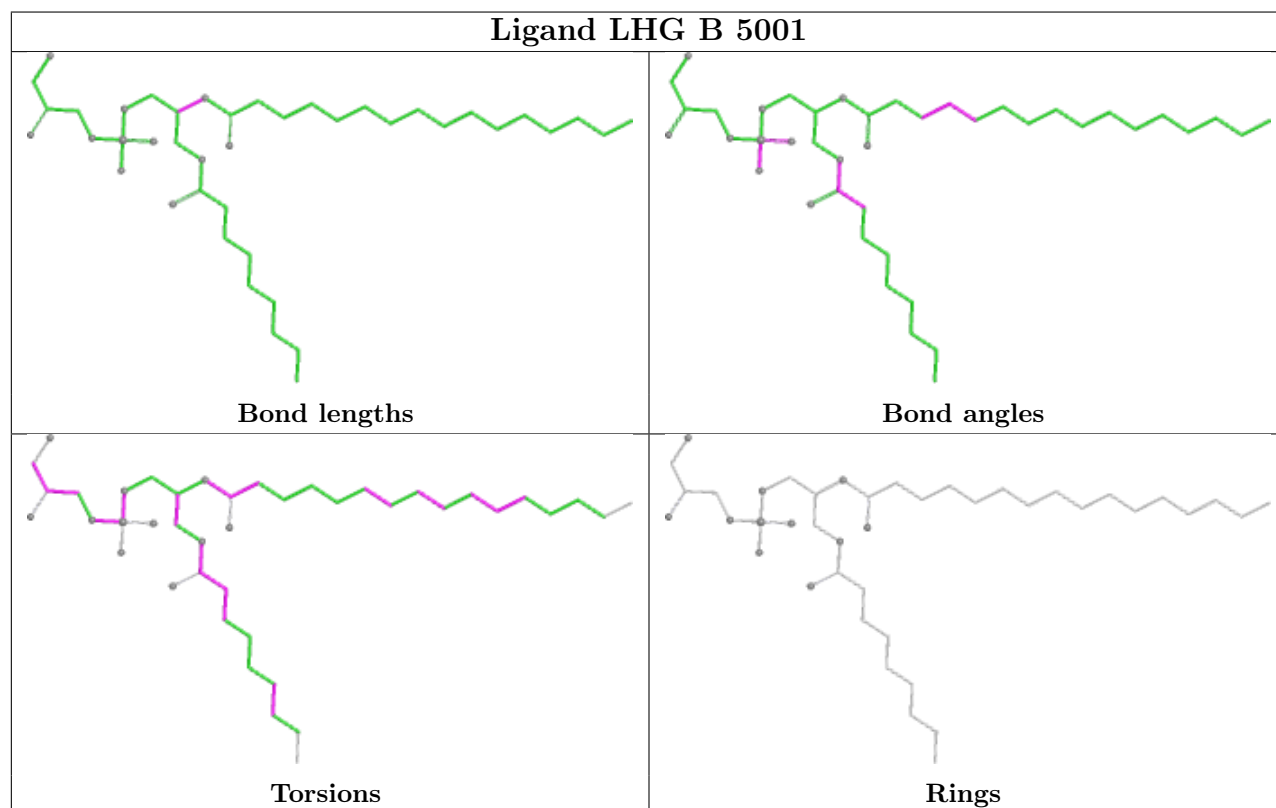
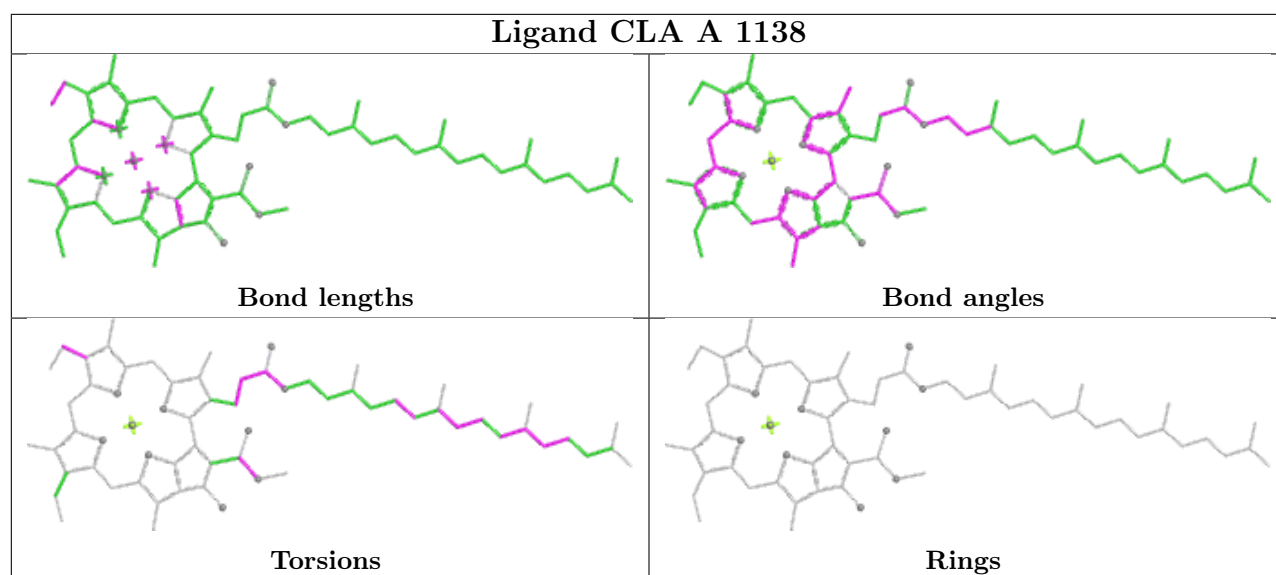


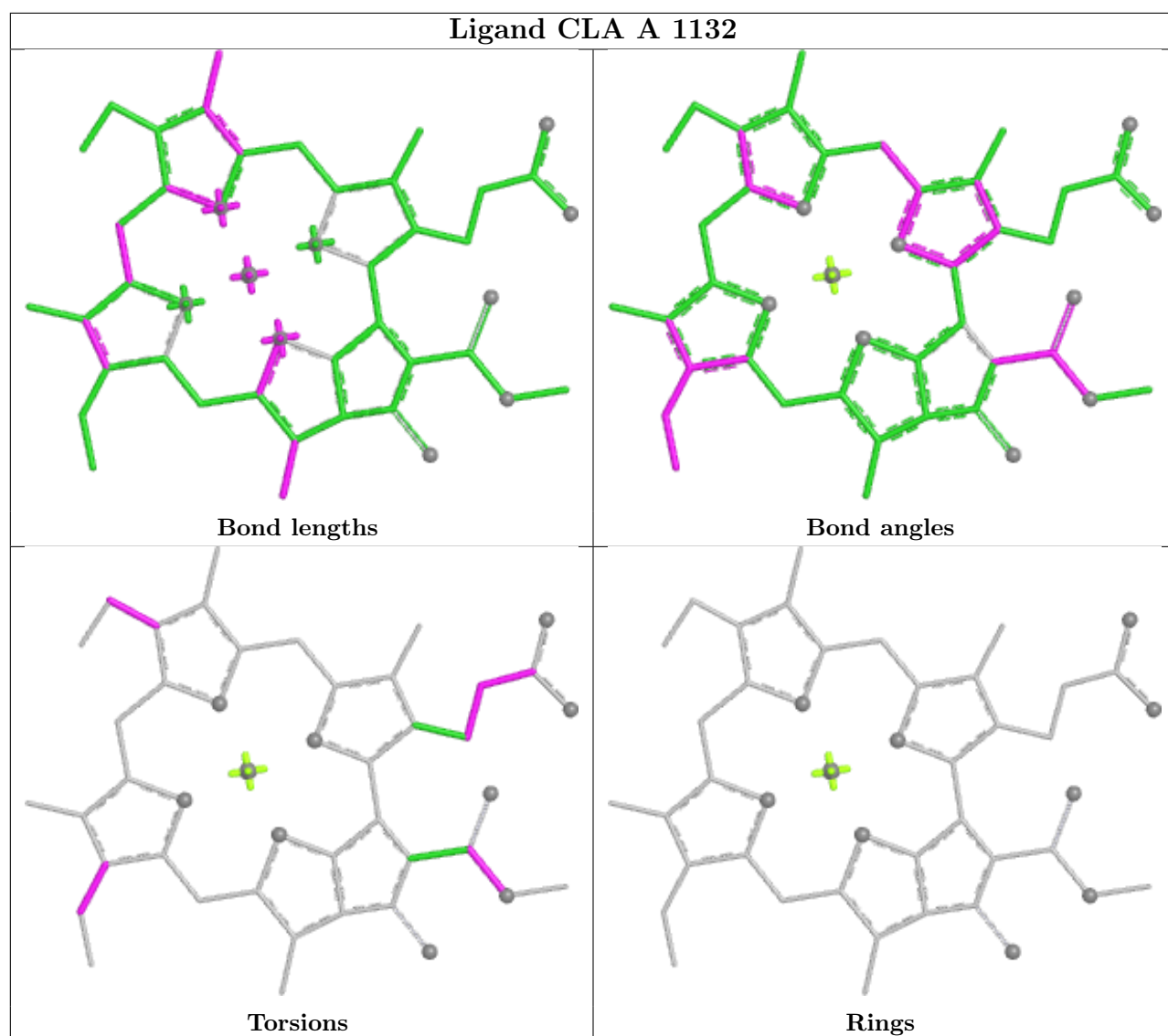
Torsions



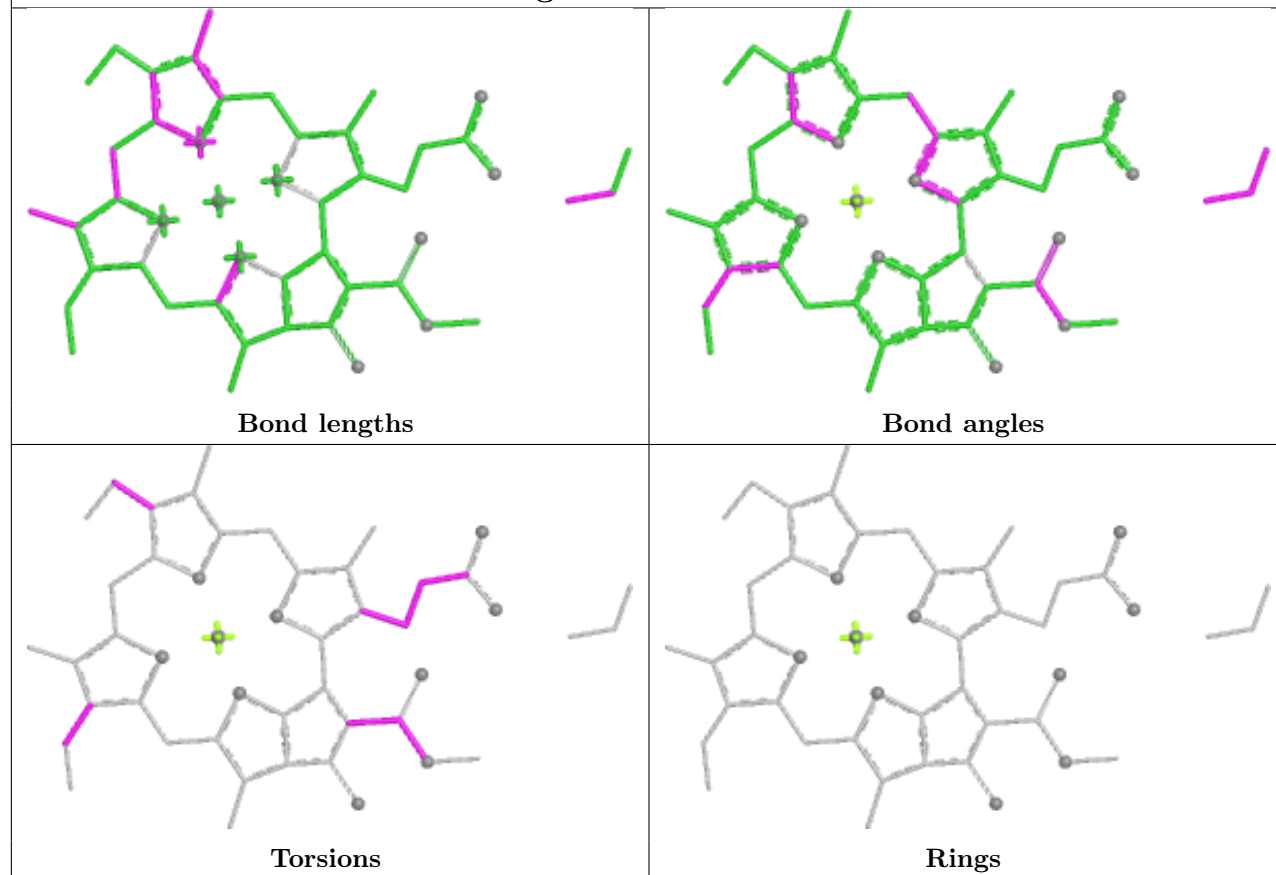
Rings



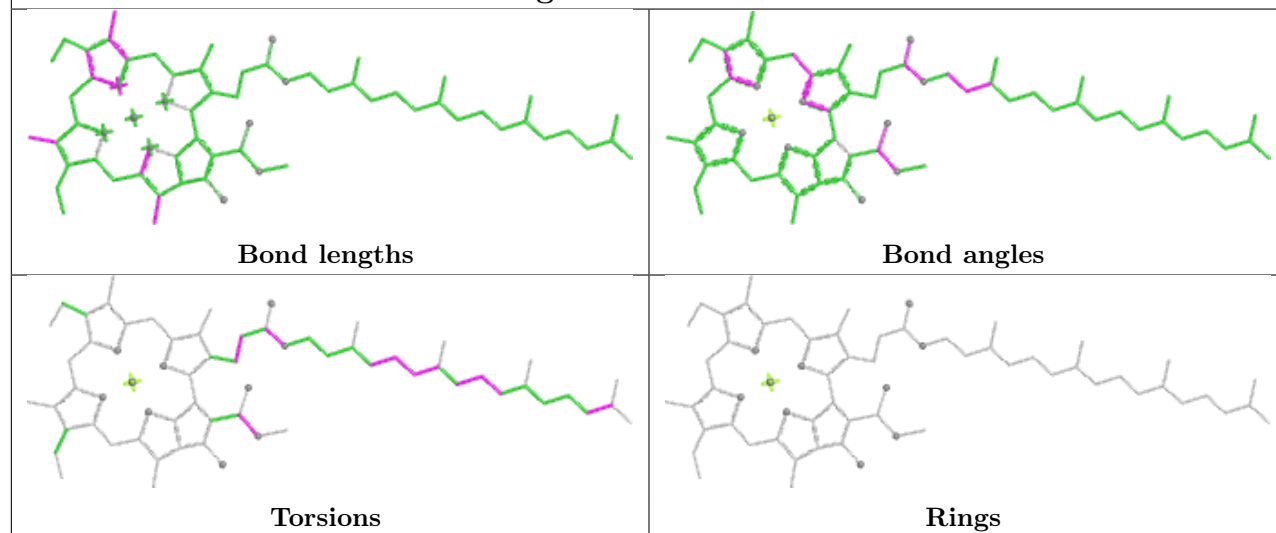


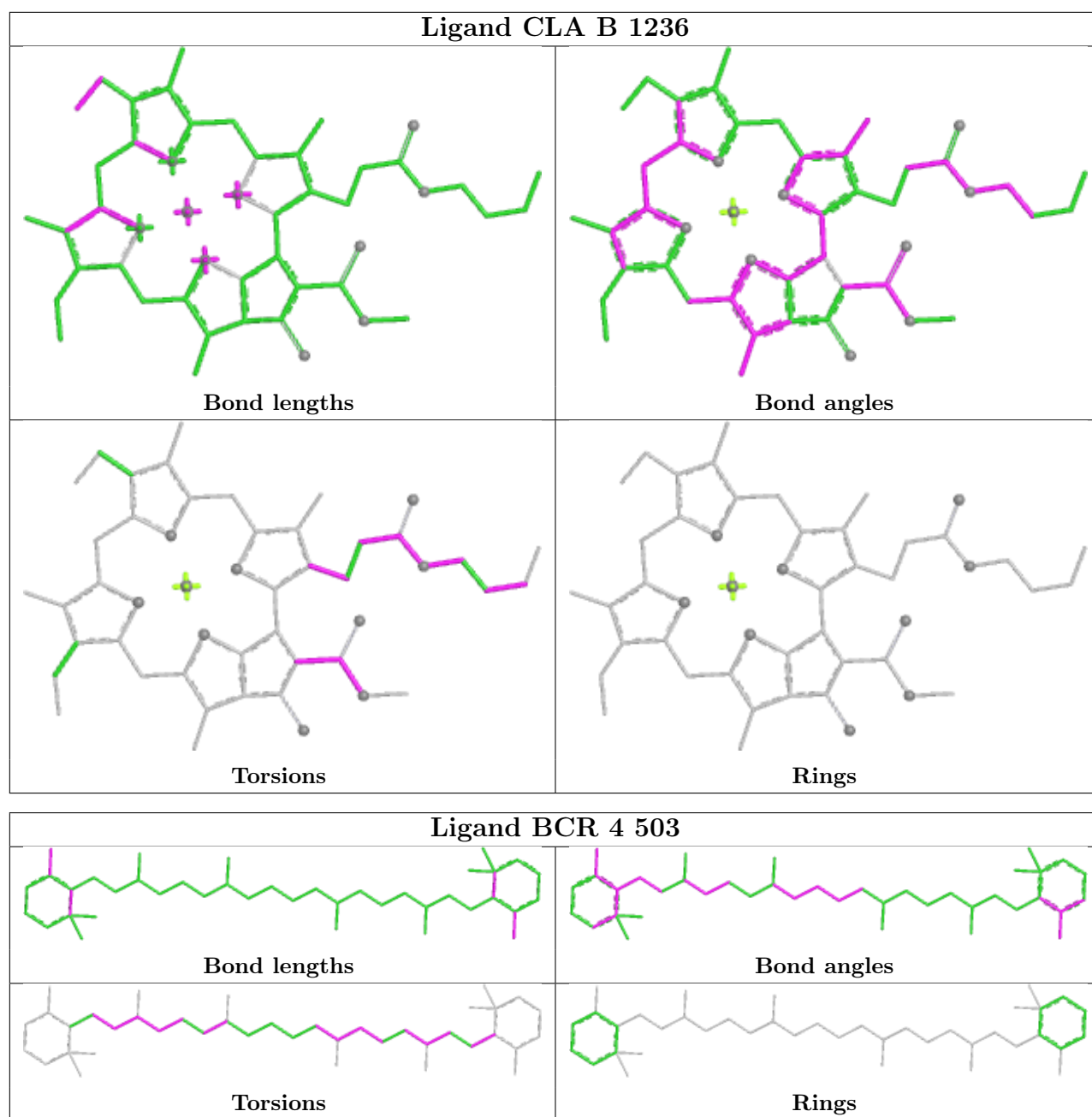


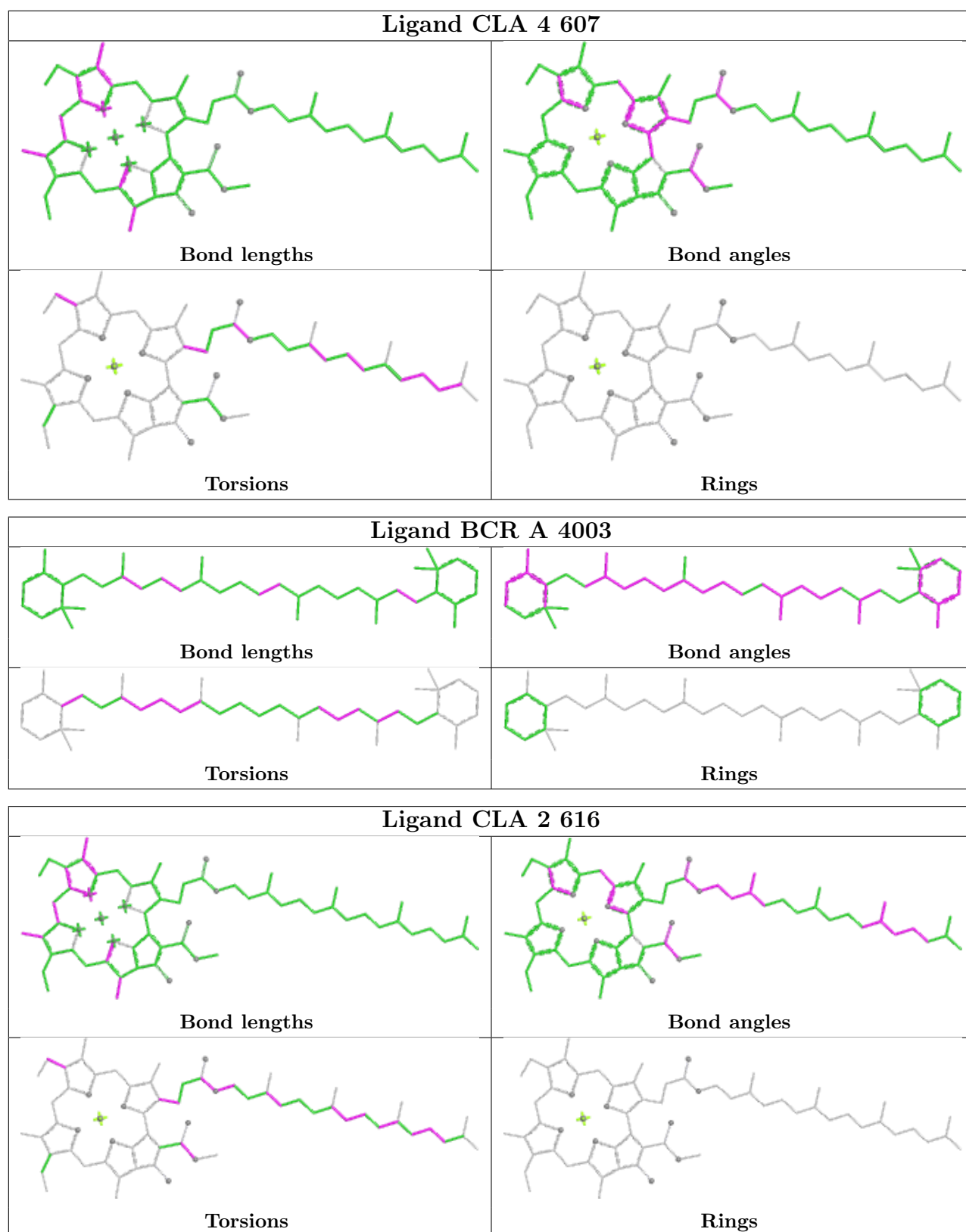
Ligand CLA 1 615

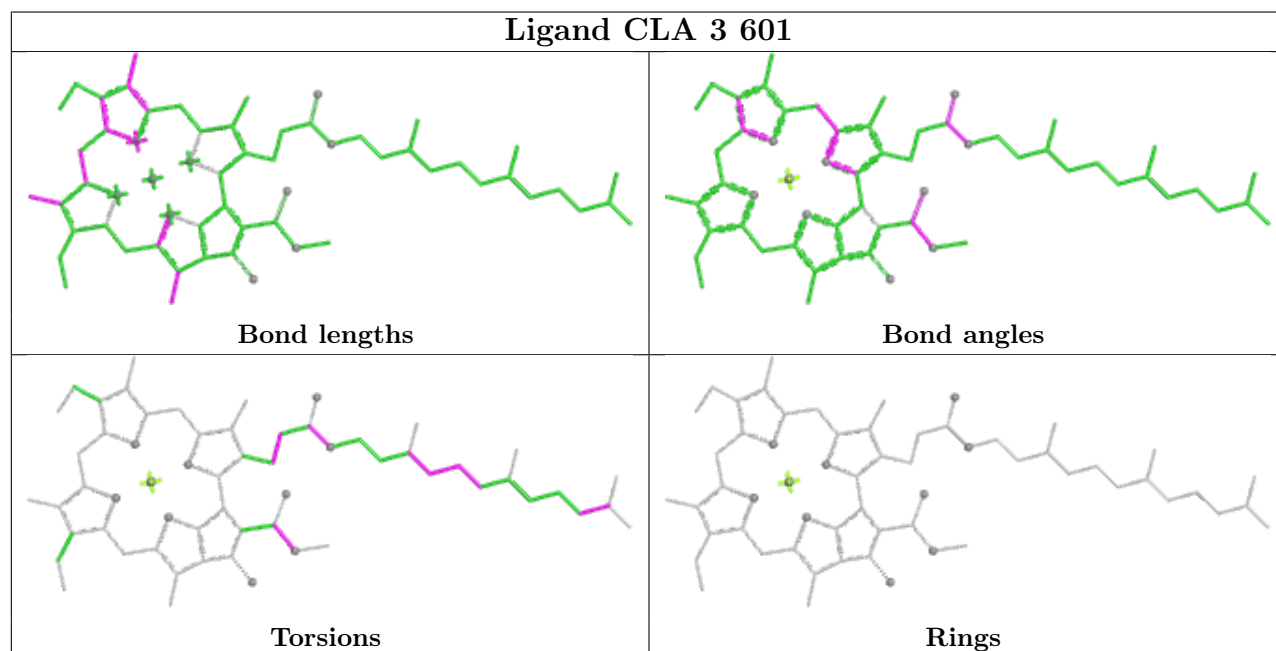
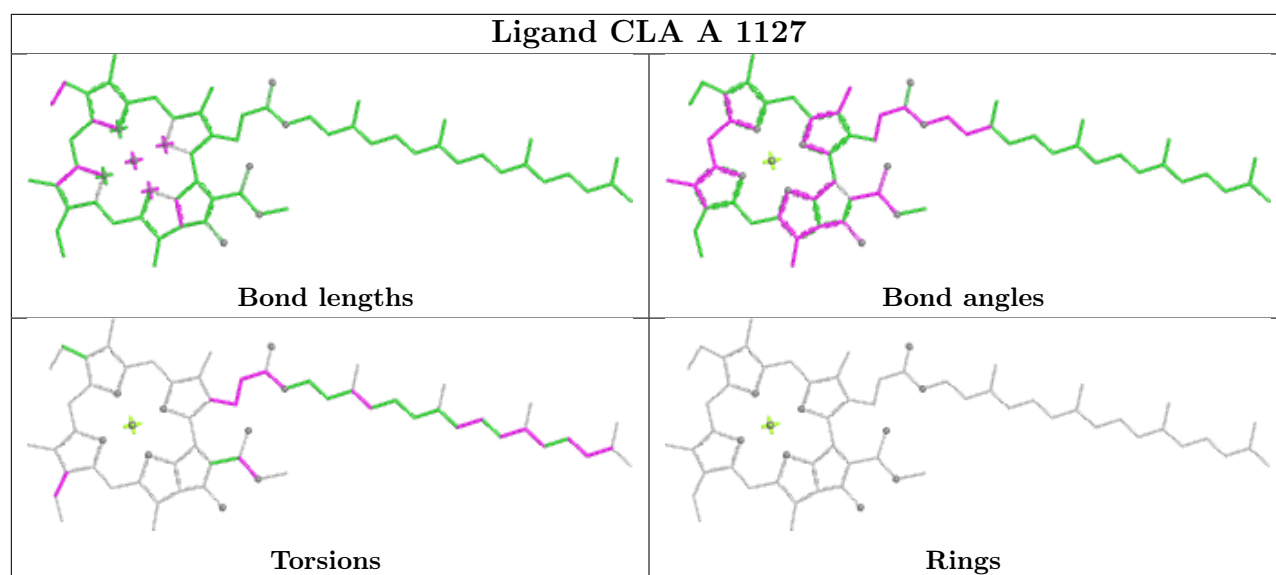


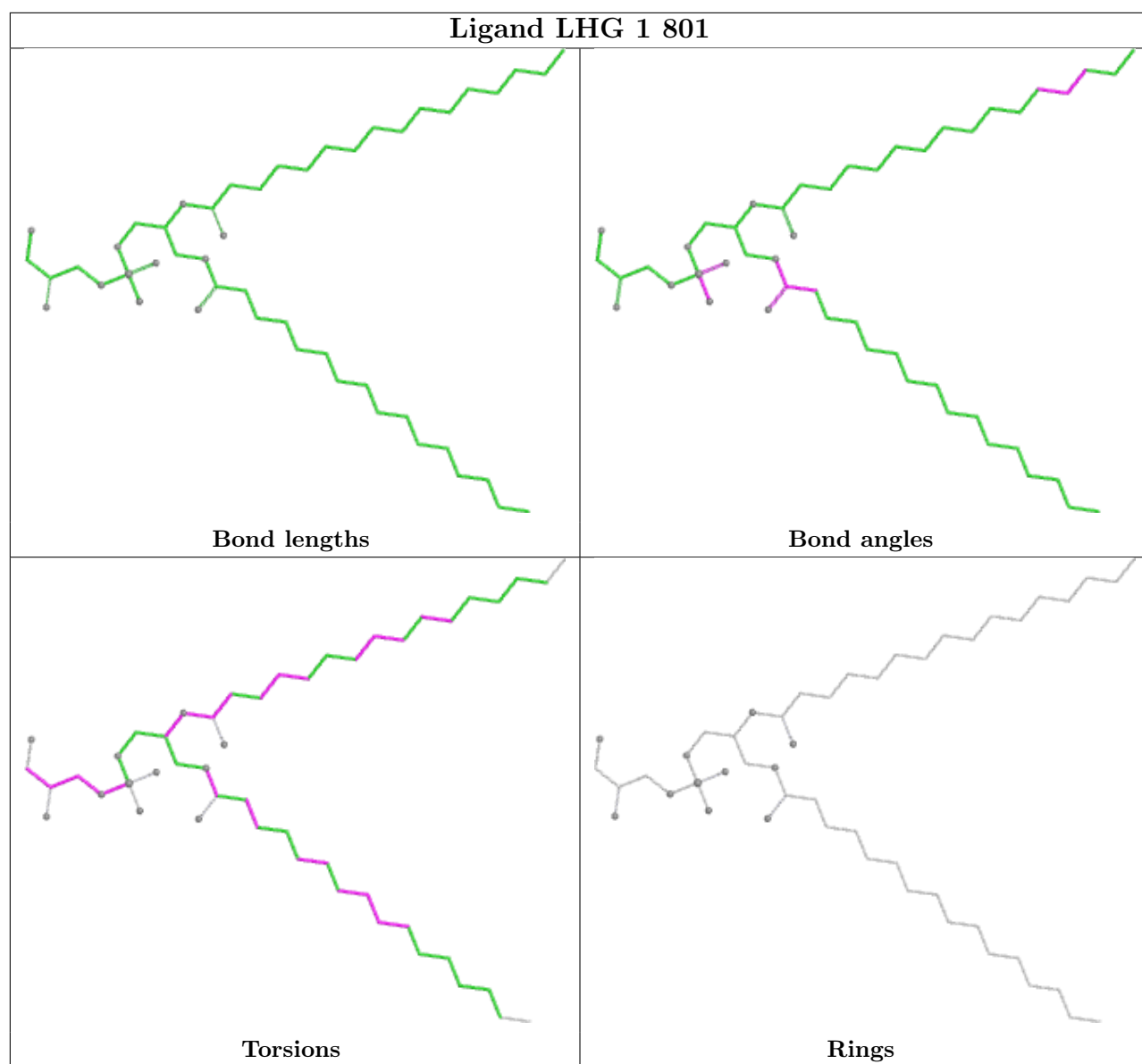
Ligand CLA 2 605

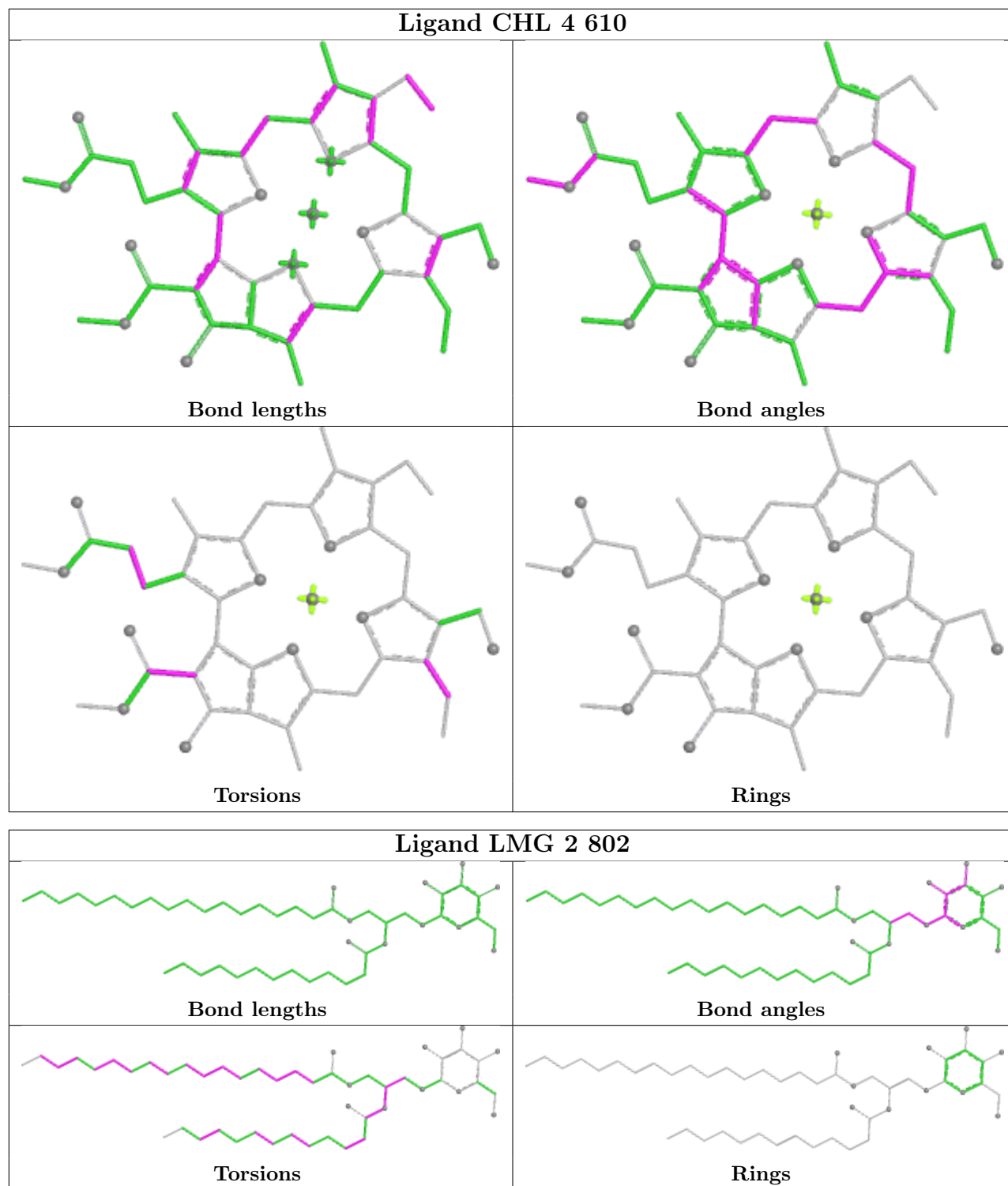




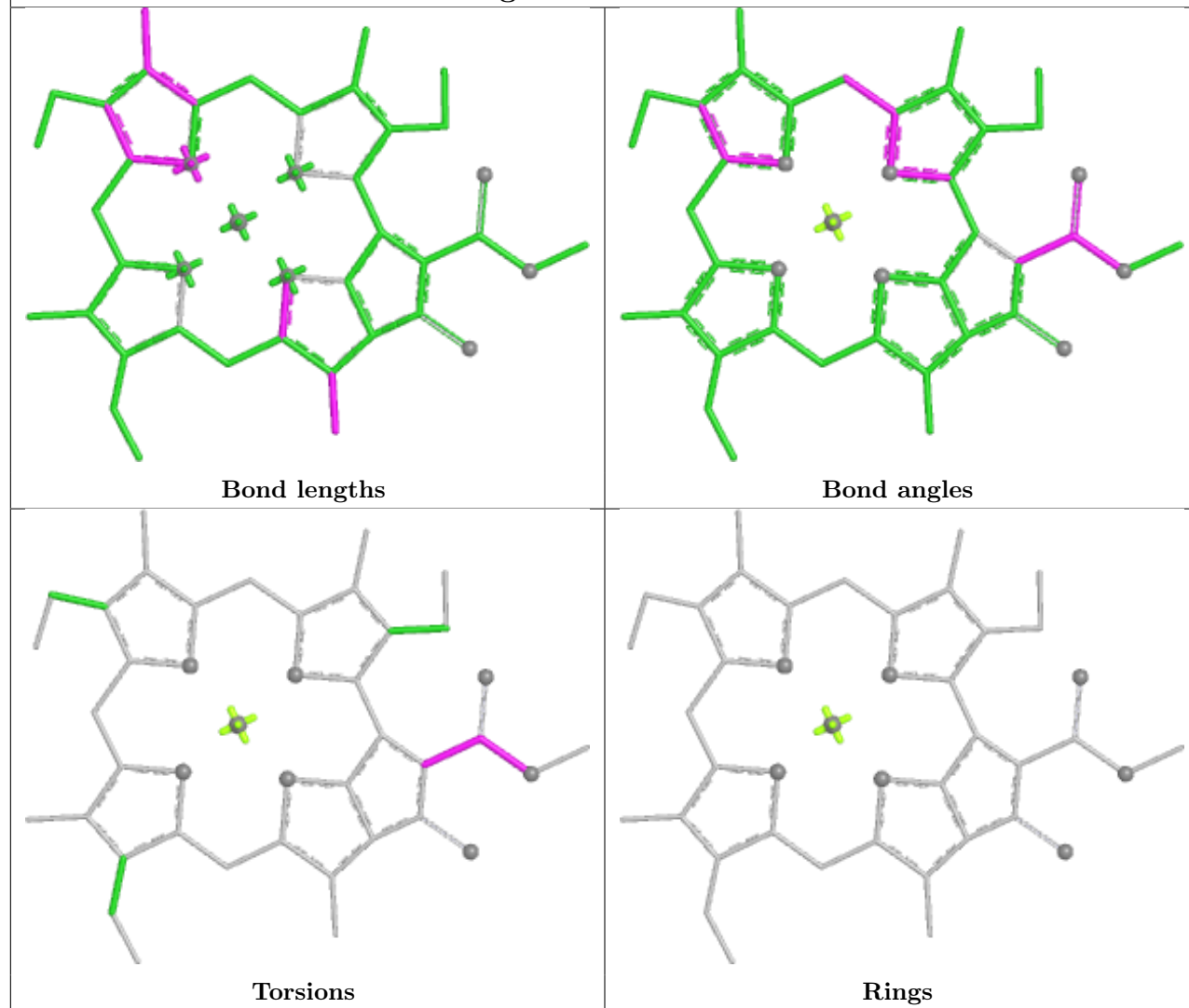




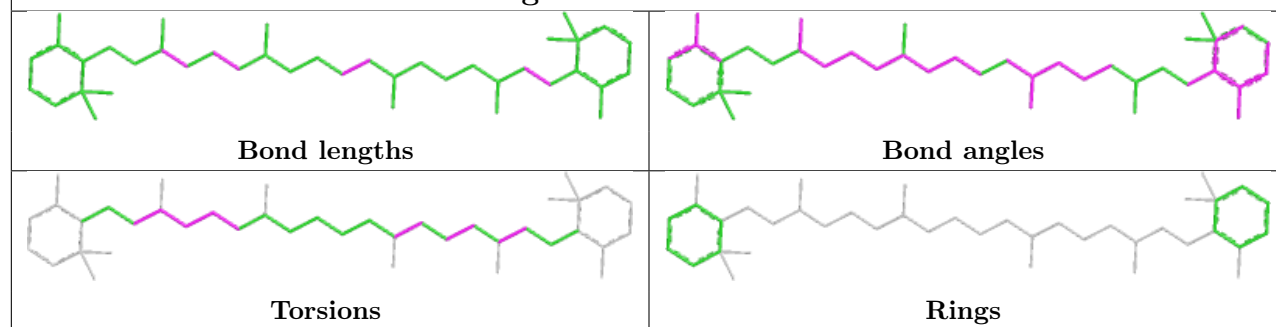


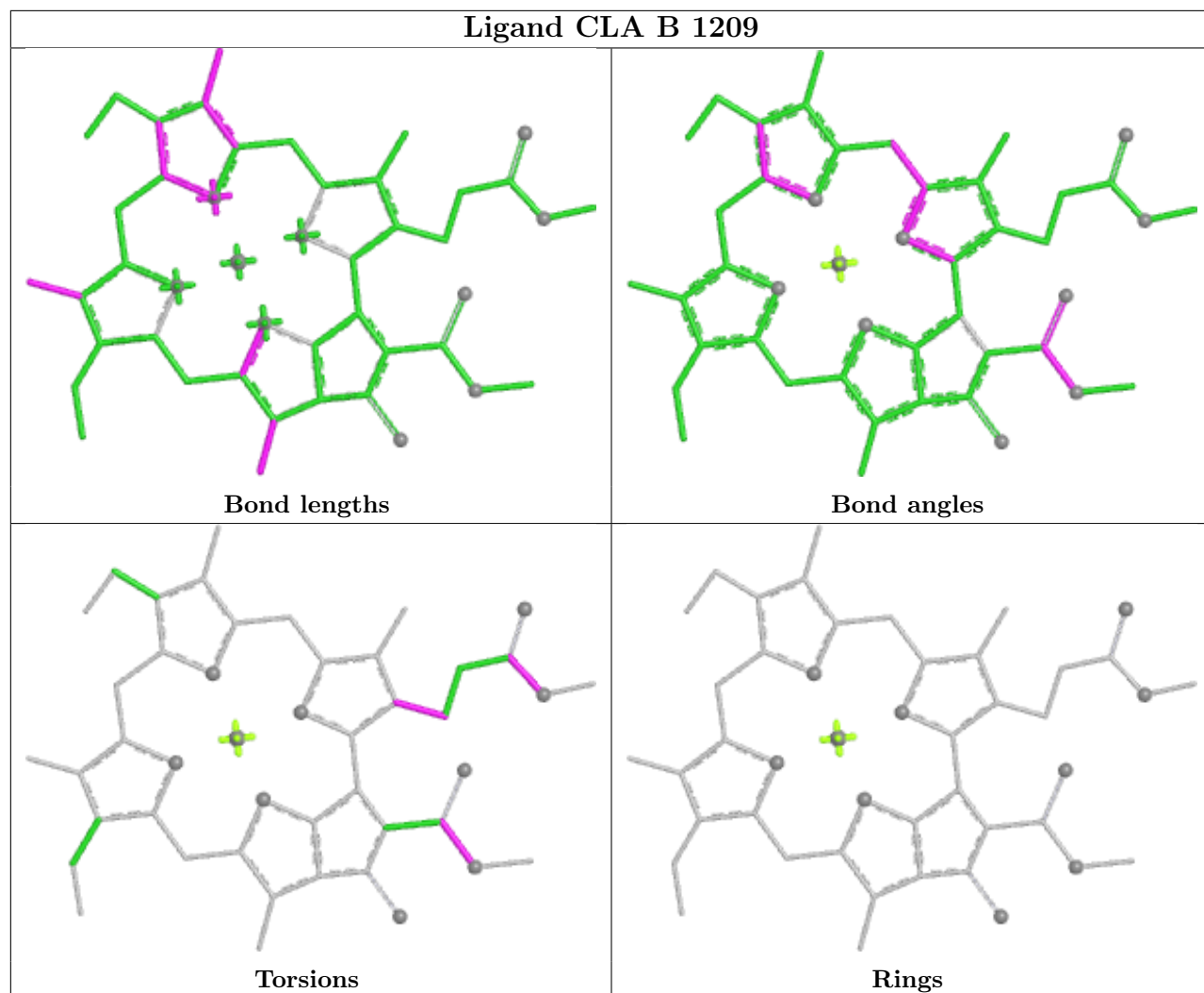


Ligand CLA 3 609

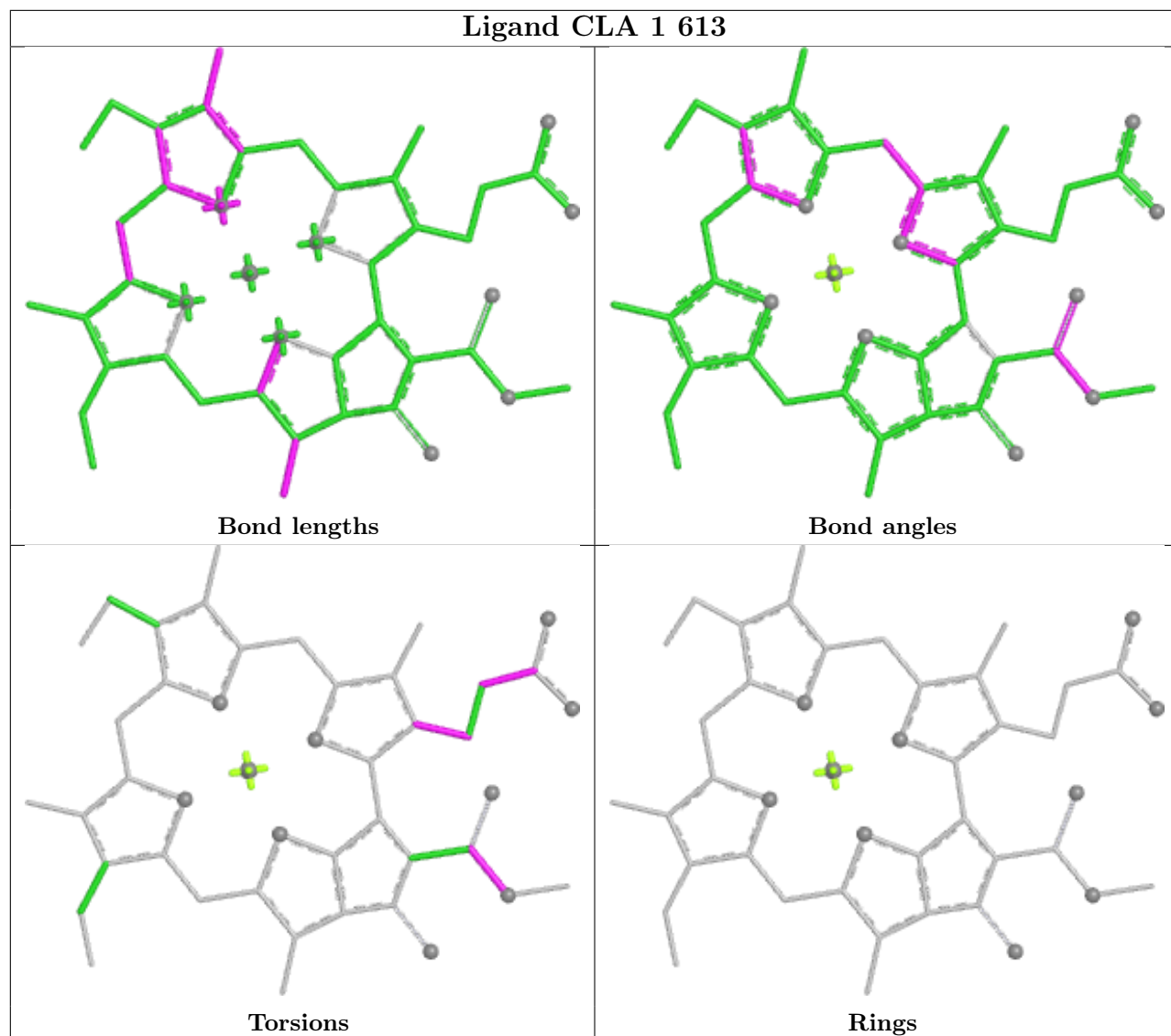


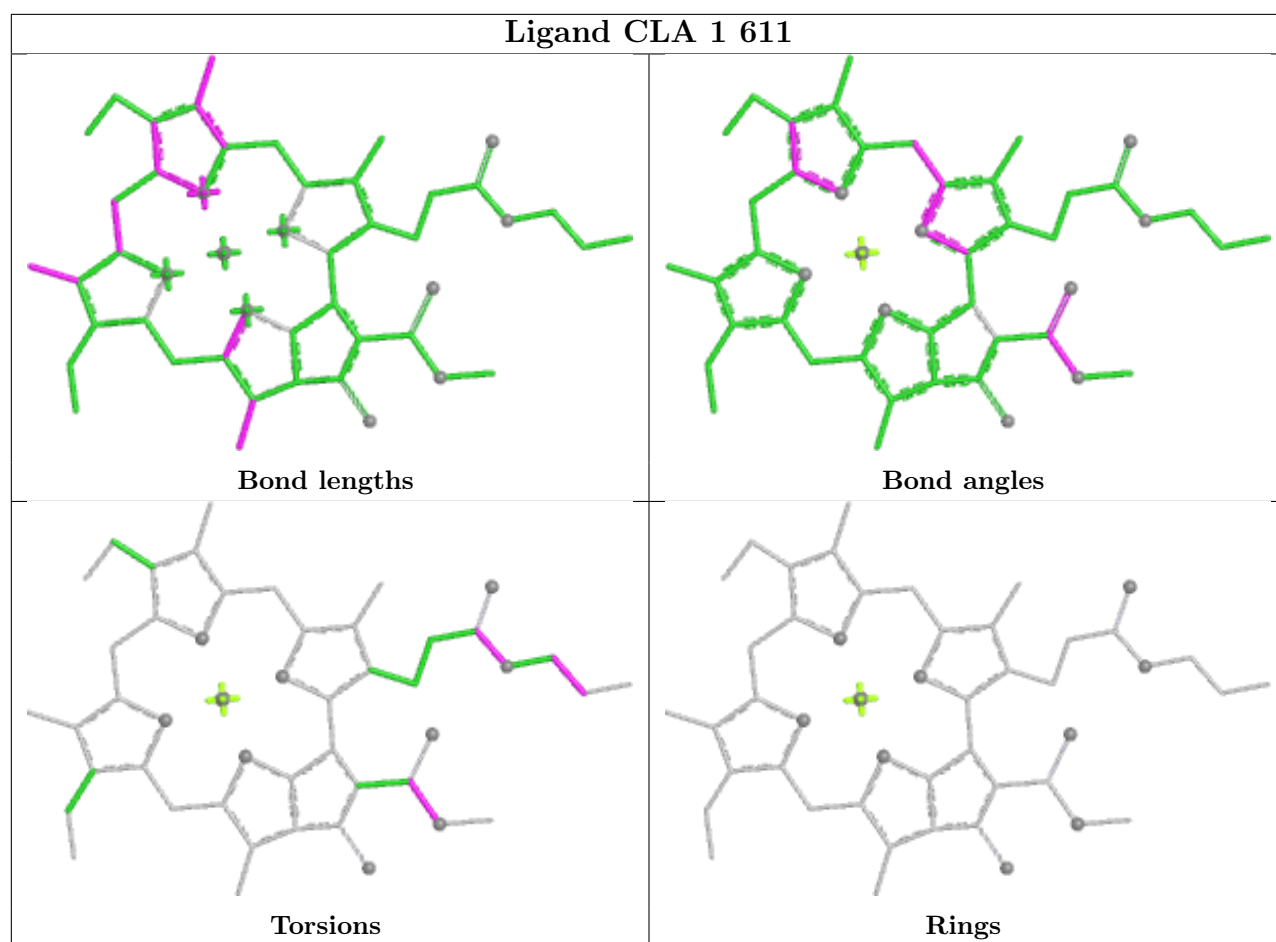
Ligand BCR B 4006

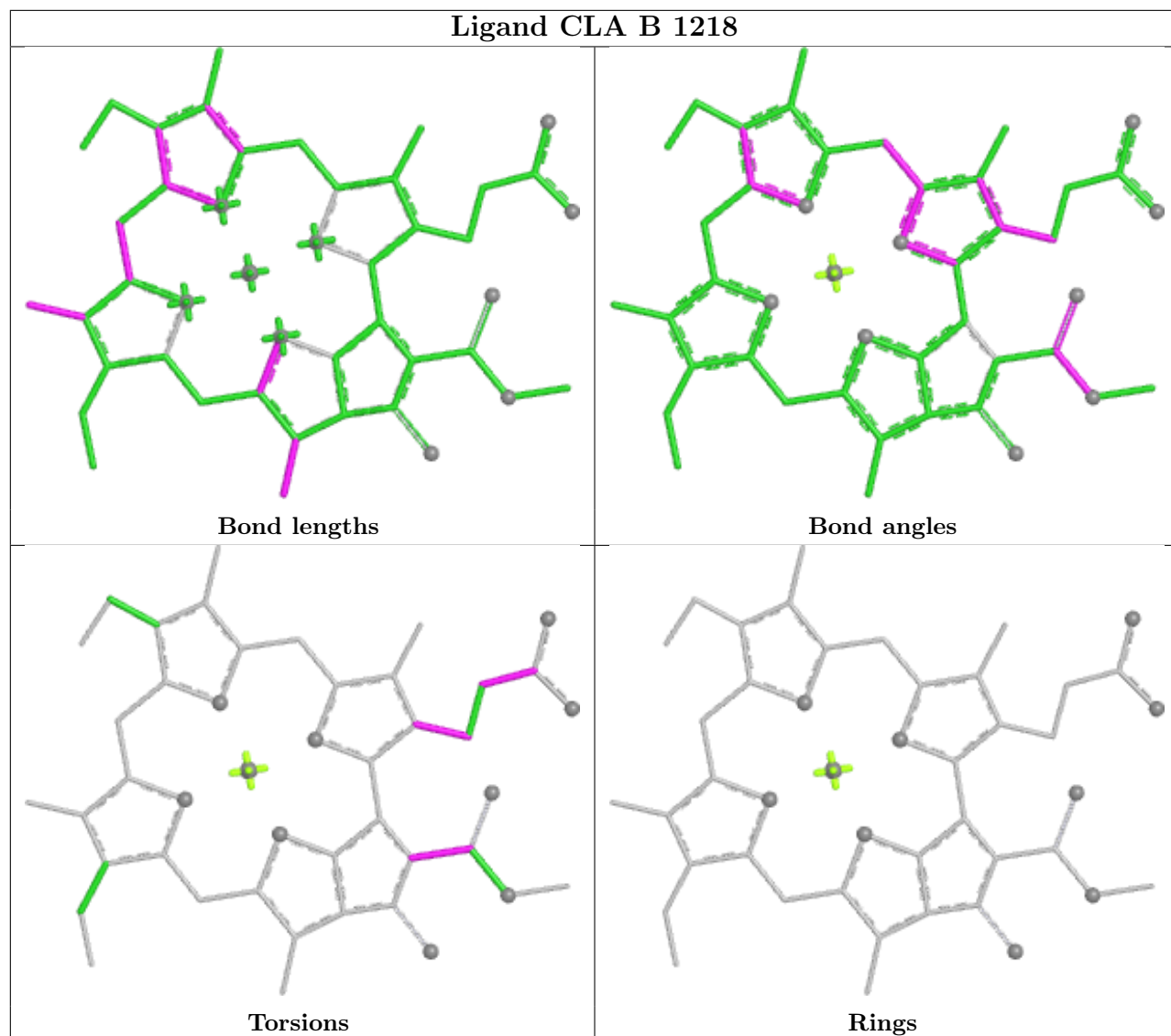


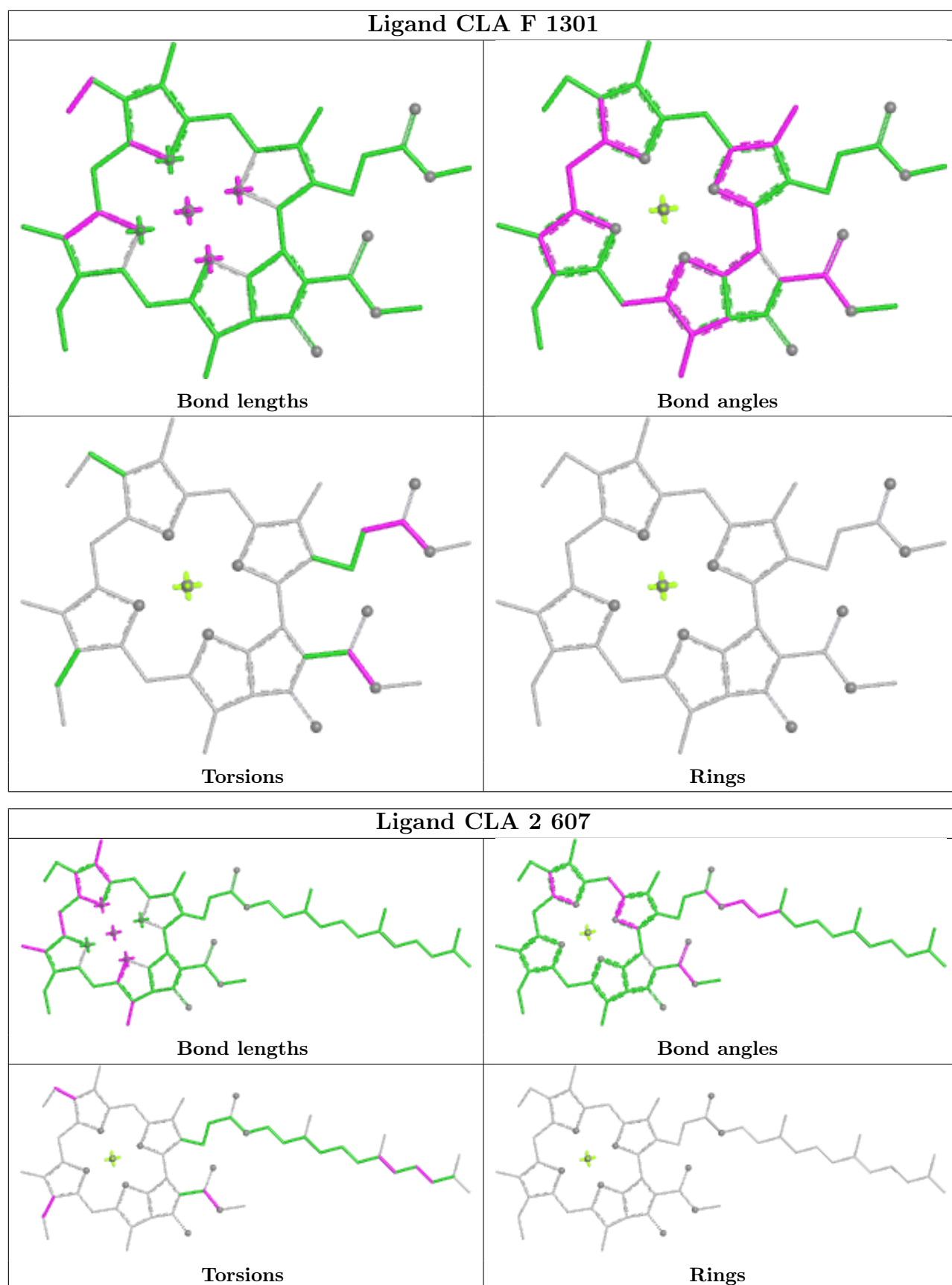


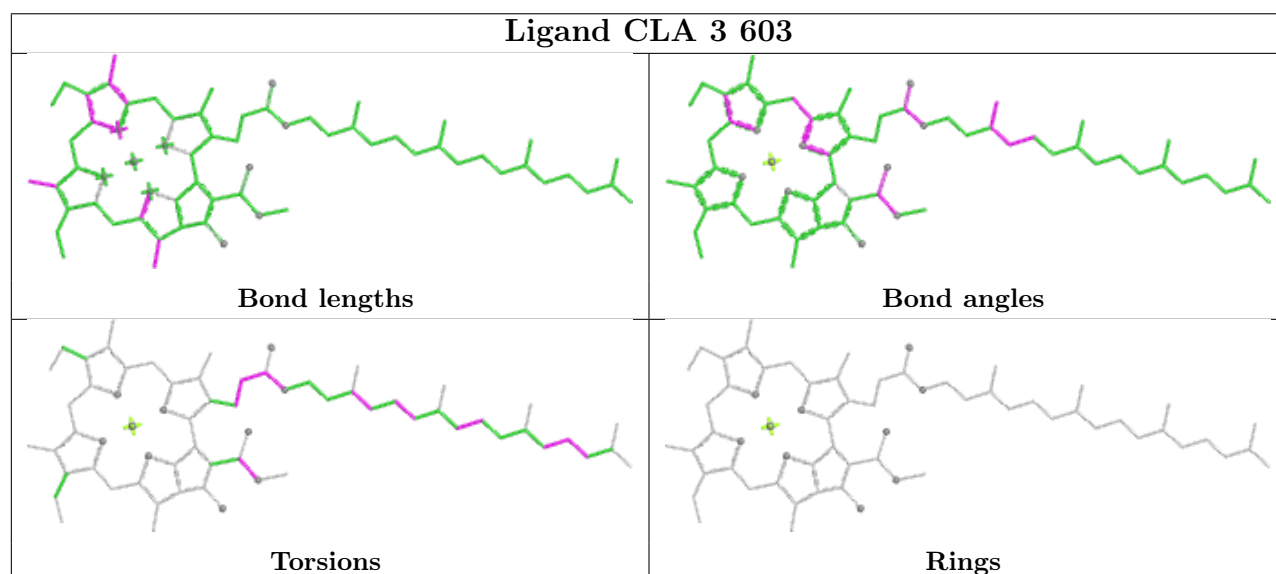
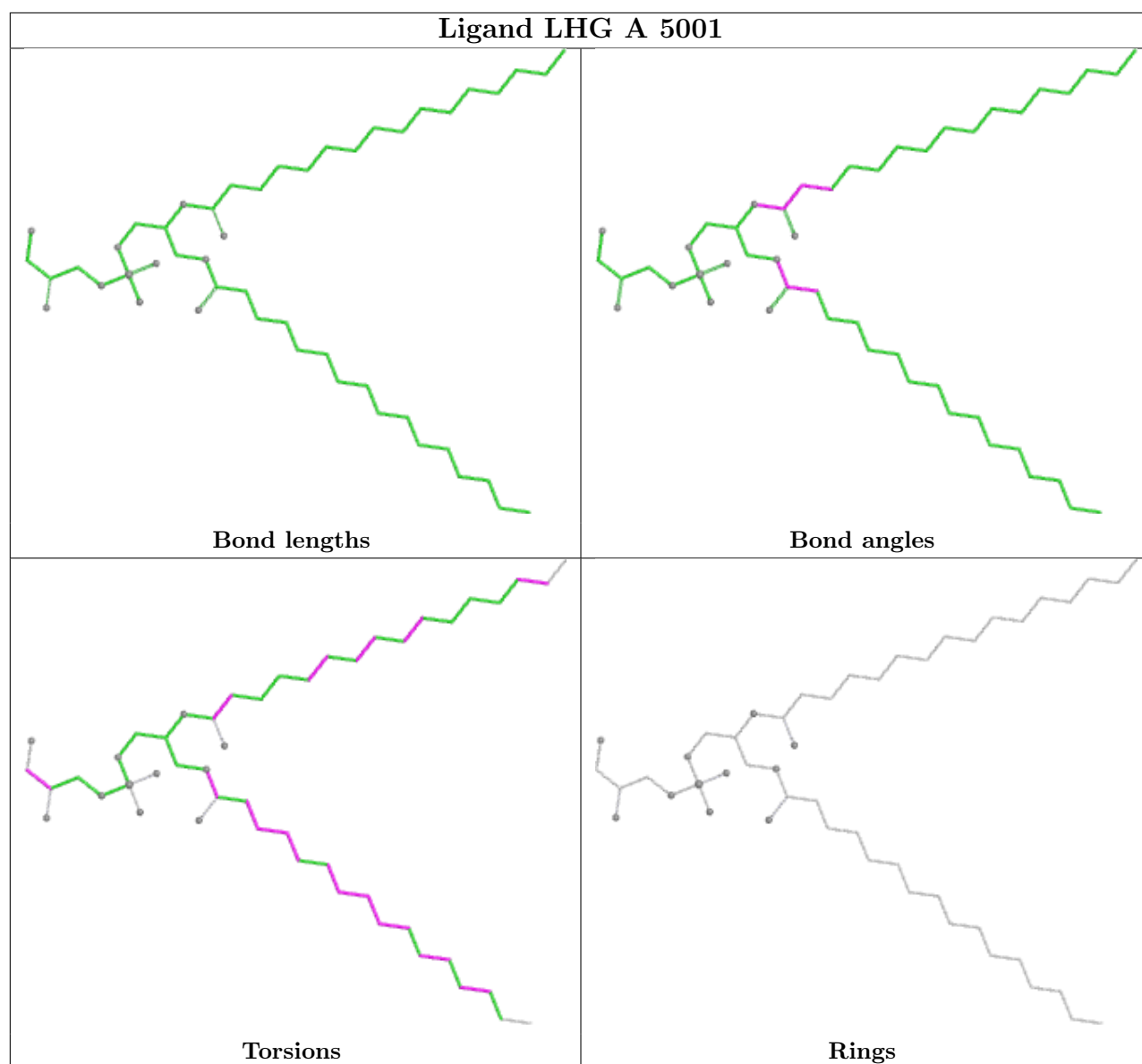
Ligand CLA 1 613



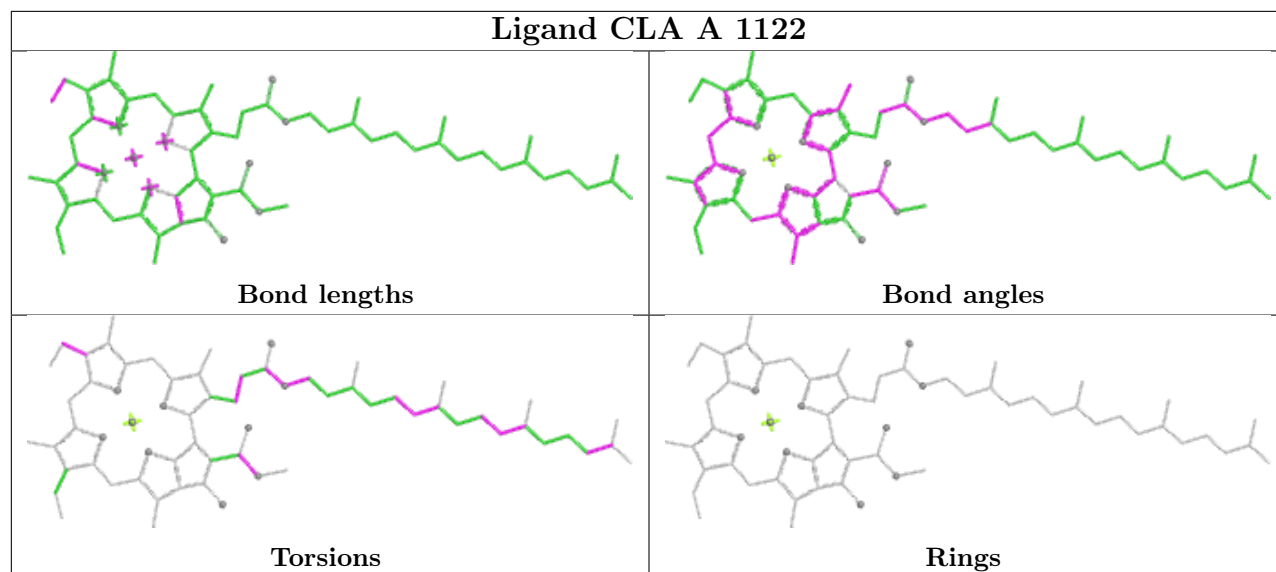




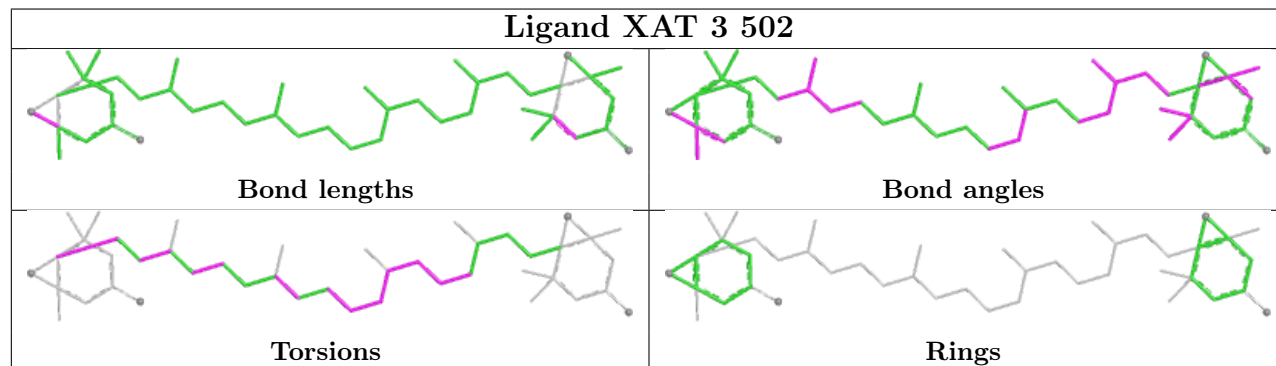




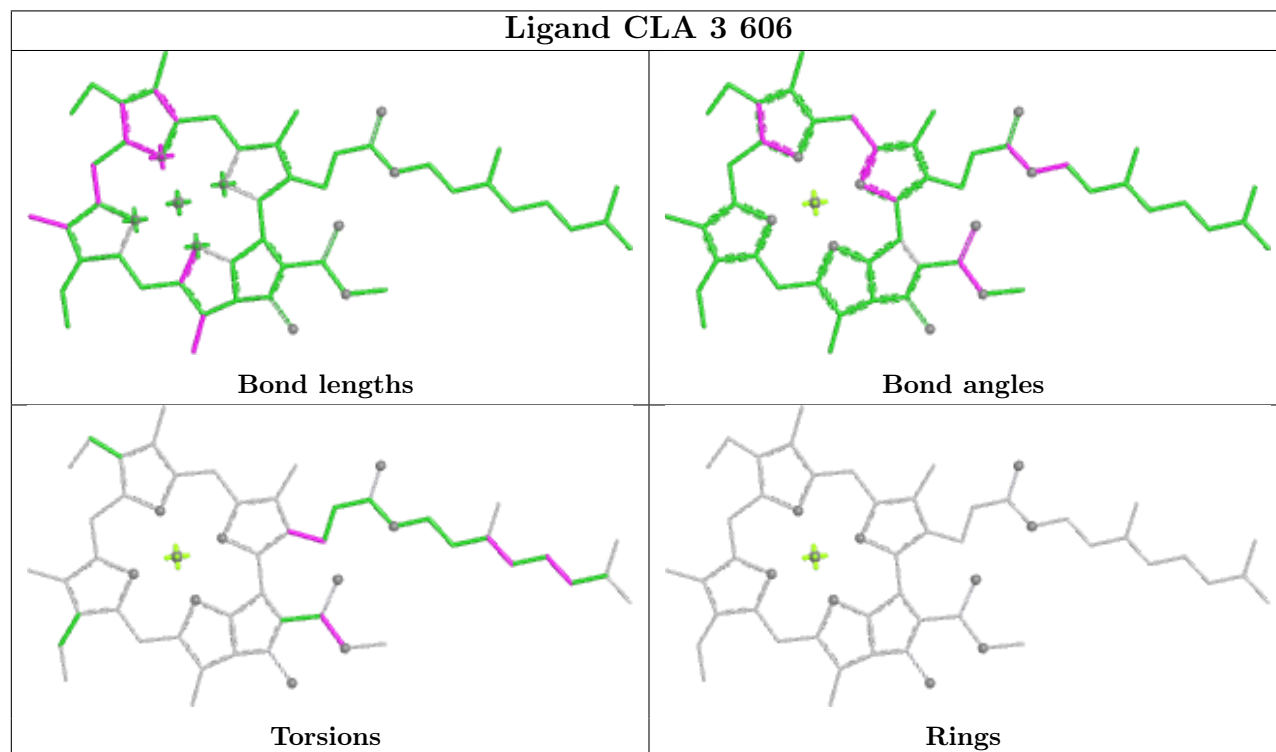
Ligand CLA A 1122

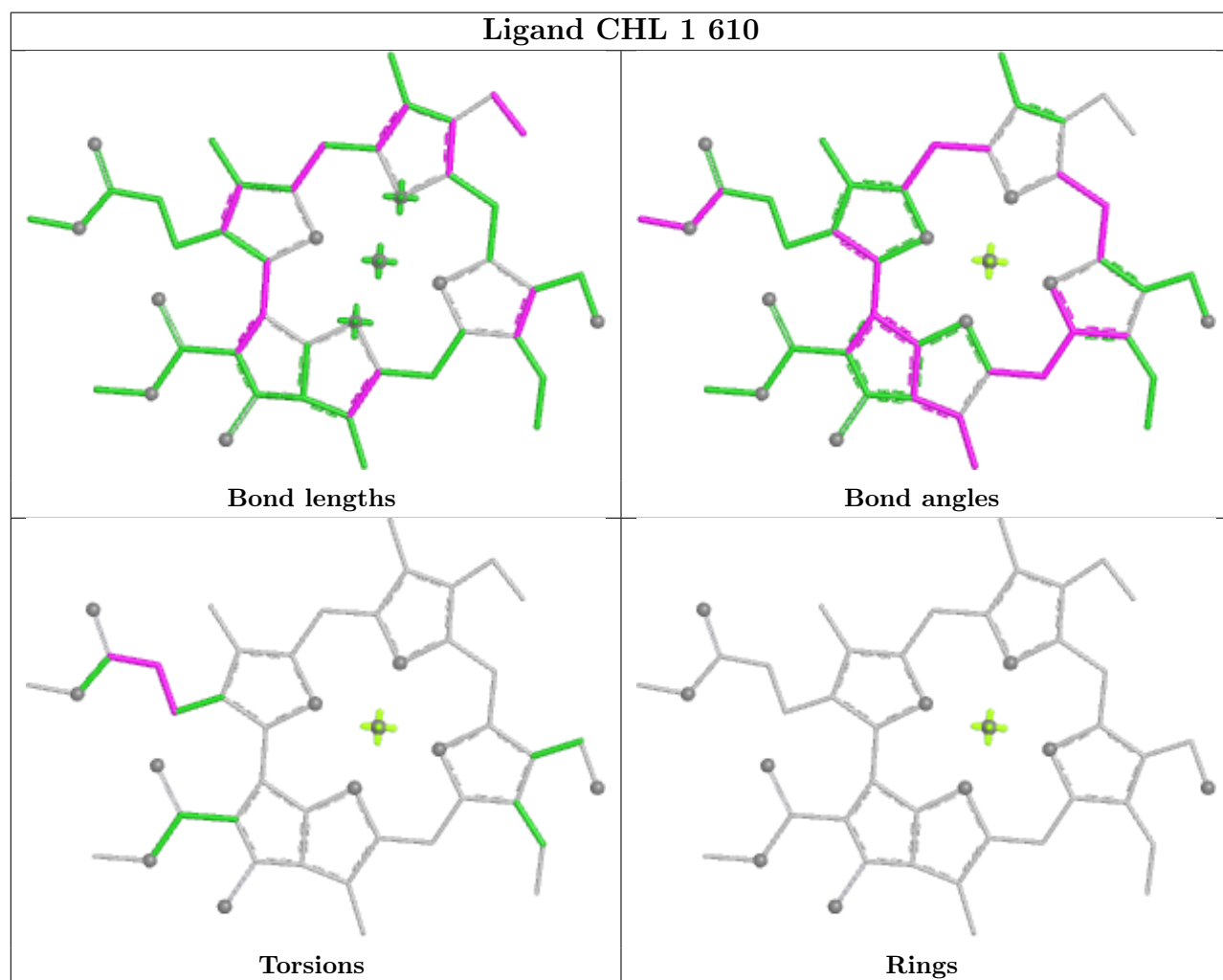
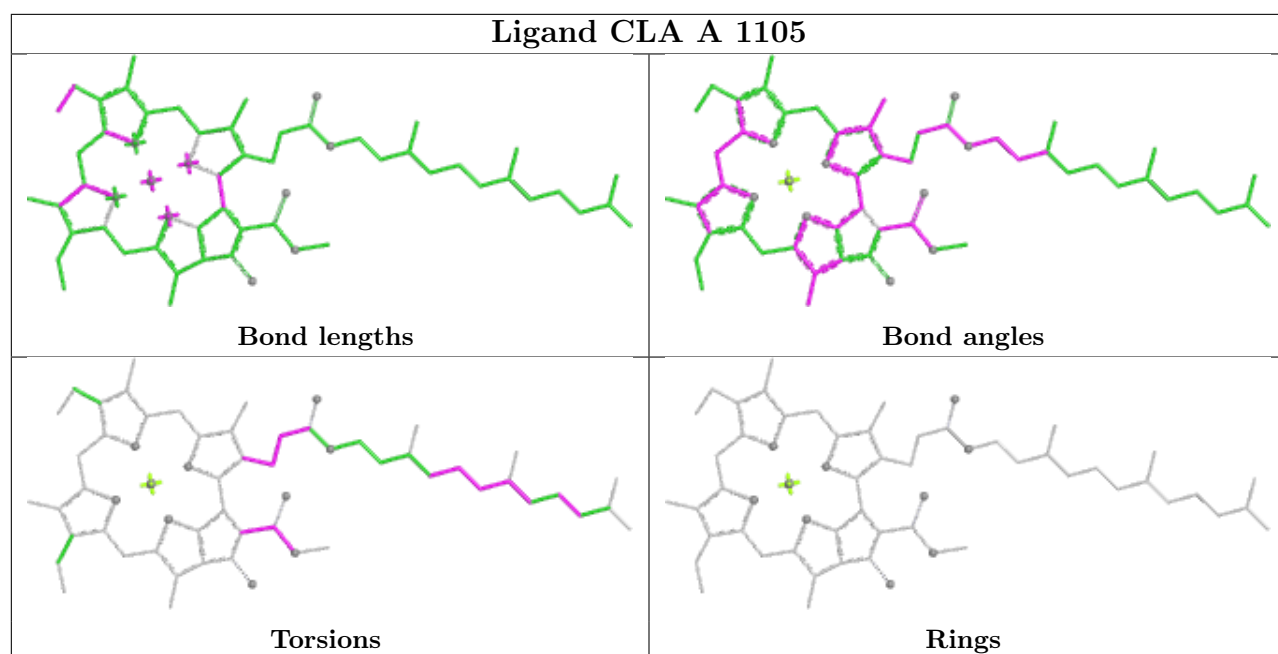


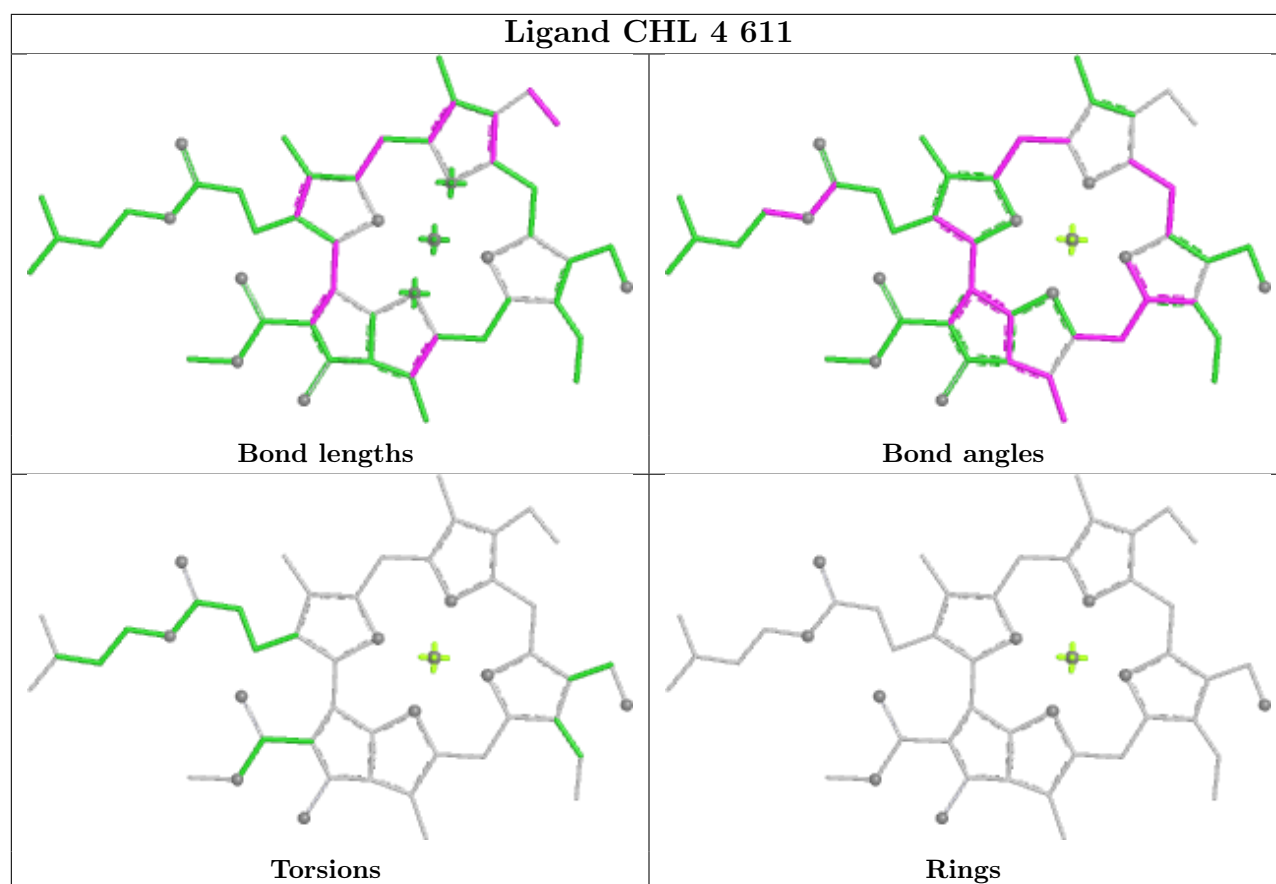
Ligand XAT 3 502

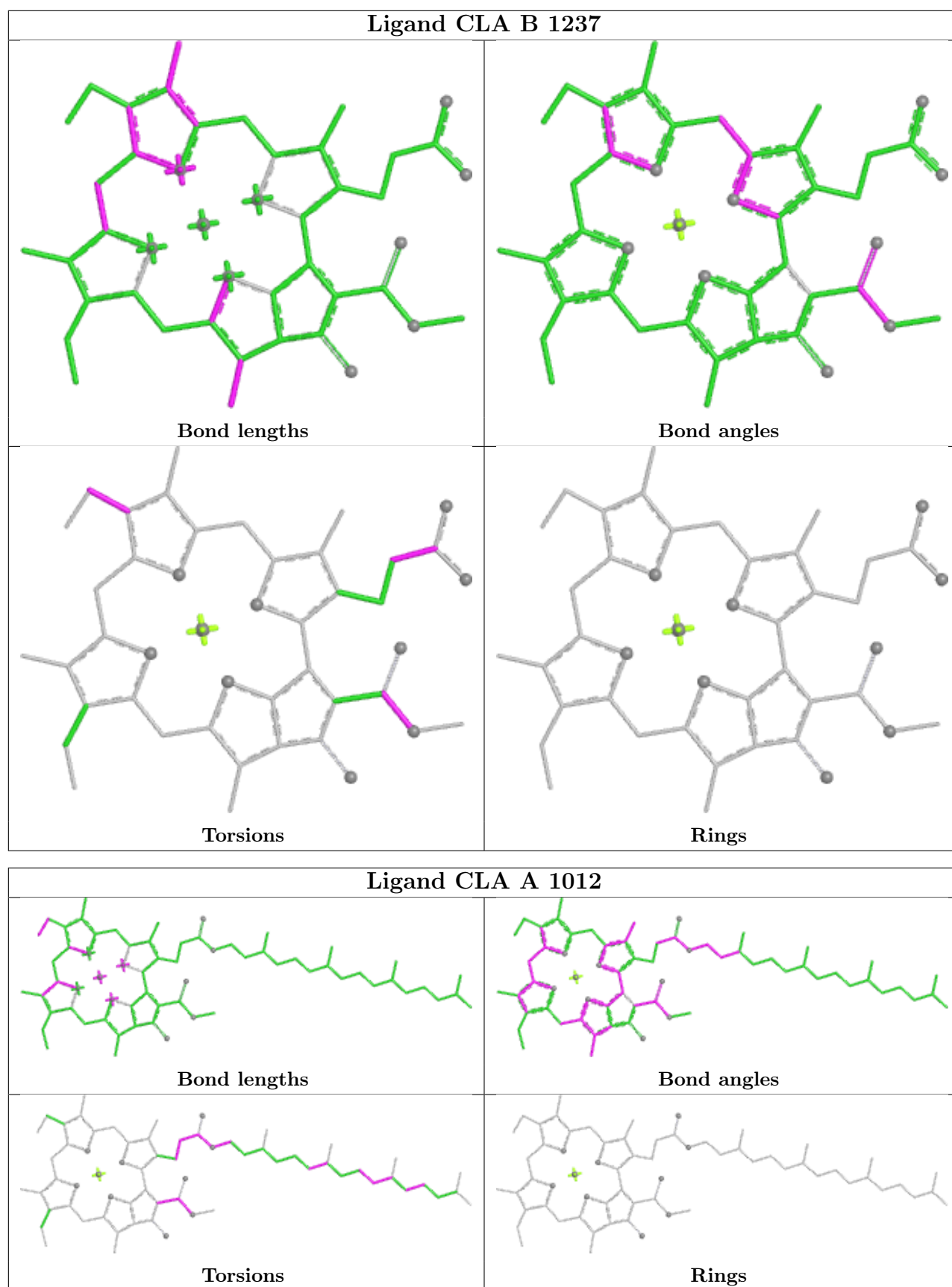


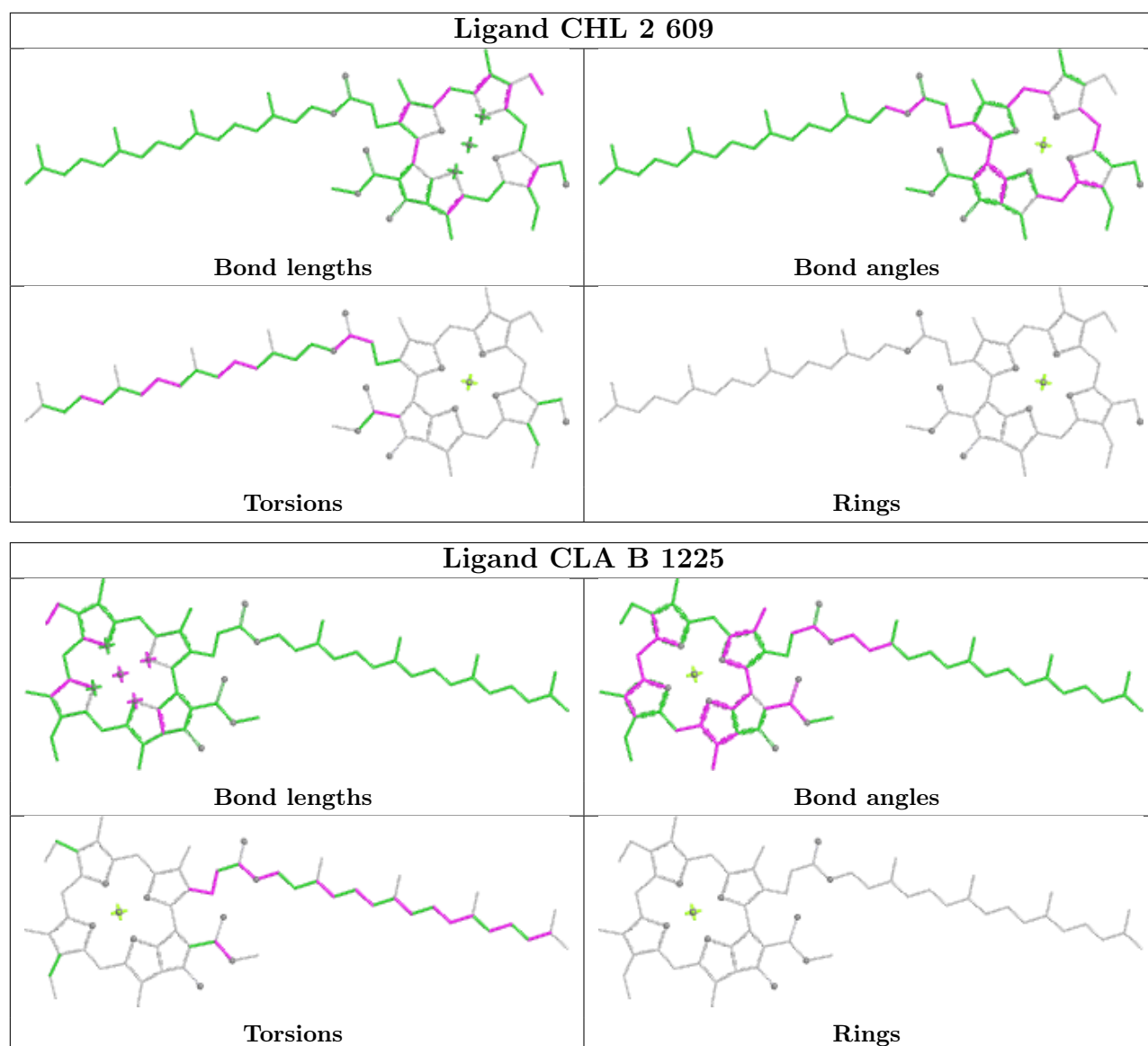
Ligand CLA 3 606



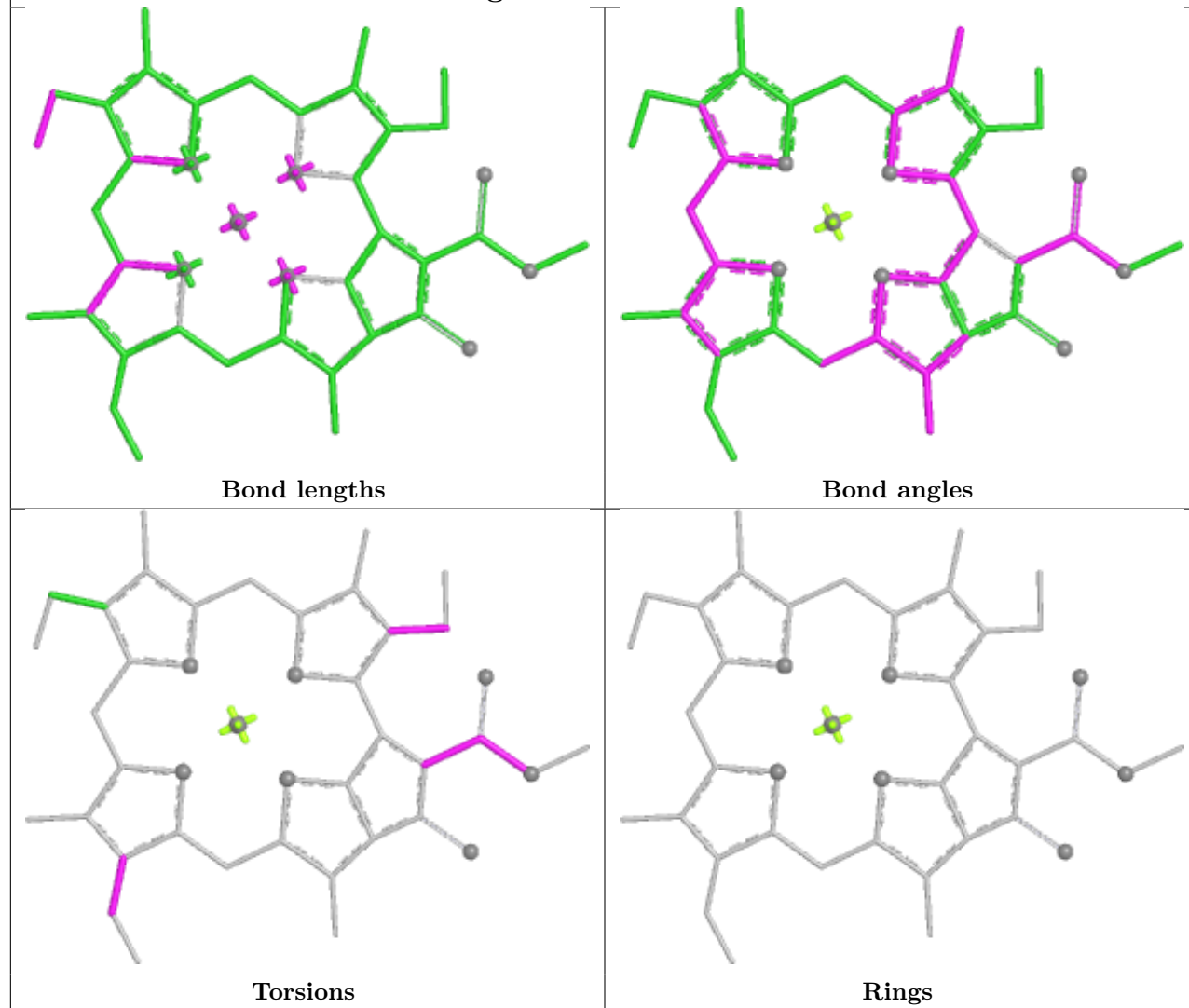




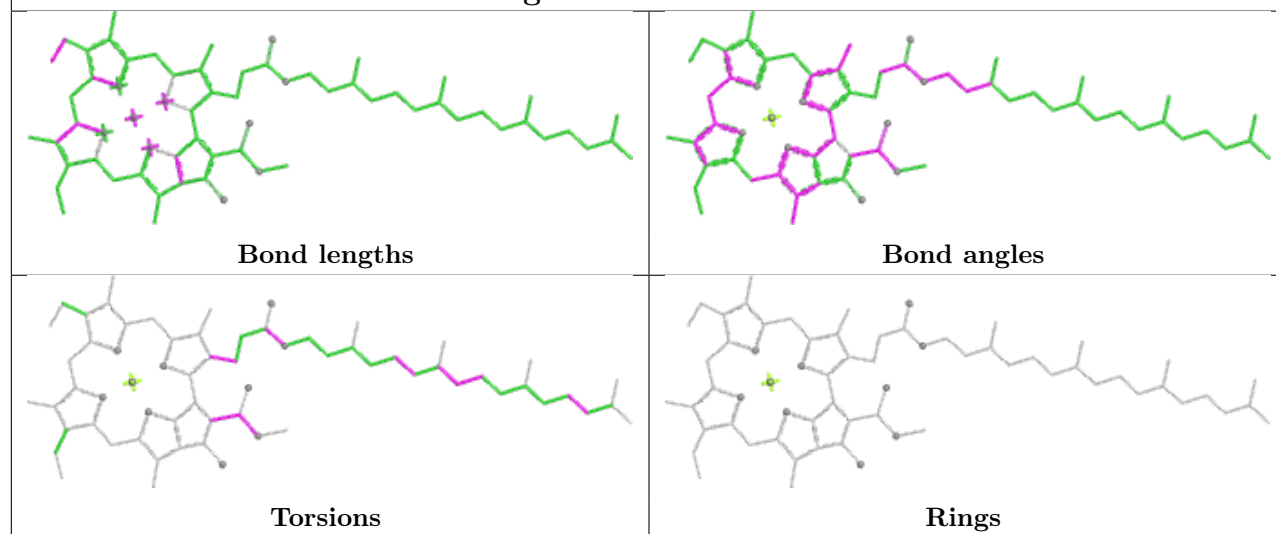


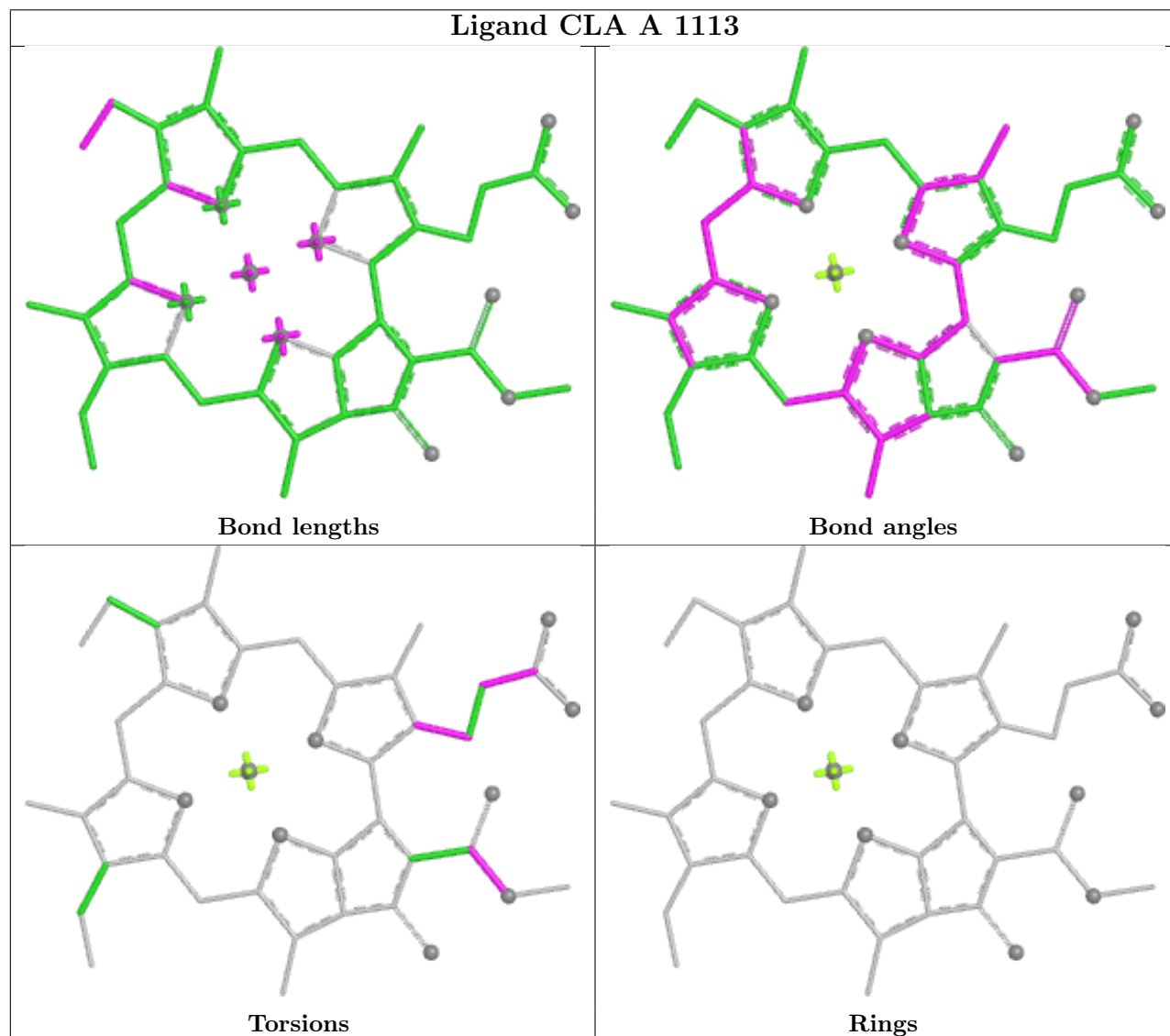
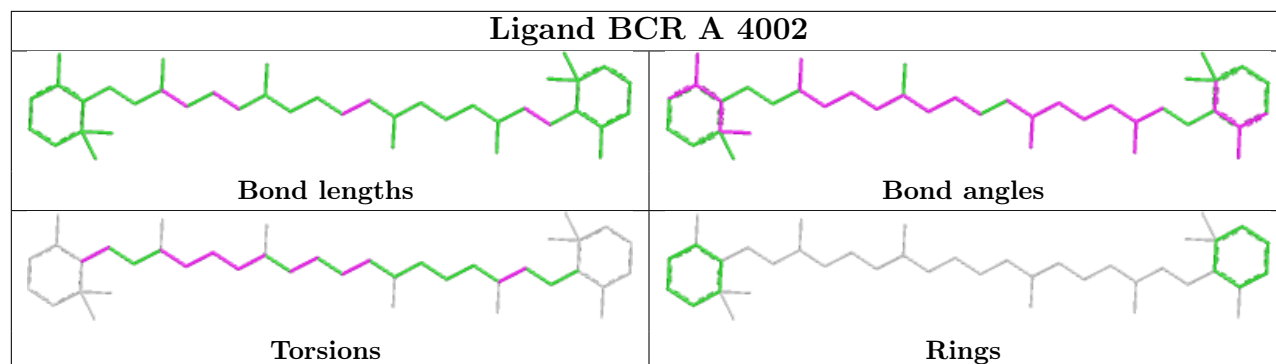


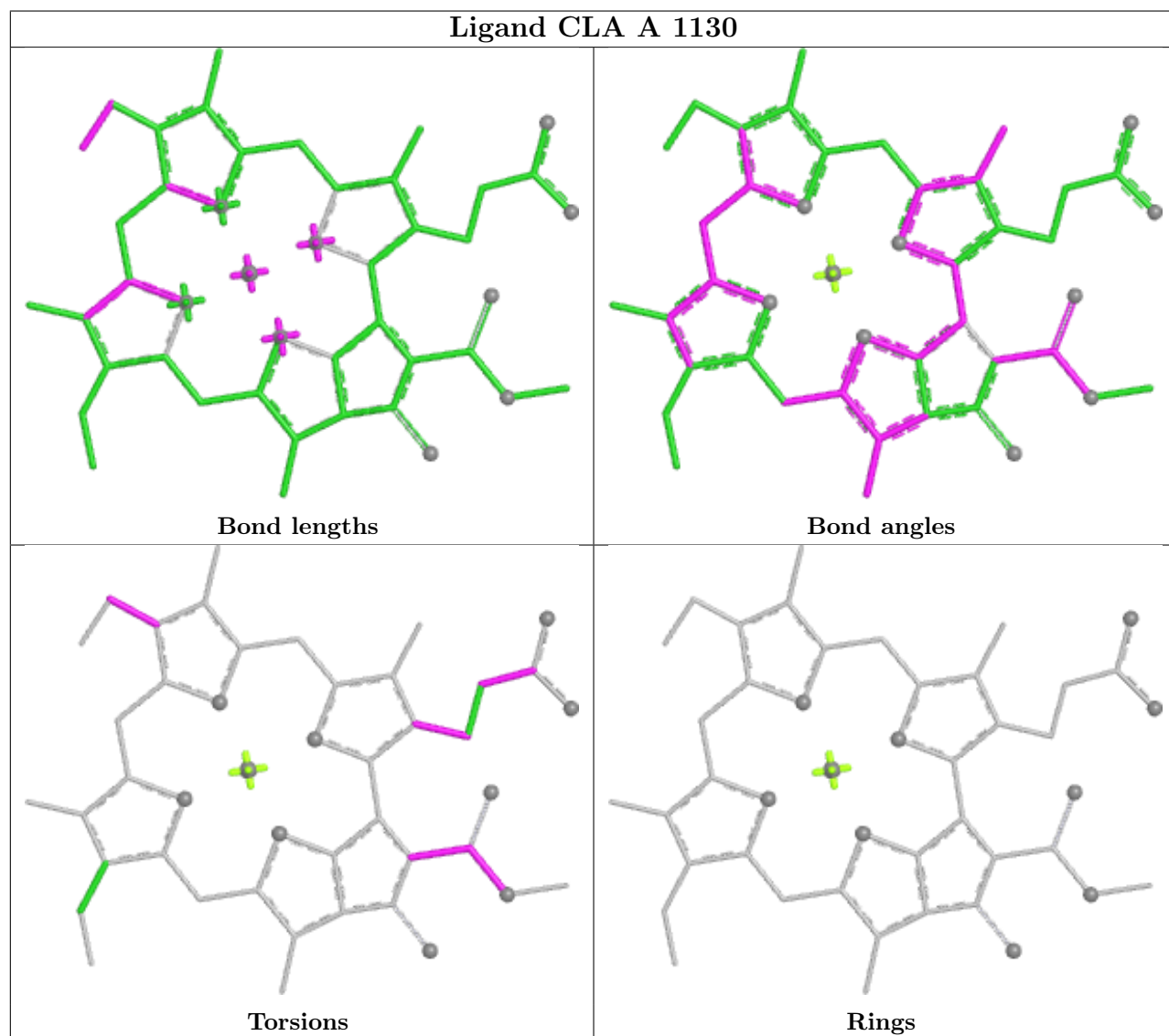
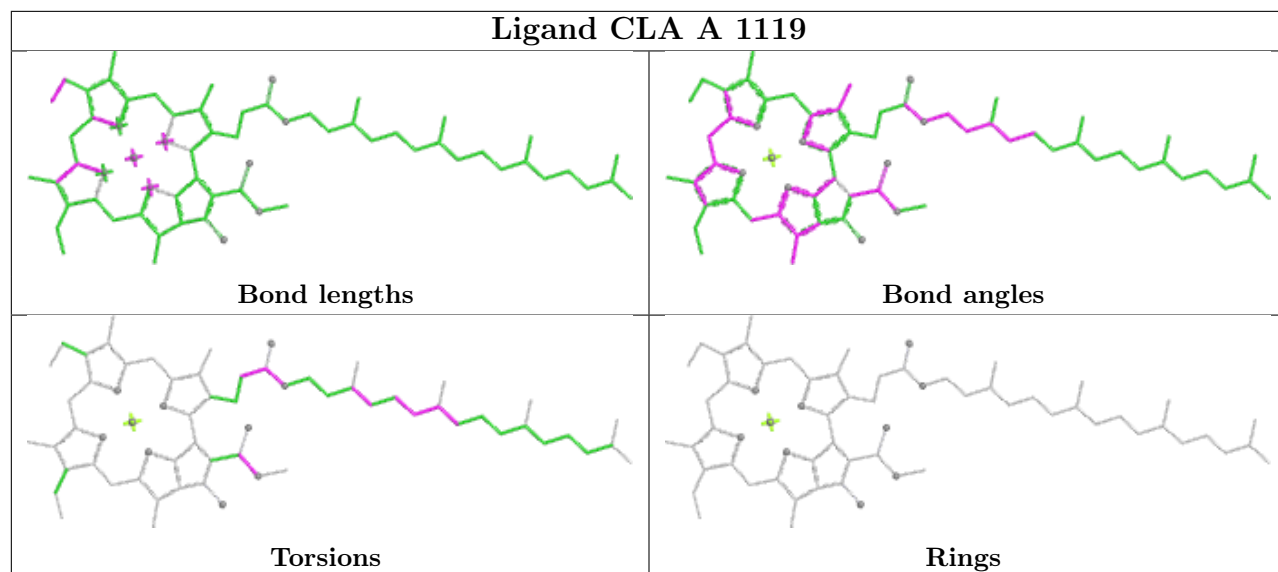
Ligand CLA A 1120

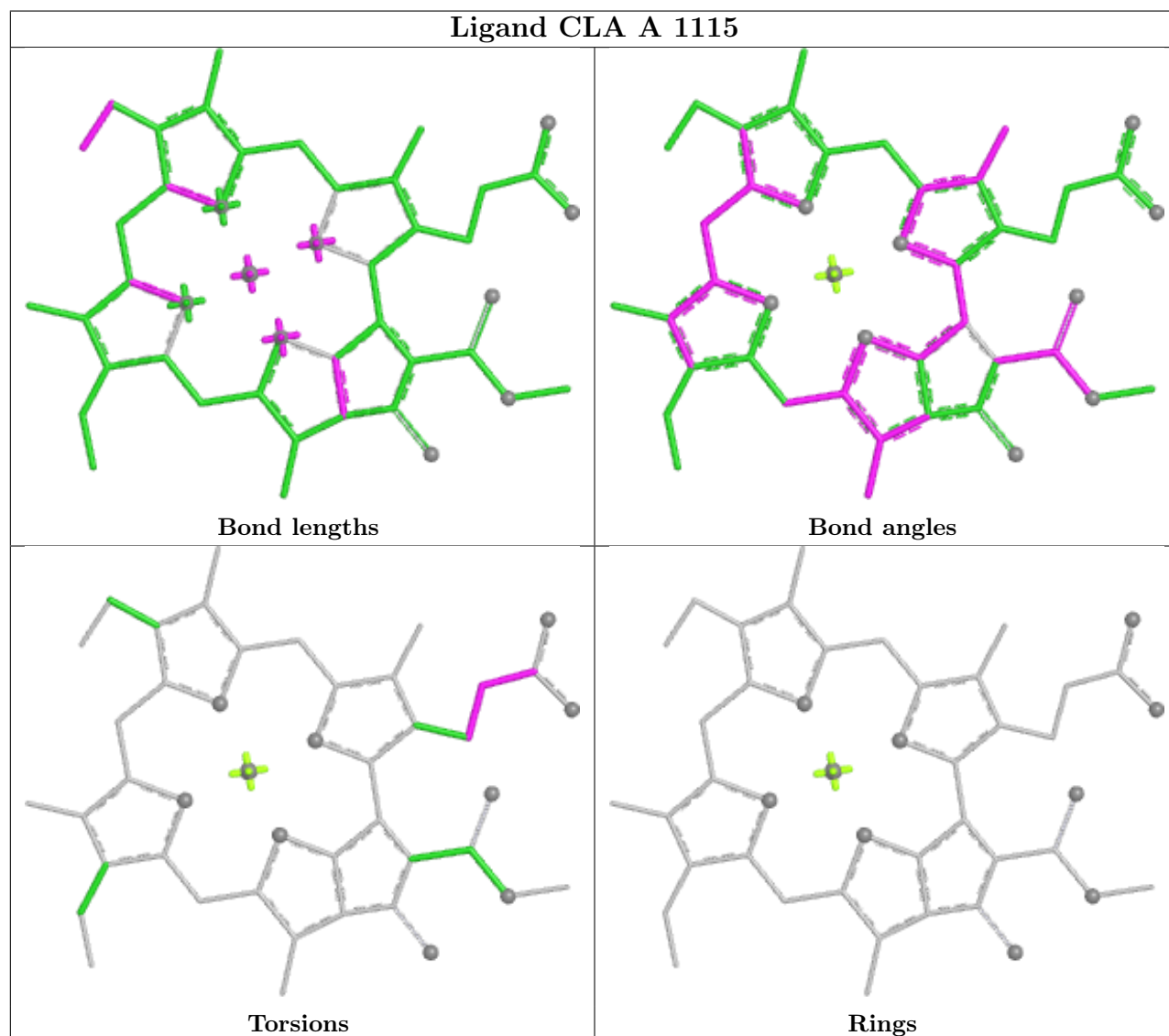
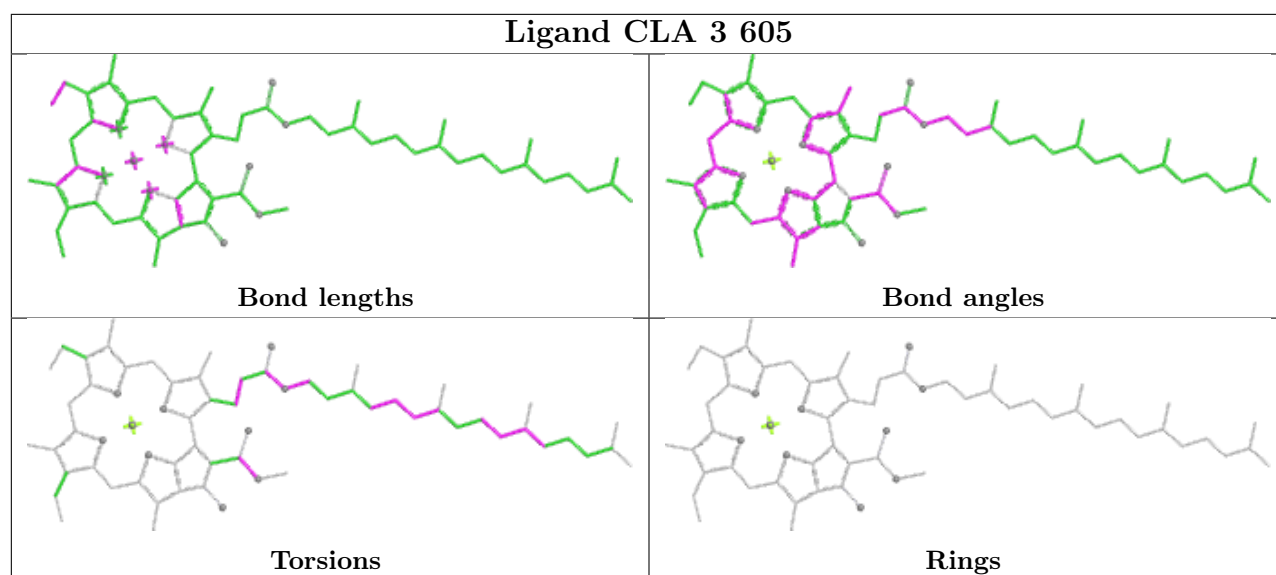


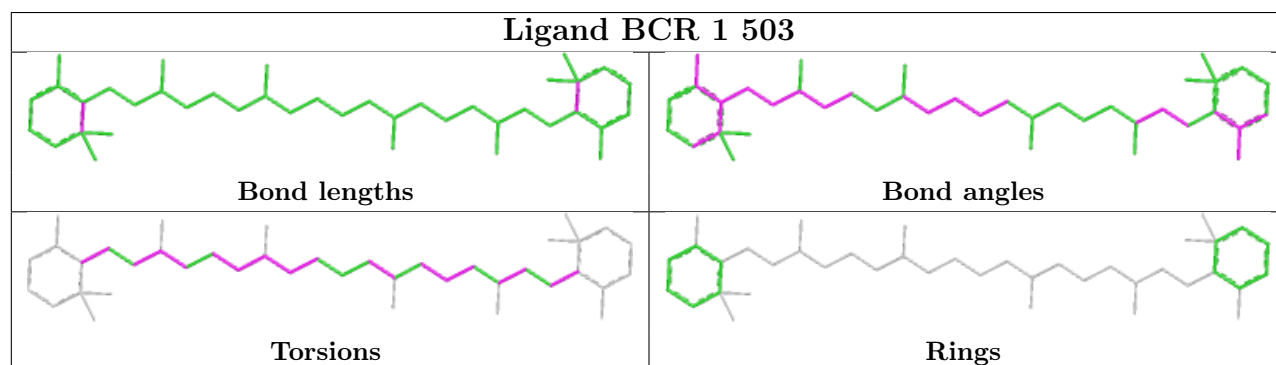
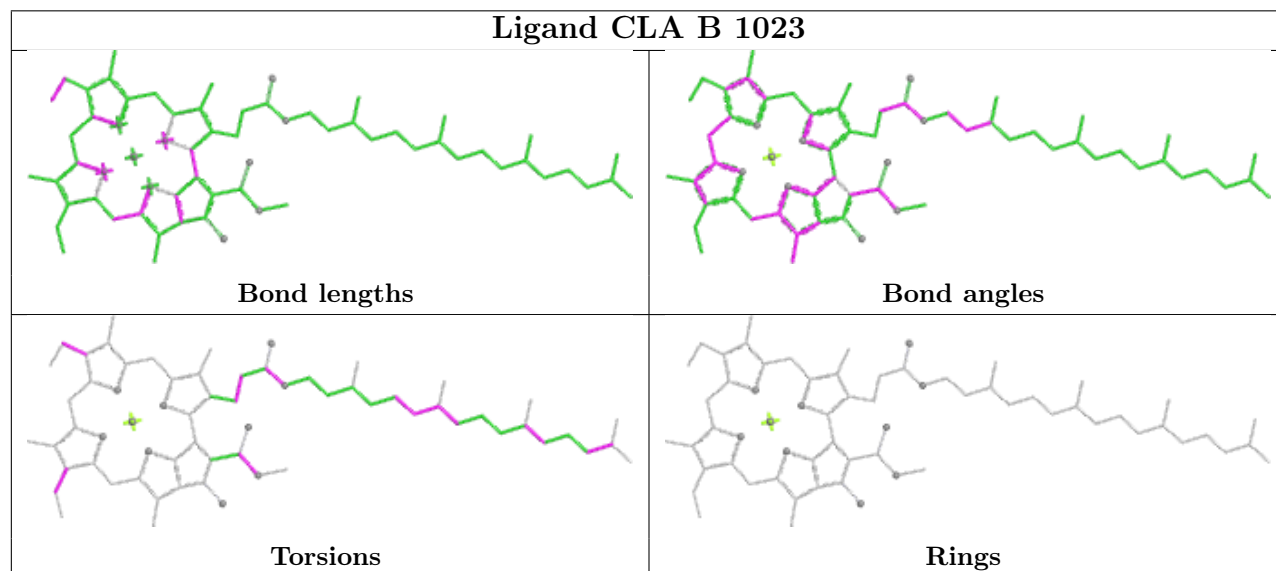
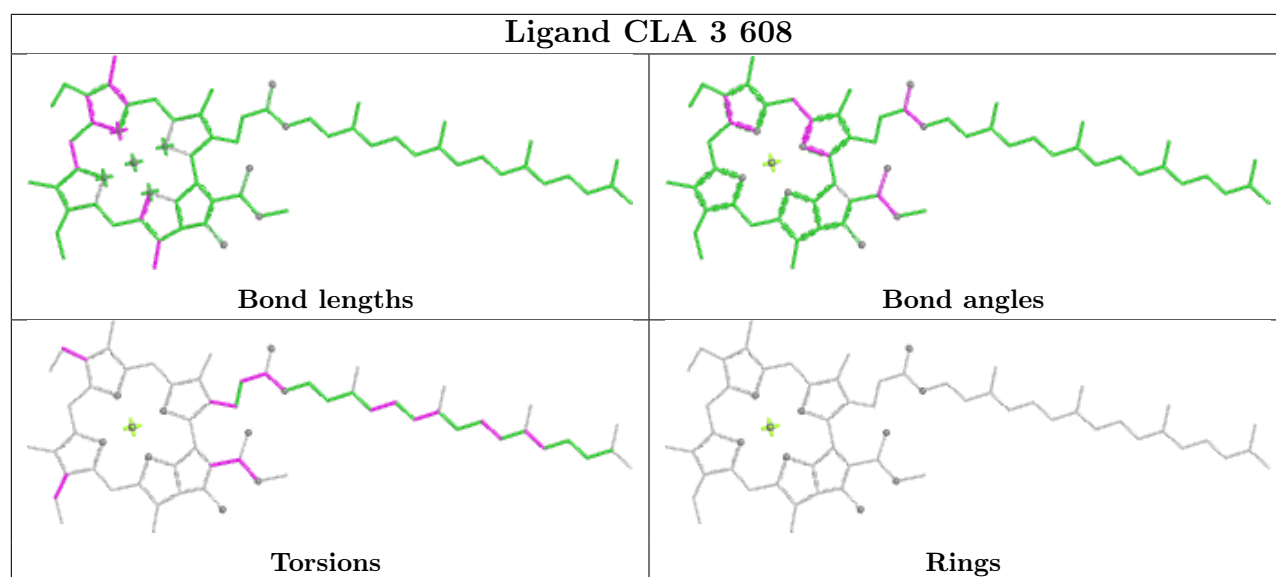
Ligand CLA B 1222

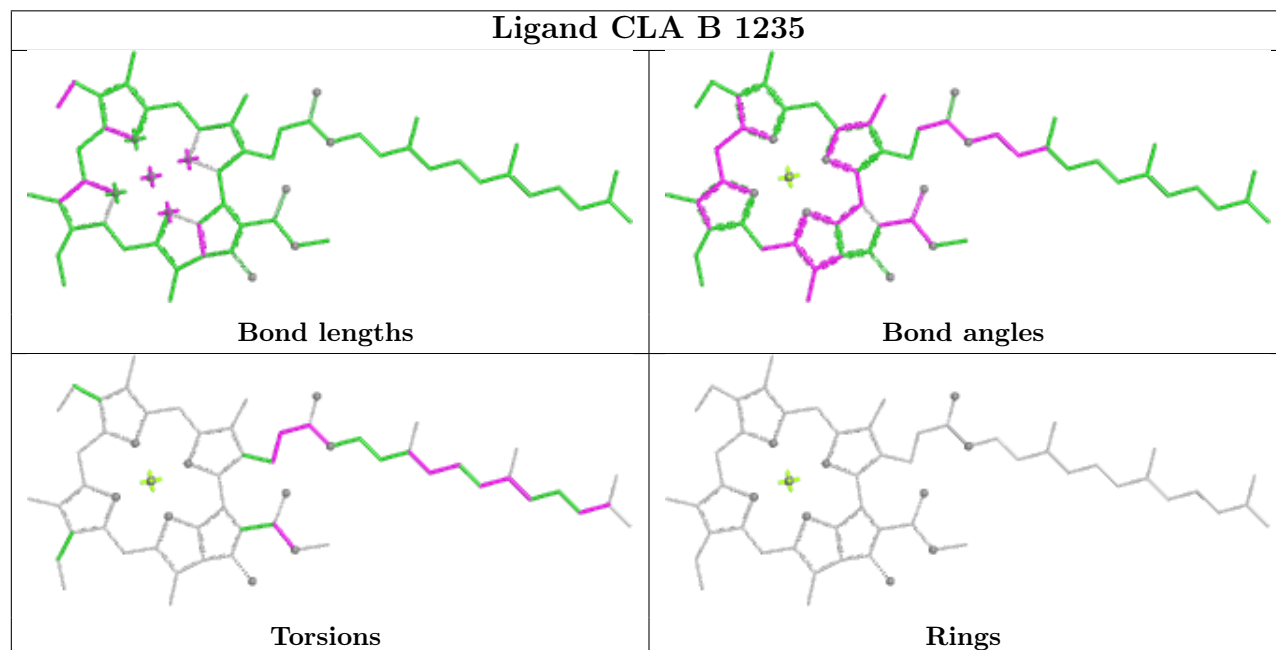
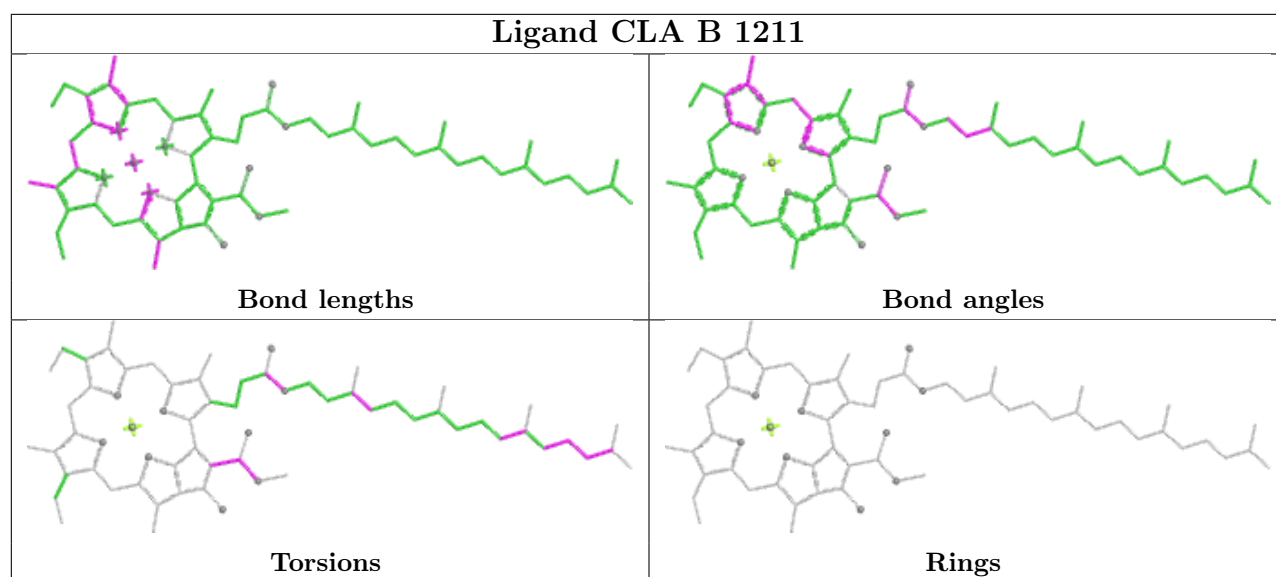


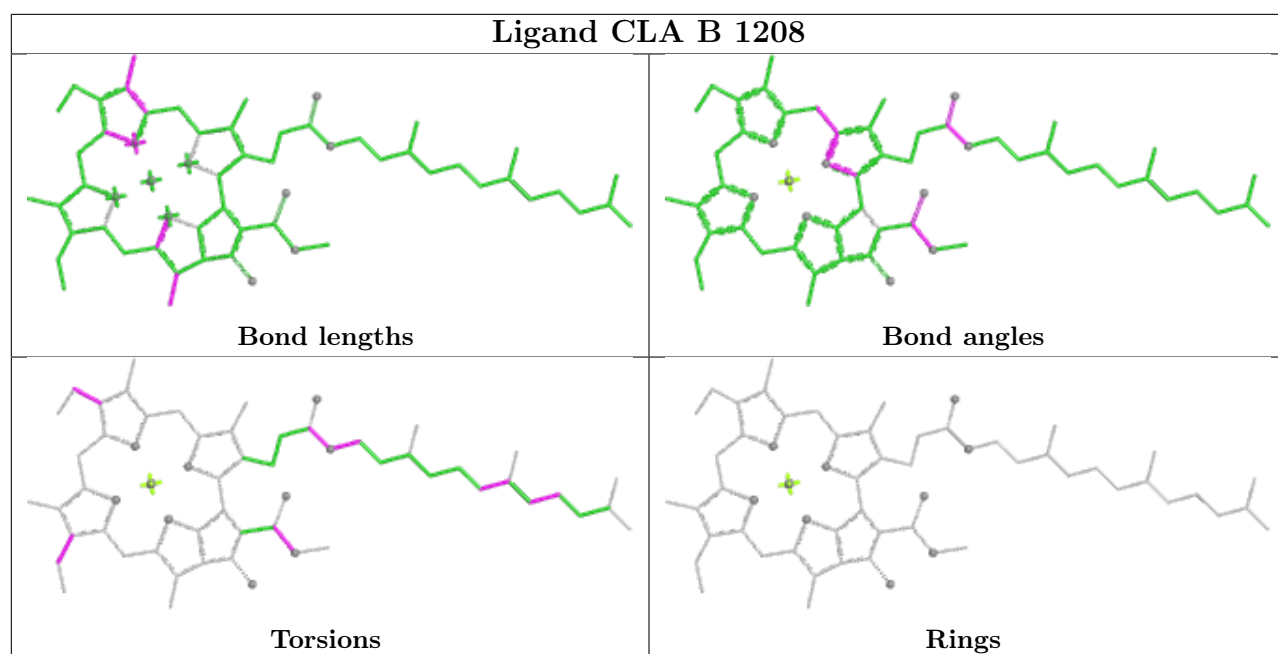


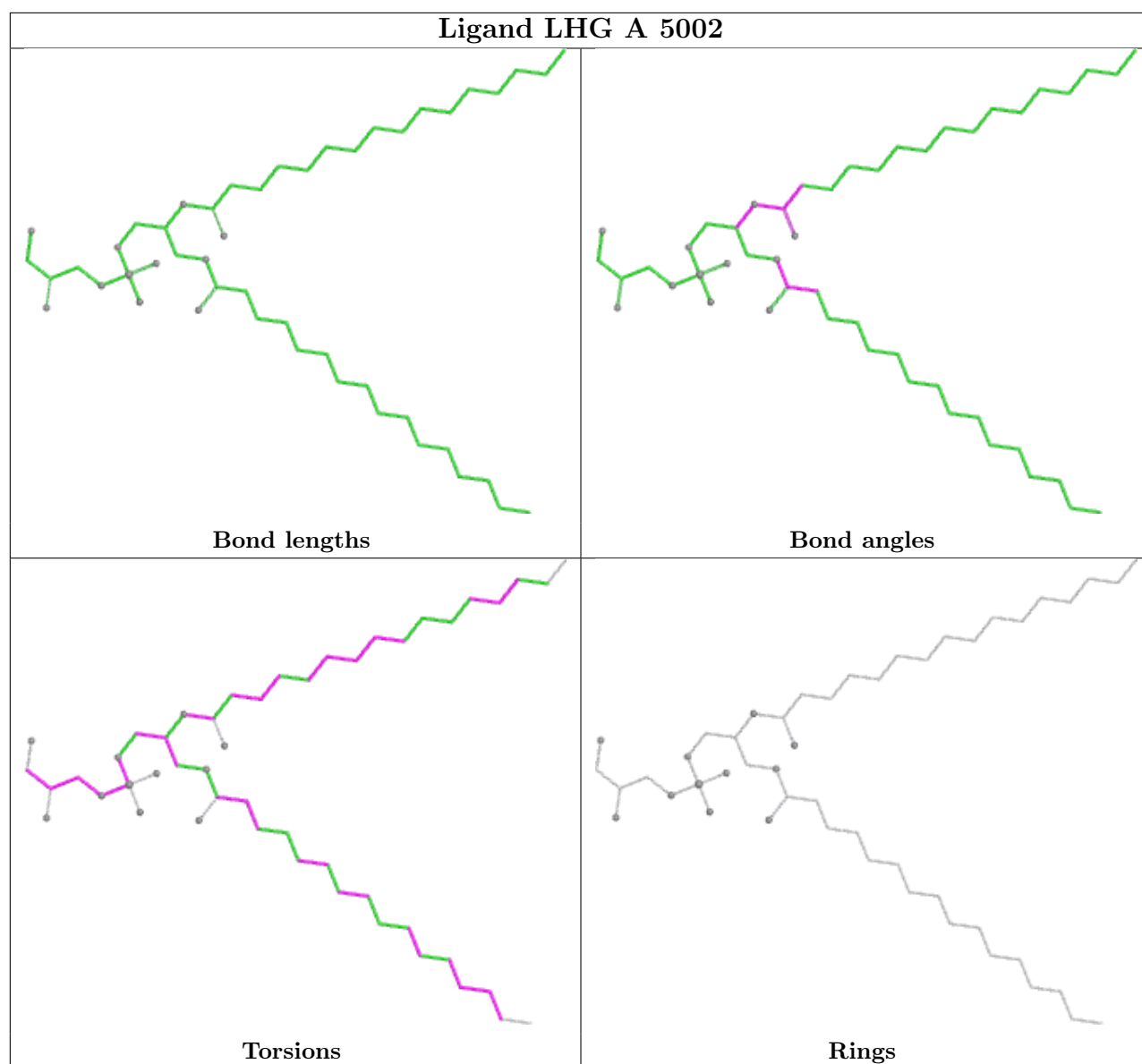




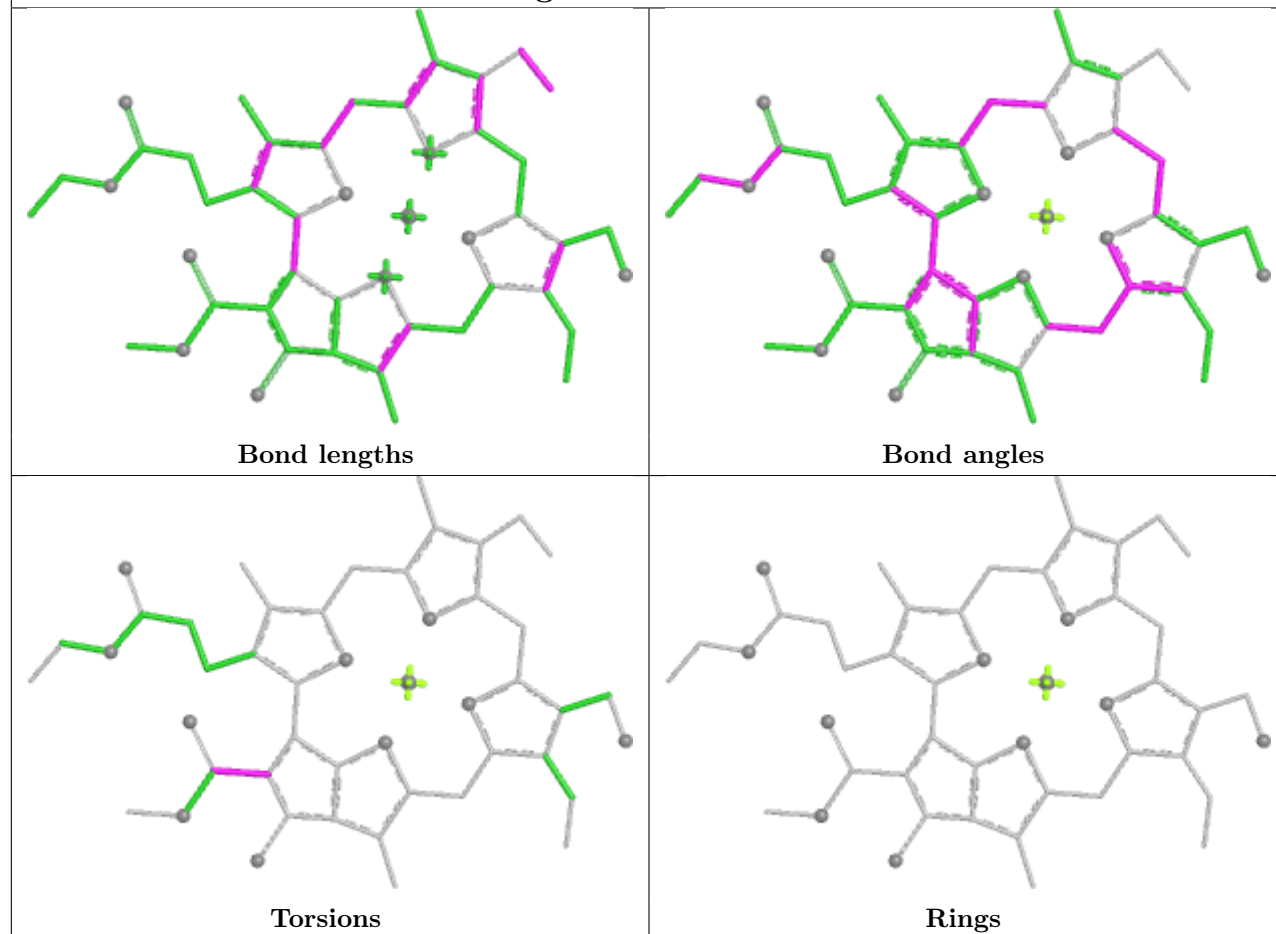




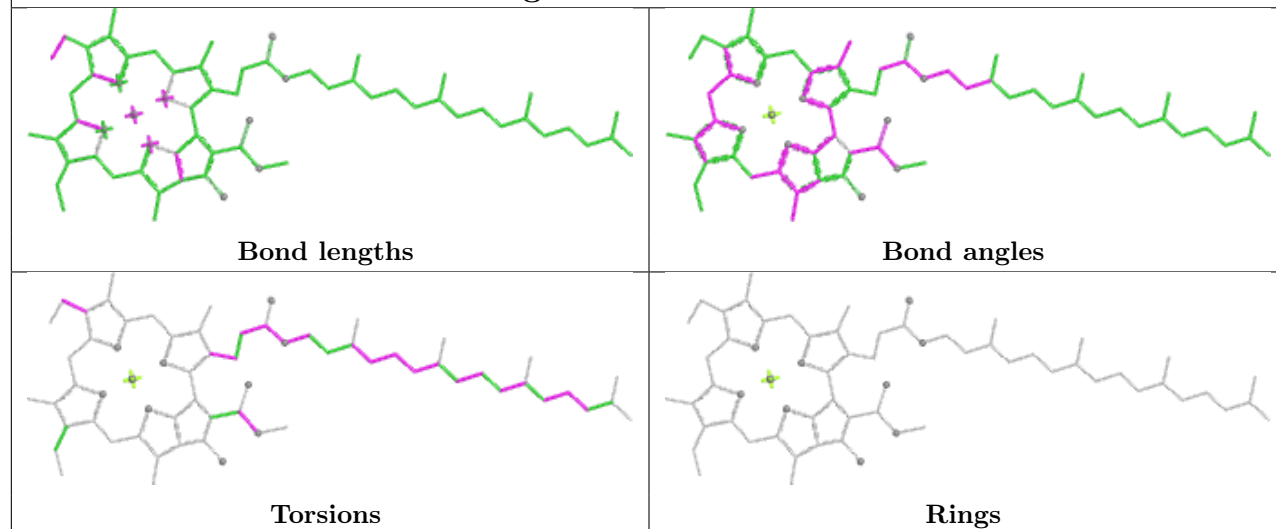


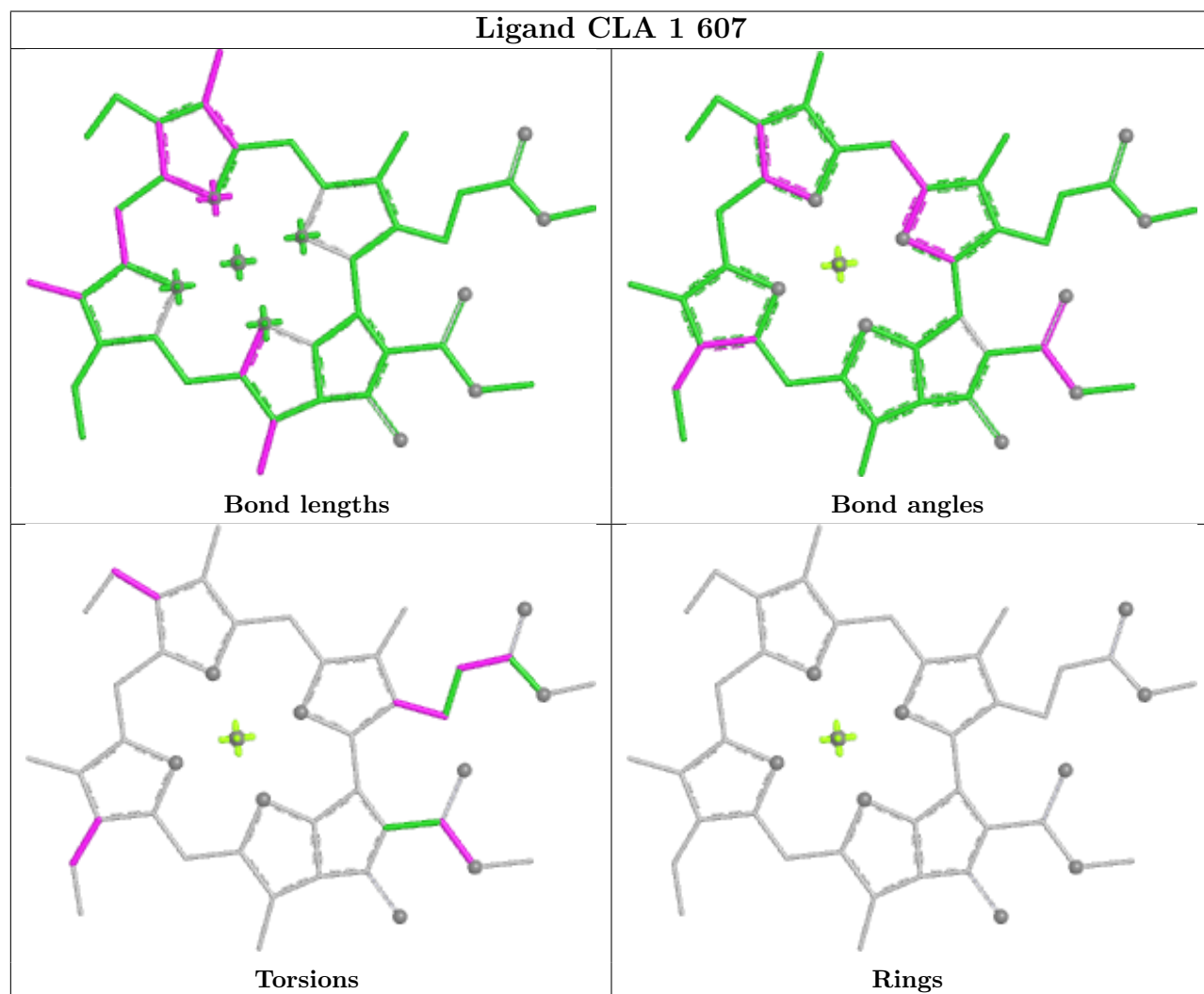
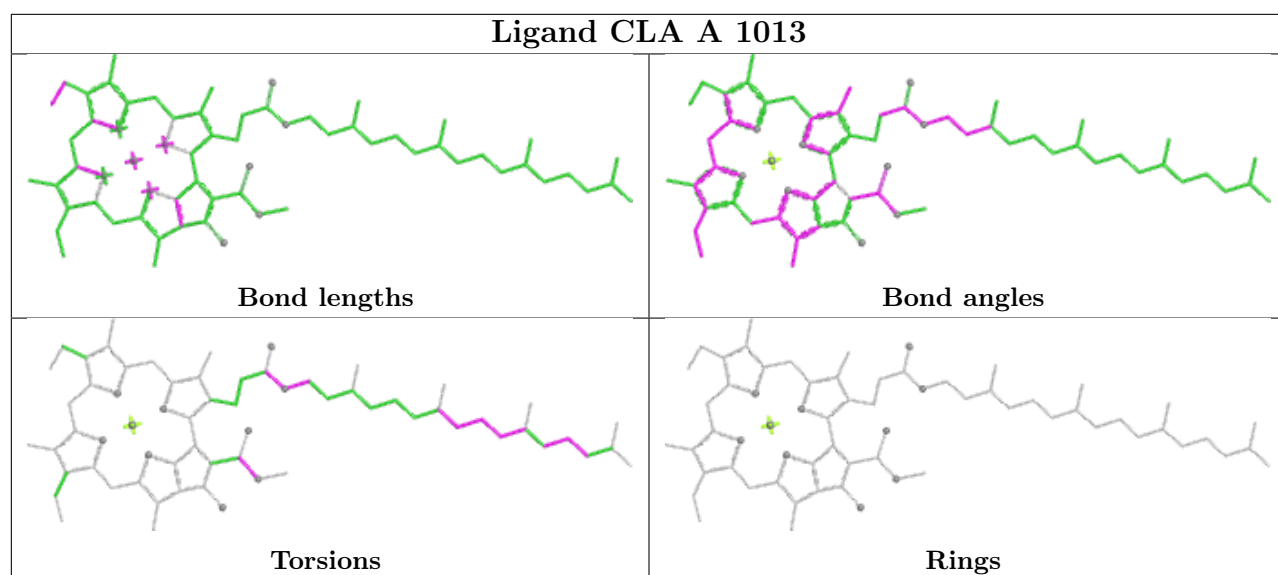


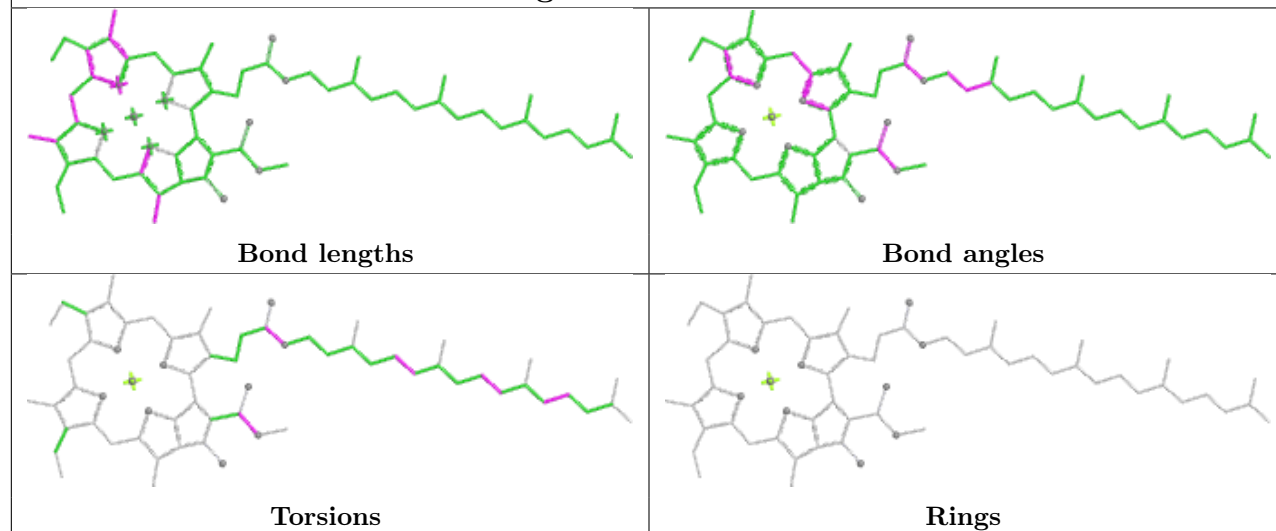
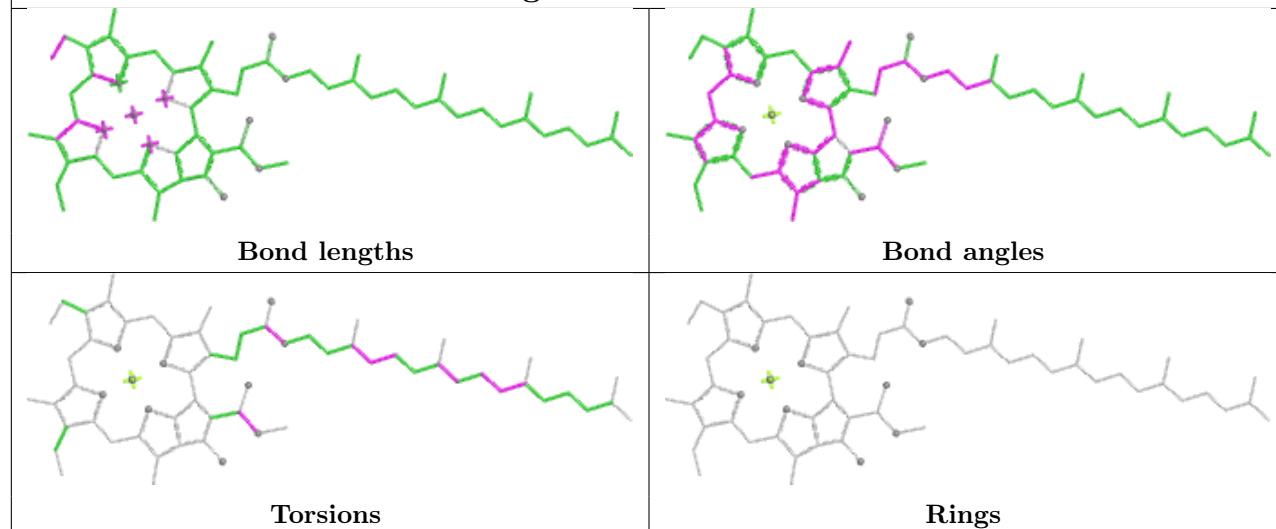
Ligand CHL 2 611



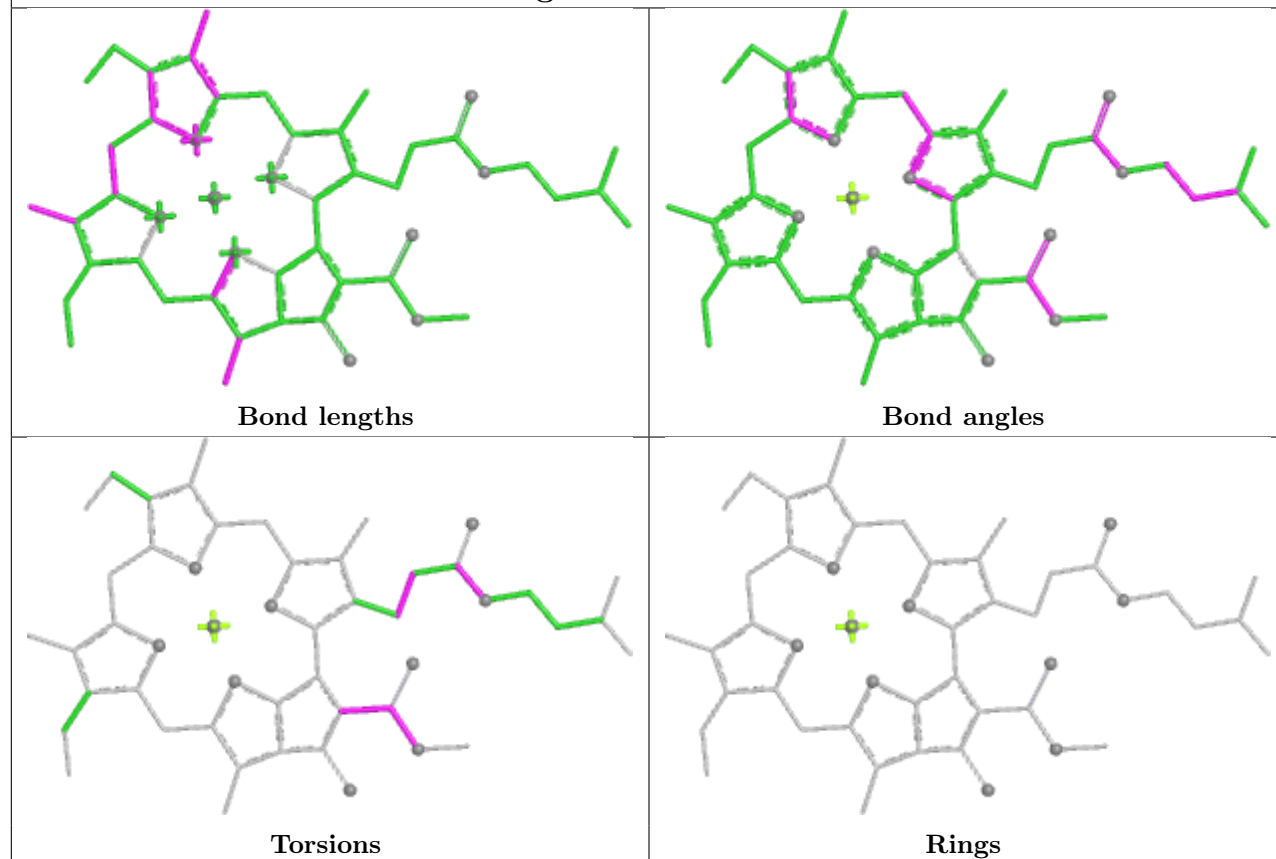
Ligand CLA B 1021



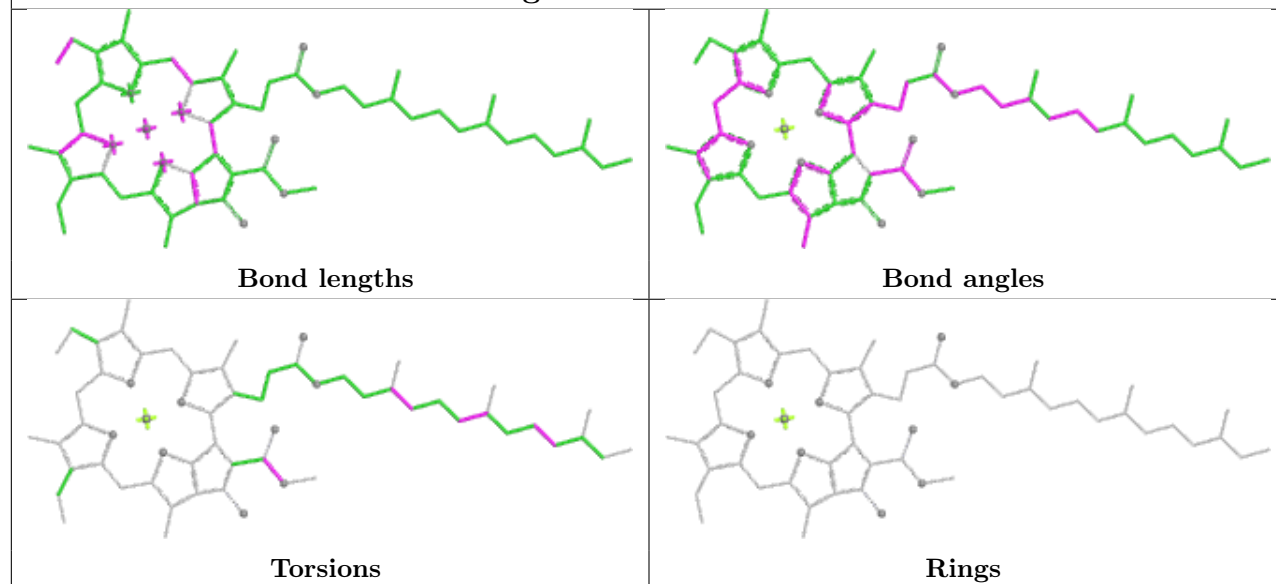


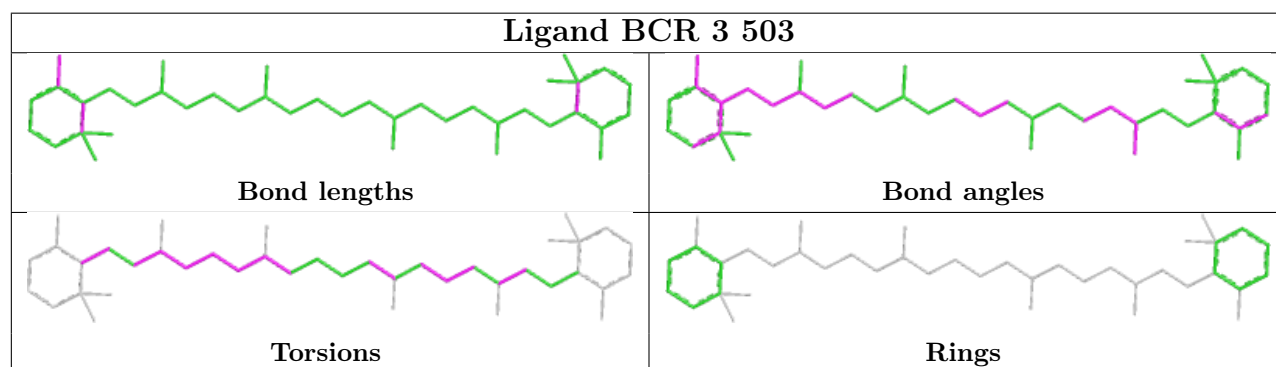
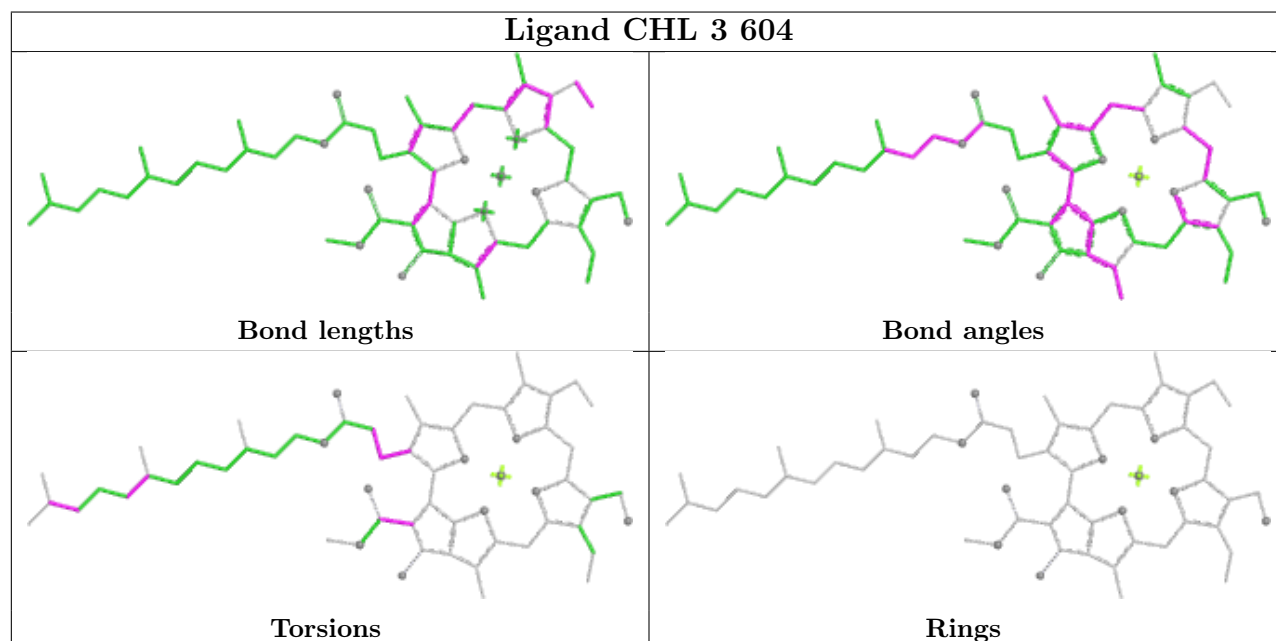
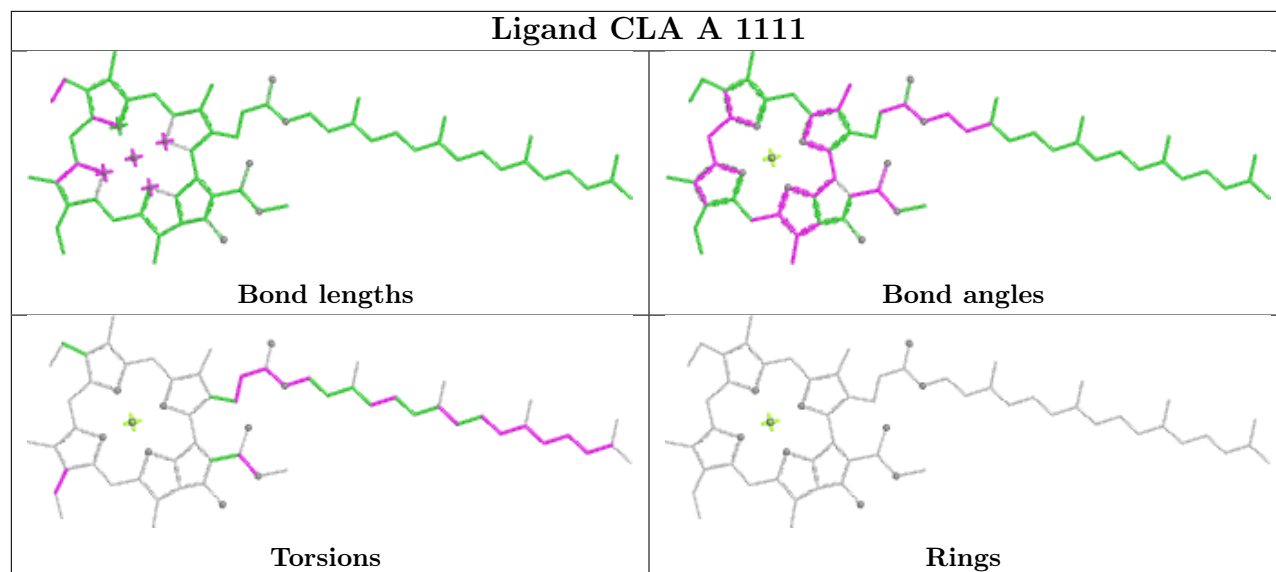
Ligand CLA 1 601**Ligand CLA A 1125**

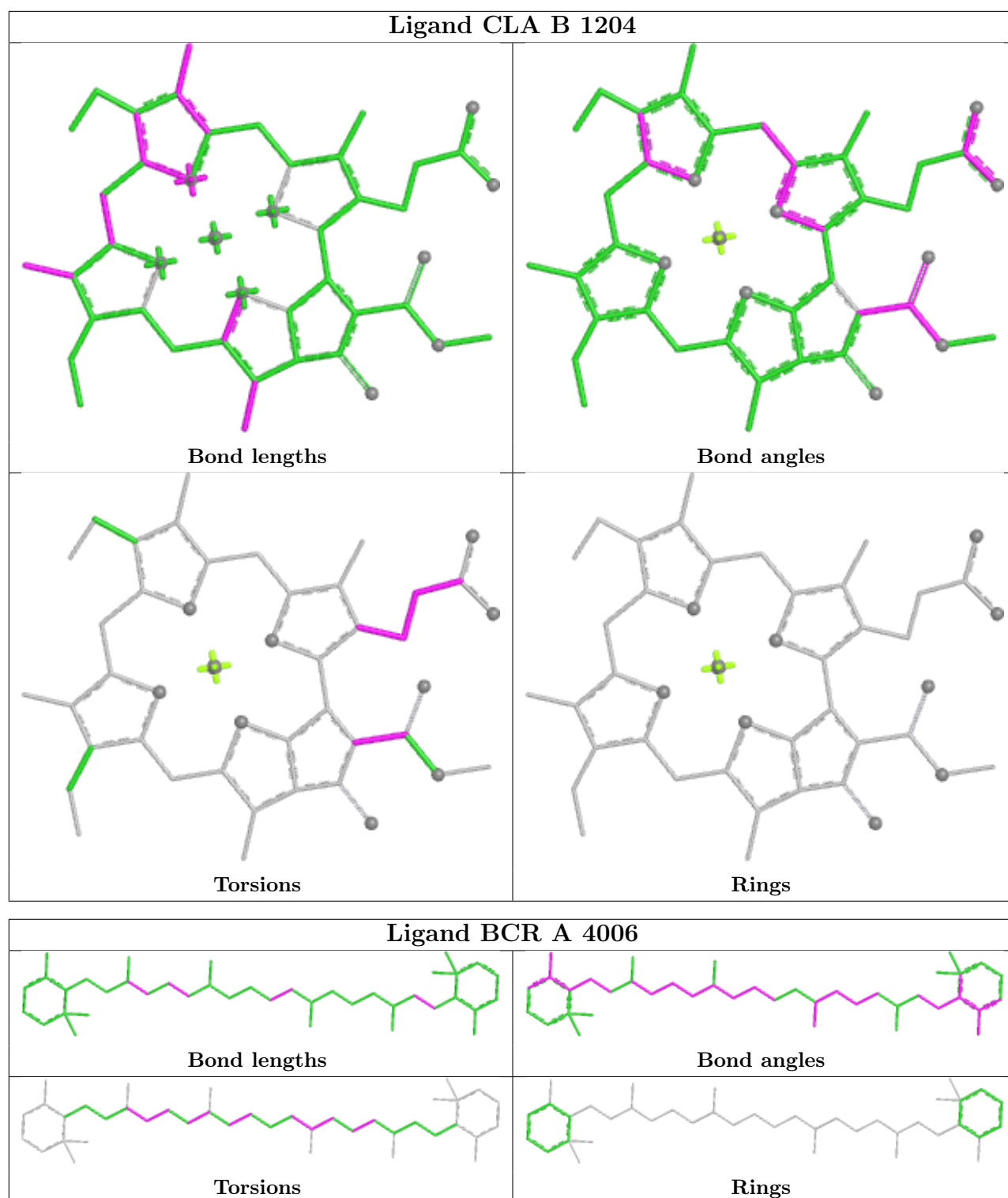
Ligand CLA 4 606



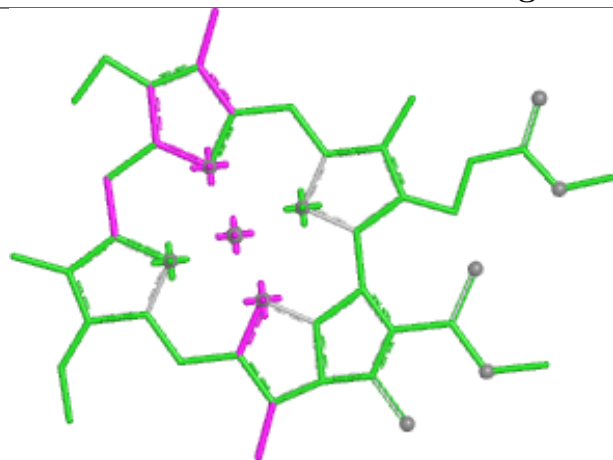
Ligand CLA A 1140



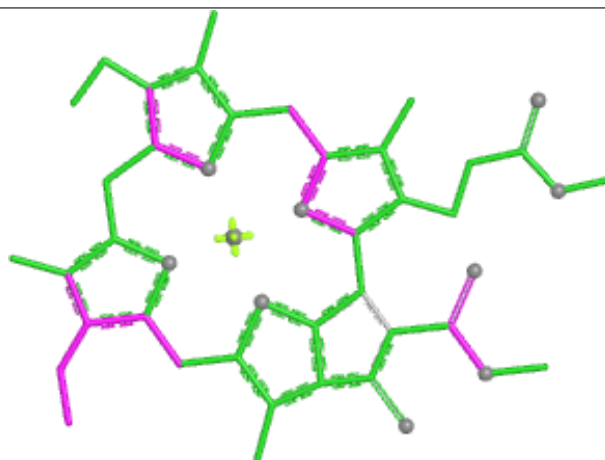




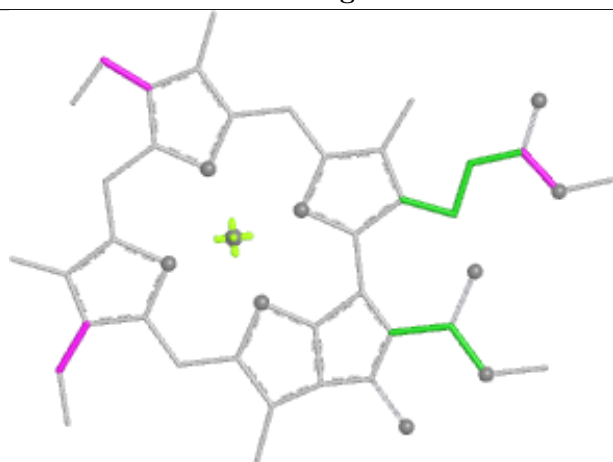
Ligand CLA 4 608



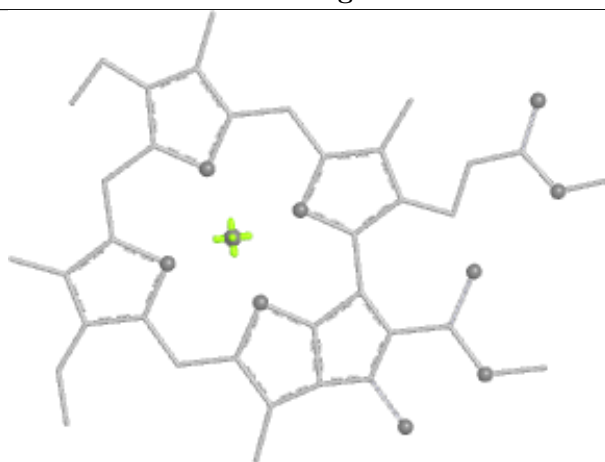
Bond lengths



Bond angles

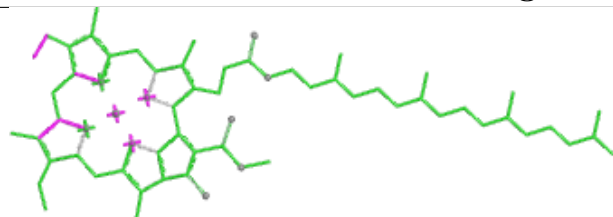


Torsions

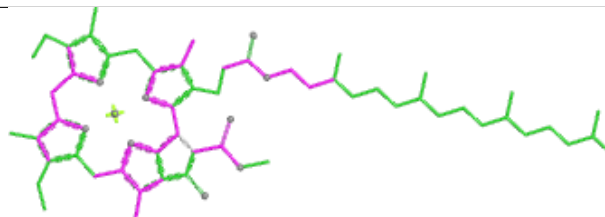


Rings

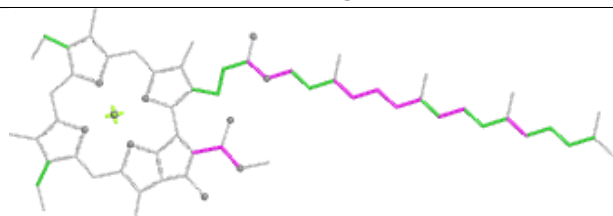
Ligand CLA 3 612



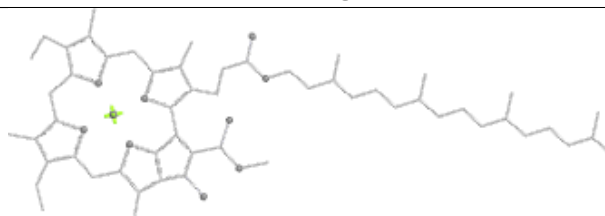
Bond lengths



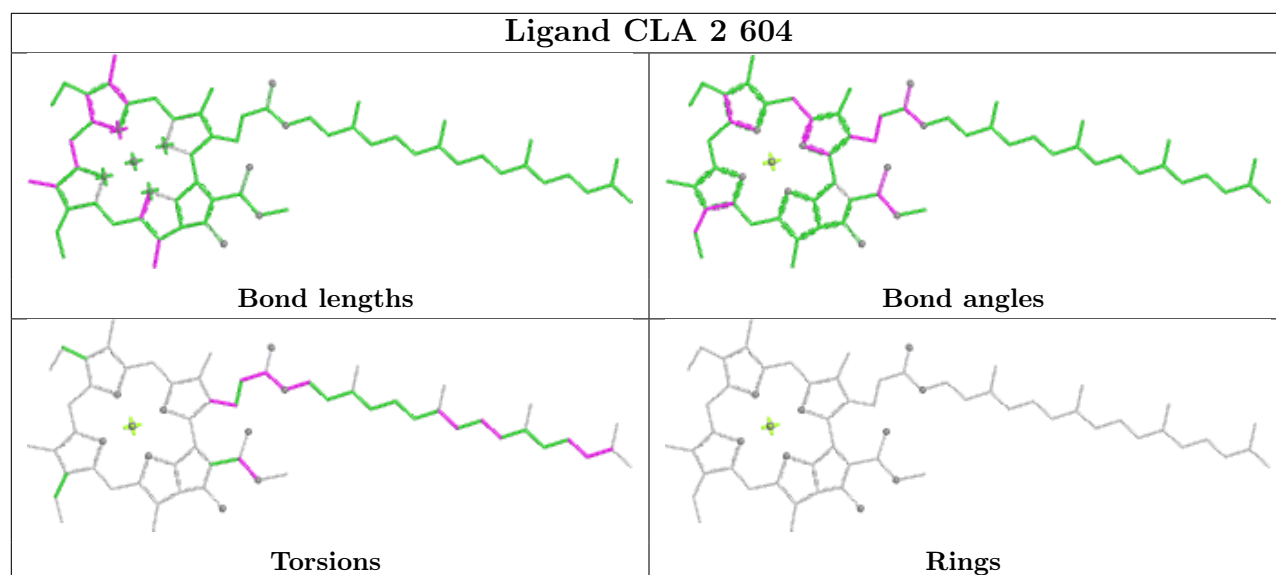
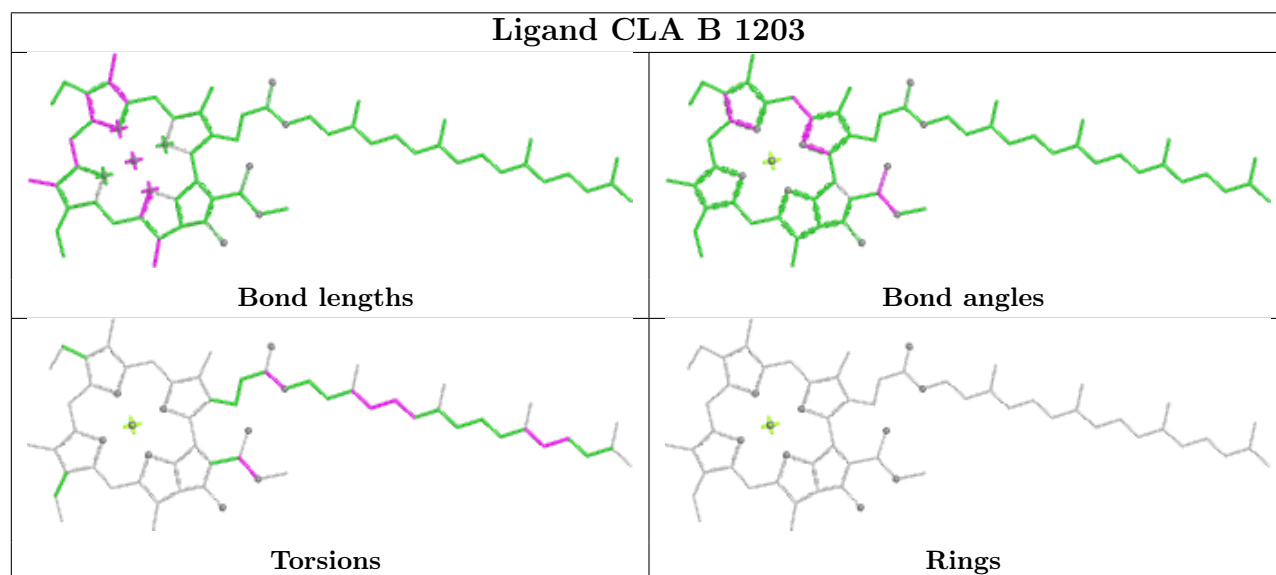
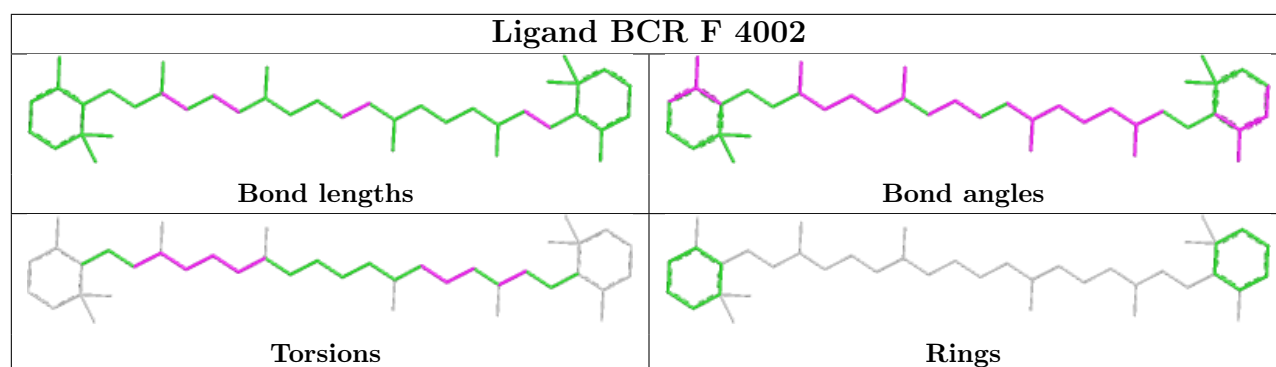
Bond angles



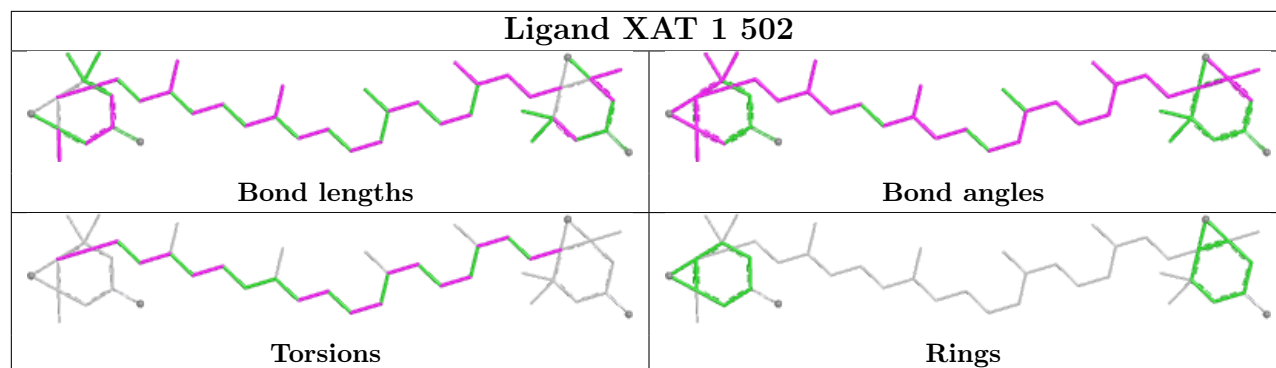
Torsions



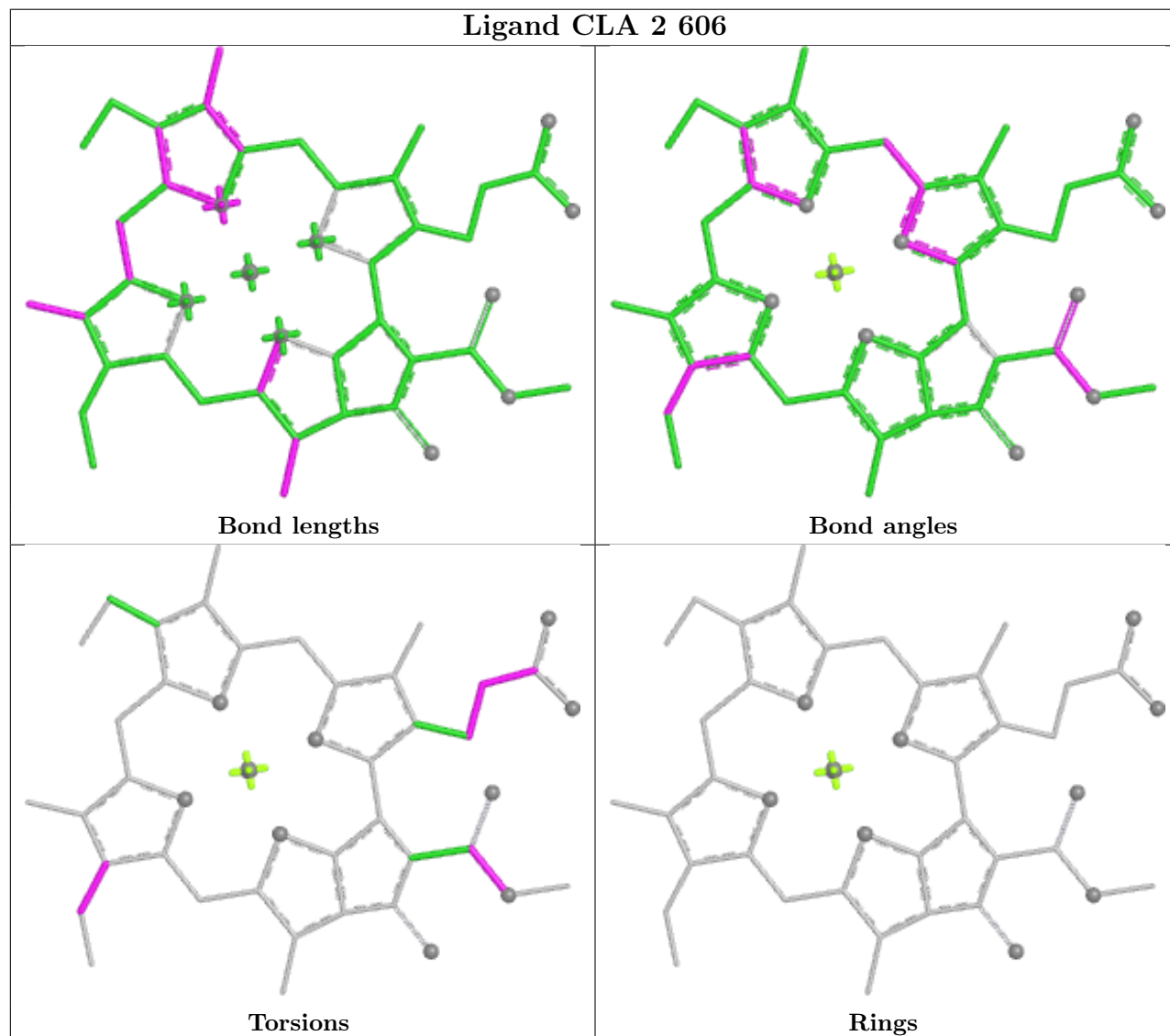
Rings



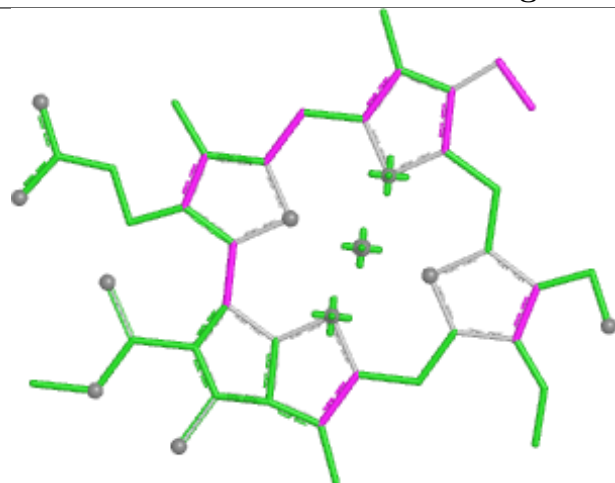
Ligand XAT 1 502



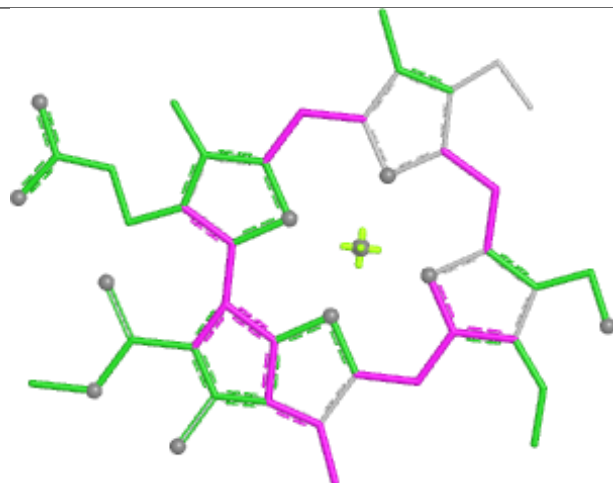
Ligand CLA 2 606



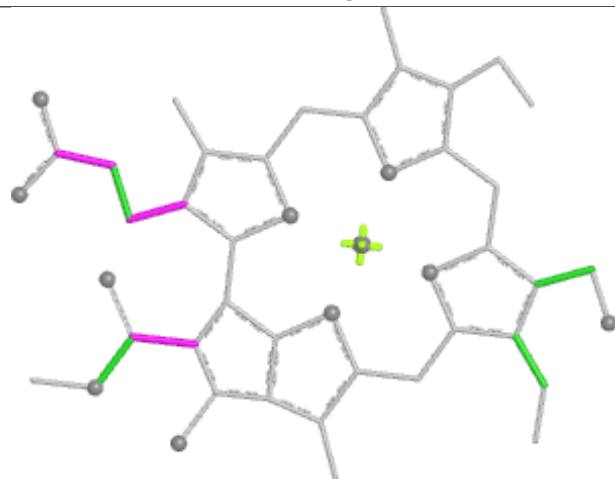
Ligand CHL 2 613



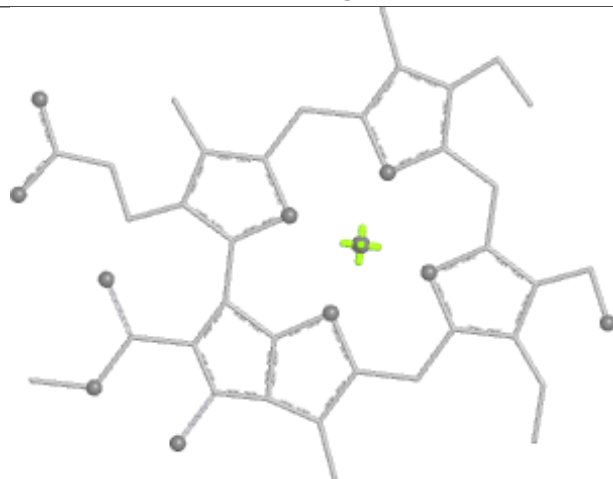
Bond lengths



Bond angles

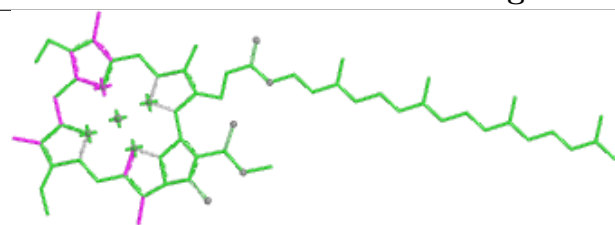


Torsions

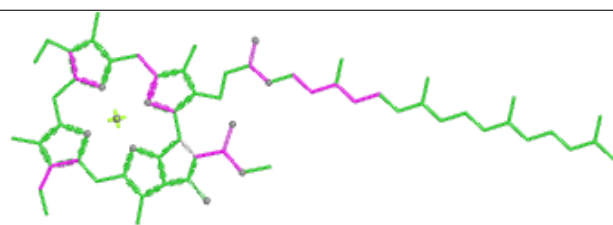


Rings

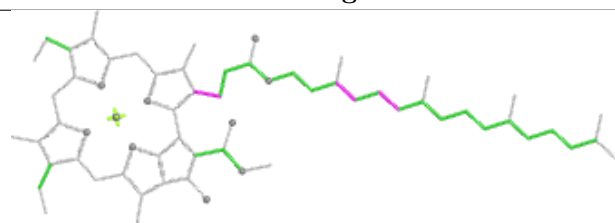
Ligand CLA B 1210



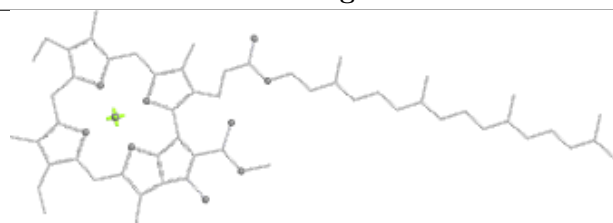
Bond lengths



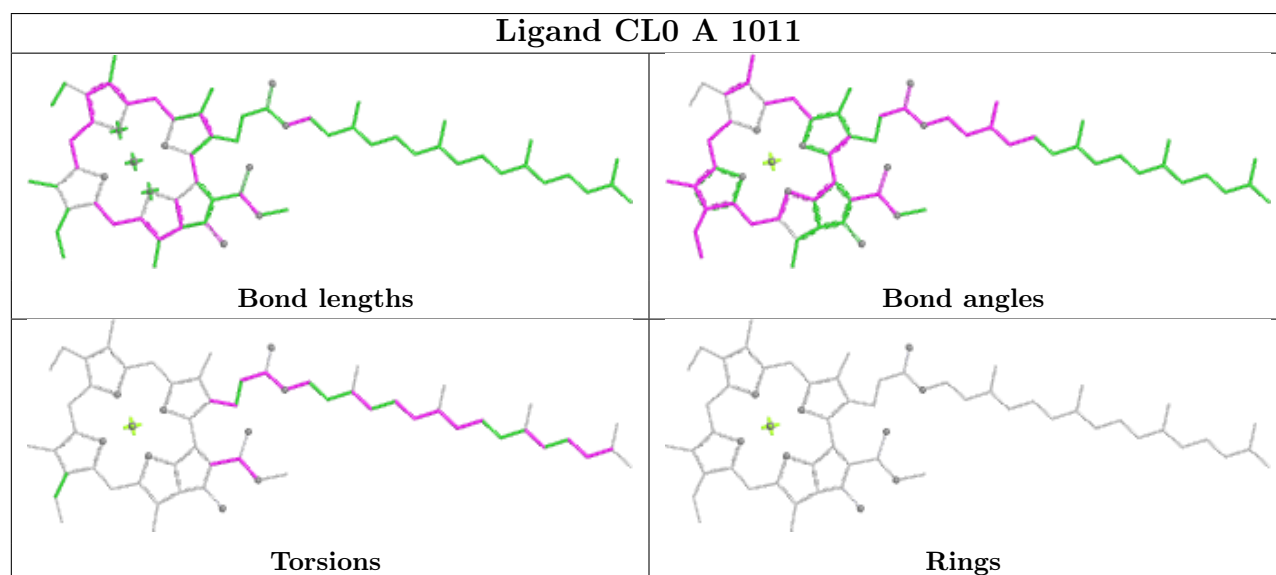
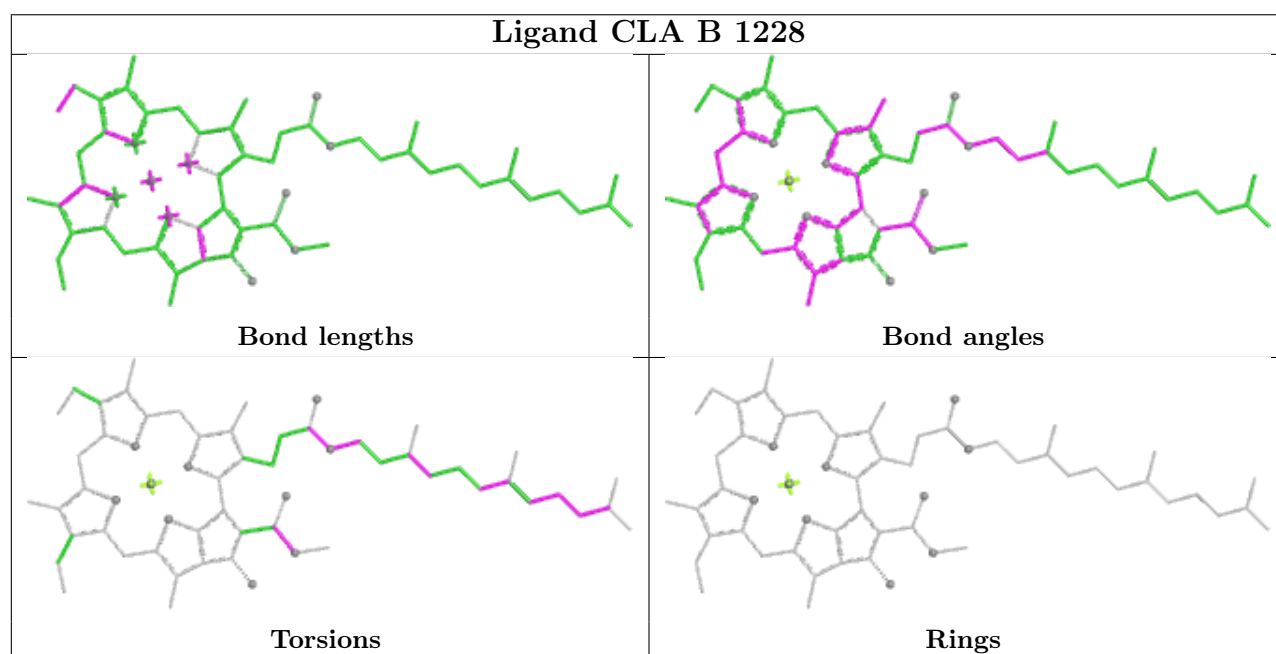
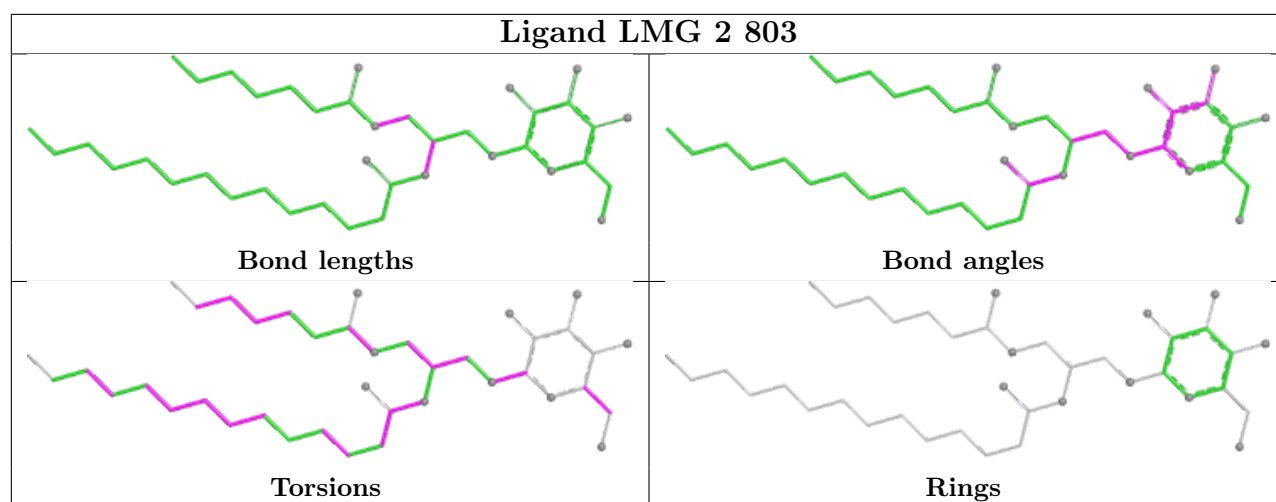
Bond angles

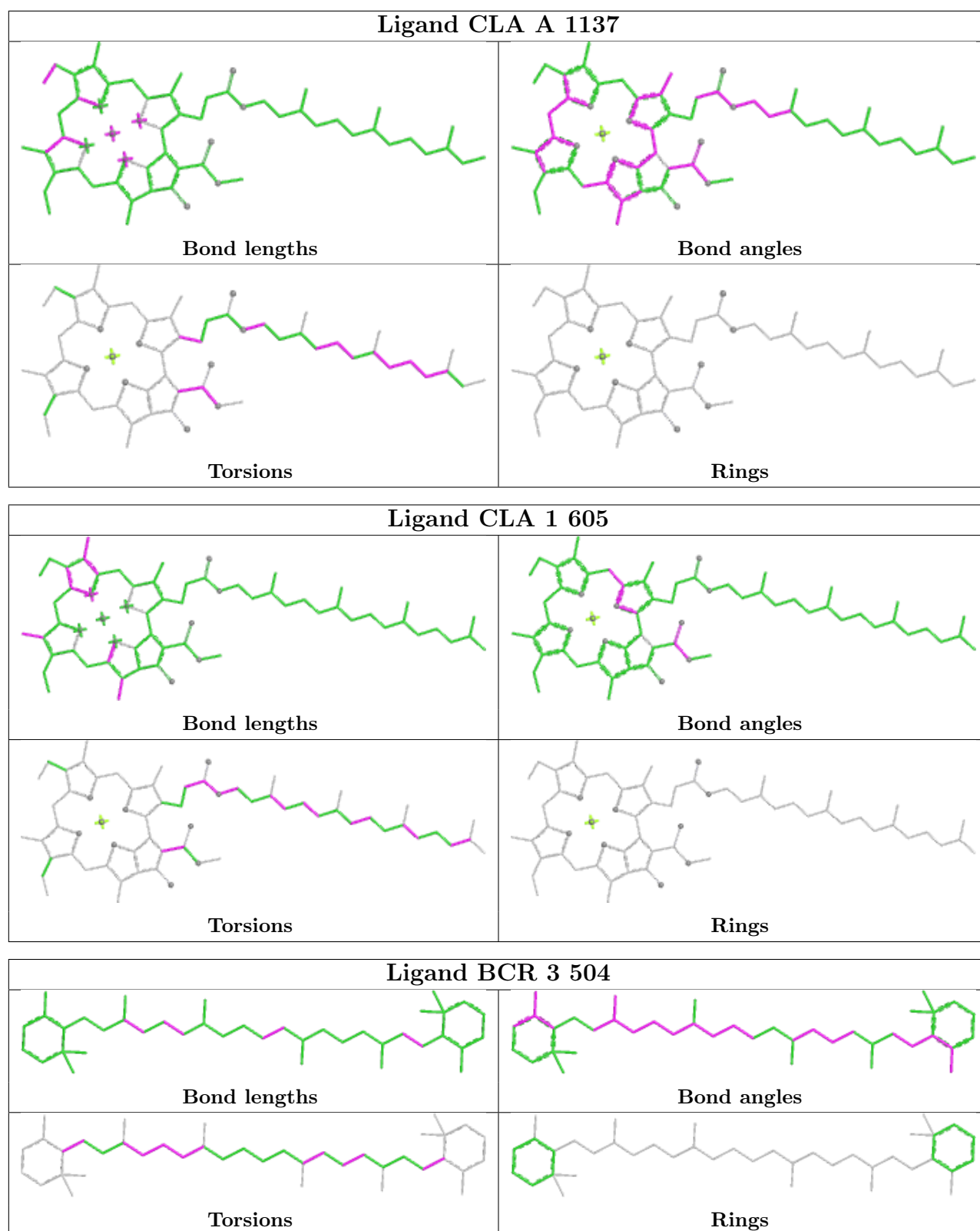


Torsions

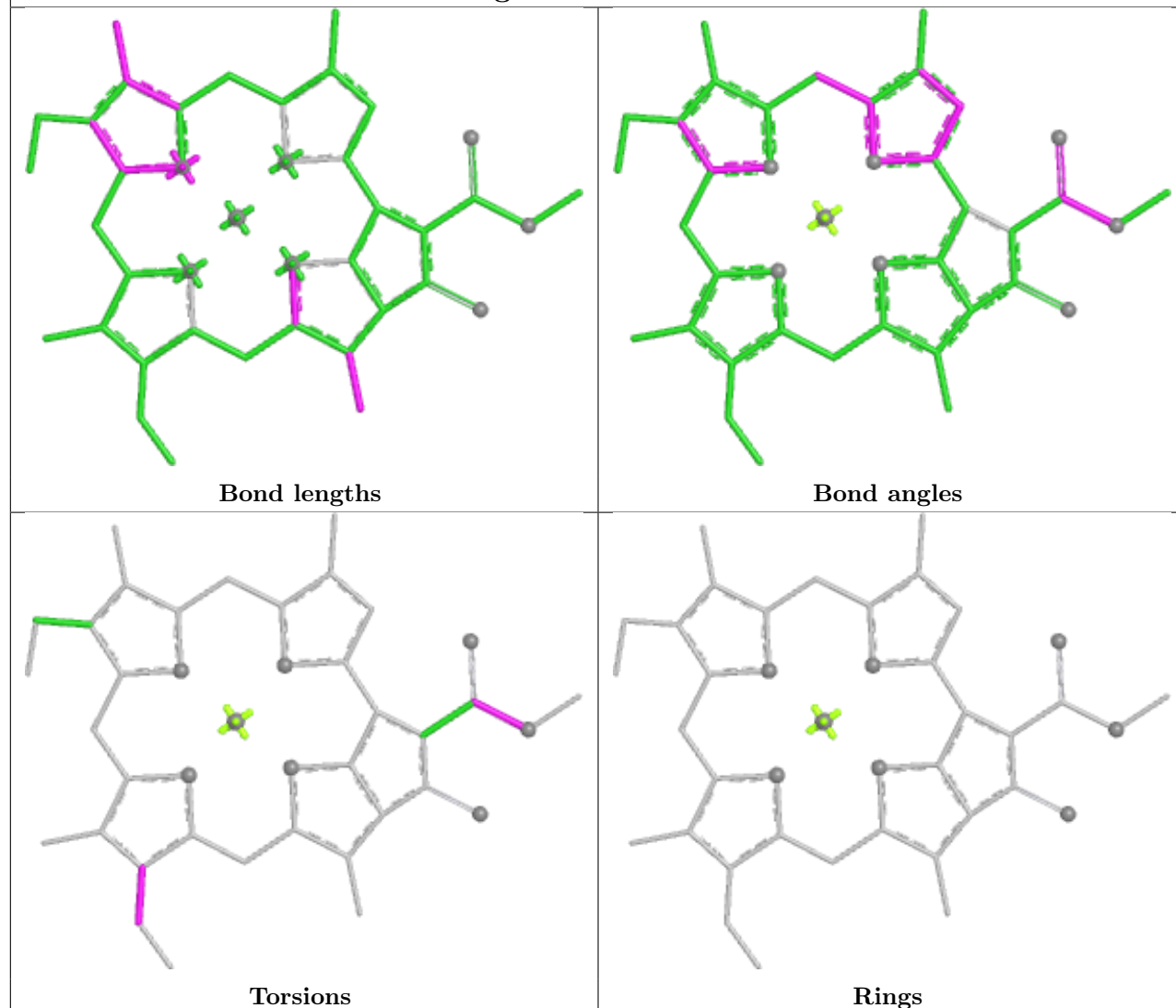


Rings

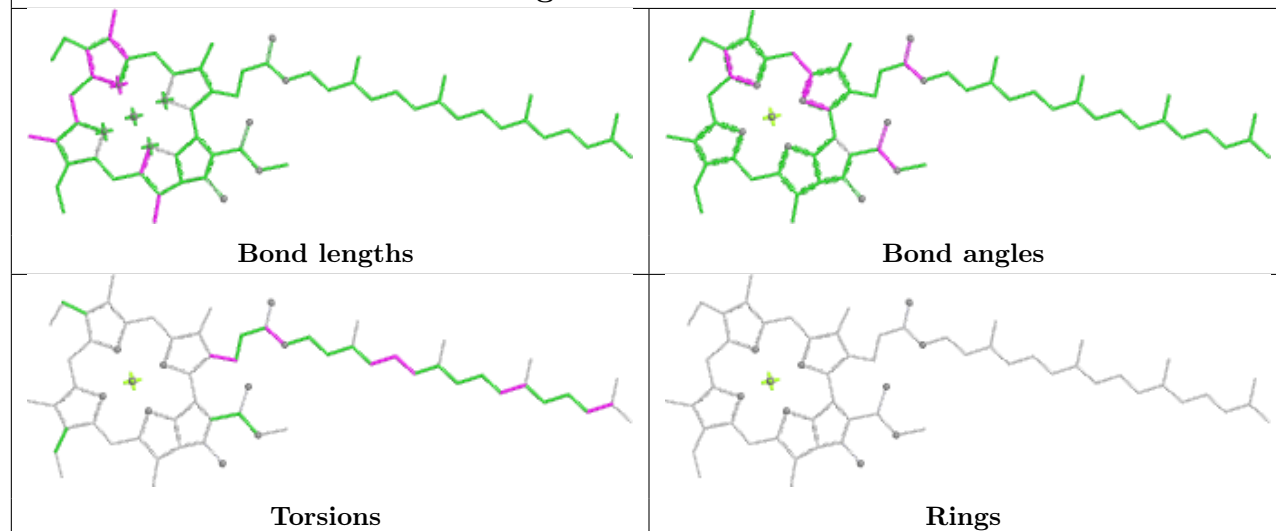


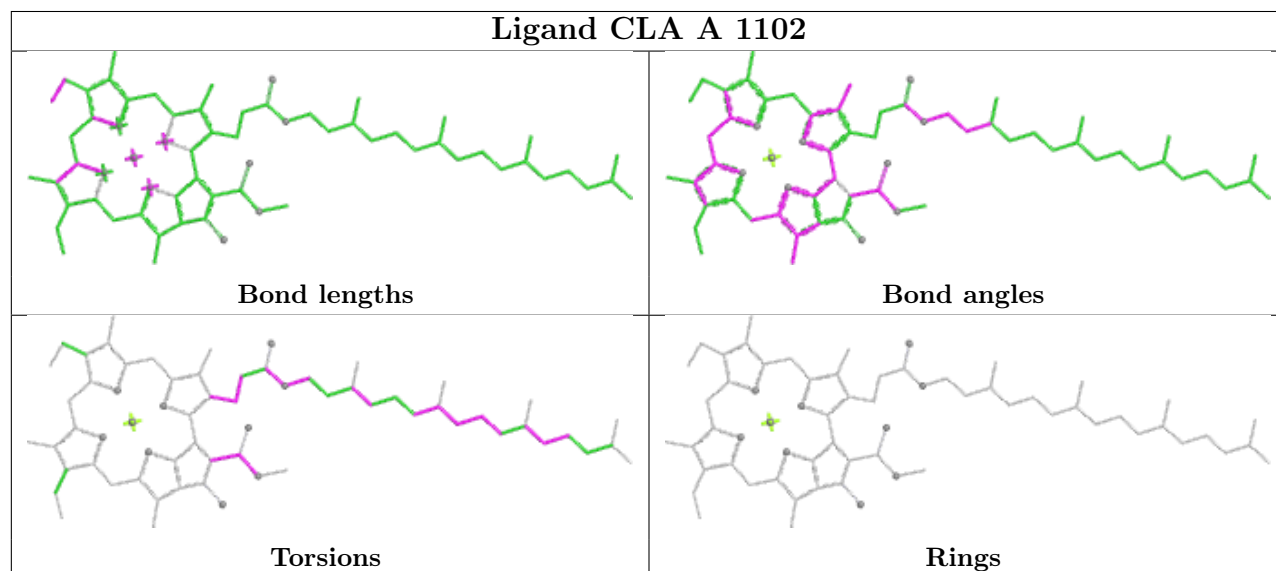
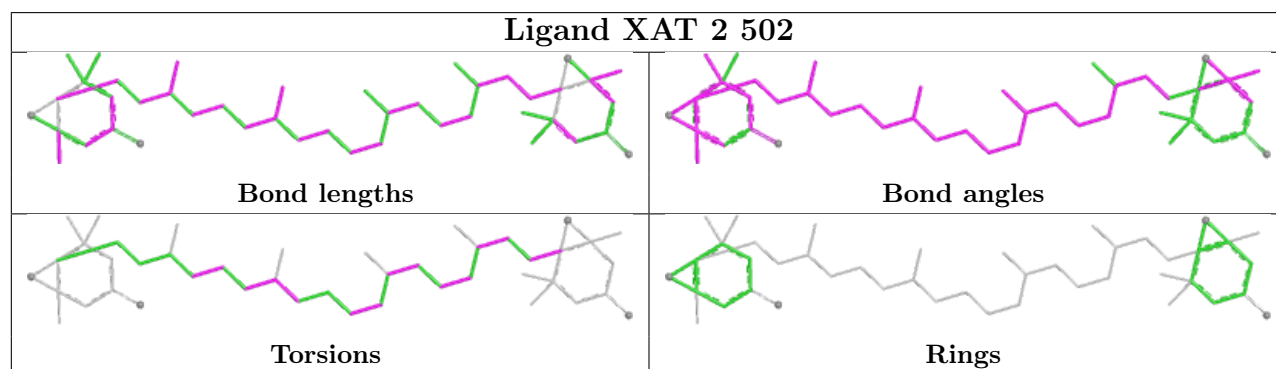
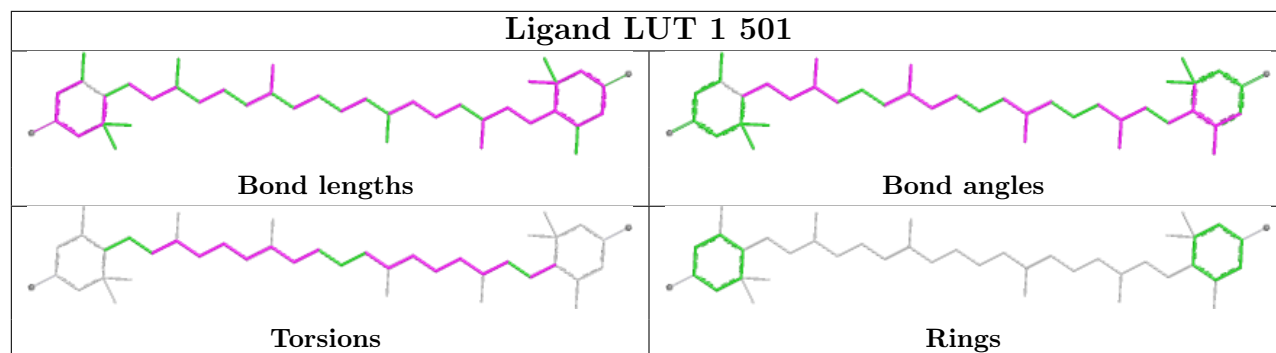


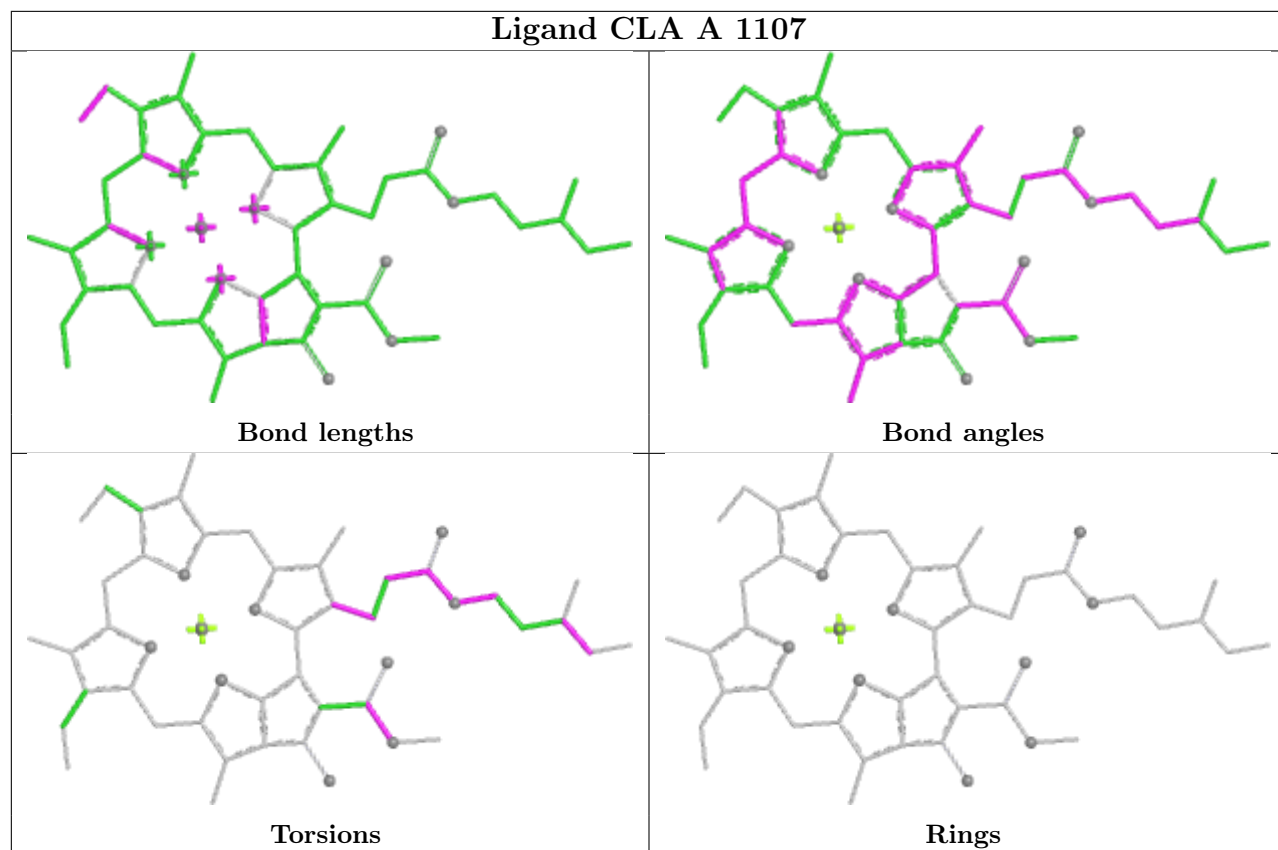
Ligand CLA 1 612



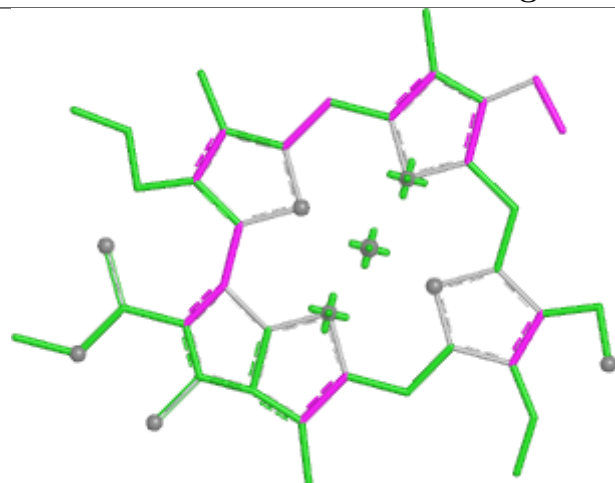
Ligand CLA 4 612



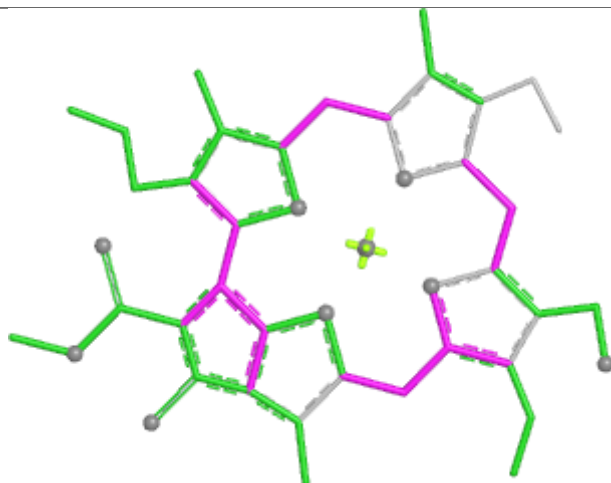




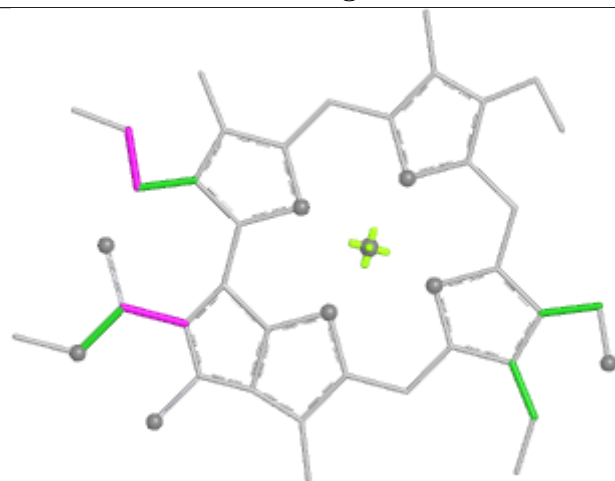
Ligand CHL 2 610



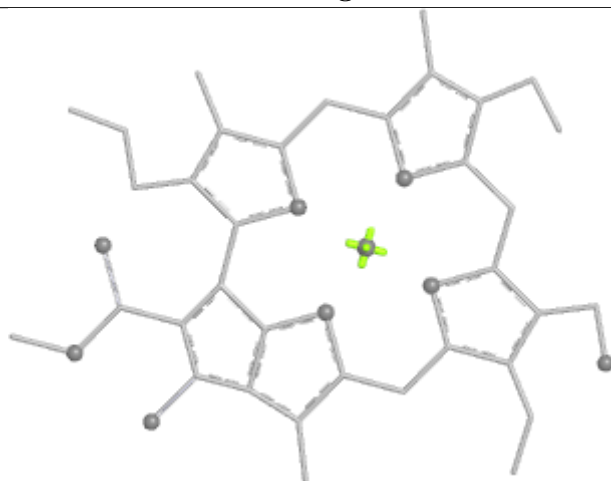
Bond lengths



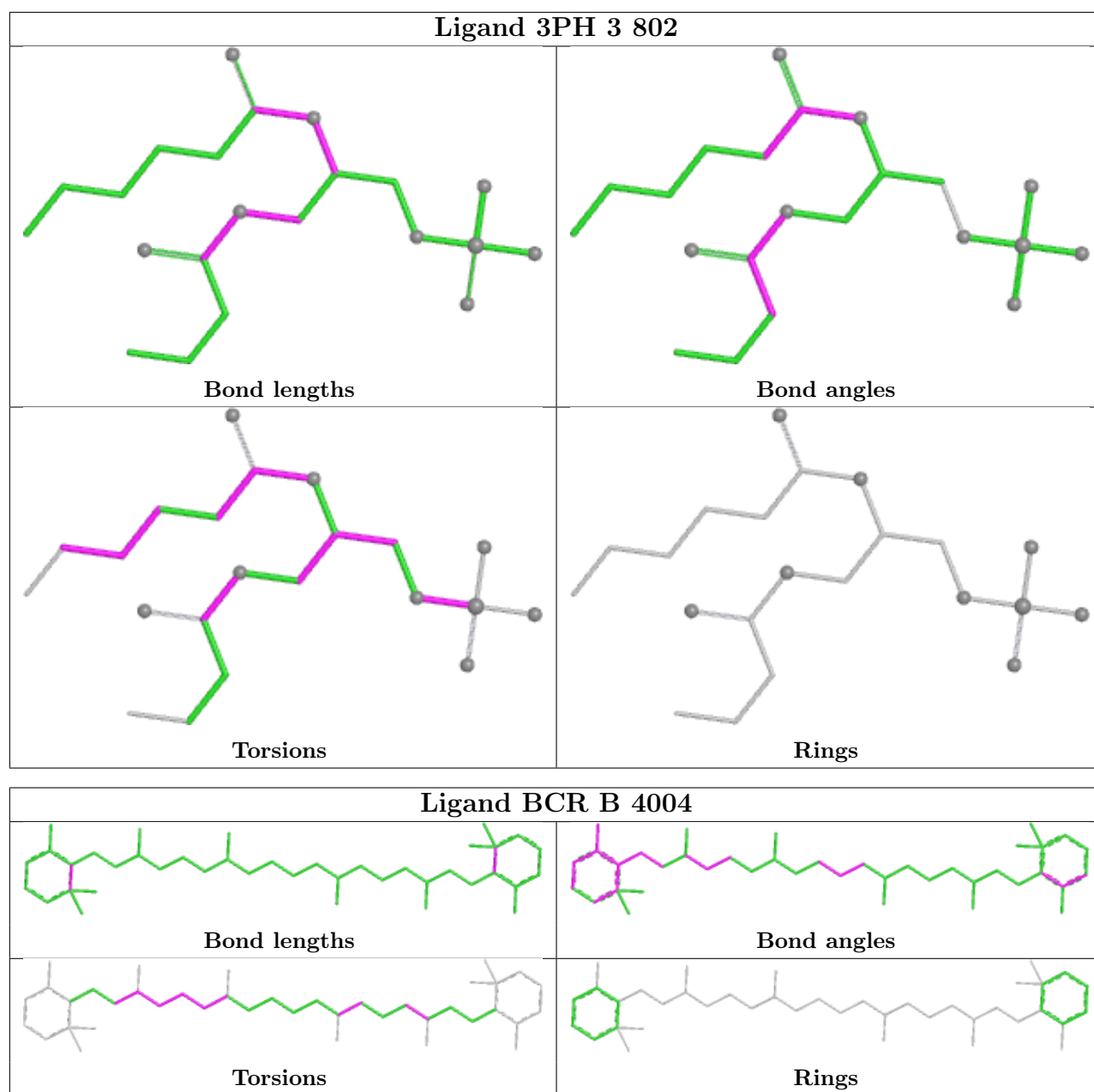
Bond angles

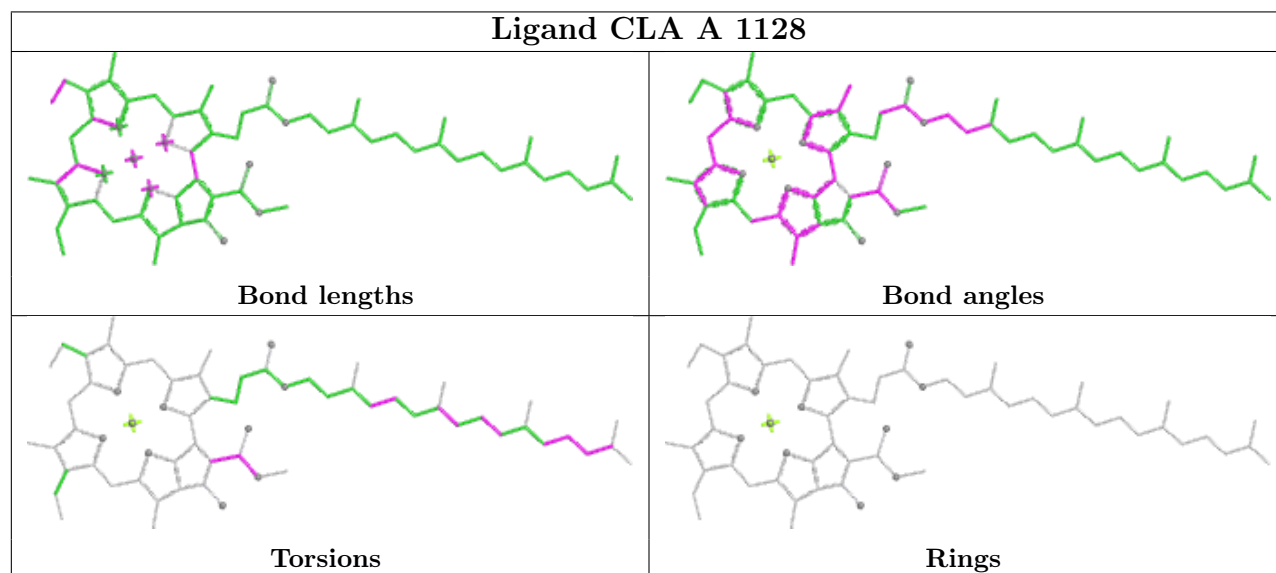
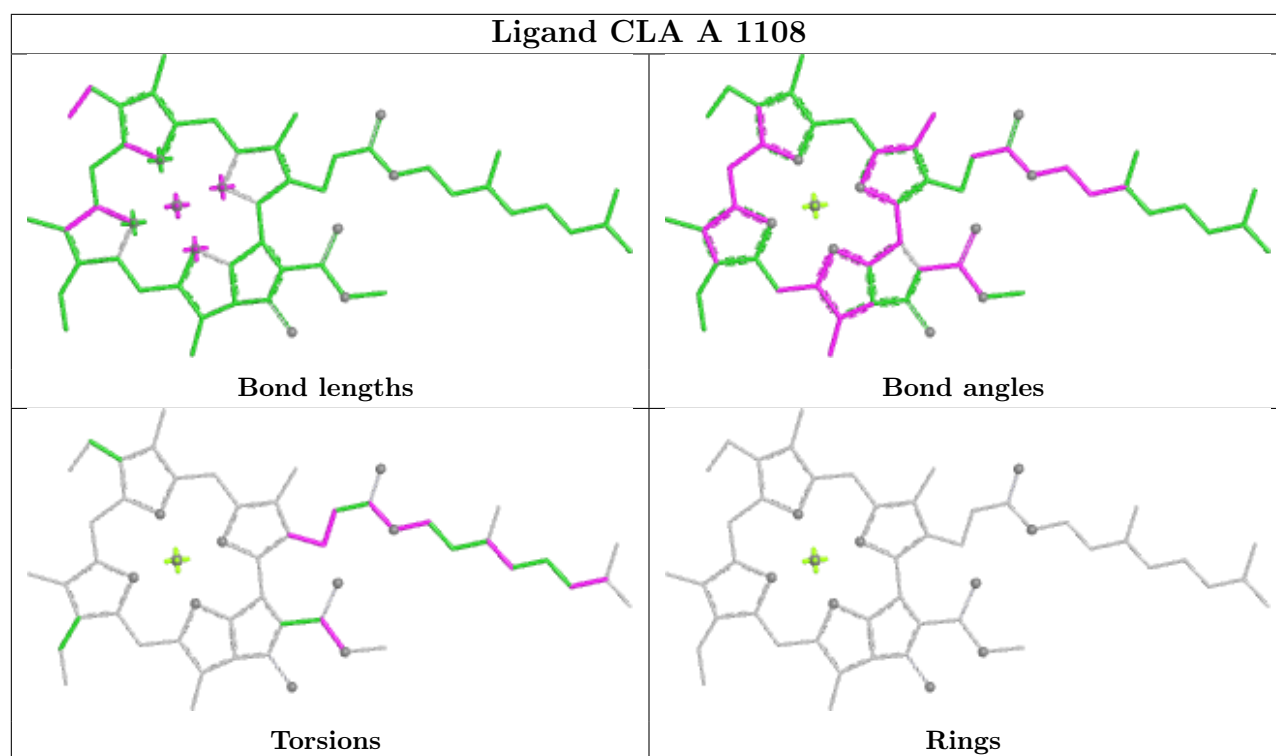


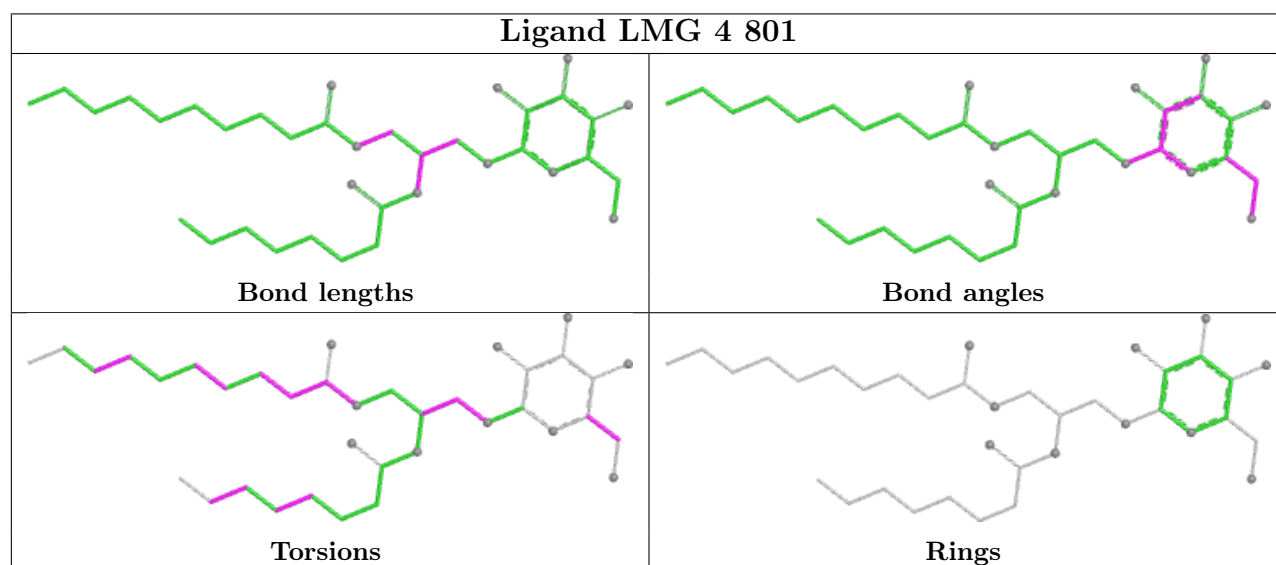
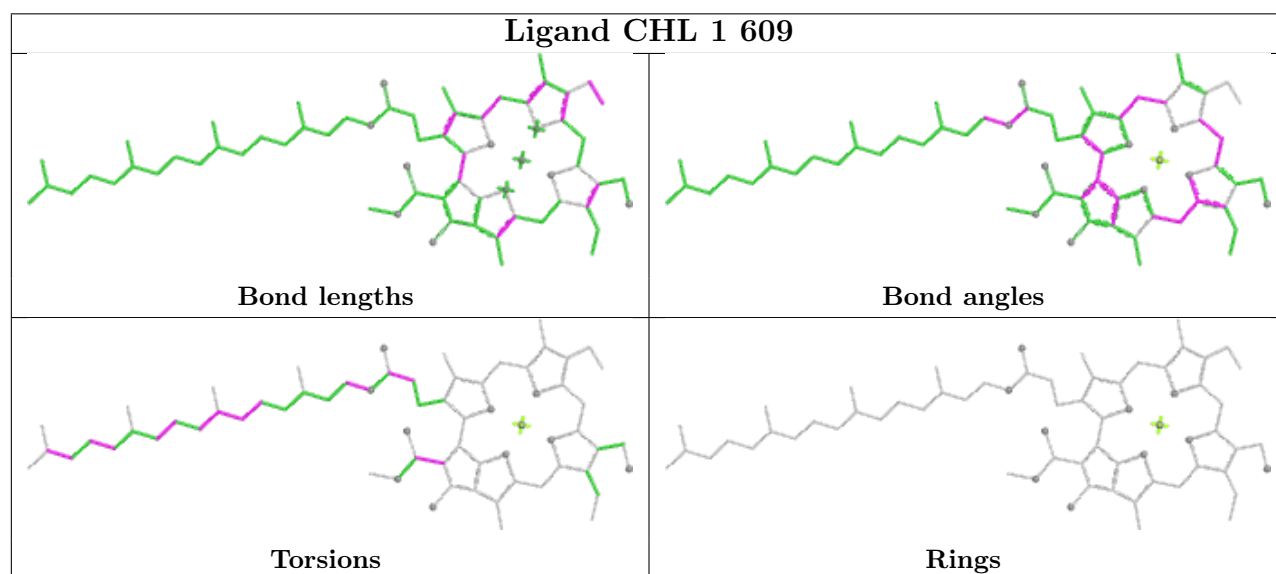
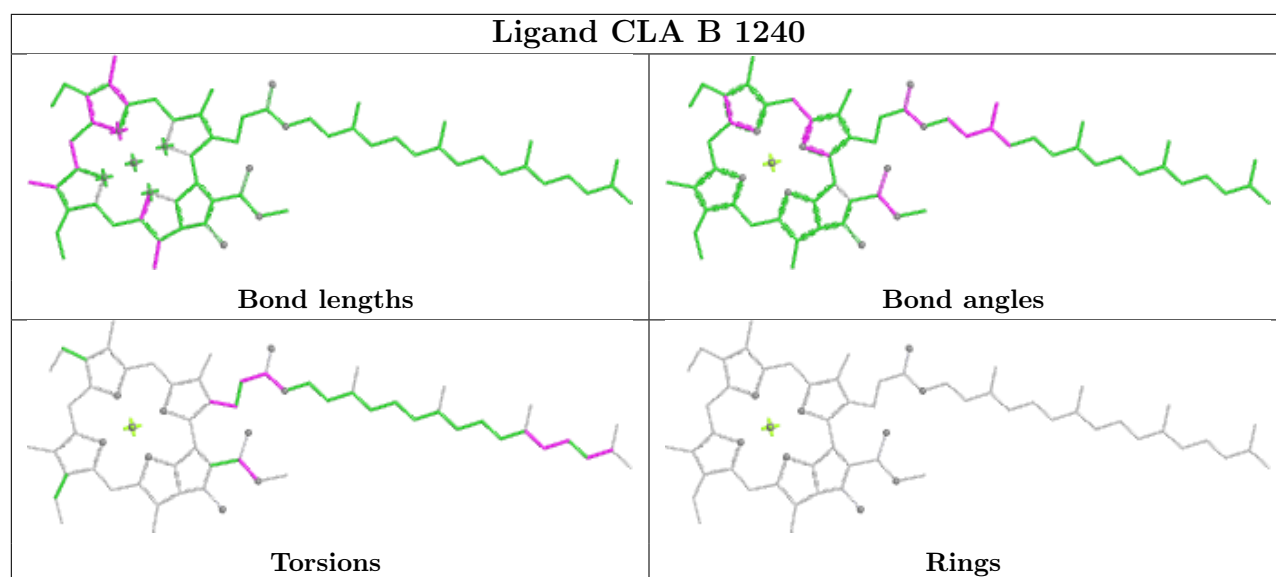
Torsions



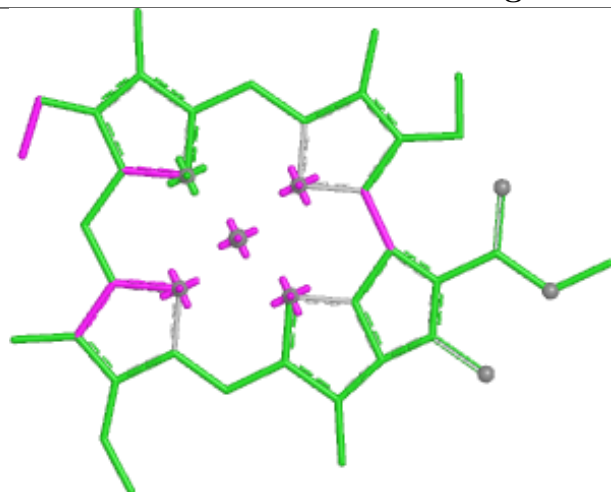
Rings



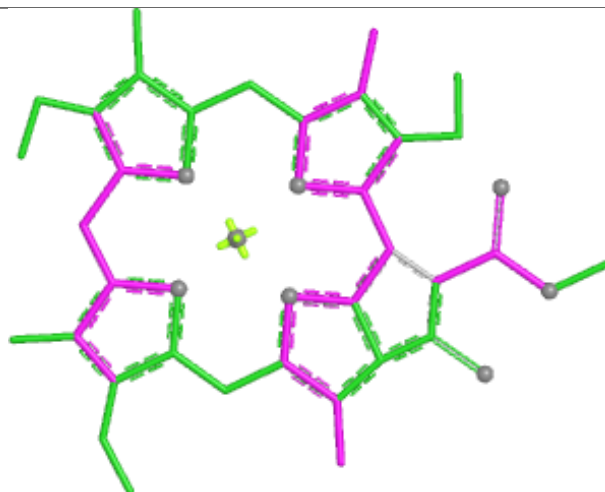




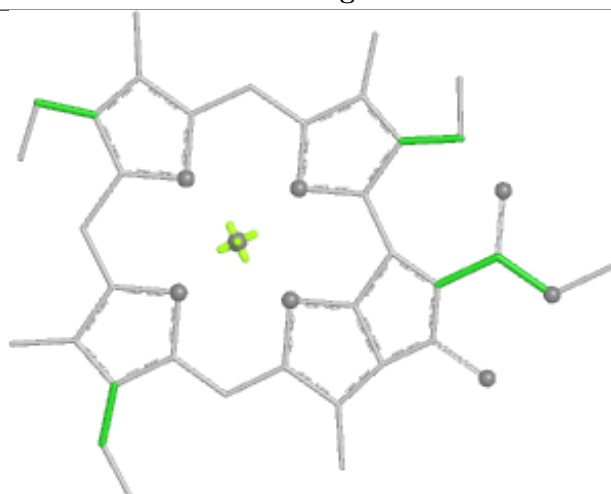
Ligand CLA A 1118



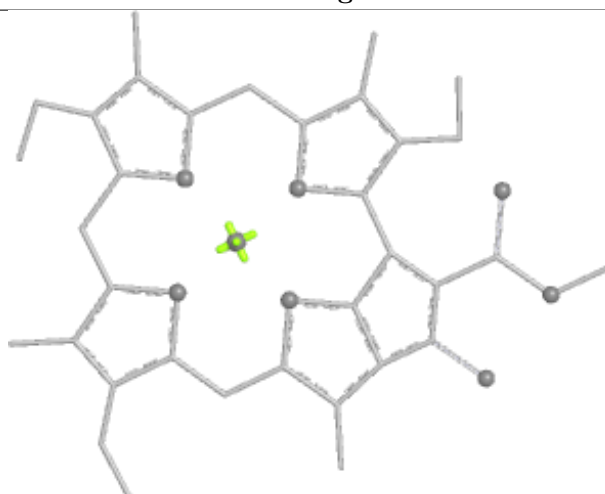
Bond lengths



Bond angles

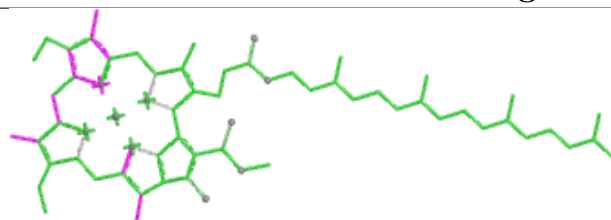


Torsions

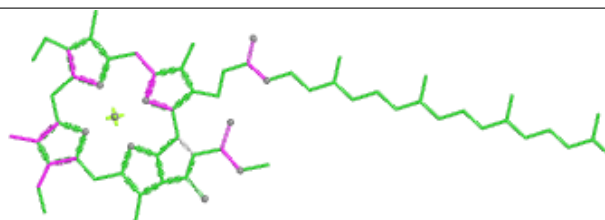


Rings

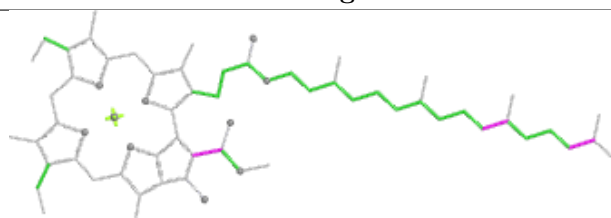
Ligand CLA 1 604



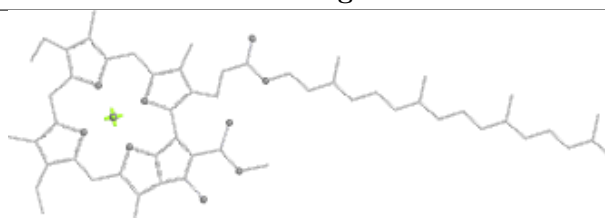
Bond lengths



Bond angles

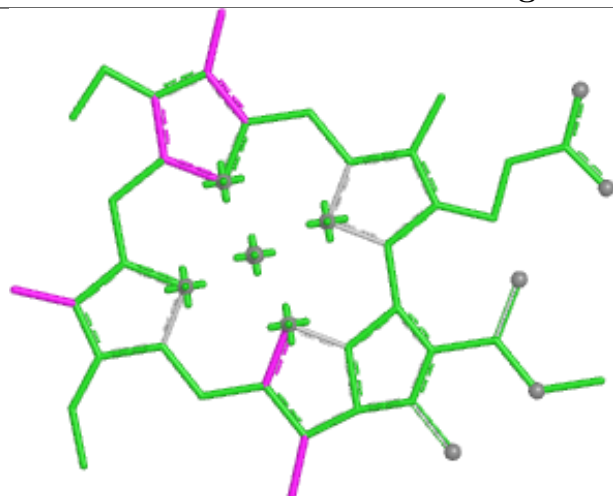


Torsions

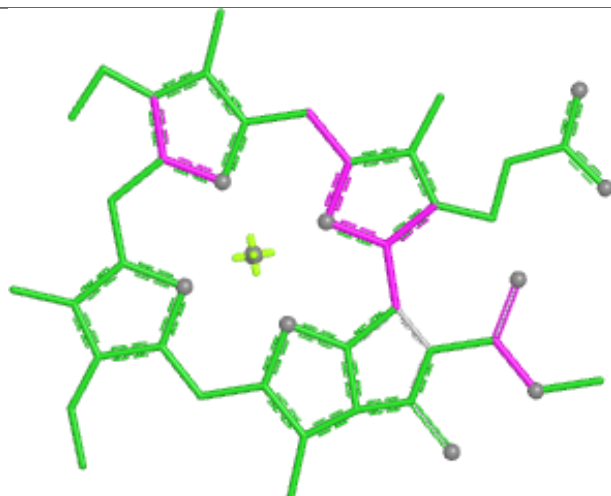


Rings

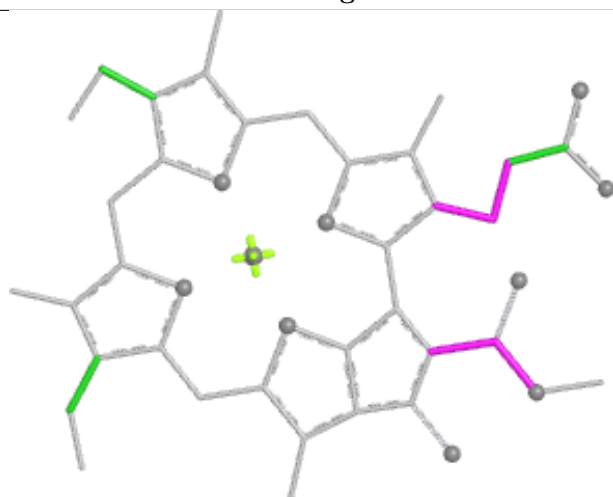
Ligand CLA 2 602



Bond lengths



Bond angles

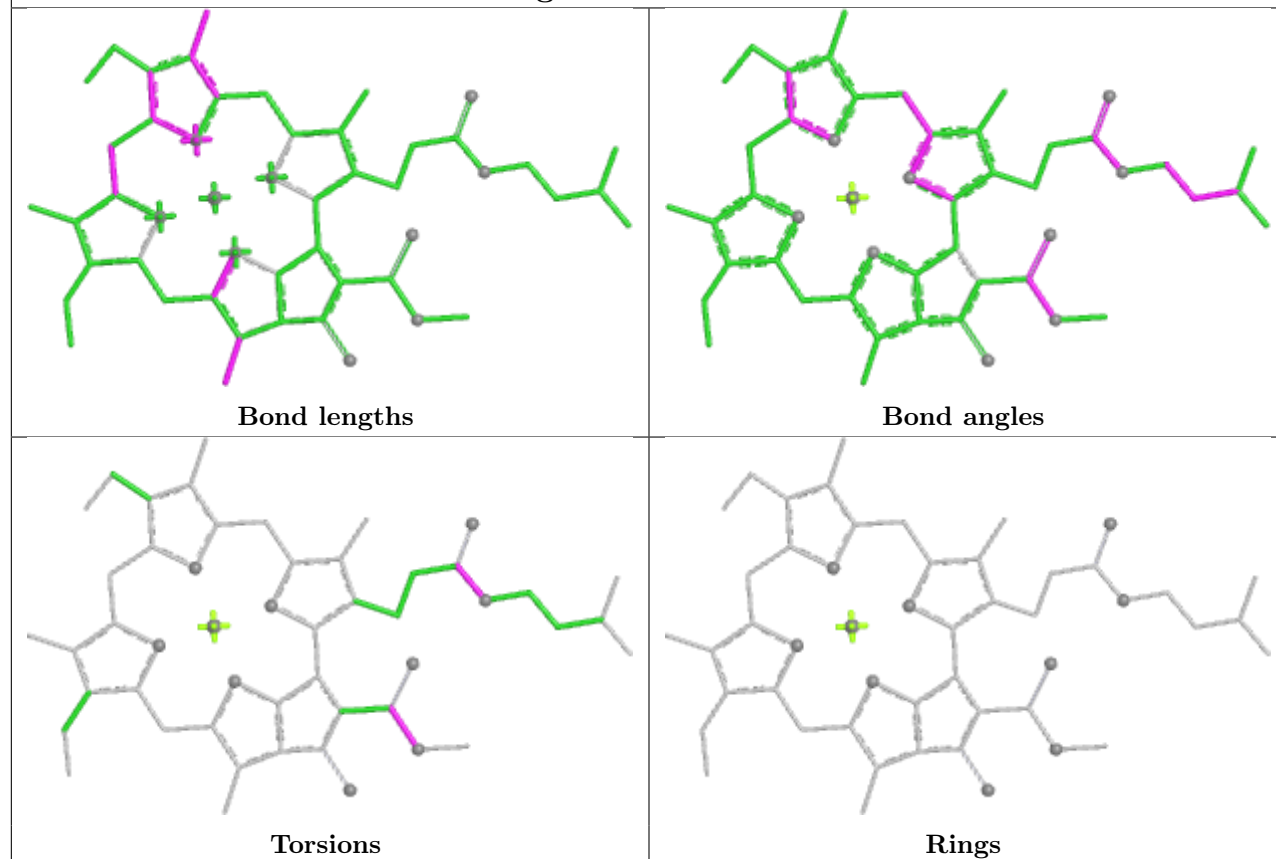


Torsions

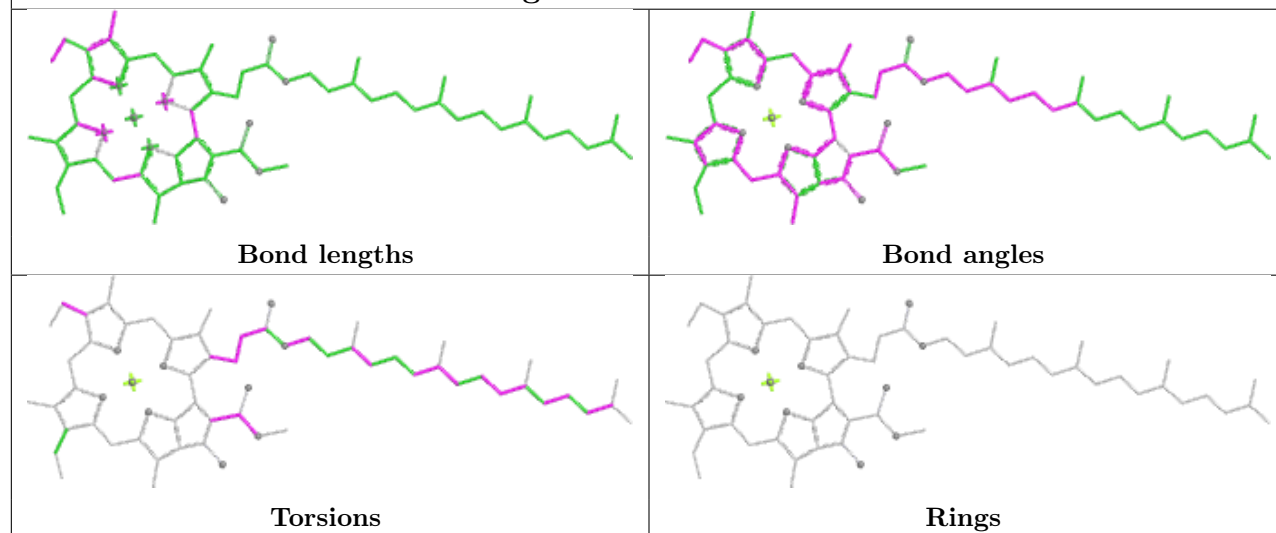


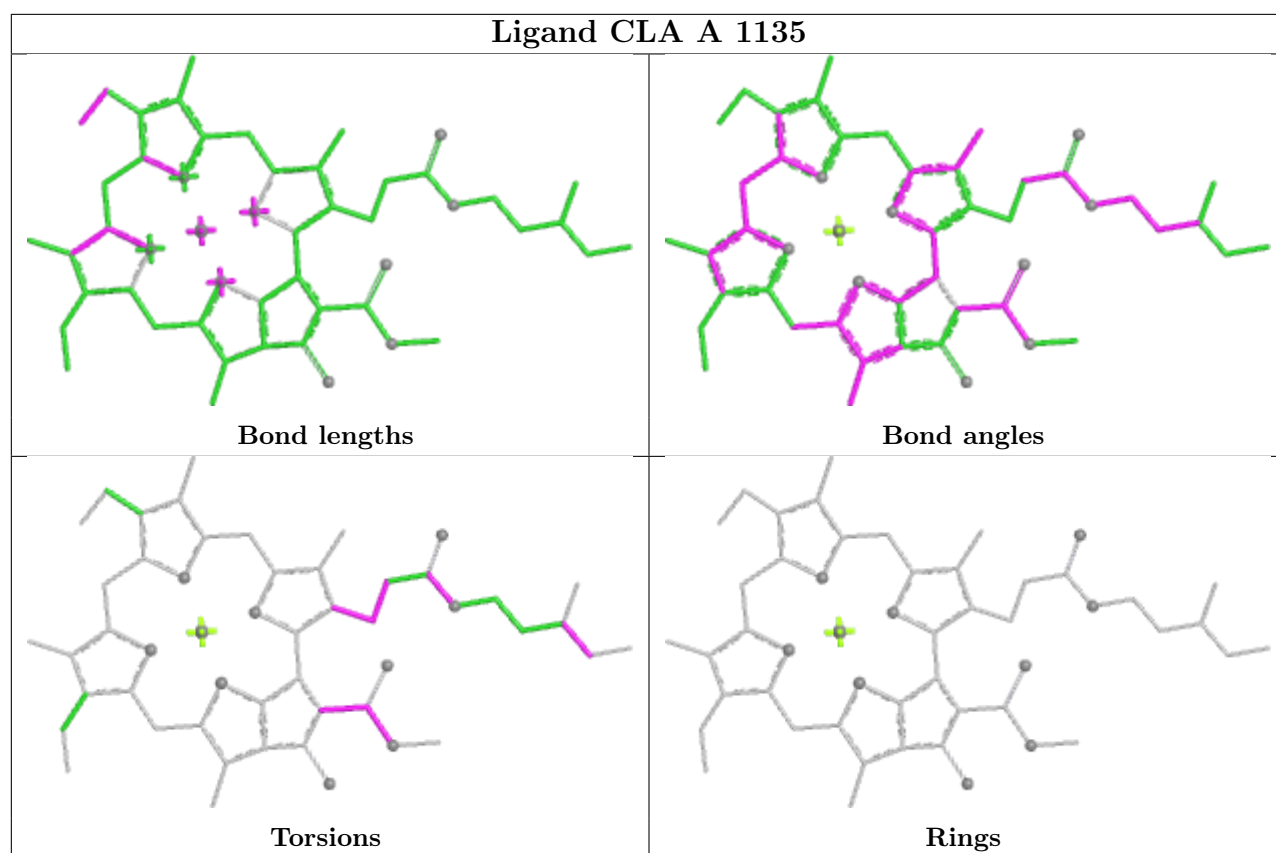
Rings

Ligand CLA 1 606

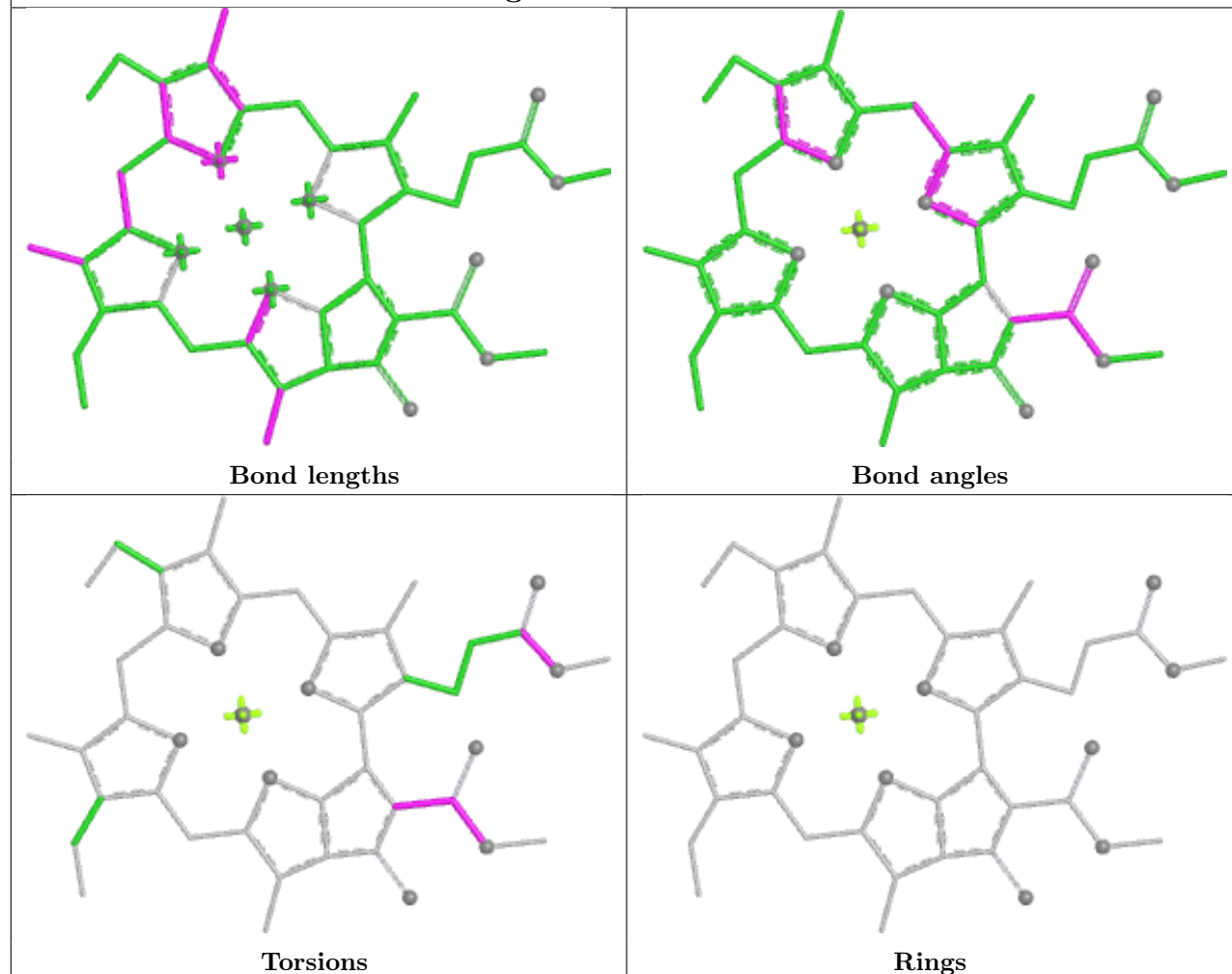


Ligand CLA A 1133

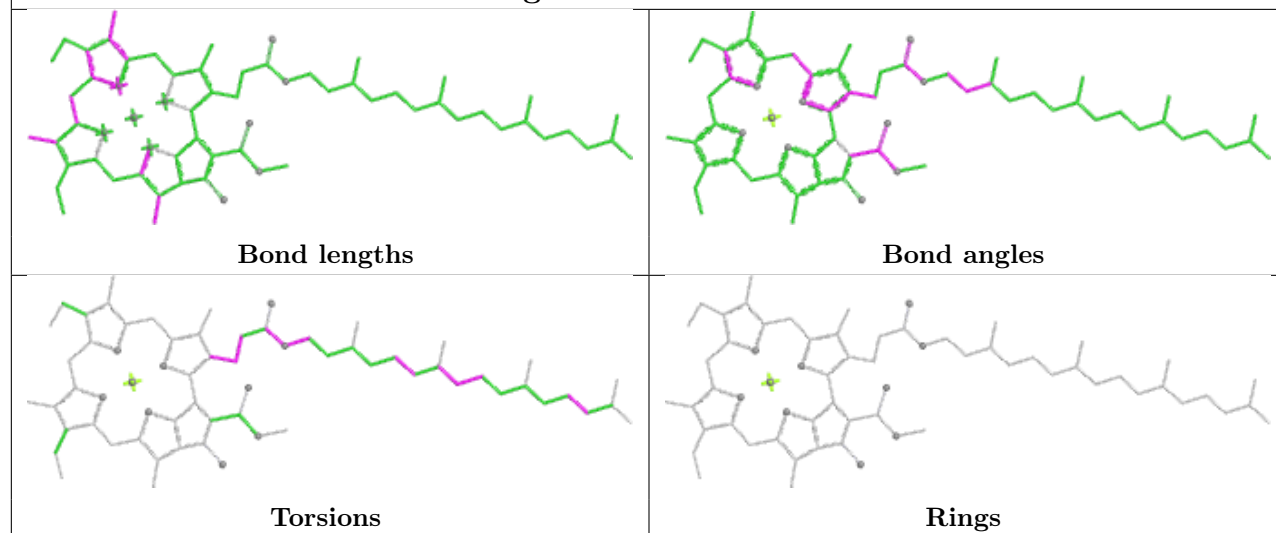




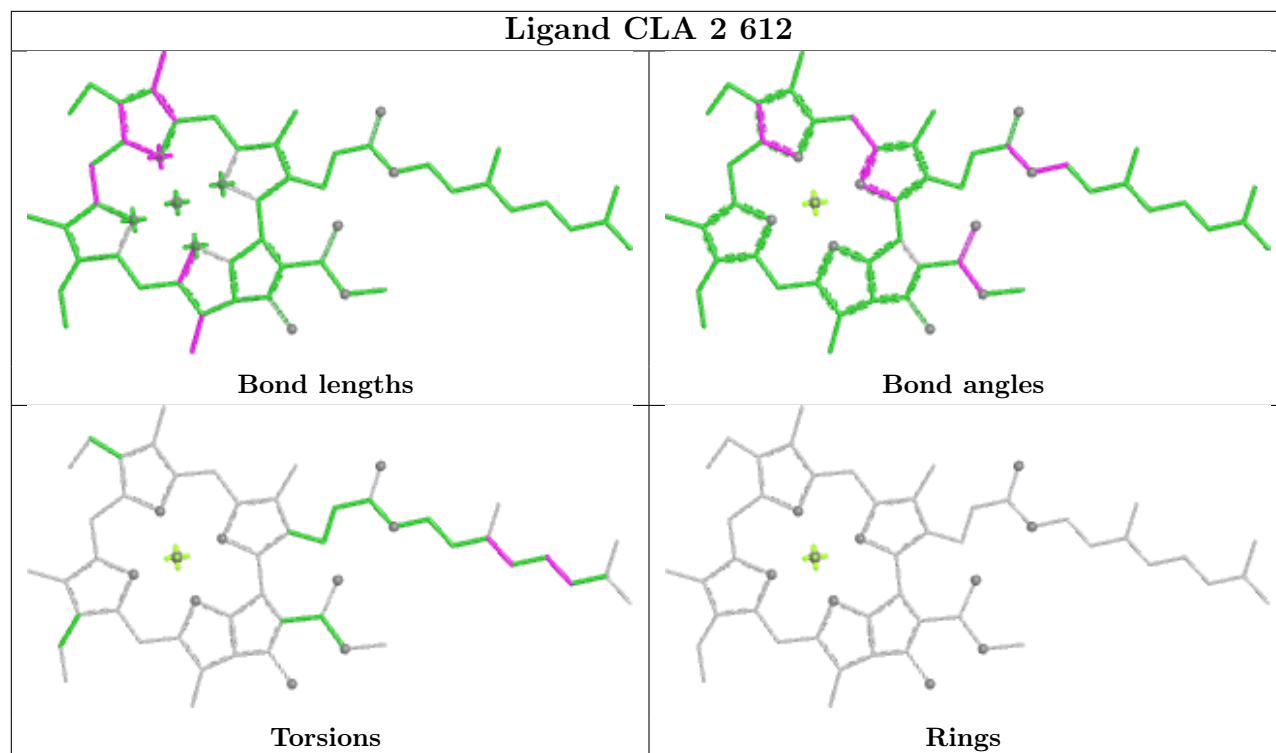
Ligand CLA B 1232



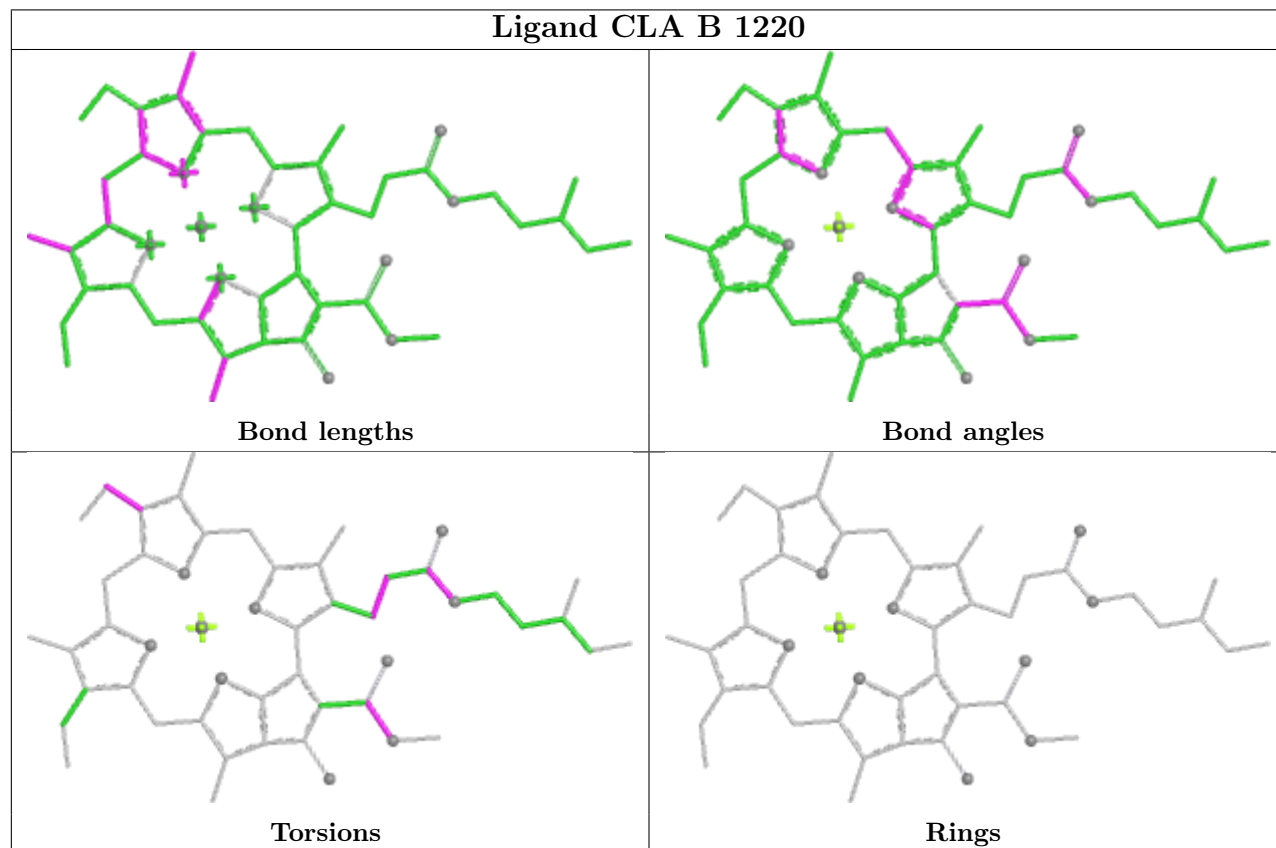
Ligand CLA B 1215

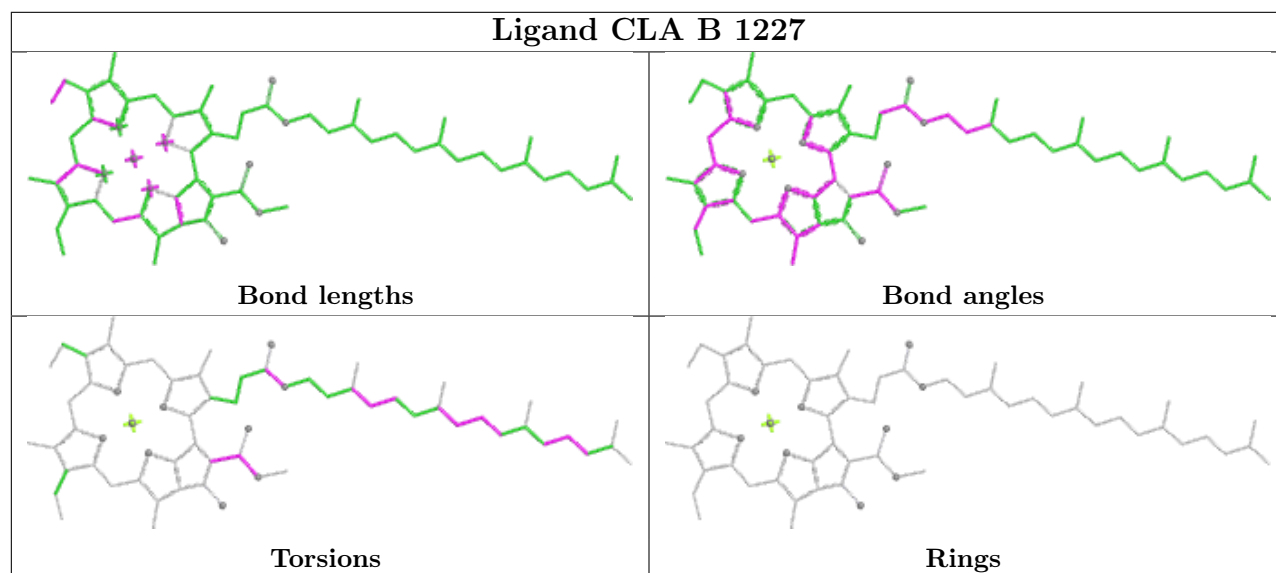
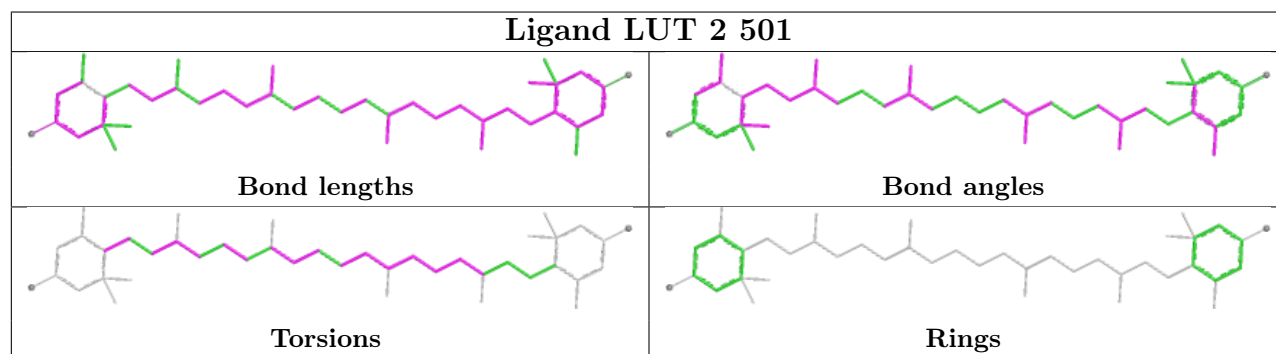
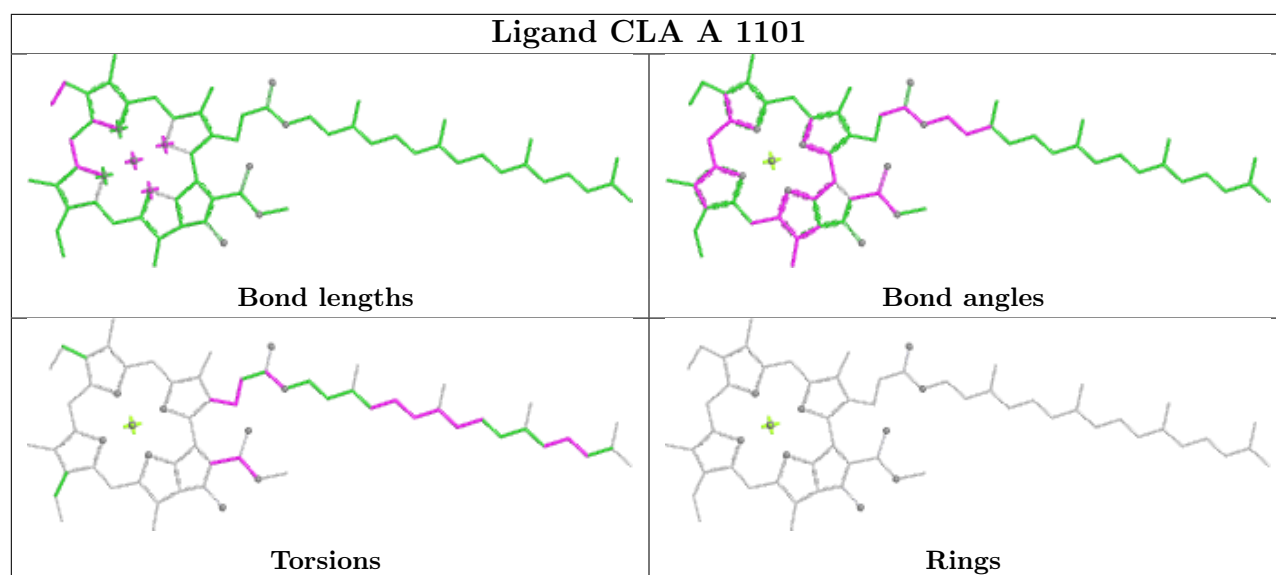


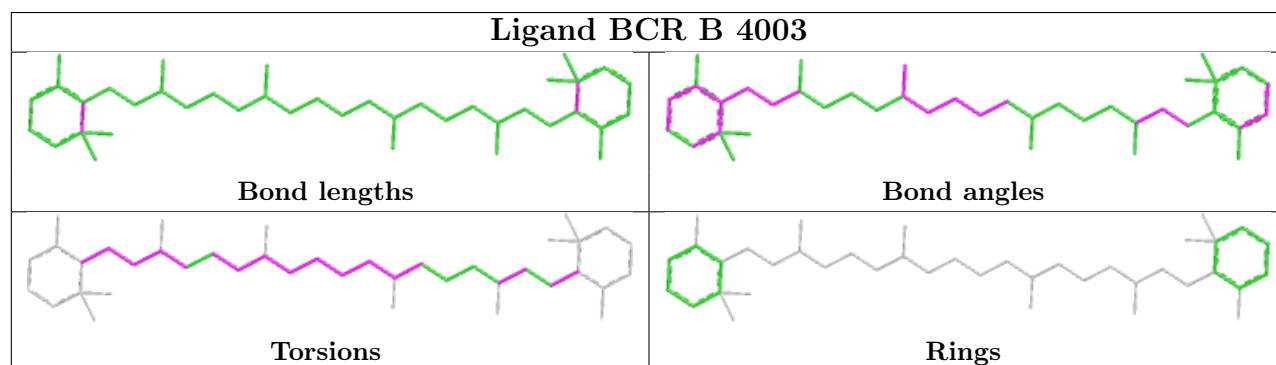
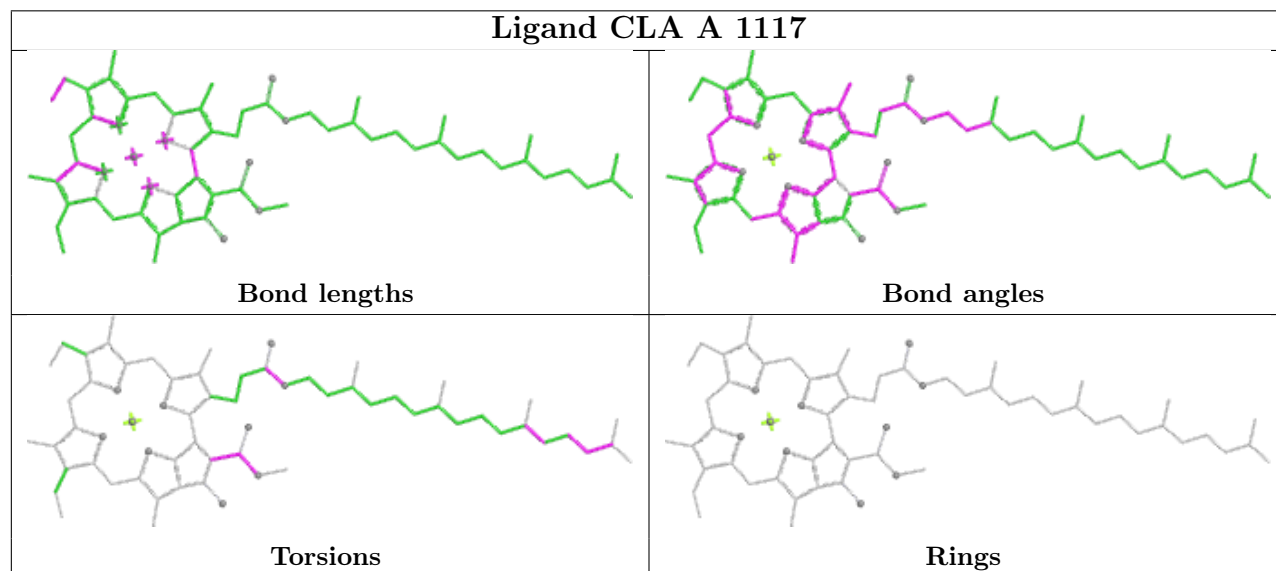
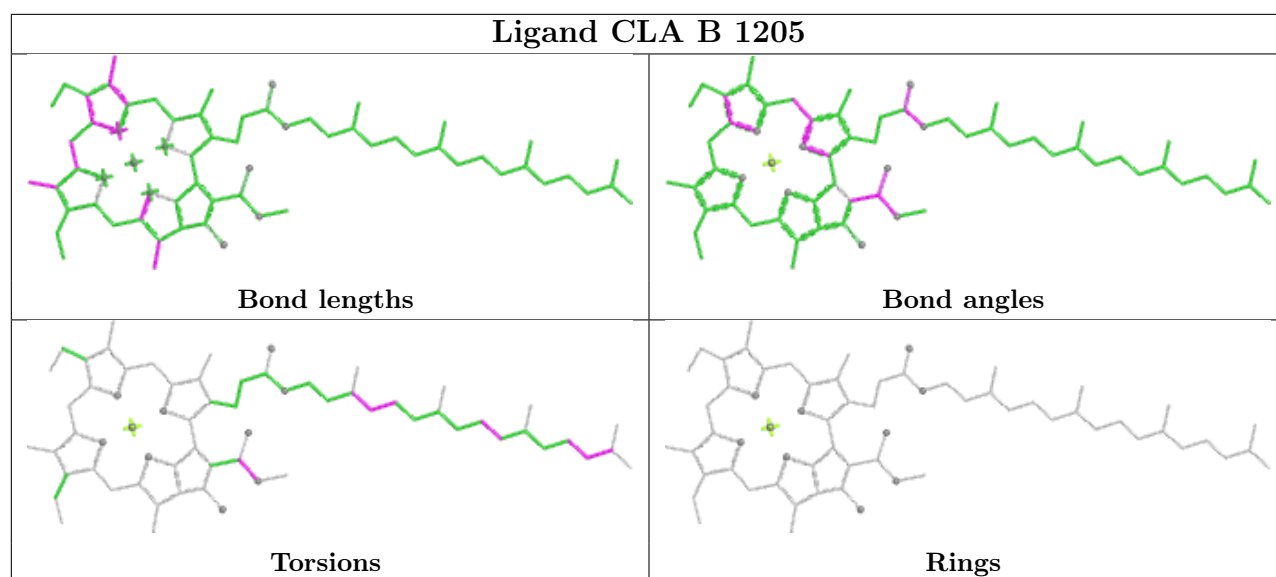
Ligand CLA 2 612



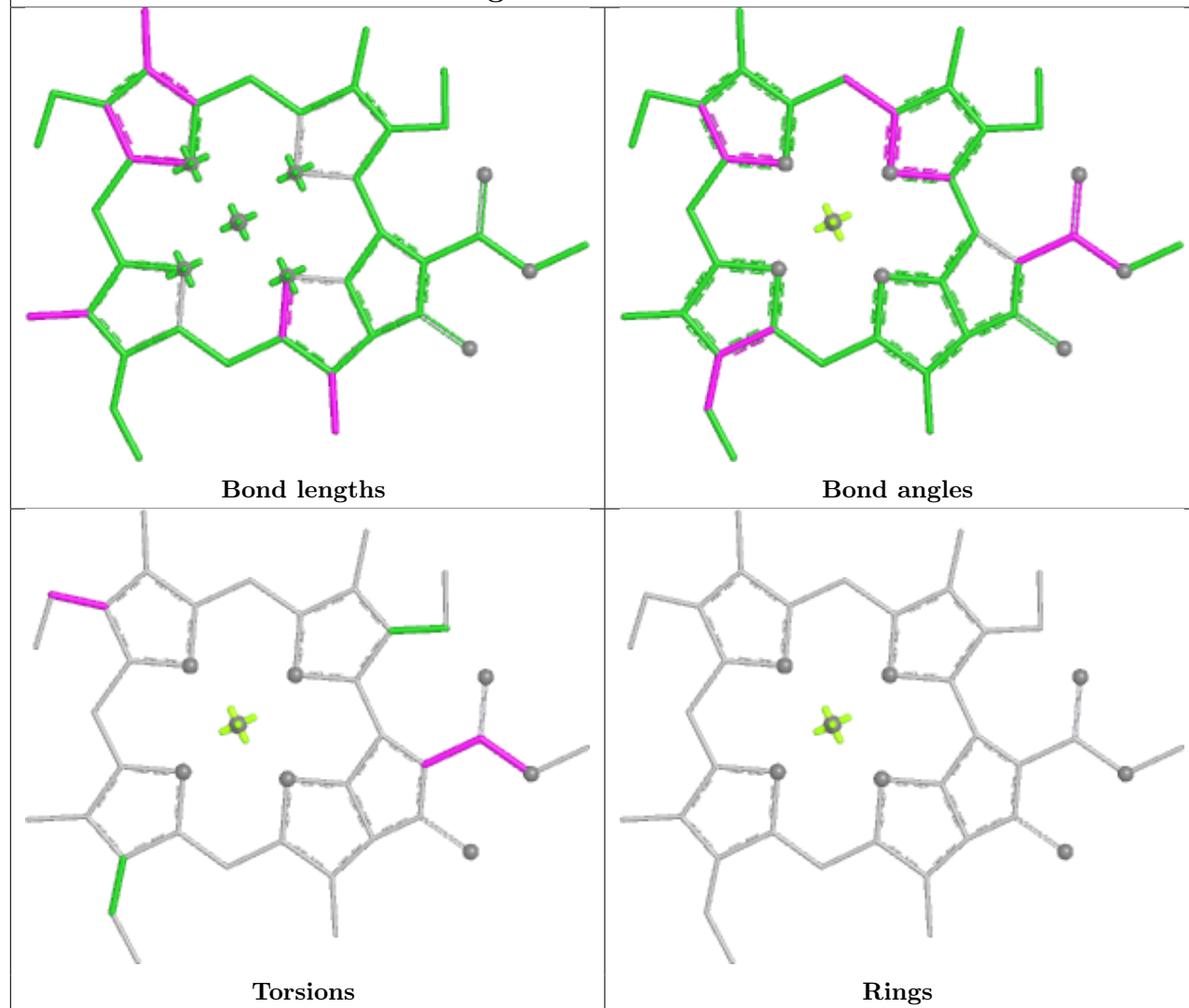
Ligand CLA B 1220



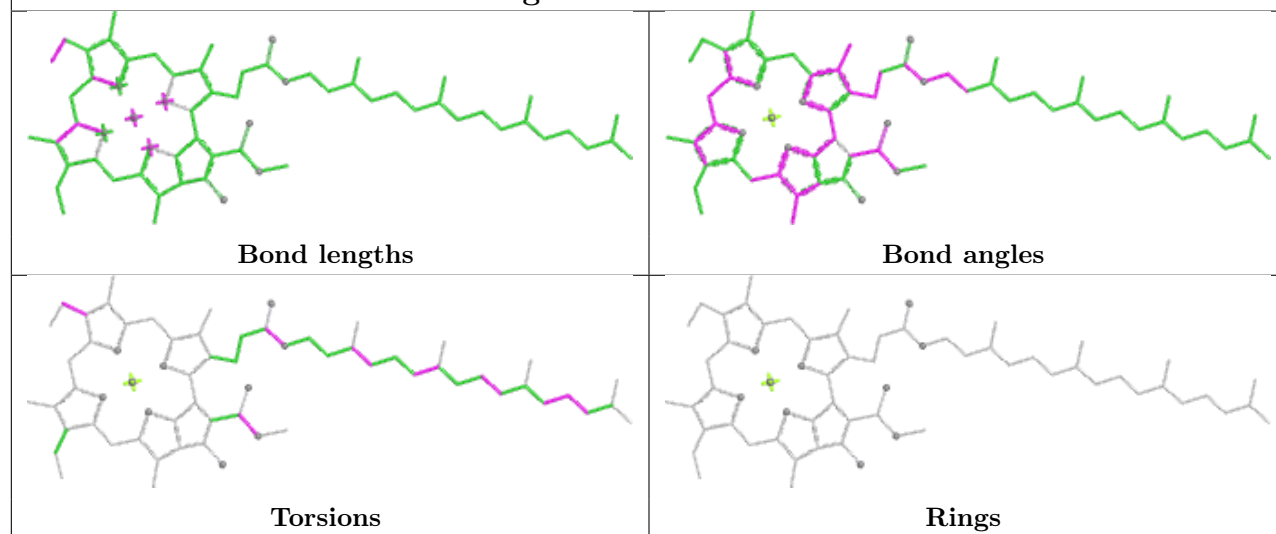


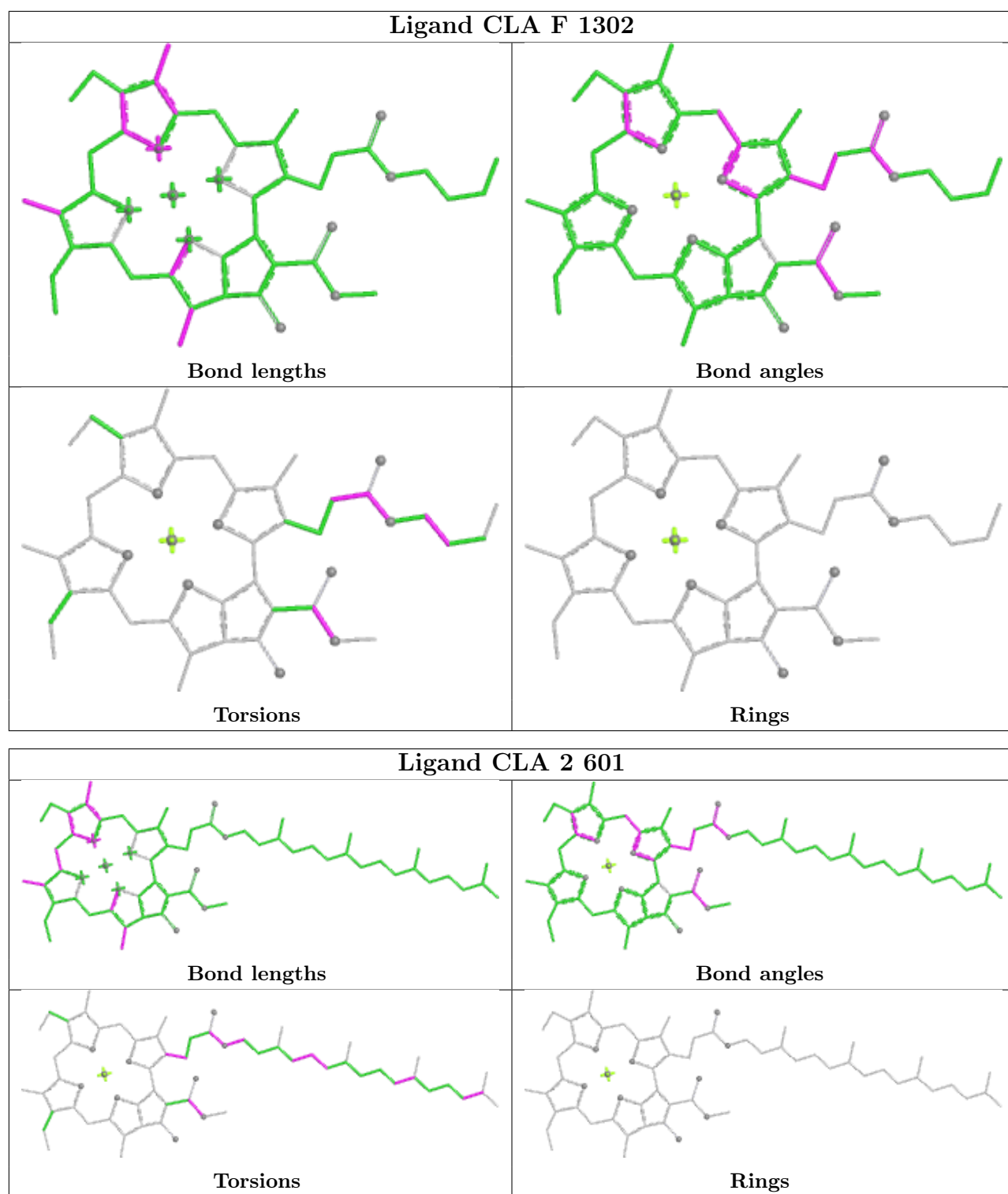


Ligand CLA B 1239

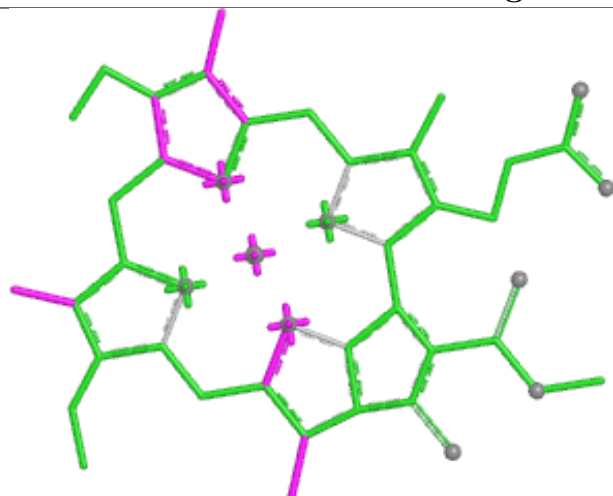


Ligand CLA A 1109

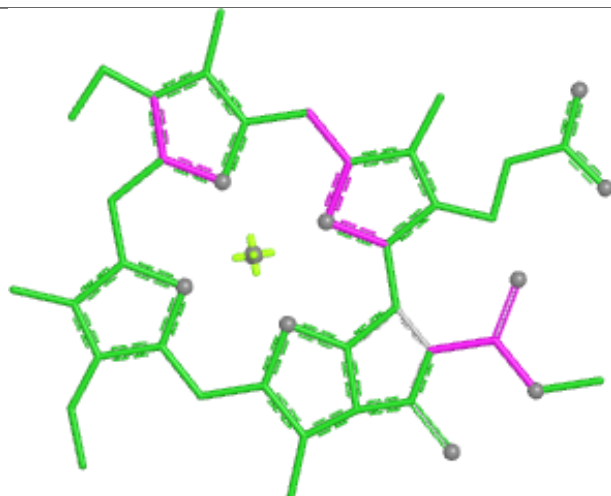




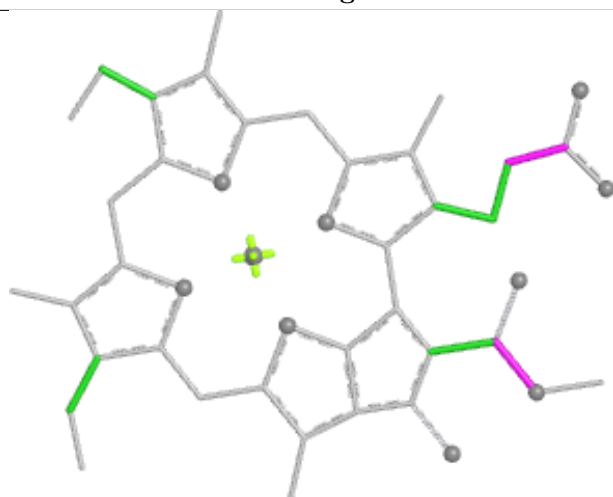
Ligand CLA B 1206



Bond lengths



Bond angles

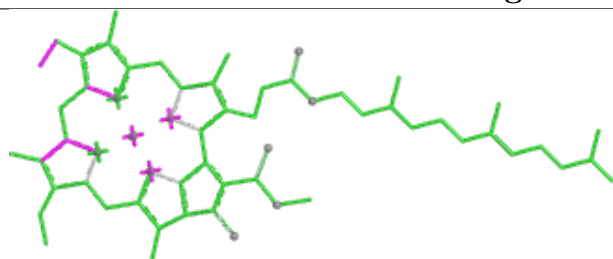


Torsions

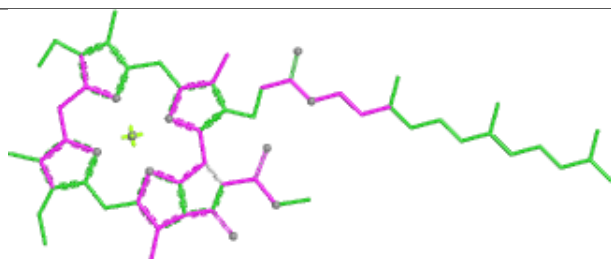


Rings

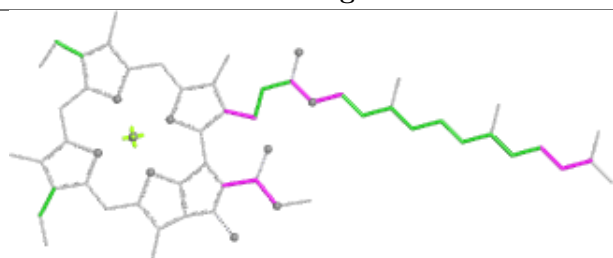
Ligand CLA A 1124



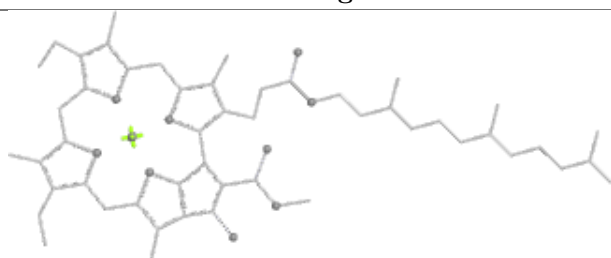
Bond lengths



Bond angles

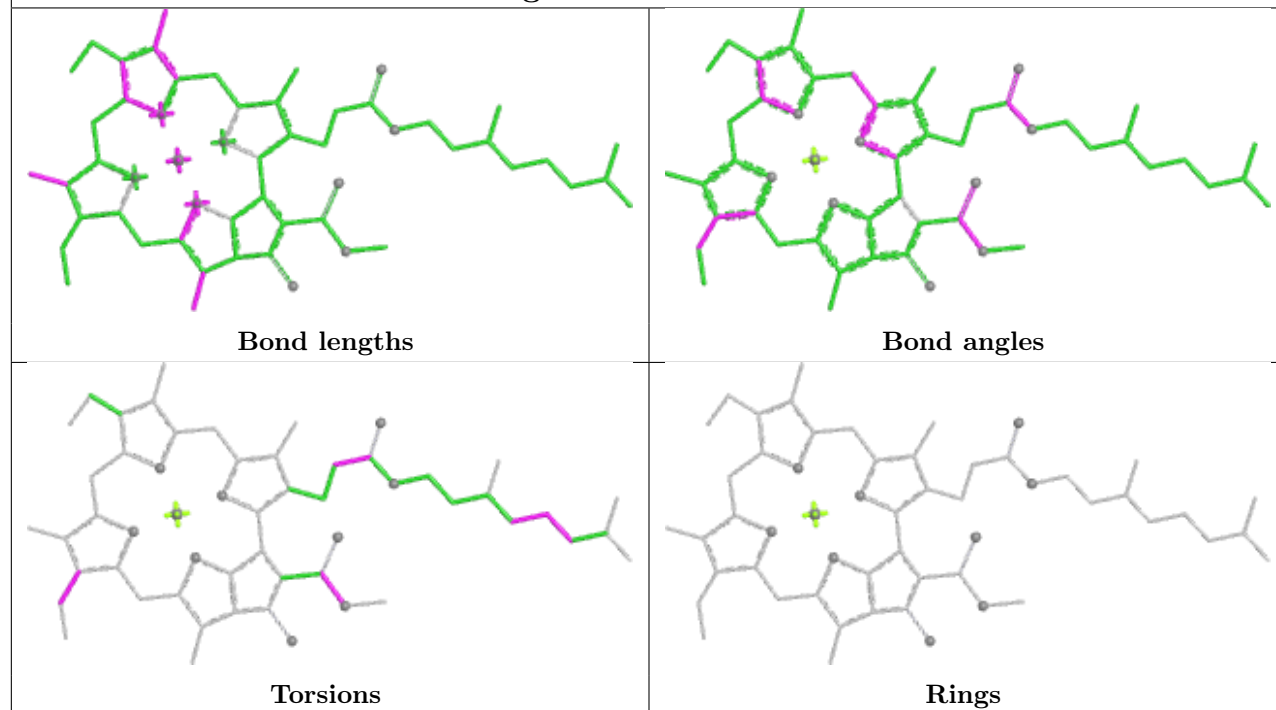


Torsions

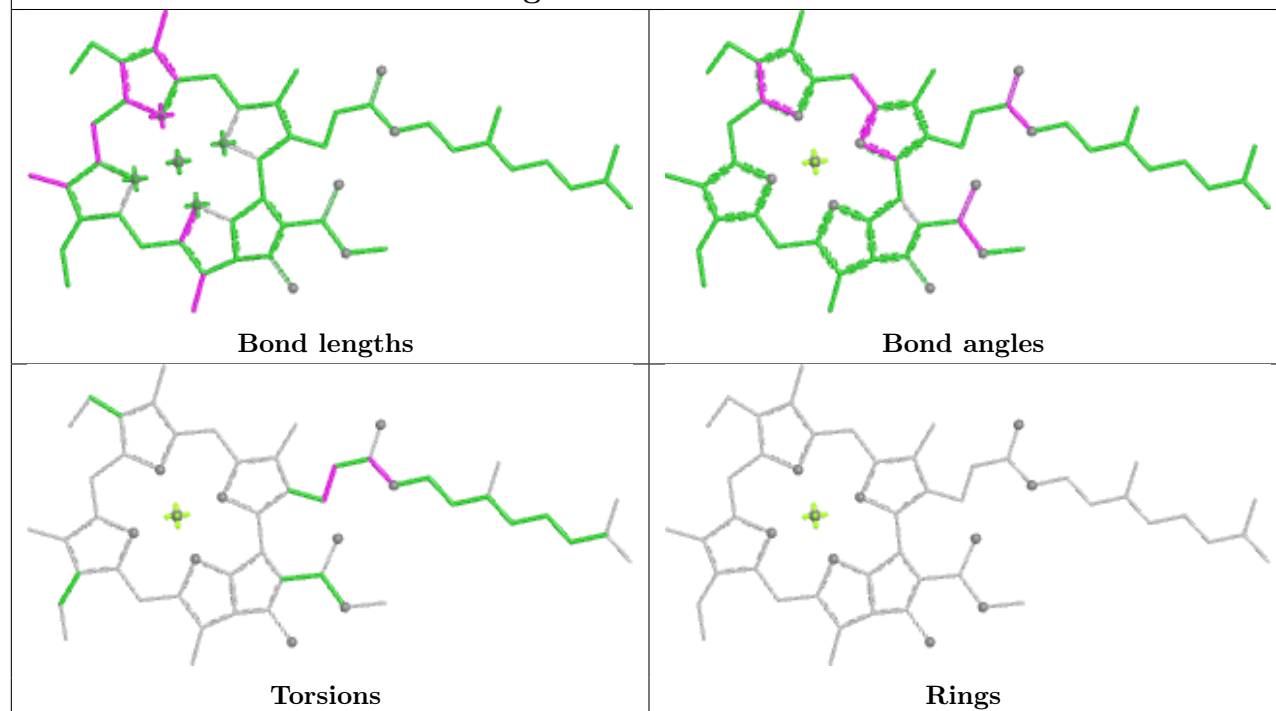


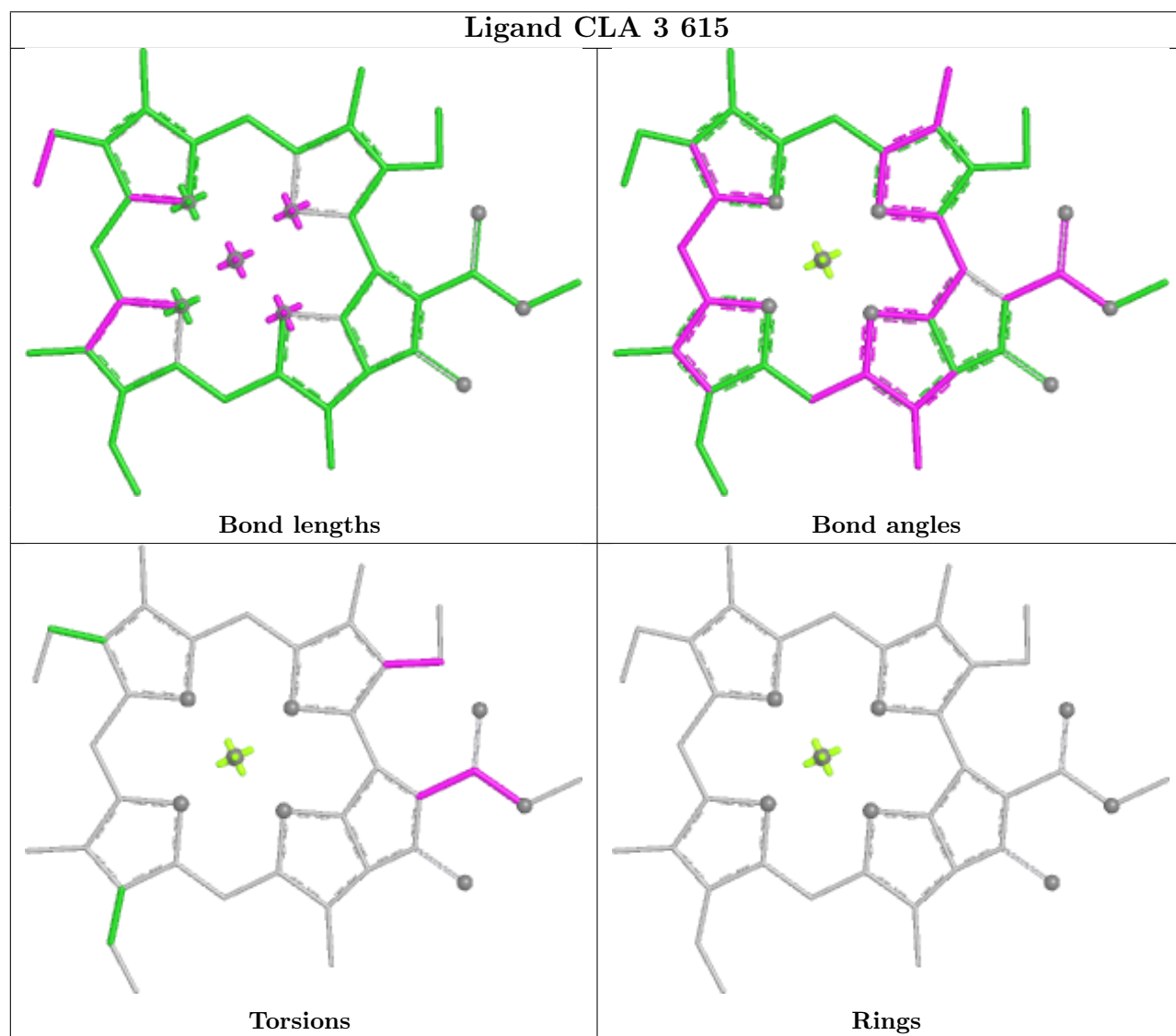
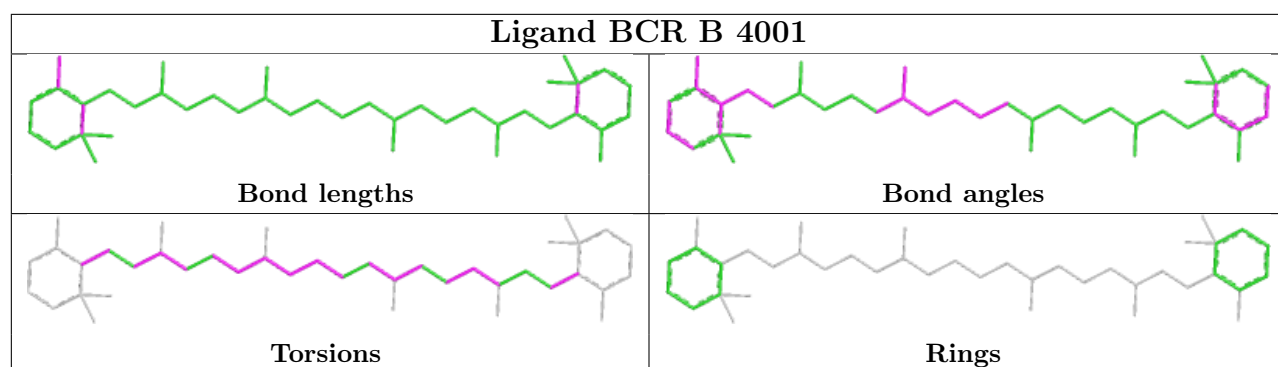
Rings

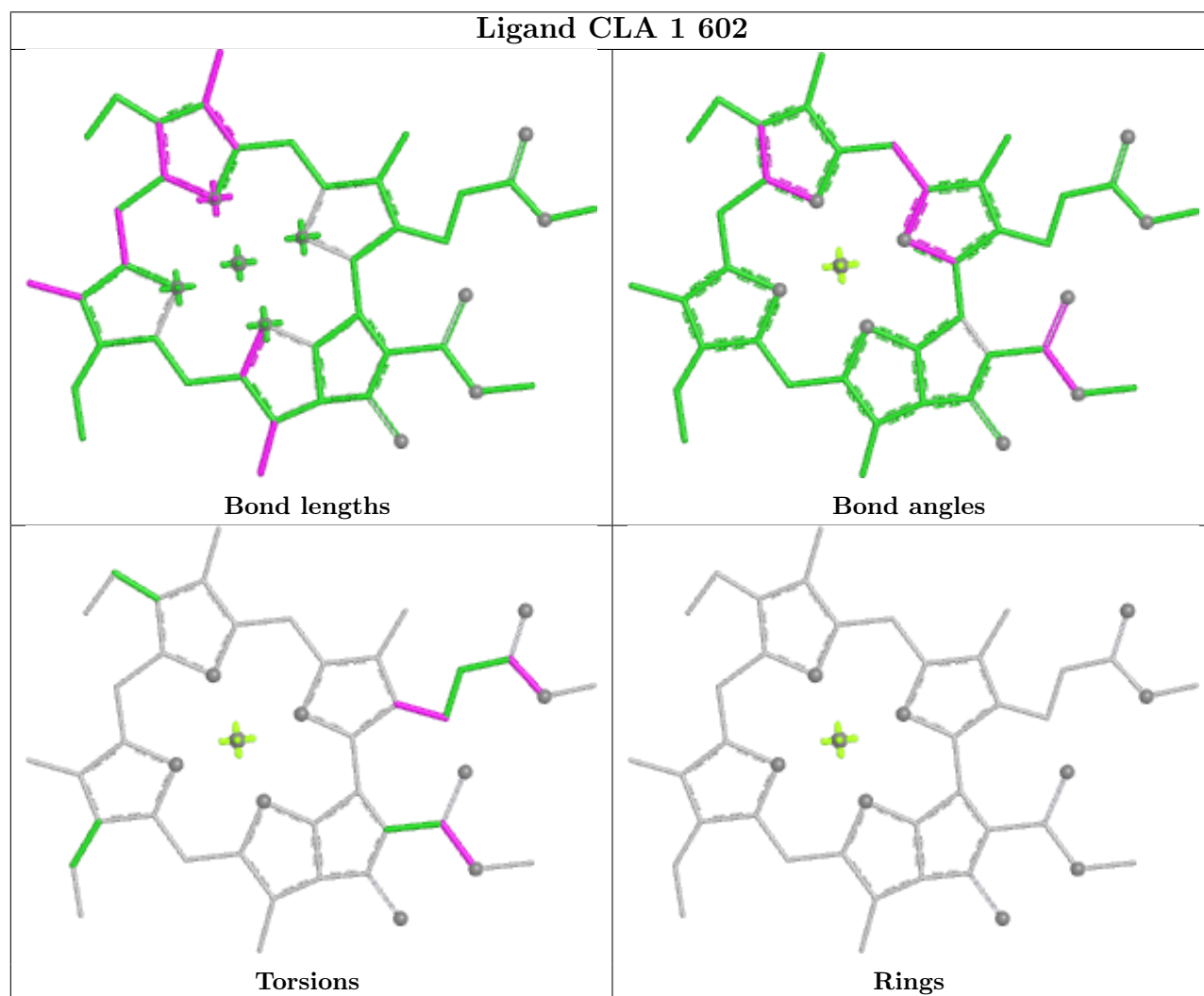
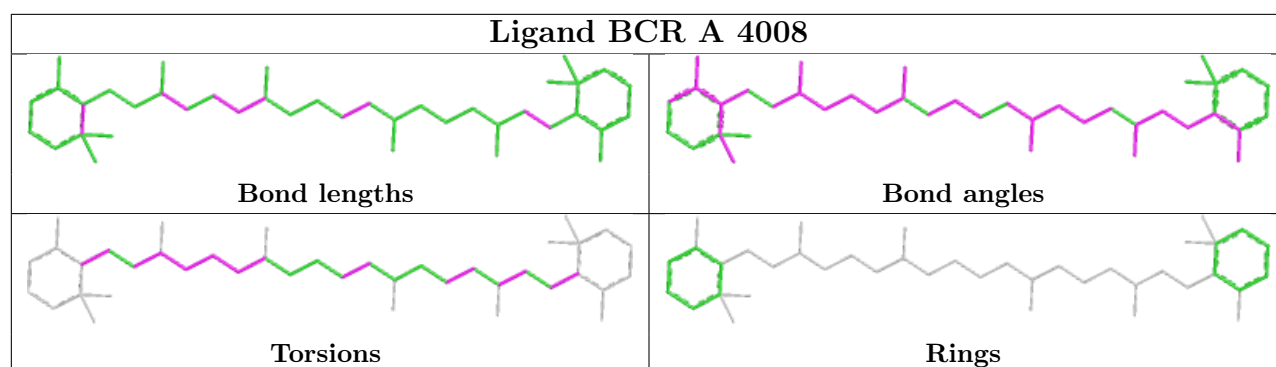
Ligand CLA A 1129

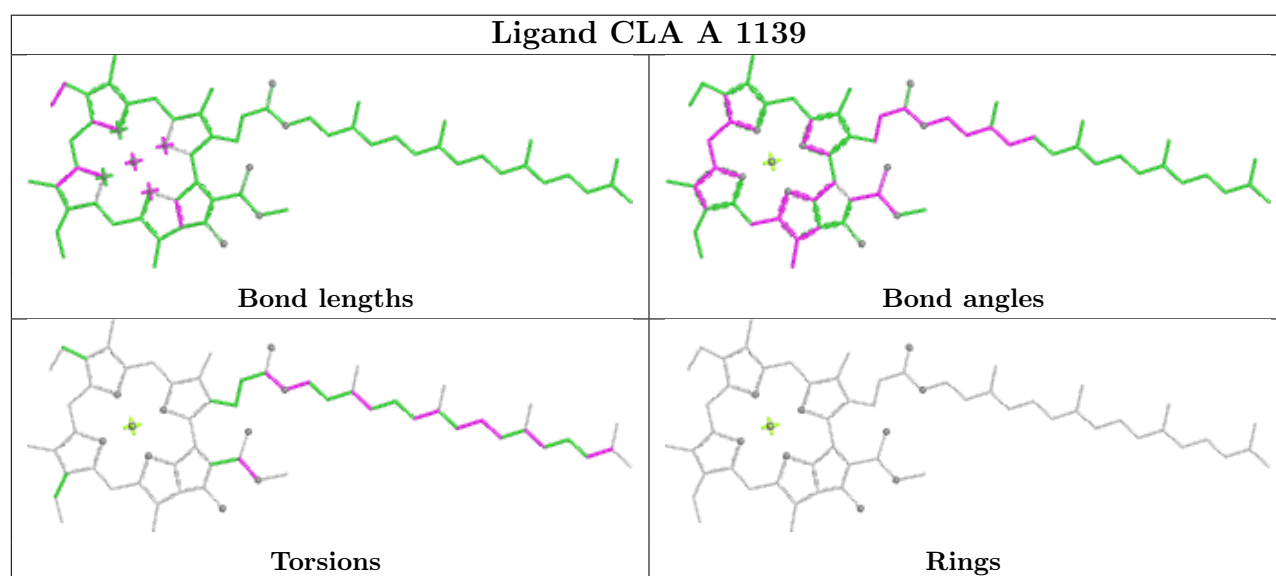
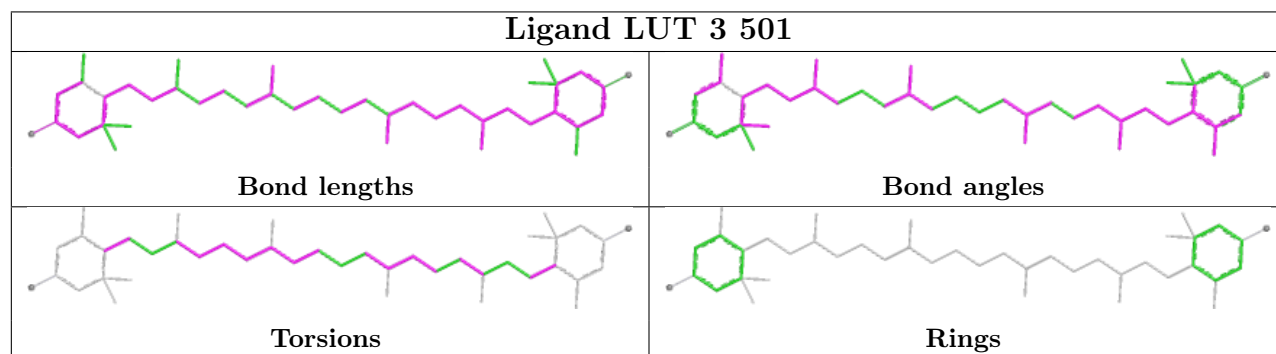
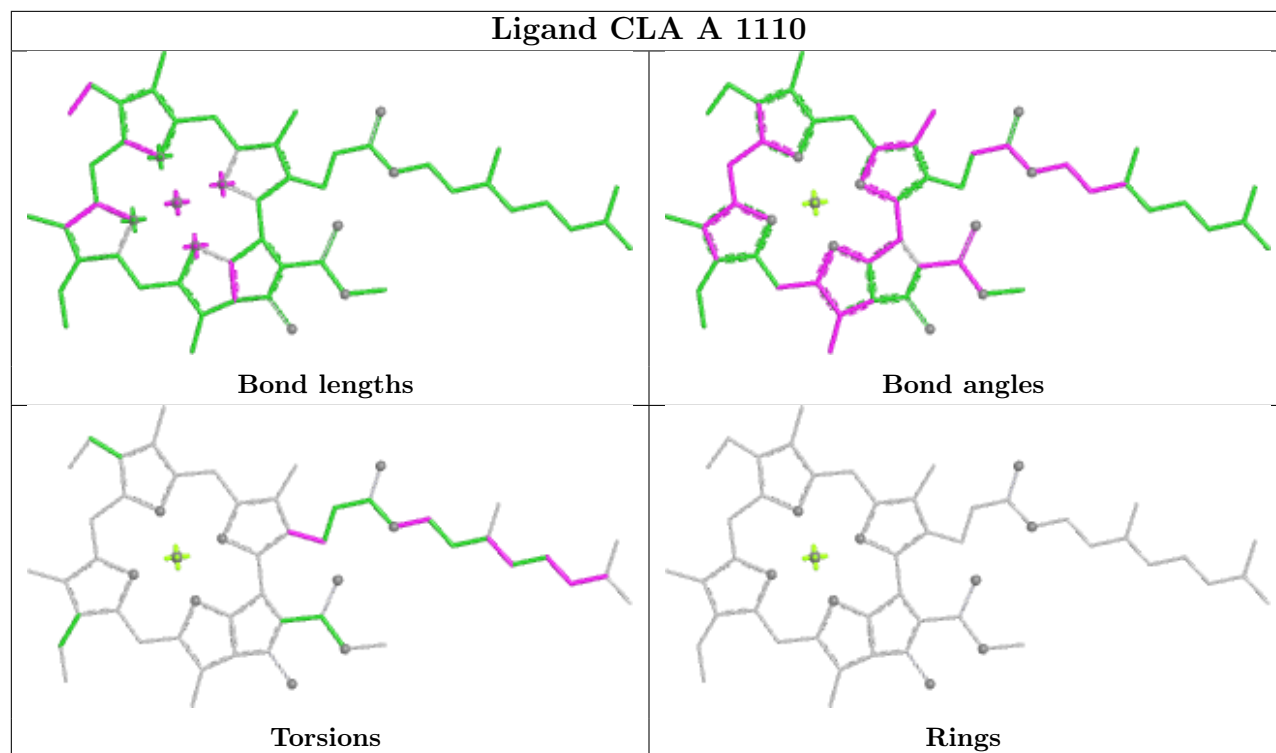


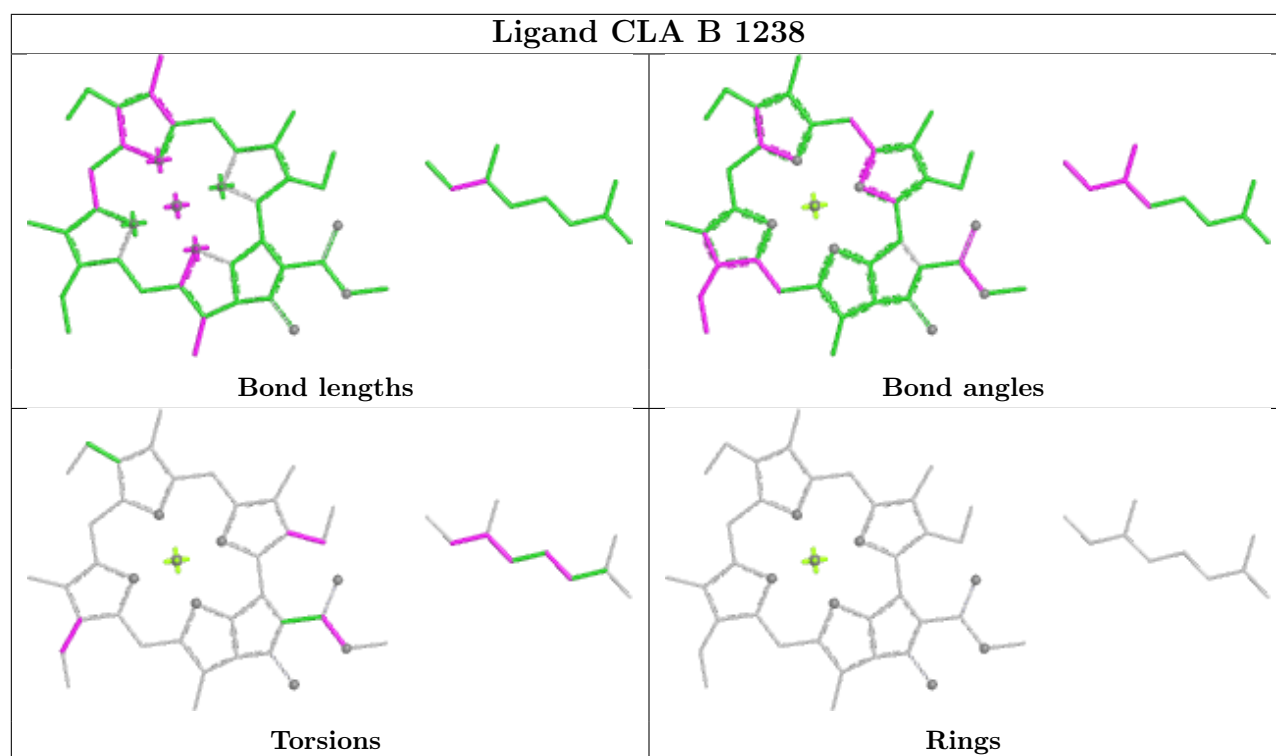
Ligand CLA B 1213

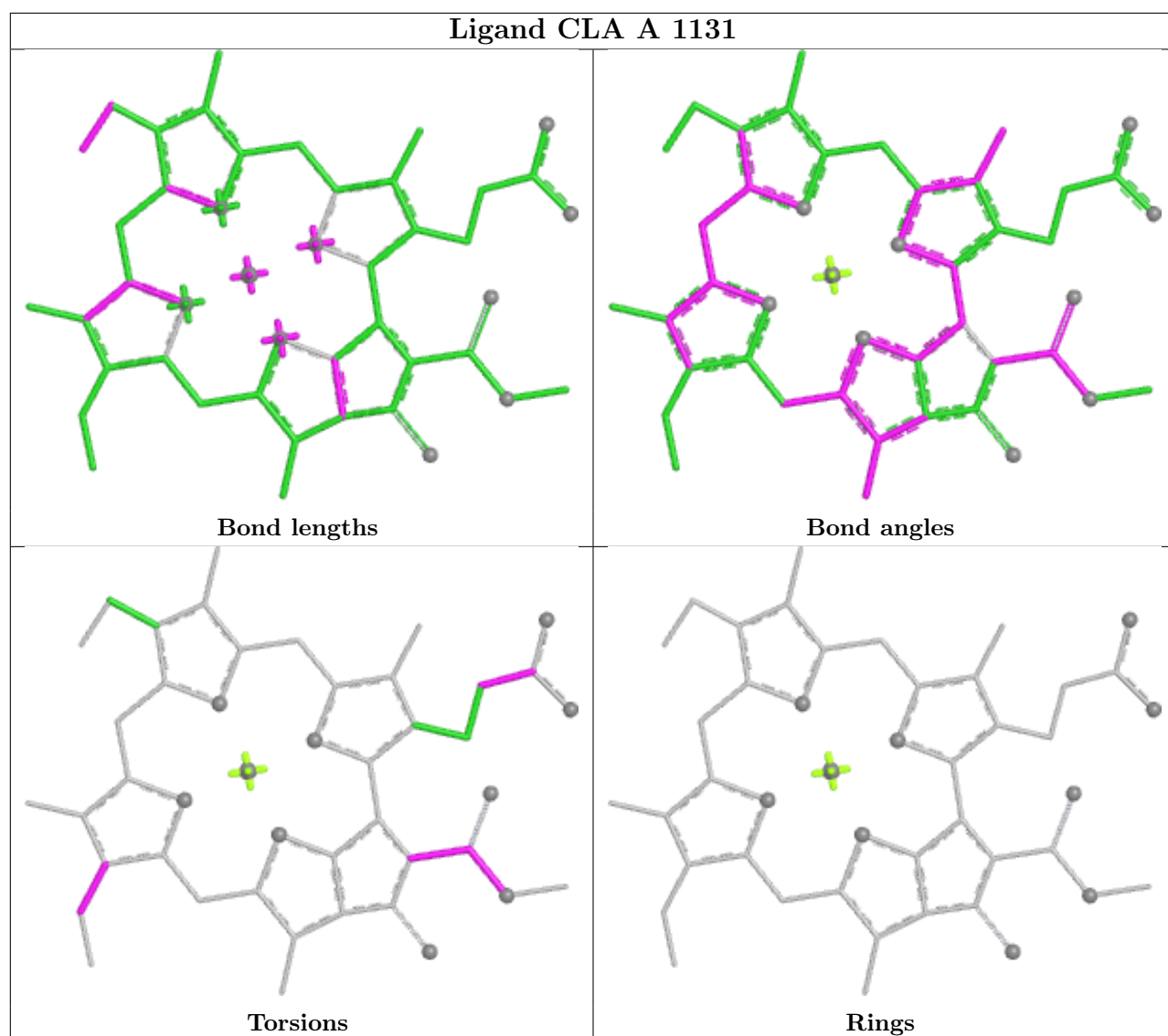


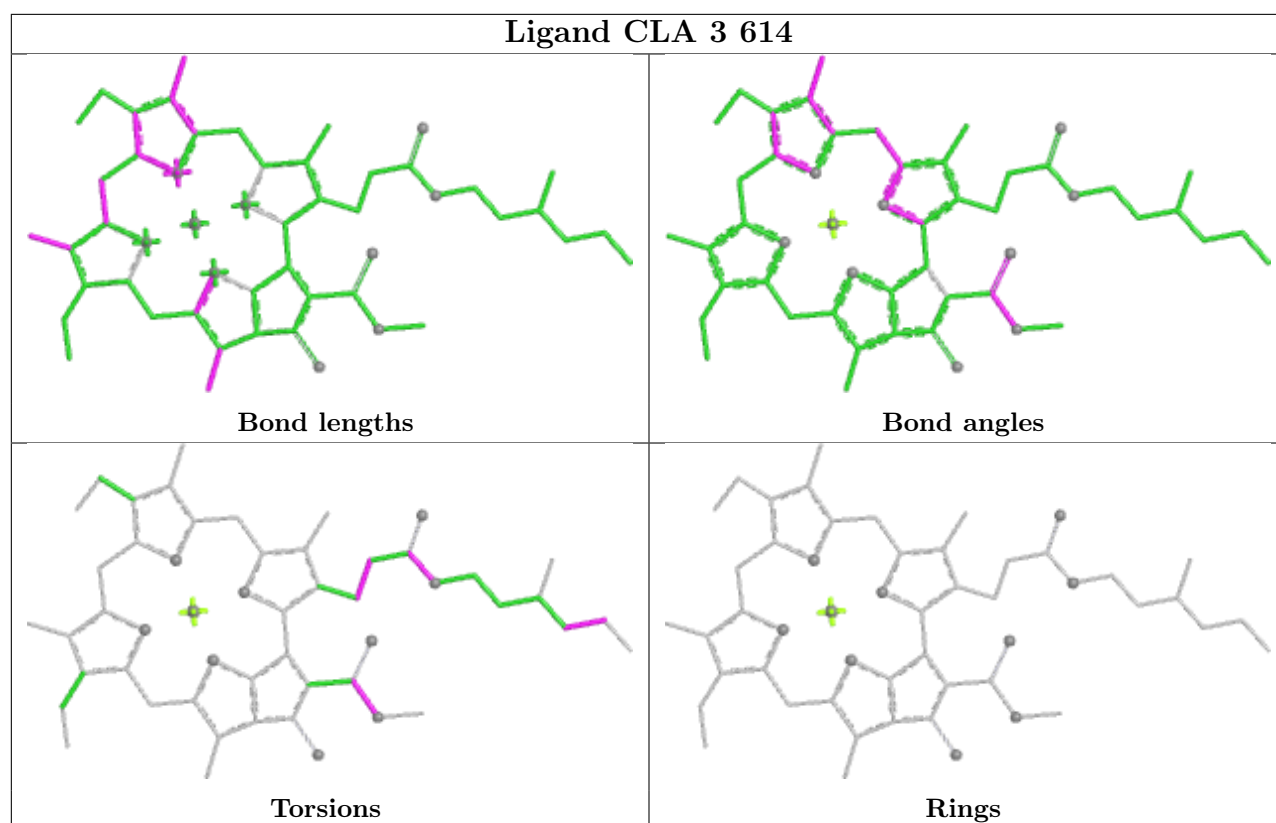


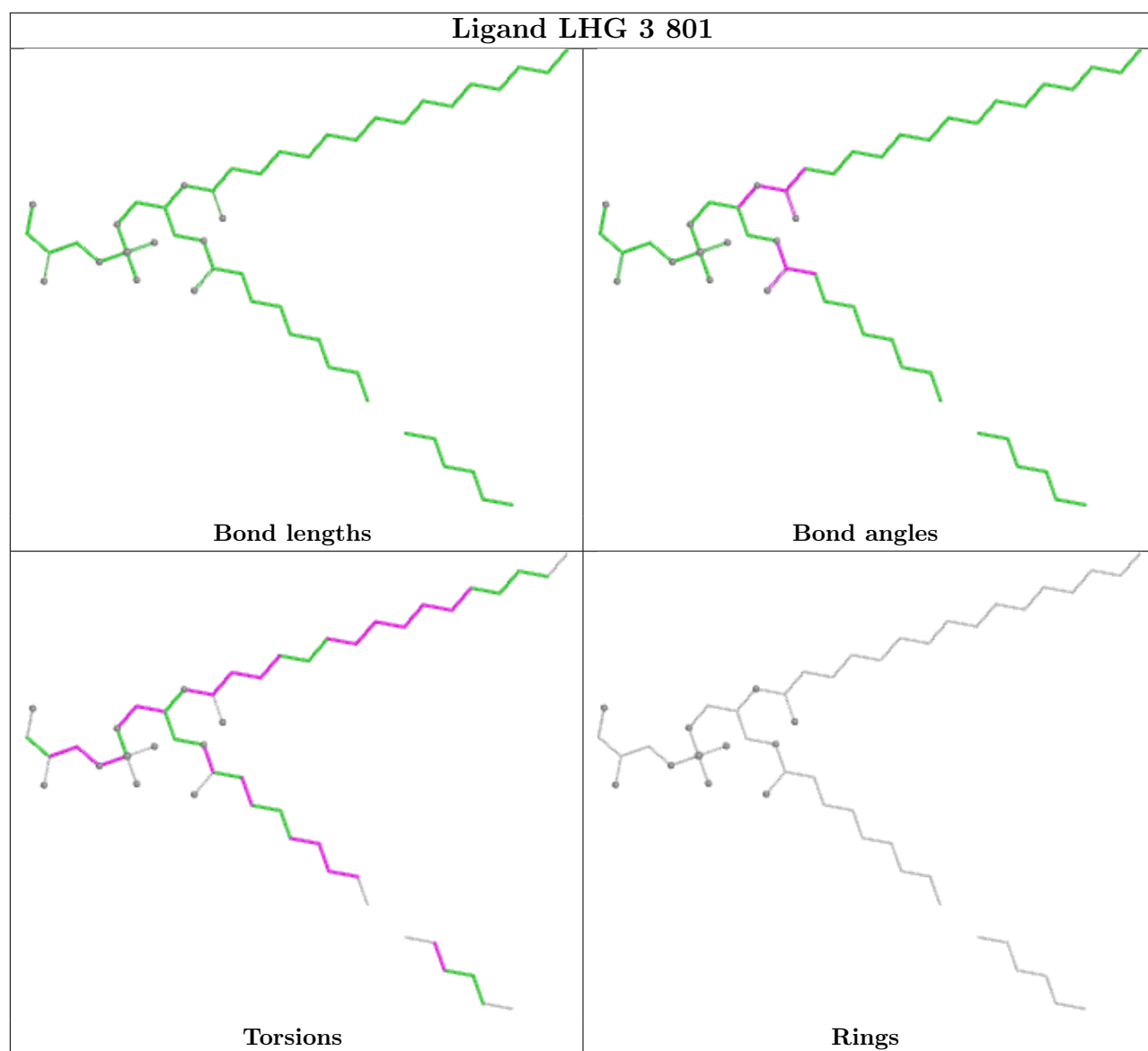


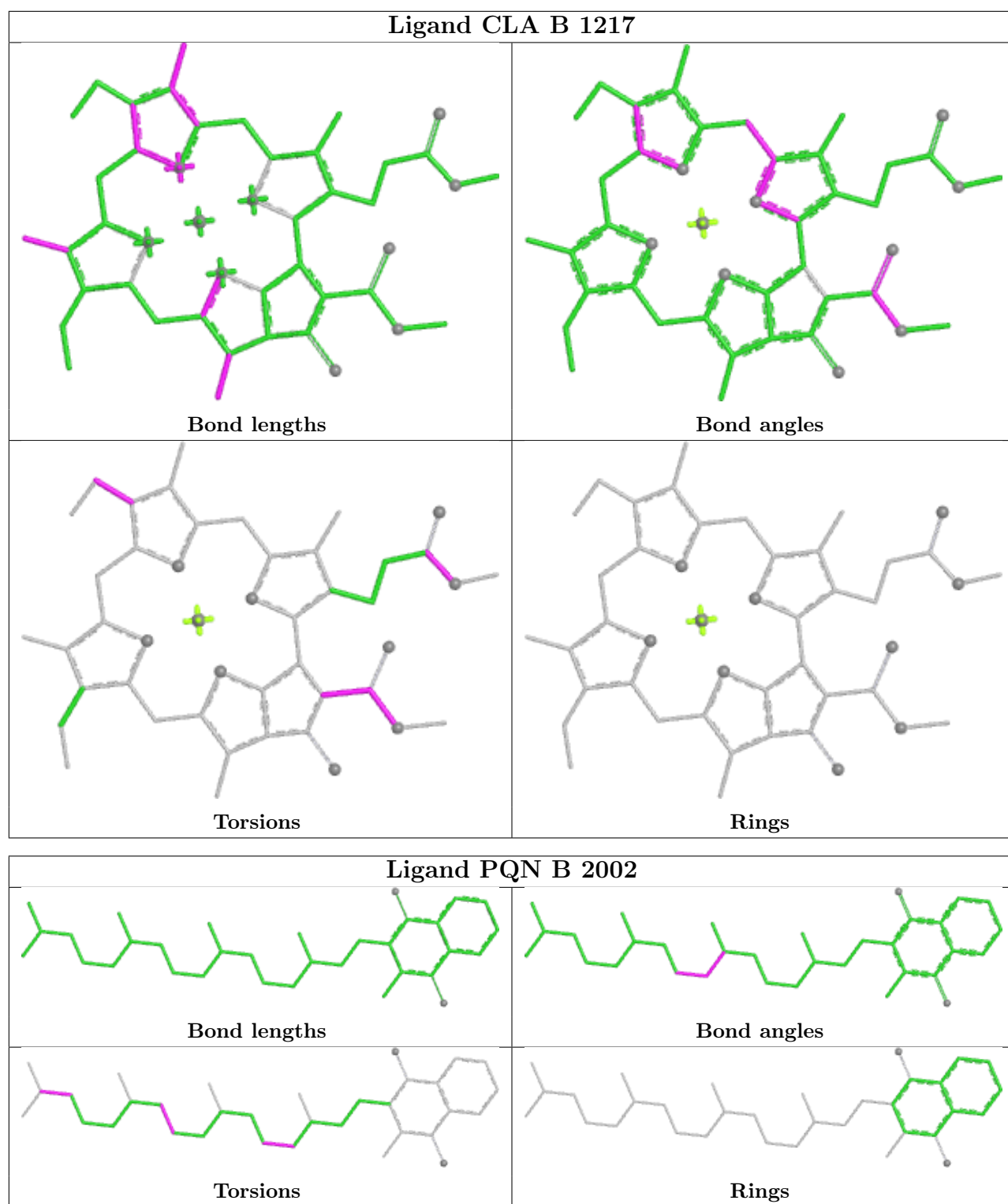




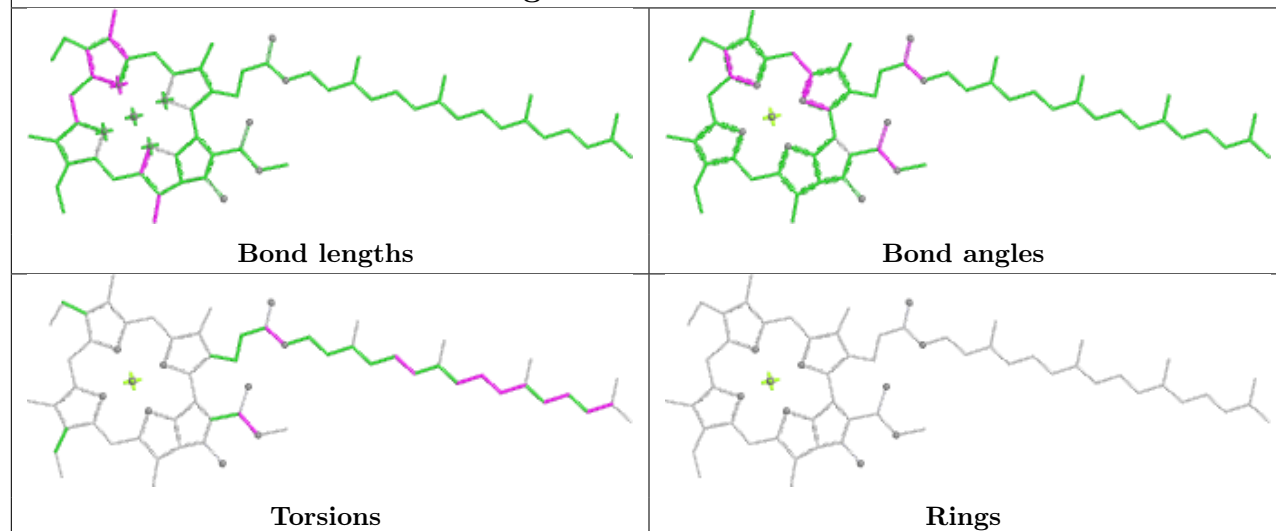




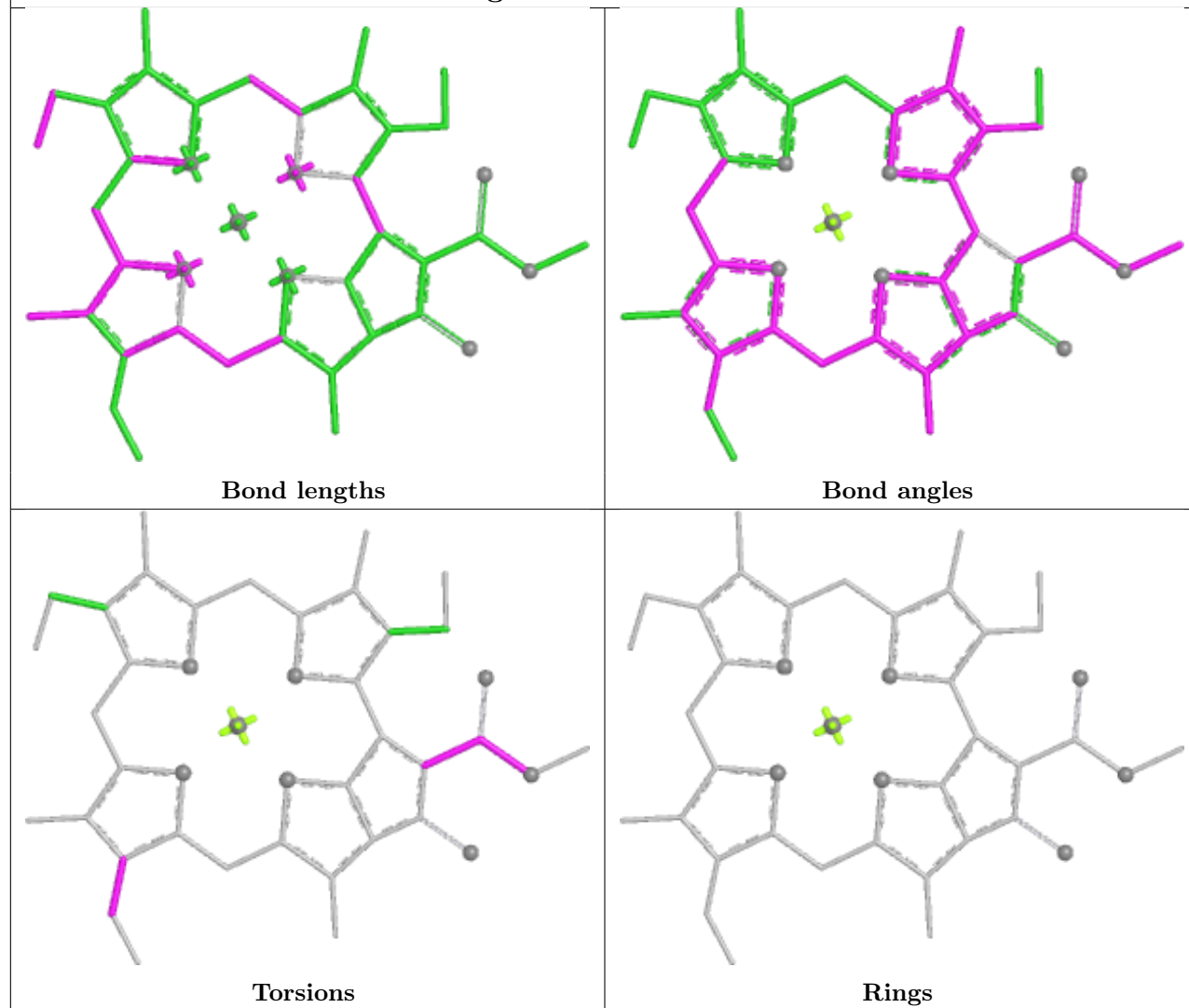




Ligand CLA B 1219



Ligand CLA A 1134



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

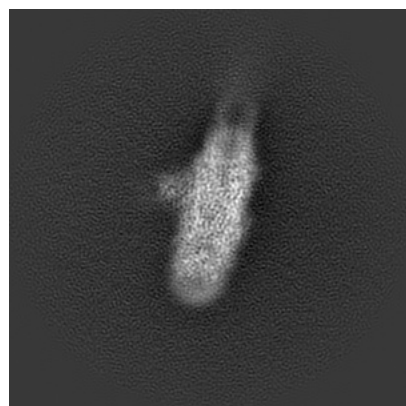
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10995. These allow visual inspection of the internal detail of the map and identification of artifacts.

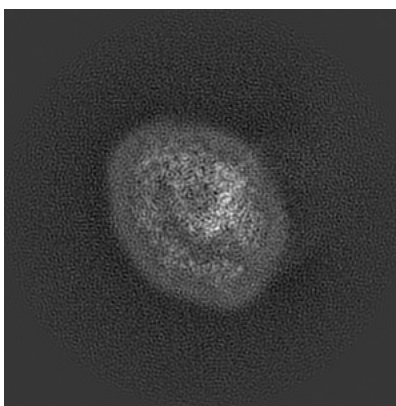
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

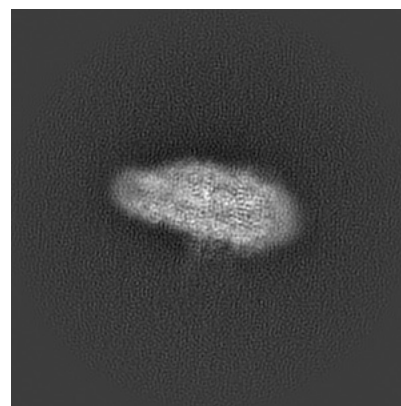
6.1.1 Primary map



X

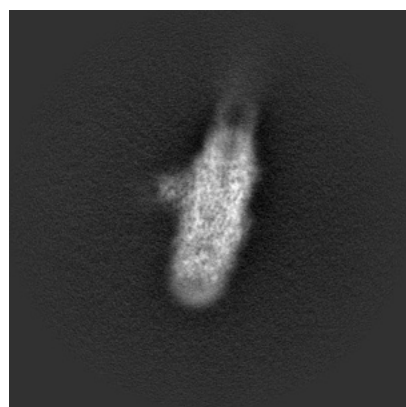


Y

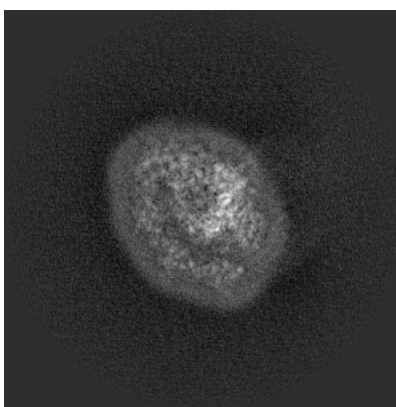


Z

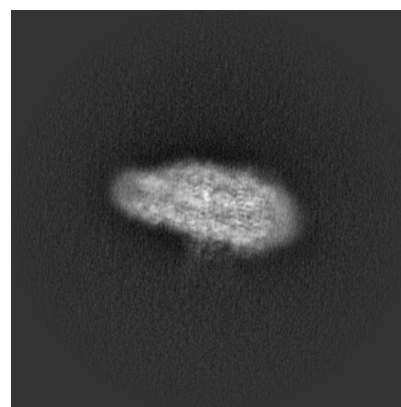
6.1.2 Raw map



X



Y

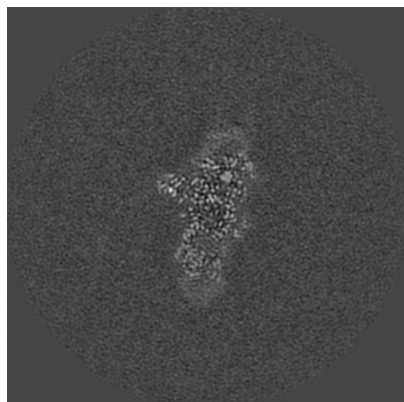


Z

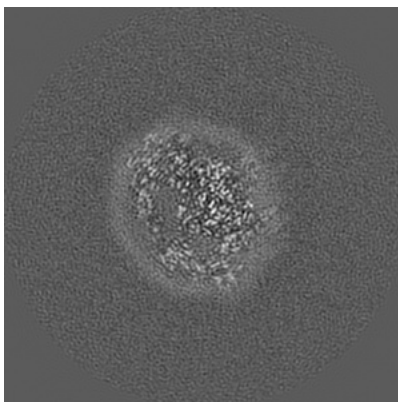
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

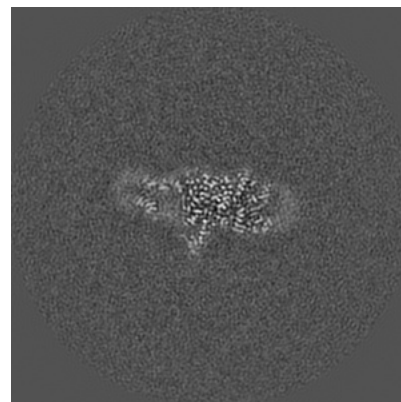
6.2.1 Primary map



X Index: 180

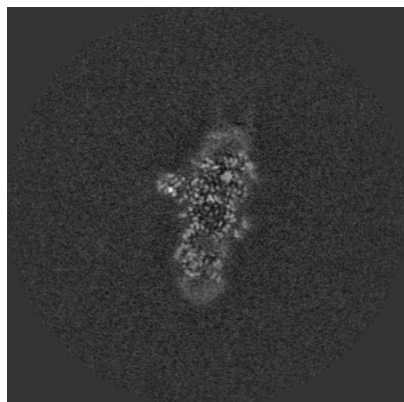


Y Index: 180

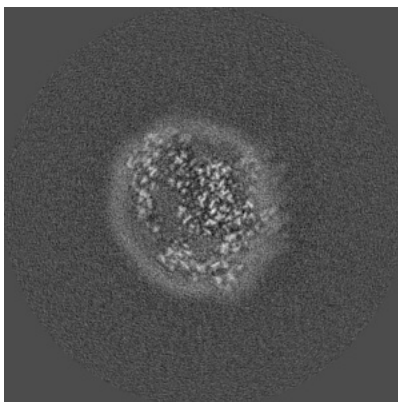


Z Index: 180

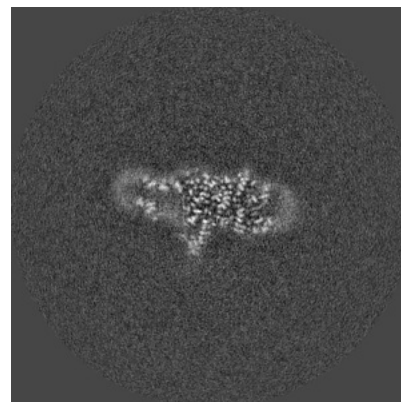
6.2.2 Raw map



X Index: 180



Y Index: 180

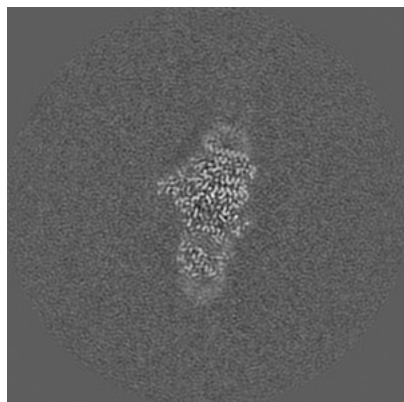


Z Index: 180

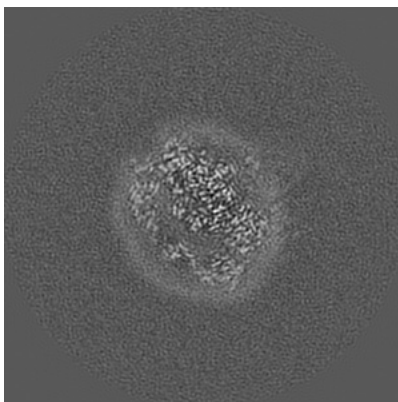
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

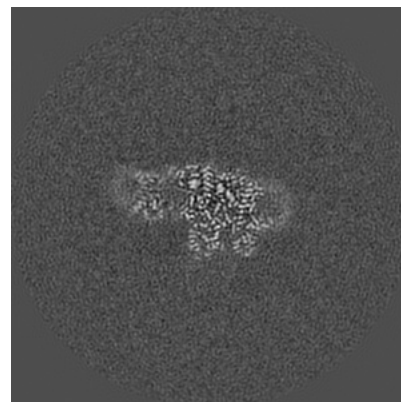
6.3.1 Primary map



X Index: 176

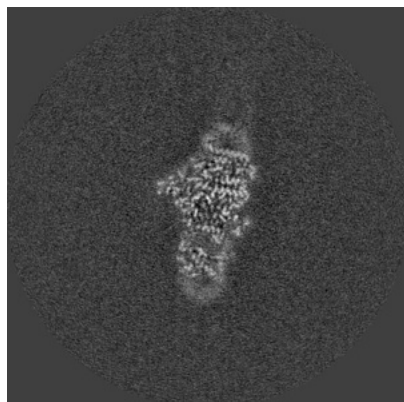


Y Index: 185

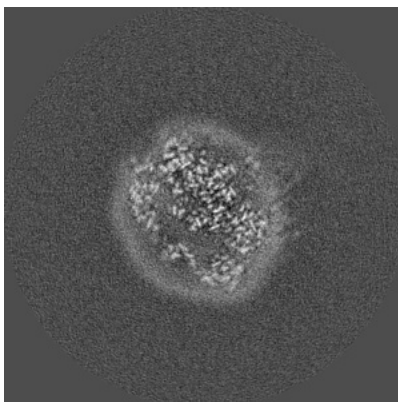


Z Index: 192

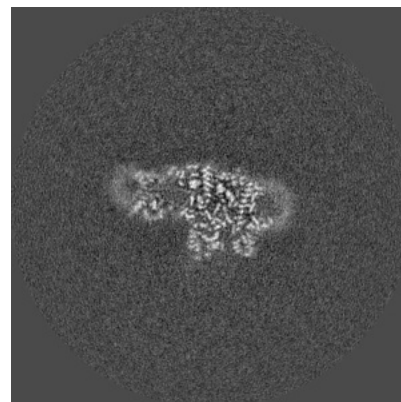
6.3.2 Raw map



X Index: 176



Y Index: 185

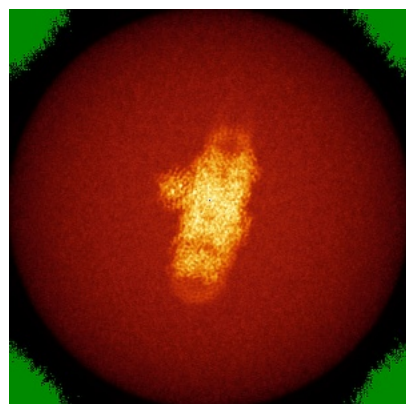


Z Index: 192

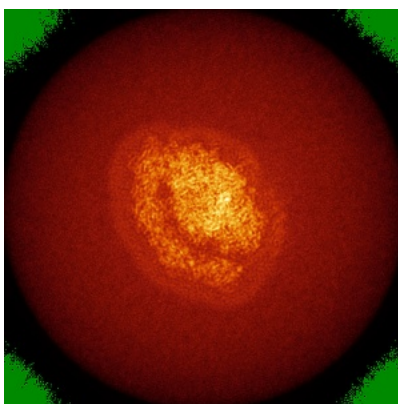
The images above show the largest variance slices of the map in three orthogonal directions.

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

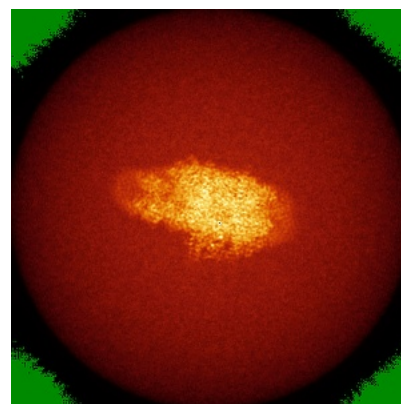
6.4.1 Primary map



X

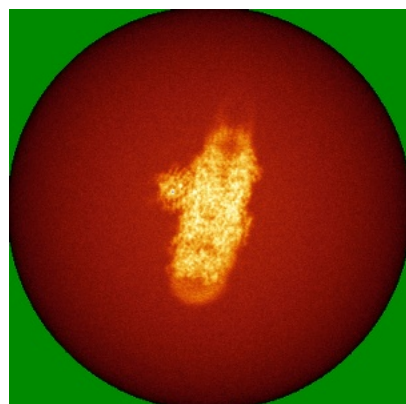


Y

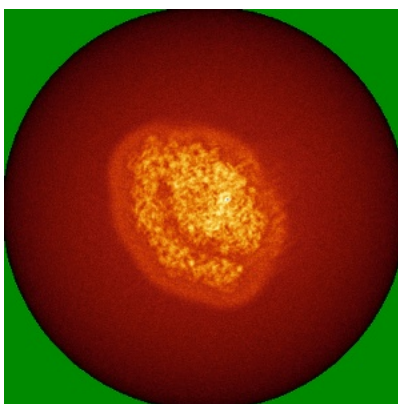


Z

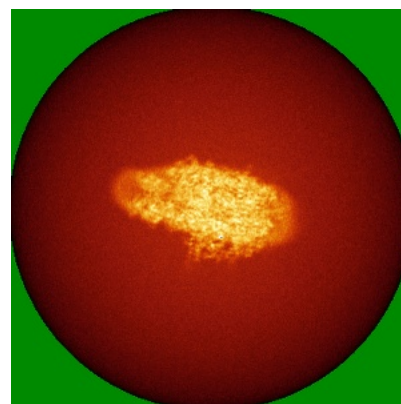
6.4.2 Raw map



X



Y

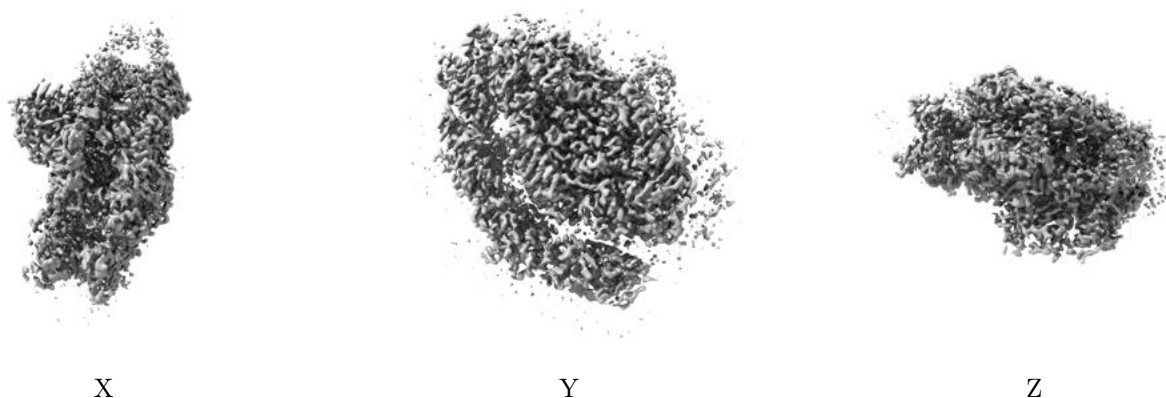


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

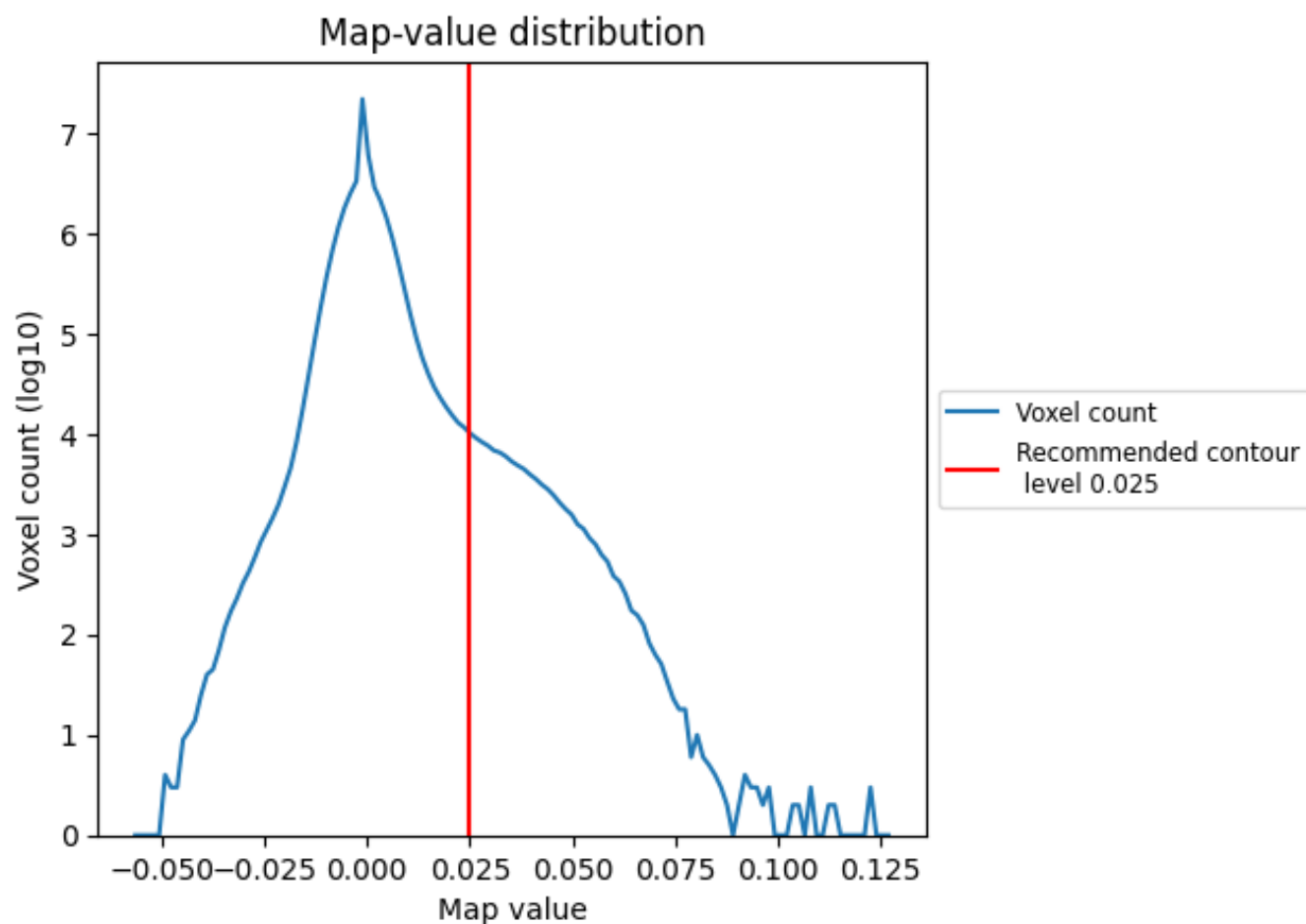
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

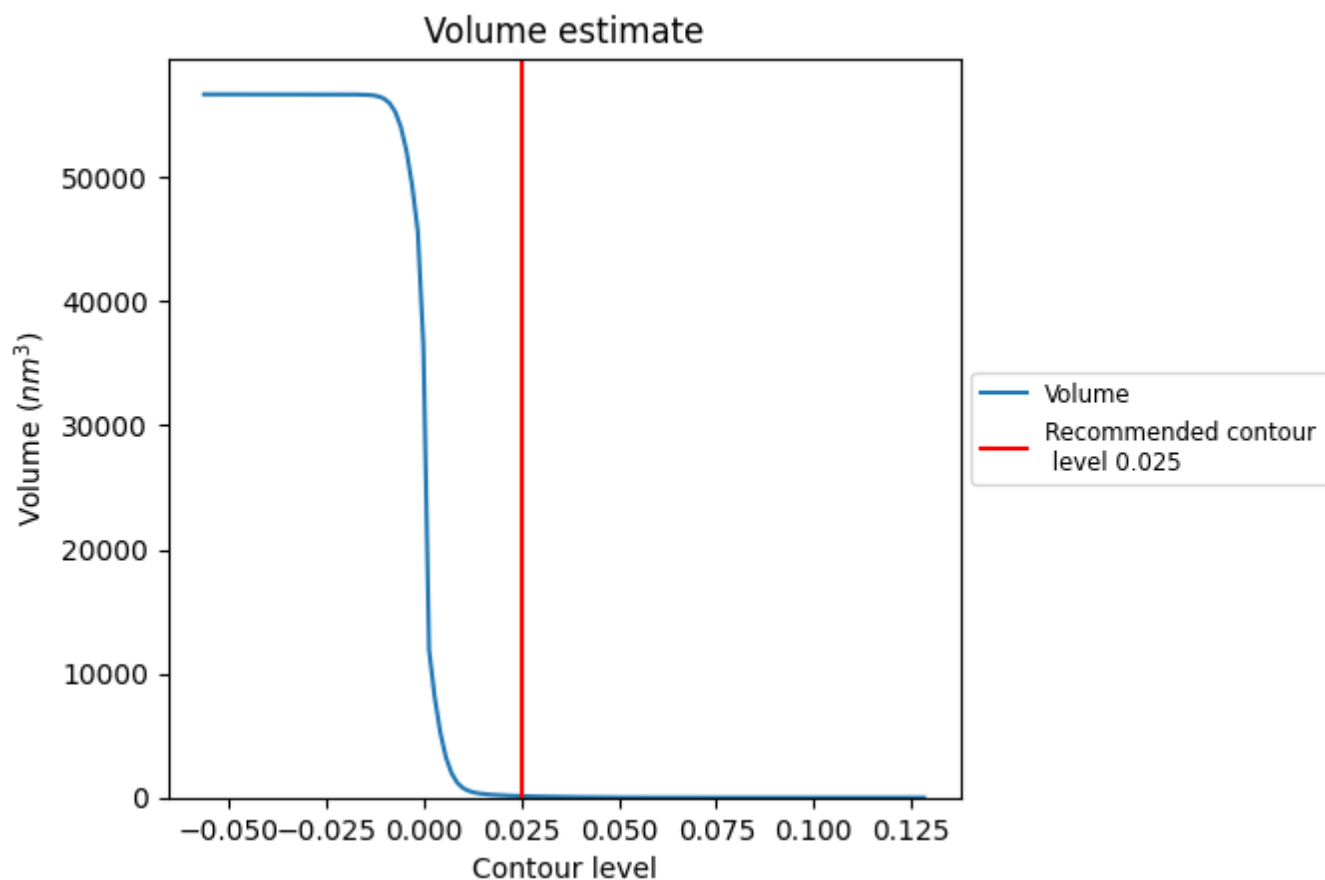
This section contains the results of statistical analysis of the map.

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.

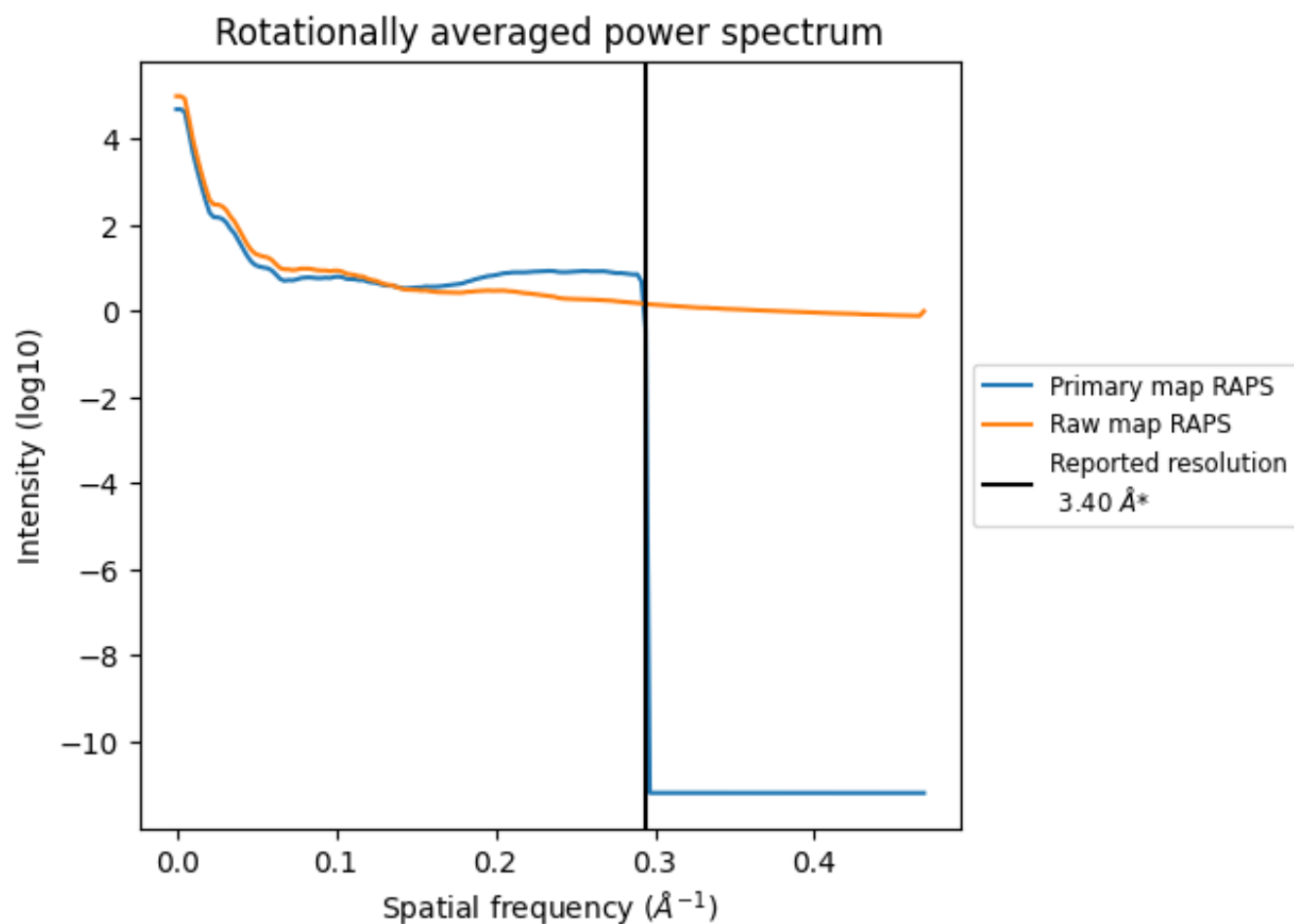
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 108 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 ⓘ

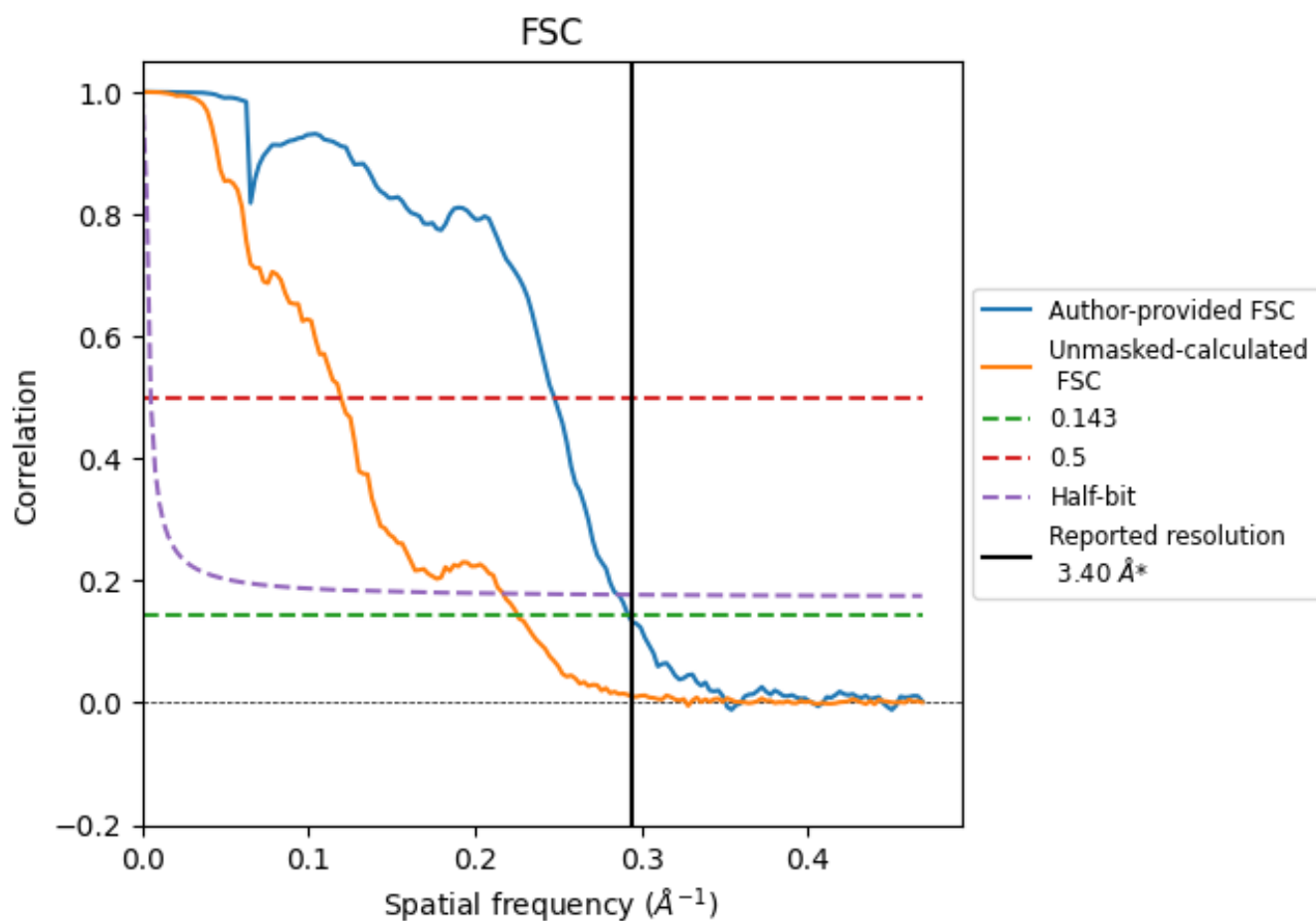


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

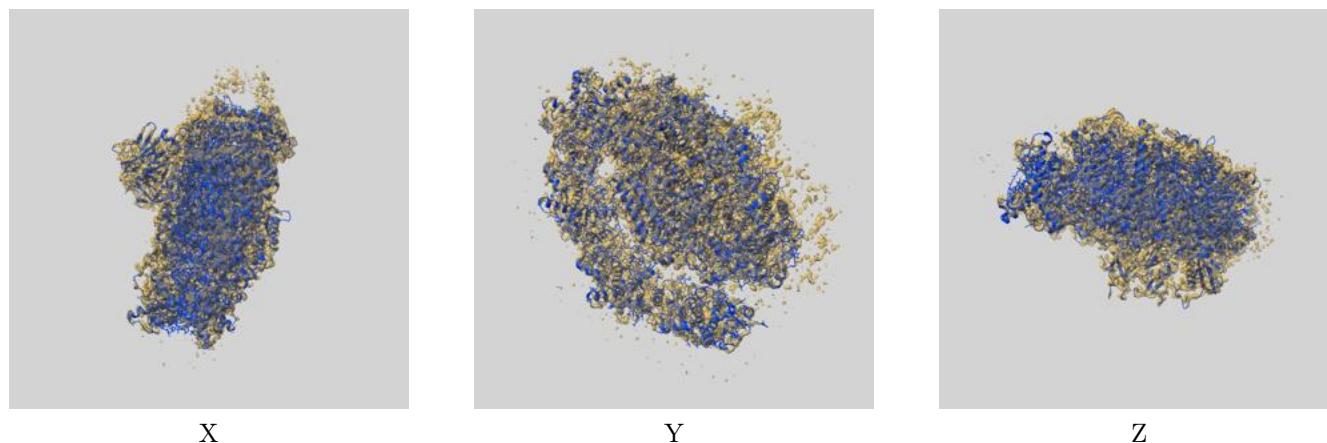
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	4.04	3.49
Unmasked-calculated*	4.43	8.38	4.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.43 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

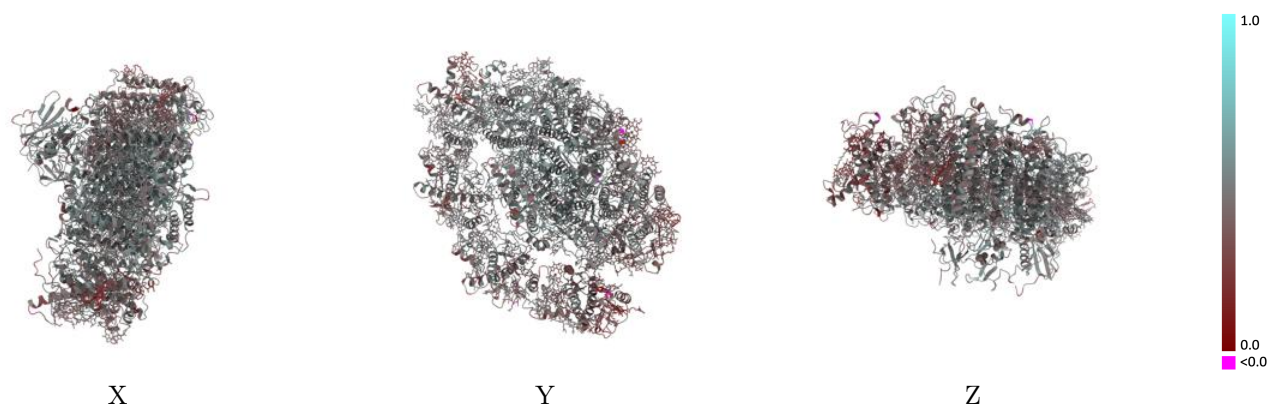
This section contains information regarding the fit between EMDB map EMD-10995 and PDB model 6YXR. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

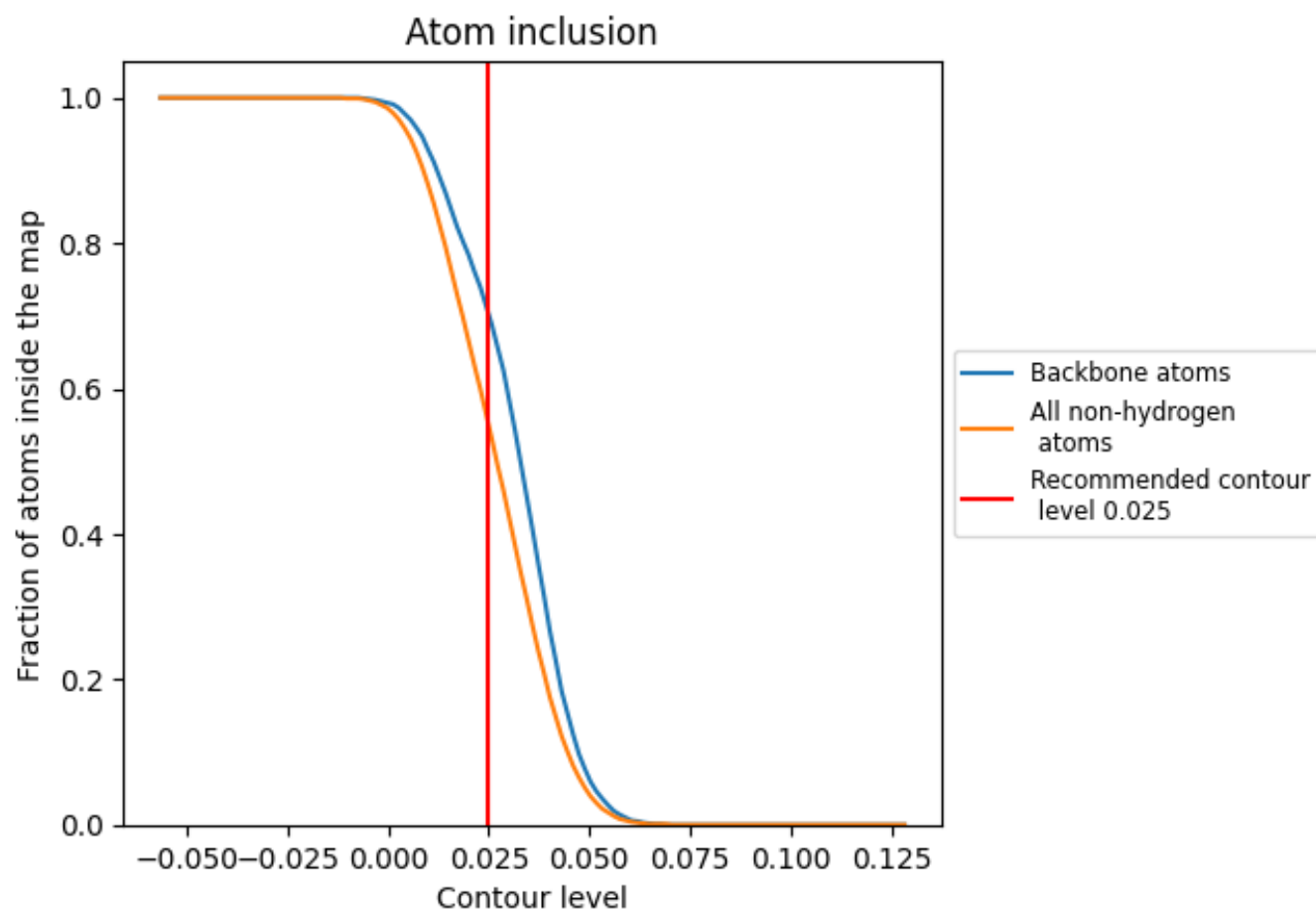


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 55% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5510	0.4530
1	0.3790	0.3630
2	0.4880	0.4320
3	0.4640	0.4200
4	0.4850	0.4160
A	0.6340	0.4970
B	0.5750	0.4530
C	0.6380	0.4890
D	0.5180	0.4550
E	0.5550	0.4630
F	0.5620	0.4680
J	0.6000	0.5000

1.0

0.0

<0.0