



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:45 PM UTC

PDB ID : 1JB0 / pdb_00001jb0
Title : Crystal Structure of Photosystem I: a Photosynthetic Reaction Center and Core Antenna System from Cyanobacteria
Authors : Jordan, P.; Fromme, P.; Witt, H.T.; Klukas, O.; Saenger, W.; Krauss, N.
Deposited on : 2001-06-01
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

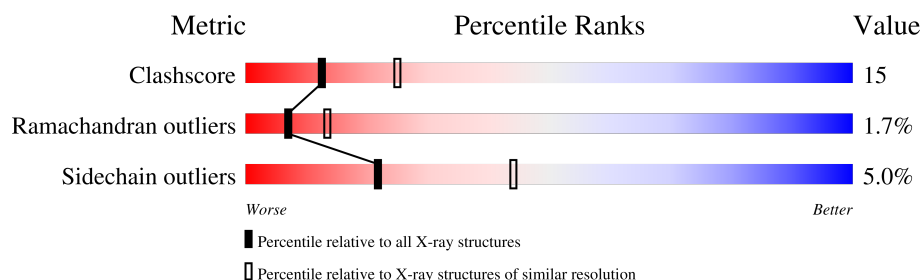
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

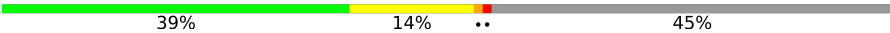
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	755	67% 26% 5% .
2	B	740	68% 27% 5% .
3	C	80	68% 28% . .
4	D	138	64% 31% . .
5	E	75	67% 21% . 8%
6	F	164	55% 27% . 14%
7	I	38	68% 26% 5%
8	J	41	54% 37% 10%

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Mol	Chain	Length	Quality of chain
9	K	83	
10	L	154	
11	M	31	
12	X	35	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	1011	X	-	-	-
13	CLA	A	1013	X	-	-	-
13	CLA	A	1022	X	-	-	-
13	CLA	A	1101	X	-	-	-
13	CLA	A	1102	X	-	-	-
13	CLA	A	1103	X	-	-	-
13	CLA	A	1104	X	-	-	-
13	CLA	A	1105	X	-	-	-
13	CLA	A	1106	X	-	-	-
13	CLA	A	1107	X	-	-	-
13	CLA	A	1109	X	-	-	-
13	CLA	A	1110	X	-	-	-
13	CLA	A	1111	X	-	-	-
13	CLA	A	1112	X	-	-	-
13	CLA	A	1113	X	-	-	-
13	CLA	A	1114	X	-	-	-
13	CLA	A	1116	X	-	-	-
13	CLA	A	1117	X	-	-	-
13	CLA	A	1118	X	-	-	-
13	CLA	A	1119	X	-	-	-
13	CLA	A	1120	X	-	-	-
13	CLA	A	1121	X	-	-	-
13	CLA	A	1122	X	-	-	-
13	CLA	A	1123	X	-	-	-
13	CLA	A	1124	X	-	-	-
13	CLA	A	1125	X	-	-	-
13	CLA	A	1126	X	-	-	-
13	CLA	A	1127	X	-	-	-
13	CLA	A	1128	X	-	-	-
13	CLA	A	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	1130	X	-	-	-
13	CLA	A	1132	X	-	-	-
13	CLA	A	1133	X	-	-	-
13	CLA	A	1134	X	-	-	-
13	CLA	A	1135	X	-	-	-
13	CLA	A	1136	X	-	-	-
13	CLA	A	1137	X	-	-	-
13	CLA	A	1138	X	-	-	-
13	CLA	A	1139	X	-	-	-
13	CLA	A	1140	X	-	-	-
13	CLA	A	1237	X	-	-	-
13	CLA	A	1402	X	-	-	-
13	CLA	A	1801	X	-	-	-
13	CLA	B	1012	X	-	-	-
13	CLA	B	1021	X	-	-	-
13	CLA	B	1201	X	-	-	-
13	CLA	B	1202	X	-	-	-
13	CLA	B	1203	X	-	-	-
13	CLA	B	1204	X	-	-	-
13	CLA	B	1205	X	-	-	-
13	CLA	B	1206	X	-	-	-
13	CLA	B	1207	X	-	-	-
13	CLA	B	1208	X	-	-	-
13	CLA	B	1209	X	-	-	-
13	CLA	B	1210	X	-	-	-
13	CLA	B	1211	X	-	-	-
13	CLA	B	1213	X	-	-	-
13	CLA	B	1214	X	-	-	-
13	CLA	B	1215	X	-	-	-
13	CLA	B	1216	X	-	-	-
13	CLA	B	1217	X	-	-	-
13	CLA	B	1218	X	-	-	-
13	CLA	B	1219	X	-	-	-
13	CLA	B	1220	X	-	-	-
13	CLA	B	1221	X	-	-	-
13	CLA	B	1222	X	-	-	-
13	CLA	B	1223	X	-	-	-
13	CLA	B	1224	X	-	-	-
13	CLA	B	1226	X	-	-	-
13	CLA	B	1227	X	-	-	-
13	CLA	B	1228	X	-	-	-
13	CLA	B	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	1230	X	-	-	-
13	CLA	B	1231	X	-	-	-
13	CLA	B	1232	X	-	-	-
13	CLA	B	1233	X	-	-	-
13	CLA	B	1234	X	-	-	-
13	CLA	B	1235	X	-	-	-
13	CLA	B	1238	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	J	1302	X	-	-	-
13	CLA	J	1303	X	-	-	-
13	CLA	L	1501	X	-	-	-
13	CLA	L	1503	X	-	-	-
13	CLA	M	1601	X	-	-	-
13	CLA	X	1701	X	-	-	-
17	LHG	A	5003	X	-	-	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 24198 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			

- Molecule 2 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

- Molecule 3 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			

- Molecule 4 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

- Molecule 5 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			539	342	93	104			

- Molecule 6 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

- Molecule 7 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

- Molecule 8 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

- Molecule 9 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	S	0	0	0
			222	130	46	46				

- Molecule 10 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ARG	PRO	conflict	UNP P25902
L	144	VAL	-	SEE REMARK 999	UNP P25902
L	145	VAL	-	SEE REMARK 999	UNP P25902
L	146	ASP	-	SEE REMARK 999	UNP P25902
L	147	GLY	-	SEE REMARK 999	UNP P25902
L	148	ILE	-	SEE REMARK 999	UNP P25902
L	149	MET	-	SEE REMARK 999	UNP P25902
L	150	THR	-	SEE REMARK 999	UNP P25902
L	151	GLY	-	SEE REMARK 999	UNP P25902
L	152	LEU	-	SEE REMARK 999	UNP P25902
L	153	PHE	-	SEE REMARK 999	UNP P25902
L	154	ASN	-	SEE REMARK 999	UNP P25902

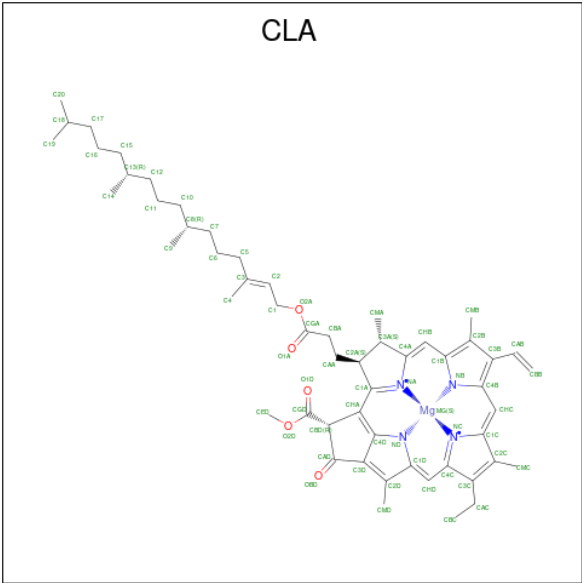
- Molecule 11 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	M	31	241	161	36	43	1	0	0	0

- Molecule 12 is a protein called PHOTOSYSTEM I SUBUNIT PSAX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	X	29	233	164	34	35	0	0	0

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	A	1	Total 65	55	1	4	5	0	0
13	A	1	Total 65	55	1	4	5	0	0
13	A	1	Total 65	55	1	4	5	0	0
13	A	1	Total 65	55	1	4	5	0	0
13	A	1	Total 59	49	1	4	5	0	0
13	A	1	Total 65	55	1	4	5	0	0
13	A	1	Total 65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
13	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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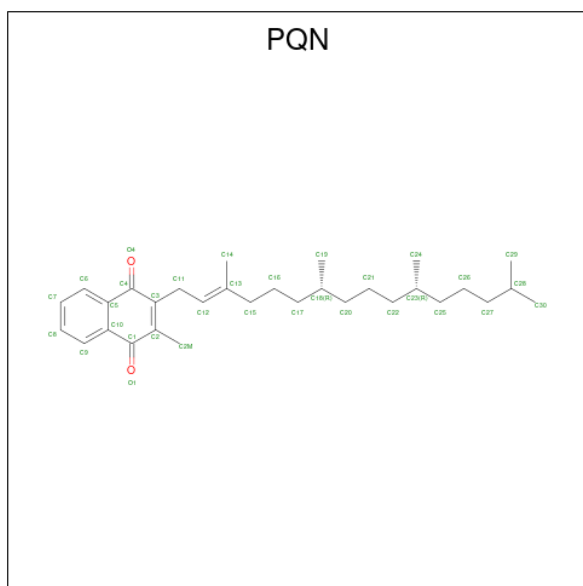
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
13	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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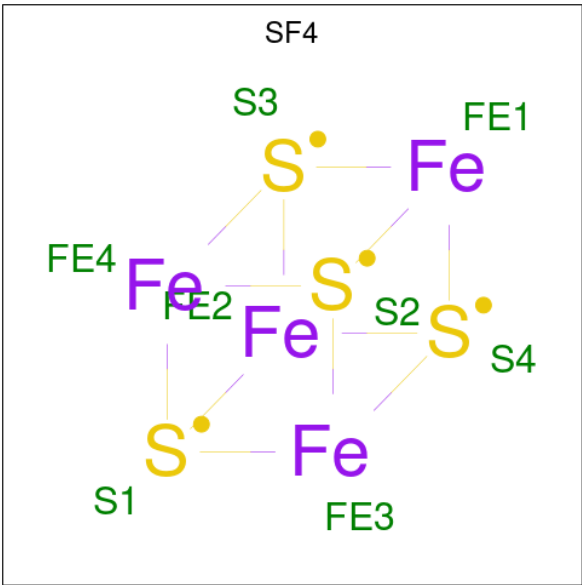
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



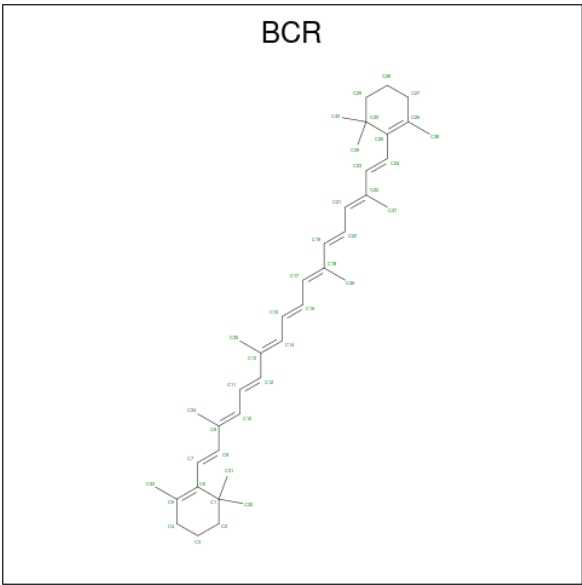
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			33	31	2		
14	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



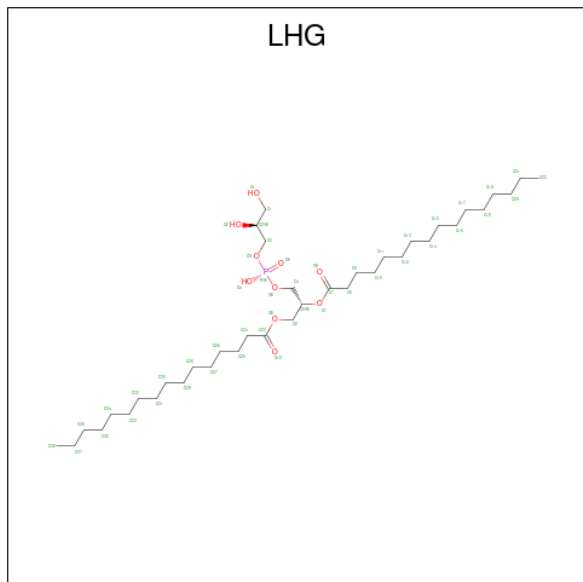
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	C	0	0
			40	40		

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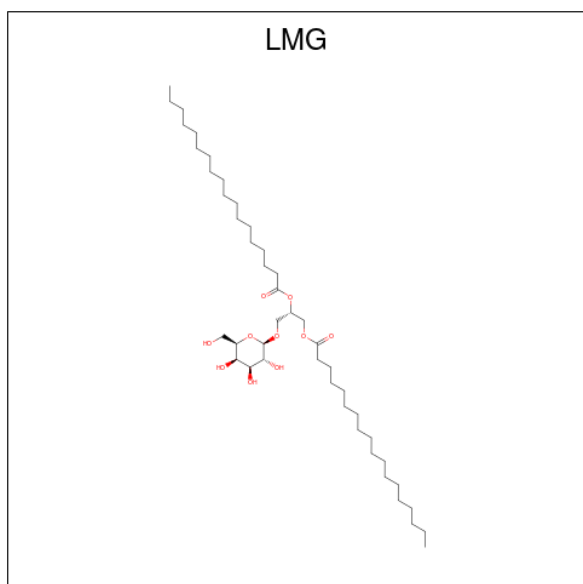
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 25 25	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	F	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	M	1	Total C 40 40	0	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			49	38	10	1		
17	A	1	Total	C	O	P	0	0
			27	16	10	1		
17	B	1	Total	C	O	P	0	0
			23	12	10	1		

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	53	Total	O	0	0
			53	53		
20	B	65	Total	O	0	0
			65	65		
20	C	21	Total	O	0	0
			21	21		
20	D	17	Total	O	0	0
			17	17		
20	E	5	Total	O	0	0
			5	5		
20	F	6	Total	O	0	0
			6	6		
20	I	3	Total	O	0	0
			3	3		
20	J	1	Total	O	0	0
			1	1		
20	L	27	Total	O	0	0
			27	27		
20	M	3	Total	O	0	0
			3	3		

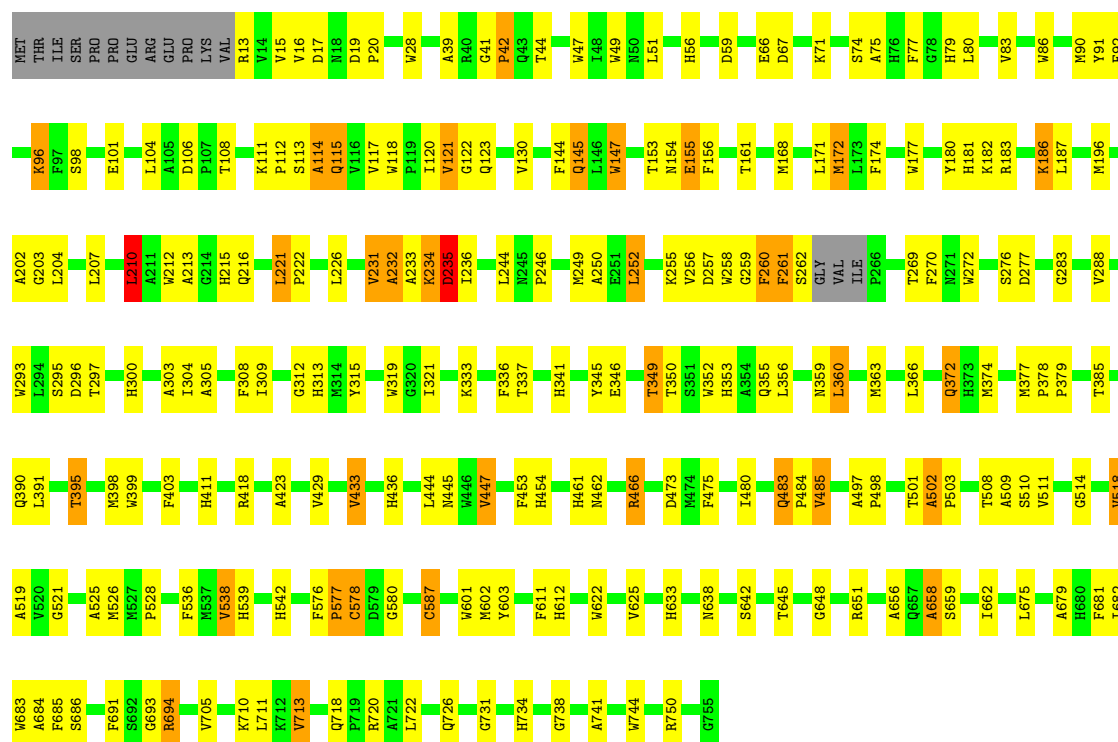
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

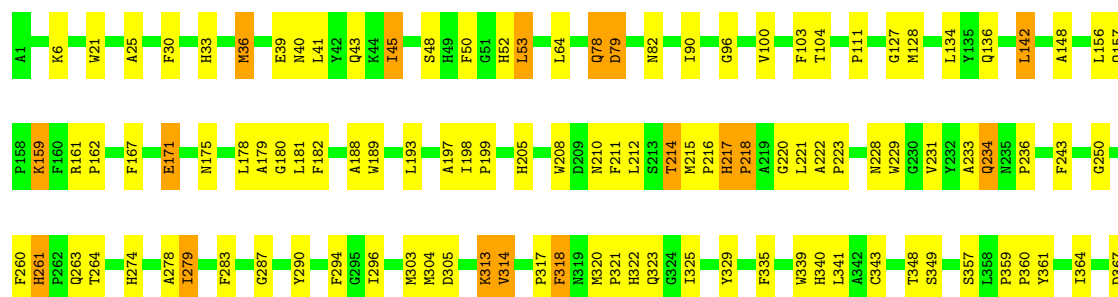
• Molecule 1: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

Chain A: 



• Molecule 2: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

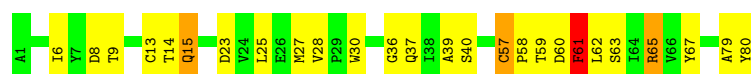
Chain B: 





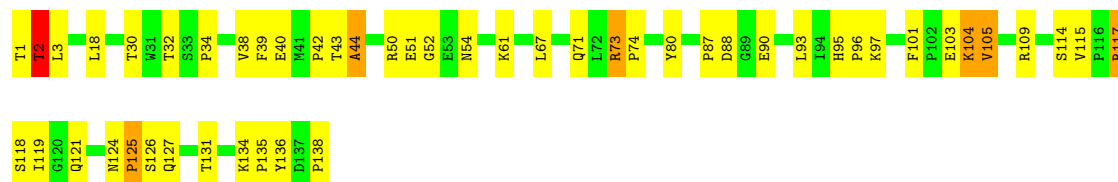
● Molecule 3: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C: 68% 28% . .



● Molecule 4: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II

Chain D: 64% 31% . .



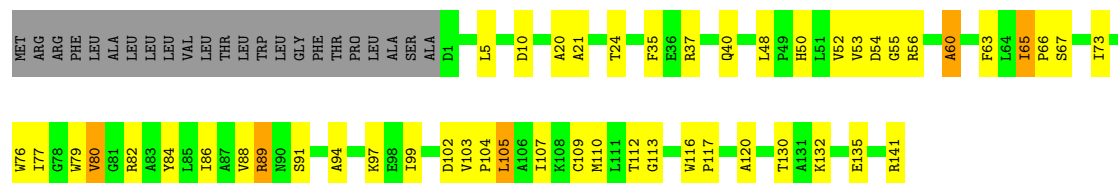
● Molecule 5: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV

Chain E: 67% 21% . 8%



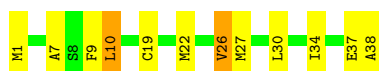
● Molecule 6: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III

Chain F: 55% 27% . 14%

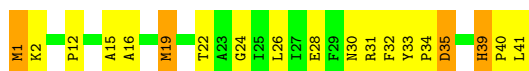


● Molecule 7: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII

Chain I: 68% 26% 5%



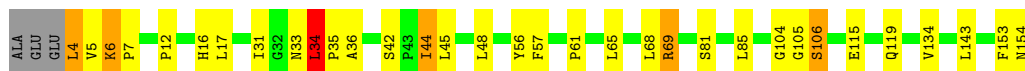
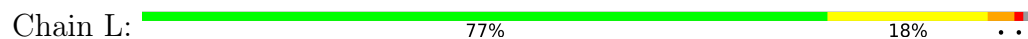
• Molecule 8: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX



• Molecule 9: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X



• Molecule 10: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI



• Molecule 11: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII



• Molecule 12: PHOTOSYSTEM I SUBUNIT PSAX



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (30.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.199 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24198	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LMG, CA, SF4, PQN, CLA, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/5983	1.04	40/8158 (0.5%)
2	B	0.66	2/6096 (0.0%)	1.02	34/8332 (0.4%)
3	C	0.91	0/608	1.30	12/824 (1.5%)
4	D	0.65	0/1101	1.19	7/1492 (0.5%)
5	E	0.64	0/551	1.26	8/750 (1.1%)
6	F	0.55	1/1087 (0.1%)	1.02	1/1476 (0.1%)
7	I	0.84	0/312	1.15	1/425 (0.2%)
8	J	0.48	0/350	1.18	4/477 (0.8%)
9	K	0.72	0/219	1.50	5/297 (1.7%)
10	L	0.77	0/1148	1.04	3/1558 (0.2%)
11	M	0.75	0/244	1.13	1/332 (0.3%)
12	X	0.52	0/242	1.09	2/332 (0.6%)
All	All	0.65	3/17941 (0.0%)	1.07	118/24453 (0.5%)

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
3	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	589	MET	SD-CE	-8.57	1.58	1.79
2	B	36	MET	SD-CE	-7.66	1.60	1.79
6	F	65	ILE	CA-CB	5.15	1.57	1.54

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	131	THR	N-CA-C	-13.95	89.86	109.95
9	K	35	GLN	N-CA-C	10.55	125.45	109.62
11	M	30	TYR	N-CA-C	10.04	132.18	110.80
2	B	482	SER	N-CA-C	-8.83	102.52	113.38
2	B	553	MET	CA-C-N	8.38	128.50	119.28
2	B	553	MET	C-N-CA	8.38	128.50	119.28
5	E	34	TYR	CA-C-N	8.33	128.02	119.19
5	E	34	TYR	C-N-CA	8.33	128.02	119.19
3	C	63	SER	N-CA-C	-8.24	103.36	113.50
2	B	651	VAL	CB-CA-C	-8.07	101.72	111.81
1	A	521	GLY	N-CA-C	-8.01	97.13	112.02
2	B	674	ARG	N-CA-C	7.94	124.40	111.37
5	E	54	GLY	N-CA-C	7.90	131.91	113.18
6	F	55	GLY	N-CA-C	-7.82	105.17	114.48
8	J	2	LYS	N-CA-C	-7.82	102.83	111.36
3	C	60	ASP	CA-C-N	7.79	136.41	121.54
3	C	60	ASP	C-N-CA	7.79	136.41	121.54
1	A	231	VAL	N-CA-C	7.39	118.16	110.62
1	A	319	TRP	N-CA-C	7.32	120.25	110.88
5	E	33	LYS	N-CA-C	7.30	119.32	111.36
5	E	55	VAL	N-CA-C	7.30	124.53	109.34
8	J	35	ASP	N-CA-C	7.30	121.47	111.54
1	A	114	ALA	N-CA-C	-7.29	95.16	108.65
1	A	577	PRO	N-CA-C	7.26	123.08	113.57
2	B	461	VAL	N-CA-C	7.02	117.78	110.62
10	L	34	LEU	N-CA-C	-7.01	100.40	110.08
8	J	39	HIS	CA-C-N	6.88	128.44	119.84
8	J	39	HIS	C-N-CA	6.88	128.44	119.84
2	B	528	ALA	N-CA-C	-6.87	103.87	111.36
2	B	261	HIS	N-CA-C	-6.82	99.66	109.48
1	A	580	GLY	CA-C-N	6.81	126.50	119.82
1	A	580	GLY	C-N-CA	6.81	126.50	119.82
1	A	418	ARG	N-CA-C	6.79	121.89	112.45
2	B	217	HIS	CA-C-N	6.79	128.32	119.84
2	B	217	HIS	C-N-CA	6.79	128.32	119.84
1	A	41	GLY	CA-C-N	6.71	128.23	119.84
1	A	41	GLY	C-N-CA	6.71	128.23	119.84
9	K	57	PRO	N-CA-CB	6.67	110.67	103.33
3	C	80	TYR	CA-C-O	6.67	140.99	121.00
9	K	41	PRO	N-CA-CB	6.66	110.24	103.25
12	X	33	ALA	N-CA-C	-6.62	104.47	112.54
2	B	525	VAL	CB-CA-C	-6.48	103.40	112.14
2	B	635	SER	N-CA-C	6.39	118.82	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	ALA	CA-C-N	6.34	127.76	119.84
1	A	502	ALA	C-N-CA	6.34	127.76	119.84
1	A	213	ALA	N-CA-C	-6.33	104.43	111.71
1	A	611	PHE	N-CA-C	-6.30	104.49	111.36
3	C	61	PHE	N-CA-CB	6.30	121.14	110.49
2	B	79	ASP	CA-C-N	6.22	125.90	119.56
2	B	79	ASP	C-N-CA	6.22	125.90	119.56
1	A	485	VAL	N-CA-C	6.17	117.66	110.62
2	B	619	SER	N-CA-C	6.15	120.39	113.01
1	A	337	THR	N-CA-C	6.12	120.06	112.59
1	A	461	HIS	N-CA-C	-6.12	104.52	111.07
1	A	96	LYS	N-CA-C	6.11	120.47	112.89
1	A	39	ALA	N-CA-C	5.99	117.81	111.28
2	B	156	LEU	N-CA-C	-5.98	105.95	113.72
2	B	220	GLY	N-CA-C	5.97	121.06	112.82
2	B	142	LEU	N-CA-C	-5.93	104.81	111.28
2	B	598	PHE	N-CA-C	-5.90	104.85	111.28
7	I	27	MET	N-CA-C	-5.89	104.94	111.36
4	D	87	PRO	CA-C-N	5.87	128.47	120.54
4	D	87	PRO	C-N-CA	5.87	128.47	120.54
1	A	694	ARG	N-CA-C	5.87	118.46	111.71
2	B	335	PHE	N-CA-C	-5.85	104.82	111.14
10	L	6	LYS	N-CA-C	5.81	113.24	108.07
1	A	658	ALA	N-CA-C	-5.81	105.96	113.16
2	B	651	VAL	N-CA-CB	5.79	116.93	110.62
1	A	106	ASP	CA-C-N	5.79	125.47	119.05
1	A	106	ASP	C-N-CA	5.79	125.47	119.05
2	B	260	PHE	N-CA-C	5.73	118.55	109.50
4	D	115	VAL	CA-C-N	5.72	126.99	119.84
4	D	115	VAL	C-N-CA	5.72	126.99	119.84
2	B	45	ILE	CB-CA-C	-5.67	104.72	111.81
9	K	73	VAL	N-CA-C	-5.67	103.96	111.05
1	A	398	MET	N-CA-C	-5.64	105.05	111.14
2	B	492	TRP	N-CA-C	5.64	122.27	109.81
1	A	538	VAL	CB-CA-C	-5.58	103.50	112.16
2	B	491	ALA	N-CA-C	-5.55	104.24	111.74
9	K	62	THR	N-CA-C	-5.55	105.77	112.54
2	B	96	GLY	N-CA-C	-5.51	103.08	112.51
3	C	9	THR	N-CA-C	-5.49	106.16	112.92
3	C	60	ASP	CA-C-O	5.49	126.91	120.98
1	A	377	MET	CA-C-N	5.49	126.03	120.38
1	A	377	MET	C-N-CA	5.49	126.03	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	42	PRO	N-CA-C	-5.46	107.32	114.03
1	A	28	TRP	N-CA-C	-5.46	105.44	111.71
10	L	5	VAL	N-CA-C	-5.39	100.56	108.11
5	E	43	VAL	CB-CA-C	-5.36	105.69	111.59
2	B	627	ARG	N-CA-C	5.34	117.92	111.40
3	C	79	ALA	N-CA-C	-5.34	106.64	112.72
1	A	483	GLN	CA-C-N	5.33	126.50	119.84
1	A	483	GLN	C-N-CA	5.33	126.50	119.84
5	E	11	ARG	CA-C-N	5.32	125.38	119.32
5	E	11	ARG	C-N-CA	5.32	125.38	119.32
2	B	425	LEU	N-CA-C	-5.32	105.48	111.28
3	C	60	ASP	O-C-N	5.30	129.67	122.57
1	A	154	ASN	N-CA-C	5.27	117.08	109.07
1	A	182	LYS	N-CA-C	5.25	118.02	111.24
1	A	272	TRP	N-CA-C	5.25	118.79	112.38
1	A	315	TYR	N-CA-C	5.23	118.33	109.76
4	D	2	THR	N-CA-C	5.21	121.91	110.80
2	B	393	GLY	N-CA-C	-5.21	106.11	112.77
12	X	21	ALA	N-CA-C	-5.19	105.52	111.07
1	A	288	VAL	N-CA-C	5.17	115.84	110.82
1	A	210	LEU	N-CA-C	-5.17	105.54	111.07
3	C	57	CYS	CA-C-N	5.14	126.26	119.84
3	C	57	CYS	C-N-CA	5.14	126.26	119.84
2	B	420	ALA	N-CA-C	-5.12	105.61	111.14
2	B	104	THR	N-CA-C	-5.11	98.72	108.17
1	A	576	PHE	CA-C-N	5.11	124.60	119.19
1	A	576	PHE	C-N-CA	5.11	124.60	119.19
3	C	59	THR	N-CA-C	5.06	117.57	110.23
1	A	454	HIS	N-CA-C	5.03	119.14	113.15
1	A	750	ARG	N-CA-C	5.03	116.61	111.03
2	B	348	THR	N-CA-C	-5.01	105.53	111.69
2	B	127	GLY	N-CA-C	5.00	122.21	115.00
2	B	739	PHE	CA-C-O	-5.00	112.30	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	61	PHE	Sidechain

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	A	5784	0	5639	219	0
2	B	5879	0	5632	239	0
3	C	598	0	580	17	0
4	D	1075	0	1077	41	0
5	E	539	0	528	10	0
6	F	1065	0	1079	45	0
7	I	301	0	306	8	0
8	J	338	0	347	23	0
9	K	222	0	110	5	0
10	L	1119	0	1125	22	0
11	M	241	0	264	13	0
12	X	233	0	231	6	0
13	A	2687	0	2675	130	0
13	B	2349	0	2304	132	0
13	F	45	0	33	1	0
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	10	0
13	M	45	0	33	1	0
13	X	45	0	33	1	0
14	A	33	0	46	1	0
14	B	33	0	46	1	0
15	A	8	0	0	0	0
15	C	16	0	0	0	0
16	A	240	0	336	21	0
16	B	265	0	369	15	0
16	F	40	0	56	2	0
16	I	80	0	112	4	0
16	J	120	0	168	16	0
16	L	80	0	112	1	0
16	M	40	0	56	2	0
17	A	76	0	98	6	0
17	B	23	0	16	1	0
18	B	55	0	86	5	0
19	L	1	0	0	0	0
20	A	53	0	0	5	0
20	B	65	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	21	0	0	3	0
20	D	17	0	0	1	0
20	E	5	0	0	0	0
20	F	6	0	0	1	0
20	I	3	0	0	0	0
20	J	1	0	0	0	0
20	L	27	0	0	1	1
20	M	3	0	0	1	0
All	All	24198	0	23804	728	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (728) 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)
8:J:31:ARG:HD3	16:J:4013:BCR:H312	1.25	1.17
2:B:622:LEU:HD12	13:B:1012:CLA:H11	1.29	1.15
1:A:508:THR:HG22	1:A:510:SER:H	1.18	1.07
2:B:159:LYS:H	2:B:159:LYS:HD2	1.18	1.05
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01
2:B:243:PHE:H	2:B:263:GLN:HE22	1.07	1.01
2:B:231:VAL:O	2:B:234:GLN:HG2	1.63	0.99
2:B:406:ASN:HD22	2:B:409:ASN:HD21	0.98	0.96
1:A:536:PHE:HA	13:A:1136:CLA:HED1	1.45	0.96
2:B:494:ASN:HD22	2:B:496:GLY:H	1.13	0.93
11:M:31:LYS:O	11:M:31:LYS:HG2	1.70	0.92
1:A:353:HIS:HD2	1:A:411:HIS:HD1	1.21	0.88
4:D:117:ARG:HG3	4:D:121:GLN:HB2	1.54	0.88
16:A:4011:BCR:H362	13:B:1012:CLA:H42	1.55	0.87
2:B:589:MET:HE2	2:B:589:MET:C	2.01	0.85
1:A:117:VAL:HG13	1:A:123:GLN:HE21	1.42	0.84
2:B:406:ASN:ND2	2:B:409:ASN:HD21	1.76	0.83
8:J:24:GLY:HA3	13:J:1302:CLA:HBB1	1.60	0.83
4:D:101:PHE:HB2	4:D:104:LYS:HE2	1.59	0.83
8:J:31:ARG:HD3	16:J:4013:BCR:C31	2.08	0.83
1:A:333:LYS:O	13:A:1801:CLA:HBC3	1.81	0.81
2:B:509:SER:O	2:B:511:THR:N	2.12	0.81
2:B:128:MET:HE3	2:B:134:LEU:HD23	1.64	0.80
1:A:203:GLY:HA2	13:A:1118:CLA:HBC1	1.63	0.80
1:A:391:LEU:O	1:A:395:THR:HG23	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:MET:HE2	13:A:1126:CLA:HED1	1.62	0.80
2:B:367:ASP:CG	2:B:370:THR:HG23	2.07	0.80
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.12	0.80
8:J:19:MET:HE3	8:J:19:MET:HA	1.63	0.79
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.63	0.79
6:F:88:VAL:HG11	6:F:97:LYS:HB2	1.64	0.79
2:B:589:MET:HE2	2:B:590:LEU:N	1.98	0.78
1:A:345:TYR:O	1:A:349:THR:HB	1.84	0.78
2:B:494:ASN:ND2	2:B:496:GLY:H	1.80	0.78
2:B:459:GLU:HG3	6:F:5:LEU:HD11	1.63	0.78
2:B:243:PHE:H	2:B:263:GLN:NE2	1.82	0.78
1:A:508:THR:HG22	1:A:510:SER:N	1.96	0.77
2:B:589:MET:HE3	2:B:593:ILE:HG13	1.65	0.77
2:B:313:LYS:O	2:B:314:VAL:HG22	1.85	0.77
3:C:37:GLN:NE2	4:D:105:VAL:HG22	1.99	0.77
2:B:278:ALA:HB2	13:B:1214:CLA:HBB1	1.66	0.77
2:B:339:TRP:HE1	13:B:1221:CLA:C2B	1.99	0.76
2:B:25:ALA:HB2	18:B:5002:LMG:H121	1.67	0.76
13:A:1011:CLA:HBB1	13:B:1012:CLA:HED1	1.67	0.75
1:A:231:VAL:O	1:A:232:ALA:HB3	1.87	0.75
13:A:1126:CLA:H192	16:J:4012:BCR:H14C	1.69	0.75
2:B:647:ASN:HD22	2:B:649:LEU:H	1.35	0.75
13:A:1126:CLA:H93	16:J:4012:BCR:H361	1.69	0.74
1:A:453:PHE:O	13:A:1132:CLA:HBB2	1.88	0.74
13:B:1222:CLA:HAA2	13:B:1223:CLA:OBD	1.87	0.74
2:B:639:ASN:HD22	2:B:642:ASN:HD22	1.36	0.74
2:B:229:TRP:HB2	13:B:1213:CLA:H12	1.70	0.73
2:B:497:ASN:O	2:B:498:VAL:HB	1.87	0.73
1:A:90:MET:HE1	13:A:1106:CLA:HED2	1.71	0.73
4:D:50:ARG:N	4:D:54:ASN:HD21	1.84	0.73
2:B:159:LYS:H	2:B:159:LYS:CD	1.92	0.73
2:B:494:ASN:HD22	2:B:496:GLY:N	1.84	0.72
2:B:181:LEU:HG	13:B:1210:CLA:H43	1.71	0.72
2:B:425:LEU:HG	13:B:1236:CLA:CBB	2.20	0.72
2:B:622:LEU:HD12	13:B:1012:CLA:C1	2.15	0.72
2:B:725:LEU:HD11	13:B:1226:CLA:H203	1.69	0.72
11:M:31:LYS:O	11:M:31:LYS:CG	2.34	0.72
2:B:329:TYR:OH	2:B:340:HIS:HE1	1.71	0.72
3:C:39:ALA:O	20:C:3012:HOH:O	2.07	0.72
2:B:343:CYS:HB3	13:B:1221:CLA:H42	1.72	0.71
13:B:1216:CLA:HAA2	13:B:1221:CLA:HBB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.71	0.71
1:A:221:LEU:HB2	1:A:222:PRO:HD3	1.73	0.71
13:B:1235:CLA:HMA2	13:B:1236:CLA:HED2	1.73	0.71
2:B:36:MET:HE2	2:B:41:LEU:N	2.06	0.70
1:A:341:HIS:HE1	17:A:5003:LHG:HC11	1.56	0.70
6:F:63:PHE:C	6:F:66:PRO:HD2	2.17	0.70
5:E:68:VAL:HG23	5:E:69:ALA:H	1.56	0.70
1:A:255:LYS:HB2	1:A:277:ASP:OD2	1.92	0.69
2:B:222:ALA:HB3	2:B:223:PRO:HD3	1.74	0.69
1:A:13:ARG:HE	1:A:15:VAL:CG2	2.05	0.68
13:A:1136:CLA:H101	13:L:1502:CLA:H191	1.75	0.68
2:B:602:TRP:HE1	2:B:614:GLN:HE21	1.40	0.68
1:A:221:LEU:HD11	1:A:295:SER:HA	1.76	0.68
1:A:399:TRP:CD1	13:A:1126:CLA:HAB	2.29	0.68
6:F:52:VAL:HG12	6:F:54:ASP:HB2	1.76	0.67
1:A:117:VAL:HG13	1:A:123:GLN:NE2	2.08	0.67
2:B:25:ALA:HA	13:B:1226:CLA:H42	1.76	0.67
1:A:101:GLU:OE2	1:A:155:GLU:HG2	1.95	0.66
2:B:480:LEU:C	2:B:482:SER:H	2.02	0.66
6:F:102:ASP:OD2	6:F:105:LEU:HB2	1.95	0.66
9:K:73:VAL:HA	13:K:1401:CLA:HBB1	1.77	0.66
1:A:336:PHE:HB2	17:A:5003:LHG:HC41	1.78	0.66
2:B:339:TRP:HZ2	13:B:1221:CLA:HAB	1.58	0.66
2:B:320:MET:HE2	13:B:1220:CLA:HBB1	1.78	0.66
3:C:65:ARG:HG2	3:C:67:TYR:CZ	2.31	0.66
14:A:2001:PQN:H172	16:B:4014:BCR:H382	1.77	0.66
4:D:50:ARG:H	4:D:54:ASN:ND2	1.89	0.66
2:B:188:ALA:HA	13:B:1212:CLA:CBB	2.27	0.65
1:A:352:TRP:HB3	13:A:1103:CLA:HAC1	1.77	0.65
2:B:210:ASN:O	2:B:214:THR:HG23	1.96	0.65
2:B:41:LEU:O	2:B:45:ILE:HG12	1.97	0.65
2:B:318:PHE:CD1	13:B:1219:CLA:HAB	2.32	0.65
1:A:249:MET:O	1:A:252:LEU:O	2.15	0.65
1:A:257:ASP:OD1	1:A:262:SER:HB3	1.96	0.65
2:B:492:TRP:CE3	2:B:493:PRO:HD3	2.32	0.65
1:A:269:THR:O	1:A:270:PHE:HB2	1.96	0.65
2:B:313:LYS:O	2:B:314:VAL:HG13	1.97	0.65
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.78	0.65
10:L:6:LYS:HB2	10:L:7:PRO:HD2	1.79	0.65
1:A:168:MET:HE2	1:A:171:LEU:HD23	1.78	0.65
13:A:1237:CLA:H191	13:L:1502:CLA:HBB1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:54:ASP:OD2	12:X:30:TYR:CE2	2.50	0.64
2:B:589:MET:HE2	2:B:590:LEU:CA	2.28	0.64
2:B:304:MET:HG3	2:B:322:HIS:O	1.97	0.64
2:B:647:ASN:ND2	2:B:649:LEU:H	1.95	0.64
1:A:473:ASP:OD1	10:L:69:ARG:NH2	2.31	0.64
10:L:61:PRO:HB3	13:L:1503:CLA:HBB1	1.78	0.64
2:B:641:TYR:HB2	2:B:646:THR:HG22	1.79	0.64
8:J:12:PRO:HB2	16:J:4013:BCR:H391	1.78	0.64
2:B:589:MET:HE3	2:B:593:ILE:CG1	2.27	0.64
13:B:1203:CLA:H162	13:B:1225:CLA:HBB2	1.80	0.64
1:A:257:ASP:CG	1:A:258:TRP:N	2.56	0.63
6:F:103:VAL:HB	6:F:104:PRO:HD3	1.79	0.63
2:B:36:MET:HE2	2:B:41:LEU:CA	2.28	0.63
3:C:23:ASP:OD2	4:D:95:HIS:HD2	1.81	0.63
13:B:1023:CLA:H111	16:B:4017:BCR:H362	1.79	0.63
6:F:63:PHE:O	6:F:66:PRO:HD2	1.98	0.63
13:A:1011:CLA:HAB	13:B:1021:CLA:NA	2.14	0.63
2:B:318:PHE:HA	13:B:1219:CLA:CAB	2.28	0.63
4:D:117:ARG:HG2	4:D:118:SER:O	1.98	0.63
2:B:622:LEU:CD1	13:B:1012:CLA:H11	2.16	0.63
6:F:60:ALA:O	6:F:65:ILE:HG12	1.98	0.62
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.80	0.62
2:B:589:MET:HE2	2:B:590:LEU:HA	1.81	0.62
11:M:29:LEU:O	11:M:30:TYR:HB2	1.99	0.62
1:A:104:LEU:HD11	1:A:153:THR:HA	1.81	0.62
1:A:651:ARG:HB2	2:B:638:ILE:HG23	1.81	0.62
1:A:86:TRP:HA	13:A:1105:CLA:HBB2	1.82	0.62
2:B:136:GLN:HE22	2:B:208:TRP:HE1	1.46	0.62
2:B:228:ASN:O	2:B:231:VAL:HG23	2.00	0.62
1:A:602:MET:HG2	13:A:1124:CLA:HBC1	1.80	0.62
2:B:647:ASN:HD21	2:B:649:LEU:HB2	1.64	0.62
1:A:356:LEU:O	1:A:360:LEU:HB2	2.00	0.62
2:B:303:MET:HE2	13:B:1220:CLA:HED1	1.81	0.62
1:A:353:HIS:CD2	1:A:411:HIS:HD1	2.11	0.61
2:B:278:ALA:CB	13:B:1214:CLA:HBB1	2.29	0.61
1:A:429:VAL:O	1:A:433:VAL:HG13	1.99	0.61
13:A:1124:CLA:HAA2	13:A:1125:CLA:OBD	2.00	0.61
1:A:42:PRO:HG2	6:F:99:ILE:HD13	1.83	0.61
2:B:438:GLY:HA3	13:B:1230:CLA:CBB	2.31	0.61
11:M:24:ARG:HG3	11:M:24:ARG:HH11	1.64	0.61
1:A:453:PHE:O	13:A:1132:CLA:CBB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:GLN:HG3	17:A:5001:LHG:O9	2.01	0.61
13:A:1801:CLA:HBD	13:A:1801:CLA:H61	1.83	0.61
1:A:518:VAL:HG22	1:A:525:ALA:HB3	1.82	0.60
1:A:601:TRP:HH2	13:A:1022:CLA:HBB1	1.66	0.60
10:L:153:PHE:O	10:L:154:ASN:HB2	1.99	0.60
13:B:1203:CLA:H102	13:B:1203:CLA:H151	1.84	0.60
3:C:30:TRP:O	3:C:36:GLY:HA2	2.00	0.60
1:A:303:ALA:HB2	13:A:1116:CLA:HBB1	1.83	0.60
9:K:32:TYR:O	9:K:34:ILE:N	2.34	0.60
9:K:40:GLY:O	9:K:41:PRO:C	2.44	0.60
1:A:484:PRO:HB3	13:A:1136:CLA:HED3	1.83	0.60
1:A:168:MET:CE	1:A:171:LEU:HD23	2.31	0.60
13:A:1011:CLA:HBB1	13:B:1012:CLA:CED	2.31	0.60
1:A:210:LEU:HD21	16:A:4001:BCR:H342	1.84	0.59
1:A:300:HIS:O	1:A:304:ILE:HG12	2.03	0.59
1:A:19:ASP:HA	1:A:181:HIS:O	2.02	0.59
1:A:231:VAL:O	1:A:232:ALA:CB	2.50	0.59
13:B:1227:CLA:HBC1	16:B:4009:BCR:H23C	1.83	0.59
1:A:259:GLY:O	1:A:261:PHE:N	2.35	0.59
2:B:181:LEU:HD21	13:B:1210:CLA:H12	1.85	0.59
13:A:1138:CLA:H43	13:B:1229:CLA:HAA2	1.84	0.59
2:B:36:MET:CE	2:B:41:LEU:N	2.66	0.59
2:B:642:ASN:HB2	2:B:643:PRO:HD2	1.84	0.59
13:B:1215:CLA:HBB1	13:B:1215:CLA:HMB3	1.83	0.59
4:D:40:GLU:H	4:D:71:GLN:NE2	2.01	0.59
7:I:7:ALA:HB1	7:I:10:LEU:HD22	1.83	0.59
7:I:37:GLU:C	7:I:38:ALA:OXT	2.41	0.59
2:B:591:ASN:HB2	13:B:1012:CLA:HBC2	1.83	0.58
1:A:16:VAL:HG12	1:A:17:ASP:N	2.17	0.58
1:A:207:LEU:HD22	16:A:4002:BCR:H361	1.84	0.58
2:B:438:GLY:HA3	13:B:1230:CLA:HBB1	1.85	0.58
1:A:86:TRP:HA	13:A:1105:CLA:CBB	2.33	0.58
13:B:1230:CLA:O1D	8:J:35:ASP:HA	2.02	0.58
2:B:243:PHE:N	2:B:263:GLN:HE22	1.90	0.58
1:A:145:GLN:H	1:A:145:GLN:NE2	2.02	0.58
1:A:744:TRP:HB2	13:A:1126:CLA:HBB1	1.86	0.58
2:B:367:ASP:OD1	2:B:370:THR:HG23	2.03	0.58
2:B:648:ASN:N	2:B:648:ASN:HD22	2.02	0.58
16:A:4011:BCR:H321	16:A:4011:BCR:HC8	1.83	0.58
2:B:380:TYR:CD1	13:B:1224:CLA:HBB1	2.39	0.57
1:A:91:TYR:CZ	1:A:147:TRP:CZ3	2.91	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:VAL:HG11	16:B:4009:BCR:H401	1.85	0.57
13:A:1119:CLA:HMD3	13:A:1120:CLA:HBB1	1.87	0.57
1:A:244:LEU:C	1:A:246:PRO:HD3	2.30	0.57
6:F:82:ARG:O	6:F:86:ILE:HG12	2.04	0.57
13:A:1013:CLA:H12	2:B:430:LEU:HD12	1.85	0.57
1:A:542:HIS:HB3	13:A:1135:CLA:HBB1	1.87	0.57
2:B:557:LYS:HD2	4:D:124:ASN:OD1	2.04	0.57
2:B:279:ILE:HD11	13:B:1214:CLA:CBC	2.35	0.57
5:E:24:ALA:O	5:E:25:SER:HB3	2.05	0.57
1:A:349:THR:HG22	1:A:350:THR:HG23	1.87	0.56
1:A:355:GLN:HG3	13:A:1123:CLA:H152	1.87	0.56
1:A:694:ARG:HD3	2:B:572:GLY:HA3	1.86	0.56
13:A:1106:CLA:H112	13:A:1128:CLA:H203	1.87	0.56
1:A:67:ASP:O	1:A:71:LYS:HG3	2.05	0.56
2:B:678:GLN:NE2	2:B:705:ALA:H	2.03	0.56
6:F:37:ARG:O	6:F:40:GLN:HG2	2.04	0.56
8:J:15:ALA:O	8:J:19:MET:HB2	2.06	0.56
1:A:233:ALA:O	1:A:235:ASP:N	2.36	0.56
2:B:234:GLN:HA	2:B:234:GLN:OE1	2.06	0.56
2:B:339:TRP:CH2	16:B:4009:BCR:H372	2.40	0.56
13:A:1124:CLA:H12	13:A:1135:CLA:HMA3	1.88	0.56
12:X:20:LEU:HD11	12:X:24:PHE:HE1	1.71	0.56
1:A:259:GLY:C	1:A:261:PHE:H	2.14	0.56
2:B:279:ILE:HG23	2:B:283:PHE:CE2	2.41	0.56
2:B:339:TRP:CZ2	13:B:1221:CLA:HAB	2.39	0.56
2:B:480:LEU:O	2:B:482:SER:N	2.38	0.56
6:F:76:TRP:CE2	6:F:113:GLY:HA3	2.40	0.56
1:A:363:MET:HE1	13:A:1127:CLA:HBC3	1.87	0.56
1:A:66:GLU:OE2	1:A:186:LYS:HG3	2.05	0.56
13:A:1011:CLA:HAB	13:B:1021:CLA:C1A	2.36	0.56
12:X:9:TYR:O	12:X:10:ALA:HB2	2.05	0.56
1:A:366:LEU:HD11	13:A:1117:CLA:H71	1.87	0.56
1:A:297:THR:O	1:A:300:HIS:HB3	2.06	0.56
1:A:741:ALA:HB2	16:A:4011:BCR:H323	1.88	0.56
1:A:79:HIS:CE1	13:A:1103:CLA:HMA2	2.41	0.55
1:A:453:PHE:C	13:A:1132:CLA:HBB2	2.31	0.55
13:A:1130:CLA:H12	13:L:1502:CLA:H93	1.86	0.55
4:D:117:ARG:CG	4:D:121:GLN:HB2	2.33	0.55
2:B:588:TRP:HH2	13:B:1012:CLA:CBB	2.19	0.55
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.41	0.55
2:B:398:VAL:CG2	2:B:547:ALA:HB1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:LEU:HD13	2:B:538:LEU:HA	1.89	0.55
1:A:681:PHE:CD2	16:A:4011:BCR:H363	2.42	0.55
13:B:1225:CLA:H51	16:B:4006:BCR:H392	1.88	0.55
2:B:261:HIS:CD2	2:B:264:THR:H	2.25	0.55
13:B:1224:CLA:HBC3	18:B:5002:LMG:H421	1.88	0.55
1:A:372:GLN:HG3	13:A:1124:CLA:CED	2.37	0.55
2:B:233:ALA:O	2:B:234:GLN:O	2.25	0.55
1:A:244:LEU:O	1:A:246:PRO:HD3	2.06	0.54
1:A:681:PHE:CG	16:A:4011:BCR:H363	2.43	0.54
13:A:1116:CLA:H41	13:A:1133:CLA:HAA2	1.88	0.54
13:B:1238:CLA:H18	16:I:4018:BCR:H362	1.89	0.54
16:A:4007:BCR:H333	16:A:4008:BCR:H333	1.89	0.54
2:B:179:ALA:HB2	2:B:287:GLY:HA3	1.89	0.54
2:B:525:VAL:HG13	13:B:1021:CLA:H141	1.89	0.54
1:A:390:GLN:HE21	1:A:390:GLN:HA	1.71	0.54
2:B:274:HIS:HB3	13:B:1214:CLA:HMB2	1.89	0.54
1:A:403:PHE:HB3	13:A:1104:CLA:H112	1.90	0.54
2:B:205:HIS:ND1	20:B:5051:HOH:O	2.24	0.54
4:D:43:THR:O	4:D:44:ALA:HB3	2.07	0.54
10:L:35:PRO:HG3	13:L:1502:CLA:HED2	1.88	0.54
2:B:413:ARG:HD3	13:B:1227:CLA:OBD	2.07	0.54
2:B:664:ALA:C	13:B:1023:CLA:HBB1	2.31	0.54
2:B:52:HIS:CE1	13:B:1202:CLA:HMA2	2.42	0.54
2:B:157:GLN:O	2:B:161:ARG:HG3	2.08	0.54
2:B:318:PHE:HA	13:B:1219:CLA:HAB	1.88	0.54
2:B:592:THR:O	2:B:596:VAL:HG13	2.08	0.54
1:A:308:PHE:HE2	13:A:1119:CLA:HAB	1.72	0.54
2:B:171:GLU:HB3	2:B:290:TYR:HB3	1.90	0.54
12:X:25:LEU:O	12:X:29:TYR:HD1	1.89	0.54
1:A:42:PRO:HG3	1:A:47:TRP:CE3	2.42	0.54
2:B:21:TRP:CG	2:B:710:GLN:HE22	2.26	0.54
2:B:103:PHE:CZ	2:B:651:VAL:HG22	2.42	0.54
2:B:614:GLN:O	2:B:618:SER:HB2	2.08	0.54
5:E:6:LYS:HD3	5:E:22:THR:HG22	1.89	0.54
2:B:212:LEU:HD21	16:B:4006:BCR:H341	1.90	0.53
2:B:548:ARG:HH22	4:D:124:ASN:CG	2.15	0.53
1:A:305:ALA:O	1:A:309:ILE:HG12	2.08	0.53
6:F:52:VAL:CG1	6:F:54:ASP:HB2	2.37	0.53
11:M:24:ARG:HH11	11:M:24:ARG:CG	2.20	0.53
13:A:1013:CLA:H142	16:A:4011:BCR:H402	1.90	0.53
13:A:1101:CLA:HED1	8:J:12:PRO:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ARG:O	2:B:646:THR:HG21	2.09	0.53
2:B:479:THR:O	2:B:480:LEU:O	2.27	0.53
13:B:1226:CLA:H143	18:B:5002:LMG:H231	1.89	0.53
6:F:53:VAL:HG12	6:F:63:PHE:HB2	1.90	0.53
6:F:88:VAL:HG11	6:F:97:LYS:CB	2.37	0.53
1:A:622:TRP:O	1:A:633:HIS:HD2	1.92	0.53
13:A:1124:CLA:H162	16:A:4007:BCR:H272	1.91	0.53
13:A:1128:CLA:H111	17:A:5001:LHG:H202	1.90	0.53
10:L:16:HIS:CD2	10:L:17:LEU:H	2.27	0.53
1:A:13:ARG:HE	1:A:15:VAL:HG22	1.72	0.53
1:A:59:ASP:OD2	1:A:353:HIS:HE1	1.91	0.52
1:A:221:LEU:HD11	1:A:295:SER:CA	2.39	0.52
13:A:1013:CLA:O1A	2:B:531:LEU:HD11	2.10	0.52
1:A:120:ILE:C	1:A:122:GLY:H	2.16	0.52
1:A:683:TRP:CD2	13:A:1011:CLA:HMA2	2.45	0.52
2:B:406:ASN:HD22	2:B:409:ASN:ND2	1.84	0.52
9:K:74:VAL:C	9:K:76:GLY:H	2.16	0.52
2:B:430:LEU:HB3	13:B:1229:CLA:HED3	1.90	0.52
6:F:40:GLN:OE1	8:J:40:PRO:O	2.26	0.52
2:B:78:GLN:OE1	2:B:78:GLN:HA	2.10	0.52
1:A:356:LEU:HG	1:A:360:LEU:HD22	1.91	0.52
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.91	0.52
6:F:79:TRP:CH2	6:F:120:ALA:HA	2.44	0.52
2:B:217:HIS:CG	2:B:218:PRO:HD2	2.44	0.52
1:A:578:CYS:HB3	1:A:587:CYS:HA	1.91	0.52
1:A:744:TRP:CZ2	13:A:1126:CLA:H43	2.44	0.52
2:B:634:SER:O	2:B:638:ILE:HB	2.10	0.52
1:A:77:PHE:CE2	13:A:1108:CLA:HBB1	2.45	0.52
1:A:718:GLN:NE2	5:E:42:LYS:HD3	2.25	0.52
1:A:16:VAL:HG11	1:A:183:ARG:HB3	1.92	0.51
1:A:83:VAL:HG11	13:A:1103:CLA:H72	1.92	0.51
8:J:28:GLU:OE1	8:J:28:GLU:HA	2.09	0.51
2:B:279:ILE:HD11	13:B:1214:CLA:HBC2	1.92	0.51
1:A:226:LEU:HD22	1:A:231:VAL:HG21	1.93	0.51
2:B:398:VAL:HG23	2:B:547:ALA:HB1	1.93	0.51
10:L:31:ILE:HA	10:L:34:LEU:HD22	1.92	0.51
1:A:71:LYS:NZ	20:A:5034:HOH:O	2.43	0.51
1:A:542:HIS:HE1	1:A:612:HIS:ND1	2.09	0.51
2:B:36:MET:HE3	2:B:40:ASN:HB2	1.92	0.51
1:A:257:ASP:O	1:A:258:TRP:HB2	2.11	0.51
2:B:456:ILE:HG22	2:B:458:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:LYS:HD2	2:B:159:LYS:N	2.03	0.51
1:A:303:ALA:CB	13:A:1116:CLA:HBB1	2.40	0.51
1:A:444:LEU:HB2	13:A:1137:CLA:CBB	2.40	0.51
2:B:453:GLU:HA	6:F:48:LEU:HD22	1.93	0.51
13:B:1238:CLA:HBB2	14:B:2002:PQN:H141	1.91	0.51
1:A:118:TRP:CB	16:J:4013:BCR:H323	2.41	0.51
1:A:90:MET:CE	13:A:1106:CLA:HED2	2.39	0.50
7:I:30:LEU:O	7:I:34:ILE:HG12	2.11	0.50
3:C:14:THR:HG22	3:C:27:MET:HG3	1.93	0.50
2:B:638:ILE:HD11	2:B:656:PHE:CE2	2.46	0.50
1:A:257:ASP:OD2	1:A:262:SER:C	2.55	0.50
2:B:464:GLN:HG2	2:B:475:TYR:CE2	2.47	0.50
11:M:30:TYR:O	11:M:31:LYS:OXT	2.29	0.50
2:B:339:TRP:HE1	13:B:1221:CLA:C3B	2.23	0.50
2:B:379:GLN:HA	2:B:379:GLN:OE1	2.11	0.50
2:B:588:TRP:HH2	13:B:1012:CLA:HBB1	1.77	0.50
4:D:32:THR:HA	4:D:52:GLY:O	2.12	0.50
13:A:1013:CLA:HBB1	13:B:1012:CLA:NB	2.27	0.50
13:B:1221:CLA:H61	13:B:1223:CLA:H42	1.94	0.50
1:A:16:VAL:CG1	1:A:17:ASP:N	2.74	0.50
2:B:431:PHE:CZ	16:J:4015:BCR:HC41	2.46	0.50
13:B:1226:CLA:H8	18:B:5002:LMG:H242	1.94	0.50
5:E:68:VAL:O	5:E:69:ALA:O	2.30	0.49
7:I:9:PHE:CE1	7:I:10:LEU:HD13	2.46	0.49
1:A:691:PHE:HB2	13:A:1013:CLA:HBC2	1.95	0.49
2:B:340:HIS:HD2	13:B:1202:CLA:OBD	1.95	0.49
4:D:101:PHE:HB3	4:D:103:GLU:OE2	2.11	0.49
2:B:459:GLU:OE2	6:F:50:HIS:ND1	2.40	0.49
2:B:548:ARG:HH22	4:D:124:ASN:ND2	2.10	0.49
6:F:80:VAL:HG22	6:F:109:CYS:O	2.13	0.49
13:A:1237:CLA:H52	13:B:1238:CLA:H43	1.93	0.49
10:L:105:GLY:O	10:L:106:SER:HB2	2.11	0.49
2:B:425:LEU:HG	13:B:1236:CLA:HBB1	1.94	0.49
2:B:458:ILE:N	2:B:458:ILE:HD12	2.28	0.49
4:D:30:THR:O	4:D:80:TYR:HA	2.13	0.49
2:B:162:PRO:HB2	2:B:167:PHE:CE1	2.48	0.49
2:B:303:MET:HE2	13:B:1220:CLA:CED	2.42	0.49
13:B:1021:CLA:H72	13:B:1012:CLA:CED	2.41	0.49
5:E:7:VAL:O	5:E:20:VAL:HA	2.13	0.49
6:F:84:TYR:O	6:F:88:VAL:HG23	2.13	0.49
1:A:293:TRP:O	1:A:296:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ILE:HD12	2:B:627:ARG:HG3	1.95	0.49
2:B:261:HIS:CD2	2:B:263:GLN:H	2.31	0.49
10:L:143:LEU:HD12	10:L:143:LEU:HA	1.61	0.49
2:B:294:PHE:O	2:B:296:ILE:HG22	2.13	0.48
2:B:390:PHE:CE1	16:B:4010:BCR:H373	2.48	0.48
13:A:1013:CLA:H71	13:A:1140:CLA:CMC	2.42	0.48
2:B:182:PHE:CE2	13:B:1210:CLA:H61	2.48	0.48
2:B:446:VAL:HG13	2:B:451:THR:O	2.13	0.48
13:B:1203:CLA:H143	13:B:1225:CLA:HBB2	1.95	0.48
1:A:399:TRP:NE1	13:A:1126:CLA:HAB	2.27	0.48
1:A:444:LEU:HB2	13:A:1137:CLA:HBB1	1.96	0.48
2:B:261:HIS:HD2	2:B:263:GLN:H	1.62	0.48
1:A:651:ARG:HG3	2:B:638:ILE:CG2	2.43	0.48
13:A:1131:CLA:HMA2	16:I:4018:BCR:H272	1.96	0.48
13:B:1221:CLA:H61	13:B:1221:CLA:H41	1.68	0.48
8:J:33:TYR:N	8:J:34:PRO:HD3	2.28	0.48
1:A:118:TRP:HB3	16:J:4013:BCR:H323	1.94	0.48
1:A:658:ALA:O	1:A:662:ILE:HG12	2.14	0.48
13:B:1203:CLA:H91	18:B:5002:LMG:H401	1.96	0.48
6:F:73:ILE:O	6:F:76:TRP:HB3	2.14	0.48
6:F:109:CYS:O	6:F:112:THR:HB	2.12	0.48
1:A:283:GLY:O	1:A:508:THR:O	2.32	0.48
6:F:88:VAL:HG13	6:F:97:LYS:HD2	1.95	0.48
8:J:31:ARG:CD	16:J:4013:BCR:H312	2.19	0.48
1:A:196:MET:HE1	13:A:1123:CLA:H142	1.94	0.48
1:A:360:LEU:CD1	13:A:1128:CLA:HBB1	2.44	0.48
13:A:1140:CLA:H172	8:J:19:MET:HE2	1.95	0.48
1:A:497:ALA:N	1:A:498:PRO:CD	2.76	0.48
1:A:693:GLY:HA3	2:B:574:CYS:HB2	1.95	0.48
2:B:180:GLY:HA3	13:B:1210:CLA:HBB1	1.96	0.48
4:D:117:ARG:HG2	4:D:118:SER:N	2.26	0.48
1:A:203:GLY:O	1:A:207:LEU:HB2	2.14	0.47
2:B:231:VAL:C	2:B:234:GLN:HG2	2.36	0.47
11:M:24:ARG:NH1	20:M:155:HOH:O	2.46	0.47
1:A:686:SER:HB3	1:A:734:HIS:HB2	1.95	0.47
6:F:10:ASP:HB3	20:F:4022:HOH:O	2.14	0.47
1:A:74:SER:OG	1:A:180:TYR:HB2	2.15	0.47
1:A:168:MET:O	1:A:172:MET:HB2	2.14	0.47
1:A:691:PHE:HB2	13:A:1013:CLA:CBC	2.44	0.47
13:A:1101:CLA:H8	8:J:16:ALA:HA	1.96	0.47
2:B:329:TYR:OH	2:B:340:HIS:CE1	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:SER:C	2:B:359:PRO:HD3	2.39	0.47
13:B:1211:CLA:HAB	13:B:1225:CLA:H13	1.96	0.47
2:B:647:ASN:HD22	2:B:649:LEU:N	2.08	0.47
4:D:124:ASN:O	4:D:127:GLN:HB2	2.13	0.47
1:A:90:MET:HE2	13:A:1126:CLA:CED	2.38	0.47
1:A:215:HIS:C	1:A:215:HIS:CD2	2.92	0.47
1:A:56:HIS:CG	13:A:1103:CLA:HAB	2.49	0.47
1:A:174:PHE:HD2	13:A:1108:CLA:CBC	2.28	0.47
1:A:683:TRP:CG	13:A:1011:CLA:HMA2	2.50	0.47
13:A:1107:CLA:HBB1	13:B:1230:CLA:HMD2	1.95	0.47
2:B:313:LYS:O	2:B:314:VAL:CG2	2.60	0.47
2:B:525:VAL:CG1	13:B:1021:CLA:H141	2.45	0.47
2:B:589:MET:C	2:B:589:MET:CE	2.83	0.47
2:B:693:LEU:HD12	13:L:1502:CLA:H11	1.97	0.47
11:M:24:ARG:CG	11:M:24:ARG:NH1	2.78	0.47
8:J:40:PRO:O	8:J:41:LEU:HB2	2.14	0.47
1:A:447:VAL:HG21	13:A:1137:CLA:C2C	2.45	0.47
1:A:379:PRO:HB2	13:A:1117:CLA:HAA2	1.96	0.47
2:B:641:TYR:CB	2:B:646:THR:HG22	2.42	0.47
2:B:696:LEU:HD11	10:L:36:ALA:HB1	1.97	0.47
1:A:145:GLN:H	1:A:145:GLN:CD	2.22	0.46
13:A:1140:CLA:H172	8:J:19:MET:HG3	1.98	0.46
2:B:198:ILE:HB	2:B:199:PRO:HD3	1.96	0.46
13:B:1207:CLA:H42	10:L:81:SER:HA	1.96	0.46
13:B:1217:CLA:HBB1	16:B:4004:BCR:H14C	1.97	0.46
3:C:65:ARG:HG2	3:C:67:TYR:OH	2.15	0.46
6:F:88:VAL:CG1	6:F:97:LYS:HB2	2.41	0.46
1:A:374:MET:HE1	13:A:1127:CLA:O1D	2.15	0.46
1:A:638:ASN:O	1:A:642:SER:HB2	2.16	0.46
1:A:603:TYR:OH	13:A:1011:CLA:HED1	2.15	0.46
13:A:1140:CLA:H2	13:A:1140:CLA:O1A	2.15	0.46
2:B:39:GLU:O	2:B:43:GLN:HG3	2.15	0.46
13:B:1225:CLA:HBA2	13:B:1225:CLA:H3A	1.64	0.46
3:C:57:CYS:HA	3:C:58:PRO:HD3	1.71	0.46
4:D:34:PRO:O	4:D:51:GLU:HG3	2.16	0.46
1:A:577:PRO:O	1:A:578:CYS:HB3	2.14	0.46
2:B:663:TRP:CD2	13:B:1021:CLA:HMA2	2.51	0.46
13:B:1235:CLA:H203	6:F:67:SER:HB3	1.98	0.46
10:L:33:ASN:HB3	13:L:1501:CLA:HAC1	1.97	0.46
1:A:656:ALA:O	1:A:659:SER:HB2	2.16	0.46
2:B:361:TYR:O	2:B:364:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1012:CLA:H41	13:B:1012:CLA:H61	1.56	0.46
3:C:61:PHE:HD2	4:D:119:ILE:HG21	1.81	0.46
11:M:17:LEU:HB3	11:M:18:PRO:CD	2.46	0.46
1:A:202:ALA:C	13:A:1118:CLA:HBC3	2.41	0.46
1:A:686:SER:HB3	1:A:734:HIS:CB	2.46	0.46
13:A:1011:CLA:HED1	20:A:5011:HOH:O	2.14	0.46
6:F:80:VAL:HG11	6:F:110:MET:HG2	1.97	0.46
1:A:19:ASP:N	1:A:20:PRO:HD3	2.31	0.46
2:B:479:THR:H	2:B:482:SER:HB3	1.79	0.46
2:B:509:SER:O	2:B:509:SER:OG	2.25	0.46
13:B:1207:CLA:HHC	13:B:1207:CLA:HBB1	1.97	0.46
1:A:445:ASN:ND2	13:B:1023:CLA:HED2	2.31	0.46
1:A:744:TRP:CG	16:A:4011:BCR:HC22	2.51	0.46
3:C:23:ASP:OD2	4:D:95:HIS:CD2	2.67	0.46
1:A:91:TYR:CZ	1:A:147:TRP:HZ3	2.33	0.46
1:A:682:ILE:HD11	13:A:1140:CLA:HMB1	1.96	0.46
2:B:36:MET:CE	2:B:40:ASN:HB2	2.45	0.46
2:B:189:TRP:CA	13:B:1211:CLA:HBB1	2.45	0.46
2:B:642:ASN:HB2	2:B:643:PRO:HD3	1.95	0.46
2:B:738:LYS:O	2:B:739:PHE:CB	2.64	0.46
13:B:1204:CLA:H102	16:I:4018:BCR:HC31	1.98	0.46
11:M:13:VAL:HG23	16:M:4021:BCR:H402	1.98	0.46
1:A:539:HIS:CG	13:A:1136:CLA:HED2	2.51	0.45
13:A:1237:CLA:HMA1	2:B:694:ALA:HB1	1.97	0.45
4:D:124:ASN:HB2	4:D:127:GLN:NE2	2.31	0.45
1:A:44:THR:HB	1:A:720:ARG:HG2	1.98	0.45
1:A:475:PHE:HA	1:A:480:ILE:O	2.16	0.45
1:A:508:THR:HG21	20:A:5033:HOH:O	2.15	0.45
2:B:468:ALA:O	2:B:482:SER:HB2	2.16	0.45
2:B:100:VAL:HG22	7:I:1:MET:HE2	1.98	0.45
2:B:339:TRP:CZ3	16:B:4009:BCR:H372	2.51	0.45
13:B:1217:CLA:H3A	13:B:1217:CLA:HBA2	1.64	0.45
13:B:1225:CLA:H12	16:B:4005:BCR:H393	1.97	0.45
13:B:1227:CLA:H3A	13:B:1227:CLA:HBA2	1.49	0.45
13:L:1501:CLA:C1B	13:L:1502:CLA:HED1	2.46	0.45
1:A:91:TYR:CE2	1:A:161:THR:HG21	2.52	0.45
1:A:313:HIS:CE1	16:A:4001:BCR:H363	2.51	0.45
13:A:1120:CLA:HBA2	13:A:1120:CLA:H3A	1.44	0.45
13:A:1123:CLA:HAB	16:A:4007:BCR:H341	1.98	0.45
2:B:64:LEU:HD11	16:B:4006:BCR:H271	1.98	0.45
2:B:471:GLY:HA3	2:B:504:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:22:THR:O	8:J:26:LEU:HD13	2.15	0.45
10:L:115:GLU:O	10:L:119:GLN:HG3	2.17	0.45
13:B:1215:CLA:H62	13:B:1215:CLA:H41	1.70	0.45
1:A:112:PRO:HB3	1:A:144:PHE:CD1	2.51	0.45
13:A:1118:CLA:HBA2	13:A:1118:CLA:H3A	1.83	0.45
2:B:570:ARG:HG3	2:B:570:ARG:HH11	1.81	0.45
13:B:1213:CLA:H41	13:B:1213:CLA:H62	1.71	0.45
4:D:39:PHE:HB2	4:D:71:GLN:HE21	1.81	0.45
1:A:508:THR:HG22	1:A:509:ALA:N	2.31	0.45
2:B:50:PHE:HB3	2:B:148:ALA:O	2.17	0.45
11:M:17:LEU:HB3	11:M:18:PRO:HD3	1.98	0.45
1:A:321:ILE:HD11	13:A:1118:CLA:H2A	1.99	0.45
13:A:1011:CLA:NA	13:B:1021:CLA:HAB	2.31	0.45
2:B:445:VAL:HG21	13:B:1230:CLA:HAC2	1.97	0.45
2:B:496:GLY:O	2:B:497:ASN:C	2.59	0.45
1:A:445:ASN:ND2	2:B:680:LEU:HD21	2.32	0.45
1:A:711:LEU:HD23	6:F:130:THR:HG22	1.98	0.45
4:D:134:LYS:HG2	4:D:136:TYR:CZ	2.52	0.45
1:A:86:TRP:HE1	13:A:1106:CLA:HBA1	1.82	0.45
1:A:250:ALA:HA	1:A:258:TRP:CD1	2.52	0.45
2:B:497:ASN:O	2:B:499:TRP:CE3	2.70	0.45
2:B:557:LYS:NZ	4:D:124:ASN:OD1	2.43	0.45
4:D:114:SER:N	20:D:144:HOH:O	2.50	0.45
6:F:20:ALA:O	6:F:21:ALA:C	2.59	0.45
1:A:75:ALA:HB1	13:A:1103:CLA:HBB1	1.99	0.44
13:A:1104:CLA:H3A	13:A:1128:CLA:HAB	1.99	0.44
2:B:215:MET:HA	2:B:216:PRO:HD3	1.83	0.44
13:B:1224:CLA:CGA	13:B:1224:CLA:H3A	2.47	0.44
1:A:92:PHE:CZ	1:A:96:LYS:HG3	2.53	0.44
2:B:531:LEU:HD21	13:B:1012:CLA:HBB1	1.99	0.44
13:B:1207:CLA:H43	13:B:1207:CLA:CED	2.47	0.44
1:A:212:TRP:N	13:A:1112:CLA:HBB1	2.32	0.44
13:A:1125:CLA:HMB3	13:A:1133:CLA:H12	1.99	0.44
2:B:370:THR:HG21	20:B:5026:HOH:O	2.16	0.44
13:B:1211:CLA:HBA1	16:B:4006:BCR:H383	2.00	0.44
3:C:6:ILE:N	3:C:6:ILE:HD12	2.33	0.44
5:E:6:LYS:CD	5:E:22:THR:HG22	2.47	0.44
2:B:48:SER:HB3	13:B:1202:CLA:HBB1	1.98	0.44
2:B:79:ASP:OD2	2:B:82:ASN:HB2	2.18	0.44
2:B:441:VAL:O	2:B:445:VAL:HG23	2.17	0.44
13:B:1228:CLA:HBC3	16:F:4016:BCR:H362	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1601:CLA:H3A	13:M:1601:CLA:HBA2	1.69	0.44
1:A:111:LYS:HB2	1:A:130:VAL:HB	2.00	0.44
1:A:484:PRO:HB3	13:A:1136:CLA:CED	2.47	0.44
4:D:125:PRO:HG3	4:D:135:PRO:HG3	2.00	0.44
8:J:1:MET:HE2	8:J:1:MET:O	2.18	0.44
8:J:32:PHE:C	8:J:34:PRO:HD3	2.42	0.44
13:A:1103:CLA:H71	16:A:4003:BCR:H402	2.00	0.44
2:B:589:MET:HE1	2:B:590:LEU:HD23	2.00	0.44
3:C:65:ARG:HD2	4:D:119:ILE:CD1	2.48	0.44
6:F:76:TRP:CD1	6:F:76:TRP:C	2.96	0.44
6:F:132:LYS:HB2	6:F:135:GLU:HG3	1.99	0.44
10:L:56:TYR:OH	13:L:1503:CLA:HED2	2.18	0.44
1:A:98:SER:HB2	1:A:113:SER:O	2.18	0.44
1:A:462:ASN:HB3	1:A:645:THR:HG22	1.99	0.44
1:A:642:SER:O	1:A:648:GLY:HA3	2.17	0.44
13:A:1107:CLA:HBC2	13:A:1126:CLA:H141	1.99	0.44
16:A:4011:BCR:H403	16:A:4011:BCR:H23C	1.99	0.44
2:B:430:LEU:HB3	13:B:1229:CLA:CED	2.48	0.44
1:A:684:ALA:C	13:A:1013:CLA:HAB	2.42	0.44
2:B:181:LEU:HD13	13:B:1210:CLA:HBB	2.00	0.44
4:D:96:PRO:O	4:D:97:LYS:C	2.59	0.44
5:E:17:TYR:O	5:E:18:ASN:HB2	2.18	0.44
13:A:1140:CLA:H41	13:A:1140:CLA:H62	1.73	0.43
2:B:211:PHE:CE2	2:B:212:LEU:HG	2.53	0.43
2:B:427:TRP:CE2	13:B:1228:CLA:HBB1	2.53	0.43
2:B:622:LEU:HD13	13:B:1012:CLA:HMA2	1.99	0.43
13:B:1206:CLA:H102	13:B:1224:CLA:H193	1.99	0.43
1:A:221:LEU:CB	1:A:222:PRO:HD3	2.44	0.43
1:A:519:ALA:HB2	1:A:625:VAL:HG21	2.00	0.43
2:B:236:PRO:O	2:B:250:GLY:HA3	2.18	0.43
2:B:317:PRO:HB3	20:B:5053:HOH:O	2.18	0.43
1:A:501:THR:C	1:A:503:PRO:HD3	2.43	0.43
2:B:439:LEU:HD11	16:J:4015:BCR:H342	2.00	0.43
2:B:492:TRP:O	2:B:493:PRO:C	2.61	0.43
2:B:529:ILE:HG21	13:B:1234:CLA:HAB	1.99	0.43
10:L:7:PRO:HB3	10:L:12:PRO:HA	2.00	0.43
2:B:431:PHE:HD2	13:B:1235:CLA:HBB2	1.84	0.43
2:B:531:LEU:HD21	13:B:1012:CLA:CBB	2.48	0.43
2:B:175:ASN:HB3	13:B:1217:CLA:HMD1	2.01	0.43
2:B:305:ASP:OD1	2:B:323:GLN:HA	2.18	0.43
2:B:339:TRP:CE2	13:B:1223:CLA:H91	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:GLN:HG3	2:B:737:ALA:CB	2.49	0.43
13:B:1203:CLA:H41	13:B:1203:CLA:H61	1.60	0.43
1:A:91:TYR:CE2	1:A:147:TRP:CZ3	3.07	0.43
1:A:212:TRP:CA	13:A:1112:CLA:HBB1	2.49	0.43
1:A:259:GLY:C	1:A:261:PHE:N	2.76	0.43
2:B:234:GLN:O	2:B:236:PRO:HD3	2.19	0.43
13:B:1215:CLA:HBA2	13:B:1215:CLA:H3A	1.92	0.43
6:F:116:TRP:CG	6:F:117:PRO:HD3	2.54	0.43
8:J:19:MET:HA	8:J:19:MET:CE	2.38	0.43
1:A:215:HIS:HB2	13:A:1112:CLA:C1C	2.48	0.43
1:A:261:PHE:O	1:A:261:PHE:CD2	2.72	0.43
13:B:1236:CLA:HBC2	13:X:1701:CLA:HBC3	2.00	0.43
6:F:21:ALA:HB2	6:F:35:PHE:CD1	2.54	0.43
1:A:120:ILE:C	1:A:122:GLY:N	2.77	0.43
1:A:359:ASN:CG	13:A:1123:CLA:HAA1	2.44	0.43
16:J:4015:BCR:H20C	16:J:4015:BCR:H361	1.89	0.43
9:K:59:LEU:C	9:K:61:ALA:H	2.25	0.43
1:A:231:VAL:HG11	1:A:236:ILE:HG12	1.99	0.43
13:B:1205:CLA:O1A	13:B:1224:CLA:HBD	2.19	0.43
4:D:18:LEU:HD23	4:D:18:LEU:HA	1.86	0.43
5:E:6:LYS:NZ	5:E:22:THR:HG21	2.34	0.43
13:A:1237:CLA:H41	13:A:1237:CLA:H62	1.62	0.42
13:A:1402:CLA:H3A	13:A:1402:CLA:HBA2	1.74	0.42
2:B:325:ILE:HD12	2:B:409:ASN:ND2	2.34	0.42
4:D:73:ARG:HB2	4:D:74:PRO:HD3	2.00	0.42
1:A:257:ASP:OD1	1:A:262:SER:CB	2.66	0.42
1:A:514:GLY:HA2	1:A:528:PRO:HB3	2.01	0.42
2:B:360:PRO:HG3	13:B:1215:CLA:HBA1	2.00	0.42
2:B:386:MET:HE1	16:B:4010:BCR:H361	2.01	0.42
13:B:1207:CLA:CBB	7:I:19:CYS:HB3	2.50	0.42
8:J:39:HIS:HA	16:J:4015:BCR:H21C	2.00	0.42
1:A:403:PHE:CB	13:A:1104:CLA:H112	2.49	0.42
1:A:711:LEU:O	1:A:713:VAL:HG22	2.20	0.42
2:B:103:PHE:HZ	2:B:651:VAL:HG22	1.82	0.42
13:B:1214:CLA:HBA2	13:B:1214:CLA:H3A	1.39	0.42
13:B:1229:CLA:H61	16:F:4016:BCR:H312	2.00	0.42
1:A:234:LYS:H	1:A:234:LYS:HG2	1.68	0.42
1:A:360:LEU:HD11	13:A:1128:CLA:HBB1	2.01	0.42
13:A:1106:CLA:HMC2	13:A:1126:CLA:H142	2.01	0.42
13:A:1107:CLA:H11	16:J:4012:BCR:H19C	2.01	0.42
1:A:679:ALA:HB1	1:A:738:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1124:CLA:H51	13:A:1135:CLA:H43	2.00	0.42
2:B:325:ILE:CD1	2:B:409:ASN:ND2	2.82	0.42
2:B:535:THR:O	2:B:539:ILE:HG13	2.20	0.42
2:B:588:TRP:CH2	13:B:1012:CLA:CBB	3.02	0.42
2:B:589:MET:CE	2:B:590:LEU:HA	2.47	0.42
10:L:4:LEU:N	10:L:4:LEU:HD22	2.35	0.42
2:B:6:LYS:HD2	11:M:31:LYS:HB3	2.02	0.42
2:B:341:LEU:HD21	13:B:1226:CLA:HAB	2.02	0.42
2:B:458:ILE:CD1	2:B:458:ILE:N	2.82	0.42
4:D:95:HIS:HA	4:D:97:LYS:N	2.35	0.42
1:A:120:ILE:O	1:A:122:GLY:N	2.52	0.42
1:A:256:VAL:HG12	1:A:257:ASP:N	2.35	0.42
1:A:542:HIS:HD2	20:A:5029:HOH:O	2.03	0.42
13:A:1128:CLA:H62	13:A:1128:CLA:H41	1.90	0.42
13:A:1122:CLA:H92	16:A:4007:BCR:H14C	2.01	0.42
13:A:1126:CLA:H93	16:J:4012:BCR:H20C	2.01	0.42
16:A:4011:BCR:H362	13:B:1012:CLA:C4	2.38	0.42
2:B:372:ALA:HA	2:B:600:TRP:CZ3	2.55	0.42
2:B:527:HIS:CD2	16:J:4015:BCR:H322	2.55	0.42
17:B:5004:LHG:HC5	12:X:12:ARG:HB3	2.02	0.42
1:A:47:TRP:CZ3	1:A:51:LEU:HD12	2.54	0.42
1:A:483:GLN:HA	1:A:484:PRO:HD3	1.70	0.42
1:A:511:VAL:HB	1:A:526:MET:HG3	2.02	0.42
2:B:261:HIS:HD2	2:B:264:THR:H	1.67	0.42
2:B:414:VAL:HG11	16:B:4009:BCR:C40	2.50	0.42
13:B:1203:CLA:H143	13:B:1225:CLA:CBB	2.50	0.42
6:F:103:VAL:O	6:F:107:ILE:HG13	2.20	0.42
1:A:346:GLU:OE1	1:A:346:GLU:N	2.47	0.42
1:A:741:ALA:CB	16:A:4011:BCR:H323	2.50	0.42
13:A:1108:CLA:H3A	13:A:1108:CLA:HBA2	1.64	0.42
2:B:136:GLN:HE21	13:B:1211:CLA:HAA1	1.85	0.42
1:A:42:PRO:CG	6:F:99:ILE:HD13	2.50	0.41
1:A:336:PHE:CD2	10:L:4:LEU:HD21	2.55	0.41
1:A:423:ALA:HA	4:D:38:VAL:HG11	2.02	0.41
2:B:586:MET:HE3	2:B:586:MET:HB3	1.96	0.41
3:C:28:VAL:HG12	4:D:109:ARG:HB3	2.02	0.41
1:A:156:PHE:CE2	13:A:1114:CLA:HAA2	2.55	0.41
1:A:203:GLY:HA3	13:A:1111:CLA:HBB1	2.02	0.41
1:A:686:SER:HB2	1:A:731:GLY:O	2.20	0.41
1:A:744:TRP:NE1	13:A:1126:CLA:H11	2.35	0.41
2:B:36:MET:HE1	2:B:40:ASN:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:TRP:HA	13:B:1211:CLA:HBB1	2.02	0.41
3:C:25:LEU:HA	3:C:40:SER:O	2.20	0.41
7:I:22:MET:O	7:I:26:VAL:HG13	2.19	0.41
11:M:9:TYR:HB3	16:M:4021:BCR:H401	2.02	0.41
1:A:177:TRP:HB2	13:A:1109:CLA:CMC	2.50	0.41
1:A:212:TRP:HA	13:A:1112:CLA:HBB1	2.01	0.41
1:A:685:PHE:HA	13:A:1013:CLA:HAB	2.01	0.41
1:A:710:LYS:HD2	1:A:710:LYS:O	2.20	0.41
13:A:1801:CLA:HBA2	13:A:1801:CLA:H12	1.86	0.41
2:B:178:LEU:O	2:B:283:PHE:HB3	2.21	0.41
4:D:50:ARG:NH1	4:D:50:ARG:HG3	2.35	0.41
1:A:49:TRP:CZ3	17:A:5001:LHG:H121	2.56	0.41
1:A:204:LEU:HD13	1:A:204:LEU:C	2.45	0.41
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.83	0.41
1:A:722:LEU:HD22	1:A:726:GLN:CD	2.46	0.41
13:A:1134:CLA:H3A	13:A:1134:CLA:HBA2	1.73	0.41
2:B:367:ASP:CG	2:B:370:THR:CG2	2.87	0.41
2:B:691:THR:HA	2:B:692:PRO:HD3	1.90	0.41
6:F:54:ASP:OD2	12:X:30:TYR:HE2	1.98	0.41
6:F:88:VAL:O	6:F:89:ARG:C	2.63	0.41
1:A:49:TRP:HZ3	17:A:5001:LHG:H121	1.86	0.41
13:A:1138:CLA:HAA2	13:B:1228:CLA:HMB1	2.02	0.41
2:B:529:ILE:HG21	13:B:1234:CLA:CAB	2.51	0.41
13:B:1213:CLA:H3A	13:B:1213:CLA:HBA2	1.68	0.41
3:C:8:ASP:OD1	3:C:8:ASP:C	2.61	0.41
1:A:161:THR:HG22	16:A:4002:BCR:HC32	2.01	0.41
1:A:186:LYS:O	1:A:187:LEU:C	2.62	0.41
1:A:257:ASP:CG	1:A:258:TRP:H	2.27	0.41
5:E:19:GLU:OE1	5:E:42:LYS:NZ	2.52	0.41
13:L:1502:CLA:H111	13:L:1502:CLA:H152	1.99	0.41
1:A:112:PRO:HA	1:A:144:PHE:CE1	2.55	0.41
1:A:360:LEU:HD12	1:A:360:LEU:HA	1.93	0.41
13:B:1023:CLA:H122	16:I:4018:BCR:H281	2.03	0.41
13:B:1202:CLA:HBA1	13:B:1202:CLA:H3A	1.74	0.41
13:B:1222:CLA:HBA2	13:B:1222:CLA:H3A	1.69	0.41
4:D:104:LYS:H	4:D:104:LYS:HG2	1.51	0.41
6:F:73:ILE:O	6:F:77:ILE:HG13	2.21	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.82	0.41
13:A:1022:CLA:O1A	13:A:1022:CLA:H3A	2.21	0.41
13:A:1117:CLA:HBA2	13:A:1117:CLA:H3A	1.89	0.41
13:A:1140:CLA:NC	13:A:1140:CLA:H52	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:PHE:CD1	2:B:45:ILE:HD13	2.56	0.41
2:B:313:LYS:C	2:B:314:VAL:HG13	2.45	0.41
2:B:440:TYR:CZ	2:B:524:LEU:HB3	2.56	0.41
2:B:442:HIS:CD2	2:B:456:ILE:HG13	2.56	0.41
13:B:1206:CLA:H203	7:I:26:VAL:CG2	2.51	0.41
13:B:1207:CLA:H2A	13:B:1207:CLA:O2A	2.20	0.41
3:C:13:CYS:SG	3:C:15:GLN:HB2	2.61	0.41
6:F:24:THR:HG21	8:J:35:ASP:OD1	2.20	0.41
10:L:44:ILE:HG23	10:L:45:LEU:N	2.36	0.41
10:L:57:PHE:CD1	10:L:57:PHE:C	2.99	0.41
1:A:118:TRP:HB3	16:J:4013:BCR:C32	2.51	0.41
13:A:1013:CLA:C14	16:A:4011:BCR:H402	2.51	0.41
13:A:1132:CLA:HED2	10:L:65:LEU:O	2.21	0.41
2:B:459:GLU:HA	2:B:460:PRO:HD3	1.81	0.41
2:B:629:TYR:O	2:B:633:ASN:HB2	2.21	0.41
4:D:43:THR:O	4:D:44:ALA:CB	2.68	0.41
1:A:502:ALA:N	1:A:503:PRO:HD3	2.36	0.40
13:A:1140:CLA:H203	13:F:1301:CLA:CBB	2.52	0.40
20:A:5047:HOH:O	10:L:16:HIS:HE1	2.04	0.40
13:B:1215:CLA:H3A	13:B:1215:CLA:CGA	2.51	0.40
6:F:80:VAL:HG21	6:F:110:MET:HA	2.03	0.40
1:A:114:ALA:O	1:A:115:GLN:O	2.39	0.40
2:B:33:HIS:HE1	13:B:1201:CLA:HED1	1.85	0.40
2:B:53:LEU:HD12	2:B:53:LEU:HA	1.83	0.40
2:B:279:ILE:HD11	13:B:1214:CLA:HBC3	2.02	0.40
2:B:490:THR:O	2:B:495:TYR:HA	2.21	0.40
2:B:605:LEU:HD12	2:B:605:LEU:HA	1.80	0.40
1:A:212:TRP:O	1:A:216:GLN:HG3	2.22	0.40
13:A:1122:CLA:HBB	13:A:1801:CLA:HBB1	2.02	0.40
13:A:1126:CLA:H62	13:A:1126:CLA:H41	1.75	0.40
2:B:193:LEU:HA	2:B:197:ALA:HB3	2.03	0.40
2:B:377:HIS:HE2	13:B:1225:CLA:C1B	2.35	0.40
2:B:564:PRO:O	2:B:565:CYS:HB3	2.22	0.40
10:L:44:ILE:HB	20:L:4045:HOH:O	2.21	0.40
16:L:4022:BCR:H20C	16:L:4022:BCR:H361	1.88	0.40
13:A:1116:CLA:CGA	13:A:1116:CLA:H3A	2.52	0.40
2:B:313:LYS:O	2:B:314:VAL:CG1	2.68	0.40
2:B:318:PHE:H	13:B:1219:CLA:C2B	2.34	0.40
2:B:548:ARG:HD3	6:F:141:ARG:O	2.21	0.40
3:C:40:SER:HA	20:C:3012:HOH:O	2.21	0.40
4:D:67:LEU:HD12	4:D:71:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:30:ASN:O	8:J:34:PRO:HG3	2.22	0.40
1:A:120:ILE:HG12	1:A:121:VAL:N	2.36	0.40
1:A:741:ALA:CB	16:A:4011:BCR:C32	2.99	0.40
13:A:1013:CLA:H71	13:A:1140:CLA:HMC2	2.03	0.40
20:C:3013:HOH:O	4:D:138:PRO:HG3	2.21	0.40
4:D:88:ASP:HB3	4:D:90:GLU:H	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:4048:HOH:O	20:L:4048:HOH:O[2_655]	1.94	0.26

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	695 (94%)	31 (4%)	10 (1%)	9	17
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	10	20
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	9	18
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	5	9
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	1	1
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	5	9
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	0
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	9	18
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	3	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	2	3
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	7	13

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE
1	A	261	PHE
2	B	234	GLN
2	B	313	LYS
2	B	314	VAL
2	B	480	LEU
2	B	492	TRP
2	B	497	ASN
2	B	510	GLY
3	C	62	LEU
4	D	2	THR
6	F	91	SER
9	K	41	PRO
9	K	42	GLY
11	M	30	TYR
12	X	10	ALA
1	A	121	VAL
1	A	578	CYS
2	B	565	CYS
4	D	3	LEU
6	F	60	ALA
6	F	89	ARG
10	L	106	SER
1	A	234	LYS
4	D	44	ALA
5	E	53	SER
10	L	104	GLY
1	A	42	PRO
1	A	232	ALA
2	B	481	LEU
5	E	25	SER
5	E	54	GLY
1	A	276	SER
5	E	55	VAL

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Mol	Chain	Res	Type
9	K	56	LEU

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/603 (98%)	563 (96%)	26 (4%)	25	50
2	B	595/597 (100%)	563 (95%)	32 (5%)	20	41
3	C	67/67 (100%)	65 (97%)	2 (3%)	36	64
4	D	115/115 (100%)	105 (91%)	10 (9%)	9	21
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	106 (97%)	3 (3%)	38	66
7	I	32/32 (100%)	30 (94%)	2 (6%)	16	34
8	J	36/36 (100%)	34 (94%)	2 (6%)	19	39
10	L	117/119 (98%)	108 (92%)	9 (8%)	12	25
11	M	26/26 (100%)	24 (92%)	2 (8%)	12	25
12	X	20/24 (83%)	19 (95%)	1 (5%)	22	44
All	All	1765/1811 (98%)	1676 (95%)	89 (5%)	22	44

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	THR
1	A	145	GLN
1	A	147	TRP
1	A	155	GLU
1	A	172	MET
1	A	186	LYS
1	A	210	LEU
1	A	221	LEU
1	A	235	ASP
1	A	252	LEU

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Mol	Chain	Res	Type
1	A	260	PHE
1	A	349	THR
1	A	360	LEU
1	A	372	GLN
1	A	385	THR
1	A	395	THR
1	A	433	VAL
1	A	447	VAL
1	A	466	ARG
1	A	485	VAL
1	A	518	VAL
1	A	538	VAL
1	A	587	CYS
1	A	675	LEU
1	A	705	VAL
1	A	713	VAL
2	B	53	LEU
2	B	78	GLN
2	B	142	LEU
2	B	159	LYS
2	B	171	GLU
2	B	214	THR
2	B	218	PRO
2	B	221	LEU
2	B	279	ILE
2	B	318	PHE
2	B	349	SER
2	B	370	THR
2	B	411	LEU
2	B	419	GLU
2	B	430	LEU
2	B	446	VAL
2	B	479	THR
2	B	480	LEU
2	B	525	VAL
2	B	574	CYS
2	B	582	PHE
2	B	589	MET
2	B	596	VAL
2	B	605	LEU
2	B	632	LEU
2	B	635	SER

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Mol	Chain	Res	Type
2	B	638	ILE
2	B	647	ASN
2	B	648	ASN
2	B	651	VAL
2	B	697	VAL
2	B	698	ARG
3	C	15	GLN
3	C	65	ARG
4	D	1	THR
4	D	2	THR
4	D	61	LYS
4	D	73	ARG
4	D	93	LEU
4	D	104	LYS
4	D	105	VAL
4	D	117	ARG
4	D	125	PRO
4	D	126	SER
6	F	56	ARG
6	F	80	VAL
6	F	105	LEU
7	I	10	LEU
7	I	26	VAL
8	J	1	MET
8	J	19	MET
10	L	4	LEU
10	L	34	LEU
10	L	42	SER
10	L	44	ILE
10	L	48	LEU
10	L	68	LEU
10	L	69	ARG
10	L	85	LEU
10	L	134	VAL
11	M	3	LEU
11	M	17	LEU
12	X	8	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS

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Mol	Chain	Res	Type
1	A	50	ASN
1	A	79	HIS
1	A	145	GLN
1	A	224	ASN
1	A	353	HIS
1	A	359	ASN
1	A	372	GLN
1	A	390	GLN
1	A	445	ASN
1	A	542	HIS
1	A	633	HIS
1	A	647	ASN
1	A	718	GLN
2	B	33	HIS
2	B	82	ASN
2	B	136	GLN
2	B	261	HIS
2	B	263	GLN
2	B	336	GLN
2	B	340	HIS
2	B	406	ASN
2	B	494	ASN
2	B	611	ASN
2	B	614	GLN
2	B	616	ASN
2	B	639	ASN
2	B	647	ASN
2	B	648	ASN
2	B	678	GLN
2	B	688	HIS
3	C	37	GLN
4	D	54	ASN
4	D	70	GLN
4	D	71	GLN
4	D	95	HIS
5	E	18	ASN
6	F	40	GLN
6	F	95	ASN
10	L	16	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
16	BCR	M	4021	-	41,41,41	1.37	7 (17%)	56,56,56	1.84	15 (26%)
13	CLA	B	1232	20	49,53,73	1.55	8 (16%)	58,89,113	1.87	10 (17%)
13	CLA	B	1207	2	69,73,73	1.34	8 (11%)	82,113,113	1.71	12 (14%)
17	LHG	A	5001	-	48,48,48	1.80	7 (14%)	51,54,54	1.30	3 (5%)
13	CLA	A	1011	-	69,73,73	1.29	6 (8%)	82,113,113	1.97	16 (19%)
13	CLA	B	1229	-	69,73,73	1.24	7 (10%)	82,113,113	1.67	7 (8%)
13	CLA	B	1224	-	69,73,73	1.39	9 (13%)	82,113,113	1.75	12 (14%)
13	CLA	A	1105	-	55,59,73	1.53	8 (14%)	64,96,113	1.87	8 (12%)
13	CLA	B	1223	-	69,73,73	1.33	6 (8%)	82,113,113	1.68	9 (10%)
15	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
13	CLA	A	1136	-	69,73,73	1.33	8 (11%)	82,113,113	1.56	7 (8%)
13	CLA	A	1109	13	69,73,73	1.25	8 (11%)	82,113,113	1.67	8 (9%)
13	CLA	A	1119	20	69,73,73	1.29	9 (13%)	82,113,113	1.71	10 (12%)
13	CLA	A	1110	-	58,62,73	1.35	7 (12%)	68,99,113	1.91	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1108	-	49,53,73	1.48	5 (10%)	58,89,113	1.83	7 (12%)
16	BCR	B	4005	-	41,41,41	1.57	7 (17%)	56,56,56	2.15	20 (35%)
13	CLA	L	1502	-	69,73,73	1.36	8 (11%)	82,113,113	1.66	8 (9%)
13	CLA	A	1126	-	69,73,73	1.24	6 (8%)	82,113,113	1.55	8 (9%)
14	PQN	A	2001	-	34,34,34	3.62	17 (50%)	43,45,45	2.11	3 (6%)
13	CLA	A	1127	-	69,73,73	1.29	6 (8%)	82,113,113	1.61	5 (6%)
13	CLA	A	1132	-	69,73,73	1.22	6 (8%)	82,113,113	1.65	9 (10%)
13	CLA	M	1601	20	49,53,73	1.49	7 (14%)	58,89,113	2.07	8 (13%)
13	CLA	F	1301	20	49,53,73	1.50	8 (16%)	58,89,113	1.93	8 (13%)
13	CLA	A	1130	-	69,73,73	1.20	7 (10%)	82,113,113	1.80	9 (10%)
13	CLA	B	1213	-	59,63,73	1.48	11 (18%)	70,101,113	1.74	7 (10%)
13	CLA	B	1228	-	53,57,73	1.37	8 (15%)	61,93,113	1.88	6 (9%)
13	CLA	B	1236	-	51,55,73	1.45	7 (13%)	60,91,113	1.74	7 (11%)
13	CLA	A	1107	1	69,73,73	1.24	7 (10%)	82,113,113	1.76	12 (14%)
18	LMG	B	5002	-	55,55,55	0.89	3 (5%)	63,63,63	1.29	3 (4%)
13	CLA	A	1111	-	64,68,73	1.24	6 (9%)	76,107,113	1.77	11 (14%)
13	CLA	A	1135	-	55,59,73	1.36	5 (9%)	64,96,113	1.94	9 (14%)
13	CLA	B	1012	20	69,73,73	1.34	6 (8%)	82,113,113	1.66	11 (13%)
16	BCR	I	4018	-	41,41,41	1.31	7 (17%)	56,56,56	1.84	16 (28%)
17	LHG	B	5004	-	22,22,48	2.87	5 (22%)	25,28,54	1.15	2 (8%)
13	CLA	L	1501	10	69,73,73	1.38	7 (10%)	82,113,113	1.68	10 (12%)
13	CLA	B	1206	2	69,73,73	1.19	4 (5%)	82,113,113	1.63	8 (9%)
13	CLA	A	1013	-	69,73,73	1.39	9 (13%)	82,113,113	1.66	11 (13%)
13	CLA	B	1203	-	69,73,73	1.28	5 (7%)	82,113,113	1.53	6 (7%)
13	CLA	B	1208	-	49,53,73	1.44	7 (14%)	58,89,113	1.86	9 (15%)
13	CLA	A	1133	-	58,62,73	1.33	7 (12%)	68,99,113	1.90	9 (13%)
16	BCR	J	4012	-	41,41,41	1.32	5 (12%)	56,56,56	1.96	17 (30%)
13	CLA	B	1225	-	69,73,73	1.44	10 (14%)	82,113,113	1.60	11 (13%)
16	BCR	B	4017	-	41,41,41	1.29	4 (9%)	56,56,56	1.78	19 (33%)
13	CLA	A	1102	13	63,67,73	1.34	6 (9%)	74,105,113	1.78	9 (12%)
13	CLA	B	1204	-	69,73,73	1.17	6 (8%)	82,113,113	1.70	9 (10%)
13	CLA	B	1211	-	69,73,73	1.27	7 (10%)	82,113,113	1.72	9 (10%)
13	CLA	B	1210	-	69,73,73	1.34	7 (10%)	82,113,113	1.59	7 (8%)
13	CLA	A	1125	-	69,73,73	1.30	6 (8%)	82,113,113	1.70	10 (12%)
13	CLA	B	1212	-	49,53,73	1.49	9 (18%)	58,89,113	1.91	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1214	-	63,67,73	1.37	8 (12%)	74,105,113	1.73	10 (13%)
13	CLA	J	1302	8	49,53,73	1.52	6 (12%)	58,89,113	2.02	7 (12%)
16	BCR	B	4014	-	41,41,41	1.25	7 (17%)	56,56,56	2.04	22 (39%)
13	CLA	J	1303	-	41,45,73	1.66	9 (21%)	50,78,113	1.99	6 (12%)
13	CLA	A	1114	20	53,57,73	1.37	8 (15%)	61,93,113	1.93	8 (13%)
14	PQN	B	2002	-	34,34,34	3.53	17 (50%)	43,45,45	2.03	6 (13%)
13	CLA	A	1022	20	69,73,73	1.29	11 (15%)	82,113,113	1.59	9 (10%)
13	CLA	B	1023	-	69,73,73	1.40	9 (13%)	82,113,113	1.58	5 (6%)
13	CLA	B	1227	-	49,53,73	1.41	7 (14%)	58,89,113	2.04	11 (18%)
16	BCR	J	4015	-	41,41,41	1.42	5 (12%)	56,56,56	1.93	15 (26%)
13	CLA	A	1138	-	69,73,73	1.23	9 (13%)	82,113,113	1.65	8 (9%)
16	BCR	A	4011	-	41,41,41	1.38	6 (14%)	56,56,56	2.09	19 (33%)
13	CLA	A	1120	-	53,57,73	1.39	6 (11%)	61,93,113	1.99	10 (16%)
13	CLA	B	1218	-	49,53,73	1.48	8 (16%)	58,89,113	2.06	9 (15%)
13	CLA	A	1112	-	49,53,73	1.53	9 (18%)	58,89,113	1.89	9 (15%)
13	CLA	B	1202	-	69,73,73	1.30	6 (8%)	82,113,113	1.56	9 (10%)
13	CLA	L	1503	20	69,73,73	1.31	6 (8%)	82,113,113	1.59	7 (8%)
13	CLA	B	1226	-	69,73,73	1.30	6 (8%)	82,113,113	1.66	10 (12%)
13	CLA	B	1215	-	64,68,73	1.38	8 (12%)	76,107,113	1.81	9 (11%)
16	BCR	L	4022	-	41,41,41	1.66	7 (17%)	56,56,56	1.77	13 (23%)
16	BCR	J	4013	-	41,41,41	1.29	4 (9%)	56,56,56	1.89	19 (33%)
16	BCR	A	4003	-	41,41,41	1.44	6 (14%)	56,56,56	1.98	21 (37%)
13	CLA	A	1122	-	63,67,73	1.25	7 (11%)	74,105,113	1.70	10 (13%)
13	CLA	B	1021	-	69,73,73	1.28	6 (8%)	82,113,113	1.64	9 (10%)
13	CLA	B	1201	-	58,62,73	1.38	9 (15%)	68,99,113	1.89	9 (13%)
13	CLA	A	1118	-	65,69,73	1.38	9 (13%)	77,108,113	1.86	10 (12%)
13	CLA	B	1221	2	58,62,73	1.60	12 (20%)	68,99,113	1.82	9 (13%)
13	CLA	A	1101	-	69,73,73	1.22	6 (8%)	82,113,113	1.67	7 (8%)
13	CLA	A	1140	-	69,73,73	1.27	8 (11%)	82,113,113	1.72	10 (12%)
13	CLA	A	1402	-	45,49,73	1.57	7 (15%)	54,83,113	1.82	5 (9%)
13	CLA	A	1801	17	56,60,73	1.50	11 (19%)	65,97,113	2.05	9 (13%)
13	CLA	A	1237	20	69,73,73	1.22	8 (11%)	82,113,113	1.58	8 (9%)
16	BCR	B	4004	-	41,41,41	1.55	5 (12%)	56,56,56	2.07	19 (33%)
16	BCR	L	4019	-	41,41,41	1.46	8 (19%)	56,56,56	1.86	15 (26%)
13	CLA	A	1104	-	69,73,73	1.37	8 (11%)	82,113,113	1.79	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1117	-	69,73,73	1.34	10 (14%)	82,113,113	1.77	11 (13%)
13	CLA	A	1124	20	69,73,73	1.21	6 (8%)	82,113,113	1.63	9 (10%)
15	SF4	C	3002	3	0,12,12	-	-	-	-	-
13	CLA	A	1121	-	55,59,73	1.49	8 (14%)	64,96,113	1.85	9 (14%)
16	BCR	A	4008	-	41,41,41	1.29	8 (19%)	56,56,56	1.94	20 (35%)
13	CLA	B	1205	-	69,73,73	1.28	6 (8%)	82,113,113	1.62	8 (9%)
17	LHG	A	5003	13	26,26,48	2.37	5 (19%)	29,32,54	1.58	5 (17%)
13	CLA	B	1235	-	69,73,73	1.25	9 (13%)	82,113,113	1.74	10 (12%)
16	BCR	A	4007	-	41,41,41	1.36	5 (12%)	56,56,56	1.84	17 (30%)
13	CLA	X	1701	12	49,53,73	1.48	5 (10%)	58,89,113	1.97	8 (13%)
16	BCR	F	4016	-	41,41,41	1.27	5 (12%)	56,56,56	1.85	16 (28%)
16	BCR	I	4020	-	41,41,41	1.27	6 (14%)	56,56,56	1.86	19 (33%)
13	CLA	B	1233	20	49,53,73	1.41	4 (8%)	58,89,113	1.96	8 (13%)
13	CLA	A	1139	20	55,59,73	1.44	6 (10%)	64,96,113	1.81	9 (14%)
16	BCR	A	4002	-	41,41,41	1.28	4 (9%)	56,56,56	1.81	18 (32%)
13	CLA	A	1116	-	58,62,73	1.47	10 (17%)	68,99,113	1.79	9 (13%)
15	SF4	C	3003	3	0,12,12	-	-	-	-	-
13	CLA	A	1134	1	49,53,73	1.42	6 (12%)	58,89,113	2.00	8 (13%)
16	BCR	B	4009	-	25,25,41	1.34	4 (16%)	33,33,56	1.89	10 (30%)
13	CLA	B	1220	-	49,53,73	1.47	5 (10%)	58,89,113	1.84	5 (8%)
13	CLA	A	1128	-	69,73,73	1.42	10 (14%)	82,113,113	1.61	8 (9%)
13	CLA	B	1239	-	69,73,73	1.17	8 (11%)	82,113,113	1.64	7 (8%)
13	CLA	B	1234	-	64,68,73	1.42	8 (12%)	76,107,113	1.68	9 (11%)
13	CLA	A	1115	-	58,62,73	1.47	10 (17%)	68,99,113	1.69	7 (10%)
13	CLA	B	1219	20	59,63,73	1.42	8 (13%)	70,101,113	1.81	5 (7%)
13	CLA	A	1113	-	49,53,73	1.42	6 (12%)	58,89,113	2.06	10 (17%)
13	CLA	A	1129	-	54,58,73	1.41	7 (12%)	64,95,113	1.98	12 (18%)
16	BCR	B	4006	-	41,41,41	1.26	5 (12%)	56,56,56	2.06	20 (35%)
13	CLA	B	1238	20	69,73,73	1.25	6 (8%)	82,113,113	1.58	8 (9%)
13	CLA	K	1401	-	49,53,73	1.48	7 (14%)	58,89,113	1.82	5 (8%)
13	CLA	A	1137	-	51,55,73	1.51	5 (9%)	60,91,113	1.83	9 (15%)
13	CLA	B	1222	20	50,54,73	1.36	7 (14%)	59,90,113	1.96	9 (15%)
13	CLA	B	1231	-	49,53,73	1.46	9 (18%)	58,89,113	1.93	11 (18%)
13	CLA	B	1209	-	49,53,73	1.45	6 (12%)	58,89,113	2.01	8 (13%)
13	CLA	B	1217	-	51,55,73	1.44	7 (13%)	60,91,113	2.09	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1123	20	69,73,73	1.32	6 (8%)	82,113,113	1.64	11 (13%)
13	CLA	A	1106	1	69,73,73	1.29	7 (10%)	82,113,113	1.71	8 (9%)
13	CLA	B	1230	-	62,66,73	1.40	12 (19%)	73,104,113	1.87	11 (15%)
16	BCR	B	4010	-	41,41,41	1.27	6 (14%)	56,56,56	1.93	19 (33%)
13	CLA	A	1103	-	69,73,73	1.17	4 (5%)	82,113,113	1.68	11 (13%)
13	CLA	A	1131	-	69,73,73	1.15	4 (5%)	82,113,113	1.59	10 (12%)
16	BCR	A	4001	-	41,41,41	1.39	6 (14%)	56,56,56	1.93	16 (28%)
13	CLA	B	1216	20	69,73,73	1.27	6 (8%)	82,113,113	1.66	8 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	M	4021	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1232	20	1/1/11/20	0/15/91/115	-
13	CLA	B	1207	2	1/1/15/20	7/39/115/115	-
17	LHG	A	5001	-	-	17/53/53/53	-
13	CLA	A	1011	-	1/1/15/20	4/39/115/115	-
13	CLA	B	1229	-	1/1/15/20	16/39/115/115	-
13	CLA	B	1224	-	1/1/15/20	15/39/115/115	-
13	CLA	A	1105	-	1/1/12/20	7/23/99/115	-
13	CLA	B	1223	-	1/1/15/20	10/39/115/115	-
15	SF4	A	3001	2,1	-	-	0/6/5/5
13	CLA	A	1136	-	1/1/15/20	7/39/115/115	-
13	CLA	A	1109	13	1/1/15/20	13/39/115/115	-
13	CLA	A	1119	20	1/1/15/20	6/39/115/115	-
13	CLA	A	1110	-	1/1/12/20	5/26/102/115	-
13	CLA	A	1108	-	-	9/15/91/115	-
16	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
13	CLA	L	1502	-	-	9/39/115/115	-
13	CLA	A	1126	-	1/1/15/20	10/39/115/115	-
14	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
13	CLA	A	1127	-	1/1/15/20	9/39/115/115	-
13	CLA	A	1132	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	M	1601	20	1/1/11/20	9/15/91/115	-
13	CLA	F	1301	20	1/1/11/20	4/15/91/115	-
13	CLA	A	1130	-	1/1/15/20	8/39/115/115	-
13	CLA	B	1213	-	1/1/13/20	9/27/103/115	-
13	CLA	B	1228	-	1/1/11/20	10/20/96/115	-
13	CLA	B	1236	-	-	6/18/94/115	-
13	CLA	A	1107	1	1/1/15/20	12/39/115/115	-
18	LMG	B	5002	-	-	8/50/70/70	0/1/1/1
13	CLA	A	1111	-	1/1/14/20	12/33/109/115	-
13	CLA	A	1135	-	1/1/12/20	6/23/99/115	-
13	CLA	B	1012	20	1/1/15/20	8/39/115/115	-
16	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
17	LHG	B	5004	-	-	6/26/26/53	-
13	CLA	L	1501	10	1/1/15/20	12/39/115/115	-
13	CLA	B	1206	2	1/1/15/20	12/39/115/115	-
13	CLA	A	1013	-	1/1/15/20	12/39/115/115	-
13	CLA	B	1203	-	1/1/15/20	16/39/115/115	-
13	CLA	B	1208	-	1/1/11/20	5/15/91/115	-
13	CLA	A	1133	-	1/1/12/20	5/26/102/115	-
16	BCR	J	4012	-	-	3/29/63/63	0/2/2/2
13	CLA	B	1225	-	-	12/39/115/115	-
16	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1102	13	1/1/13/20	13/32/108/115	-
13	CLA	B	1204	-	1/1/15/20	0/39/115/115	-
13	CLA	B	1211	-	1/1/15/20	12/39/115/115	-
13	CLA	B	1210	-	1/1/15/20	14/39/115/115	-
13	CLA	A	1125	-	1/1/15/20	7/39/115/115	-
13	CLA	B	1212	-	-	7/15/91/115	-
13	CLA	B	1214	-	1/1/13/20	7/32/108/115	-
13	CLA	J	1302	8	1/1/11/20	10/15/91/115	-
16	BCR	B	4014	-	-	1/29/63/63	0/2/2/2
13	CLA	J	1303	-	1/1/8/20	1/4/76/115	-
13	CLA	A	1114	20	1/1/11/20	9/20/96/115	-
14	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
13	CLA	A	1022	20	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1023	-	-	2/39/115/115	-
13	CLA	B	1227	-	1/1/11/20	9/15/91/115	-
16	BCR	J	4015	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1138	-	1/1/15/20	6/39/115/115	-
16	BCR	A	4011	-	-	8/29/63/63	0/2/2/2
13	CLA	A	1120	-	1/1/11/20	11/20/96/115	-
13	CLA	B	1218	-	1/1/11/20	6/15/91/115	-
13	CLA	A	1112	-	1/1/11/20	3/15/91/115	-
13	CLA	B	1202	-	1/1/15/20	14/39/115/115	-
13	CLA	L	1503	20	1/1/15/20	10/39/115/115	-
13	CLA	B	1226	-	1/1/15/20	9/39/115/115	-
13	CLA	B	1215	-	1/1/14/20	8/33/109/115	-
16	BCR	L	4022	-	-	1/29/63/63	0/2/2/2
16	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	A	1122	-	1/1/13/20	10/32/108/115	-
13	CLA	B	1021	-	1/1/15/20	8/39/115/115	-
13	CLA	B	1201	-	1/1/12/20	5/26/102/115	-
13	CLA	A	1118	-	1/1/14/20	15/35/111/115	-
13	CLA	B	1221	2	1/1/12/20	9/26/102/115	-
13	CLA	A	1101	-	1/1/15/20	6/39/115/115	-
13	CLA	A	1140	-	1/1/15/20	8/39/115/115	-
13	CLA	A	1402	-	1/1/9/20	4/9/81/115	-
13	CLA	A	1801	17	1/1/12/20	13/24/100/115	-
13	CLA	A	1237	20	1/1/15/20	9/39/115/115	-
16	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
16	BCR	L	4019	-	-	1/29/63/63	0/2/2/2
13	CLA	A	1104	-	1/1/15/20	16/39/115/115	-
13	CLA	A	1117	-	1/1/15/20	11/39/115/115	-
13	CLA	A	1124	20	1/1/15/20	13/39/115/115	-
15	SF4	C	3002	3	-	-	0/6/5/5
13	CLA	A	1121	-	1/1/12/20	10/23/99/115	-
16	BCR	A	4008	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1205	-	1/1/15/20	9/39/115/115	-
17	LHG	A	5003	13	1/1/5/5	10/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1235	-	1/1/15/20	3/39/115/115	-
16	BCR	A	4007	-	-	2/29/63/63	0/2/2/2
13	CLA	X	1701	12	1/1/11/20	8/15/91/115	-
16	BCR	F	4016	-	-	5/29/63/63	0/2/2/2
16	BCR	I	4020	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1233	20	1/1/11/20	4/15/91/115	-
13	CLA	A	1139	20	1/1/12/20	8/23/99/115	-
16	BCR	A	4002	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1116	-	1/1/12/20	12/26/102/115	-
15	SF4	C	3003	3	-	-	0/6/5/5
13	CLA	A	1134	1	1/1/11/20	3/15/91/115	-
16	BCR	B	4009	-	-	4/18/35/63	0/1/1/2
13	CLA	B	1220	-	1/1/11/20	4/15/91/115	-
13	CLA	A	1128	-	1/1/15/20	9/39/115/115	-
13	CLA	B	1239	-	-	5/39/115/115	-
13	CLA	B	1234	-	1/1/14/20	8/33/109/115	-
13	CLA	A	1115	-	-	1/26/102/115	-
13	CLA	B	1219	20	1/1/13/20	11/27/103/115	-
13	CLA	A	1113	-	1/1/11/20	4/15/91/115	-
13	CLA	A	1129	-	1/1/12/20	3/21/97/115	-
16	BCR	B	4006	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1238	20	1/1/15/20	2/39/115/115	-
13	CLA	K	1401	-	-	7/15/91/115	-
13	CLA	A	1137	-	1/1/11/20	5/18/94/115	-
13	CLA	B	1222	20	1/1/11/20	8/17/93/115	-
13	CLA	B	1231	-	1/1/11/20	6/15/91/115	-
13	CLA	B	1209	-	1/1/11/20	2/15/91/115	-
13	CLA	B	1217	-	1/1/11/20	6/18/94/115	-
13	CLA	A	1123	20	1/1/15/20	13/39/115/115	-
13	CLA	A	1106	1	1/1/15/20	17/39/115/115	-
13	CLA	B	1230	-	1/1/13/20	8/31/107/115	-
16	BCR	B	4010	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1103	-	1/1/15/20	16/39/115/115	-
13	CLA	A	1131	-	-	7/39/115/115	-
16	BCR	A	4001	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1216	20	1/1/15/20	4/39/115/115	-

All (883) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	2001	PQN	O4-C4	9.40	1.42	1.23
14	B	2002	PQN	O4-C4	9.07	1.42	1.23
14	A	2001	PQN	O1-C1	9.05	1.42	1.23
17	B	5004	LHG	P-O5	8.83	1.81	1.50
14	A	2001	PQN	C12-C13	8.57	1.52	1.33
14	B	2002	PQN	C12-C13	8.57	1.52	1.33
14	B	2002	PQN	O1-C1	8.53	1.41	1.23
17	A	5001	LHG	P-O5	8.39	1.79	1.50
17	A	5003	LHG	P-O5	7.87	1.78	1.50
14	A	2001	PQN	C2M-C2	-6.98	1.36	1.50
13	L	1501	CLA	MG-NA	6.74	2.22	2.06
13	B	1221	CLA	MG-NA	6.69	2.22	2.06
13	A	1123	CLA	MG-NA	6.64	2.22	2.06
14	B	2002	PQN	C2M-C2	-6.62	1.37	1.50
13	B	1210	CLA	MG-NA	6.51	2.21	2.06
14	A	2001	PQN	C3-C2	6.51	1.46	1.35
13	A	1137	CLA	MG-NA	6.46	2.21	2.06
14	B	2002	PQN	C3-C2	6.46	1.46	1.35
13	B	1207	CLA	MG-NA	6.43	2.21	2.06
13	B	1225	CLA	MG-NA	6.30	2.21	2.06
13	A	1115	CLA	MG-NA	6.29	2.21	2.06
13	A	1402	CLA	MG-NA	6.26	2.21	2.06
13	A	1121	CLA	MG-NA	6.26	2.21	2.06
13	A	1128	CLA	MG-NA	6.25	2.21	2.06
13	A	1112	CLA	MG-NA	6.22	2.21	2.06
13	B	1213	CLA	MG-NA	6.22	2.21	2.06
13	B	1238	CLA	MG-NA	6.22	2.21	2.06
13	B	1220	CLA	MG-NA	6.18	2.20	2.06
13	J	1303	CLA	MG-NA	6.16	2.20	2.06
13	B	1234	CLA	MG-NA	6.15	2.20	2.06
13	A	1108	CLA	MG-NA	6.15	2.20	2.06
13	B	1232	CLA	MG-NA	6.14	2.20	2.06
13	A	1105	CLA	MG-NA	6.12	2.20	2.06
17	B	5004	LHG	P-O6	6.07	1.83	1.59
13	A	1116	CLA	MG-NA	6.02	2.20	2.06
13	B	1226	CLA	MG-NA	6.01	2.20	2.06
13	A	1135	CLA	MG-NA	5.98	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1127	CLA	MG-NA	5.96	2.20	2.06
13	B	1012	CLA	MG-NA	5.94	2.20	2.06
13	J	1302	CLA	MG-NA	5.94	2.20	2.06
13	A	1131	CLA	MG-NA	5.93	2.20	2.06
13	X	1701	CLA	MG-NA	5.91	2.20	2.06
13	A	1139	CLA	MG-NA	5.90	2.20	2.06
13	A	1126	CLA	MG-NA	5.86	2.20	2.06
13	B	1206	CLA	MG-NA	5.85	2.20	2.06
13	B	1224	CLA	MG-NA	5.85	2.20	2.06
13	B	1236	CLA	MG-NA	5.82	2.20	2.06
13	B	1223	CLA	MG-NA	5.82	2.20	2.06
13	A	1102	CLA	MG-NA	5.80	2.20	2.06
13	B	1218	CLA	MG-NA	5.79	2.20	2.06
13	A	1104	CLA	MG-NA	5.77	2.20	2.06
13	A	1117	CLA	MG-NA	5.76	2.20	2.06
13	L	1503	CLA	MG-NA	5.76	2.20	2.06
13	B	1202	CLA	MG-NA	5.74	2.19	2.06
13	B	1203	CLA	MG-NA	5.74	2.19	2.06
13	K	1401	CLA	MG-NA	5.73	2.19	2.06
13	A	1113	CLA	MG-NA	5.73	2.19	2.06
13	B	1233	CLA	MG-NA	5.73	2.19	2.06
13	B	1212	CLA	MG-NA	5.73	2.19	2.06
13	B	1216	CLA	MG-NA	5.72	2.19	2.06
13	A	1114	CLA	MG-NA	5.72	2.19	2.06
13	B	1217	CLA	MG-NA	5.72	2.19	2.06
13	A	1136	CLA	MG-NA	5.69	2.19	2.06
13	B	1208	CLA	MG-NA	5.68	2.19	2.06
13	A	1101	CLA	MG-NA	5.63	2.19	2.06
13	A	1801	CLA	MG-NA	5.62	2.19	2.06
13	A	1120	CLA	MG-NA	5.61	2.19	2.06
13	B	1209	CLA	MG-NA	5.60	2.19	2.06
13	F	1301	CLA	MG-NA	5.59	2.19	2.06
13	A	1134	CLA	MG-NA	5.53	2.19	2.06
13	M	1601	CLA	MG-NA	5.52	2.19	2.06
13	B	1227	CLA	MG-NA	5.50	2.19	2.06
13	B	1211	CLA	MG-NA	5.50	2.19	2.06
13	A	1118	CLA	MG-NA	5.50	2.19	2.06
13	B	1215	CLA	MG-NA	5.48	2.19	2.06
17	B	5004	LHG	P-O3	5.46	1.80	1.59
13	A	1011	CLA	MG-NA	5.45	2.19	2.06
13	B	1219	CLA	MG-NA	5.41	2.19	2.06
13	B	1021	CLA	MG-NA	5.39	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1125	CLA	MG-NA	5.39	2.19	2.06
17	A	5001	LHG	P-O3	5.37	1.80	1.59
13	A	1107	CLA	MG-NA	5.36	2.19	2.06
13	A	1109	CLA	MG-NA	5.33	2.18	2.06
13	B	1201	CLA	MG-NA	5.33	2.18	2.06
16	L	4022	BCR	C1-C6	5.31	1.60	1.53
13	L	1502	CLA	MG-NA	5.26	2.18	2.06
13	B	1230	CLA	MG-NA	5.22	2.18	2.06
13	B	1222	CLA	MG-NA	5.20	2.18	2.06
13	A	1122	CLA	MG-NA	5.20	2.18	2.06
16	B	4005	BCR	C1-C6	5.15	1.60	1.53
13	A	1110	CLA	MG-NA	5.15	2.18	2.06
13	A	1111	CLA	MG-NA	5.12	2.18	2.06
13	A	1119	CLA	MG-NA	5.11	2.18	2.06
13	A	1022	CLA	MG-NA	5.09	2.18	2.06
13	A	1133	CLA	MG-NA	5.09	2.18	2.06
16	L	4019	BCR	C30-C25	5.08	1.60	1.53
17	A	5003	LHG	P-O6	5.08	1.79	1.59
16	B	4004	BCR	C30-C25	5.04	1.60	1.53
13	A	1106	CLA	MG-NA	5.02	2.18	2.06
13	B	1229	CLA	MG-NA	5.02	2.18	2.06
13	B	1228	CLA	MG-NA	5.02	2.18	2.06
13	B	1214	CLA	MG-NA	5.00	2.18	2.06
13	B	1205	CLA	MG-NA	4.98	2.18	2.06
13	B	1023	CLA	MG-NA	4.98	2.18	2.06
13	A	1013	CLA	MG-NA	4.95	2.18	2.06
16	L	4022	BCR	C30-C25	4.90	1.60	1.53
13	A	1138	CLA	MG-NA	4.88	2.17	2.06
16	A	4007	BCR	C30-C25	4.78	1.59	1.53
13	A	1129	CLA	MG-NA	4.74	2.17	2.06
13	B	1235	CLA	MG-NA	4.72	2.17	2.06
14	B	2002	PQN	C16-C15	-4.71	1.34	1.52
13	A	1140	CLA	MG-NA	4.69	2.17	2.06
13	A	1132	CLA	MG-NA	4.63	2.17	2.06
13	A	1124	CLA	MG-NA	4.61	2.17	2.06
14	A	2001	PQN	C16-C15	-4.59	1.35	1.52
17	A	5003	LHG	P-O3	4.59	1.77	1.59
13	B	1231	CLA	MG-NA	4.57	2.17	2.06
13	A	1130	CLA	MG-NA	4.49	2.16	2.06
13	B	1205	CLA	MG-NB	4.46	2.14	2.05
13	A	1103	CLA	MG-NA	4.42	2.16	2.06
13	B	1239	CLA	MG-NA	4.34	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1237	CLA	MG-NA	4.34	2.16	2.06
17	A	5001	LHG	P-O6	4.24	1.76	1.59
13	A	1013	CLA	MG-NB	4.24	2.14	2.05
13	B	1204	CLA	MG-NA	4.00	2.15	2.06
16	A	4003	BCR	C1-C6	3.95	1.58	1.53
16	A	4003	BCR	C30-C25	3.91	1.58	1.53
13	A	1128	CLA	MG-NB	3.88	2.13	2.05
16	J	4015	BCR	C30-C25	3.87	1.58	1.53
16	A	4001	BCR	C30-C25	3.84	1.58	1.53
17	A	5003	LHG	O7-C7	3.81	1.45	1.34
16	J	4013	BCR	C29-C30	3.80	1.62	1.54
16	A	4001	BCR	C1-C6	3.76	1.58	1.53
14	B	2002	PQN	C10-C5	3.75	1.46	1.40
16	A	4011	BCR	C30-C25	3.72	1.58	1.53
16	A	4002	BCR	C30-C25	3.67	1.58	1.53
16	J	4013	BCR	C2-C1	3.66	1.62	1.54
13	L	1502	CLA	MG-NB	3.64	2.13	2.05
13	A	1136	CLA	MG-NB	3.63	2.13	2.05
16	M	4021	BCR	C1-C6	3.61	1.58	1.53
13	A	1115	CLA	MG-NB	3.61	2.12	2.05
17	B	5004	LHG	O7-C7	3.59	1.44	1.34
13	B	1214	CLA	MG-NB	3.57	2.12	2.05
16	F	4016	BCR	C2-C1	3.57	1.62	1.54
13	B	1203	CLA	MG-NB	3.56	2.12	2.05
13	A	1105	CLA	MG-NB	3.55	2.12	2.05
13	B	1224	CLA	MG-NC	3.55	2.14	2.06
13	A	1103	CLA	MG-NB	3.54	2.12	2.05
16	B	4004	BCR	C1-C6	3.53	1.58	1.53
16	A	4011	BCR	C1-C6	3.51	1.58	1.53
13	A	1135	CLA	MG-NB	3.49	2.12	2.05
16	I	4020	BCR	C30-C25	3.48	1.58	1.53
16	J	4015	BCR	C1-C6	3.47	1.58	1.53
16	A	4008	BCR	C1-C6	3.47	1.58	1.53
13	B	1207	CLA	MG-NC	3.44	2.14	2.06
13	B	1235	CLA	CHC-C1C	3.42	1.45	1.38
16	L	4022	BCR	C2-C1	3.40	1.61	1.54
13	A	1108	CLA	MG-NB	3.40	2.12	2.05
13	B	1202	CLA	MG-NB	3.38	2.12	2.05
13	B	1210	CLA	MG-NB	3.38	2.12	2.05
13	A	1129	CLA	C1D-ND	-3.38	1.33	1.37
16	J	4013	BCR	C30-C25	3.38	1.58	1.53
13	B	1212	CLA	MG-NB	3.37	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	4010	BCR	C30-C25	3.37	1.58	1.53
13	L	1501	CLA	MG-NB	3.34	2.12	2.05
13	B	1231	CLA	MG-NB	3.33	2.12	2.05
13	L	1501	CLA	CHC-C1C	3.31	1.45	1.38
16	F	4016	BCR	C30-C25	3.29	1.58	1.53
14	B	2002	PQN	C11-C12	3.29	1.55	1.50
13	A	1104	CLA	MG-NB	3.28	2.12	2.05
16	B	4004	BCR	C2-C1	3.27	1.61	1.54
16	B	4004	BCR	C26-C25	3.27	1.40	1.34
13	B	1225	CLA	C2-C3	3.27	1.40	1.33
13	A	1140	CLA	C1D-ND	-3.27	1.33	1.37
14	A	2001	PQN	C10-C5	3.26	1.46	1.40
13	B	1215	CLA	C1D-ND	-3.25	1.33	1.37
13	B	1223	CLA	MG-NC	3.23	2.13	2.06
13	B	1226	CLA	MG-NC	3.23	2.13	2.06
13	B	1208	CLA	MG-NB	3.23	2.12	2.05
14	B	2002	PQN	C6-C5	3.23	1.44	1.39
13	B	1012	CLA	MG-NC	3.22	2.13	2.06
13	B	1023	CLA	CHC-C1C	3.21	1.44	1.38
13	B	1236	CLA	MG-NB	3.20	2.12	2.05
13	B	1235	CLA	MG-NB	3.20	2.12	2.05
13	B	1234	CLA	MG-NB	3.19	2.12	2.05
16	B	4005	BCR	C30-C25	3.18	1.57	1.53
16	A	4007	BCR	C29-C30	3.18	1.61	1.54
16	J	4012	BCR	C29-C30	3.18	1.61	1.54
13	B	1206	CLA	MG-NC	3.18	2.13	2.06
13	B	1210	CLA	MG-NC	3.18	2.13	2.06
16	B	4017	BCR	C2-C1	3.17	1.61	1.54
14	A	2001	PQN	C6-C5	3.16	1.44	1.39
13	B	1219	CLA	MG-NB	3.15	2.12	2.05
16	J	4015	BCR	C2-C1	3.15	1.61	1.54
13	B	1218	CLA	CHC-C1C	3.15	1.44	1.38
13	F	1301	CLA	MG-NC	3.14	2.13	2.06
16	J	4012	BCR	C1-C6	3.13	1.57	1.53
16	A	4002	BCR	C2-C1	3.13	1.61	1.54
16	A	4011	BCR	C2-C1	3.13	1.61	1.54
13	A	1118	CLA	C1D-ND	-3.12	1.33	1.37
13	A	1106	CLA	CAA-C2A	3.12	1.59	1.54
13	A	1135	CLA	MG-NC	3.12	2.13	2.06
13	A	1138	CLA	MG-NB	3.11	2.12	2.05
13	L	1503	CLA	MG-NB	3.10	2.11	2.05
13	A	1125	CLA	C5-C3	3.09	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1119	CLA	C1D-ND	-3.08	1.33	1.37
13	B	1220	CLA	MG-NB	3.07	2.11	2.05
13	B	1230	CLA	MG-NB	3.07	2.11	2.05
13	A	1022	CLA	MG-NC	3.07	2.13	2.06
13	B	1239	CLA	C1D-ND	-3.06	1.33	1.37
16	A	4003	BCR	C2-C1	3.06	1.61	1.54
16	B	4014	BCR	C29-C30	3.06	1.61	1.54
13	A	1128	CLA	CHC-C1C	3.06	1.44	1.38
16	A	4002	BCR	C29-C30	3.06	1.61	1.54
16	B	4017	BCR	C30-C25	3.05	1.57	1.53
13	X	1701	CLA	MG-NB	3.04	2.11	2.05
13	A	1116	CLA	CAA-C2A	3.04	1.59	1.54
16	B	4006	BCR	C1-C6	3.03	1.57	1.53
16	M	4021	BCR	C2-C1	3.03	1.61	1.54
16	B	4006	BCR	C30-C25	3.03	1.57	1.53
16	J	4012	BCR	C30-C25	3.03	1.57	1.53
13	B	1225	CLA	MG-NB	3.02	2.11	2.05
13	A	1138	CLA	CHC-C1C	3.02	1.44	1.38
13	B	1224	CLA	CHC-C1C	3.02	1.44	1.38
13	A	1107	CLA	C1D-ND	-3.01	1.33	1.37
16	M	4021	BCR	C29-C30	3.01	1.61	1.54
13	L	1502	CLA	CHC-C1C	3.01	1.44	1.38
13	B	1221	CLA	CHC-C1C	3.01	1.44	1.38
13	A	1801	CLA	CHC-C1C	3.00	1.44	1.38
13	A	1121	CLA	MG-NB	3.00	2.11	2.05
13	A	1106	CLA	CHC-C1C	3.00	1.44	1.38
13	A	1127	CLA	MG-NC	2.99	2.13	2.06
13	B	1219	CLA	CAA-C2A	2.98	1.59	1.54
13	A	1108	CLA	MG-NC	2.98	2.13	2.06
16	B	4005	BCR	C2-C1	2.98	1.60	1.54
16	B	4009	BCR	C29-C30	2.98	1.60	1.54
13	A	1237	CLA	CMD-C2D	2.98	1.56	1.50
16	B	4017	BCR	C29-C30	2.97	1.60	1.54
16	F	4016	BCR	C29-C30	2.97	1.60	1.54
13	B	1231	CLA	CHC-C1C	2.97	1.44	1.38
16	B	4006	BCR	C2-C1	2.96	1.60	1.54
13	A	1113	CLA	MG-NB	2.96	2.11	2.05
13	B	1213	CLA	C5-C3	2.96	1.57	1.51
13	A	1125	CLA	CHC-C1C	2.96	1.44	1.38
13	A	1137	CLA	MG-NB	2.96	2.11	2.05
16	B	4009	BCR	C30-C25	2.96	1.57	1.53
13	A	1109	CLA	MG-NB	2.96	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1137	CLA	CAA-C2A	2.95	1.59	1.54
13	X	1701	CLA	CHC-C1C	2.94	1.44	1.38
16	M	4021	BCR	C30-C25	2.94	1.57	1.53
16	B	4010	BCR	C2-C1	2.94	1.60	1.54
16	A	4001	BCR	C29-C30	2.94	1.60	1.54
13	A	1139	CLA	MG-NB	2.93	2.11	2.05
13	B	1021	CLA	MG-NC	2.93	2.13	2.06
13	B	1221	CLA	C5-C3	2.93	1.57	1.51
13	A	1402	CLA	MG-NB	2.93	2.11	2.05
16	J	4015	BCR	C29-C30	2.93	1.60	1.54
13	B	1209	CLA	MG-NB	2.92	2.11	2.05
13	A	1112	CLA	CHC-C1C	2.92	1.44	1.38
13	B	1205	CLA	CHB-C1B	-2.92	1.32	1.39
16	B	4006	BCR	C29-C30	2.92	1.60	1.54
13	B	1213	CLA	CAA-C2A	2.92	1.59	1.54
13	A	1801	CLA	CAA-C2A	2.92	1.59	1.54
13	B	1220	CLA	CHC-C1C	2.91	1.44	1.38
16	A	4002	BCR	C1-C6	2.90	1.57	1.53
13	F	1301	CLA	MG-NB	2.90	2.11	2.05
16	B	4004	BCR	C29-C30	2.90	1.60	1.54
13	B	1211	CLA	MG-NB	2.90	2.11	2.05
13	B	1232	CLA	CAA-C2A	2.89	1.59	1.54
16	A	4007	BCR	C1-C6	2.89	1.57	1.53
13	B	1224	CLA	CAA-C2A	2.89	1.59	1.54
13	B	1228	CLA	CHB-C1B	-2.88	1.32	1.39
13	B	1212	CLA	CHC-C1C	2.88	1.44	1.38
16	I	4020	BCR	C2-C1	2.88	1.60	1.54
17	A	5003	LHG	O8-C23	2.88	1.41	1.33
16	A	4011	BCR	C29-C30	2.88	1.60	1.54
16	A	4008	BCR	C30-C25	2.87	1.57	1.53
13	A	1118	CLA	CHC-C1C	2.87	1.44	1.38
16	B	4005	BCR	C26-C25	2.87	1.39	1.34
13	A	1119	CLA	CAA-C2A	2.86	1.59	1.54
13	A	1130	CLA	MG-NC	2.86	2.13	2.06
13	B	1226	CLA	CAA-C2A	2.85	1.59	1.54
13	B	1232	CLA	CHC-C1C	2.84	1.44	1.38
13	A	1119	CLA	CHC-C1C	2.84	1.44	1.38
16	J	4012	BCR	C2-C1	2.84	1.60	1.54
13	K	1401	CLA	MG-NB	2.83	2.11	2.05
16	L	4019	BCR	C29-C30	2.82	1.60	1.54
13	A	1013	CLA	CHB-C1B	-2.82	1.33	1.39
13	B	1221	CLA	MG-NB	2.82	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1123	CLA	CHC-C1C	2.82	1.44	1.38
13	A	1120	CLA	CHC-C1C	2.82	1.44	1.38
13	B	1205	CLA	MG-NC	2.82	2.13	2.06
13	B	1218	CLA	MG-NB	2.82	2.11	2.05
13	A	1022	CLA	MG-NB	2.82	2.11	2.05
13	A	1105	CLA	MG-NC	2.81	2.13	2.06
16	B	4010	BCR	C1-C6	2.81	1.57	1.53
13	B	1223	CLA	MG-NB	2.81	2.11	2.05
13	A	1124	CLA	C1D-ND	-2.81	1.34	1.37
13	B	1234	CLA	CHC-C1C	2.81	1.44	1.38
13	B	1023	CLA	CHD-C1D	2.80	1.43	1.38
13	B	1201	CLA	MG-NB	2.79	2.11	2.05
13	J	1302	CLA	MG-NC	2.79	2.12	2.06
13	B	1214	CLA	CAA-C2A	2.79	1.59	1.54
16	I	4018	BCR	C29-C30	2.78	1.60	1.54
13	J	1303	CLA	MG-NB	2.78	2.11	2.05
13	B	1225	CLA	MG-NC	2.78	2.12	2.06
13	A	1129	CLA	CHB-C1B	-2.77	1.33	1.39
13	A	1119	CLA	CHB-C1B	-2.77	1.33	1.39
13	A	1129	CLA	CHC-C1C	2.77	1.44	1.38
13	B	1207	CLA	MG-NB	2.77	2.11	2.05
13	B	1212	CLA	MG-NC	2.77	2.12	2.06
13	A	1116	CLA	MG-NB	2.77	2.11	2.05
13	A	1106	CLA	MG-NB	2.77	2.11	2.05
13	A	1134	CLA	MG-NB	2.76	2.11	2.05
18	B	5002	LMG	O8-C28	2.76	1.41	1.33
14	A	2001	PQN	C8-C9	2.75	1.43	1.38
16	A	4001	BCR	C2-C1	2.75	1.60	1.54
13	B	1230	CLA	C5-C3	2.75	1.57	1.51
13	L	1503	CLA	CHC-C1C	2.75	1.44	1.38
13	A	1140	CLA	C1-C2	2.75	1.57	1.49
14	A	2001	PQN	C15-C13	2.74	1.56	1.51
13	B	1012	CLA	CHC-C1C	2.74	1.44	1.38
17	A	5001	LHG	O8-C23	2.74	1.41	1.33
13	A	1104	CLA	MG-ND	-2.74	2.00	2.05
13	J	1302	CLA	CHC-C1C	2.73	1.44	1.38
13	B	1023	CLA	CHB-C1B	-2.73	1.33	1.39
13	A	1124	CLA	MG-NB	2.73	2.11	2.05
13	B	1204	CLA	CHD-C1D	2.73	1.43	1.38
16	I	4020	BCR	C29-C30	2.73	1.60	1.54
13	B	1209	CLA	C1D-ND	-2.73	1.34	1.37
13	B	1215	CLA	CAA-C2A	2.72	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2002	PQN	C8-C9	2.71	1.43	1.38
16	L	4022	BCR	C29-C30	2.71	1.60	1.54
13	J	1302	CLA	MG-NB	2.71	2.11	2.05
13	B	1239	CLA	MG-NB	2.71	2.11	2.05
13	A	1237	CLA	C1D-ND	-2.71	1.34	1.37
13	A	1137	CLA	MG-NC	2.70	2.12	2.06
13	B	1203	CLA	MG-NC	2.69	2.12	2.06
13	B	1204	CLA	CHB-C1B	-2.69	1.33	1.39
13	F	1301	CLA	CHC-C1C	2.69	1.43	1.38
13	J	1303	CLA	CHD-C1D	2.69	1.43	1.38
13	A	1126	CLA	MG-NC	2.69	2.12	2.06
13	L	1502	CLA	CMD-C2D	2.68	1.56	1.50
13	B	1023	CLA	C3B-C4B	2.68	1.50	1.42
13	L	1501	CLA	MG-NC	2.67	2.12	2.06
13	B	1223	CLA	C1D-C2D	-2.67	1.40	1.45
13	A	1102	CLA	CHC-C1C	2.67	1.43	1.38
16	A	4007	BCR	C2-C1	2.67	1.60	1.54
13	A	1102	CLA	MG-NB	2.67	2.11	2.05
16	B	4014	BCR	C2-C1	2.67	1.60	1.54
13	A	1112	CLA	MG-NB	2.67	2.11	2.05
13	B	1225	CLA	C5-C3	2.66	1.56	1.51
13	A	1237	CLA	CAA-C2A	2.66	1.58	1.54
18	B	5002	LMG	O7-C8	-2.66	1.40	1.46
13	A	1137	CLA	CHC-C1C	2.66	1.43	1.38
13	M	1601	CLA	MG-NB	2.65	2.11	2.05
17	A	5001	LHG	O7-C7	2.65	1.41	1.34
13	B	1023	CLA	MG-NB	2.65	2.11	2.05
13	A	1011	CLA	C4D-CHA	2.65	1.47	1.38
13	M	1601	CLA	C1D-ND	-2.65	1.34	1.37
13	B	1217	CLA	MG-NB	2.65	2.11	2.05
13	A	1136	CLA	CHC-C1C	2.65	1.43	1.38
13	A	1107	CLA	MG-NC	2.64	2.12	2.06
13	A	1102	CLA	CAA-C2A	2.64	1.58	1.54
13	A	1124	CLA	CHB-C1B	-2.64	1.33	1.39
16	A	4011	BCR	C23-C22	-2.63	1.40	1.46
13	B	1021	CLA	CHB-C1B	-2.63	1.33	1.39
13	A	1125	CLA	MG-NB	2.62	2.11	2.05
13	B	1214	CLA	C1D-ND	-2.62	1.34	1.37
13	A	1801	CLA	MG-NB	2.62	2.11	2.05
13	L	1502	CLA	CHB-C1B	-2.62	1.33	1.39
13	B	1223	CLA	CHC-C1C	2.61	1.43	1.38
13	A	1117	CLA	MG-NB	2.61	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1201	CLA	CHC-C1C	2.61	1.43	1.38
14	A	2001	PQN	C8-C7	2.61	1.44	1.38
13	A	1126	CLA	MG-NB	2.61	2.11	2.05
13	B	1202	CLA	CMD-C2D	2.60	1.56	1.50
14	A	2001	PQN	C11-C12	2.60	1.54	1.50
13	B	1214	CLA	CHB-C1B	-2.60	1.33	1.39
13	B	1236	CLA	CHB-C1B	-2.60	1.33	1.39
13	B	1216	CLA	MG-NC	2.60	2.12	2.06
13	A	1106	CLA	CHB-C1B	-2.60	1.33	1.39
13	B	1208	CLA	CHB-C1B	-2.60	1.33	1.39
13	A	1140	CLA	CHC-C1C	2.60	1.43	1.38
13	A	1104	CLA	MG-NC	2.59	2.12	2.06
13	B	1203	CLA	CHD-C1D	2.59	1.43	1.38
14	A	2001	PQN	C10-C1	-2.59	1.43	1.48
13	A	1013	CLA	C1D-ND	-2.59	1.34	1.37
13	B	1228	CLA	CHC-C1C	2.59	1.43	1.38
13	A	1117	CLA	C1-C2	2.58	1.56	1.49
13	B	1213	CLA	MG-NB	2.58	2.10	2.05
16	A	4008	BCR	C29-C30	2.58	1.60	1.54
14	A	2001	PQN	C7-C6	2.58	1.43	1.38
13	A	1116	CLA	C5-C3	2.57	1.56	1.51
13	A	1106	CLA	C1D-ND	-2.57	1.34	1.37
13	B	1012	CLA	C1D-ND	-2.57	1.34	1.37
14	B	2002	PQN	C9-C10	2.57	1.43	1.39
13	A	1013	CLA	CAA-C2A	2.56	1.58	1.54
16	I	4018	BCR	C30-C25	2.56	1.57	1.53
13	B	1236	CLA	MG-NC	2.56	2.12	2.06
13	A	1121	CLA	CHD-C1D	2.56	1.43	1.38
13	M	1601	CLA	CAA-C2A	2.56	1.58	1.54
13	A	1138	CLA	CHB-C1B	-2.56	1.33	1.39
13	A	1120	CLA	MG-NB	2.56	2.10	2.05
13	B	1221	CLA	CHB-C1B	-2.55	1.33	1.39
13	B	1217	CLA	CAA-C2A	2.55	1.58	1.54
13	A	1117	CLA	C2-C3	2.55	1.38	1.33
13	A	1133	CLA	C5-C3	2.55	1.56	1.51
16	J	4015	BCR	C5-C6	2.55	1.38	1.34
13	A	1109	CLA	C1D-ND	-2.54	1.34	1.37
13	A	1402	CLA	CBD-CAD	2.54	1.57	1.51
13	M	1601	CLA	CHC-C1C	2.54	1.43	1.38
13	B	1234	CLA	C1D-ND	-2.54	1.34	1.37
13	A	1128	CLA	C5-C3	2.54	1.56	1.51
13	B	1233	CLA	MG-NB	2.53	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1116	CLA	CHC-C1C	2.53	1.43	1.38
13	B	1232	CLA	MG-NB	2.53	2.10	2.05
13	B	1214	CLA	CHC-C1C	2.53	1.43	1.38
13	B	1202	CLA	MG-NC	2.52	2.12	2.06
13	B	1221	CLA	MG-NC	2.52	2.12	2.06
13	A	1110	CLA	CHD-C1D	2.52	1.43	1.38
13	A	1118	CLA	C5-C3	2.52	1.56	1.51
13	B	1209	CLA	CHD-C1D	2.52	1.43	1.38
13	A	1111	CLA	MG-NB	2.52	2.10	2.05
13	B	1238	CLA	MG-NC	2.52	2.12	2.06
13	A	1022	CLA	MG-ND	-2.52	2.00	2.05
13	B	1202	CLA	C1D-ND	-2.51	1.34	1.37
16	L	4019	BCR	C2-C1	2.51	1.59	1.54
16	I	4018	BCR	C2-C1	2.51	1.59	1.54
13	A	1108	CLA	CAA-C2A	2.51	1.58	1.54
16	B	4005	BCR	C29-C30	2.51	1.59	1.54
13	L	1502	CLA	CAA-C2A	2.50	1.58	1.54
13	A	1013	CLA	CMD-C2D	2.50	1.55	1.50
13	B	1207	CLA	MG-ND	-2.50	2.00	2.05
13	A	1117	CLA	CAA-C2A	2.50	1.58	1.54
13	A	1105	CLA	CHC-C1C	2.50	1.43	1.38
13	A	1139	CLA	C5-C3	2.49	1.58	1.51
13	A	1139	CLA	MG-NC	2.49	2.12	2.06
13	A	1121	CLA	CAA-C2A	2.49	1.58	1.54
13	A	1103	CLA	CHC-C1C	2.49	1.43	1.38
13	A	1112	CLA	CHB-C1B	-2.49	1.33	1.39
13	A	1107	CLA	MG-ND	-2.49	2.00	2.05
13	J	1303	CLA	MG-NC	2.49	2.12	2.06
13	L	1503	CLA	MG-NC	2.49	2.12	2.06
16	L	4022	BCR	C38-C26	2.49	1.54	1.50
13	A	1101	CLA	CHB-C1B	-2.49	1.33	1.39
16	B	4005	BCR	C38-C26	2.49	1.54	1.50
13	B	1235	CLA	CHB-C1B	-2.48	1.33	1.39
13	B	1210	CLA	CMD-C2D	2.48	1.55	1.50
13	A	1101	CLA	C1D-ND	-2.48	1.34	1.37
13	A	1132	CLA	CHB-C1B	-2.48	1.33	1.39
13	B	1225	CLA	CAA-C2A	2.48	1.58	1.54
14	B	2002	PQN	C8-C7	2.47	1.43	1.38
13	A	1011	CLA	MG-NB	2.47	2.10	2.05
16	B	4010	BCR	C29-C30	2.47	1.59	1.54
13	B	1023	CLA	MG-NC	2.47	2.12	2.06
13	A	1124	CLA	MG-NC	2.47	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1217	CLA	C1D-ND	-2.46	1.34	1.37
13	A	1123	CLA	MG-NC	2.46	2.12	2.06
16	M	4021	BCR	C23-C22	-2.46	1.40	1.46
13	L	1501	CLA	CMD-C2D	2.46	1.55	1.50
13	B	1225	CLA	C1-C2	2.45	1.56	1.49
16	L	4019	BCR	C19-C18	-2.45	1.40	1.46
13	A	1136	CLA	CHB-C1B	-2.45	1.33	1.39
13	A	1128	CLA	MG-NC	2.45	2.12	2.06
13	B	1204	CLA	CAA-C2A	2.45	1.58	1.54
13	A	1115	CLA	C1D-ND	-2.45	1.34	1.37
13	A	1110	CLA	CAA-C2A	2.44	1.58	1.54
13	A	1118	CLA	MG-NB	2.44	2.10	2.05
16	A	4003	BCR	C29-C30	2.44	1.59	1.54
13	A	1111	CLA	CHB-C1B	-2.44	1.33	1.39
13	A	1103	CLA	CHB-C1B	-2.44	1.34	1.39
13	B	1210	CLA	CHB-C1B	-2.44	1.34	1.39
13	B	1232	CLA	CHB-C1B	-2.44	1.34	1.39
13	B	1217	CLA	CHC-C1C	2.44	1.43	1.38
13	B	1219	CLA	CHC-C1C	2.44	1.43	1.38
13	J	1303	CLA	CHC-C1C	2.43	1.43	1.38
16	A	4001	BCR	C26-C25	2.43	1.38	1.34
13	B	1021	CLA	MG-NB	2.43	2.10	2.05
13	A	1118	CLA	CAA-C2A	2.43	1.58	1.54
13	B	1012	CLA	MG-NB	2.43	2.10	2.05
13	B	1224	CLA	CMD-C2D	2.43	1.55	1.50
13	J	1302	CLA	CHD-C1D	2.42	1.43	1.38
13	B	1227	CLA	CHC-C1C	2.42	1.43	1.38
13	A	1115	CLA	MG-NC	2.42	2.12	2.06
13	A	1134	CLA	CHC-C1C	2.42	1.43	1.38
13	A	1115	CLA	CHB-C1B	-2.42	1.34	1.39
13	A	1109	CLA	CHB-C1B	-2.42	1.34	1.39
13	B	1221	CLA	CHD-C1D	2.42	1.43	1.38
13	B	1216	CLA	MG-NB	2.42	2.10	2.05
13	L	1501	CLA	CAA-C2A	2.42	1.58	1.54
13	L	1503	CLA	CMD-C2D	2.42	1.55	1.50
13	K	1401	CLA	MG-NC	2.42	2.12	2.06
13	B	1232	CLA	C3B-C4B	2.42	1.49	1.42
13	B	1229	CLA	CHC-C1C	2.41	1.43	1.38
16	I	4018	BCR	C33-C5	2.41	1.54	1.50
13	B	1231	CLA	CHD-C1D	2.41	1.43	1.38
13	X	1701	CLA	MG-NC	2.41	2.12	2.06
14	B	2002	PQN	C11-C3	2.41	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1127	CLA	CHD-C1D	2.41	1.43	1.38
13	A	1122	CLA	CHB-C1B	-2.41	1.34	1.39
13	A	1132	CLA	C1D-ND	-2.40	1.34	1.37
13	A	1237	CLA	C4-C3	2.40	1.56	1.50
13	B	1216	CLA	CHB-C1B	-2.40	1.34	1.39
14	A	2001	PQN	C9-C10	2.40	1.43	1.39
13	A	1128	CLA	C3B-C4B	2.40	1.49	1.42
13	B	1229	CLA	C1D-ND	-2.40	1.34	1.37
13	B	1230	CLA	CAA-C2A	2.39	1.58	1.54
13	A	1130	CLA	CMD-C2D	2.39	1.55	1.50
13	B	1206	CLA	C1D-ND	-2.39	1.34	1.37
13	A	1115	CLA	CHC-C1C	2.39	1.43	1.38
13	B	1231	CLA	CHB-C1B	-2.39	1.34	1.39
13	A	1131	CLA	MG-NC	2.38	2.11	2.06
13	A	1128	CLA	C1D-ND	-2.38	1.34	1.37
13	A	1114	CLA	MG-NB	2.38	2.10	2.05
16	L	4022	BCR	C26-C25	2.38	1.38	1.34
13	B	1227	CLA	CHB-C1B	-2.38	1.34	1.39
13	A	1123	CLA	CHD-C1D	2.38	1.43	1.38
13	A	1104	CLA	CHC-C1C	2.37	1.43	1.38
13	B	1215	CLA	MG-NB	2.37	2.10	2.05
13	B	1232	CLA	C1D-ND	-2.37	1.34	1.37
13	A	1121	CLA	MG-NC	2.37	2.11	2.06
16	B	4005	BCR	C29-C28	-2.37	1.47	1.52
16	B	4009	BCR	C23-C22	-2.36	1.40	1.46
16	B	4017	BCR	C23-C22	-2.36	1.40	1.46
13	J	1303	CLA	CBD-CAD	2.36	1.57	1.51
13	B	1229	CLA	MG-NB	2.36	2.10	2.05
16	I	4018	BCR	C2-C3	-2.36	1.47	1.52
13	B	1211	CLA	CHB-C1B	-2.36	1.34	1.39
13	B	1238	CLA	CAA-C2A	2.36	1.58	1.54
13	B	1227	CLA	C1D-ND	-2.35	1.34	1.37
13	B	1207	CLA	CMD-C2D	2.35	1.55	1.50
13	A	1109	CLA	MG-NC	2.35	2.11	2.06
13	K	1401	CLA	CMD-C2D	2.35	1.55	1.50
13	B	1222	CLA	MG-NC	2.35	2.11	2.06
16	B	4014	BCR	C23-C22	-2.35	1.40	1.46
13	A	1801	CLA	C5-C3	2.35	1.56	1.51
13	B	1216	CLA	C1D-ND	-2.35	1.34	1.37
13	A	1127	CLA	MG-NB	2.35	2.10	2.05
13	B	1208	CLA	CAA-C2A	2.35	1.58	1.54
13	A	1102	CLA	C1D-ND	-2.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1122	CLA	CHC-C1C	2.34	1.43	1.38
16	L	4019	BCR	C38-C26	2.34	1.54	1.50
13	B	1209	CLA	CHC-C1C	2.34	1.43	1.38
13	B	1211	CLA	C5-C3	2.34	1.56	1.51
13	A	1022	CLA	CHC-C1C	2.33	1.43	1.38
13	K	1401	CLA	CHB-C1B	-2.33	1.34	1.39
13	B	1239	CLA	CAA-CBA	-2.33	1.45	1.52
13	A	1132	CLA	MG-ND	-2.33	2.01	2.05
13	B	1224	CLA	C1D-ND	-2.33	1.34	1.37
13	A	1105	CLA	C1D-ND	-2.32	1.34	1.37
16	I	4020	BCR	C33-C5	2.32	1.54	1.50
13	B	1012	CLA	CMD-C2D	2.32	1.55	1.50
13	B	1222	CLA	MG-NB	2.32	2.10	2.05
13	A	1120	CLA	CHD-C1D	2.32	1.42	1.38
13	B	1227	CLA	MG-NB	2.31	2.10	2.05
13	A	1022	CLA	CHB-C1B	-2.31	1.34	1.39
13	A	1123	CLA	MG-NB	2.31	2.10	2.05
13	B	1211	CLA	CHC-C1C	2.31	1.43	1.38
13	A	1126	CLA	CHB-C1B	-2.31	1.34	1.39
13	A	1138	CLA	CAA-C2A	2.31	1.58	1.54
13	A	1124	CLA	CAA-C2A	2.30	1.58	1.54
13	B	1236	CLA	CHC-C1C	2.30	1.43	1.38
13	A	1116	CLA	C1D-C2D	-2.30	1.40	1.45
13	A	1116	CLA	MG-NC	2.30	2.11	2.06
13	A	1133	CLA	C1-C2	2.30	1.55	1.49
13	A	1237	CLA	CHB-C1B	-2.29	1.34	1.39
13	A	1136	CLA	CHD-C1D	2.29	1.42	1.38
13	B	1222	CLA	CHD-C1D	2.29	1.42	1.38
13	B	1235	CLA	MG-NC	2.29	2.11	2.06
13	A	1105	CLA	C1-C2	2.29	1.55	1.49
13	B	1224	CLA	OBD-CAD	2.29	1.26	1.22
14	B	2002	PQN	C5-C4	-2.29	1.43	1.48
13	B	1212	CLA	CHB-C1B	-2.29	1.34	1.39
13	A	1801	CLA	CHB-C1B	-2.29	1.34	1.39
13	A	1402	CLA	MG-NC	2.29	2.11	2.06
13	B	1213	CLA	C4-C3	2.29	1.56	1.50
13	B	1212	CLA	C3B-C4B	2.29	1.49	1.42
16	B	4014	BCR	C5-C6	2.29	1.38	1.34
13	B	1238	CLA	CMD-C2D	2.28	1.55	1.50
16	I	4020	BCR	C19-C18	-2.28	1.41	1.46
13	K	1401	CLA	CHC-C1C	2.28	1.43	1.38
13	B	1211	CLA	MG-NC	2.28	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2002	PQN	C7-C6	2.27	1.42	1.38
13	B	1207	CLA	C1B-C2B	2.27	1.48	1.43
13	B	1213	CLA	C1-C2	2.27	1.55	1.49
13	A	1125	CLA	MG-NC	2.27	2.11	2.06
13	A	1113	CLA	CHD-C1D	2.27	1.42	1.38
13	A	1115	CLA	C3B-C4B	2.27	1.49	1.42
16	A	4008	BCR	C2-C1	2.27	1.59	1.54
13	A	1119	CLA	CHD-C1D	2.27	1.42	1.38
13	B	1213	CLA	CHC-C1C	2.27	1.43	1.38
13	A	1119	CLA	C1-C2	2.27	1.55	1.49
13	B	1224	CLA	MG-NB	2.27	2.10	2.05
13	B	1221	CLA	C1-C2	2.27	1.55	1.49
13	A	1022	CLA	CHD-C1D	2.27	1.42	1.38
13	A	1111	CLA	MG-NC	2.27	2.11	2.06
13	A	1112	CLA	C3B-C4B	2.26	1.49	1.42
16	A	4003	BCR	C29-C28	-2.26	1.47	1.52
13	A	1134	CLA	CAA-C2A	2.26	1.58	1.54
13	B	1210	CLA	CHD-C1D	2.26	1.42	1.38
13	A	1101	CLA	MG-NB	2.26	2.10	2.05
13	B	1023	CLA	CMD-C2D	2.25	1.55	1.50
16	L	4019	BCR	C29-C28	-2.25	1.47	1.52
13	A	1140	CLA	MG-NB	2.25	2.10	2.05
13	B	1202	CLA	C5-C3	2.25	1.55	1.51
13	A	1114	CLA	MG-NC	2.25	2.11	2.06
16	M	4021	BCR	C2-C3	-2.25	1.47	1.52
16	A	4008	BCR	C33-C5	2.25	1.54	1.50
13	B	1219	CLA	MG-NC	2.25	2.11	2.06
13	A	1114	CLA	C1D-ND	-2.25	1.34	1.37
13	A	1011	CLA	MG-ND	-2.24	2.01	2.05
13	B	1216	CLA	CHC-C1C	2.24	1.43	1.38
13	A	1135	CLA	CHB-C4A	2.24	1.43	1.37
13	B	1239	CLA	CMD-C2D	2.24	1.55	1.50
13	A	1107	CLA	CHC-C1C	2.24	1.43	1.38
13	B	1208	CLA	CHC-C1C	2.24	1.43	1.38
13	J	1302	CLA	CAA-C2A	2.24	1.58	1.54
13	A	1112	CLA	C1D-ND	-2.24	1.34	1.37
13	A	1117	CLA	CMD-C2D	2.23	1.55	1.50
13	A	1138	CLA	CMD-C2D	2.23	1.55	1.50
13	A	1801	CLA	MG-NC	2.23	2.11	2.06
13	B	1226	CLA	CHD-C1D	2.23	1.42	1.38
13	A	1136	CLA	C3B-C4B	2.23	1.49	1.42
13	B	1230	CLA	CMD-C2D	2.23	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1134	CLA	C1D-ND	-2.23	1.34	1.37
13	B	1231	CLA	C1D-ND	-2.23	1.34	1.37
13	A	1114	CLA	CHB-C1B	-2.23	1.34	1.39
13	A	1136	CLA	MG-NC	2.23	2.11	2.06
13	A	1022	CLA	C3B-C4B	2.23	1.49	1.42
16	L	4022	BCR	C23-C22	-2.22	1.41	1.46
13	A	1104	CLA	CAA-CBA	-2.22	1.46	1.52
13	B	1228	CLA	MG-ND	-2.22	2.01	2.05
13	A	1109	CLA	CAA-C2A	2.22	1.58	1.54
13	A	1117	CLA	C1D-ND	-2.22	1.34	1.37
13	B	1207	CLA	C1D-C2D	-2.22	1.40	1.45
13	B	1218	CLA	CHD-C1D	2.22	1.42	1.38
16	B	4014	BCR	C29-C28	-2.22	1.47	1.52
13	B	1227	CLA	CAA-C2A	2.21	1.58	1.54
13	A	1121	CLA	CHB-C1B	-2.21	1.34	1.39
13	B	1222	CLA	CAA-C2A	2.21	1.58	1.54
13	K	1401	CLA	CHD-C1D	2.21	1.42	1.38
13	B	1230	CLA	MG-NC	2.21	2.11	2.06
13	A	1102	CLA	MG-ND	-2.21	2.01	2.05
13	A	1131	CLA	MG-NB	2.21	2.10	2.05
13	B	1231	CLA	CAA-C2A	2.21	1.58	1.54
13	A	1135	CLA	C1B-C2B	2.21	1.48	1.43
13	A	1116	CLA	C1D-ND	-2.21	1.35	1.37
13	B	1221	CLA	C3B-C4B	2.21	1.49	1.42
16	J	4013	BCR	C1-C6	2.21	1.56	1.53
13	B	1239	CLA	MG-NC	2.20	2.11	2.06
13	B	1229	CLA	MG-NC	2.20	2.11	2.06
13	A	1133	CLA	MG-NC	2.20	2.11	2.06
13	A	1128	CLA	CAA-C2A	2.20	1.58	1.54
16	I	4018	BCR	C19-C18	-2.20	1.41	1.46
13	B	1231	CLA	CMD-C2D	2.20	1.55	1.50
13	A	1237	CLA	MG-NB	2.20	2.10	2.05
16	J	4012	BCR	C26-C25	2.20	1.38	1.34
13	B	1234	CLA	MG-NC	2.20	2.11	2.06
13	B	1239	CLA	C1C-NC	-2.19	1.34	1.37
13	B	1229	CLA	CHB-C1B	-2.19	1.34	1.39
16	L	4019	BCR	C26-C25	2.19	1.38	1.34
13	B	1201	CLA	C1-C2	2.19	1.55	1.49
13	A	1120	CLA	CHB-C1B	-2.19	1.34	1.39
13	B	1213	CLA	CHB-C1B	-2.19	1.34	1.39
13	B	1227	CLA	CHD-C1D	2.19	1.42	1.38
13	A	1118	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1234	CLA	C5-C3	2.19	1.55	1.51
13	B	1228	CLA	MG-NB	2.19	2.10	2.05
13	A	1136	CLA	CAA-C2A	2.19	1.58	1.54
13	A	1402	CLA	CAA-C2A	2.19	1.58	1.54
13	A	1801	CLA	C4-C3	2.19	1.56	1.50
13	A	1140	CLA	C5-C3	2.19	1.55	1.51
13	B	1225	CLA	CHB-C1B	-2.18	1.34	1.39
13	B	1204	CLA	C5-C3	2.18	1.55	1.51
13	A	1130	CLA	C1B-C2B	2.18	1.48	1.43
16	B	4006	BCR	C5-C6	2.18	1.38	1.34
13	B	1201	CLA	CAA-C2A	2.18	1.58	1.54
13	A	1132	CLA	MG-NC	2.18	2.11	2.06
13	A	1011	CLA	CHC-C1C	2.18	1.42	1.38
13	A	1125	CLA	C3B-C4B	2.18	1.49	1.42
13	A	1126	CLA	C4-C3	2.18	1.56	1.50
13	A	1113	CLA	CHC-C1C	2.17	1.42	1.38
13	B	1225	CLA	C1D-ND	-2.17	1.35	1.37
14	A	2001	PQN	C5-C4	-2.17	1.43	1.48
13	A	1112	CLA	CAA-C2A	2.17	1.58	1.54
13	B	1233	CLA	CHC-C1C	2.17	1.42	1.38
13	A	1110	CLA	CHB-C1B	-2.17	1.34	1.39
14	A	2001	PQN	C11-C3	2.17	1.55	1.51
13	A	1132	CLA	C1-C2	2.17	1.55	1.49
16	A	4008	BCR	C29-C28	-2.17	1.47	1.52
13	A	1108	CLA	CHB-C1B	-2.17	1.34	1.39
13	B	1023	CLA	C4-C3	2.17	1.56	1.50
13	B	1211	CLA	CHD-C1D	2.17	1.42	1.38
13	A	1117	CLA	CHB-C1B	-2.16	1.34	1.39
13	A	1011	CLA	MG-NC	2.16	2.11	2.06
17	A	5001	LHG	O7-C5	-2.16	1.41	1.46
13	A	1113	CLA	MG-NC	2.16	2.11	2.06
13	A	1110	CLA	C5-C3	2.16	1.55	1.51
13	B	1210	CLA	CHC-C1C	2.16	1.42	1.38
13	B	1208	CLA	MG-NC	2.16	2.11	2.06
13	A	1101	CLA	CHC-C1C	2.16	1.42	1.38
16	I	4020	BCR	C26-C25	2.16	1.38	1.34
13	A	1138	CLA	C1D-ND	-2.16	1.35	1.37
13	B	1224	CLA	C3B-C4B	2.16	1.49	1.42
13	A	1134	CLA	CMD-C2D	2.16	1.55	1.50
16	A	4003	BCR	C26-C25	2.16	1.38	1.34
13	A	1130	CLA	C1D-ND	-2.16	1.35	1.37
13	B	1235	CLA	C3B-C4B	2.16	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1122	CLA	MG-NB	2.15	2.10	2.05
13	A	1121	CLA	C1-C2	2.15	1.55	1.49
16	L	4019	BCR	C2-C3	-2.15	1.47	1.52
13	B	1215	CLA	C1B-NB	-2.15	1.35	1.37
13	B	1221	CLA	CMD-C2D	2.14	1.55	1.50
13	A	1122	CLA	CHD-C1D	2.14	1.42	1.38
13	A	1118	CLA	MG-ND	-2.14	2.01	2.05
13	A	1119	CLA	MG-NB	2.14	2.10	2.05
14	B	2002	PQN	C15-C13	2.14	1.55	1.51
13	B	1238	CLA	C1-C2	2.14	1.55	1.49
13	A	1107	CLA	CHB-C1B	-2.14	1.34	1.39
16	A	4008	BCR	C19-C18	-2.14	1.41	1.46
13	A	1101	CLA	C3B-C4B	2.14	1.49	1.42
13	A	1111	CLA	CMD-C2D	2.13	1.55	1.50
13	B	1218	CLA	C3B-C4B	2.13	1.49	1.42
13	B	1205	CLA	CHC-C1C	2.13	1.42	1.38
14	B	2002	PQN	C10-C1	-2.13	1.44	1.48
16	A	4007	BCR	C2-C3	-2.13	1.47	1.52
13	X	1701	CLA	C3B-C4B	2.13	1.49	1.42
13	B	1230	CLA	C1D-ND	-2.13	1.35	1.37
13	B	1208	CLA	CHD-C1D	2.13	1.42	1.38
13	B	1207	CLA	CHB-C1B	-2.13	1.34	1.39
13	A	1013	CLA	MG-NC	2.13	2.11	2.06
13	B	1230	CLA	C4-C3	2.13	1.55	1.50
13	B	1213	CLA	CMD-C2D	2.12	1.55	1.50
13	B	1215	CLA	CMD-C2D	2.12	1.55	1.50
13	B	1201	CLA	C1D-ND	-2.12	1.35	1.37
13	A	1129	CLA	CMD-C2D	2.12	1.55	1.50
13	B	1203	CLA	CAA-C2A	2.12	1.57	1.54
13	A	1133	CLA	C1D-ND	-2.12	1.35	1.37
13	B	1218	CLA	CAA-C2A	2.12	1.57	1.54
13	A	1110	CLA	C4-C3	2.12	1.55	1.50
13	A	1127	CLA	C5-C3	2.12	1.55	1.51
13	A	1133	CLA	CHC-C1C	2.12	1.42	1.38
13	B	1230	CLA	CHC-C1C	2.12	1.42	1.38
13	A	1117	CLA	MG-NC	2.12	2.11	2.06
13	A	1127	CLA	C1D-C2D	-2.12	1.41	1.45
13	B	1234	CLA	C4-C3	2.12	1.55	1.50
13	A	1104	CLA	CHD-C1D	2.11	1.42	1.38
13	A	1115	CLA	CAA-C2A	2.11	1.57	1.54
13	B	1226	CLA	C1D-ND	-2.11	1.35	1.37
13	A	1105	CLA	CMD-C2D	2.11	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1233	CLA	C1D-ND	-2.11	1.35	1.37
16	B	4014	BCR	C30-C25	2.11	1.56	1.53
13	B	1204	CLA	C3B-C4B	2.10	1.48	1.42
13	A	1013	CLA	CHC-C1C	2.10	1.42	1.38
13	B	1212	CLA	CMD-C2D	2.10	1.55	1.50
13	A	1237	CLA	C5-C3	2.10	1.55	1.51
13	A	1122	CLA	C1D-ND	-2.10	1.35	1.37
13	L	1502	CLA	C1D-ND	-2.10	1.35	1.37
13	J	1303	CLA	C3B-C4B	2.10	1.48	1.42
13	A	1114	CLA	CHC-C1C	2.10	1.42	1.38
16	B	4014	BCR	C1-C6	2.10	1.56	1.53
13	A	1105	CLA	C1D-C2D	-2.10	1.41	1.45
13	B	1221	CLA	CAA-C2A	2.09	1.57	1.54
13	A	1126	CLA	C1D-ND	-2.09	1.35	1.37
17	B	5004	LHG	O8-C23	2.09	1.43	1.33
13	A	1121	CLA	CHC-C1C	2.09	1.42	1.38
13	B	1230	CLA	C1-C2	2.09	1.55	1.49
13	B	1235	CLA	CHD-C1D	2.09	1.42	1.38
13	A	1013	CLA	CHD-C1D	2.09	1.42	1.38
13	F	1301	CLA	C1D-C2D	-2.08	1.41	1.45
13	B	1218	CLA	C1D-ND	-2.08	1.35	1.37
13	B	1225	CLA	CHD-C1D	2.08	1.42	1.38
13	A	1112	CLA	CMD-C2D	2.08	1.55	1.50
13	A	1111	CLA	CHC-C1C	2.08	1.42	1.38
13	B	1220	CLA	C3B-C4B	2.08	1.48	1.42
13	A	1115	CLA	C1-C2	2.08	1.55	1.49
13	B	1219	CLA	C1-C2	2.08	1.55	1.49
13	A	1112	CLA	CHD-C1D	2.08	1.42	1.38
13	A	1801	CLA	CMD-C2D	2.08	1.55	1.50
13	B	1222	CLA	C1D-ND	-2.08	1.35	1.37
13	B	1206	CLA	CMD-C2D	2.07	1.55	1.50
13	A	1122	CLA	C5-C3	2.07	1.55	1.51
16	I	4018	BCR	C26-C25	2.07	1.38	1.34
13	A	1131	CLA	CHD-C1D	2.07	1.42	1.38
13	A	1118	CLA	C1-C2	2.07	1.55	1.49
13	B	1223	CLA	CHB-C4A	2.07	1.42	1.37
13	B	1235	CLA	CMD-C2D	2.07	1.55	1.50
13	A	1119	CLA	C3B-C4B	2.07	1.48	1.42
13	M	1601	CLA	MG-NC	2.07	2.11	2.06
16	B	4010	BCR	C5-C6	2.07	1.38	1.34
13	B	1228	CLA	CHD-C1D	2.07	1.42	1.38
13	A	1022	CLA	C1D-C2D	-2.07	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1201	CLA	CHB-C1B	-2.07	1.34	1.39
13	F	1301	CLA	C3B-C4B	2.07	1.48	1.42
13	B	1212	CLA	CAA-C2A	2.06	1.57	1.54
13	A	1116	CLA	CHB-C1B	-2.06	1.34	1.39
13	B	1238	CLA	CHB-C1B	-2.06	1.34	1.39
13	A	1022	CLA	C1D-ND	-2.06	1.35	1.37
13	J	1303	CLA	CMD-C2D	2.06	1.55	1.50
13	B	1213	CLA	C3B-C4B	2.06	1.48	1.42
13	A	1129	CLA	MG-NB	2.06	2.09	2.05
13	B	1209	CLA	CHB-C4A	2.06	1.42	1.37
13	A	1123	CLA	C3B-C4B	2.06	1.48	1.42
13	A	1138	CLA	C4-C3	2.06	1.55	1.50
13	B	1230	CLA	CHD-C1D	2.06	1.42	1.38
13	B	1228	CLA	C3B-C4B	2.06	1.48	1.42
13	B	1217	CLA	CHD-C1D	2.06	1.42	1.38
13	A	1114	CLA	CMD-C2D	2.05	1.55	1.50
13	B	1219	CLA	CHB-C1B	-2.05	1.34	1.39
13	A	1115	CLA	CMD-C2D	2.05	1.55	1.50
13	A	1402	CLA	CHD-C1D	2.05	1.42	1.38
13	A	1801	CLA	CHD-C1D	2.05	1.42	1.38
13	A	1104	CLA	C4-C3	2.05	1.55	1.50
13	B	1236	CLA	C3D-C4D	-2.05	1.39	1.44
13	B	1219	CLA	C3B-C4B	2.05	1.48	1.42
13	B	1213	CLA	MG-NC	2.05	2.11	2.06
13	A	1117	CLA	CHD-C1D	2.05	1.42	1.38
13	A	1113	CLA	CMD-C2D	2.05	1.55	1.50
13	A	1109	CLA	CMD-C2D	2.05	1.55	1.50
13	A	1133	CLA	CAA-C2A	2.05	1.57	1.54
13	B	1214	CLA	MG-NC	2.05	2.11	2.06
13	B	1228	CLA	CAA-C2A	2.05	1.57	1.54
13	B	1021	CLA	CAA-CBA	-2.05	1.46	1.52
13	A	1801	CLA	C3B-C4B	2.05	1.48	1.42
13	L	1501	CLA	C3B-C4B	2.05	1.48	1.42
13	F	1301	CLA	CHB-C1B	-2.04	1.34	1.39
13	B	1215	CLA	CHB-C1B	-2.04	1.34	1.39
13	A	1140	CLA	C3B-C4B	2.04	1.48	1.42
13	B	1230	CLA	CHB-C4A	2.04	1.42	1.37
13	A	1138	CLA	C3B-C4B	2.04	1.48	1.42
13	B	1201	CLA	MG-NC	2.04	2.11	2.06
13	F	1301	CLA	CHD-C1D	2.04	1.42	1.38
13	A	1022	CLA	C3D-C4D	-2.04	1.39	1.44
16	A	4008	BCR	C26-C25	2.03	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1130	CLA	CHD-C1D	2.03	1.42	1.38
13	B	1235	CLA	C1D-ND	-2.03	1.35	1.37
13	B	1229	CLA	C3B-C4B	2.03	1.48	1.42
13	A	1139	CLA	CHB-C4A	2.03	1.42	1.37
13	A	1129	CLA	C3B-C4B	2.03	1.48	1.42
13	A	1110	CLA	MG-NB	2.03	2.09	2.05
13	A	1106	CLA	C1-C2	2.03	1.54	1.49
16	F	4016	BCR	C29-C28	-2.03	1.47	1.52
16	F	4016	BCR	C23-C22	-2.03	1.41	1.46
13	B	1218	CLA	MG-NC	2.03	2.11	2.06
13	A	1402	CLA	C1D-ND	-2.03	1.35	1.37
13	A	1139	CLA	C4-C3	2.03	1.55	1.50
16	B	4010	BCR	C29-C28	-2.03	1.47	1.52
13	J	1303	CLA	CHB-C4A	2.03	1.42	1.37
13	B	1215	CLA	C5-C3	2.03	1.55	1.51
13	B	1221	CLA	C1D-ND	-2.03	1.35	1.37
13	B	1232	CLA	MG-NC	2.02	2.11	2.06
13	B	1220	CLA	CHB-C1B	-2.02	1.34	1.39
13	M	1601	CLA	C3B-C4B	2.02	1.48	1.42
13	L	1503	CLA	CBA-CGA	-2.02	1.44	1.50
16	M	4021	BCR	C38-C26	2.02	1.54	1.50
13	B	1212	CLA	C1D-C2D	-2.02	1.41	1.45
13	A	1130	CLA	C1-C2	2.02	1.54	1.49
13	A	1140	CLA	CAA-C2A	2.02	1.57	1.54
17	A	5001	LHG	O8-C6	-2.02	1.40	1.45
13	B	1226	CLA	MG-ND	-2.02	2.01	2.05
18	B	5002	LMG	O1-C7	-2.02	1.40	1.43
13	B	1231	CLA	C3B-C4B	2.02	1.48	1.42
13	A	1114	CLA	CAA-C2A	2.02	1.57	1.54
13	A	1116	CLA	C1-C2	2.02	1.54	1.49
13	B	1214	CLA	C3B-C4B	2.02	1.48	1.42
13	B	1236	CLA	C1D-C2D	-2.01	1.41	1.45
13	B	1222	CLA	CHC-C1C	2.01	1.42	1.38
13	A	1109	CLA	CHC-C1C	2.01	1.42	1.38
13	L	1502	CLA	C1-C2	2.01	1.54	1.49
13	A	1120	CLA	CAA-C2A	2.01	1.57	1.54
13	B	1234	CLA	C3B-C4B	2.01	1.48	1.42
13	A	1128	CLA	C4-C3	2.01	1.55	1.50
13	B	1021	CLA	C4-C3	2.01	1.55	1.50
16	A	4001	BCR	C19-C18	-2.01	1.41	1.46
13	A	1107	CLA	CHD-C1D	2.01	1.42	1.38
16	A	4011	BCR	C39-C30	-2.01	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1201	CLA	CMD-C2D	2.01	1.54	1.50
13	B	1217	CLA	MG-NC	2.01	2.11	2.06
13	B	1205	CLA	CAA-C2A	2.00	1.57	1.54
13	A	1128	CLA	CHB-C1B	-2.00	1.34	1.39
16	B	4009	BCR	C14-C13	2.00	1.40	1.34
13	B	1239	CLA	CHB-C1B	-2.00	1.34	1.39

All (1247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1217	CLA	C4A-NA-C1A	12.19	112.24	106.68
13	A	1130	CLA	C4A-NA-C1A	12.12	112.21	106.68
13	M	1601	CLA	C4A-NA-C1A	12.07	112.18	106.68
13	A	1113	CLA	C4A-NA-C1A	11.89	112.10	106.68
13	A	1118	CLA	C4A-NA-C1A	11.79	112.06	106.68
13	B	1209	CLA	C4A-NA-C1A	11.75	112.04	106.68
13	A	1110	CLA	C4A-NA-C1A	11.75	112.04	106.68
13	B	1218	CLA	C4A-NA-C1A	11.72	112.03	106.68
13	J	1302	CLA	C4A-NA-C1A	11.65	112.00	106.68
13	A	1801	CLA	C4A-NA-C1A	11.58	111.96	106.68
13	X	1701	CLA	C4A-NA-C1A	11.58	111.96	106.68
13	B	1233	CLA	C4A-NA-C1A	11.57	111.96	106.68
13	A	1134	CLA	C4A-NA-C1A	11.53	111.94	106.68
13	B	1227	CLA	C4A-NA-C1A	11.40	111.88	106.68
13	F	1301	CLA	C4A-NA-C1A	11.34	111.85	106.68
13	A	1114	CLA	C4A-NA-C1A	11.26	111.82	106.68
13	A	1109	CLA	C4A-NA-C1A	11.26	111.82	106.68
13	J	1303	CLA	C4A-NA-C1A	11.23	111.80	106.68
13	B	1230	CLA	C4A-NA-C1A	11.21	111.79	106.68
13	B	1215	CLA	C4A-NA-C1A	11.17	111.78	106.68
13	A	1120	CLA	C4A-NA-C1A	11.17	111.77	106.68
13	B	1219	CLA	C4A-NA-C1A	11.10	111.74	106.68
13	A	1107	CLA	C4A-NA-C1A	11.07	111.73	106.68
13	A	1133	CLA	C4A-NA-C1A	11.05	111.72	106.68
13	B	1204	CLA	C4A-NA-C1A	11.04	111.72	106.68
13	A	1117	CLA	C4A-NA-C1A	11.00	111.70	106.68
13	A	1129	CLA	C4A-NA-C1A	11.00	111.70	106.68
13	A	1111	CLA	C4A-NA-C1A	10.98	111.69	106.68
13	B	1207	CLA	C4A-NA-C1A	10.97	111.68	106.68
13	B	1222	CLA	C4A-NA-C1A	10.95	111.67	106.68
13	B	1201	CLA	C4A-NA-C1A	10.93	111.67	106.68
13	A	1135	CLA	C4A-NA-C1A	10.86	111.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1223	CLA	C4A-NA-C1A	10.85	111.63	106.68
13	A	1105	CLA	C4A-NA-C1A	10.85	111.63	106.68
13	B	1235	CLA	C4A-NA-C1A	10.85	111.63	106.68
13	A	1106	CLA	C4A-NA-C1A	10.81	111.61	106.68
13	A	1402	CLA	C4A-NA-C1A	10.81	111.61	106.68
13	A	1102	CLA	C4A-NA-C1A	10.76	111.59	106.68
13	A	1125	CLA	C4A-NA-C1A	10.75	111.58	106.68
13	A	1138	CLA	C4A-NA-C1A	10.71	111.56	106.68
13	B	1239	CLA	C4A-NA-C1A	10.68	111.55	106.68
13	B	1216	CLA	C4A-NA-C1A	10.64	111.53	106.68
13	B	1228	CLA	C4A-NA-C1A	10.61	111.52	106.68
13	A	1116	CLA	C4A-NA-C1A	10.59	111.51	106.68
13	B	1212	CLA	C4A-NA-C1A	10.58	111.50	106.68
13	B	1231	CLA	C4A-NA-C1A	10.57	111.50	106.68
13	A	1124	CLA	C4A-NA-C1A	10.56	111.50	106.68
13	B	1214	CLA	C4A-NA-C1A	10.51	111.47	106.68
13	B	1211	CLA	C4A-NA-C1A	10.49	111.47	106.68
13	B	1021	CLA	C4A-NA-C1A	10.46	111.45	106.68
13	A	1101	CLA	C4A-NA-C1A	10.44	111.44	106.68
13	B	1220	CLA	C4A-NA-C1A	10.34	111.40	106.68
13	B	1229	CLA	C4A-NA-C1A	10.34	111.40	106.68
13	A	1122	CLA	C4A-NA-C1A	10.34	111.39	106.68
13	A	1112	CLA	C4A-NA-C1A	10.31	111.38	106.68
13	L	1502	CLA	C4A-NA-C1A	10.30	111.38	106.68
13	A	1119	CLA	C4A-NA-C1A	10.28	111.37	106.68
13	A	1140	CLA	C4A-NA-C1A	10.27	111.37	106.68
13	A	1139	CLA	C4A-NA-C1A	10.26	111.36	106.68
13	B	1221	CLA	C4A-NA-C1A	10.26	111.36	106.68
13	B	1232	CLA	C4A-NA-C1A	10.24	111.35	106.68
13	B	1208	CLA	C4A-NA-C1A	10.20	111.33	106.68
13	A	1127	CLA	C4A-NA-C1A	10.19	111.33	106.68
13	B	1206	CLA	C4A-NA-C1A	10.17	111.32	106.68
13	L	1501	CLA	C4A-NA-C1A	10.12	111.30	106.68
13	A	1136	CLA	C4A-NA-C1A	10.12	111.30	106.68
13	A	1108	CLA	C4A-NA-C1A	10.09	111.28	106.68
13	A	1123	CLA	C4A-NA-C1A	10.08	111.28	106.68
13	K	1401	CLA	C4A-NA-C1A	10.04	111.26	106.68
13	B	1224	CLA	C4A-NA-C1A	10.04	111.26	106.68
13	B	1213	CLA	C4A-NA-C1A	10.01	111.25	106.68
13	A	1104	CLA	C4A-NA-C1A	9.96	111.22	106.68
13	A	1121	CLA	C4A-NA-C1A	9.94	111.22	106.68
13	B	1234	CLA	C4A-NA-C1A	9.89	111.19	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	1503	CLA	C4A-NA-C1A	9.85	111.17	106.68
13	B	1226	CLA	C4A-NA-C1A	9.79	111.15	106.68
13	A	1131	CLA	C4A-NA-C1A	9.75	111.13	106.68
13	A	1115	CLA	C4A-NA-C1A	9.75	111.12	106.68
13	B	1238	CLA	C4A-NA-C1A	9.73	111.12	106.68
13	A	1103	CLA	C4A-NA-C1A	9.72	111.11	106.68
13	B	1023	CLA	C4A-NA-C1A	9.69	111.10	106.68
13	A	1128	CLA	C4A-NA-C1A	9.66	111.09	106.68
13	B	1236	CLA	C4A-NA-C1A	9.52	111.02	106.68
13	A	1132	CLA	C4A-NA-C1A	9.49	111.01	106.68
13	A	1013	CLA	C4A-NA-C1A	9.48	111.00	106.68
13	B	1203	CLA	C4A-NA-C1A	9.47	111.00	106.68
13	B	1012	CLA	C4A-NA-C1A	9.46	111.00	106.68
13	A	1137	CLA	C4A-NA-C1A	9.46	110.99	106.68
13	A	1126	CLA	C4A-NA-C1A	9.43	110.98	106.68
13	A	1237	CLA	C4A-NA-C1A	9.38	110.96	106.68
13	B	1210	CLA	C4A-NA-C1A	9.32	110.93	106.68
13	B	1202	CLA	C4A-NA-C1A	9.13	110.84	106.68
13	A	1011	CLA	C4A-NA-C1A	9.05	110.81	106.68
13	A	1022	CLA	C4A-NA-C1A	8.99	110.78	106.68
13	B	1225	CLA	C4A-NA-C1A	8.79	110.69	106.68
13	A	1011	CLA	O2D-CGD-CBD	8.72	126.47	111.23
13	B	1205	CLA	C4A-NA-C1A	8.70	110.65	106.68
14	B	2002	PQN	C11-C12-C13	-7.95	113.14	126.83
14	A	2001	PQN	C11-C12-C13	-7.83	113.34	126.83
14	A	2001	PQN	C14-C13-C15	7.22	127.76	115.23
14	A	2001	PQN	C15-C13-C12	-6.57	106.41	121.17
14	B	2002	PQN	C14-C13-C15	6.21	126.01	115.23
16	B	4004	BCR	C38-C26-C25	6.17	131.22	124.48
17	A	5001	LHG	C25-C24-C23	6.14	136.18	113.69
18	B	5002	LMG	C30-C29-C28	6.08	135.97	113.69
16	B	4005	BCR	C38-C26-C25	5.96	130.99	124.48
16	A	4008	BCR	C38-C26-C25	5.68	130.68	124.48
14	B	2002	PQN	C15-C13-C12	-5.59	108.62	121.17
13	A	1011	CLA	O1D-CGD-CBD	-5.51	113.64	124.52
16	L	4022	BCR	C33-C5-C6	5.33	130.31	124.48
16	A	4001	BCR	C38-C26-C25	5.31	130.28	124.48
16	B	4014	BCR	C33-C5-C6	5.26	130.22	124.48
16	J	4012	BCR	C38-C26-C25	5.24	130.20	124.48
16	L	4019	BCR	C33-C5-C6	5.07	130.02	124.48
13	B	1012	CLA	O2D-CGD-CBD	4.98	119.94	111.23
13	A	1132	CLA	O2D-CGD-CBD	4.96	119.91	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1226	CLA	O2D-CGD-CBD	4.96	119.90	111.23
17	A	5003	LHG	C25-C24-C23	4.95	137.56	114.11
16	J	4015	BCR	C33-C5-C6	4.94	129.88	124.48
16	B	4006	BCR	C33-C5-C6	4.92	129.85	124.48
13	A	1104	CLA	CAA-C2A-C3A	-4.87	99.84	113.00
16	B	4010	BCR	C33-C5-C6	4.85	129.78	124.48
13	B	1201	CLA	O2D-CGD-CBD	4.84	119.70	111.23
16	I	4018	BCR	C33-C5-C6	4.82	129.75	124.48
16	B	4004	BCR	C33-C5-C6	4.82	129.74	124.48
13	A	1104	CLA	O2A-CGA-CBA	4.80	126.48	111.83
16	J	4015	BCR	C38-C26-C25	4.77	129.69	124.48
13	L	1501	CLA	O2D-CGD-CBD	4.76	119.55	111.23
16	A	4003	BCR	C38-C26-C25	4.73	129.65	124.48
16	L	4022	BCR	C38-C26-C25	4.67	129.57	124.48
13	A	1102	CLA	O2D-CGD-CBD	4.66	119.38	111.23
16	F	4016	BCR	C38-C26-C25	4.64	129.55	124.48
13	B	1205	CLA	O2D-CGD-CBD	4.62	119.31	111.23
13	B	1230	CLA	O2D-CGD-CBD	4.61	119.29	111.23
16	A	4002	BCR	C38-C26-C25	4.61	129.51	124.48
16	B	4006	BCR	C29-C30-C25	4.60	117.11	110.44
16	I	4018	BCR	C38-C26-C25	4.58	129.49	124.48
13	A	1801	CLA	O2D-CGD-CBD	4.57	119.22	111.23
16	B	4014	BCR	C38-C26-C25	4.56	129.46	124.48
13	B	1211	CLA	O2D-CGD-CBD	4.56	119.20	111.23
16	M	4021	BCR	C38-C26-C25	4.54	129.43	124.48
13	B	1224	CLA	O2A-CGA-CBA	4.53	125.66	111.83
16	B	4006	BCR	C7-C8-C9	4.52	132.93	126.23
16	A	4001	BCR	C33-C5-C6	4.47	129.36	124.48
16	A	4003	BCR	C33-C5-C6	4.46	129.35	124.48
16	A	4007	BCR	C38-C26-C25	4.45	129.34	124.48
13	B	1212	CLA	O2D-CGD-CBD	4.42	118.96	111.23
16	B	4006	BCR	C38-C26-C25	4.42	129.30	124.48
16	I	4018	BCR	C2-C1-C6	4.38	116.81	110.44
16	L	4019	BCR	C38-C26-C25	4.37	129.25	124.48
16	A	4011	BCR	C7-C8-C9	4.35	132.68	126.23
13	A	1123	CLA	O2D-CGD-CBD	4.34	118.82	111.23
13	A	1113	CLA	O2D-CGD-CBD	4.34	118.81	111.23
13	A	1125	CLA	O2D-CGD-CBD	4.32	118.78	111.23
13	B	1222	CLA	O2D-CGD-CBD	4.31	118.77	111.23
16	J	4015	BCR	C8-C7-C6	4.30	138.50	127.00
16	B	4009	BCR	C38-C26-C25	4.30	129.18	124.48
16	B	4005	BCR	C33-C5-C6	4.28	129.16	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1101	CLA	O2D-CGD-CBD	4.26	118.69	111.23
16	A	4011	BCR	C33-C5-C6	4.26	129.13	124.48
13	A	1106	CLA	O2D-CGD-CBD	4.24	118.64	111.23
16	I	4020	BCR	C38-C26-C25	4.21	129.08	124.48
16	J	4012	BCR	C33-C5-C6	4.21	129.08	124.48
13	A	1128	CLA	O2D-CGD-CBD	4.20	118.57	111.23
13	A	1135	CLA	O2A-CGA-CBA	4.19	124.62	111.83
13	M	1601	CLA	O2D-CGD-CBD	4.18	118.54	111.23
13	A	1013	CLA	O2A-CGA-CBA	4.17	124.56	111.83
13	A	1137	CLA	O2A-CGA-CBA	4.16	124.53	111.83
13	B	1217	CLA	O2D-CGD-CBD	4.16	118.50	111.23
13	A	1129	CLA	O2D-CGD-CBD	4.15	118.48	111.23
13	B	1229	CLA	O2D-CGD-CBD	4.12	118.44	111.23
13	B	1227	CLA	O2D-CGD-CBD	4.12	118.43	111.23
16	F	4016	BCR	C33-C5-C6	4.12	128.98	124.48
13	B	1225	CLA	O2A-CGA-CBA	4.09	124.32	111.83
16	A	4011	BCR	C38-C26-C25	4.09	128.95	124.48
16	A	4002	BCR	C33-C5-C6	4.09	128.95	124.48
16	B	4010	BCR	C38-C26-C25	4.09	128.94	124.48
13	B	1234	CLA	O2D-CGD-CBD	4.07	118.35	111.23
16	I	4020	BCR	C24-C23-C22	4.07	132.26	126.23
13	B	1218	CLA	O2D-CGD-CBD	4.05	118.31	111.23
13	A	1121	CLA	O2D-CGD-CBD	4.05	118.30	111.23
16	B	4017	BCR	C33-C5-C6	4.04	128.89	124.48
16	J	4015	BCR	C2-C1-C6	4.04	116.31	110.44
13	J	1302	CLA	O2D-CGD-CBD	4.04	118.29	111.23
16	B	4017	BCR	C38-C26-C25	4.04	128.89	124.48
16	A	4007	BCR	C33-C5-C6	4.01	128.86	124.48
16	A	4011	BCR	C2-C1-C6	4.01	116.26	110.44
13	B	1210	CLA	O2D-CGD-CBD	3.99	118.21	111.23
16	J	4012	BCR	C29-C30-C25	3.99	116.24	110.44
13	B	1202	CLA	O2D-CGD-CBD	3.99	118.20	111.23
16	B	4004	BCR	C2-C1-C6	3.99	116.23	110.44
16	B	4005	BCR	C7-C8-C9	3.97	132.12	126.23
13	A	1140	CLA	O2A-CGA-CBA	3.97	123.93	111.83
13	A	1107	CLA	O2A-CGA-CBA	3.96	123.91	111.83
13	B	1223	CLA	O2D-CGD-CBD	3.95	118.14	111.23
13	B	1205	CLA	O2A-CGA-CBA	3.94	123.86	111.83
16	A	4003	BCR	C29-C30-C25	3.94	116.17	110.44
13	K	1401	CLA	O2D-CGD-CBD	3.94	118.11	111.23
13	A	1103	CLA	O2D-CGD-CBD	3.93	118.11	111.23
13	A	1120	CLA	O2A-CGA-CBA	3.93	123.81	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1117	CLA	O2A-CGA-CBA	3.92	123.80	111.83
13	A	1120	CLA	O2D-CGD-CBD	3.92	118.08	111.23
13	B	1215	CLA	O2A-CGA-CBA	3.92	123.78	111.83
16	A	4011	BCR	C40-C30-C25	3.92	116.39	110.24
13	A	1237	CLA	O2A-CGA-CBA	3.91	123.76	111.83
16	A	4011	BCR	C24-C23-C22	3.90	132.01	126.23
13	B	1221	CLA	O2D-CGD-CBD	3.90	118.05	111.23
13	A	1118	CLA	O2A-CGA-CBA	3.90	123.71	111.83
13	A	1801	CLA	O2A-CGA-CBA	3.89	123.71	111.83
13	B	1211	CLA	C1-C2-C3	3.88	132.56	126.20
13	B	1228	CLA	O2D-CGD-CBD	3.87	118.00	111.23
16	B	4014	BCR	C7-C8-C9	3.87	131.96	126.23
13	A	1801	CLA	C1-C2-C3	3.87	132.53	126.20
13	A	1022	CLA	C3B-C4B-NB	-3.85	107.09	110.53
13	A	1139	CLA	O2A-CGA-CBA	3.85	123.57	111.83
16	M	4021	BCR	C24-C23-C22	3.85	131.93	126.23
13	A	1111	CLA	O2D-CGD-CBD	3.84	117.94	111.23
13	B	1231	CLA	O2D-CGD-CBD	3.82	117.91	111.23
16	J	4013	BCR	C2-C1-C6	3.82	115.98	110.44
13	B	1224	CLA	CBA-CAA-C2A	3.81	125.12	113.79
13	A	1121	CLA	O2A-CGA-CBA	3.80	123.42	111.83
16	J	4013	BCR	C29-C30-C25	3.80	115.95	110.44
16	M	4021	BCR	C33-C5-C6	3.79	128.62	124.48
13	A	1127	CLA	O2A-CGA-CBA	3.78	123.37	111.83
16	J	4013	BCR	C33-C5-C6	3.78	128.61	124.48
13	B	1217	CLA	O2A-CGA-CBA	3.77	123.34	111.83
16	B	4005	BCR	C30-C25-C26	-3.77	117.49	122.64
16	B	4005	BCR	C24-C23-C22	3.74	131.77	126.23
16	I	4020	BCR	C33-C5-C6	3.73	128.56	124.48
13	B	1214	CLA	O2A-CGA-CBA	3.73	123.21	111.83
13	A	1116	CLA	O2A-CGA-CBA	3.70	123.13	111.83
16	A	4008	BCR	C33-C5-C6	3.70	128.53	124.48
13	A	1110	CLA	O2A-CGA-CBA	3.70	123.12	111.83
16	B	4010	BCR	C7-C8-C9	3.70	131.71	126.23
16	B	4005	BCR	C29-C30-C25	3.70	115.81	110.44
13	A	1127	CLA	O2D-CGD-CBD	3.69	117.68	111.23
13	B	1204	CLA	O2D-CGD-CBD	3.69	117.68	111.23
13	A	1114	CLA	O2D-CGD-CBD	3.67	117.64	111.23
16	A	4007	BCR	C24-C23-C22	3.67	131.66	126.23
16	J	4012	BCR	C2-C1-C6	3.66	115.75	110.44
13	A	1137	CLA	O2D-CGD-CBD	3.65	117.62	111.23
13	A	1105	CLA	O2A-CGA-CBA	3.65	122.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1106	CLA	O2A-CGA-CBA	3.65	122.95	111.83
13	A	1130	CLA	O2D-CGD-CBD	3.64	117.60	111.23
13	B	1201	CLA	O2A-CGA-CBA	3.64	122.92	111.83
13	B	1209	CLA	O2D-CGD-CBD	3.63	117.58	111.23
16	A	4003	BCR	C24-C23-C22	3.63	131.60	126.23
13	L	1503	CLA	O2D-CGD-CBD	3.62	117.55	111.23
16	A	4011	BCR	C29-C30-C25	3.61	115.69	110.44
13	X	1701	CLA	O2D-CGD-CBD	3.60	117.52	111.23
16	J	4015	BCR	C24-C23-C22	3.60	131.56	126.23
13	B	1213	CLA	O2D-CGD-CBD	3.60	117.52	111.23
16	A	4002	BCR	C2-C1-C6	3.59	115.66	110.44
16	J	4012	BCR	C23-C24-C25	3.59	136.60	127.00
13	B	1213	CLA	O2A-CGA-CBA	3.59	122.79	111.83
13	A	1118	CLA	O2D-CGD-CBD	3.59	117.51	111.23
13	A	1130	CLA	C1-C2-C3	3.59	132.08	126.20
16	A	4008	BCR	C38-C26-C27	-3.59	105.95	113.60
16	B	4014	BCR	C2-C1-C6	3.58	115.64	110.44
16	B	4014	BCR	C29-C30-C25	3.58	115.64	110.44
16	A	4001	BCR	C29-C30-C25	3.57	115.62	110.44
13	A	1131	CLA	O2D-CGD-CBD	3.56	117.46	111.23
16	B	4004	BCR	C23-C24-C25	3.55	136.49	127.00
13	B	1224	CLA	O2D-CGD-CBD	3.55	117.44	111.23
16	B	4017	BCR	C2-C1-C6	3.55	115.59	110.44
16	M	4021	BCR	C2-C1-C6	3.54	115.59	110.44
13	A	1112	CLA	O2D-CGD-CBD	3.54	117.42	111.23
16	B	4006	BCR	C2-C1-C6	3.54	115.58	110.44
13	L	1502	CLA	O2D-CGD-CBD	3.54	117.42	111.23
13	A	1125	CLA	O2A-CGA-CBA	3.54	122.62	111.83
16	B	4010	BCR	C2-C1-C6	3.53	115.57	110.44
13	A	1124	CLA	O2D-CGD-CBD	3.53	117.39	111.23
16	J	4015	BCR	C29-C30-C25	3.53	115.56	110.44
13	B	1239	CLA	O2D-CGD-CBD	3.52	117.38	111.23
13	A	1011	CLA	C4D-CHA-C1A	-3.51	117.06	121.24
13	B	1235	CLA	O2D-CGD-CBD	3.51	117.36	111.23
13	A	1133	CLA	C1-C2-C3	3.50	131.93	126.20
16	B	4004	BCR	C38-C26-C27	-3.50	106.14	113.60
13	A	1139	CLA	O2D-CGD-CBD	3.50	117.34	111.23
16	F	4016	BCR	C15-C14-C13	3.50	132.18	127.28
13	A	1109	CLA	O2A-CGA-CBA	3.50	122.50	111.83
16	L	4022	BCR	C2-C1-C6	3.50	115.52	110.44
16	F	4016	BCR	C2-C1-C6	3.49	115.51	110.44
16	B	4009	BCR	C20-C21-C22	3.49	132.17	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1220	CLA	O2D-CGD-CBD	3.48	117.31	111.23
13	A	1135	CLA	O2D-CGD-CBD	3.48	117.31	111.23
13	B	1215	CLA	O2D-CGD-CBD	3.46	117.29	111.23
16	A	4008	BCR	C29-C30-C25	3.45	115.46	110.44
13	A	1022	CLA	O2D-CGD-CBD	3.45	117.26	111.23
16	A	4008	BCR	C24-C23-C22	3.45	131.34	126.23
13	A	1801	CLA	C3B-C4B-NB	-3.45	107.45	110.53
13	A	1102	CLA	O2A-CGA-CBA	3.44	122.31	111.83
13	L	1501	CLA	O2A-CGA-CBA	3.43	122.30	111.83
16	M	4021	BCR	C29-C30-C25	3.42	115.41	110.44
13	B	1235	CLA	O2A-CGA-CBA	3.42	122.26	111.83
16	F	4016	BCR	C29-C30-C25	3.41	115.40	110.44
13	B	1234	CLA	C1-C2-C3	3.40	131.78	126.20
13	A	1135	CLA	C1-C2-C3	3.40	131.76	126.20
13	A	1101	CLA	O2A-CGA-CBA	3.38	122.14	111.83
13	A	1114	CLA	O2A-CGA-CBA	3.38	122.14	111.83
13	B	1219	CLA	C1-C2-C3	3.38	131.73	126.20
13	A	1110	CLA	O2D-CGD-CBD	3.38	117.13	111.23
13	A	1129	CLA	O2A-CGA-CBA	3.37	122.12	111.83
13	A	1126	CLA	O2A-CGA-CBA	3.37	122.11	111.83
13	A	1134	CLA	O2D-CGD-CBD	3.37	117.12	111.23
13	A	1115	CLA	O2D-CGD-CBD	3.37	117.12	111.23
16	A	4007	BCR	C29-C30-C25	3.37	115.33	110.44
16	B	4004	BCR	C29-C30-C25	3.36	115.33	110.44
13	A	1105	CLA	O2D-CGD-CBD	3.36	117.11	111.23
13	B	1238	CLA	C1-C2-C3	3.36	131.70	126.20
13	B	1207	CLA	O2A-CGA-CBA	3.35	122.06	111.83
13	B	1204	CLA	O2A-CGA-CBA	3.35	122.05	111.83
17	A	5001	LHG	O8-C23-C24	3.35	122.04	111.83
13	A	1138	CLA	O2A-CGA-CBA	3.35	122.04	111.83
16	J	4013	BCR	C38-C26-C25	3.34	128.13	124.48
13	B	1202	CLA	C1-C2-C3	3.34	131.67	126.20
13	A	1011	CLA	O2A-CGA-CBA	3.34	122.02	111.83
16	B	4004	BCR	C30-C25-C26	-3.34	118.08	122.64
13	A	1130	CLA	O2A-CGA-CBA	3.33	121.99	111.83
16	A	4003	BCR	C2-C1-C6	3.33	115.27	110.44
13	A	1133	CLA	O2D-CGD-CBD	3.32	117.04	111.23
13	B	1224	CLA	C3B-C4B-NB	-3.32	107.57	110.53
13	A	1129	CLA	C3B-C4B-NB	-3.31	107.57	110.53
13	A	1133	CLA	O2A-CGA-CBA	3.31	121.92	111.83
13	B	1228	CLA	C3B-C4B-NB	-3.31	107.58	110.53
16	B	4004	BCR	C24-C23-C22	3.31	131.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	4007	BCR	C2-C1-C6	3.31	115.24	110.44
13	A	1011	CLA	C4D-C3D-CAD	-3.30	104.52	108.11
13	B	1223	CLA	O2A-CGA-CBA	3.29	121.88	111.83
13	A	1111	CLA	O2A-CGA-CBA	3.29	121.86	111.83
13	A	1103	CLA	O2A-CGA-CBA	3.28	121.84	111.83
16	B	4014	BCR	C33-C5-C4	-3.28	106.61	113.60
13	A	1136	CLA	O2A-CGA-CBA	3.28	121.82	111.83
16	B	4005	BCR	C38-C26-C27	-3.26	106.64	113.60
16	A	4001	BCR	C30-C25-C26	-3.26	118.17	122.64
13	B	1229	CLA	O2A-CGA-CBA	3.26	121.78	111.83
13	B	1202	CLA	O2A-CGA-CBA	3.26	121.77	111.83
13	B	1210	CLA	O2A-CGA-CBA	3.26	121.77	111.83
13	A	1237	CLA	O2A-CGA-O1A	-3.25	115.50	123.63
16	A	4001	BCR	C2-C1-C6	3.25	115.16	110.44
16	B	4005	BCR	C2-C1-C6	3.24	115.14	110.44
13	B	1012	CLA	O2A-CGA-CBA	3.24	121.70	111.83
13	B	1229	CLA	C3B-C4B-NB	-3.24	107.64	110.53
16	J	4013	BCR	C7-C8-C9	3.23	131.02	126.23
13	B	1221	CLA	C3B-C4B-NB	-3.23	107.65	110.53
13	B	1233	CLA	O2D-CGD-CBD	3.23	116.87	111.23
13	A	1022	CLA	C1-C2-C3	3.23	131.48	126.20
16	J	4012	BCR	C30-C25-C26	-3.22	118.23	122.64
13	A	1107	CLA	O2D-CGD-CBD	3.22	116.85	111.23
16	A	4003	BCR	C38-C26-C27	-3.21	106.74	113.60
13	B	1206	CLA	O2D-CGD-CBD	3.21	116.85	111.23
13	B	1236	CLA	O2A-CGA-CBA	3.21	121.61	111.83
13	B	1232	CLA	C3B-C4B-NB	-3.21	107.67	110.53
13	B	1205	CLA	O1D-CGD-CBD	-3.20	118.20	124.52
13	B	1230	CLA	C1-C2-C3	3.20	131.44	126.20
18	B	5002	LMG	O8-C28-C29	3.20	121.60	111.83
16	B	4009	BCR	C29-C30-C25	3.20	115.08	110.44
13	A	1121	CLA	C1-C2-C3	3.20	131.43	126.20
16	A	4008	BCR	C30-C25-C26	-3.19	118.27	122.64
16	A	4001	BCR	C38-C26-C27	-3.19	106.80	113.60
13	B	1227	CLA	C3B-C4B-NB	-3.19	107.68	110.53
16	J	4012	BCR	C38-C26-C27	-3.18	106.81	113.60
13	B	1238	CLA	CED-O2D-CGD	3.18	123.13	115.92
13	B	1023	CLA	O2A-CGA-CBA	3.18	121.53	111.83
13	F	1301	CLA	O2D-CGD-CBD	3.18	116.78	111.23
13	A	1119	CLA	CED-O2D-CGD	3.16	123.09	115.92
13	B	1012	CLA	C3B-C4B-NB	-3.16	107.70	110.53
16	B	4006	BCR	C38-C26-C27	-3.16	106.86	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1118	CLA	C1-C2-C3	3.16	131.37	126.20
13	B	1226	CLA	O2A-CGA-CBA	3.15	121.45	111.83
13	B	1207	CLA	O2D-CGD-CBD	3.15	116.74	111.23
16	L	4019	BCR	C2-C1-C6	3.15	115.02	110.44
13	J	1303	CLA	CAA-C2A-C3A	-3.15	109.01	116.23
13	B	1235	CLA	C3B-C4B-NB	-3.15	107.72	110.53
16	B	4005	BCR	C23-C24-C25	3.15	135.40	127.00
13	A	1122	CLA	O2D-CGD-CBD	3.15	116.73	111.23
13	A	1123	CLA	O2A-CGA-CBA	3.15	121.43	111.83
13	A	1013	CLA	O2A-CGA-O1A	-3.15	115.76	123.63
13	B	1021	CLA	O2A-CGA-CBA	3.14	121.40	111.83
13	B	1023	CLA	C3B-C4B-NB	-3.14	107.73	110.53
13	A	1138	CLA	CED-O2D-CGD	3.14	123.03	115.92
13	B	1216	CLA	O2D-CGD-CBD	3.13	116.71	111.23
16	J	4015	BCR	C1-C6-C5	-3.13	118.35	122.64
13	A	1103	CLA	CAA-C2A-C3A	-3.13	104.53	113.00
13	B	1221	CLA	O2A-CGA-CBA	3.13	121.38	111.83
13	B	1021	CLA	C7-C6-C5	-3.12	104.94	113.26
16	L	4019	BCR	C24-C23-C22	3.11	130.84	126.23
16	J	4012	BCR	C8-C7-C6	3.11	135.31	127.00
17	A	5003	LHG	O8-C23-C24	3.11	120.59	111.15
16	B	4017	BCR	C29-C30-C25	3.11	114.95	110.44
13	B	1216	CLA	O2A-CGA-CBA	3.11	121.31	111.83
13	B	1219	CLA	O2A-CGA-CBA	3.11	121.31	111.83
16	A	4002	BCR	C29-C30-C25	3.11	114.95	110.44
16	L	4019	BCR	C30-C25-C24	3.10	124.05	115.65
13	B	1219	CLA	O2D-CGD-CBD	3.10	116.64	111.23
16	A	4001	BCR	C23-C24-C25	3.09	135.26	127.00
16	I	4020	BCR	C33-C5-C4	-3.09	107.00	113.60
16	I	4020	BCR	C38-C26-C27	-3.09	107.01	113.60
13	A	1116	CLA	O2D-CGD-CBD	3.09	116.63	111.23
16	B	4017	BCR	C7-C8-C9	3.09	130.80	126.23
16	B	4004	BCR	C7-C8-C9	3.09	130.80	126.23
16	A	4002	BCR	C38-C26-C27	-3.08	107.02	113.60
13	B	1239	CLA	O2A-CGA-CBA	3.08	121.23	111.83
16	B	4005	BCR	C1-C6-C5	-3.07	118.45	122.64
13	B	1228	CLA	O2A-CGA-CBA	3.06	121.18	111.83
13	A	1122	CLA	O2A-CGA-CBA	3.06	121.17	111.83
13	A	1108	CLA	O2D-CGD-CBD	3.06	116.58	111.23
16	B	4004	BCR	C1-C6-C5	-3.06	118.46	122.64
13	A	1013	CLA	CED-O2D-CGD	3.06	122.85	115.92
16	A	4003	BCR	C40-C30-C25	3.06	115.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1206	CLA	O2A-CGA-CBA	3.05	121.15	111.83
13	B	1205	CLA	CAA-C2A-C3A	-3.05	104.75	113.00
13	B	1230	CLA	O2A-CGA-CBA	3.05	121.14	111.83
16	L	4019	BCR	C33-C5-C4	-3.05	107.09	113.60
16	A	4008	BCR	C2-C1-C6	3.04	114.86	110.44
16	B	4009	BCR	C24-C23-C22	3.04	130.73	126.23
16	M	4021	BCR	C1-C6-C7	3.04	123.89	115.65
13	A	1115	CLA	O2A-CGA-CBA	3.03	121.09	111.83
13	A	1135	CLA	O2A-CGA-O1A	-3.03	116.04	123.63
13	L	1502	CLA	O2A-CGA-CBA	3.03	121.08	111.83
16	A	4007	BCR	C30-C25-C26	-3.02	118.50	122.64
16	J	4013	BCR	C30-C25-C24	3.02	123.85	115.65
16	A	4011	BCR	C16-C17-C18	3.02	131.51	127.28
13	A	1114	CLA	CED-O2D-CGD	3.02	122.77	115.92
16	B	4010	BCR	C33-C5-C4	-3.02	107.16	113.60
13	B	1236	CLA	O2D-CGD-CBD	3.02	116.51	111.23
13	L	1503	CLA	O2A-CGA-CBA	3.02	121.04	111.83
16	B	4010	BCR	C24-C23-C22	3.02	130.70	126.23
13	A	1119	CLA	C1-C2-C3	3.02	131.14	126.20
16	B	4006	BCR	C33-C5-C4	-3.02	107.17	113.60
16	J	4015	BCR	C33-C5-C4	-3.01	107.19	113.60
13	M	1601	CLA	CED-O2D-CGD	3.00	122.73	115.92
17	B	5004	LHG	O7-C7-C8	3.00	117.98	111.48
13	M	1601	CLA	O2A-CGA-CBA	3.00	123.48	114.00
16	B	4006	BCR	C24-C23-C22	3.00	130.67	126.23
16	L	4022	BCR	C8-C7-C6	2.99	134.97	127.00
13	A	1104	CLA	CED-O2D-CGD	2.99	122.69	115.92
13	B	1226	CLA	C1-C2-C3	2.98	131.09	126.20
13	B	1211	CLA	O2A-CGA-CBA	2.98	120.93	111.83
16	B	4009	BCR	C38-C26-C27	-2.98	107.24	113.60
13	A	1140	CLA	O2D-CGD-CBD	2.98	116.44	111.23
16	I	4018	BCR	C7-C8-C9	2.98	130.64	126.23
13	A	1135	CLA	C4-C3-C5	-2.98	112.62	116.13
16	I	4018	BCR	C38-C26-C27	-2.98	107.25	113.60
13	A	1110	CLA	C1-C2-C3	2.98	131.07	126.20
13	B	1235	CLA	CED-O2D-CGD	2.97	122.66	115.92
13	B	1203	CLA	O2D-CGD-CBD	2.97	116.43	111.23
16	J	4015	BCR	C38-C26-C27	-2.97	107.26	113.60
16	A	4007	BCR	C30-C25-C24	2.97	123.70	115.65
16	M	4021	BCR	C1-C6-C5	-2.97	118.58	122.64
13	A	1132	CLA	C3B-C4B-NB	-2.96	107.89	110.53
13	A	1124	CLA	O2A-CGA-CBA	2.96	120.87	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1208	CLA	O2D-CGD-CBD	2.96	116.41	111.23
16	B	4006	BCR	C1-C6-C5	-2.96	118.59	122.64
16	B	4014	BCR	C8-C9-C10	-2.95	114.36	119.01
13	A	1104	CLA	C2A-C3A-C4A	2.95	106.64	101.87
16	B	4006	BCR	C30-C25-C26	-2.95	118.60	122.64
13	B	1214	CLA	O2D-CGD-CBD	2.95	116.38	111.23
16	A	4008	BCR	C23-C24-C25	2.95	134.87	127.00
17	A	5001	LHG	O7-C7-C8	2.95	117.86	111.48
16	L	4022	BCR	C29-C30-C25	2.94	114.72	110.44
13	A	1137	CLA	O2A-CGA-O1A	-2.94	116.26	123.63
13	A	1120	CLA	C3B-C4B-NB	-2.94	107.90	110.53
13	A	1117	CLA	O2D-CGD-CBD	2.94	116.37	111.23
16	B	4014	BCR	C38-C26-C27	-2.94	107.33	113.60
16	J	4012	BCR	C36-C18-C19	2.94	122.58	118.09
13	A	1131	CLA	O2A-CGA-CBA	2.94	120.80	111.83
16	A	4001	BCR	C8-C7-C6	2.94	134.85	127.00
13	B	1023	CLA	CED-O2D-CGD	2.94	122.58	115.92
13	B	1210	CLA	C1-C2-C3	2.94	131.01	126.20
13	B	1208	CLA	CED-O2D-CGD	2.93	122.57	115.92
13	J	1302	CLA	C3B-C4B-NB	-2.93	107.91	110.53
16	B	4005	BCR	C1-C6-C7	2.93	123.60	115.65
16	L	4019	BCR	C8-C7-C6	2.93	134.83	127.00
13	A	1104	CLA	C1-C2-C3	2.92	130.99	126.20
16	A	4003	BCR	C7-C8-C9	2.92	130.56	126.23
16	F	4016	BCR	C24-C23-C22	2.92	130.56	126.23
16	I	4018	BCR	C23-C24-C25	2.92	134.79	127.00
13	B	1207	CLA	C4D-CHA-C1A	2.92	124.72	121.24
16	B	4009	BCR	C40-C30-C25	2.91	114.81	110.24
16	B	4010	BCR	C29-C30-C25	2.91	114.67	110.44
13	B	1213	CLA	C1-C2-C3	2.91	130.97	126.20
13	B	1221	CLA	CED-O2D-CGD	2.91	122.51	115.92
16	B	4004	BCR	C33-C5-C4	-2.91	107.40	113.60
16	I	4020	BCR	C32-C1-C6	2.90	114.80	110.24
16	L	4022	BCR	C33-C5-C4	-2.90	107.41	113.60
16	A	4011	BCR	C32-C1-C6	2.89	114.78	110.24
13	B	1217	CLA	CED-O2D-CGD	2.89	122.48	115.92
16	A	4001	BCR	C1-C6-C5	-2.89	118.69	122.64
16	A	4007	BCR	C38-C26-C27	-2.89	107.44	113.60
16	A	4002	BCR	C30-C25-C26	-2.89	118.69	122.64
16	A	4001	BCR	C24-C23-C22	2.89	130.51	126.23
13	A	1118	CLA	C3B-C4B-NB	-2.89	107.95	110.53
13	A	1126	CLA	O2D-CGD-CBD	2.89	116.27	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1119	CLA	CAA-C2A-C3A	-2.88	105.20	113.00
13	B	1209	CLA	O2A-CGA-CBA	2.88	123.11	114.00
13	B	1216	CLA	C3B-C4B-NB	-2.88	107.96	110.53
13	B	1230	CLA	CED-O2D-CGD	2.87	122.44	115.92
13	B	1218	CLA	C3B-C4B-NB	-2.87	107.97	110.53
16	F	4016	BCR	C33-C5-C4	-2.87	107.47	113.60
17	A	5003	LHG	O7-C7-C8	2.87	117.69	111.48
17	A	5003	LHG	C6-C5-C4	-2.87	105.09	111.78
16	B	4014	BCR	C15-C14-C13	2.87	131.30	127.28
13	B	1225	CLA	O2D-CGD-CBD	2.86	116.24	111.23
13	B	1231	CLA	CED-O2D-CGD	2.86	122.41	115.92
16	A	4011	BCR	C30-C25-C24	2.86	123.42	115.65
16	B	4014	BCR	C12-C13-C14	-2.86	114.50	119.01
13	A	1123	CLA	C3B-C4B-NB	-2.86	107.98	110.53
13	B	1205	CLA	O2A-CGA-O1A	-2.86	116.48	123.63
16	L	4019	BCR	C38-C26-C27	-2.86	107.50	113.60
13	A	1132	CLA	O2A-CGA-CBA	2.85	120.54	111.83
16	A	4003	BCR	C1-C6-C5	-2.85	118.74	122.64
16	F	4016	BCR	C38-C26-C27	-2.85	107.51	113.60
16	I	4020	BCR	C30-C25-C26	-2.85	118.74	122.64
13	A	1116	CLA	C3B-C4B-NB	-2.85	107.98	110.53
13	B	1219	CLA	CED-O2D-CGD	2.85	122.38	115.92
13	J	1303	CLA	C2A-C3A-C4A	2.85	104.93	101.59
13	A	1104	CLA	CBA-CAA-C2A	2.85	122.26	113.79
16	J	4015	BCR	C30-C25-C26	-2.85	118.75	122.64
13	B	1210	CLA	O1D-CGD-CBD	-2.84	118.91	124.52
16	I	4020	BCR	C7-C8-C9	2.84	130.44	126.23
13	A	1138	CLA	C3B-C4B-NB	-2.84	107.99	110.53
16	J	4013	BCR	C23-C24-C25	2.84	134.57	127.00
13	B	1218	CLA	CED-O2D-CGD	2.84	122.35	115.92
16	A	4003	BCR	C33-C5-C4	-2.84	107.55	113.60
13	J	1302	CLA	CED-O2D-CGD	2.83	122.34	115.92
16	I	4018	BCR	C29-C30-C25	2.83	114.56	110.44
13	B	1203	CLA	O2A-CGA-CBA	2.83	120.47	111.83
13	B	1212	CLA	C3B-C4B-NB	-2.83	108.00	110.53
16	A	4011	BCR	C33-C5-C4	-2.83	107.56	113.60
16	A	4001	BCR	C33-C5-C4	-2.83	107.56	113.60
13	A	1117	CLA	CED-O2D-CGD	2.83	122.33	115.92
16	L	4019	BCR	C30-C25-C26	-2.83	118.78	122.64
16	I	4018	BCR	C36-C18-C19	2.82	122.40	118.09
16	L	4019	BCR	C40-C30-C25	2.82	114.66	110.24
13	A	1140	CLA	C3B-C4B-NB	-2.82	108.02	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1125	CLA	C1-C2-C3	2.81	130.80	126.20
16	B	4005	BCR	C20-C21-C22	2.81	131.22	127.28
13	B	1208	CLA	CAA-C2A-C3A	-2.81	105.41	113.00
13	A	1108	CLA	O2A-CGA-CBA	2.81	122.87	114.00
13	B	1021	CLA	CED-O2D-CGD	2.81	122.28	115.92
13	B	1232	CLA	CED-O2D-CGD	2.81	122.28	115.92
13	A	1237	CLA	O2D-CGD-CBD	2.80	116.13	111.23
16	B	4014	BCR	C32-C1-C6	2.80	114.63	110.24
16	J	4012	BCR	C1-C6-C7	2.80	123.24	115.65
13	B	1234	CLA	O2A-CGA-CBA	2.80	120.36	111.83
13	A	1130	CLA	CED-O2D-CGD	2.79	122.25	115.92
13	A	1107	CLA	C3B-C4B-NB	-2.79	108.04	110.53
13	A	1103	CLA	CED-O2D-CGD	2.79	122.23	115.92
16	B	4005	BCR	C33-C5-C4	-2.78	107.66	113.60
13	A	1801	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
16	L	4019	BCR	C29-C30-C25	2.78	114.47	110.44
13	A	1140	CLA	CED-O2D-CGD	2.78	122.21	115.92
13	B	1230	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
13	A	1109	CLA	CED-O2D-CGD	2.77	122.21	115.92
13	B	1233	CLA	O2A-CGA-CBA	2.77	122.75	114.00
16	F	4016	BCR	C1-C6-C5	-2.77	118.85	122.64
16	A	4003	BCR	C30-C25-C26	-2.77	118.86	122.64
16	B	4010	BCR	C30-C25-C24	2.77	123.15	115.65
13	A	1102	CLA	O1D-CGD-CBD	-2.76	119.06	124.52
13	A	1116	CLA	CED-O2D-CGD	2.76	122.19	115.92
16	B	4010	BCR	C30-C25-C26	-2.76	118.86	122.64
13	A	1237	CLA	CAA-C2A-C3A	-2.76	105.53	113.00
13	A	1112	CLA	CED-O2D-CGD	2.76	122.18	115.92
13	B	1203	CLA	C1-C2-C3	2.76	130.72	126.20
13	A	1128	CLA	O2A-CGA-CBA	2.75	120.23	111.83
16	L	4022	BCR	C30-C25-C26	-2.75	118.88	122.64
16	B	4010	BCR	C38-C26-C27	-2.75	107.73	113.60
16	M	4021	BCR	C38-C26-C27	-2.75	107.73	113.60
16	B	4010	BCR	C36-C18-C19	2.75	122.28	118.09
16	B	4014	BCR	C30-C25-C26	-2.75	118.88	122.64
13	B	1225	CLA	C4-C3-C5	-2.74	110.47	115.23
16	M	4021	BCR	C8-C7-C6	2.74	134.33	127.00
13	A	1123	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
13	B	1204	CLA	C3B-C4B-NB	-2.74	108.08	110.53
13	A	1111	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
13	A	1104	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
16	I	4020	BCR	C37-C22-C23	2.74	122.27	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	1701	CLA	O2A-CGA-CBA	2.74	122.64	114.00
13	B	1211	CLA	O1D-CGD-CBD	-2.73	119.13	124.52
16	F	4016	BCR	C30-C25-C26	-2.73	118.90	122.64
13	B	1227	CLA	O1D-CGD-CBD	-2.73	119.13	124.52
13	A	1112	CLA	O2A-CGA-CBA	2.73	122.62	114.00
13	F	1301	CLA	O2A-CGA-CBA	2.73	122.62	114.00
16	B	4017	BCR	C38-C26-C27	-2.73	107.78	113.60
13	A	1133	CLA	CED-O2D-CGD	2.73	122.10	115.92
16	A	4002	BCR	C33-C5-C4	-2.73	107.78	113.60
13	B	1207	CLA	C2A-C1A-CHA	2.72	128.60	123.87
16	B	4006	BCR	C23-C24-C25	2.72	134.27	127.00
13	B	1021	CLA	C1-C2-C3	2.72	130.66	126.20
13	A	1109	CLA	O2D-CGD-CBD	2.72	115.98	111.23
16	B	4014	BCR	C23-C24-C25	2.72	134.26	127.00
13	A	1108	CLA	CED-O2D-CGD	2.72	122.08	115.92
13	B	1214	CLA	CED-O2D-CGD	2.72	122.08	115.92
13	B	1221	CLA	C1-C2-C3	2.72	130.65	126.20
13	B	1238	CLA	O2D-CGD-CBD	2.71	115.98	111.23
16	A	4011	BCR	C38-C26-C27	-2.71	107.81	113.60
13	A	1132	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
16	J	4012	BCR	C1-C6-C5	-2.70	118.94	122.64
13	A	1106	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
13	B	1217	CLA	C3B-C4B-NB	-2.70	108.12	110.53
16	A	4008	BCR	C11-C10-C9	2.69	131.05	127.28
16	J	4013	BCR	C30-C25-C26	-2.69	118.96	122.64
13	A	1101	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	A	1129	CLA	O1D-CGD-CBD	-2.69	119.21	124.52
13	A	1125	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	X	1701	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	A	1011	CLA	OBD-CAD-C3D	2.68	134.69	128.42
13	B	1238	CLA	O2A-CGA-CBA	2.68	120.02	111.83
13	B	1216	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
13	A	1115	CLA	CED-O2D-CGD	2.68	122.00	115.92
13	A	1133	CLA	C3B-C4B-NB	-2.68	108.14	110.53
13	B	1212	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
13	B	1206	CLA	CED-O2D-CGD	2.68	122.00	115.92
13	A	1134	CLA	C3B-C4B-NB	-2.68	108.14	110.53
16	B	4014	BCR	C34-C9-C8	2.68	122.18	118.09
13	A	1110	CLA	C3B-C4B-NB	-2.68	108.14	110.53
13	L	1502	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
13	B	1216	CLA	CED-O2D-CGD	2.68	121.99	115.92
13	A	1129	CLA	CAA-C2A-C3A	-2.68	105.77	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	4011	BCR	C30-C25-C26	-2.68	118.98	122.64
13	F	1301	CLA	C3B-C4B-NB	-2.67	108.14	110.53
13	A	1107	CLA	C2A-C1A-CHA	2.67	128.50	123.87
13	A	1801	CLA	CED-O2D-CGD	2.67	121.97	115.92
13	A	1134	CLA	CED-O2D-CGD	2.67	121.96	115.92
13	A	1113	CLA	O2A-CGA-CBA	2.67	122.42	114.00
13	B	1235	CLA	C1-C2-C3	2.66	130.56	126.20
13	A	1119	CLA	C3B-C4B-NB	-2.66	108.15	110.53
16	L	4022	BCR	C1-C6-C5	-2.66	119.00	122.64
13	A	1124	CLA	C1-C2-C3	2.66	130.56	126.20
16	B	4009	BCR	C35-C13-C12	2.66	120.71	114.59
16	M	4021	BCR	C30-C25-C26	-2.66	119.00	122.64
13	A	1106	CLA	C3B-C4B-NB	-2.66	108.16	110.53
13	B	1225	CLA	CED-O2D-CGD	2.66	121.94	115.92
13	A	1114	CLA	C3B-C4B-NB	-2.65	108.16	110.53
13	A	1119	CLA	CAA-CBA-CGA	2.65	120.74	113.21
16	J	4013	BCR	C33-C5-C4	-2.65	107.94	113.60
13	M	1601	CLA	C3B-C4B-NB	-2.65	108.17	110.53
13	A	1128	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
16	A	4011	BCR	C1-C6-C7	2.65	122.83	115.65
13	B	1220	CLA	O2A-CGA-CBA	2.65	122.36	114.00
13	B	1213	CLA	C3B-C4B-NB	-2.64	108.17	110.53
16	J	4013	BCR	C1-C6-C5	-2.64	119.02	122.64
16	B	4010	BCR	C16-C17-C18	2.64	130.98	127.28
13	B	1218	CLA	O1D-CGD-CBD	-2.64	119.31	124.52
16	A	4002	BCR	C1-C6-C5	-2.64	119.03	122.64
13	B	1223	CLA	C1-C2-C3	2.64	130.52	126.20
13	A	1022	CLA	C4D-CHA-C1A	2.64	124.39	121.24
13	A	1119	CLA	O2D-CGD-CBD	2.63	115.84	111.23
13	B	1210	CLA	CED-O2D-CGD	2.63	121.89	115.92
13	B	1218	CLA	O2A-CGA-CBA	2.63	122.30	114.00
16	B	4010	BCR	C32-C1-C6	2.62	114.36	110.24
13	J	1302	CLA	O2A-CGA-CBA	2.62	122.29	114.00
16	I	4018	BCR	C1-C6-C5	-2.62	119.05	122.64
13	A	1013	CLA	C1-O2A-CGA	2.62	123.00	116.65
16	A	4008	BCR	C1-C6-C7	2.62	122.76	115.65
16	B	4006	BCR	C35-C13-C12	2.62	122.09	118.09
13	B	1216	CLA	C1-C2-C3	2.62	130.49	126.20
13	A	1129	CLA	CED-O2D-CGD	2.62	121.86	115.92
16	B	4005	BCR	C32-C1-C6	2.62	114.35	110.24
13	B	1224	CLA	C1-C2-C3	2.62	130.49	126.20
13	B	1012	CLA	C4D-CHA-C1A	2.62	124.37	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	4011	BCR	C15-C14-C13	2.62	130.95	127.28
16	A	4007	BCR	C33-C5-C4	-2.62	108.02	113.60
16	A	4003	BCR	C1-C6-C7	2.61	122.73	115.65
13	B	1207	CLA	CED-O2D-CGD	2.61	121.84	115.92
13	A	1125	CLA	O1D-CGD-CBD	-2.61	119.37	124.52
16	B	4017	BCR	C33-C5-C4	-2.61	108.03	113.60
13	A	1105	CLA	CED-O2D-CGD	2.60	121.82	115.92
13	L	1501	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
16	A	4002	BCR	C30-C25-C24	2.60	122.69	115.65
13	J	1303	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	J	4013	BCR	C36-C18-C19	2.60	122.05	118.09
16	I	4020	BCR	C30-C25-C24	2.60	122.69	115.65
13	B	1209	CLA	CED-O2D-CGD	2.60	121.80	115.92
16	A	4003	BCR	C30-C25-C24	2.59	122.68	115.65
13	B	1227	CLA	O2A-CGA-CBA	2.59	122.19	114.00
16	J	4012	BCR	C33-C5-C4	-2.59	108.07	113.60
13	A	1140	CLA	C1-O2A-CGA	2.59	122.92	116.65
13	A	1112	CLA	C3B-C4B-NB	-2.59	108.22	110.53
13	A	1111	CLA	CED-O2D-CGD	2.59	121.79	115.92
13	A	1011	CLA	C1-C2-C3	2.59	130.44	126.20
16	B	4017	BCR	C8-C9-C10	-2.59	114.94	119.01
13	A	1133	CLA	O2A-CGA-O1A	-2.58	117.16	123.63
13	B	1220	CLA	C3B-C4B-NB	-2.58	108.23	110.53
13	A	1402	CLA	O2A-CGA-CBA	2.58	122.15	114.00
13	B	1208	CLA	O2A-CGA-CBA	2.58	122.14	114.00
13	B	1228	CLA	CED-O2D-CGD	2.58	121.76	115.92
13	A	1111	CLA	C1-C2-C3	2.57	130.41	126.20
13	B	1212	CLA	O2A-CGA-CBA	2.57	122.13	114.00
13	B	1211	CLA	C3B-C4B-NB	-2.57	108.23	110.53
13	B	1209	CLA	C3B-C4B-NB	-2.57	108.23	110.53
16	B	4014	BCR	C35-C13-C12	2.57	122.01	118.09
16	B	4017	BCR	C34-C9-C8	2.57	122.01	118.09
13	A	1105	CLA	C1-C2-C3	2.57	130.41	126.20
13	A	1138	CLA	O2D-CGD-CBD	2.57	115.72	111.23
13	A	1022	CLA	O2A-CGA-CBA	2.57	119.66	111.83
13	A	1120	CLA	CED-O2D-CGD	2.56	121.73	115.92
13	A	1126	CLA	CAA-C2A-C3A	-2.56	106.08	113.00
13	B	1226	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
13	B	1234	CLA	C3B-C4B-NB	-2.56	108.25	110.53
13	A	1134	CLA	O2A-CGA-CBA	2.56	122.08	114.00
13	A	1111	CLA	C4D-CHA-C1A	2.55	124.29	121.24
16	M	4021	BCR	C33-C5-C4	-2.55	108.15	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1226	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
13	B	1233	CLA	C3B-C4B-NB	-2.55	108.25	110.53
13	B	1229	CLA	C1-C2-C3	2.55	130.38	126.20
13	A	1117	CLA	C4D-CHA-C1A	2.55	124.28	121.24
13	A	1119	CLA	O2A-CGA-CBA	2.55	119.61	111.83
13	A	1132	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
13	B	1238	CLA	C4D-CHA-C1A	2.55	124.28	121.24
16	I	4020	BCR	C29-C30-C25	2.55	114.14	110.44
13	L	1501	CLA	C3B-C4B-NB	-2.55	108.26	110.53
13	A	1113	CLA	O1D-CGD-CBD	-2.55	119.50	124.52
16	I	4020	BCR	C36-C18-C19	2.55	121.98	118.09
13	A	1113	CLA	CED-O2D-CGD	2.54	121.67	115.92
16	I	4018	BCR	C33-C5-C4	-2.54	108.18	113.60
13	A	1139	CLA	C1-C2-C3	2.54	130.36	126.20
13	A	1140	CLA	C1-C2-C3	2.53	130.35	126.20
13	B	1215	CLA	CED-O2D-CGD	2.53	121.66	115.92
13	B	1201	CLA	O1D-CGD-CBD	-2.53	119.53	124.52
16	B	4009	BCR	C30-C25-C26	-2.53	119.18	122.64
16	A	4007	BCR	C32-C1-C6	2.53	114.20	110.24
16	L	4022	BCR	C38-C26-C27	-2.53	108.21	113.60
13	B	1232	CLA	O2D-CGD-CBD	2.52	115.64	111.23
13	A	1119	CLA	C12-C11-C10	-2.52	101.97	113.28
13	B	1207	CLA	C1-C2-C3	2.52	130.32	126.20
13	L	1503	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	J	4012	BCR	C35-C13-C12	2.52	121.94	118.09
13	B	1012	CLA	C2A-C1A-CHA	2.52	128.24	123.87
13	A	1119	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
16	A	4002	BCR	C23-C24-C25	2.52	133.72	127.00
13	A	1137	CLA	CED-O2D-CGD	2.52	121.62	115.92
13	B	1225	CLA	C5-C3-C2	2.51	126.81	121.17
13	A	1117	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
13	B	1214	CLA	C1-C2-C3	2.51	130.31	126.20
13	A	1132	CLA	CED-O2D-CGD	2.51	121.60	115.92
16	J	4013	BCR	C38-C26-C27	-2.51	108.25	113.60
13	A	1103	CLA	CHD-C1D-ND	-2.51	121.28	124.80
16	A	4002	BCR	C7-C8-C9	2.51	129.94	126.23
13	A	1103	CLA	O1D-CGD-CBD	-2.51	119.58	124.52
16	A	4008	BCR	C37-C22-C23	2.50	121.91	118.09
13	A	1126	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
13	B	1222	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
13	B	1208	CLA	C3B-C4B-NB	-2.50	108.30	110.53
13	B	1213	CLA	O2A-CGA-O1A	-2.50	117.38	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	4007	BCR	C23-C24-C25	2.50	133.67	127.00
18	B	5002	LMG	C7-O1-C1	2.50	119.15	113.80
13	A	1128	CLA	C3B-C4B-NB	-2.50	108.30	110.53
13	B	1213	CLA	CED-O2D-CGD	2.50	121.58	115.92
16	A	4011	BCR	C1-C6-C5	-2.50	119.22	122.64
13	B	1202	CLA	CED-O2D-CGD	2.49	121.57	115.92
16	I	4018	BCR	C30-C25-C26	-2.49	119.23	122.64
16	B	4010	BCR	C1-C6-C5	-2.49	119.23	122.64
13	B	1012	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
13	A	1106	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
16	A	4007	BCR	C1-C6-C7	2.49	122.40	115.65
13	B	1211	CLA	CED-O2D-CGD	2.49	121.56	115.92
16	L	4019	BCR	C36-C18-C19	2.49	121.89	118.09
13	B	1222	CLA	C2A-C3A-C4A	2.49	105.89	101.87
13	A	1801	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
16	A	4002	BCR	C24-C23-C22	2.48	129.91	126.23
13	A	1104	CLA	C2A-C1A-CHA	2.48	128.18	123.87
13	B	1217	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
13	B	1236	CLA	CED-O2D-CGD	2.48	121.54	115.92
13	K	1401	CLA	CED-O2D-CGD	2.48	121.54	115.92
16	A	4001	BCR	C1-C6-C7	2.48	122.37	115.65
13	A	1108	CLA	C3B-C4B-NB	-2.47	108.32	110.53
13	A	1013	CLA	C1-C2-C3	2.47	130.24	126.20
16	J	4015	BCR	C30-C25-C24	2.47	122.34	115.65
16	B	4014	BCR	C36-C18-C19	2.46	121.85	118.09
13	A	1117	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
16	B	4004	BCR	C8-C7-C6	2.46	133.57	127.00
13	A	1118	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
13	B	1206	CLA	C12-C11-C10	-2.46	102.26	113.28
13	A	1122	CLA	C3B-C4B-NB	-2.46	108.34	110.53
13	B	1021	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
13	A	1123	CLA	CED-O2D-CGD	2.46	121.49	115.92
13	A	1126	CLA	CED-O2D-CGD	2.46	121.49	115.92
13	F	1301	CLA	CED-O2D-CGD	2.46	121.48	115.92
16	A	4011	BCR	C23-C22-C21	-2.46	115.15	119.01
13	B	1232	CLA	O2A-CGA-CBA	2.45	121.75	114.00
13	B	1215	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
16	I	4020	BCR	C1-C6-C5	-2.45	119.29	122.64
16	B	4017	BCR	C23-C24-C25	2.45	133.53	127.00
13	B	1231	CLA	C3B-C4B-NB	-2.44	108.35	110.53
13	B	1215	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
13	A	1135	CLA	C4D-CHA-C1A	2.44	124.15	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	4007	BCR	C40-C30-C25	2.44	114.06	110.24
13	B	1204	CLA	CED-O2D-CGD	2.43	121.44	115.92
13	A	1013	CLA	CHD-C1D-ND	-2.43	121.38	124.80
13	A	1109	CLA	C1-C2-C3	2.43	130.18	126.20
13	B	1214	CLA	C3B-C4B-NB	-2.43	108.36	110.53
13	B	1201	CLA	CMD-C2D-C1D	2.43	129.01	124.73
13	B	1234	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
13	K	1401	CLA	O2A-CGA-CBA	2.43	121.67	114.00
13	A	1137	CLA	C3B-C4B-NB	-2.43	108.36	110.53
16	A	4008	BCR	C34-C9-C8	2.43	121.79	118.09
16	A	4002	BCR	C1-C6-C7	2.42	122.23	115.65
13	A	1130	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
13	B	1233	CLA	CED-O2D-CGD	2.42	121.40	115.92
13	L	1502	CLA	C4D-CHA-C1A	2.42	124.13	121.24
13	A	1136	CLA	O2D-CGD-CBD	2.42	115.46	111.23
13	B	1211	CLA	CMD-C2D-C1D	2.42	128.98	124.73
16	A	4007	BCR	C1-C6-C5	-2.41	119.34	122.64
13	A	1127	CLA	CED-O2D-CGD	2.41	121.39	115.92
16	F	4016	BCR	C7-C8-C9	2.41	129.81	126.23
13	B	1205	CLA	C7-C6-C5	-2.41	106.83	113.26
13	A	1103	CLA	C1-C2-C3	2.41	130.15	126.20
16	J	4012	BCR	C24-C23-C22	2.41	129.80	126.23
13	B	1229	CLA	C12-C11-C10	-2.41	102.47	113.28
13	A	1128	CLA	CED-O2D-CGD	2.41	121.38	115.92
13	B	1218	CLA	C4D-CHA-C1A	2.41	124.12	121.24
13	A	1237	CLA	CED-O2D-CGD	2.41	121.38	115.92
13	A	1122	CLA	CAA-C2A-C3A	-2.40	106.50	113.00
13	B	1203	CLA	CED-O2D-CGD	2.40	121.36	115.92
13	L	1501	CLA	C4D-CHA-C1A	2.40	124.10	121.24
13	A	1013	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
13	B	1231	CLA	O2A-CGA-CBA	2.39	121.55	114.00
16	A	4003	BCR	C8-C7-C6	2.39	133.38	127.00
13	A	1137	CLA	CMD-C2D-C1D	2.38	128.93	124.73
16	I	4020	BCR	C1-C6-C7	2.38	122.12	115.65
16	J	4013	BCR	C40-C30-C25	2.38	113.98	110.24
13	B	1221	CLA	C2A-C1A-CHA	2.38	128.00	123.87
13	B	1227	CLA	CED-O2D-CGD	2.38	121.31	115.92
16	B	4006	BCR	C28-C27-C26	2.38	118.29	114.06
13	K	1401	CLA	C3B-C4B-NB	-2.38	108.41	110.53
16	B	4017	BCR	C30-C25-C26	-2.38	119.39	122.64
16	L	4019	BCR	C1-C6-C5	-2.38	119.39	122.64
13	A	1103	CLA	C2A-C3A-C4A	2.37	105.70	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1225	CLA	C3B-C4B-NB	-2.37	108.42	110.53
13	B	1232	CLA	O2A-CGA-O1A	-2.37	117.24	123.33
16	L	4022	BCR	C30-C25-C24	2.37	122.07	115.65
13	B	1231	CLA	C2A-C3A-C4A	2.37	105.69	101.87
13	A	1011	CLA	CAA-C2A-C3A	-2.37	106.61	113.00
13	A	1120	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
16	L	4019	BCR	C23-C24-C25	2.36	133.31	127.00
16	F	4016	BCR	C30-C25-C24	2.36	122.04	115.65
13	B	1211	CLA	CAA-C2A-C3A	-2.36	106.63	113.00
13	A	1136	CLA	CED-O2D-CGD	2.36	121.26	115.92
13	A	1110	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
13	B	1201	CLA	C1-C2-C3	2.36	130.06	126.20
13	A	1129	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
13	A	1011	CLA	C2A-C3A-C4A	2.35	105.67	101.87
13	B	1224	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
13	A	1103	CLA	CMD-C2D-C1D	2.35	128.87	124.73
16	A	4008	BCR	C8-C9-C10	-2.35	115.32	119.01
16	B	4004	BCR	C1-C6-C7	2.35	122.02	115.65
13	A	1801	CLA	C2A-C1A-CHA	2.35	127.94	123.87
16	B	4009	BCR	C30-C25-C24	2.34	122.01	115.65
13	A	1237	CLA	C3B-C4B-NB	-2.34	108.44	110.53
13	A	1237	CLA	CMA-C3A-C2A	-2.34	104.92	113.98
16	B	4005	BCR	C35-C13-C12	2.34	121.67	118.09
13	B	1227	CLA	CMD-C2D-C1D	2.34	128.85	124.73
13	B	1234	CLA	C4D-CHA-C1A	2.34	124.03	121.24
13	A	1101	CLA	C1-C2-C3	2.34	130.03	126.20
13	B	1222	CLA	O2A-CGA-CBA	2.34	120.97	112.14
13	B	1234	CLA	CED-O2D-CGD	2.34	121.22	115.92
16	B	4017	BCR	C24-C23-C22	2.34	129.69	126.23
13	A	1130	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
13	B	1023	CLA	C12-C11-C10	-2.34	102.81	113.28
13	B	1221	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
16	B	4006	BCR	C30-C25-C24	2.33	121.98	115.65
13	A	1118	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
13	B	1222	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
13	B	1225	CLA	CBA-CAA-C2A	2.33	120.73	113.79
16	A	4008	BCR	C1-C6-C5	-2.33	119.45	122.64
13	A	1104	CLA	CAA-CBA-CGA	2.33	119.81	113.21
13	F	1301	CLA	C2A-C1A-CHA	2.33	127.90	123.87
13	B	1222	CLA	CED-O2D-CGD	2.32	121.19	115.92
16	B	4005	BCR	C34-C9-C8	2.32	121.64	118.09
16	J	4013	BCR	C1-C6-C7	2.32	121.95	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1214	CLA	CAA-C2A-C3A	-2.32	106.72	113.00
13	J	1302	CLA	C2A-C1A-CHA	2.32	127.89	123.87
13	A	1011	CLA	C2D-C1D-ND	2.32	112.42	110.13
13	B	1021	CLA	C3B-C4B-NB	-2.32	108.46	110.53
13	A	1128	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
13	A	1112	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
13	A	1125	CLA	C4D-CHA-C1A	2.31	124.00	121.24
16	B	4005	BCR	C36-C18-C19	2.31	121.62	118.09
16	I	4018	BCR	C1-C6-C7	2.31	121.92	115.65
13	A	1121	CLA	C3B-C4B-NB	-2.31	108.47	110.53
13	A	1118	CLA	CED-O2D-CGD	2.31	121.15	115.92
13	J	1303	CLA	CMA-C3A-C2A	-2.31	110.94	116.23
13	B	1230	CLA	C4D-CHA-C1A	2.31	124.00	121.24
13	A	1118	CLA	C4D-CHA-C1A	2.30	123.99	121.24
16	A	4008	BCR	C33-C5-C4	-2.30	108.68	113.60
16	A	4008	BCR	C8-C7-C6	2.30	133.15	127.00
13	B	1217	CLA	C2A-C1A-CHA	2.30	127.86	123.87
13	L	1502	CLA	CHD-C1D-ND	-2.30	121.56	124.80
13	A	1105	CLA	C4-C3-C5	-2.30	113.42	116.13
16	I	4018	BCR	C34-C9-C8	2.30	121.60	118.09
13	A	1121	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
13	A	1125	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
13	A	1136	CLA	CHD-C1D-ND	-2.30	121.57	124.80
13	A	1117	CLA	C1-C2-C3	2.30	129.96	126.20
16	A	4001	BCR	C37-C22-C23	2.29	121.59	118.09
16	B	4014	BCR	C1-C6-C5	-2.29	119.50	122.64
16	A	4001	BCR	C35-C13-C12	2.29	121.59	118.09
16	B	4017	BCR	C1-C6-C5	-2.29	119.51	122.64
16	B	4010	BCR	C1-C6-C7	2.29	121.86	115.65
16	B	4006	BCR	C34-C9-C8	2.29	121.58	118.09
13	A	1013	CLA	O2D-CGD-CBD	2.29	115.23	111.23
13	A	1011	CLA	CHA-C4D-ND	2.29	137.27	132.55
13	A	1116	CLA	C1-C2-C3	2.29	129.94	126.20
16	A	4001	BCR	C32-C1-C6	2.29	113.83	110.24
16	I	4020	BCR	C3-C4-C5	2.28	118.13	114.06
16	B	4006	BCR	C36-C18-C19	2.28	121.58	118.09
13	B	1230	CLA	CMD-C2D-C1D	2.28	128.75	124.73
13	B	1208	CLA	O2A-CGA-O1A	-2.28	117.46	123.33
16	A	4011	BCR	C34-C9-C8	2.28	121.57	118.09
16	B	4009	BCR	C36-C18-C19	2.28	121.57	118.09
13	B	1218	CLA	C2A-C1A-CHA	2.28	127.83	123.87
13	A	1122	CLA	O2A-CGA-O1A	-2.28	117.92	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	1502	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
16	B	4006	BCR	C1-C6-C7	2.28	121.83	115.65
13	B	1227	CLA	C4D-CHA-C1A	2.28	123.96	121.24
13	A	1138	CLA	C4D-CHA-C1A	2.28	123.96	121.24
13	A	1112	CLA	O2A-CGA-O1A	-2.27	117.49	123.33
16	J	4012	BCR	C37-C22-C23	2.27	121.56	118.09
13	A	1402	CLA	O2A-CGA-O1A	-2.27	117.49	123.33
13	A	1139	CLA	CED-O2D-CGD	2.27	121.07	115.92
13	A	1123	CLA	C4D-CHA-C1A	2.27	123.95	121.24
16	J	4013	BCR	C24-C23-C22	2.27	129.59	126.23
13	B	1226	CLA	CED-O2D-CGD	2.27	121.06	115.92
13	X	1701	CLA	CED-O2D-CGD	2.27	121.06	115.92
13	B	1236	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
13	A	1122	CLA	C4D-CHA-C1A	2.27	123.95	121.24
13	A	1102	CLA	C3B-C4B-NB	-2.27	108.51	110.53
13	A	1107	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
13	B	1221	CLA	C4D-CHA-C1A	2.26	123.94	121.24
13	A	1110	CLA	C4D-CHA-C1A	2.26	123.94	121.24
13	A	1105	CLA	C3B-C4B-NB	-2.26	108.51	110.53
13	B	1230	CLA	C3B-C4B-NB	-2.26	108.51	110.53
13	B	1207	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
13	B	1223	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
13	A	1113	CLA	C4D-CHA-C1A	2.26	123.94	121.24
13	B	1232	CLA	C2A-C1A-CHA	2.26	127.79	123.87
13	A	1022	CLA	C6-C5-C3	-2.26	107.97	113.47
16	L	4022	BCR	C23-C24-C25	2.26	133.03	127.00
13	A	1115	CLA	C3B-C4B-NB	-2.26	108.52	110.53
13	A	1102	CLA	CED-O2D-CGD	2.26	121.03	115.92
16	J	4013	BCR	C35-C13-C12	2.26	121.53	118.09
16	F	4016	BCR	C8-C7-C6	2.25	133.02	127.00
16	J	4013	BCR	C34-C9-C8	2.25	121.53	118.09
13	M	1601	CLA	O2A-CGA-O1A	-2.25	117.53	123.33
13	B	1234	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
13	A	1120	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
13	A	1129	CLA	C1-C2-C3	2.25	130.40	126.76
16	A	4002	BCR	C40-C30-C25	2.25	113.77	110.24
13	B	1227	CLA	CHD-C1D-ND	-2.25	121.64	124.80
13	B	1217	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
16	A	4008	BCR	C23-C22-C21	-2.25	115.47	119.01
16	F	4016	BCR	C1-C6-C7	2.24	121.74	115.65
13	A	1129	CLA	CHD-C1D-ND	-2.24	121.65	124.80
13	A	1134	CLA	O2A-CGA-O1A	-2.24	117.57	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1117	CLA	C4-C3-C5	-2.24	111.34	115.23
13	B	1012	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
13	B	1224	CLA	CAA-CBA-CGA	2.23	119.55	113.21
13	A	1135	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
16	L	4019	BCR	C37-C22-C23	2.23	121.49	118.09
14	B	2002	PQN	C17-C16-C15	-2.23	107.33	113.26
13	A	1139	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
13	A	1110	CLA	CED-O2D-CGD	2.22	120.96	115.92
13	L	1501	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
16	B	4010	BCR	C23-C24-C25	2.22	132.93	127.00
13	B	1235	CLA	C4D-CHA-C1A	2.22	123.89	121.24
16	A	4008	BCR	C7-C8-C9	2.22	129.52	126.23
16	B	4017	BCR	C23-C22-C21	-2.22	115.52	119.01
16	A	4011	BCR	C37-C22-C23	2.22	121.47	118.09
16	I	4018	BCR	C19-C18-C17	-2.22	115.52	119.01
16	A	4003	BCR	C35-C13-C12	2.21	121.47	118.09
13	B	1230	CLA	CHD-C1D-ND	-2.21	121.69	124.80
13	L	1501	CLA	CHB-C1B-NB	2.21	127.37	124.05
16	B	4014	BCR	C24-C23-C22	2.21	129.50	126.23
13	B	1236	CLA	C3B-C4B-NB	-2.21	108.56	110.53
13	J	1302	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
16	I	4020	BCR	C19-C18-C17	-2.21	115.54	119.01
13	A	1116	CLA	CBA-CAA-C2A	2.21	120.36	113.79
16	M	4021	BCR	C35-C13-C12	2.21	121.46	118.09
16	B	4006	BCR	C40-C30-C25	2.21	113.70	110.24
13	B	1206	CLA	C1-C2-C3	2.20	129.81	126.20
13	B	1231	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
16	M	4021	BCR	C30-C25-C24	2.20	121.62	115.65
16	B	4005	BCR	C8-C7-C6	2.20	132.88	127.00
13	A	1133	CLA	C4D-CHA-C1A	2.20	123.87	121.24
13	A	1123	CLA	C1-C2-C3	2.20	129.80	126.20
13	A	1102	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
14	B	2002	PQN	C11-C3-C2	-2.20	121.12	124.89
13	A	1109	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
13	A	1126	CLA	CMD-C2D-C1D	2.19	128.59	124.73
13	B	1223	CLA	CED-O2D-CGD	2.19	120.89	115.92
13	B	1231	CLA	CHD-C1D-ND	-2.19	121.72	124.80
13	B	1220	CLA	C4D-CHA-C1A	2.19	123.86	121.24
13	L	1501	CLA	C12-C11-C10	-2.19	103.46	113.28
13	B	1205	CLA	CED-O2D-CGD	2.19	120.89	115.92
13	A	1118	CLA	C2A-C1A-CHA	2.19	127.67	123.87
13	A	1121	CLA	C4-C3-C5	-2.19	113.55	116.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1235	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
16	A	4001	BCR	C30-C25-C24	2.19	121.58	115.65
13	B	1233	CLA	C2A-C1A-CHA	2.19	127.66	123.87
13	B	1239	CLA	CED-O2D-CGD	2.18	120.87	115.92
13	B	1201	CLA	CAA-C2A-C3A	-2.18	107.10	113.00
13	B	1239	CLA	CBA-CAA-C2A	2.18	120.29	113.79
13	A	1131	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	B	4010	BCR	C34-C9-C8	2.18	121.42	118.09
13	B	1204	CLA	C1-C2-C3	2.18	129.77	126.20
13	A	1140	CLA	C12-C11-C10	-2.18	103.52	113.28
16	B	4014	BCR	C40-C30-C25	2.18	113.66	110.24
13	B	1207	CLA	CAA-C2A-C1A	2.18	119.11	111.97
16	L	4022	BCR	C32-C1-C6	2.18	113.65	110.24
13	A	1022	CLA	CED-O2D-CGD	2.17	120.84	115.92
16	B	4017	BCR	C15-C14-C13	2.17	130.32	127.28
16	B	4017	BCR	C30-C25-C24	2.17	121.53	115.65
13	A	1106	CLA	CED-O2D-CGD	2.17	120.83	115.92
13	B	1209	CLA	C4D-CHA-C1A	2.17	123.83	121.24
13	B	1214	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
13	A	1120	CLA	CHD-C1D-ND	-2.17	121.75	124.80
16	I	4018	BCR	C32-C1-C6	2.16	113.64	110.24
16	B	4004	BCR	C34-C9-C8	2.16	121.39	118.09
13	B	1206	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
13	A	1116	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
13	A	1112	CLA	C4D-CHA-C1A	2.16	123.82	121.24
13	A	1137	CLA	C4D-CHA-C1A	2.16	123.82	121.24
16	B	4017	BCR	C11-C10-C9	2.15	130.30	127.28
13	A	1131	CLA	CED-O2D-CGD	2.15	120.80	115.92
13	B	1223	CLA	C4D-CHA-C1A	2.15	123.81	121.24
13	M	1601	CLA	C2A-C1A-CHA	2.15	127.60	123.87
13	B	1202	CLA	C2A-C3A-C4A	2.15	105.34	101.87
13	L	1502	CLA	C6-C5-C3	-2.15	108.23	113.47
13	A	1138	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
13	B	1235	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
13	A	1105	CLA	C4D-CHA-C1A	2.15	123.80	121.24
16	F	4016	BCR	C36-C18-C19	2.15	121.36	118.09
13	B	1238	CLA	C12-C11-C10	-2.14	103.67	113.28
13	A	1135	CLA	C2A-C1A-CHA	2.14	127.59	123.87
16	B	4004	BCR	C37-C22-C23	2.14	121.36	118.09
13	A	1130	CLA	C2A-C3A-C4A	2.14	105.33	101.87
13	B	1231	CLA	CMA-C3A-C2A	-2.14	105.69	113.98
13	B	1201	CLA	O2A-CGA-O1A	-2.14	118.27	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	1301	CLA	O2A-CGA-O1A	-2.14	117.82	123.33
13	A	1122	CLA	C1-C2-C3	2.14	129.71	126.20
13	A	1136	CLA	CMD-C2D-C1D	2.14	128.50	124.73
13	B	1224	CLA	CED-O2D-CGD	2.14	120.77	115.92
16	M	4021	BCR	C37-C22-C23	2.14	121.36	118.09
13	A	1134	CLA	C2A-C1A-CHA	2.14	127.58	123.87
13	A	1113	CLA	CAA-C2A-C3A	-2.14	107.23	113.00
16	J	4013	BCR	C15-C14-C13	2.13	130.27	127.28
13	A	1134	CLA	CHD-C1D-ND	-2.13	121.80	124.80
13	B	1207	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
13	B	1238	CLA	CMD-C2D-C1D	2.13	128.49	124.73
16	A	4002	BCR	C35-C13-C12	2.13	121.34	118.09
13	A	1131	CLA	CMD-C2D-C1D	2.13	128.48	124.73
16	A	4002	BCR	C32-C1-C6	2.13	113.58	110.24
13	A	1107	CLA	C1-C2-C3	2.13	129.69	126.20
13	A	1122	CLA	CED-O2D-CGD	2.13	120.75	115.92
13	A	1117	CLA	CBA-CAA-C2A	2.13	120.13	113.79
13	A	1111	CLA	C2A-C1A-CHA	2.13	127.56	123.87
13	A	1107	CLA	C4D-CHA-C1A	2.13	123.78	121.24
13	A	1112	CLA	C2A-C1A-CHA	2.13	127.56	123.87
16	J	4015	BCR	C40-C30-C25	2.13	113.58	110.24
16	M	4021	BCR	C32-C1-C6	2.13	113.58	110.24
16	I	4020	BCR	C35-C13-C12	2.12	121.33	118.09
16	F	4016	BCR	C40-C30-C25	2.12	113.58	110.24
13	B	1210	CLA	C2A-C1A-CHA	2.12	127.55	123.87
13	A	1138	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
16	B	4004	BCR	C20-C21-C22	2.12	130.25	127.28
16	A	4002	BCR	C15-C14-C13	2.12	130.25	127.28
13	A	1131	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
13	A	1131	CLA	C4D-CHA-C1A	2.12	123.77	121.24
16	J	4015	BCR	C16-C17-C18	2.12	130.25	127.28
13	B	1239	CLA	C3B-C4B-NB	-2.12	108.64	110.53
13	A	1011	CLA	CMA-C3A-C2A	-2.12	105.80	113.98
16	B	4006	BCR	C20-C21-C22	2.11	130.24	127.28
13	B	1224	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
13	A	1120	CLA	C2A-C3A-C4A	2.11	105.28	101.87
13	A	1102	CLA	C1-C2-C3	2.11	129.66	126.20
13	B	1232	CLA	C4D-CHA-C1A	2.11	123.77	121.24
16	I	4018	BCR	C30-C25-C24	2.11	121.38	115.65
16	J	4015	BCR	C37-C22-C23	2.11	121.31	118.09
13	X	1701	CLA	O2A-CGA-O1A	-2.11	117.91	123.33
13	A	1102	CLA	C2A-C1A-CHA	2.11	127.53	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	4005	BCR	C15-C14-C13	2.11	130.23	127.28
13	B	1230	CLA	CBA-CAA-C2A	2.11	120.06	113.79
13	J	1303	CLA	OBD-CAD-CBD	-2.11	121.71	125.94
13	A	1123	CLA	C2A-C1A-CHA	2.11	127.52	123.87
16	B	4006	BCR	C32-C1-C6	2.11	113.55	110.24
13	B	1233	CLA	O2A-CGA-O1A	-2.10	117.92	123.33
13	A	1124	CLA	CED-O2D-CGD	2.10	120.69	115.92
13	A	1104	CLA	O2D-CGD-CBD	2.10	114.91	111.23
16	J	4013	BCR	C19-C18-C17	-2.10	115.70	119.01
13	A	1107	CLA	CMD-C2D-C1D	2.10	128.43	124.73
13	A	1140	CLA	CMD-C2D-C1D	2.10	128.43	124.73
16	B	4014	BCR	C30-C25-C24	2.10	121.35	115.65
13	B	1209	CLA	O2A-CGA-O1A	-2.10	117.93	123.33
13	B	1203	CLA	CMD-C2D-C1D	2.10	128.42	124.73
13	A	1402	CLA	C2A-C3A-C4A	2.10	105.26	101.87
13	A	1108	CLA	O2A-CGA-O1A	-2.10	117.94	123.33
16	B	4010	BCR	C19-C18-C17	-2.10	115.71	119.01
13	B	1229	CLA	CHD-C1D-ND	-2.09	121.86	124.80
13	B	1226	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
13	A	1120	CLA	C2A-C1A-CHA	2.09	127.50	123.87
13	A	1122	CLA	CMD-C2D-C1D	2.09	128.41	124.73
13	B	1222	CLA	CMD-C2D-C1D	2.09	128.41	124.73
13	B	1224	CLA	CHB-C1B-NB	2.09	127.19	124.05
13	B	1215	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
13	A	1140	CLA	CBA-CAA-C2A	2.09	120.01	113.79
13	A	1107	CLA	CBA-CAA-C2A	2.09	120.00	113.79
16	I	4020	BCR	C23-C24-C25	2.09	132.57	127.00
13	B	1216	CLA	C4D-CHA-C1A	2.09	123.73	121.24
13	A	1128	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
13	B	1227	CLA	O2A-CGA-O1A	-2.08	117.98	123.33
13	A	1013	CLA	C2A-C3A-C4A	2.08	105.23	101.87
16	B	4005	BCR	C30-C25-C24	2.08	121.29	115.65
13	A	1139	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
13	B	1224	CLA	C12-C11-C10	-2.08	103.96	113.28
16	B	4014	BCR	C11-C10-C9	2.08	130.19	127.28
13	B	1239	CLA	C4D-CHA-C1A	2.08	123.72	121.24
13	A	1132	CLA	CMD-C2D-C1D	2.07	128.38	124.73
16	L	4022	BCR	C1-C6-C7	2.07	121.27	115.65
13	A	1013	CLA	CMA-C3A-C2A	-2.07	105.97	113.98
16	J	4015	BCR	C23-C24-C25	2.07	132.53	127.00
13	B	1212	CLA	C2A-C1A-CHA	2.07	127.46	123.87
13	A	1123	CLA	C7-C6-C5	-2.07	107.74	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1202	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
13	L	1501	CLA	CMD-C2D-C1D	2.07	128.37	124.73
13	A	1132	CLA	C1-C2-C3	2.07	129.59	126.20
13	A	1131	CLA	C2A-C3A-C4A	2.07	105.21	101.87
13	A	1136	CLA	C3B-C4B-NB	-2.07	108.68	110.53
13	A	1109	CLA	C2D-C1D-ND	2.07	112.17	110.13
13	A	1121	CLA	CMD-C2D-C1D	2.07	128.37	124.73
13	A	1109	CLA	CHD-C1D-ND	-2.07	121.89	124.80
16	J	4012	BCR	C32-C1-C2	-2.07	101.02	108.95
13	A	1127	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
13	X	1701	CLA	C2A-C1A-CHA	2.06	127.45	123.87
13	A	1117	CLA	C2A-C1A-CHA	2.06	127.45	123.87
16	A	4003	BCR	C37-C22-C23	2.06	121.24	118.09
16	A	4007	BCR	C8-C7-C6	2.06	132.51	127.00
16	A	4003	BCR	C15-C14-C13	2.06	130.17	127.28
13	B	1235	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
13	B	1223	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	A	4008	BCR	C30-C25-C24	2.06	121.24	115.65
13	A	1402	CLA	C3B-C4B-NB	-2.06	108.69	110.53
13	A	1114	CLA	C2A-C1A-CHA	2.06	127.44	123.87
13	B	1012	CLA	C1-C2-C3	2.06	129.57	126.20
13	A	1103	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
13	L	1503	CLA	CHD-C1D-ND	-2.06	121.91	124.80
13	B	1227	CLA	C3C-C4C-NC	-2.06	107.80	110.43
13	A	1111	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
13	B	1218	CLA	O2A-CGA-O1A	-2.05	118.05	123.33
13	A	1107	CLA	CHB-C1B-NB	2.05	127.13	124.05
13	L	1503	CLA	C4D-CHA-C1A	2.05	123.69	121.24
16	B	4010	BCR	C20-C21-C22	2.05	130.16	127.28
13	B	1207	CLA	C3A-C2A-C1A	2.05	104.41	101.34
13	B	1212	CLA	C2D-C1D-ND	2.05	112.16	110.13
13	B	1012	CLA	CHA-C1A-NA	-2.05	121.75	126.39
13	B	1202	CLA	CHD-C1D-ND	-2.05	121.92	124.80
13	A	1113	CLA	C2A-C1A-CHA	2.05	127.42	123.87
13	A	1022	CLA	CHB-C1B-NB	2.05	127.12	124.05
13	B	1214	CLA	C2A-C1A-CHA	2.05	127.42	123.87
13	B	1225	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
13	B	1233	CLA	C4D-CHA-C1A	2.05	123.69	121.24
13	B	1021	CLA	O2D-CGD-CBD	2.05	114.81	111.23
13	A	1124	CLA	C4D-CHA-C1A	2.05	123.69	121.24
13	A	1101	CLA	CMD-C2D-C1D	2.05	128.33	124.73
13	B	1231	CLA	O2A-CGA-O1A	-2.05	118.07	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1114	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
13	A	1139	CLA	C3B-C4B-NB	-2.05	108.70	110.53
13	A	1125	CLA	C2A-C3A-C4A	2.05	105.17	101.87
16	B	4004	BCR	C40-C30-C25	2.05	113.45	110.24
13	A	1114	CLA	C4D-CHA-C1A	2.04	123.68	121.24
13	A	1125	CLA	CMD-C2D-C1D	2.04	128.33	124.73
13	B	1208	CLA	CMD-C2D-C1D	2.04	128.33	124.73
13	A	1137	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
13	A	1139	CLA	C2A-C1A-CHA	2.04	127.41	123.87
13	A	1011	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
13	A	1113	CLA	O2A-CGA-O1A	-2.04	118.08	123.33
13	A	1101	CLA	C2A-C1A-CHA	2.04	127.41	123.87
13	A	1011	CLA	CGD-CBD-CAD	2.04	117.46	110.85
13	B	1208	CLA	CHD-C1D-ND	-2.04	121.93	124.80
16	A	4003	BCR	C34-C9-C8	2.04	121.21	118.09
13	A	1106	CLA	C4D-CHA-C1A	2.04	123.68	121.24
17	B	5004	LHG	O8-C23-C24	2.04	121.03	112.38
16	B	4004	BCR	C35-C13-C12	2.04	121.20	118.09
16	J	4012	BCR	C19-C18-C17	-2.04	115.80	119.01
16	A	4007	BCR	C36-C18-C19	2.04	121.20	118.09
13	A	1124	CLA	CHD-C1D-ND	-2.04	121.94	124.80
13	A	1133	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
13	B	1223	CLA	C12-C11-C10	-2.04	104.15	113.28
13	B	1204	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
13	B	1209	CLA	CHD-C1D-ND	-2.03	121.94	124.80
13	A	1116	CLA	C2A-C1A-CHA	2.03	127.40	123.87
13	B	1215	CLA	C1-C2-C3	2.03	129.53	126.20
13	A	1111	CLA	CMD-C2D-C1D	2.03	128.30	124.73
13	B	1021	CLA	CMA-C3A-C2A	-2.03	106.14	113.98
13	A	1123	CLA	CMD-C2D-C1D	2.03	128.30	124.73
13	B	1226	CLA	CAA-C2A-C3A	-2.03	107.53	113.00
13	A	1121	CLA	CED-O2D-CGD	2.03	120.51	115.92
16	B	4017	BCR	C8-C7-C6	2.03	132.41	127.00
16	I	4020	BCR	C2-C1-C6	2.02	113.38	110.44
16	A	4003	BCR	C32-C1-C6	2.02	113.42	110.24
13	B	1207	CLA	CMD-C2D-C1D	2.02	128.29	124.73
13	A	1011	CLA	C3B-C4B-NB	-2.02	108.72	110.53
13	A	1115	CLA	CHD-C1D-ND	-2.02	121.95	124.80
13	F	1301	CLA	C4D-CHA-C1A	2.02	123.66	121.24
14	B	2002	PQN	C22-C21-C20	-2.02	104.22	113.28
13	L	1503	CLA	CED-O2D-CGD	2.02	120.50	115.92
16	B	4014	BCR	C1-C6-C7	2.02	121.13	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	4003	BCR	C36-C18-C19	2.02	121.17	118.09
13	B	1225	CLA	CHD-C1D-ND	-2.02	121.96	124.80
13	B	1214	CLA	C2A-C3A-C4A	2.02	105.13	101.87
13	M	1601	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
13	A	1113	CLA	CHD-C1D-ND	-2.02	121.96	124.80
16	A	4002	BCR	C8-C7-C6	2.02	132.39	127.00
13	A	1124	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
16	A	4007	BCR	C40-C30-C29	-2.02	101.20	108.95
13	X	1701	CLA	C2A-C3A-C4A	2.02	105.13	101.87
16	A	4003	BCR	C23-C24-C25	2.02	132.39	127.00
13	B	1204	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
13	B	1202	CLA	CMA-C3A-C2A	-2.01	106.19	113.98
13	B	1231	CLA	CMA-C3A-C4A	-2.01	106.36	111.77
13	B	1204	CLA	C3C-C4C-NC	-2.01	107.85	110.43
16	B	4004	BCR	C30-C25-C24	2.01	121.11	115.65
13	A	1130	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
16	B	4017	BCR	C37-C22-C23	2.01	121.16	118.09
17	A	5003	LHG	P-O6-C4	-2.01	109.82	121.35
13	B	1236	CLA	CMD-C2D-C1D	2.01	128.27	124.73
13	B	1232	CLA	C2A-C3A-C4A	2.01	105.12	101.87
13	B	1201	CLA	CHD-C1D-ND	-2.01	121.98	124.80
13	B	1206	CLA	C2B-C1B-NB	-2.01	108.24	110.33
13	A	1129	CLA	CMD-C2D-C1D	2.01	128.26	124.73
13	B	1222	CLA	C2A-C1A-CHA	2.01	127.35	123.87
13	B	1012	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
13	A	1107	CLA	CED-O2D-CGD	2.00	120.46	115.92
13	A	1131	CLA	CHD-C1D-ND	-2.00	121.98	124.80
13	A	1124	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
13	A	1108	CLA	CMD-C2D-C1D	2.00	128.26	124.73
13	B	1215	CLA	CMD-C2D-C1D	2.00	128.26	124.73
13	A	1126	CLA	CHD-C1D-ND	-2.00	121.98	124.80
13	B	1226	CLA	C2A-C3A-C4A	2.00	105.10	101.87
16	A	4008	BCR	C32-C1-C6	2.00	113.38	110.24
13	A	1115	CLA	CMD-C2D-C1D	2.00	128.25	124.73
13	A	1111	CLA	C2A-C3A-C4A	2.00	105.10	101.87
13	B	1232	CLA	CHB-C1B-NB	2.00	127.05	124.05
13	B	1228	CLA	CHD-C1D-ND	-2.00	121.99	124.80
13	A	1129	CLA	C2C-C1C-NC	-2.00	107.88	109.98
13	B	1225	CLA	C3A-C2A-C1A	2.00	104.33	101.34

All (87) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	1011	CLA	ND
13	A	1022	CLA	ND
13	A	1013	CLA	ND
13	A	1101	CLA	ND
13	A	1102	CLA	ND
13	A	1103	CLA	ND
13	A	1104	CLA	ND
13	A	1105	CLA	ND
13	A	1106	CLA	ND
13	A	1107	CLA	ND
13	A	1109	CLA	ND
13	A	1110	CLA	ND
13	A	1111	CLA	ND
13	A	1112	CLA	ND
13	A	1113	CLA	ND
13	A	1114	CLA	ND
13	A	1116	CLA	ND
13	A	1117	CLA	ND
13	A	1118	CLA	ND
13	A	1119	CLA	ND
13	A	1120	CLA	ND
13	A	1121	CLA	ND
13	A	1122	CLA	ND
13	A	1123	CLA	ND
13	A	1124	CLA	ND
13	A	1125	CLA	ND
13	A	1126	CLA	ND
13	A	1127	CLA	ND
13	A	1128	CLA	ND
13	A	1129	CLA	ND
13	A	1130	CLA	ND
13	A	1132	CLA	ND
13	A	1133	CLA	ND
13	A	1134	CLA	ND
13	A	1135	CLA	ND
13	A	1136	CLA	ND
13	A	1137	CLA	ND
13	A	1138	CLA	ND
13	A	1139	CLA	ND
13	A	1140	CLA	ND
13	A	1237	CLA	ND
13	A	1402	CLA	ND
13	A	1801	CLA	ND

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Mol	Chain	Res	Type	Atom
13	B	1021	CLA	ND
13	B	1012	CLA	ND
13	B	1201	CLA	ND
13	B	1202	CLA	ND
13	B	1203	CLA	ND
13	B	1204	CLA	ND
13	B	1205	CLA	ND
13	B	1206	CLA	ND
13	B	1207	CLA	ND
13	B	1208	CLA	ND
13	B	1209	CLA	ND
13	B	1210	CLA	ND
13	B	1211	CLA	ND
13	B	1213	CLA	ND
13	B	1214	CLA	ND
13	B	1215	CLA	ND
13	B	1216	CLA	ND
13	B	1217	CLA	ND
13	B	1218	CLA	ND
13	B	1219	CLA	ND
13	B	1220	CLA	ND
13	B	1221	CLA	ND
13	B	1222	CLA	ND
13	B	1223	CLA	ND
13	B	1224	CLA	ND
13	B	1226	CLA	ND
13	B	1227	CLA	ND
13	B	1228	CLA	ND
13	B	1229	CLA	ND
13	B	1230	CLA	ND
13	B	1231	CLA	ND
13	B	1232	CLA	ND
13	B	1233	CLA	ND
13	B	1234	CLA	ND
13	B	1235	CLA	ND
13	B	1238	CLA	ND
13	F	1301	CLA	ND
13	J	1302	CLA	ND
13	J	1303	CLA	ND
13	L	1501	CLA	ND
13	L	1503	CLA	ND
13	M	1601	CLA	ND

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Mol	Chain	Res	Type	Atom
13	X	1701	CLA	ND
17	A	5003	LHG	C2

All (900) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1011	CLA	C2B-C3B-CAB-CBB
13	A	1011	CLA	C4B-C3B-CAB-CBB
13	A	1022	CLA	C4B-C3B-CAB-CBB
13	A	1102	CLA	C3A-C2A-CAA-CBA
13	A	1102	CLA	C2B-C3B-CAB-CBB
13	A	1103	CLA	C1A-C2A-CAA-CBA
13	A	1103	CLA	C3A-C2A-CAA-CBA
13	A	1103	CLA	CBA-CGA-O2A-C1
13	A	1103	CLA	CAD-CBD-CGD-O1D
13	A	1103	CLA	CAD-CBD-CGD-O2D
13	A	1104	CLA	C1A-C2A-CAA-CBA
13	A	1104	CLA	C2-C3-C5-C6
13	A	1104	CLA	C4-C3-C5-C6
13	A	1106	CLA	C3A-C2A-CAA-CBA
13	A	1106	CLA	CHA-CBD-CGD-O1D
13	A	1106	CLA	CHA-CBD-CGD-O2D
13	A	1107	CLA	C2B-C3B-CAB-CBB
13	A	1107	CLA	C4B-C3B-CAB-CBB
13	A	1108	CLA	C1A-C2A-CAA-CBA
13	A	1108	CLA	C3A-C2A-CAA-CBA
13	A	1109	CLA	C1A-C2A-CAA-CBA
13	A	1109	CLA	C3A-C2A-CAA-CBA
13	A	1110	CLA	CBD-CGD-O2D-CED
13	A	1114	CLA	C1A-C2A-CAA-CBA
13	A	1114	CLA	C3A-C2A-CAA-CBA
13	A	1114	CLA	CBD-CGD-O2D-CED
13	A	1116	CLA	C3A-C2A-CAA-CBA
13	A	1117	CLA	C1A-C2A-CAA-CBA
13	A	1117	CLA	C3A-C2A-CAA-CBA
13	A	1118	CLA	C1A-C2A-CAA-CBA
13	A	1118	CLA	C3A-C2A-CAA-CBA
13	A	1118	CLA	CBD-CGD-O2D-CED
13	A	1120	CLA	C1A-C2A-CAA-CBA
13	A	1120	CLA	C3A-C2A-CAA-CBA
13	A	1120	CLA	C4B-C3B-CAB-CBB
13	A	1120	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
13	A	1121	CLA	C4-C3-C5-C6
13	A	1122	CLA	C2B-C3B-CAB-CBB
13	A	1122	CLA	C4B-C3B-CAB-CBB
13	A	1128	CLA	CHA-CBD-CGD-O1D
13	A	1128	CLA	CHA-CBD-CGD-O2D
13	A	1131	CLA	C2B-C3B-CAB-CBB
13	A	1131	CLA	C4B-C3B-CAB-CBB
13	A	1132	CLA	CHA-CBD-CGD-O1D
13	A	1132	CLA	CHA-CBD-CGD-O2D
13	A	1134	CLA	C1A-C2A-CAA-CBA
13	A	1135	CLA	C4-C3-C5-C6
13	A	1138	CLA	C4B-C3B-CAB-CBB
13	A	1139	CLA	C1A-C2A-CAA-CBA
13	A	1139	CLA	C2-C3-C5-C6
13	A	1139	CLA	C4-C3-C5-C6
13	A	1801	CLA	C1A-C2A-CAA-CBA
13	A	1801	CLA	CBA-CGA-O2A-C1
13	A	1801	CLA	O1A-CGA-O2A-C1
13	A	1801	CLA	CAD-CBD-CGD-O1D
13	A	1801	CLA	CAD-CBD-CGD-O2D
13	A	1801	CLA	CBD-CGD-O2D-CED
13	B	1021	CLA	C2B-C3B-CAB-CBB
13	B	1021	CLA	C4B-C3B-CAB-CBB
13	B	1012	CLA	C2B-C3B-CAB-CBB
13	B	1012	CLA	C4B-C3B-CAB-CBB
13	B	1201	CLA	C2B-C3B-CAB-CBB
13	B	1201	CLA	C4B-C3B-CAB-CBB
13	B	1202	CLA	C1A-C2A-CAA-CBA
13	B	1202	CLA	C3A-C2A-CAA-CBA
13	B	1205	CLA	CHA-CBD-CGD-O1D
13	B	1205	CLA	CHA-CBD-CGD-O2D
13	B	1206	CLA	C2B-C3B-CAB-CBB
13	B	1206	CLA	C4B-C3B-CAB-CBB
13	B	1208	CLA	CBD-CGD-O2D-CED
13	B	1210	CLA	C1A-C2A-CAA-CBA
13	B	1211	CLA	C2B-C3B-CAB-CBB
13	B	1211	CLA	C4B-C3B-CAB-CBB
13	B	1211	CLA	CHA-CBD-CGD-O1D
13	B	1211	CLA	CHA-CBD-CGD-O2D
13	B	1212	CLA	C1A-C2A-CAA-CBA
13	B	1212	CLA	C3A-C2A-CAA-CBA
13	B	1213	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	B	1213	CLA	C3A-C2A-CAA-CBA
13	B	1214	CLA	C1A-C2A-CAA-CBA
13	B	1214	CLA	C3A-C2A-CAA-CBA
13	B	1214	CLA	C4B-C3B-CAB-CBB
13	B	1215	CLA	C3A-C2A-CAA-CBA
13	B	1217	CLA	C3A-C2A-CAA-CBA
13	B	1218	CLA	C4B-C3B-CAB-CBB
13	B	1218	CLA	CBD-CGD-O2D-CED
13	B	1219	CLA	CBD-CGD-O2D-CED
13	B	1220	CLA	C4B-C3B-CAB-CBB
13	B	1221	CLA	C4B-C3B-CAB-CBB
13	B	1221	CLA	CHA-CBD-CGD-O1D
13	B	1221	CLA	CHA-CBD-CGD-O2D
13	B	1222	CLA	C1A-C2A-CAA-CBA
13	B	1222	CLA	CHA-CBD-CGD-O1D
13	B	1222	CLA	CHA-CBD-CGD-O2D
13	B	1224	CLA	C3A-C2A-CAA-CBA
13	B	1225	CLA	C1A-C2A-CAA-CBA
13	B	1225	CLA	C3A-C2A-CAA-CBA
13	B	1225	CLA	C4B-C3B-CAB-CBB
13	B	1226	CLA	CHA-CBD-CGD-O1D
13	B	1226	CLA	CHA-CBD-CGD-O2D
13	B	1227	CLA	C3A-C2A-CAA-CBA
13	B	1227	CLA	C4B-C3B-CAB-CBB
13	B	1227	CLA	CBD-CGD-O2D-CED
13	B	1229	CLA	C1A-C2A-CAA-CBA
13	B	1229	CLA	C3A-C2A-CAA-CBA
13	B	1230	CLA	C4B-C3B-CAB-CBB
13	B	1230	CLA	CHA-CBD-CGD-O1D
13	B	1230	CLA	CHA-CBD-CGD-O2D
13	B	1231	CLA	CHA-CBD-CGD-O1D
13	B	1231	CLA	CHA-CBD-CGD-O2D
13	B	1233	CLA	CBD-CGD-O2D-CED
13	B	1239	CLA	C1A-C2A-CAA-CBA
13	B	1239	CLA	C3A-C2A-CAA-CBA
13	J	1302	CLA	C1A-C2A-CAA-CBA
13	J	1302	CLA	C3A-C2A-CAA-CBA
13	J	1302	CLA	CAD-CBD-CGD-O1D
13	J	1302	CLA	CAD-CBD-CGD-O2D
13	J	1302	CLA	CBD-CGD-O2D-CED
13	K	1401	CLA	CBD-CGD-O2D-CED
13	L	1501	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	L	1501	CLA	C3A-C2A-CAA-CBA
13	L	1502	CLA	C2B-C3B-CAB-CBB
13	L	1502	CLA	C4B-C3B-CAB-CBB
13	L	1503	CLA	C2B-C3B-CAB-CBB
13	L	1503	CLA	C4B-C3B-CAB-CBB
13	M	1601	CLA	C1A-C2A-CAA-CBA
13	M	1601	CLA	C3A-C2A-CAA-CBA
13	M	1601	CLA	CAD-CBD-CGD-O1D
13	M	1601	CLA	CAD-CBD-CGD-O2D
13	M	1601	CLA	CBD-CGD-O2D-CED
13	X	1701	CLA	CHA-CBD-CGD-O2D
16	A	4002	BCR	C23-C24-C25-C26
16	A	4007	BCR	C23-C24-C25-C26
16	A	4007	BCR	C23-C24-C25-C30
16	B	4010	BCR	C23-C24-C25-C26
16	B	4010	BCR	C23-C24-C25-C30
16	J	4012	BCR	C1-C6-C7-C8
16	J	4012	BCR	C5-C6-C7-C8
16	J	4013	BCR	C23-C24-C25-C26
16	J	4013	BCR	C23-C24-C25-C30
17	A	5001	LHG	C4-O6-P-O3
17	A	5001	LHG	C4-O6-P-O4
17	B	5004	LHG	O1-C1-C2-C3
13	A	1114	CLA	O1D-CGD-O2D-CED
13	A	1139	CLA	O1D-CGD-O2D-CED
13	B	1231	CLA	O1D-CGD-O2D-CED
13	A	1107	CLA	CBD-CGD-O2D-CED
13	A	1108	CLA	CBD-CGD-O2D-CED
13	A	1109	CLA	CBD-CGD-O2D-CED
13	A	1113	CLA	CBD-CGD-O2D-CED
13	A	1139	CLA	CBD-CGD-O2D-CED
13	B	1021	CLA	CBD-CGD-O2D-CED
13	B	1201	CLA	CBD-CGD-O2D-CED
13	B	1212	CLA	CBD-CGD-O2D-CED
13	B	1231	CLA	CBD-CGD-O2D-CED
13	F	1301	CLA	CBD-CGD-O2D-CED
13	A	1103	CLA	O1A-CGA-O2A-C1
13	A	1118	CLA	O1A-CGA-O2A-C1
13	A	1133	CLA	O1A-CGA-O2A-C1
13	A	1133	CLA	CBA-CGA-O2A-C1
13	A	1237	CLA	CBA-CGA-O2A-C1
13	B	1228	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	1013	CLA	O1A-CGA-O2A-C1
13	A	1110	CLA	O1A-CGA-O2A-C1
13	A	1130	CLA	O1A-CGA-O2A-C1
13	A	1135	CLA	O1A-CGA-O2A-C1
13	A	1237	CLA	O1A-CGA-O2A-C1
13	B	1219	CLA	O1D-CGD-O2D-CED
13	K	1401	CLA	O1D-CGD-O2D-CED
13	A	1801	CLA	O1D-CGD-O2D-CED
13	B	1208	CLA	O1D-CGD-O2D-CED
13	A	1104	CLA	CBD-CGD-O2D-CED
13	A	1103	CLA	C3-C5-C6-C7
13	A	1107	CLA	C3-C5-C6-C7
13	A	1110	CLA	C3-C5-C6-C7
13	B	1206	CLA	C3-C5-C6-C7
13	A	1114	CLA	CBA-CGA-O2A-C1
13	A	1117	CLA	CBA-CGA-O2A-C1
13	A	1118	CLA	CBA-CGA-O2A-C1
13	A	1135	CLA	CBA-CGA-O2A-C1
13	A	1137	CLA	CBA-CGA-O2A-C1
13	L	1501	CLA	CBA-CGA-O2A-C1
13	A	1102	CLA	CBD-CGD-O2D-CED
13	A	1105	CLA	CBD-CGD-O2D-CED
13	A	1106	CLA	CBD-CGD-O2D-CED
13	A	1120	CLA	CBD-CGD-O2D-CED
13	A	1126	CLA	CBD-CGD-O2D-CED
13	A	1132	CLA	CBD-CGD-O2D-CED
13	A	1140	CLA	CBD-CGD-O2D-CED
13	B	1230	CLA	CBD-CGD-O2D-CED
13	L	1503	CLA	CBD-CGD-O2D-CED
13	X	1701	CLA	CBD-CGD-O2D-CED
13	A	1110	CLA	O1D-CGD-O2D-CED
13	A	1118	CLA	O1D-CGD-O2D-CED
13	B	1233	CLA	O1D-CGD-O2D-CED
13	J	1302	CLA	O1D-CGD-O2D-CED
13	M	1601	CLA	O1D-CGD-O2D-CED
13	B	1218	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	C4-C3-C5-C6
13	A	1140	CLA	C4-C3-C5-C6
13	A	1237	CLA	C4-C3-C5-C6
13	B	1203	CLA	C4-C3-C5-C6
13	B	1215	CLA	C4-C3-C5-C6
14	A	2001	PQN	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	A	1126	CLA	C2-C3-C5-C6
13	B	1215	CLA	C2-C3-C5-C6
17	B	5004	LHG	C24-C23-O8-C6
13	B	1021	CLA	O1D-CGD-O2D-CED
13	B	1227	CLA	O1D-CGD-O2D-CED
13	B	1212	CLA	C2A-CAA-CBA-CGA
13	A	1013	CLA	CBA-CGA-O2A-C1
13	A	1110	CLA	CBA-CGA-O2A-C1
13	A	1122	CLA	CBA-CGA-O2A-C1
13	A	1130	CLA	CBA-CGA-O2A-C1
13	B	1217	CLA	CBA-CGA-O2A-C1
13	A	1114	CLA	O1A-CGA-O2A-C1
13	A	1121	CLA	O1A-CGA-O2A-C1
13	B	1213	CLA	O1A-CGA-O2A-C1
13	L	1501	CLA	O1A-CGA-O2A-C1
17	B	5004	LHG	O9-C7-O7-C5
13	B	1201	CLA	O1D-CGD-O2D-CED
13	A	1123	CLA	C3-C5-C6-C7
13	A	1122	CLA	CBD-CGD-O2D-CED
13	A	1127	CLA	CBD-CGD-O2D-CED
13	A	1108	CLA	O1D-CGD-O2D-CED
13	A	1109	CLA	O1D-CGD-O2D-CED
13	A	1106	CLA	CBA-CGA-O2A-C1
13	A	1129	CLA	CBA-CGA-O2A-C1
13	L	1502	CLA	CBA-CGA-O2A-C1
18	B	5002	LMG	O6-C5-C6-O5
13	A	1117	CLA	O1A-CGA-O2A-C1
13	A	1137	CLA	O1A-CGA-O2A-C1
13	F	1301	CLA	O1D-CGD-O2D-CED
17	B	5004	LHG	C8-C7-O7-C5
13	A	1106	CLA	C3-C5-C6-C7
13	B	1203	CLA	C3-C5-C6-C7
13	B	1205	CLA	C3-C5-C6-C7
13	B	1238	CLA	C3-C5-C6-C7
13	A	1121	CLA	CBD-CGD-O2D-CED
13	B	1236	CLA	CBD-CGD-O2D-CED
13	A	1113	CLA	O1D-CGD-O2D-CED
13	B	1212	CLA	O1D-CGD-O2D-CED
13	B	1228	CLA	O1D-CGD-O2D-CED
13	A	1121	CLA	CBA-CGA-O2A-C1
13	B	1213	CLA	CBA-CGA-O2A-C1
13	A	1133	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	B	1012	CLA	C4-C3-C5-C6
13	B	1213	CLA	C4-C3-C5-C6
13	A	1133	CLA	C2-C3-C5-C6
13	A	1140	CLA	C2-C3-C5-C6
13	B	1012	CLA	C2-C3-C5-C6
13	B	1203	CLA	C2-C3-C5-C6
13	B	1213	CLA	C2-C3-C5-C6
13	A	1106	CLA	O1A-CGA-O2A-C1
13	B	1217	CLA	O1A-CGA-O2A-C1
13	L	1502	CLA	O1A-CGA-O2A-C1
13	B	1203	CLA	CBD-CGD-O2D-CED
13	A	1107	CLA	O1D-CGD-O2D-CED
13	A	1122	CLA	O1A-CGA-O2A-C1
13	A	1129	CLA	O1A-CGA-O2A-C1
13	B	1221	CLA	C3-C5-C6-C7
13	B	1215	CLA	CBA-CGA-O2A-C1
13	B	1226	CLA	CBA-CGA-O2A-C1
13	B	1205	CLA	CBD-CGD-O2D-CED
13	B	1207	CLA	CBD-CGD-O2D-CED
13	B	1229	CLA	CBD-CGD-O2D-CED
13	A	1126	CLA	O1A-CGA-O2A-C1
13	A	1104	CLA	O1D-CGD-O2D-CED
13	B	1215	CLA	O1A-CGA-O2A-C1
17	A	5003	LHG	C1-C2-C3-O3
13	A	1102	CLA	CBA-CGA-O2A-C1
13	A	1109	CLA	CBA-CGA-O2A-C1
13	A	1120	CLA	CBA-CGA-O2A-C1
13	A	1126	CLA	CBA-CGA-O2A-C1
13	B	1210	CLA	CBA-CGA-O2A-C1
13	B	1223	CLA	CBA-CGA-O2A-C1
13	B	1234	CLA	CBA-CGA-O2A-C1
13	A	1103	CLA	CBD-CGD-O2D-CED
13	A	1120	CLA	O1D-CGD-O2D-CED
13	A	1140	CLA	O1D-CGD-O2D-CED
13	A	1132	CLA	O1D-CGD-O2D-CED
13	B	1221	CLA	C4-C3-C5-C6
13	A	1237	CLA	C2-C3-C5-C6
13	B	1221	CLA	C2-C3-C5-C6
14	A	2001	PQN	C12-C13-C15-C16
17	B	5004	LHG	O10-C23-O8-C6
13	A	1102	CLA	O1D-CGD-O2D-CED
13	B	1230	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	A	5003	LHG	O2-C2-C3-O3
13	A	1105	CLA	O1D-CGD-O2D-CED
13	A	1120	CLA	O1A-CGA-O2A-C1
13	B	1210	CLA	O1A-CGA-O2A-C1
13	B	1239	CLA	CBD-CGD-O2D-CED
13	A	1127	CLA	C2A-CAA-CBA-CGA
13	A	1109	CLA	O1A-CGA-O2A-C1
13	A	1140	CLA	C2-C1-O2A-CGA
13	L	1503	CLA	O1D-CGD-O2D-CED
13	A	1125	CLA	C10-C11-C12-C13
13	A	1140	CLA	C13-C15-C16-C17
13	B	1203	CLA	C13-C15-C16-C17
13	X	1701	CLA	O1D-CGD-O2D-CED
17	B	5004	LHG	O1-C1-C2-O2
13	B	1202	CLA	CBD-CGD-O2D-CED
13	L	1503	CLA	C5-C6-C7-C8
13	A	1106	CLA	O1D-CGD-O2D-CED
13	A	1104	CLA	C3-C5-C6-C7
13	A	1102	CLA	O1A-CGA-O2A-C1
13	B	1223	CLA	O1A-CGA-O2A-C1
13	A	1402	CLA	C2A-CAA-CBA-CGA
13	B	1201	CLA	C2A-CAA-CBA-CGA
13	B	1227	CLA	C2A-CAA-CBA-CGA
13	B	1228	CLA	C2A-CAA-CBA-CGA
13	B	1238	CLA	C2A-CAA-CBA-CGA
13	A	1104	CLA	C15-C16-C17-C18
13	A	1136	CLA	C8-C10-C11-C12
18	B	5002	LMG	C4-C5-C6-O5
13	B	1226	CLA	O1A-CGA-O2A-C1
13	B	1207	CLA	C15-C16-C17-C18
13	B	1234	CLA	O1A-CGA-O2A-C1
14	A	2001	PQN	C13-C15-C16-C17
13	A	1126	CLA	O1D-CGD-O2D-CED
14	B	2002	PQN	C25-C26-C27-C28
13	A	1130	CLA	CBD-CGD-O2D-CED
13	A	1128	CLA	CBA-CGA-O2A-C1
13	A	1139	CLA	CBA-CGA-O2A-C1
13	B	1236	CLA	CBA-CGA-O2A-C1
13	A	1116	CLA	CBD-CGD-O2D-CED
13	B	1202	CLA	CBA-CGA-O2A-C1
13	A	1107	CLA	C8-C10-C11-C12
13	B	1205	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	B	1223	CLA	C10-C11-C12-C13
13	B	1225	CLA	C15-C16-C17-C18
13	B	1234	CLA	C8-C10-C11-C12
13	A	1107	CLA	C13-C15-C16-C17
13	A	1124	CLA	C5-C6-C7-C8
13	B	1225	CLA	C5-C6-C7-C8
13	A	1109	CLA	C15-C16-C17-C18
13	A	1127	CLA	O1D-CGD-O2D-CED
13	L	1502	CLA	C8-C10-C11-C12
13	A	1122	CLA	O1D-CGD-O2D-CED
16	B	4009	BCR	C16-C17-C18-C36
16	B	4009	BCR	C20-C21-C22-C37
13	B	1226	CLA	C13-C15-C16-C17
13	B	1229	CLA	C10-C11-C12-C13
13	A	1128	CLA	O1A-CGA-O2A-C1
13	A	1139	CLA	O1A-CGA-O2A-C1
13	B	1236	CLA	O1A-CGA-O2A-C1
13	A	1107	CLA	C2A-CAA-CBA-CGA
13	A	1120	CLA	C2A-CAA-CBA-CGA
13	A	1013	CLA	O2A-C1-C2-C3
13	A	1103	CLA	O2A-C1-C2-C3
14	B	2002	PQN	C26-C27-C28-C29
14	B	2002	PQN	C26-C27-C28-C30
13	A	1121	CLA	O1D-CGD-O2D-CED
13	B	1203	CLA	O1D-CGD-O2D-CED
13	B	1236	CLA	O1D-CGD-O2D-CED
13	B	1203	CLA	C10-C11-C12-C13
16	B	4005	BCR	C11-C10-C9-C8
16	B	4009	BCR	C16-C17-C18-C19
16	I	4020	BCR	C20-C21-C22-C23
13	A	1106	CLA	C5-C6-C7-C8
13	A	1130	CLA	C8-C10-C11-C12
13	B	1219	CLA	C6-C7-C8-C9
13	B	1219	CLA	C6-C7-C8-C10
17	A	5001	LHG	C24-C25-C26-C27
13	A	1103	CLA	C10-C11-C12-C13
13	A	1102	CLA	C4B-C3B-CAB-CBB
13	A	1111	CLA	C4B-C3B-CAB-CBB
13	A	1113	CLA	C4B-C3B-CAB-CBB
13	A	1123	CLA	C4B-C3B-CAB-CBB
13	A	1126	CLA	C4B-C3B-CAB-CBB
13	B	1023	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	B	1203	CLA	C4B-C3B-CAB-CBB
13	B	1210	CLA	C4B-C3B-CAB-CBB
13	B	1219	CLA	C4B-C3B-CAB-CBB
13	B	1222	CLA	C4B-C3B-CAB-CBB
13	B	1235	CLA	C4B-C3B-CAB-CBB
13	B	1202	CLA	C13-C15-C16-C17
13	B	1229	CLA	C15-C16-C17-C18
13	B	1202	CLA	O1A-CGA-O2A-C1
13	B	1012	CLA	C3-C5-C6-C7
13	A	1101	CLA	C3A-C2A-CAA-CBA
13	A	1104	CLA	C3A-C2A-CAA-CBA
13	A	1134	CLA	C3A-C2A-CAA-CBA
13	A	1139	CLA	C3A-C2A-CAA-CBA
13	B	1210	CLA	C3A-C2A-CAA-CBA
13	B	1205	CLA	O1D-CGD-O2D-CED
13	A	1101	CLA	CBD-CGD-O2D-CED
13	A	1022	CLA	C2B-C3B-CAB-CBB
13	A	1120	CLA	C2B-C3B-CAB-CBB
13	B	1218	CLA	C2B-C3B-CAB-CBB
16	A	4002	BCR	C1-C6-C7-C8
16	A	4002	BCR	C5-C6-C7-C8
16	A	4002	BCR	C23-C24-C25-C30
16	A	4008	BCR	C1-C6-C7-C8
16	A	4011	BCR	C1-C6-C7-C8
16	A	4011	BCR	C5-C6-C7-C8
16	A	4011	BCR	C23-C24-C25-C26
16	A	4011	BCR	C23-C24-C25-C30
16	B	4005	BCR	C1-C6-C7-C8
16	B	4005	BCR	C5-C6-C7-C8
16	B	4005	BCR	C23-C24-C25-C26
16	I	4020	BCR	C23-C24-C25-C30
16	J	4013	BCR	C1-C6-C7-C8
16	M	4021	BCR	C1-C6-C7-C8
16	M	4021	BCR	C5-C6-C7-C8
13	B	1234	CLA	C5-C6-C7-C8
13	B	1215	CLA	C3-C5-C6-C7
16	B	4009	BCR	C18-C19-C20-C21
13	A	1118	CLA	C4C-C3C-CAC-CBC
13	B	1207	CLA	O1D-CGD-O2D-CED
17	A	5001	LHG	C28-C29-C30-C31
17	A	5003	LHG	C9-C10-C11-C12
13	A	1103	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	A	1123	CLA	C4-C3-C5-C6
13	B	1021	CLA	C13-C15-C16-C17
13	B	1216	CLA	C10-C11-C12-C13
13	A	1103	CLA	O1D-CGD-O2D-CED
13	A	1111	CLA	C3-C5-C6-C7
13	B	1224	CLA	CBD-CGD-O2D-CED
13	B	1239	CLA	O1D-CGD-O2D-CED
13	B	1230	CLA	C4-C3-C5-C6
13	A	1123	CLA	C2-C3-C5-C6
13	B	1229	CLA	O1D-CGD-O2D-CED
13	B	1202	CLA	O1D-CGD-O2D-CED
13	A	1140	CLA	C5-C6-C7-C8
13	B	1213	CLA	C3-C5-C6-C7
13	A	1101	CLA	C1A-C2A-CAA-CBA
13	A	1102	CLA	C1A-C2A-CAA-CBA
13	A	1106	CLA	C1A-C2A-CAA-CBA
13	A	1116	CLA	C1A-C2A-CAA-CBA
13	A	1137	CLA	C1A-C2A-CAA-CBA
13	B	1208	CLA	C1A-C2A-CAA-CBA
13	B	1215	CLA	C1A-C2A-CAA-CBA
13	B	1216	CLA	C1A-C2A-CAA-CBA
13	B	1217	CLA	C1A-C2A-CAA-CBA
13	B	1224	CLA	C1A-C2A-CAA-CBA
13	B	1227	CLA	C1A-C2A-CAA-CBA
13	B	1228	CLA	C1A-C2A-CAA-CBA
13	K	1401	CLA	C1A-C2A-CAA-CBA
13	B	1210	CLA	C8-C10-C11-C12
13	A	1237	CLA	C3-C5-C6-C7
13	A	1106	CLA	C11-C10-C8-C7
13	B	1223	CLA	C11-C12-C13-C15
13	A	1022	CLA	C15-C16-C17-C18
13	B	1224	CLA	C10-C11-C12-C13
13	A	1131	CLA	C2-C3-C5-C6
13	A	1106	CLA	C11-C10-C8-C9
13	B	1223	CLA	C11-C12-C13-C14
13	B	1214	CLA	CBA-CGA-O2A-C1
13	B	1228	CLA	CBA-CGA-O2A-C1
13	A	1114	CLA	C1-C2-C3-C4
13	A	1138	CLA	C5-C6-C7-C8
17	A	5001	LHG	C10-C11-C12-C13
17	A	5001	LHG	C24-C23-O8-C6
13	A	1130	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	I	4020	BCR	C20-C21-C22-C37
13	A	1131	CLA	C4-C3-C5-C6
13	A	1109	CLA	C2A-CAA-CBA-CGA
13	A	1134	CLA	C2A-CAA-CBA-CGA
13	B	1222	CLA	CBA-CGA-O2A-C1
13	A	1125	CLA	CBA-CGA-O2A-C1
13	B	1221	CLA	O2A-C1-C2-C3
13	B	1229	CLA	O2A-C1-C2-C3
13	A	1136	CLA	C5-C6-C7-C8
16	B	4014	BCR	C11-C10-C9-C8
13	A	1801	CLA	C2-C3-C5-C6
13	B	1206	CLA	C16-C17-C18-C20
18	B	5002	LMG	C30-C31-C32-C33
13	A	1130	CLA	C3-C5-C6-C7
13	A	1119	CLA	CBA-CGA-O2A-C1
13	B	1223	CLA	CBD-CGD-O2D-CED
17	A	5003	LHG	C11-C10-C9-C8
13	A	1124	CLA	C15-C16-C17-C18
13	A	1111	CLA	C8-C10-C11-C12
13	A	1127	CLA	C4-C3-C5-C6
13	A	1801	CLA	C4-C3-C5-C6
13	A	1123	CLA	CBA-CGA-O2A-C1
13	A	1124	CLA	CBA-CGA-O2A-C1
13	A	1127	CLA	C14-C13-C15-C16
13	B	1012	CLA	C14-C13-C15-C16
13	A	1013	CLA	C4B-C3B-CAB-CBB
13	A	1112	CLA	C4B-C3B-CAB-CBB
13	A	1116	CLA	C4B-C3B-CAB-CBB
13	A	1124	CLA	C4B-C3B-CAB-CBB
13	A	1129	CLA	C4B-C3B-CAB-CBB
13	A	1132	CLA	C4B-C3B-CAB-CBB
13	B	1208	CLA	C4B-C3B-CAB-CBB
13	B	1231	CLA	C4B-C3B-CAB-CBB
13	A	1123	CLA	C8-C10-C11-C12
13	A	1123	CLA	C13-C15-C16-C17
13	B	1203	CLA	C15-C16-C17-C18
13	B	1206	CLA	C16-C17-C18-C19
13	A	1106	CLA	C8-C10-C11-C12
13	A	1106	CLA	C15-C16-C17-C18
13	A	1116	CLA	CAA-CBA-CGA-O2A
13	A	1127	CLA	C12-C13-C15-C16
13	A	1132	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	B	1012	CLA	C12-C13-C15-C16
13	B	1202	CLA	C12-C13-C15-C16
13	B	1228	CLA	O1A-CGA-O2A-C1
13	A	1402	CLA	C3A-C2A-CAA-CBA
13	A	1801	CLA	C3A-C2A-CAA-CBA
13	B	1211	CLA	C4-C3-C5-C6
13	B	1222	CLA	C3A-C2A-CAA-CBA
13	B	1228	CLA	C3A-C2A-CAA-CBA
13	B	1230	CLA	C2-C3-C5-C6
13	A	1125	CLA	O1A-CGA-O2A-C1
13	A	1013	CLA	C15-C16-C17-C18
13	A	1124	CLA	C8-C10-C11-C12
13	A	1105	CLA	C4-C3-C5-C6
13	B	1214	CLA	O1A-CGA-O2A-C1
17	A	5001	LHG	O10-C23-O8-C6
13	A	1101	CLA	O1D-CGD-O2D-CED
13	A	1127	CLA	C5-C6-C7-C8
13	A	1114	CLA	O2A-C1-C2-C3
13	A	1116	CLA	O1D-CGD-O2D-CED
13	B	1215	CLA	C5-C6-C7-C8
13	L	1501	CLA	C13-C15-C16-C17
13	B	1225	CLA	C4-C3-C5-C6
13	A	1127	CLA	C2-C3-C5-C6
13	B	1211	CLA	C2-C3-C5-C6
13	A	1138	CLA	C2B-C3B-CAB-CBB
13	B	1220	CLA	C2B-C3B-CAB-CBB
13	B	1230	CLA	C2B-C3B-CAB-CBB
16	J	4013	BCR	C5-C6-C7-C8
13	A	1124	CLA	O1A-CGA-O2A-C1
13	A	1104	CLA	C16-C17-C18-C19
13	B	1229	CLA	C2A-CAA-CBA-CGA
13	B	1225	CLA	C2-C3-C5-C6
13	A	1104	CLA	C16-C17-C18-C20
13	L	1501	CLA	C11-C10-C8-C9
13	B	1021	CLA	C5-C6-C7-C8
16	L	4019	BCR	C22-C23-C24-C25
13	A	1120	CLA	O2A-C1-C2-C3
13	B	1229	CLA	C2-C3-C5-C6
16	F	4016	BCR	C20-C21-C22-C37
16	J	4012	BCR	C35-C13-C14-C15
16	L	4022	BCR	C35-C13-C14-C15
13	A	1138	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	B	1206	CLA	C6-C7-C8-C10
13	B	1210	CLA	C11-C10-C8-C7
13	B	1225	CLA	C12-C13-C15-C16
13	L	1501	CLA	C11-C10-C8-C7
14	A	2001	PQN	C15-C16-C17-C18
13	B	1211	CLA	CBA-CGA-O2A-C1
13	A	1013	CLA	C2A-CAA-CBA-CGA
13	A	1108	CLA	C2A-CAA-CBA-CGA
13	A	1117	CLA	C16-C17-C18-C20
13	B	1234	CLA	C4-C3-C5-C6
13	A	1123	CLA	O1A-CGA-O2A-C1
13	A	1119	CLA	O1A-CGA-O2A-C1
13	B	1228	CLA	O2A-C1-C2-C3
13	B	1229	CLA	C4-C3-C5-C6
13	L	1503	CLA	C4-C3-C5-C6
13	B	1225	CLA	C2A-CAA-CBA-CGA
13	A	1132	CLA	C14-C13-C15-C16
13	B	1234	CLA	C2-C3-C5-C6
13	A	1140	CLA	C3-C5-C6-C7
13	B	1211	CLA	C3-C5-C6-C7
13	L	1501	CLA	C3-C5-C6-C7
13	B	1211	CLA	O1A-CGA-O2A-C1
13	A	1106	CLA	C4B-C3B-CAB-CBB
13	A	1107	CLA	C1A-C2A-CAA-CBA
13	A	1108	CLA	C4B-C3B-CAB-CBB
13	A	1118	CLA	C4B-C3B-CAB-CBB
13	A	1119	CLA	C1A-C2A-CAA-CBA
13	A	1122	CLA	C1A-C2A-CAA-CBA
13	A	1125	CLA	C4B-C3B-CAB-CBB
13	A	1128	CLA	C4B-C3B-CAB-CBB
13	A	1136	CLA	C4B-C3B-CAB-CBB
13	A	1137	CLA	C4B-C3B-CAB-CBB
13	A	1237	CLA	C1A-C2A-CAA-CBA
13	A	1402	CLA	C1A-C2A-CAA-CBA
13	B	1216	CLA	C4B-C3B-CAB-CBB
13	B	1224	CLA	C4B-C3B-CAB-CBB
13	B	1228	CLA	C4B-C3B-CAB-CBB
13	B	1236	CLA	C4B-C3B-CAB-CBB
13	K	1401	CLA	C4B-C3B-CAB-CBB
13	L	1501	CLA	C4B-C3B-CAB-CBB
13	A	1102	CLA	C4-C3-C5-C6
16	B	4006	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
13	L	1503	CLA	C2-C3-C5-C6
13	A	1121	CLA	C2-C3-C5-C6
13	A	1135	CLA	C2-C3-C5-C6
13	A	1103	CLA	C11-C10-C8-C7
13	B	1224	CLA	C6-C7-C8-C10
13	B	1224	CLA	C11-C12-C13-C15
13	B	1229	CLA	C11-C10-C8-C7
18	B	5002	LMG	C41-C42-C43-C44
13	A	1117	CLA	C16-C17-C18-C19
13	B	1229	CLA	C16-C17-C18-C20
13	B	1203	CLA	C5-C6-C7-C8
13	A	1138	CLA	C11-C10-C8-C9
13	B	1210	CLA	C11-C10-C8-C9
13	L	1502	CLA	C11-C10-C8-C9
13	A	1237	CLA	O1D-CGD-O2D-CED
13	B	1228	CLA	C1-C2-C3-C4
13	B	1210	CLA	C4-C3-C5-C6
13	B	1224	CLA	C4-C3-C5-C6
13	B	1202	CLA	CAD-CBD-CGD-O2D
13	A	1116	CLA	CBA-CGA-O2A-C1
13	B	1209	CLA	C2A-CAA-CBA-CGA
13	B	1217	CLA	C2A-CAA-CBA-CGA
17	A	5001	LHG	C27-C28-C29-C30
13	A	1101	CLA	CHA-CBD-CGD-O1D
13	A	1101	CLA	CHA-CBD-CGD-O2D
13	A	1123	CLA	CHA-CBD-CGD-O1D
13	A	1123	CLA	CHA-CBD-CGD-O2D
13	B	1202	CLA	CAD-CBD-CGD-O1D
13	X	1701	CLA	CHA-CBD-CGD-O1D
17	A	5003	LHG	C3-O3-P-O5
13	B	1207	CLA	C4-C3-C5-C6
13	L	1501	CLA	C4-C3-C5-C6
13	A	1111	CLA	C2B-C3B-CAB-CBB
13	A	1113	CLA	C2B-C3B-CAB-CBB
13	A	1118	CLA	C2B-C3B-CAB-CBB
13	A	1126	CLA	C2B-C3B-CAB-CBB
13	B	1203	CLA	C2B-C3B-CAB-CBB
13	B	1210	CLA	C2B-C3B-CAB-CBB
13	B	1219	CLA	C2B-C3B-CAB-CBB
13	B	1222	CLA	C2B-C3B-CAB-CBB
16	B	4005	BCR	C23-C24-C25-C30
16	B	4017	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	B	1223	CLA	O1D-CGD-O2D-CED
13	B	1226	CLA	C10-C11-C12-C13
13	B	1234	CLA	CBD-CGD-O2D-CED
13	A	1104	CLA	C11-C12-C13-C14
13	A	1124	CLA	C14-C13-C15-C16
13	A	1131	CLA	C14-C13-C15-C16
13	B	1203	CLA	C14-C13-C15-C16
13	B	1224	CLA	C6-C7-C8-C9
13	B	1225	CLA	C14-C13-C15-C16
13	B	1229	CLA	C11-C10-C8-C9
13	A	1104	CLA	C11-C12-C13-C15
13	A	1131	CLA	C12-C13-C15-C16
13	L	1502	CLA	C11-C10-C8-C7
13	L	1502	CLA	C12-C13-C15-C16
16	B	4006	BCR	C20-C21-C22-C23
13	B	1222	CLA	O1A-CGA-O2A-C1
13	A	1136	CLA	C4-C3-C5-C6
13	B	1229	CLA	C16-C17-C18-C19
13	A	1116	CLA	O1A-CGA-O2A-C1
13	A	1132	CLA	C2A-CAA-CBA-CGA
13	B	1202	CLA	C15-C16-C17-C18
13	B	1023	CLA	C10-C11-C12-C13
13	A	1104	CLA	CAA-CBA-CGA-O2A
13	L	1503	CLA	C3-C5-C6-C7
13	A	1114	CLA	C2A-CAA-CBA-CGA
18	B	5002	LMG	C34-C35-C36-C37
13	A	1117	CLA	C4-C3-C5-C6
13	B	1207	CLA	C13-C15-C16-C17
17	A	5001	LHG	C1-C2-C3-O3
13	A	1103	CLA	C11-C10-C8-C9
13	A	1117	CLA	C11-C12-C13-C14
13	B	1202	CLA	C14-C13-C15-C16
13	A	1103	CLA	C4B-C3B-CAB-CBB
13	A	1115	CLA	C4B-C3B-CAB-CBB
13	B	1213	CLA	C4B-C3B-CAB-CBB
13	J	1303	CLA	C4B-C3B-CAB-CBB
13	A	1237	CLA	C5-C6-C7-C8
13	B	1012	CLA	C13-C15-C16-C17
13	A	1125	CLA	C4-C3-C5-C6
13	A	1102	CLA	C2-C3-C5-C6
13	B	1210	CLA	C2-C3-C5-C6
13	L	1501	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	B	1021	CLA	C12-C13-C15-C16
13	B	1206	CLA	C12-C13-C15-C16
13	A	1121	CLA	C3A-C2A-CAA-CBA
13	A	1133	CLA	C3A-C2A-CAA-CBA
13	A	1107	CLA	C10-C11-C12-C13
16	A	4011	BCR	C11-C10-C9-C34
16	A	4011	BCR	C16-C17-C18-C36
16	B	4005	BCR	C11-C10-C9-C34
16	F	4016	BCR	C35-C13-C14-C15
13	A	1111	CLA	C2-C1-O2A-CGA
13	B	1207	CLA	C2-C3-C5-C6
13	B	1224	CLA	C2-C3-C5-C6
13	A	1109	CLA	C10-C11-C12-C13
17	A	5001	LHG	C26-C27-C28-C29
13	A	1138	CLA	C3-C5-C6-C7
13	A	1122	CLA	C6-C7-C8-C9
13	A	1128	CLA	C11-C10-C8-C9
13	B	1206	CLA	C14-C13-C15-C16
13	B	1211	CLA	C11-C12-C13-C14
13	J	1302	CLA	CAA-CBA-CGA-O1A
13	A	1117	CLA	C2-C3-C5-C6
13	A	1136	CLA	C2-C3-C5-C6
13	B	1220	CLA	CAA-CBA-CGA-O2A
13	B	1227	CLA	CAA-CBA-CGA-O2A
13	B	1224	CLA	O1D-CGD-O2D-CED
13	A	1106	CLA	C2A-CAA-CBA-CGA
13	M	1601	CLA	C2A-CAA-CBA-CGA
13	A	1124	CLA	C1A-C2A-CAA-CBA
16	A	4011	BCR	C11-C10-C9-C8
16	A	4011	BCR	C16-C17-C18-C19
16	F	4016	BCR	C12-C13-C14-C15
18	B	5002	LMG	C15-C16-C17-C18
13	A	1103	CLA	C2B-C3B-CAB-CBB
13	A	1108	CLA	C2B-C3B-CAB-CBB
13	A	1112	CLA	C2B-C3B-CAB-CBB
13	A	1116	CLA	C2B-C3B-CAB-CBB
13	A	1123	CLA	C2B-C3B-CAB-CBB
13	A	1130	CLA	C2B-C3B-CAB-CBB
13	A	1137	CLA	C2B-C3B-CAB-CBB
13	B	1202	CLA	C2B-C3B-CAB-CBB
13	B	1208	CLA	C2B-C3B-CAB-CBB
13	B	1214	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	B	1216	CLA	C2B-C3B-CAB-CBB
13	B	1221	CLA	C2B-C3B-CAB-CBB
13	B	1225	CLA	C2B-C3B-CAB-CBB
13	B	1227	CLA	C2B-C3B-CAB-CBB
13	B	1231	CLA	C2B-C3B-CAB-CBB
13	B	1235	CLA	C2B-C3B-CAB-CBB
13	B	1236	CLA	C2B-C3B-CAB-CBB
13	K	1401	CLA	C2B-C3B-CAB-CBB
16	A	4008	BCR	C5-C6-C7-C8
16	F	4016	BCR	C23-C24-C25-C30
16	I	4020	BCR	C23-C24-C25-C26
16	M	4021	BCR	C23-C24-C25-C30
13	B	1233	CLA	CAA-CBA-CGA-O2A
13	X	1701	CLA	CAA-CBA-CGA-O2A
17	A	5001	LHG	C19-C20-C21-C22
13	B	1227	CLA	CAA-CBA-CGA-O1A
13	M	1601	CLA	CAA-CBA-CGA-O1A
13	A	1022	CLA	C4-C3-C5-C6
13	A	1107	CLA	C4-C3-C5-C6
13	A	1111	CLA	C4-C3-C5-C6
13	B	1205	CLA	C4-C3-C5-C6
13	B	1206	CLA	C4-C3-C5-C6
13	B	1223	CLA	C4-C3-C5-C6
13	A	1125	CLA	C2-C3-C5-C6
13	A	1013	CLA	C8-C10-C11-C12
13	A	1111	CLA	C11-C10-C8-C7
13	A	1117	CLA	C11-C12-C13-C15
13	A	1124	CLA	C12-C13-C15-C16
13	A	1128	CLA	C11-C10-C8-C7
13	B	1223	CLA	C6-C7-C8-C10
13	B	1233	CLA	CAA-CBA-CGA-O1A
13	X	1701	CLA	CAA-CBA-CGA-O1A
18	B	5002	LMG	C31-C32-C33-C34
13	B	1218	CLA	CAA-CBA-CGA-O1A
13	B	1218	CLA	CAA-CBA-CGA-O2A
13	A	1106	CLA	C4-C3-C5-C6
13	A	1107	CLA	C2-C3-C5-C6
13	B	1206	CLA	C2-C3-C5-C6
13	B	1220	CLA	CAA-CBA-CGA-O1A
13	J	1302	CLA	CAA-CBA-CGA-O2A
13	B	1219	CLA	C5-C6-C7-C8
13	A	1125	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	A	5001	LHG	O9-C7-O7-C5
13	A	1109	CLA	C4-C3-C5-C6
13	A	1122	CLA	C4-C3-C5-C6
13	B	1226	CLA	C4-C3-C5-C6
13	M	1601	CLA	CAA-CBA-CGA-O2A
13	B	1226	CLA	C2-C3-C5-C6
13	B	1214	CLA	C8-C10-C11-C12
14	B	2002	PQN	C23-C25-C26-C27
13	A	1131	CLA	C13-C15-C16-C17
13	A	1124	CLA	O1D-CGD-O2D-CED
13	A	1013	CLA	C4-C3-C5-C6
13	A	1116	CLA	C4-C3-C5-C6
13	B	1207	CLA	C10-C11-C12-C13
13	B	1202	CLA	C4B-C3B-CAB-CBB
13	X	1701	CLA	C4B-C3B-CAB-CBB
13	F	1301	CLA	CAA-CBA-CGA-O2A
16	B	4006	BCR	C11-C10-C9-C34
16	B	4006	BCR	C20-C21-C22-C37
16	J	4015	BCR	C20-C21-C22-C37
13	B	1219	CLA	C4-C3-C5-C6
13	A	1111	CLA	C2-C3-C5-C6
13	A	1116	CLA	CAA-CBA-CGA-O1A
13	B	1021	CLA	C14-C13-C15-C16
13	B	1205	CLA	C14-C13-C15-C16
13	B	1223	CLA	C6-C7-C8-C9
13	A	1119	CLA	C4-C3-C5-C6
13	A	1124	CLA	C3A-C2A-CAA-CBA
13	A	1022	CLA	C2-C3-C5-C6
13	B	1205	CLA	C2-C3-C5-C6
13	F	1301	CLA	CAA-CBA-CGA-O1A
17	A	5001	LHG	C11-C10-C9-C8
16	B	4006	BCR	C11-C10-C9-C8
13	A	1118	CLA	C8-C10-C11-C12
13	B	1203	CLA	C16-C17-C18-C20
13	A	1124	CLA	C4-C3-C5-C6
13	J	1302	CLA	C2A-CAA-CBA-CGA
13	A	1237	CLA	CBD-CGD-O2D-CED
13	K	1401	CLA	CAA-CBA-CGA-O1A
13	A	1118	CLA	C6-C7-C8-C9
13	B	1206	CLA	C6-C7-C8-C9
13	K	1401	CLA	CAA-CBA-CGA-O2A
13	A	1013	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	1108	CLA	CAA-CBA-CGA-O1A
13	A	1118	CLA	C6-C7-C8-C10
13	B	1210	CLA	C6-C7-C8-C10
14	A	2001	PQN	C16-C17-C18-C20
13	A	1013	CLA	C2B-C3B-CAB-CBB
13	A	1104	CLA	C2B-C3B-CAB-CBB
13	A	1124	CLA	C2B-C3B-CAB-CBB
13	A	1128	CLA	C2B-C3B-CAB-CBB
16	B	4017	BCR	C5-C6-C7-C8
16	F	4016	BCR	C23-C24-C25-C26
16	J	4015	BCR	C23-C24-C25-C30
16	M	4021	BCR	C23-C24-C25-C26
13	B	1206	CLA	C2-C1-O2A-CGA
13	B	1224	CLA	C2-C1-O2A-CGA
13	B	1225	CLA	C2-C1-O2A-CGA
13	B	1239	CLA	C2-C1-O2A-CGA
17	A	5001	LHG	C11-C12-C13-C14
17	A	5001	LHG	C13-C14-C15-C16
17	A	5003	LHG	O7-C7-C8-C9
13	B	1213	CLA	C2A-CAA-CBA-CGA
13	X	1701	CLA	C2A-CAA-CBA-CGA
17	A	5001	LHG	C8-C7-O7-C5
13	A	1122	CLA	C11-C12-C13-C14
13	A	1013	CLA	CAA-CBA-CGA-O2A
13	A	1102	CLA	CAA-CBA-CGA-O2A
13	A	1126	CLA	CAA-CBA-CGA-O2A
13	B	1221	CLA	C6-C7-C8-C9
13	A	1111	CLA	O1A-CGA-O2A-C1
13	A	1118	CLA	C4-C3-C5-C6
13	A	1123	CLA	CAA-CBA-CGA-O2A
13	B	1203	CLA	CAA-CBA-CGA-O2A
13	B	1224	CLA	C2A-CAA-CBA-CGA
13	A	1132	CLA	C13-C15-C16-C17
13	A	1109	CLA	CAA-CBA-CGA-O2A
13	B	1229	CLA	CAA-CBA-CGA-O2A
17	A	5001	LHG	C25-C26-C27-C28
13	B	1212	CLA	CAA-CBA-CGA-O2A
13	B	1219	CLA	CAA-CBA-CGA-O2A
13	B	1203	CLA	C16-C17-C18-C19
13	A	1104	CLA	C4B-C3B-CAB-CBB
13	A	1105	CLA	C4B-C3B-CAB-CBB
13	A	1109	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	A	1111	CLA	C1A-C2A-CAA-CBA
13	A	1121	CLA	C1A-C2A-CAA-CBA
13	A	1130	CLA	C4B-C3B-CAB-CBB
13	A	1135	CLA	C1A-C2A-CAA-CBA
13	A	1402	CLA	C4B-C3B-CAB-CBB
13	A	1801	CLA	C4B-C3B-CAB-CBB
13	B	1217	CLA	C4B-C3B-CAB-CBB
13	B	1234	CLA	C1A-C2A-CAA-CBA
13	J	1302	CLA	C4B-C3B-CAB-CBB
13	L	1503	CLA	C1A-C2A-CAA-CBA
13	B	1210	CLA	CAA-CBA-CGA-O2A
13	A	1119	CLA	C13-C15-C16-C17
17	A	5003	LHG	O10-C23-O8-C6
13	A	1105	CLA	CAA-CBA-CGA-O2A
13	A	1801	CLA	CAA-CBA-CGA-O2A
13	A	1102	CLA	C2-C1-O2A-CGA
13	A	1119	CLA	C2-C1-O2A-CGA
13	B	1211	CLA	C2-C1-O2A-CGA
13	A	1136	CLA	C12-C13-C15-C16
13	A	1116	CLA	C2-C3-C5-C6
13	A	1108	CLA	CAA-CBA-CGA-O2A
13	A	1022	CLA	C2A-CAA-CBA-CGA
13	A	1104	CLA	C2A-CAA-CBA-CGA
13	L	1503	CLA	C2A-CAA-CBA-CGA
13	B	1226	CLA	C8-C10-C11-C12
17	A	5003	LHG	O8-C23-C24-C25
13	A	1128	CLA	C4-C3-C5-C6
13	B	1219	CLA	C2-C3-C5-C6
13	B	1212	CLA	CAA-CBA-CGA-O1A
17	A	5003	LHG	C24-C23-O8-C6
13	L	1501	CLA	C8-C10-C11-C12
13	A	1102	CLA	CAA-CBA-CGA-O1A
13	A	1127	CLA	C13-C15-C16-C17
13	A	1105	CLA	C2A-CAA-CBA-CGA
13	A	1111	CLA	CBA-CGA-O2A-C1
13	A	1111	CLA	C11-C10-C8-C9
13	A	1117	CLA	C11-C10-C8-C9
13	A	1136	CLA	C14-C13-C15-C16
13	B	1210	CLA	C6-C7-C8-C9
13	B	1224	CLA	C11-C12-C13-C14
13	L	1502	CLA	C14-C13-C15-C16
14	A	2001	PQN	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	B	1224	CLA	C5-C6-C7-C8
13	B	1203	CLA	CAA-CBA-CGA-O1A
13	A	1013	CLA	CAA-CBA-CGA-O1A
13	A	1105	CLA	CAA-CBA-CGA-O1A
13	A	1126	CLA	CAA-CBA-CGA-O1A
18	B	5002	LMG	C16-C17-C18-C19
13	B	1229	CLA	CAA-CBA-CGA-O1A
17	A	5003	LHG	O9-C7-C8-C9
13	A	1011	CLA	CAD-CBD-CGD-O2D
13	A	1118	CLA	CAA-CBA-CGA-O2A
13	B	1209	CLA	CAA-CBA-CGA-O1A
13	A	1123	CLA	CAA-CBA-CGA-O1A
13	A	1135	CLA	C2-C1-O2A-CGA
13	A	1801	CLA	C2-C1-O2A-CGA
13	A	1109	CLA	CAA-CBA-CGA-O1A
13	B	1219	CLA	CAA-CBA-CGA-O1A
13	A	1121	CLA	CAA-CBA-CGA-O2A
13	A	1121	CLA	CAA-CBA-CGA-O1A
13	B	1235	CLA	C11-C12-C13-C15
13	A	1011	CLA	CAA-CBA-CGA-O2A
13	B	1211	CLA	CAA-CBA-CGA-O2A
13	A	1022	CLA	C16-C17-C18-C19
13	A	1118	CLA	CAA-CBA-CGA-O1A
13	A	1112	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

107 monomers are involved in 306 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	4021	BCR	2	0
13	B	1207	CLA	5	0
17	A	5001	LHG	4	0
13	A	1011	CLA	9	0
13	B	1229	CLA	4	0
13	B	1224	CLA	5	0
13	A	1105	CLA	2	0
13	B	1223	CLA	3	0
13	A	1136	CLA	5	0
13	A	1109	CLA	1	0
13	A	1119	CLA	2	0
13	A	1108	CLA	3	0
16	B	4005	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	1502	CLA	7	0
13	A	1126	CLA	13	0
14	A	2001	PQN	1	0
13	A	1127	CLA	2	0
13	A	1132	CLA	4	0
13	M	1601	CLA	1	0
13	F	1301	CLA	1	0
13	A	1130	CLA	1	0
13	B	1213	CLA	3	0
13	B	1228	CLA	3	0
13	B	1236	CLA	4	0
13	A	1107	CLA	3	0
18	B	5002	LMG	5	0
13	A	1111	CLA	1	0
13	A	1135	CLA	3	0
13	B	1012	CLA	17	0
16	I	4018	BCR	4	0
17	B	5004	LHG	1	0
13	L	1501	CLA	2	0
13	B	1206	CLA	2	0
13	A	1013	CLA	11	0
13	B	1203	CLA	6	0
13	A	1133	CLA	2	0
16	J	4012	BCR	4	0
13	B	1225	CLA	8	0
16	B	4017	BCR	1	0
13	B	1204	CLA	1	0
13	B	1211	CLA	5	0
13	B	1210	CLA	5	0
13	A	1125	CLA	2	0
13	B	1212	CLA	1	0
13	B	1214	CLA	7	0
13	J	1302	CLA	1	0
16	B	4014	BCR	1	0
13	A	1114	CLA	1	0
14	B	2002	PQN	1	0
13	A	1022	CLA	2	0
13	B	1023	CLA	4	0
13	B	1227	CLA	3	0
16	J	4015	BCR	5	0
13	A	1138	CLA	2	0
16	A	4011	BCR	12	0

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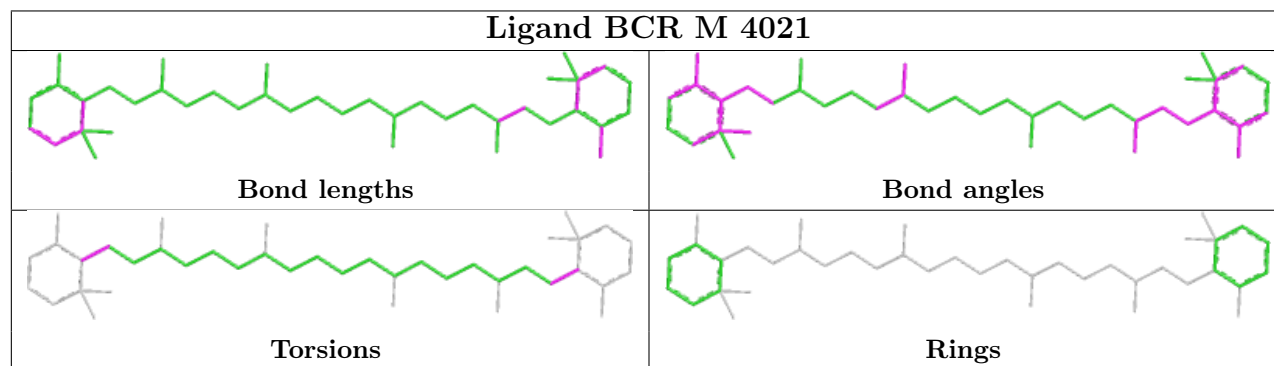
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1120	CLA	2	0
13	A	1112	CLA	4	0
13	B	1202	CLA	4	0
13	L	1503	CLA	2	0
13	B	1226	CLA	5	0
13	B	1215	CLA	5	0
16	L	4022	BCR	1	0
16	J	4013	BCR	7	0
16	A	4003	BCR	1	0
13	A	1122	CLA	2	0
13	B	1021	CLA	7	0
13	B	1201	CLA	1	0
13	A	1118	CLA	4	0
13	B	1221	CLA	8	0
13	A	1101	CLA	2	0
13	A	1140	CLA	9	0
13	A	1402	CLA	1	0
13	A	1801	CLA	4	0
13	A	1237	CLA	4	0
16	B	4004	BCR	1	0
13	A	1104	CLA	3	0
13	A	1117	CLA	3	0
13	A	1124	CLA	6	0
16	A	4008	BCR	1	0
13	B	1205	CLA	1	0
17	A	5003	LHG	2	0
13	B	1235	CLA	3	0
16	A	4007	BCR	4	0
13	X	1701	CLA	1	0
16	F	4016	BCR	2	0
16	A	4002	BCR	2	0
13	A	1116	CLA	4	0
13	A	1134	CLA	1	0
16	B	4009	BCR	5	0
13	B	1220	CLA	3	0
13	A	1128	CLA	6	0
13	B	1234	CLA	2	0
13	B	1219	CLA	4	0
16	B	4006	BCR	4	0
13	B	1238	CLA	3	0
13	K	1401	CLA	1	0
13	A	1137	CLA	3	0

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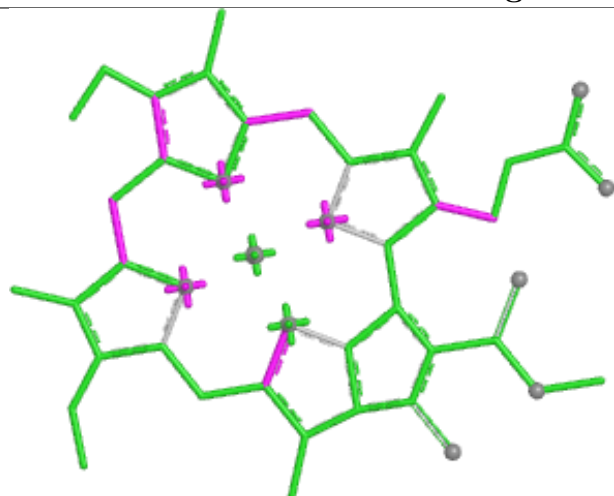
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1222	CLA	2	0
13	B	1217	CLA	3	0
13	A	1123	CLA	4	0
13	A	1106	CLA	5	0
13	B	1230	CLA	5	0
16	B	4010	BCR	2	0
13	A	1103	CLA	6	0
13	A	1131	CLA	1	0
16	A	4001	BCR	2	0
13	B	1216	CLA	1	0

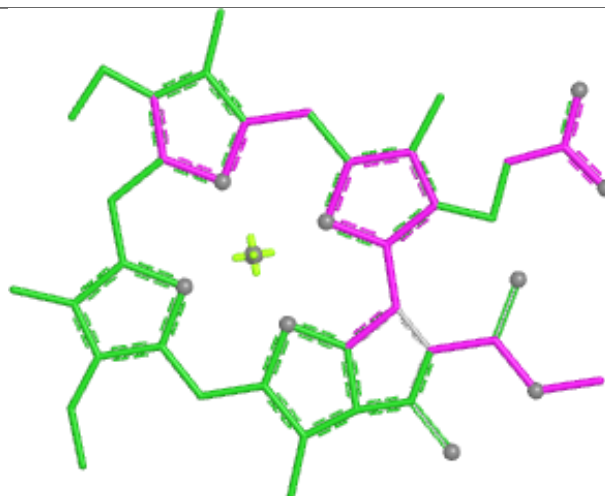
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



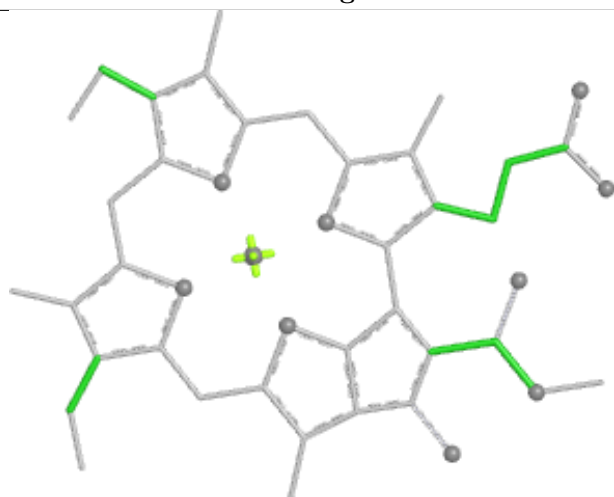
Ligand CLA B 1232



Bond lengths



Bond angles

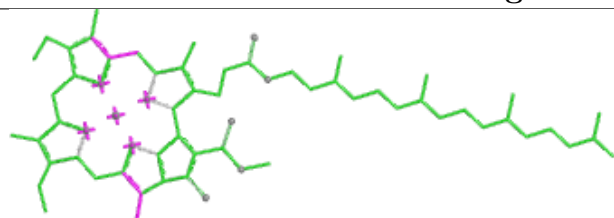


Torsions

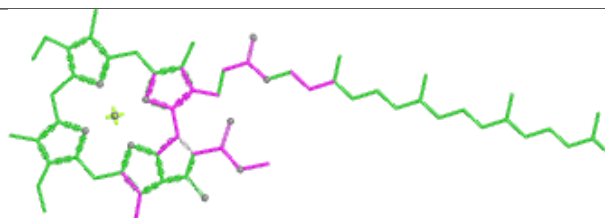


Rings

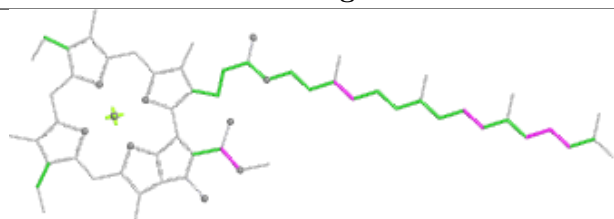
Ligand CLA B 1207



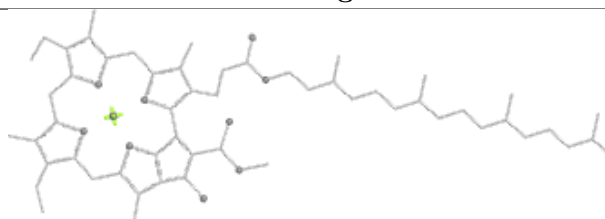
Bond lengths



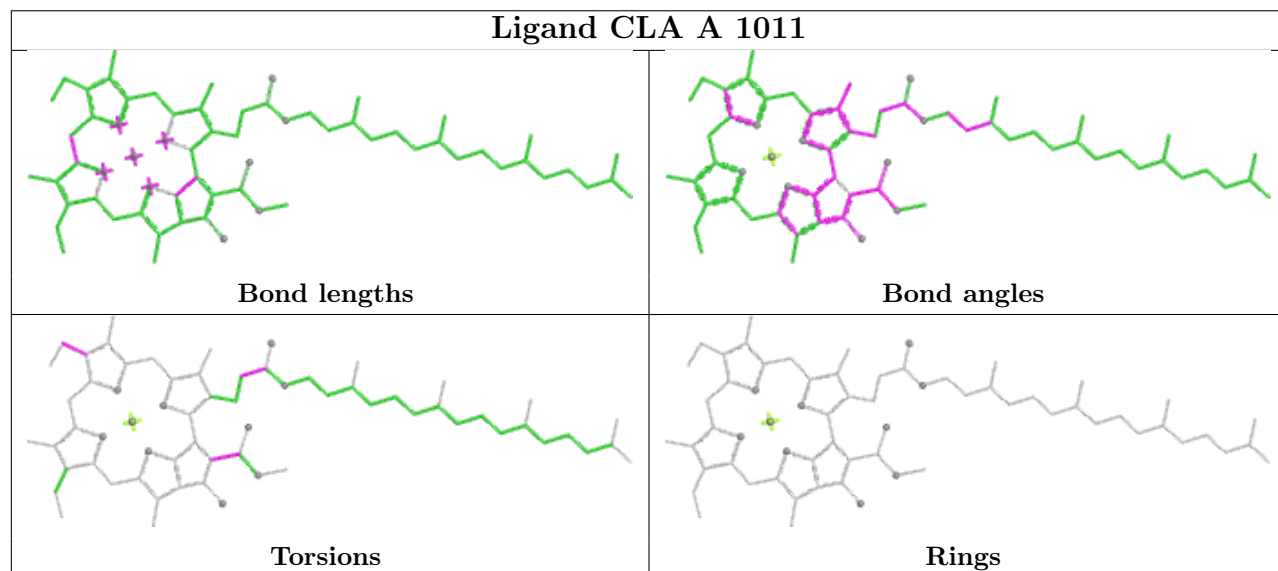
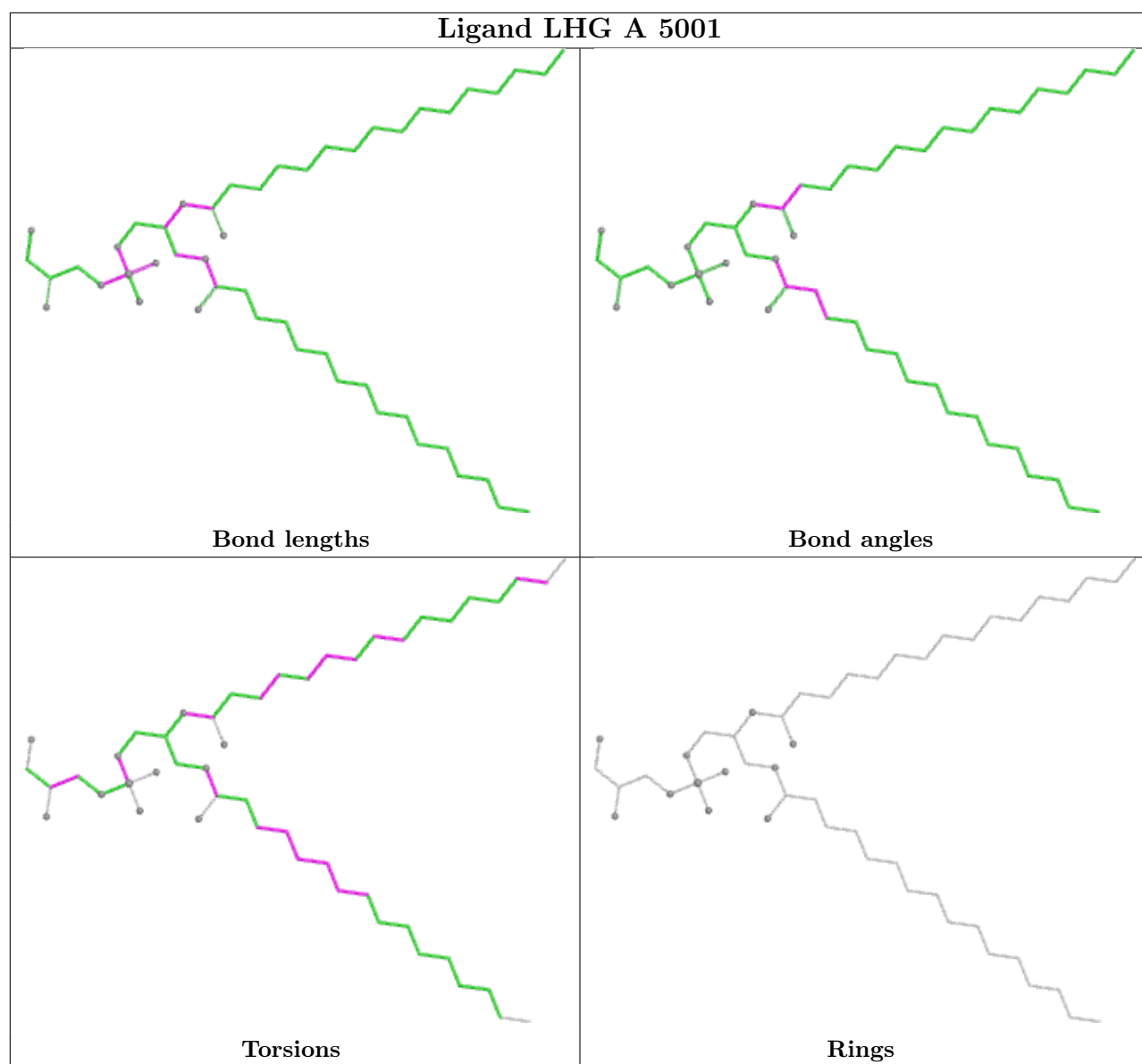
Bond angles

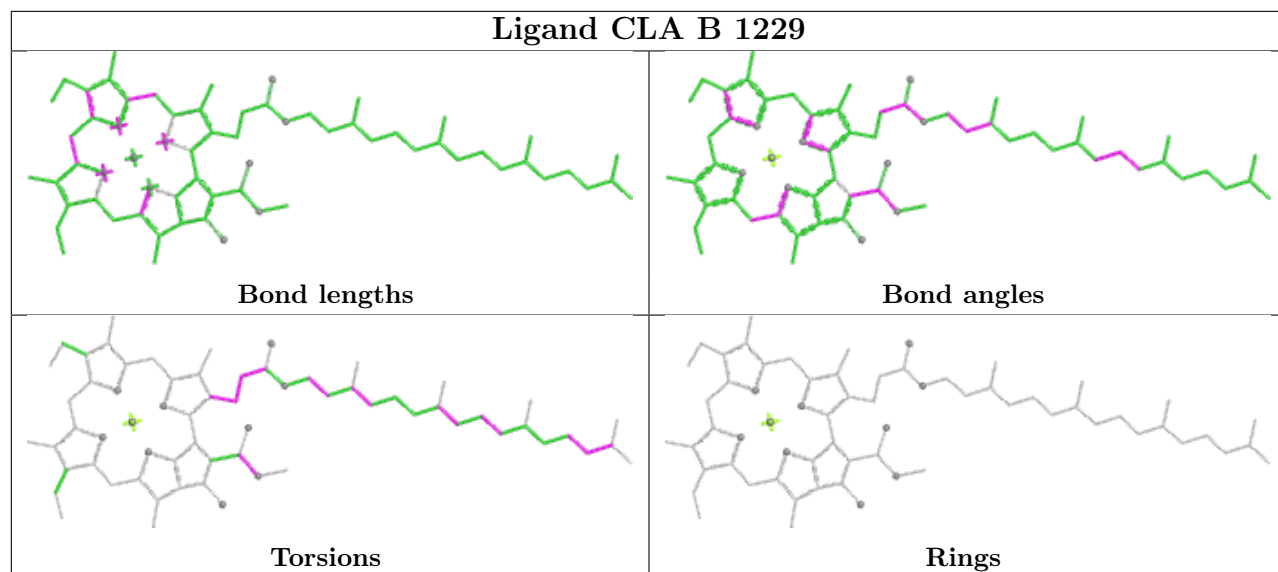
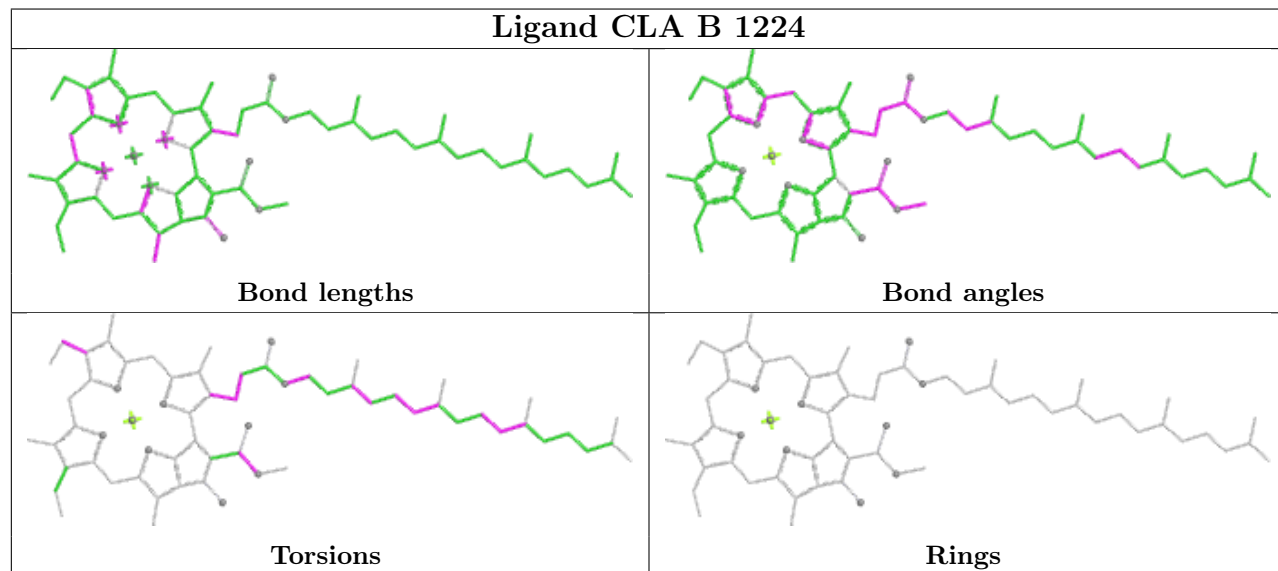


Torsions

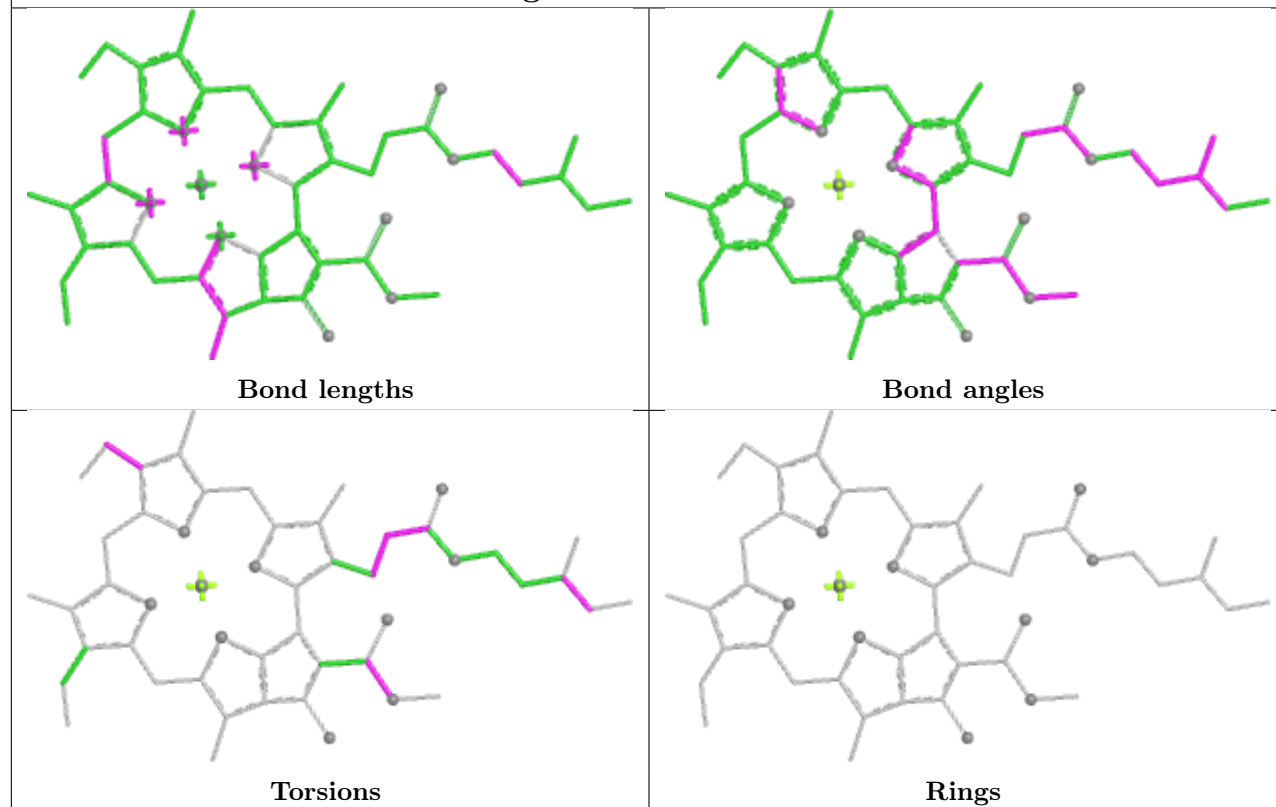


Rings

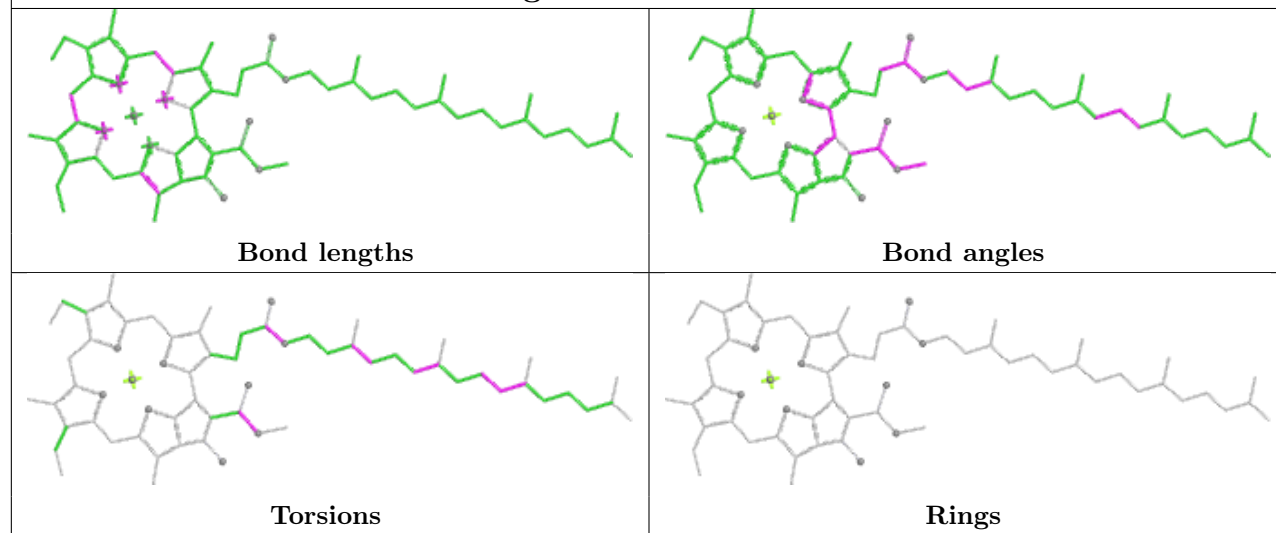


Ligand CLA B 1229**Ligand CLA B 1224**

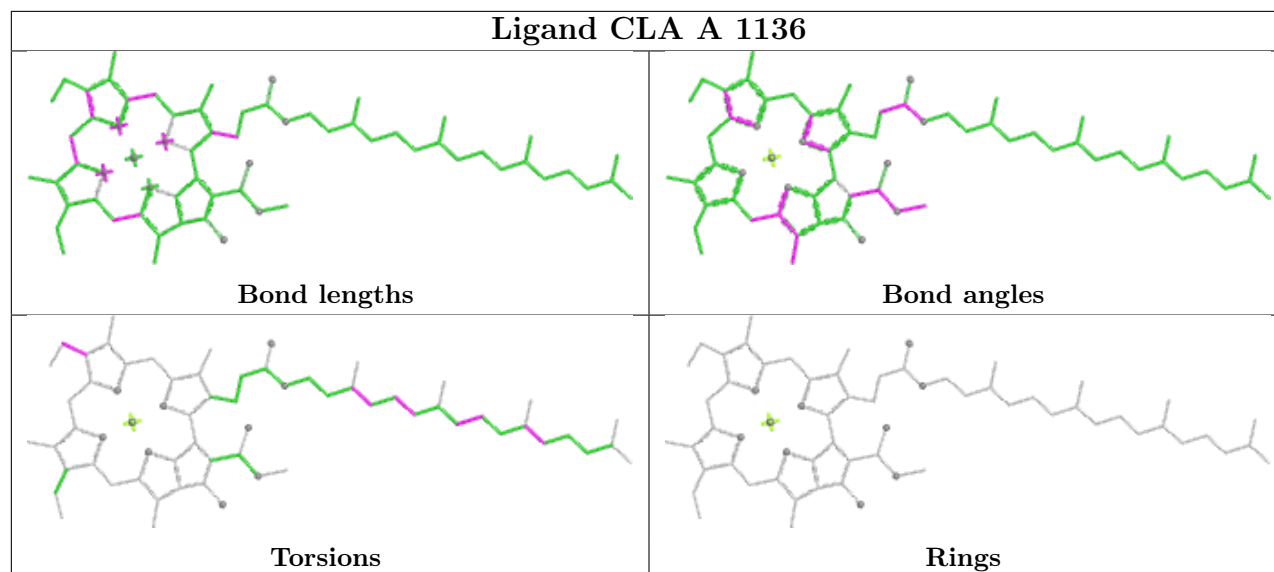
Ligand CLA A 1105



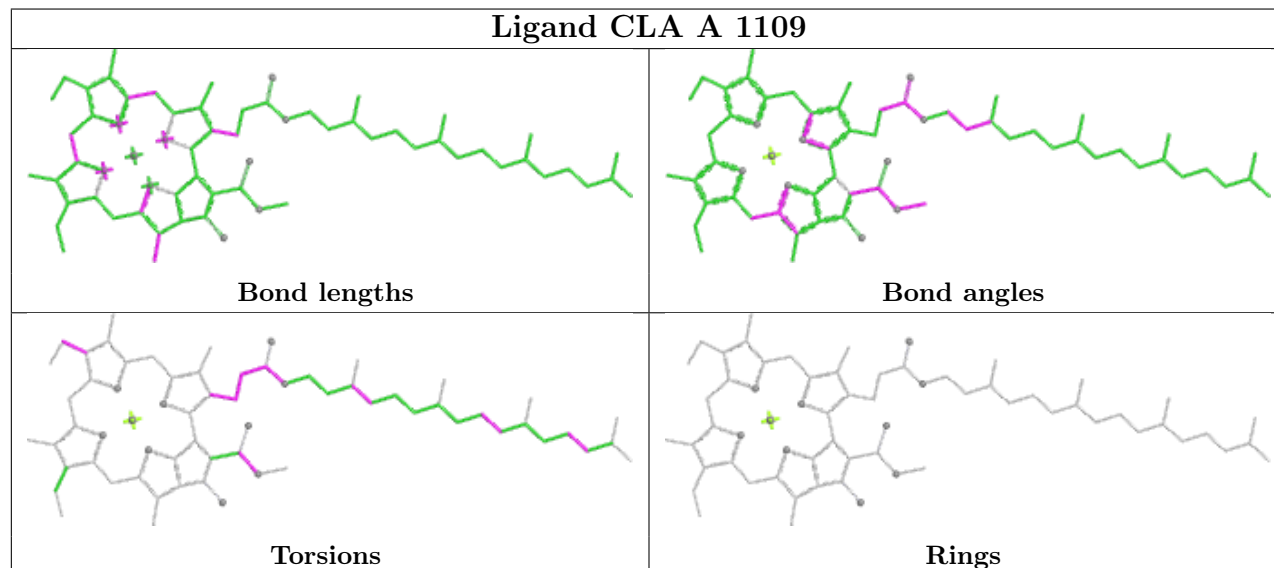
Ligand CLA B 1223



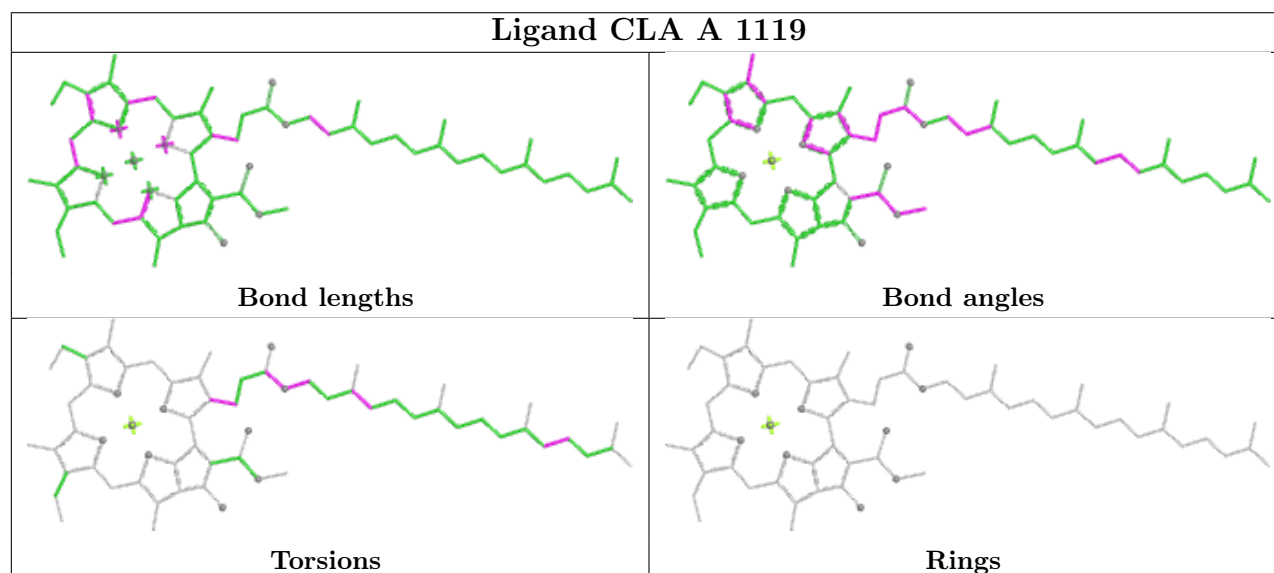
Ligand CLA A 1136

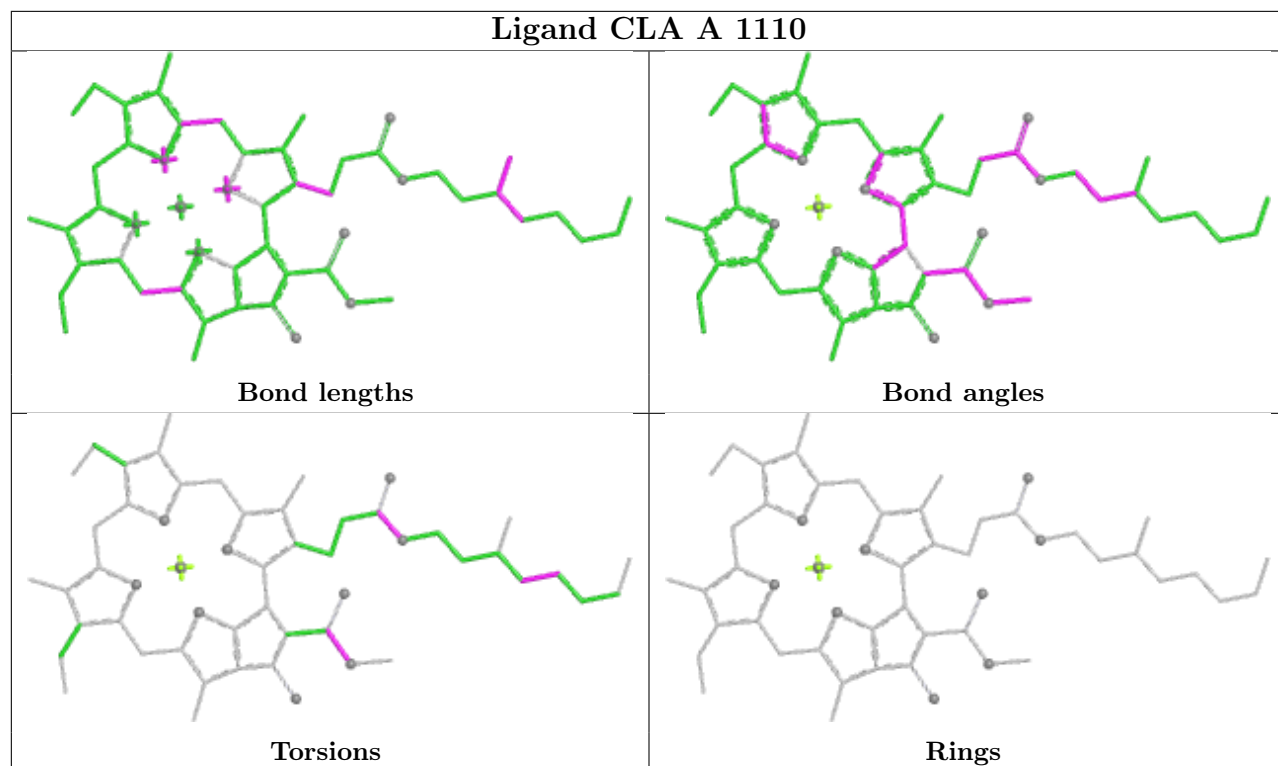


Ligand CLA A 1109

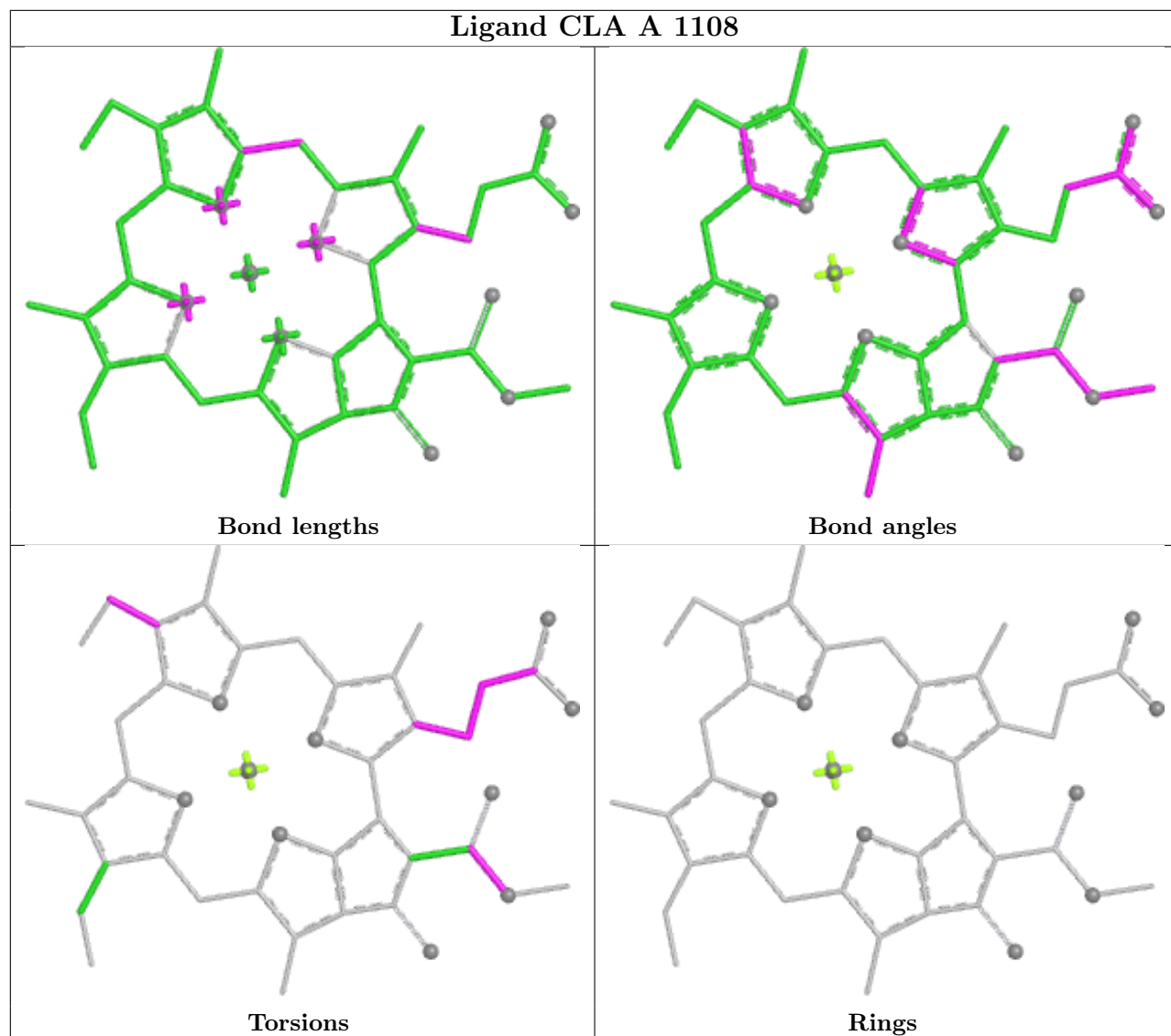


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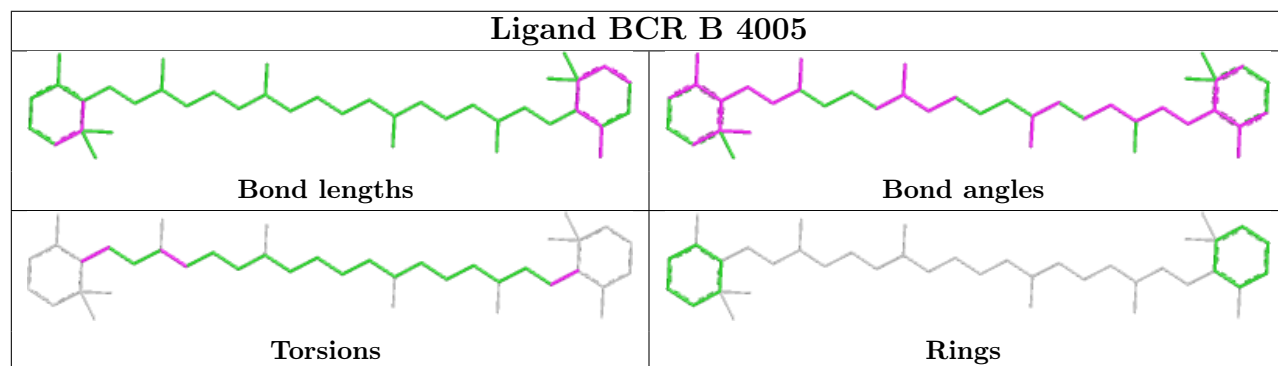


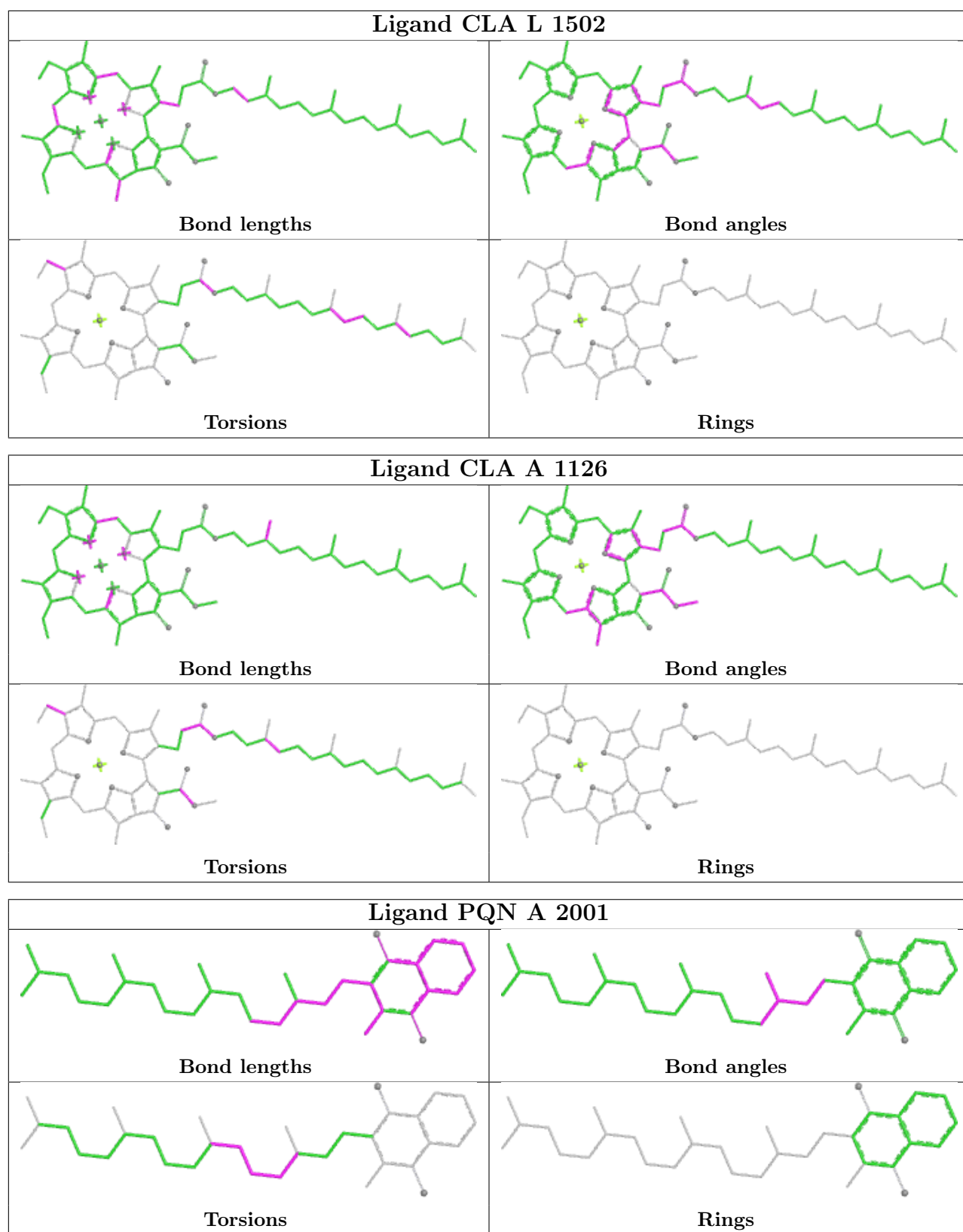


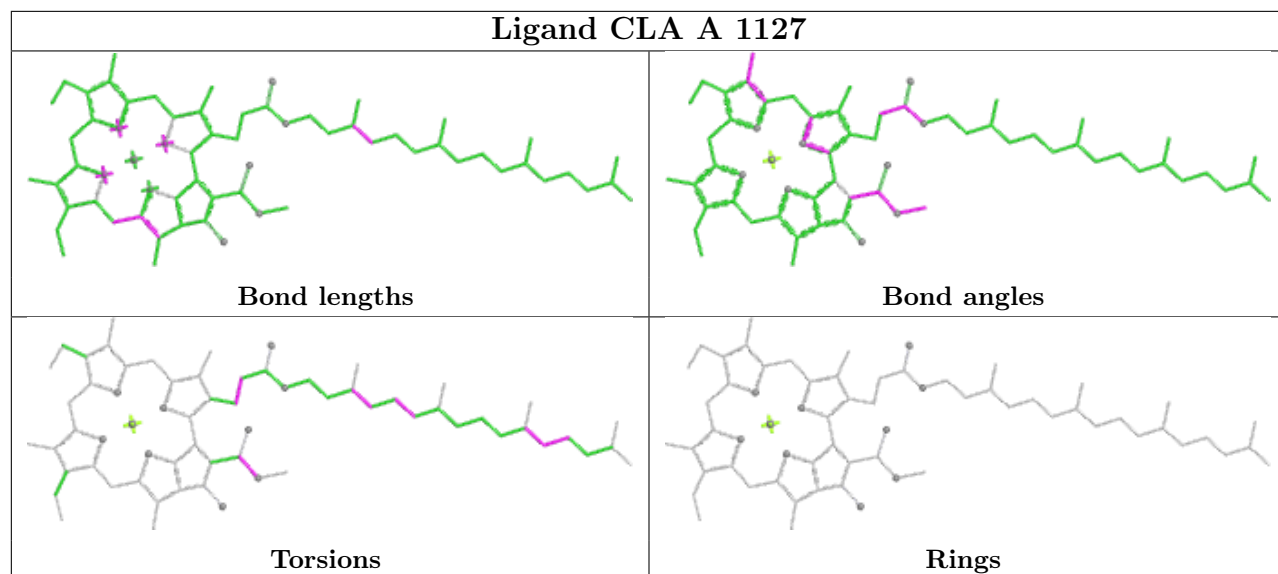
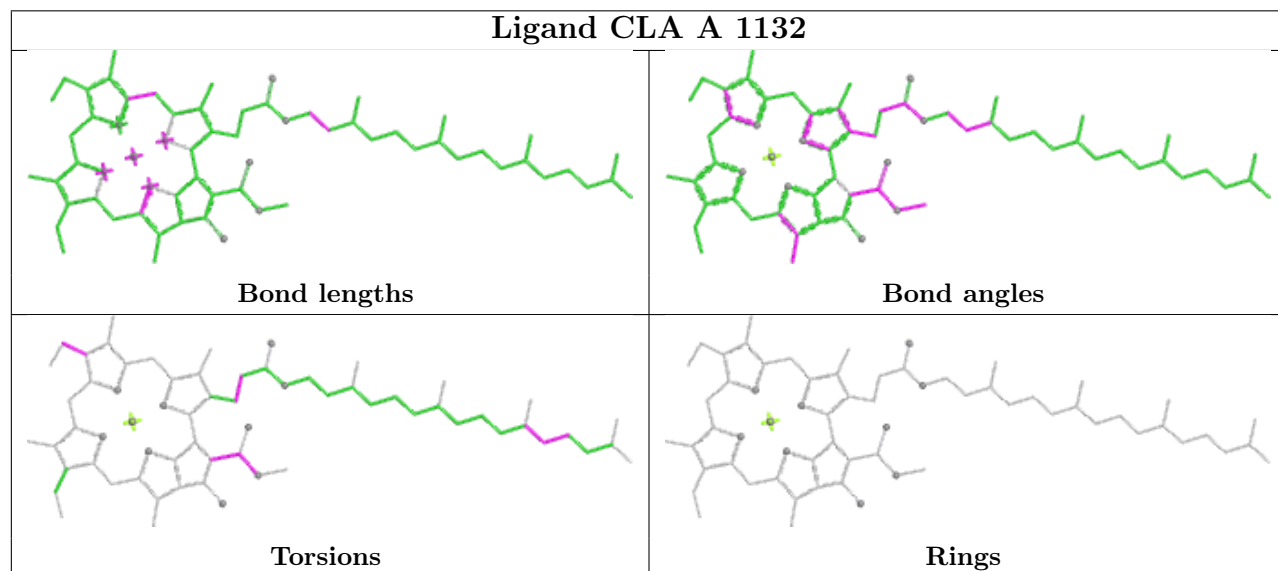
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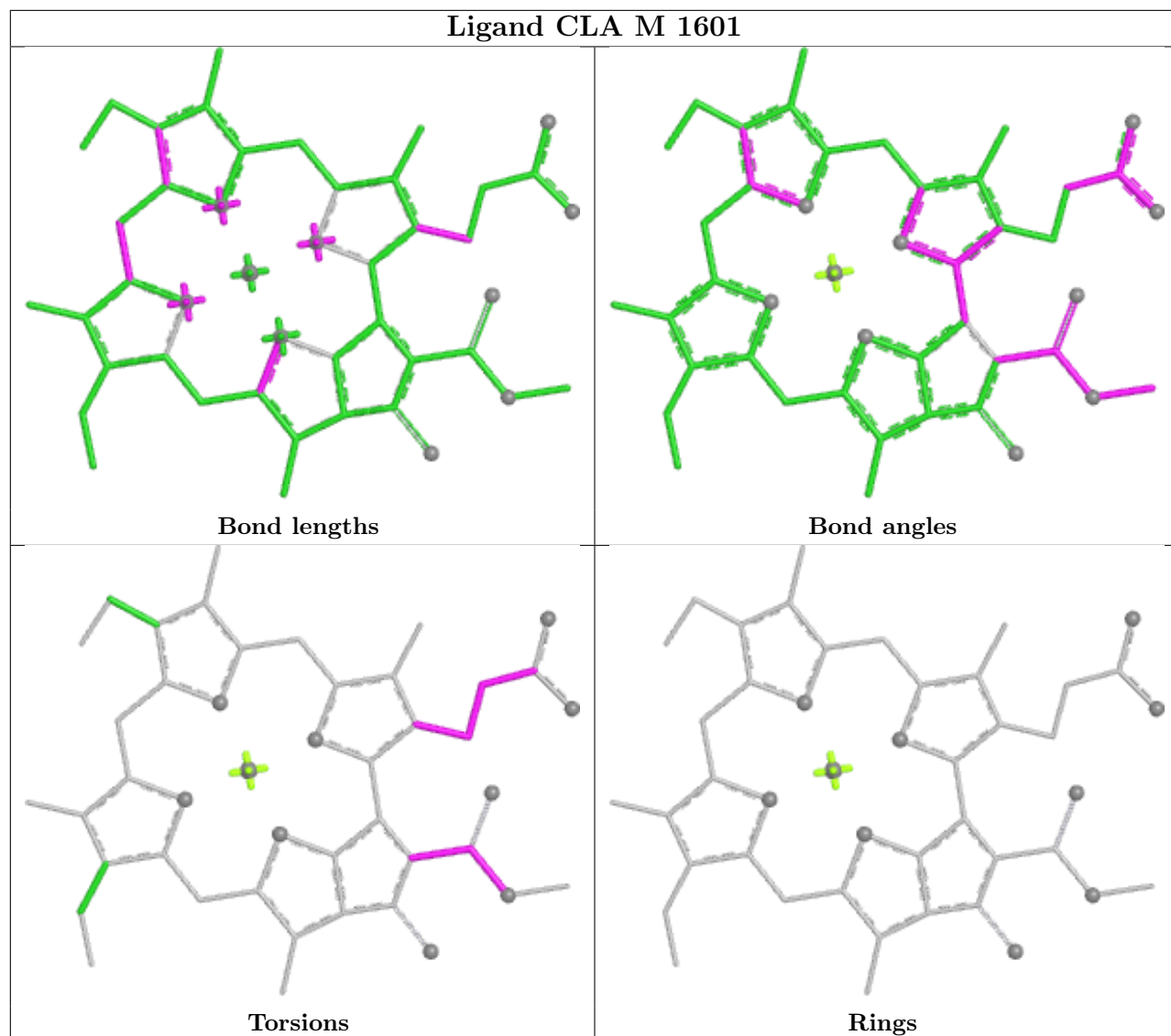
Ligand BCR B 4005



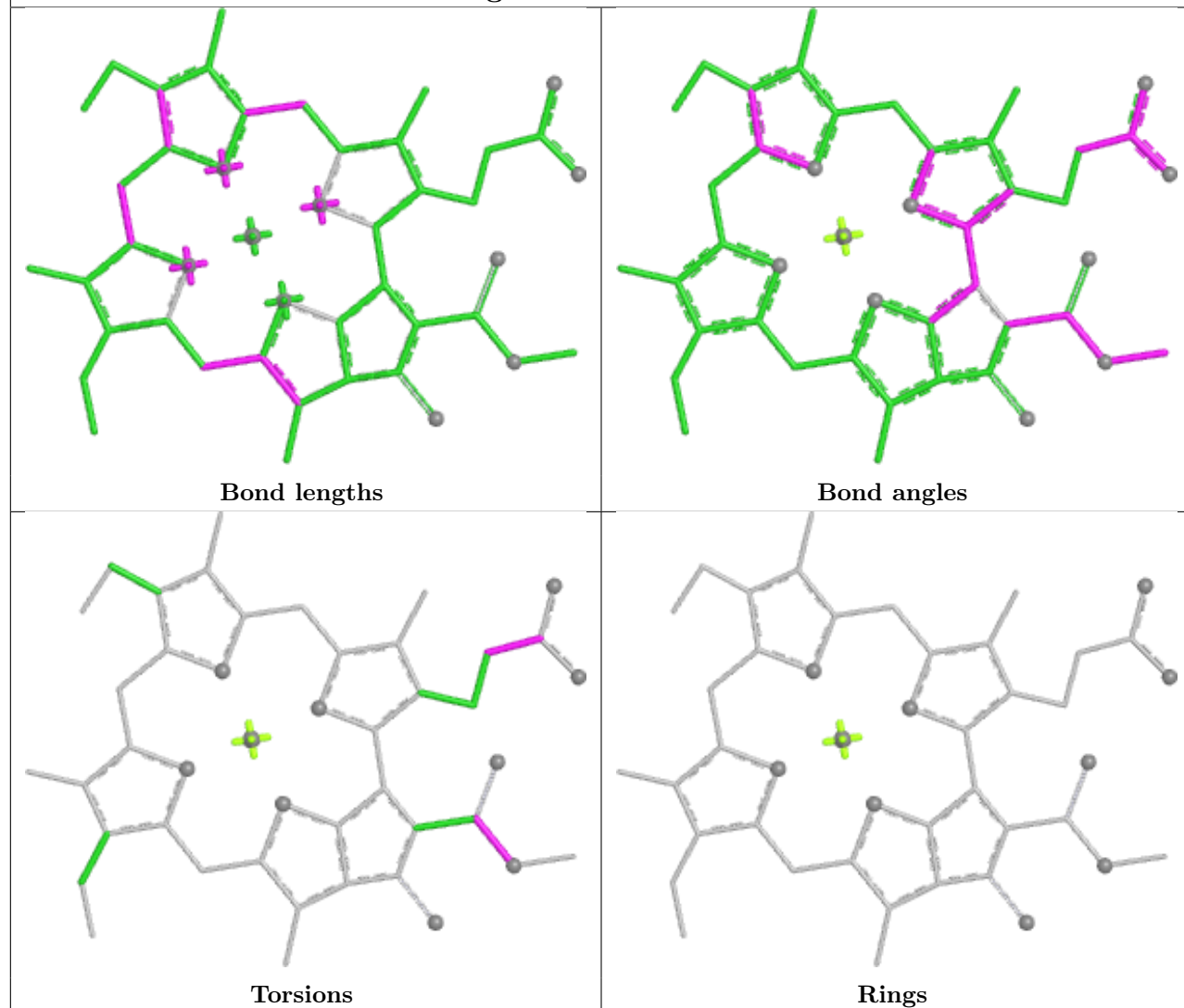


Ligand CLA A 1127**Ligand CLA A 1132**

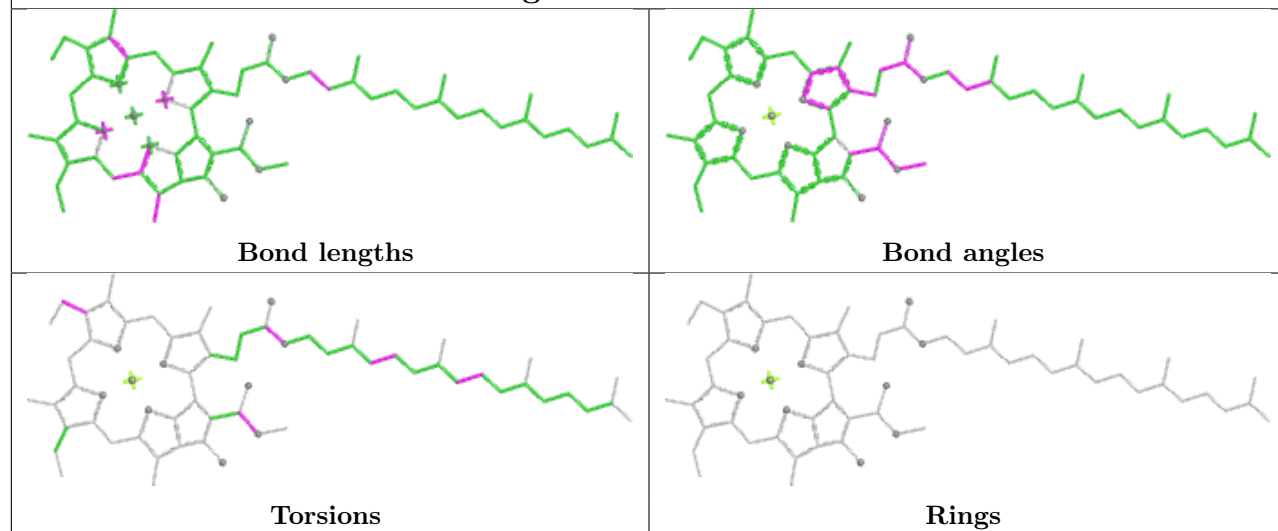
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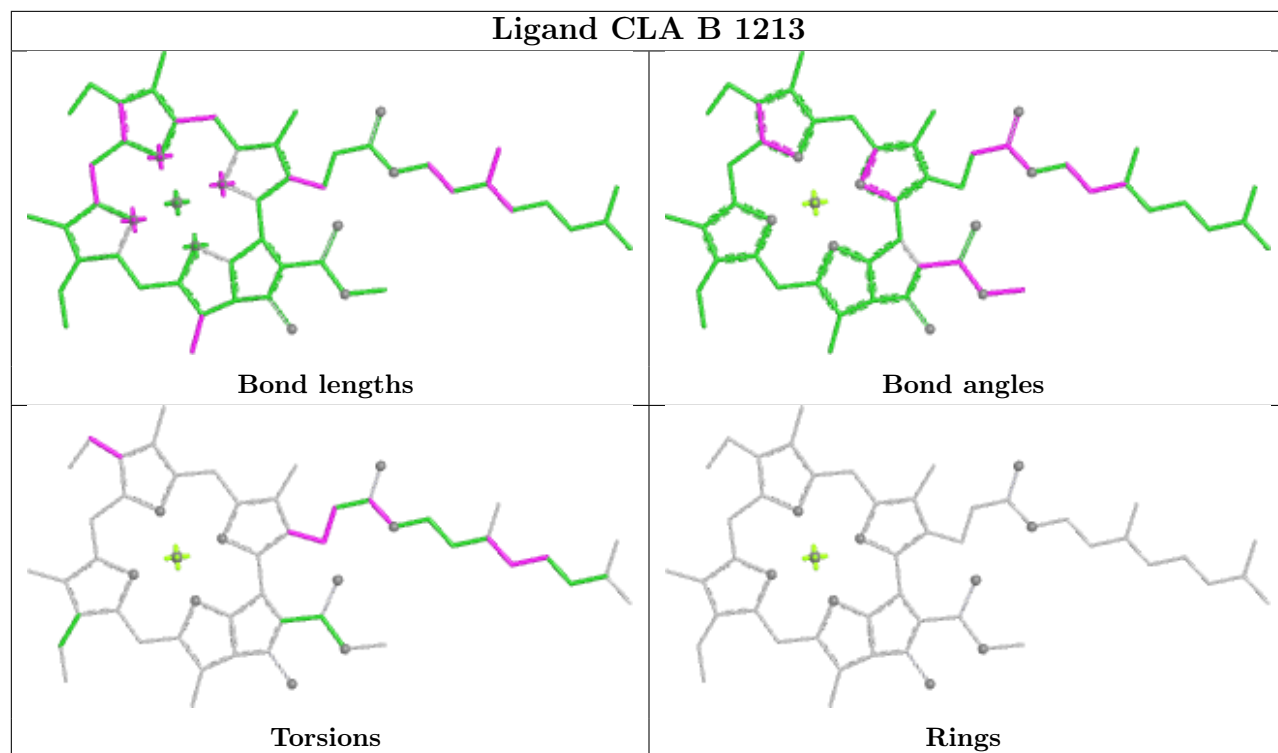
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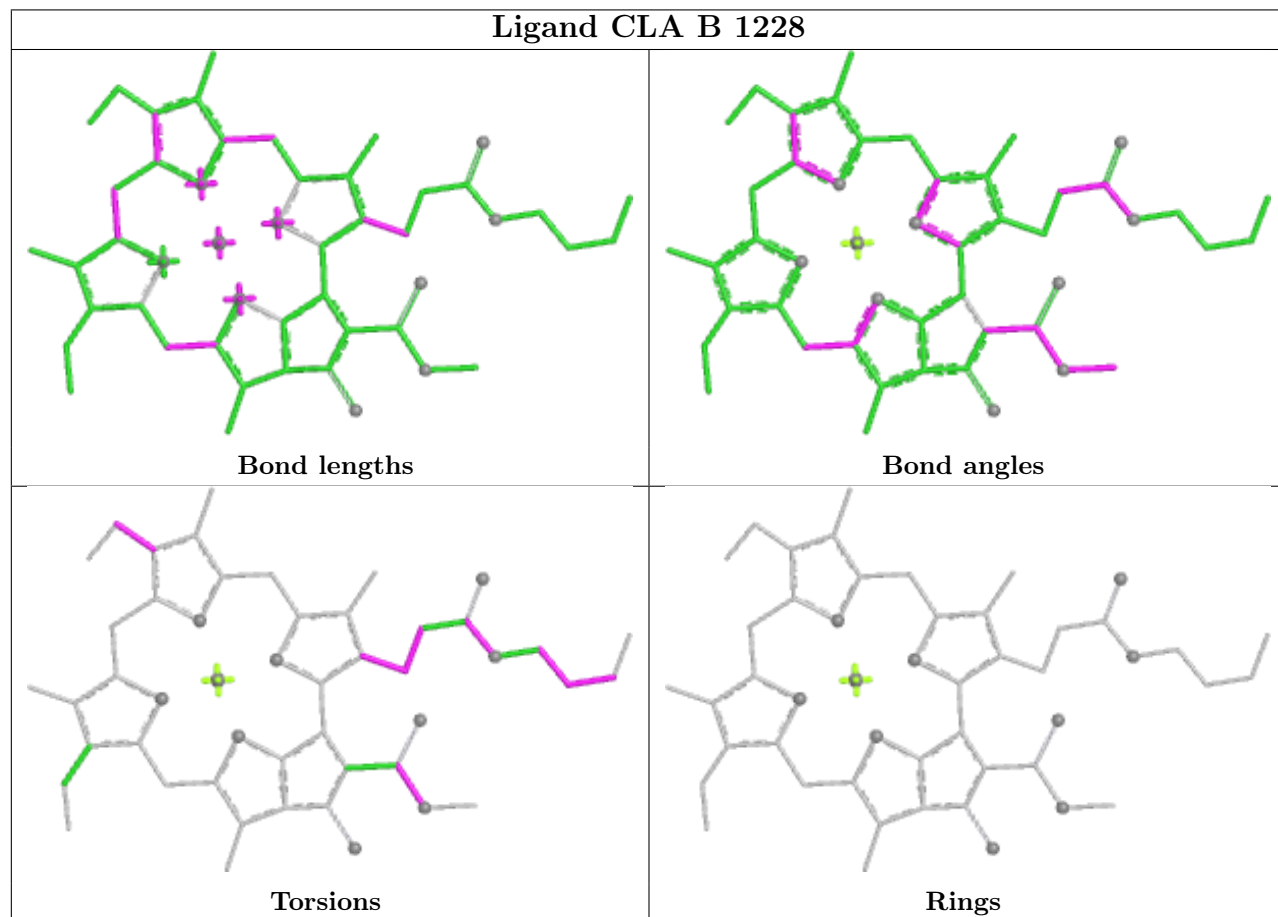
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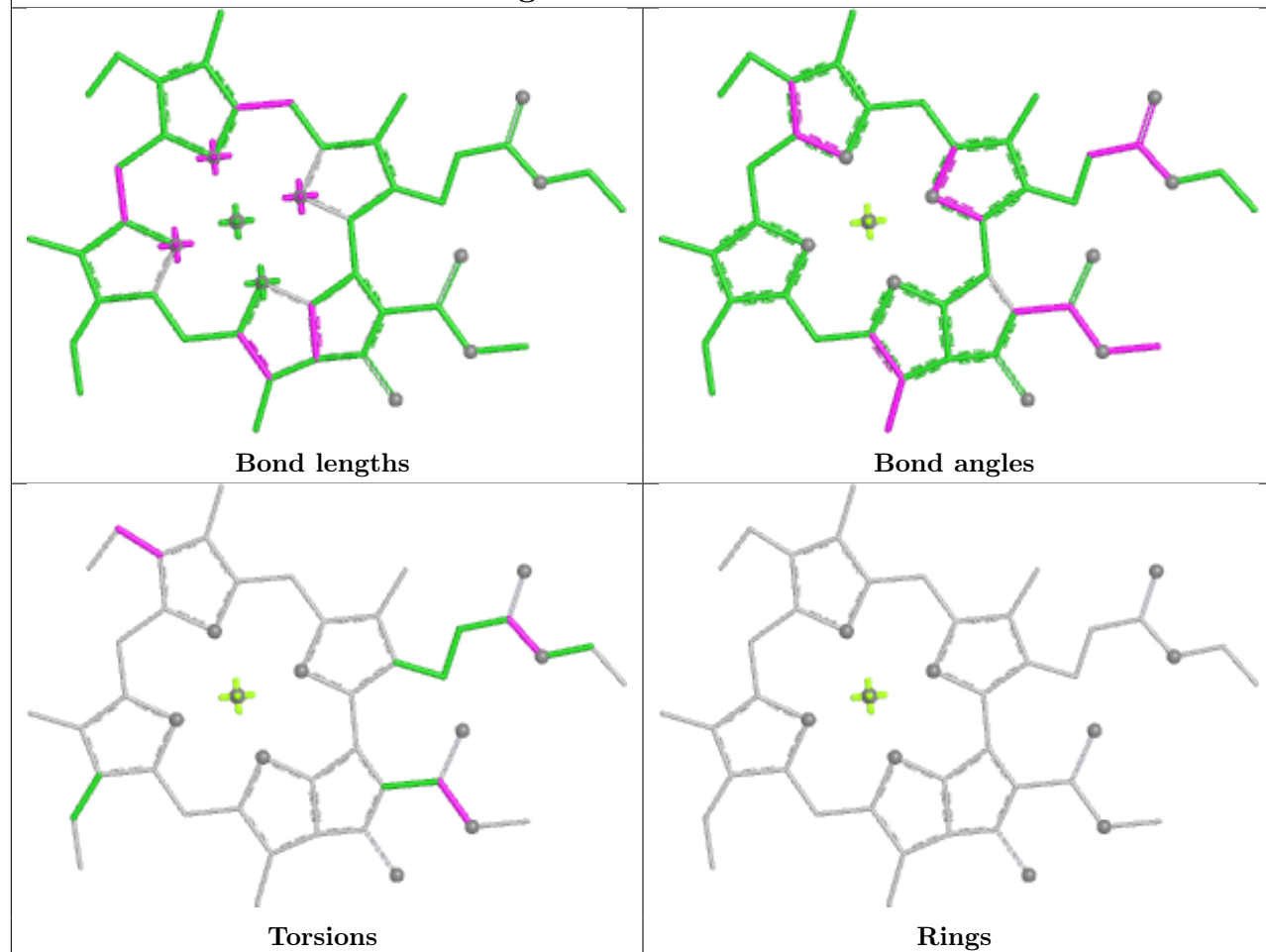
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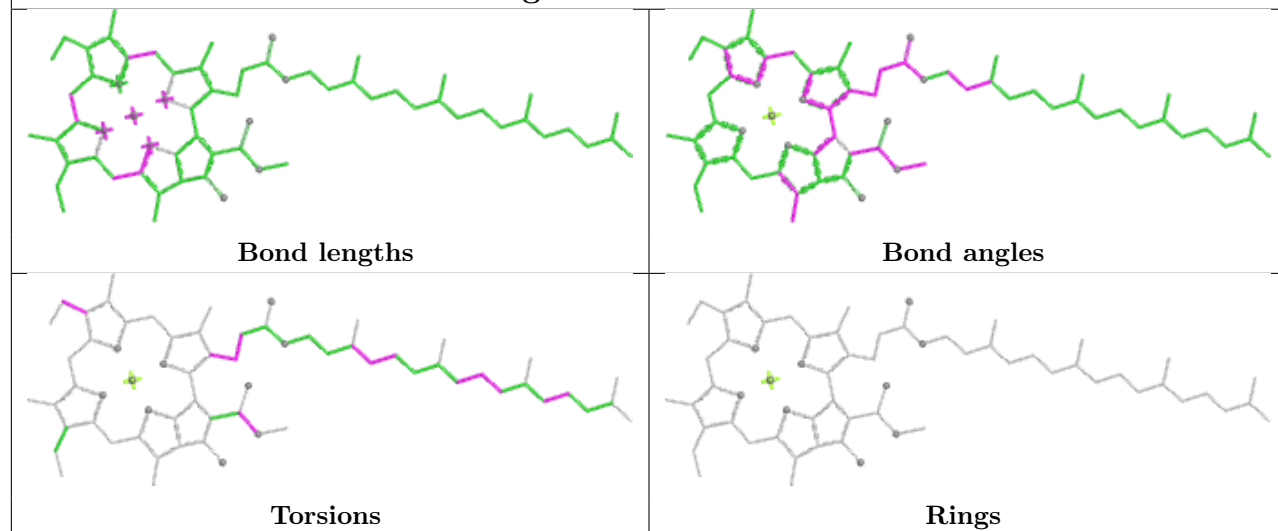
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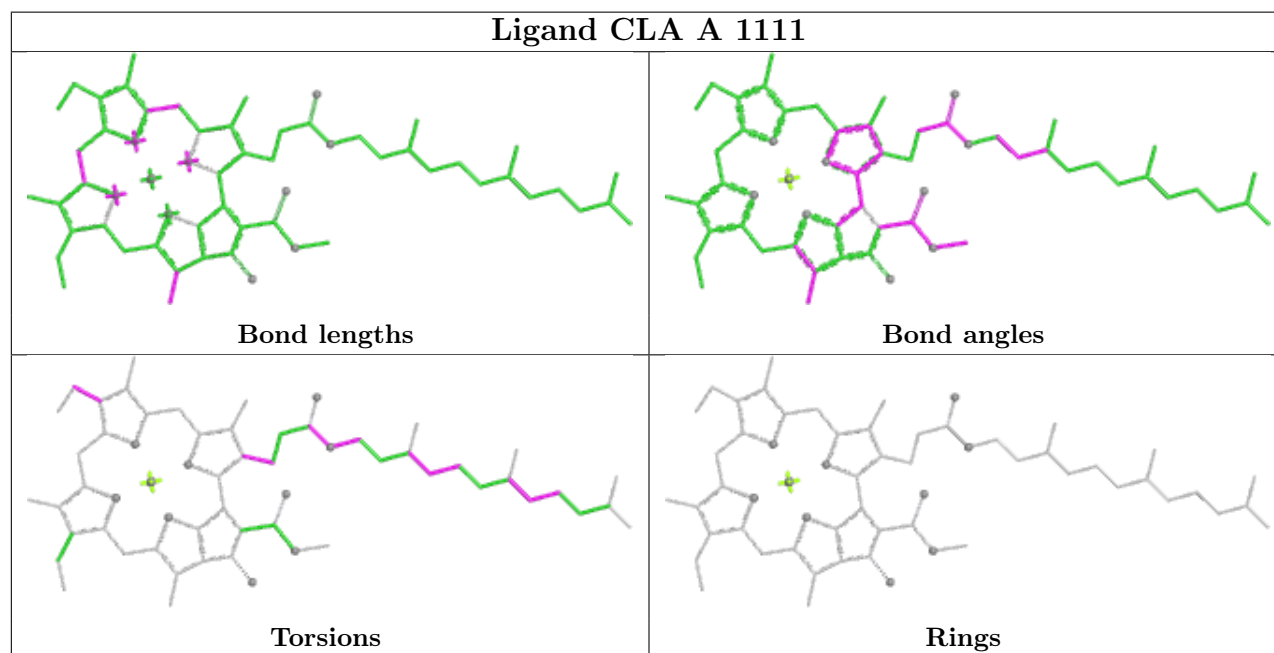
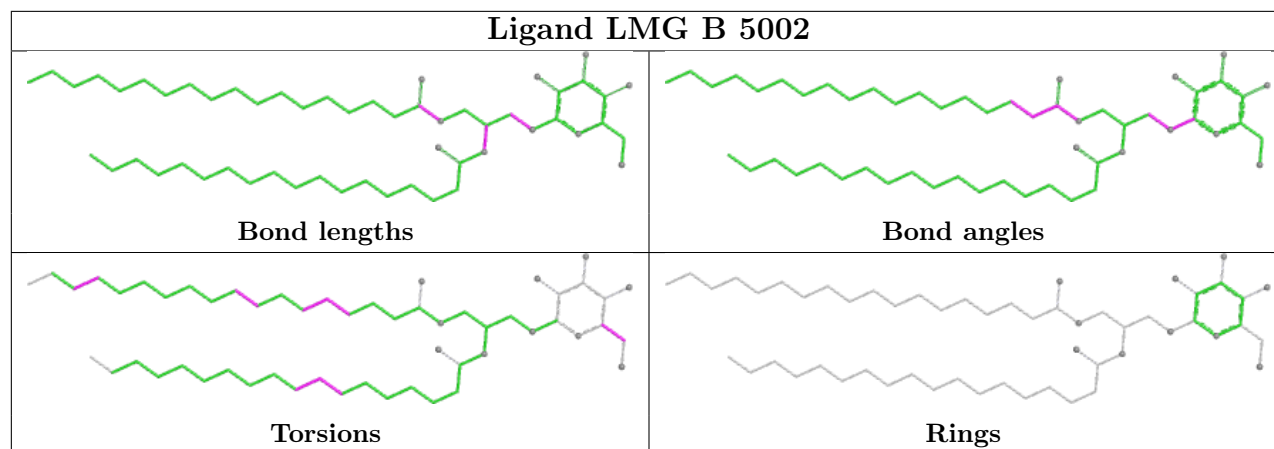


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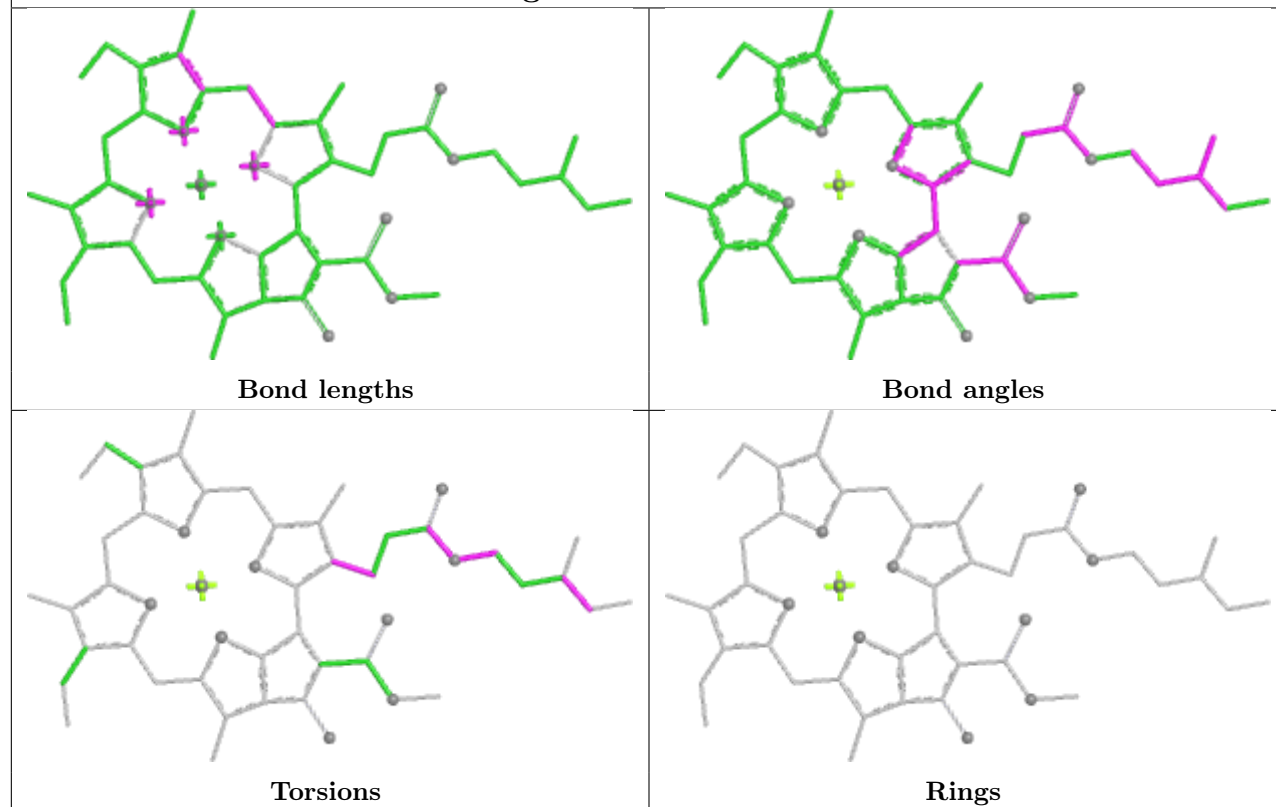


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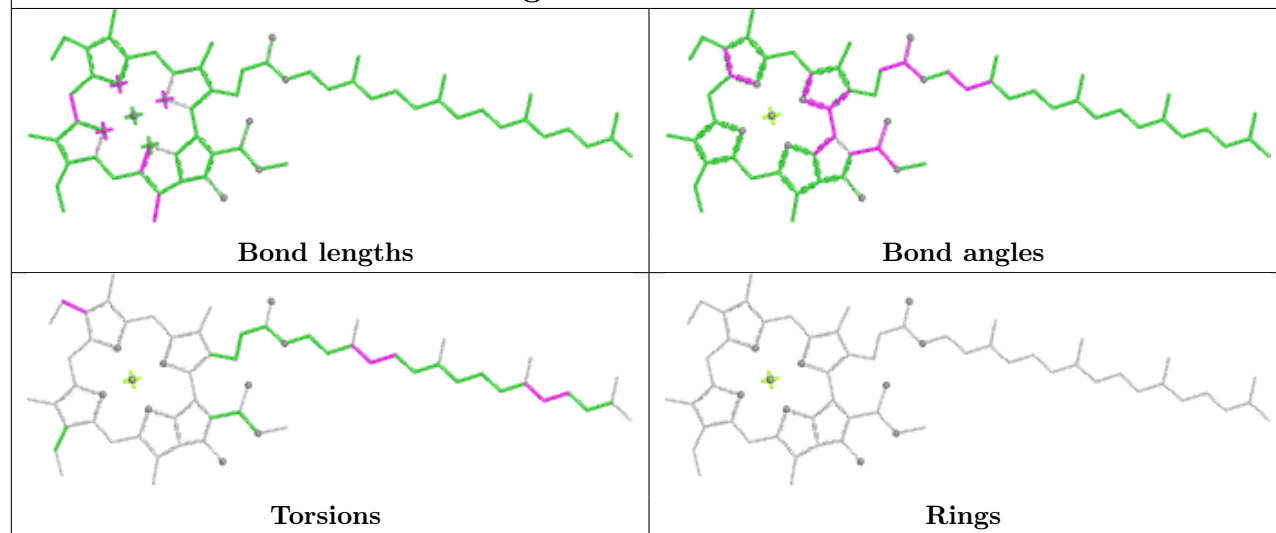


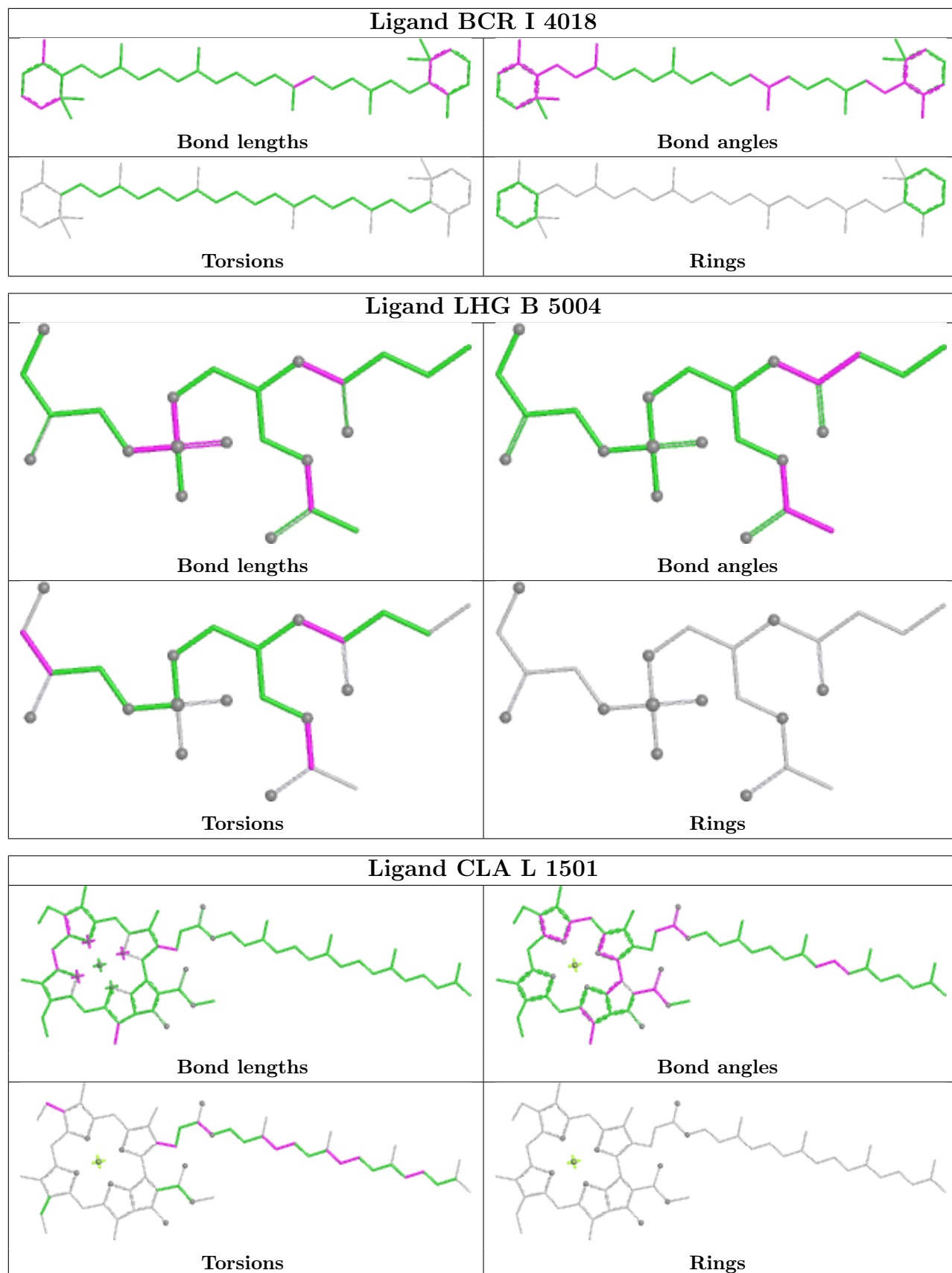


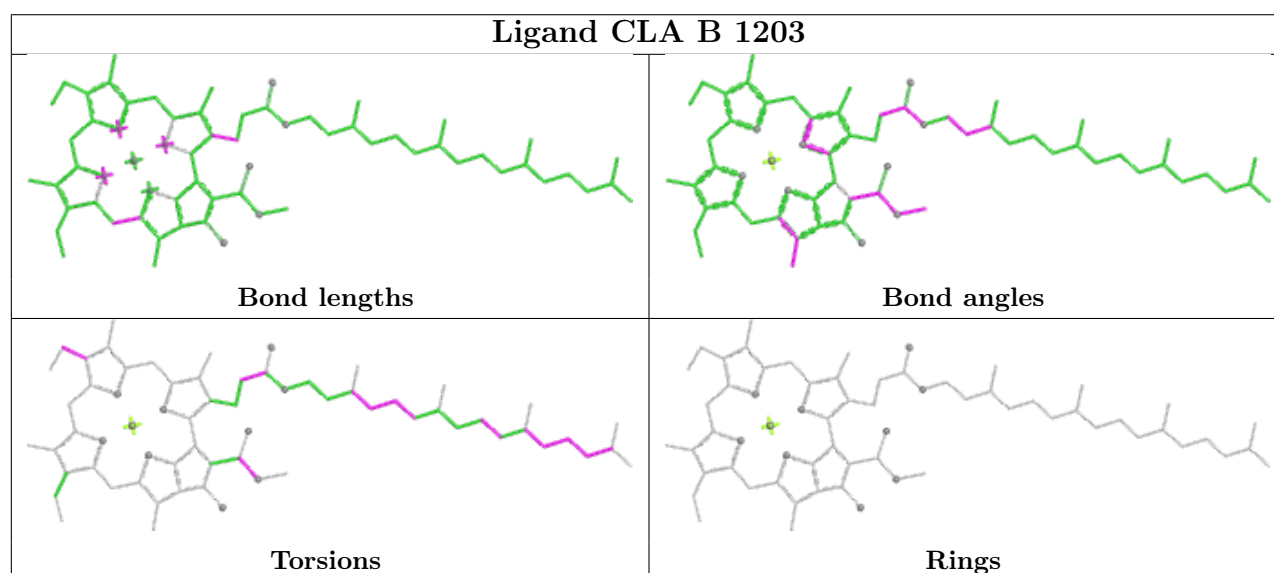
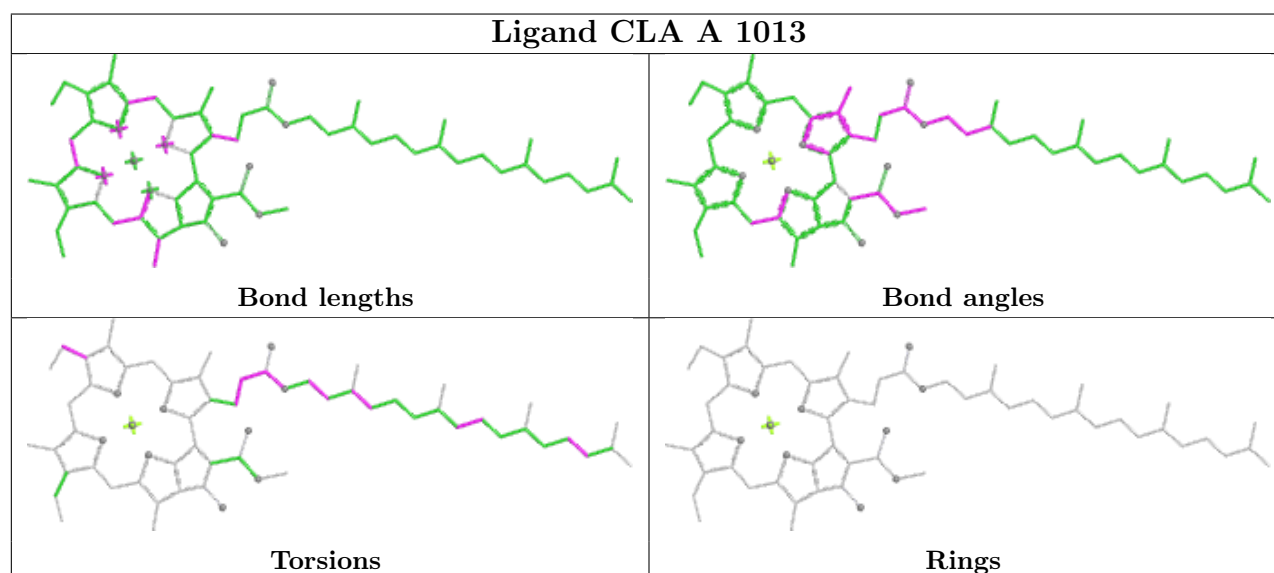
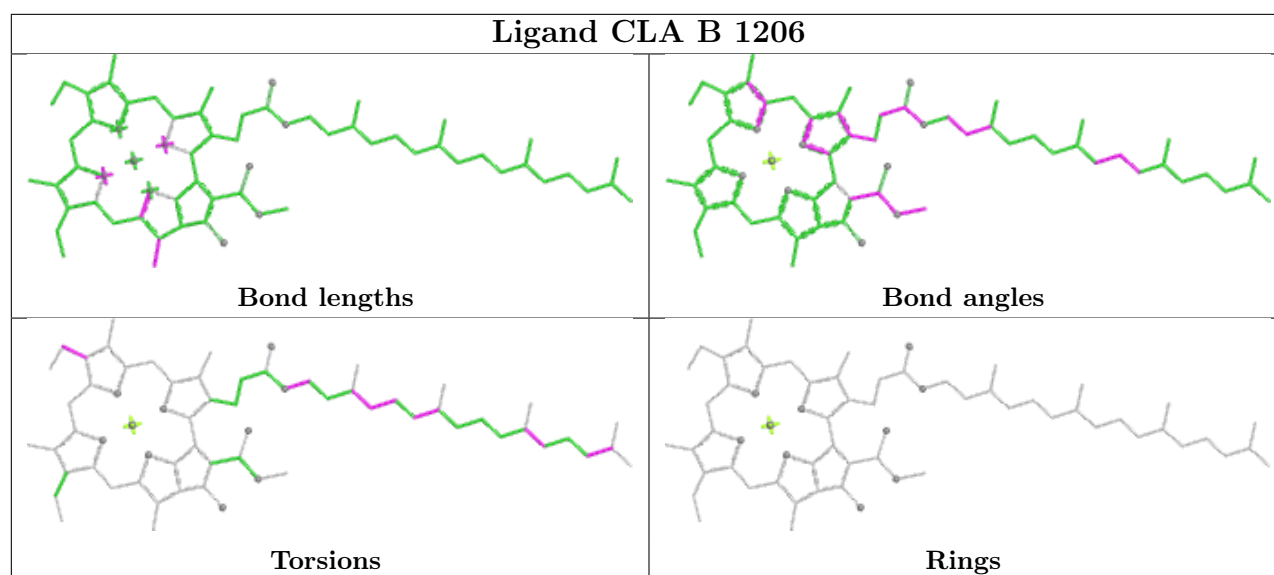
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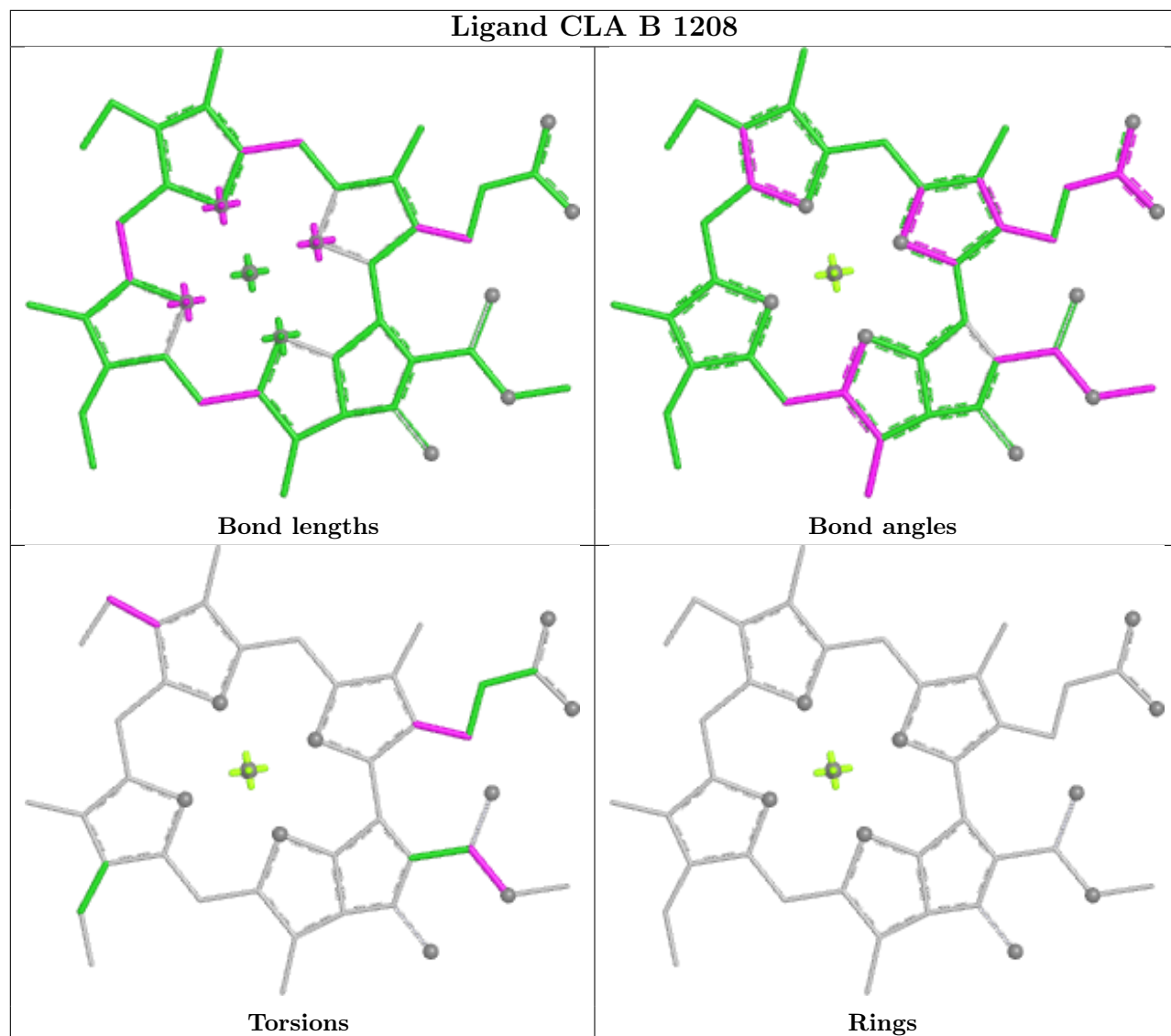
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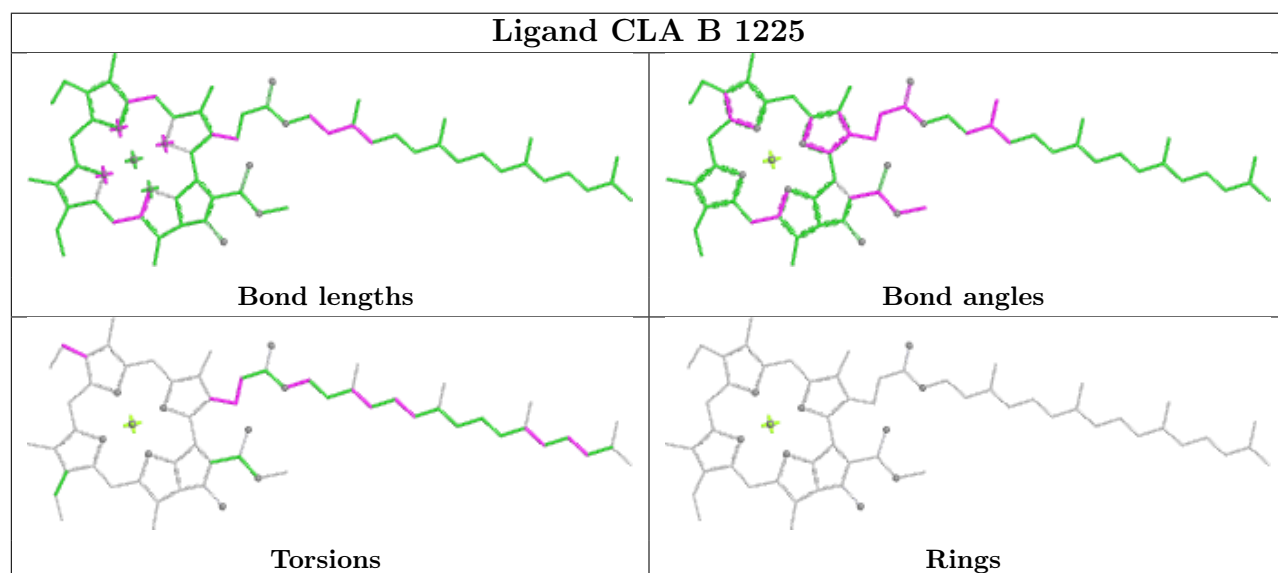
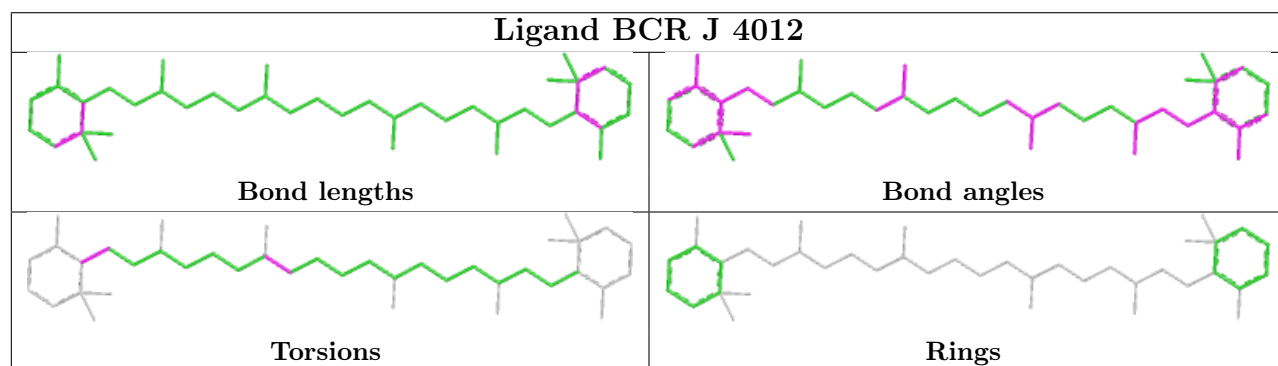
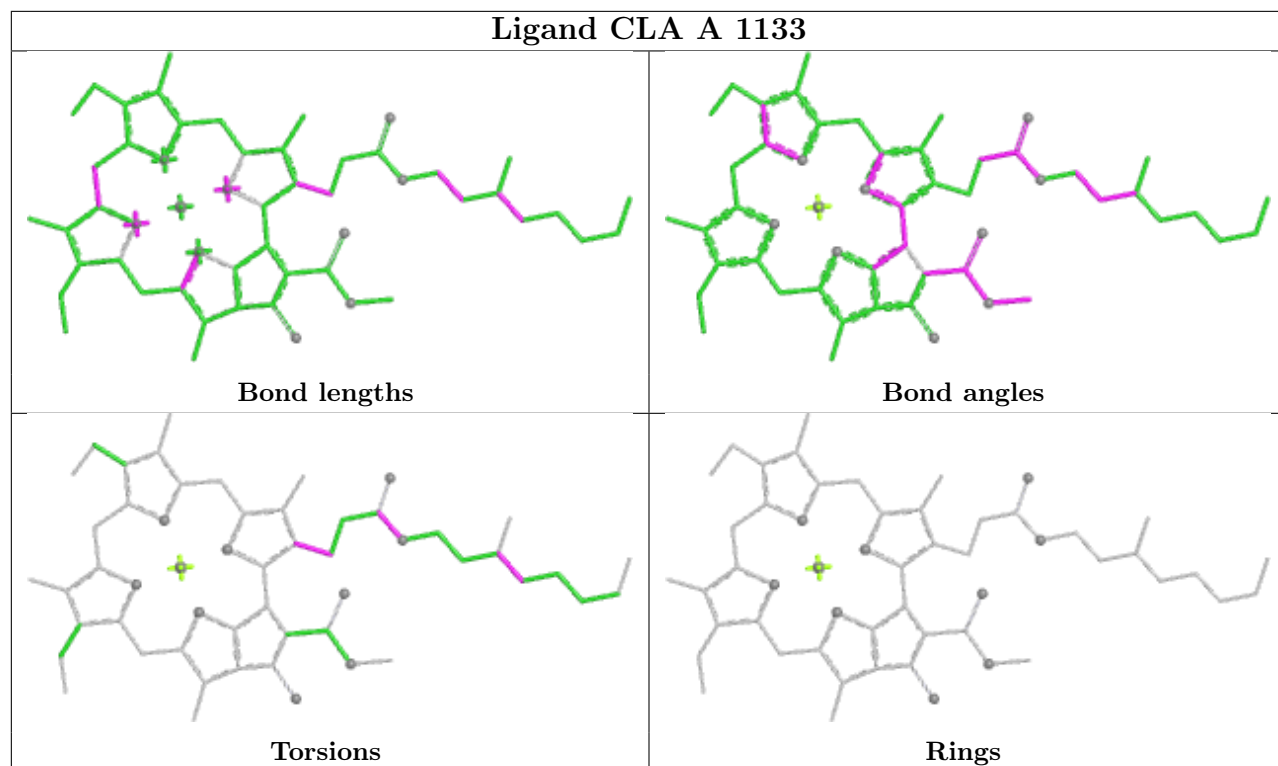




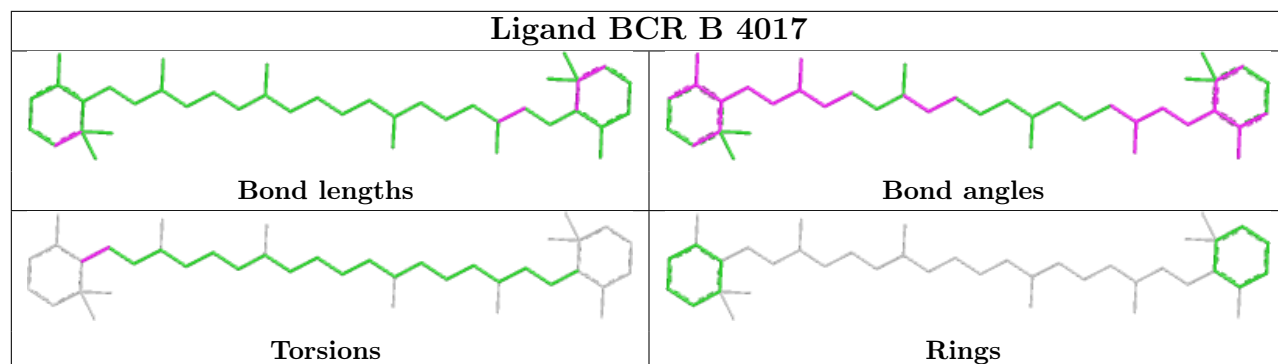


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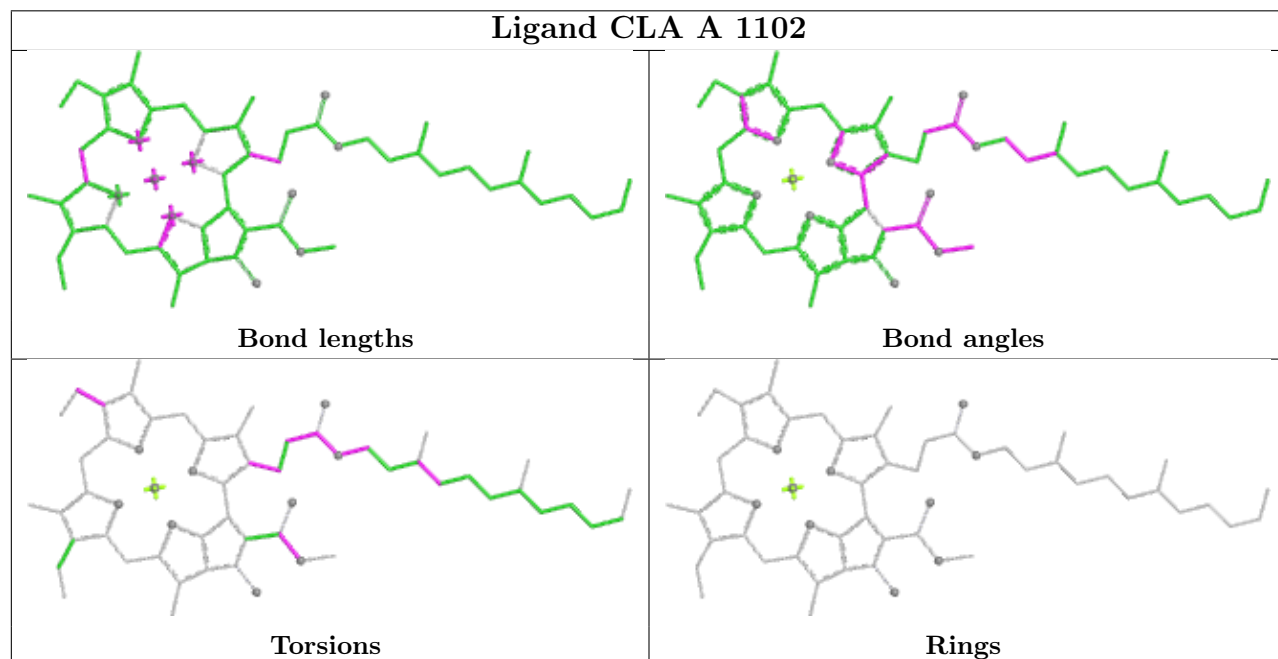




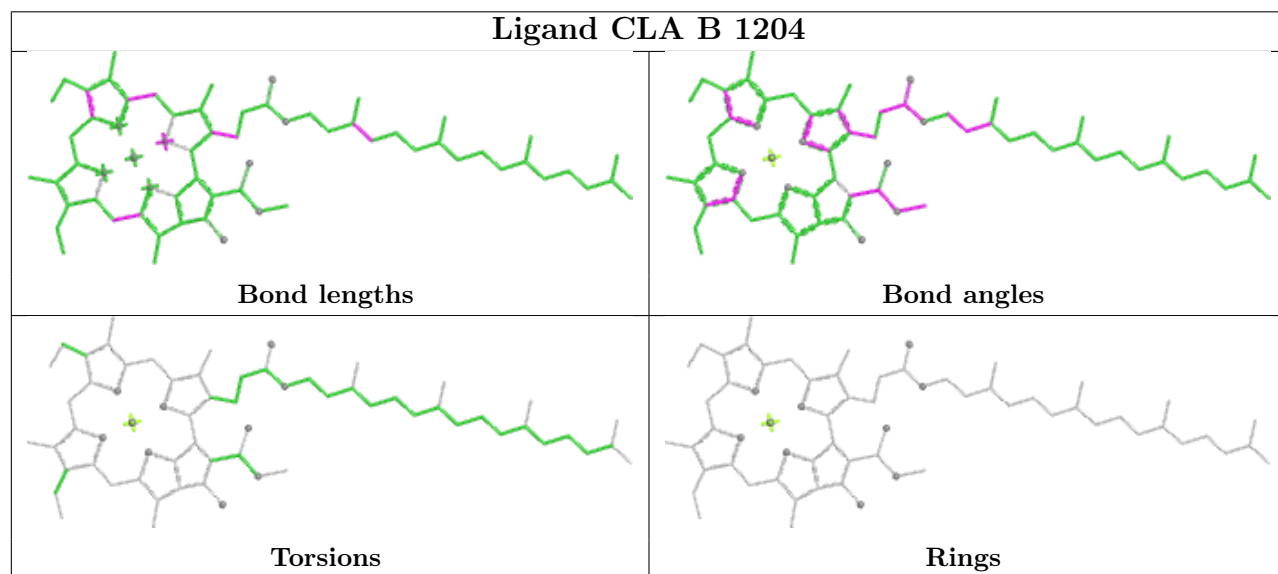
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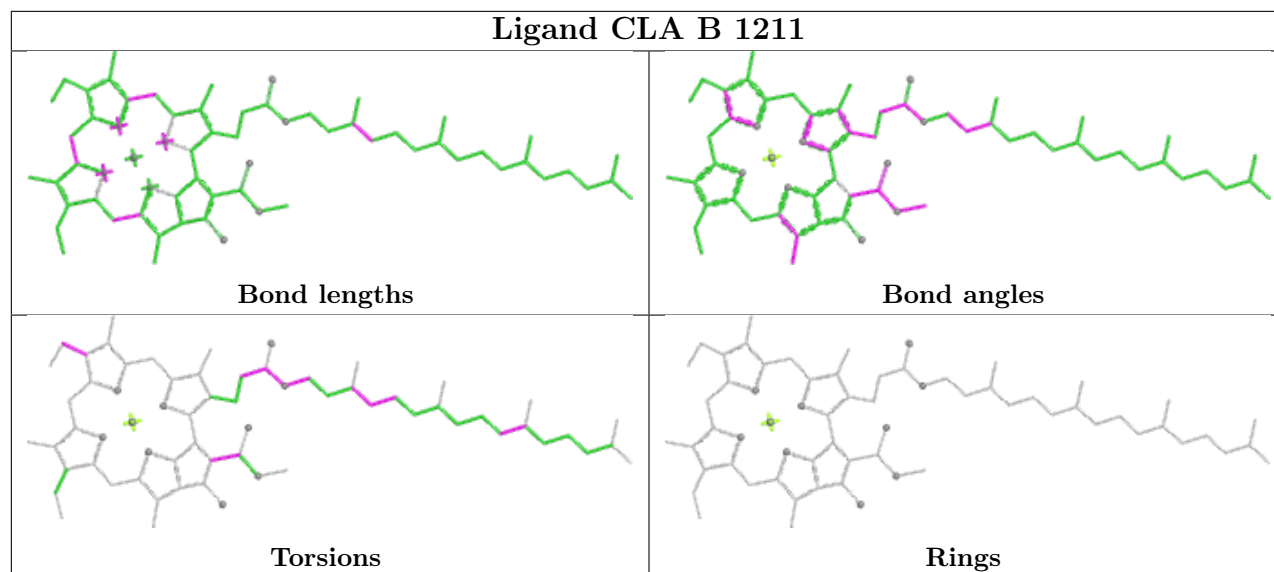
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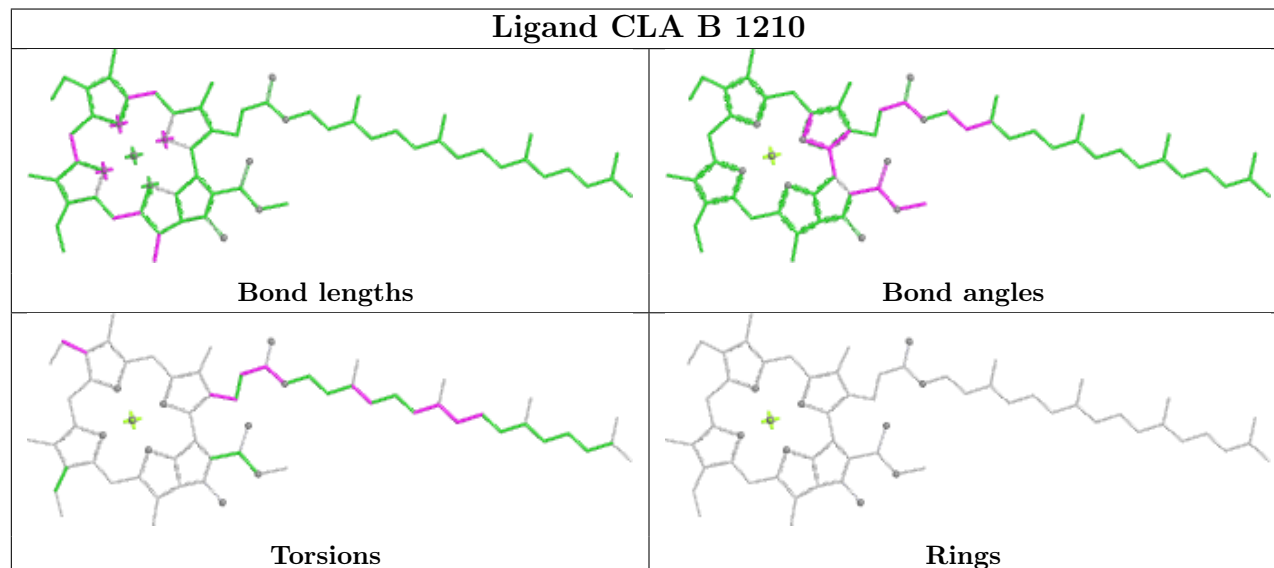
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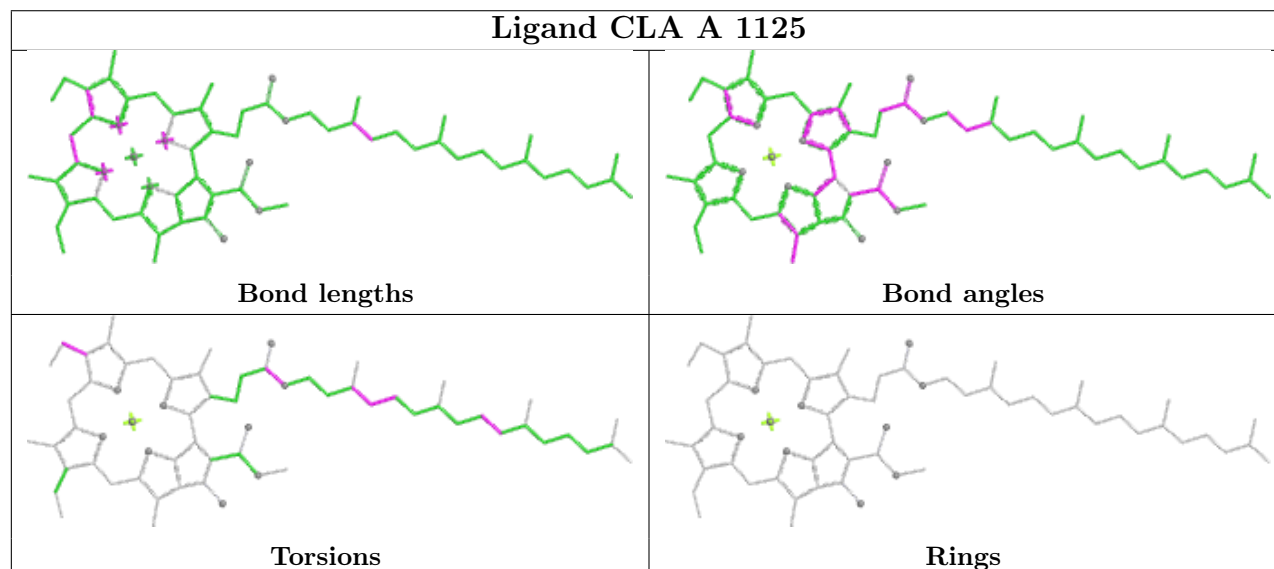
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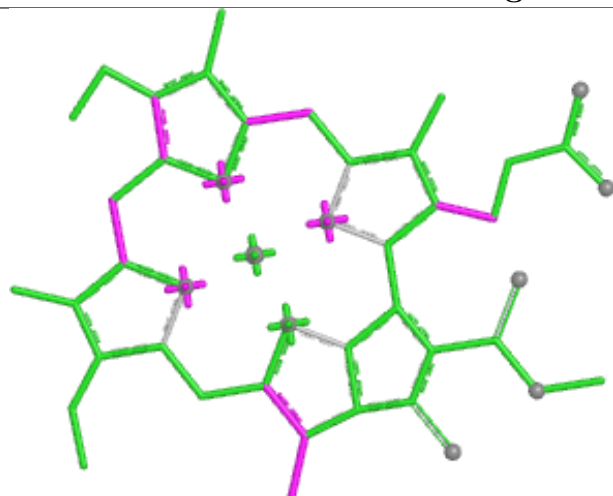
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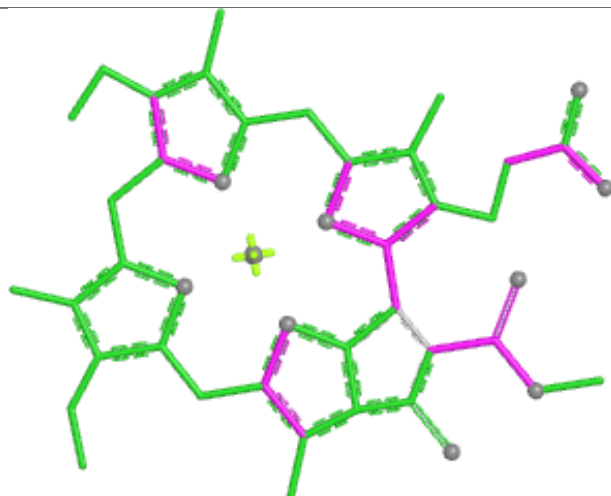
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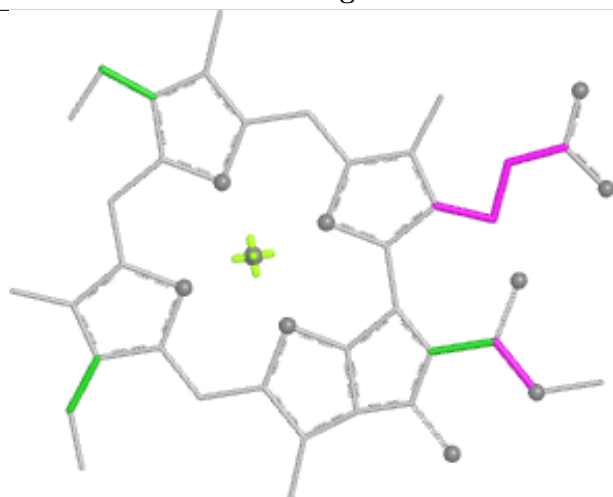
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Bond lengths



Bond angles

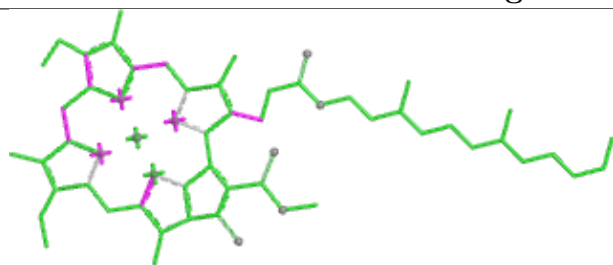


Torsions

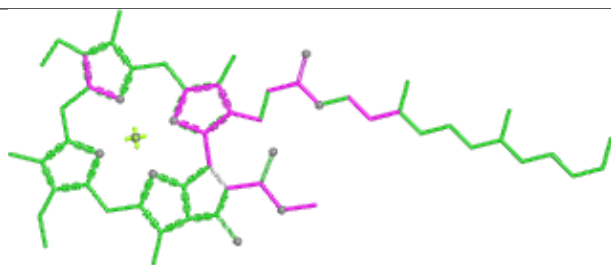


Rings

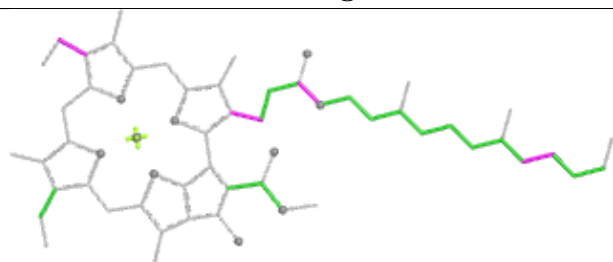
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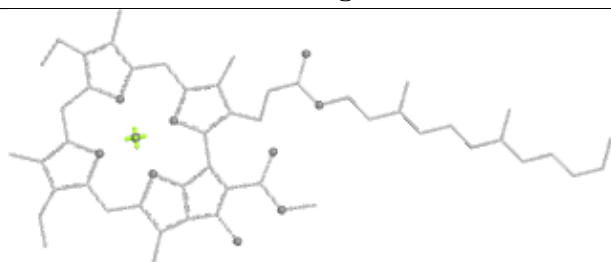
Bond lengths



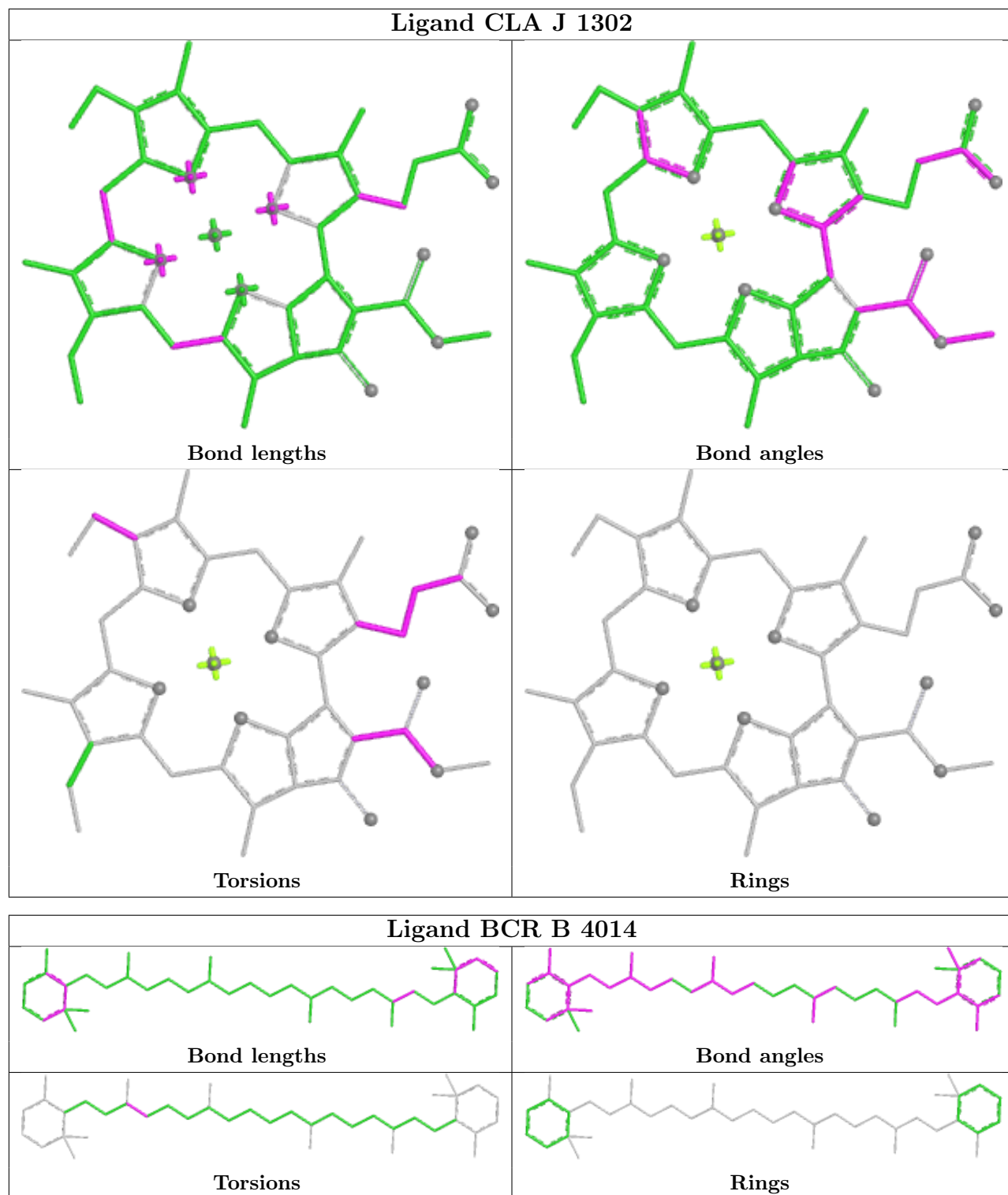
Bond angles



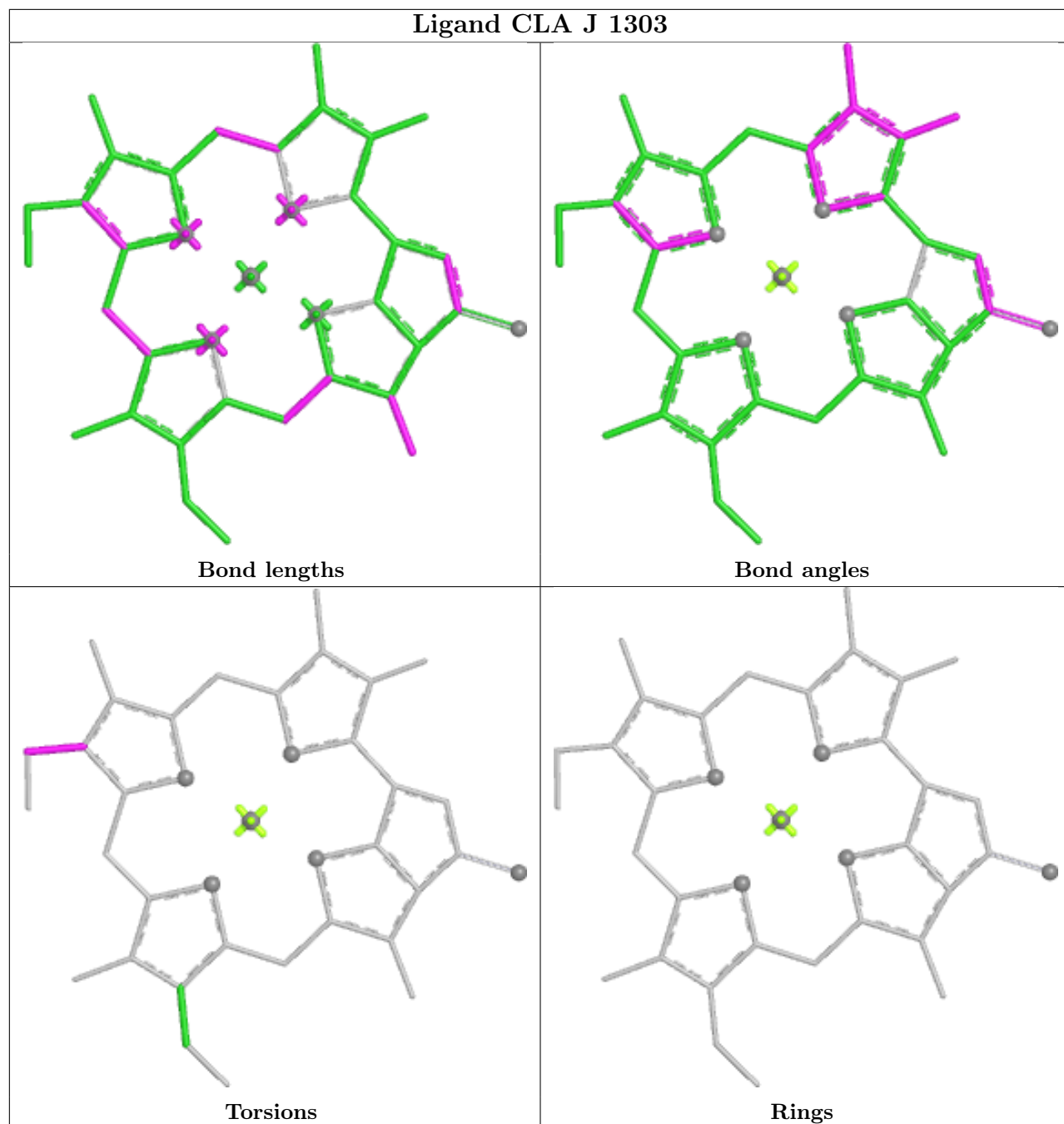
Torsions



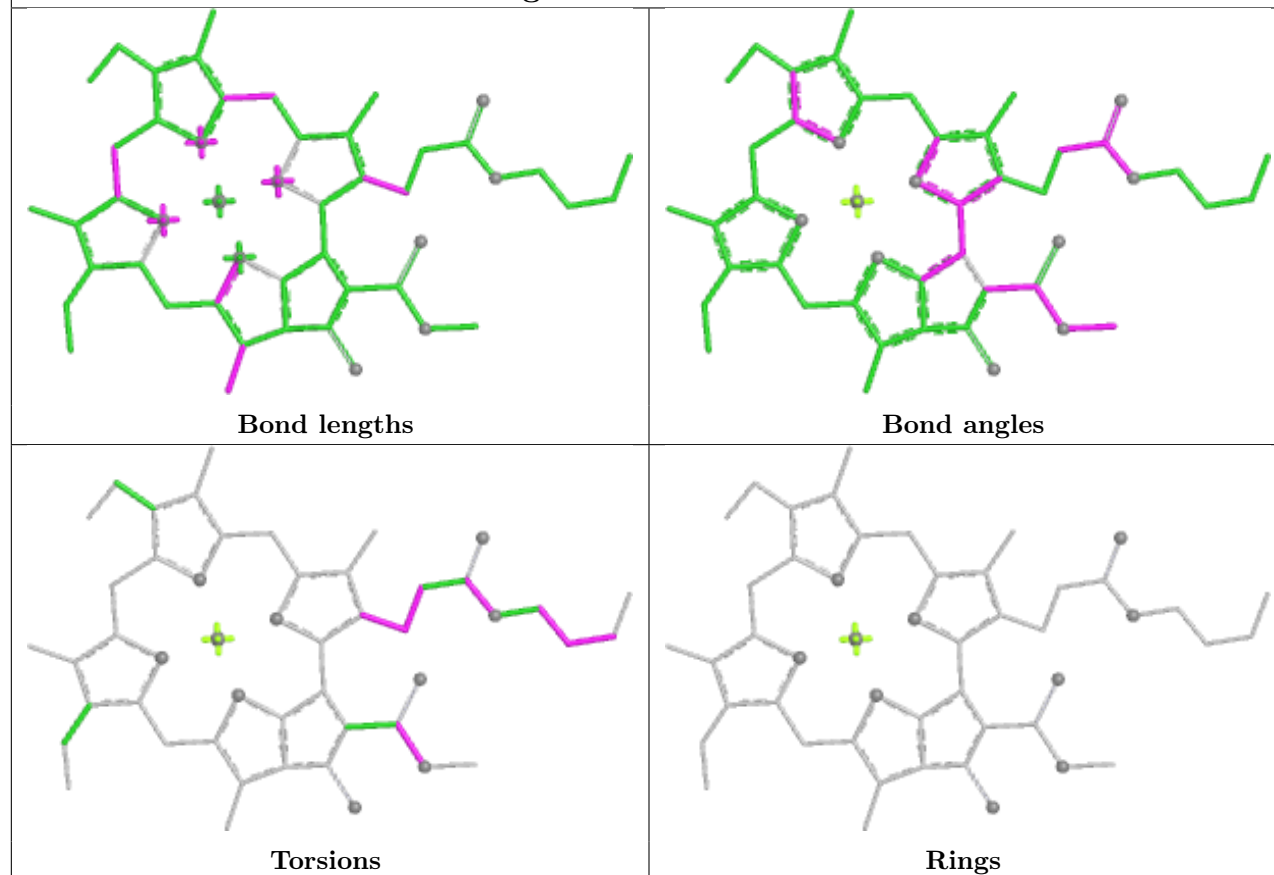
Rings



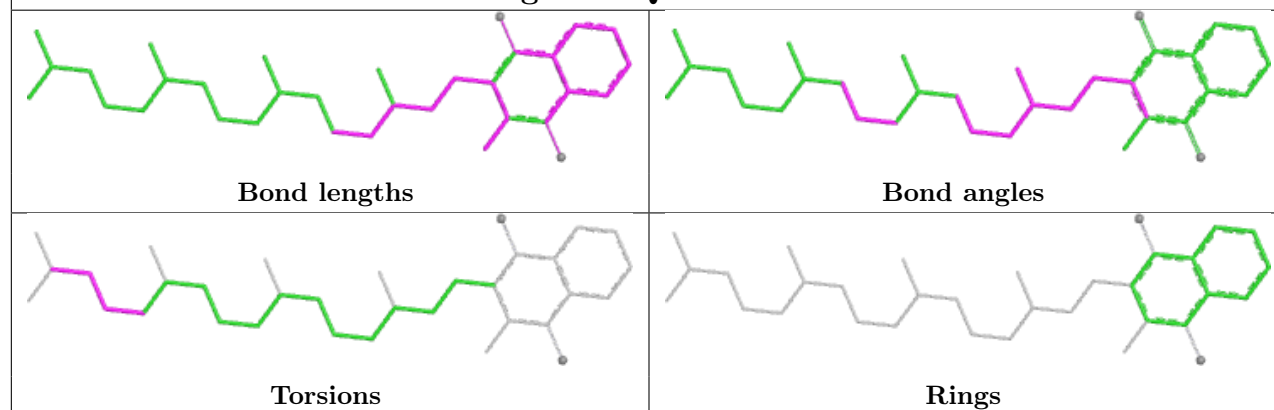
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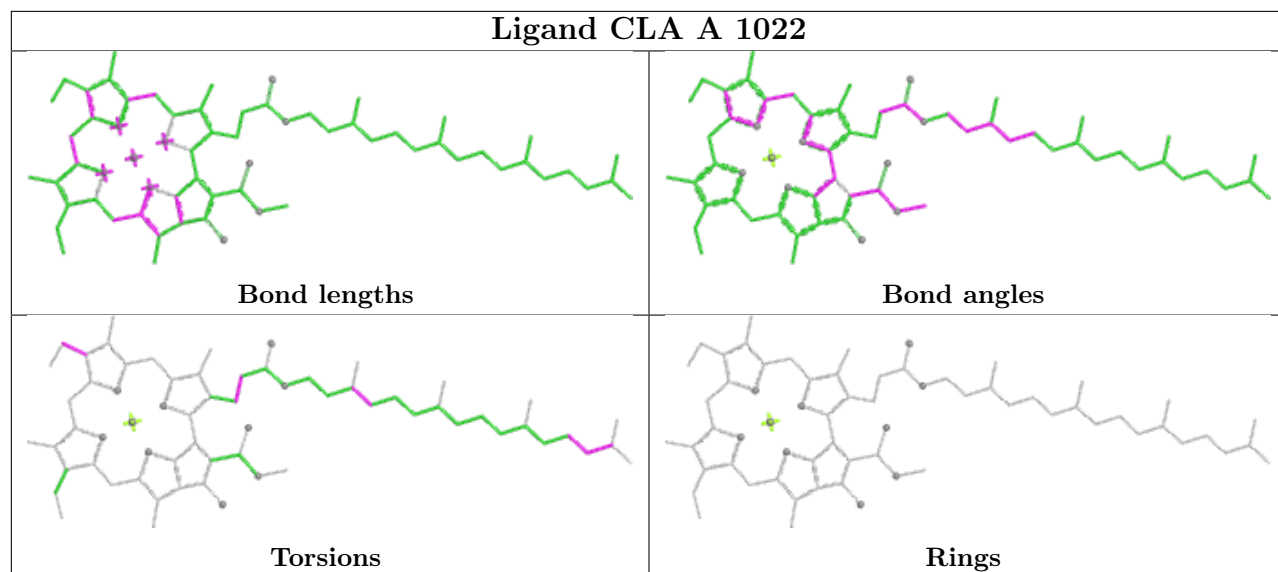
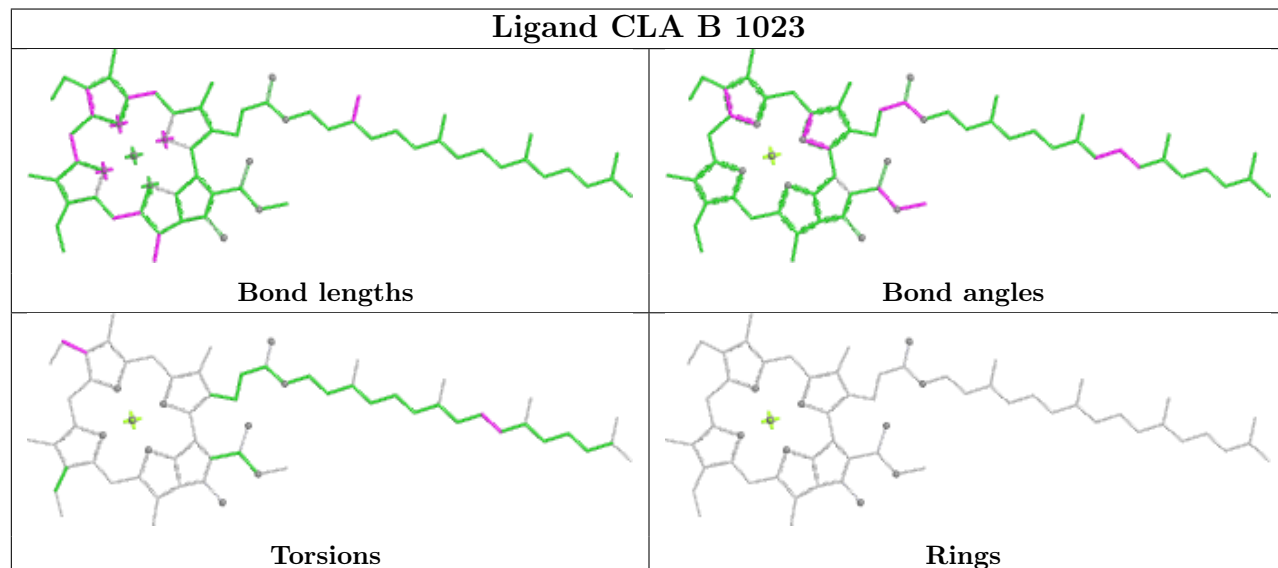


Ligand CLA A 1114

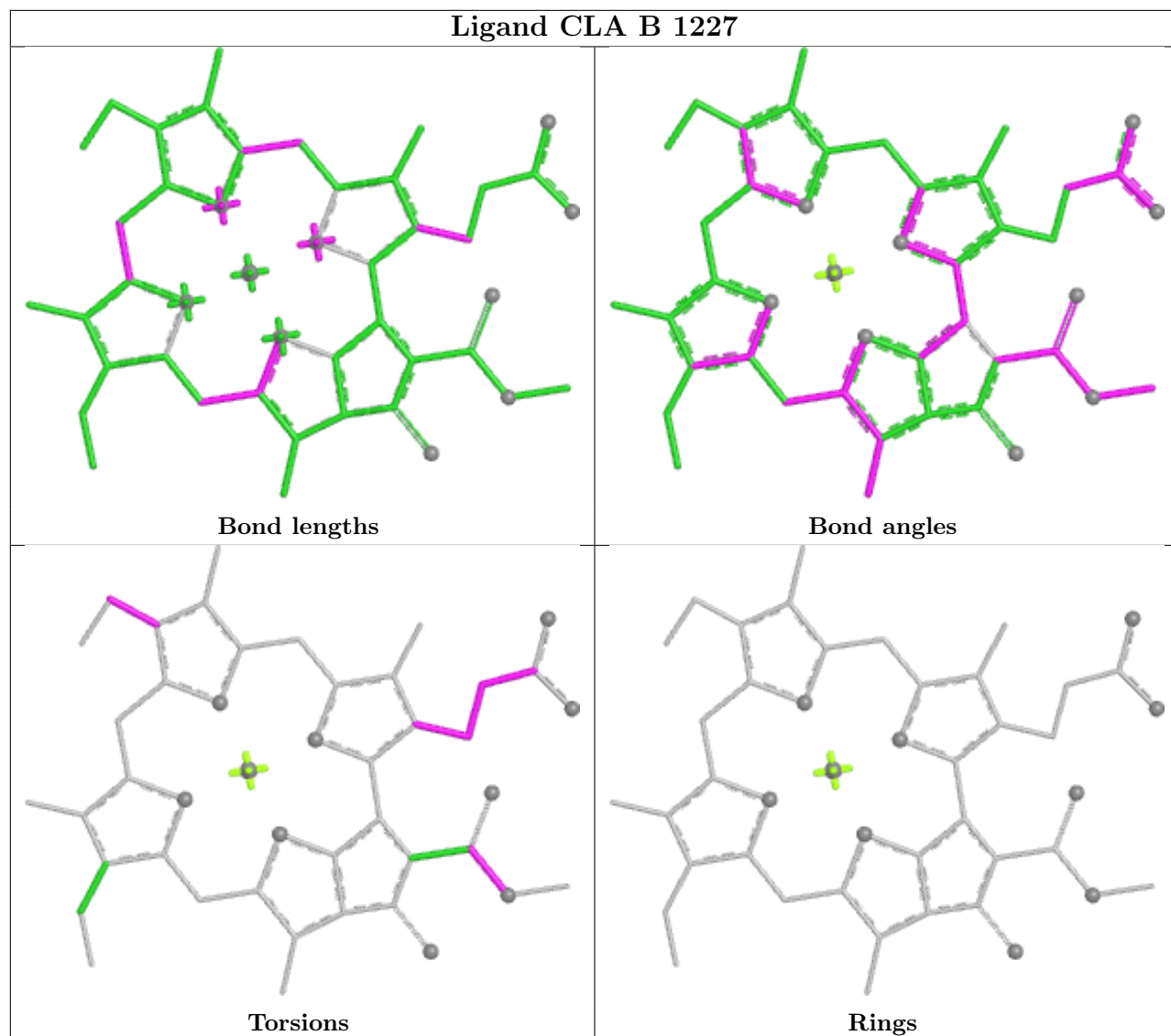


Ligand PQN B 2002

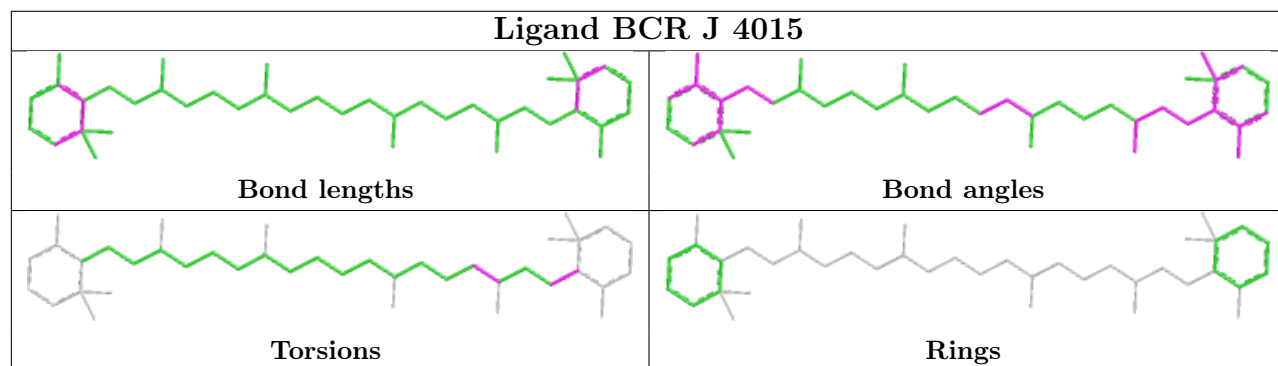


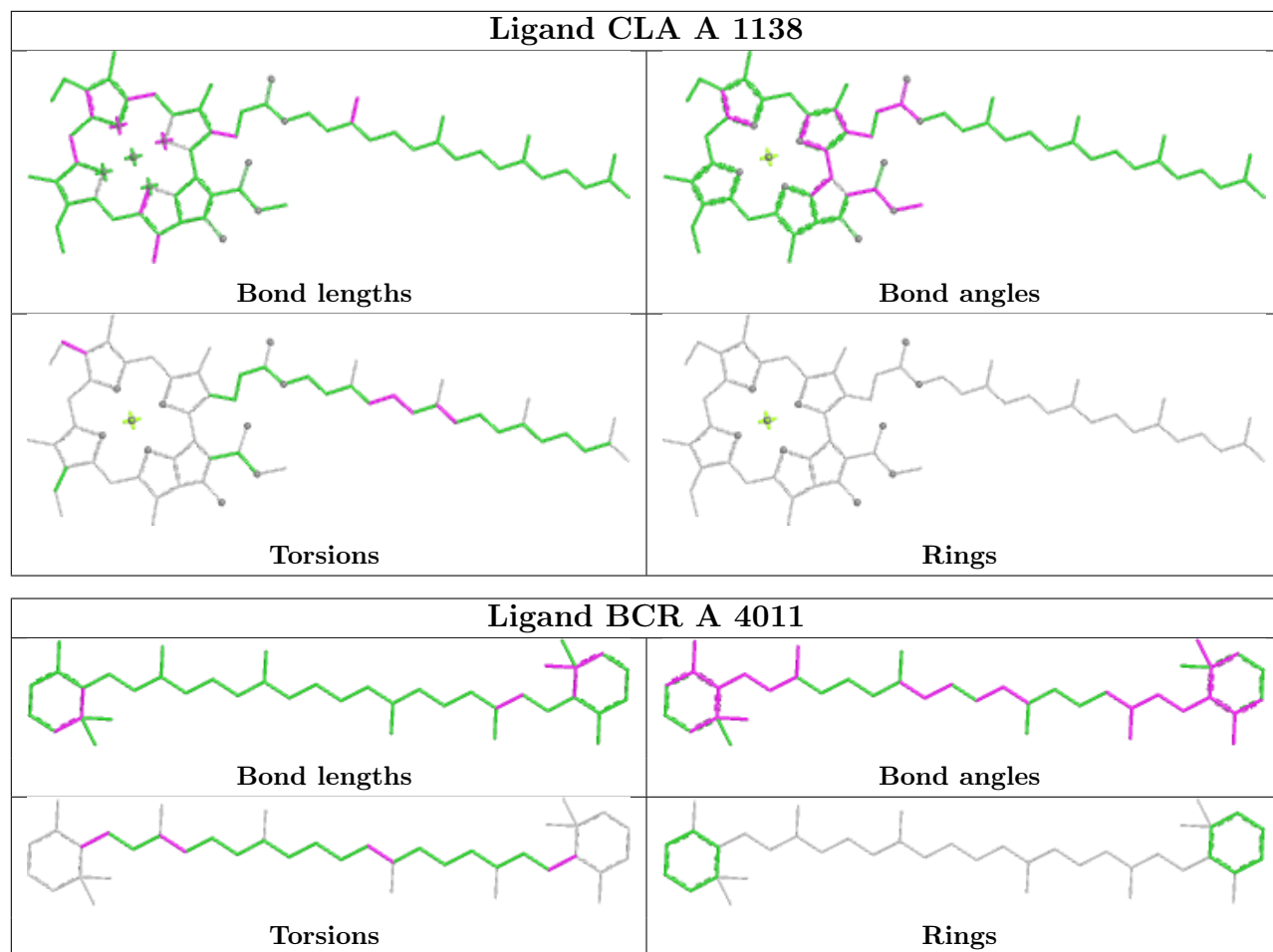
Ligand CLA A 1022**Ligand CLA B 1023**

Ligand CLA B 1227

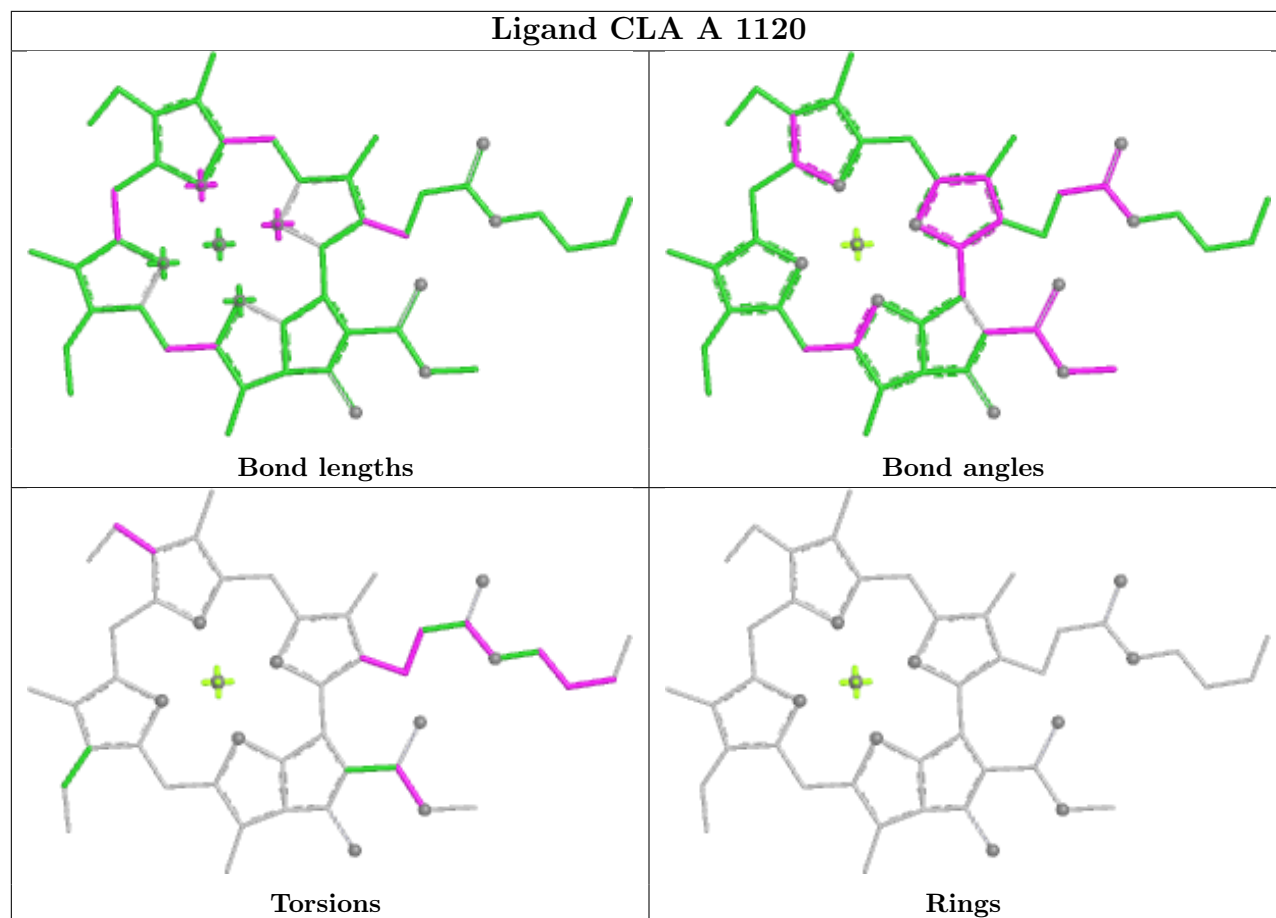


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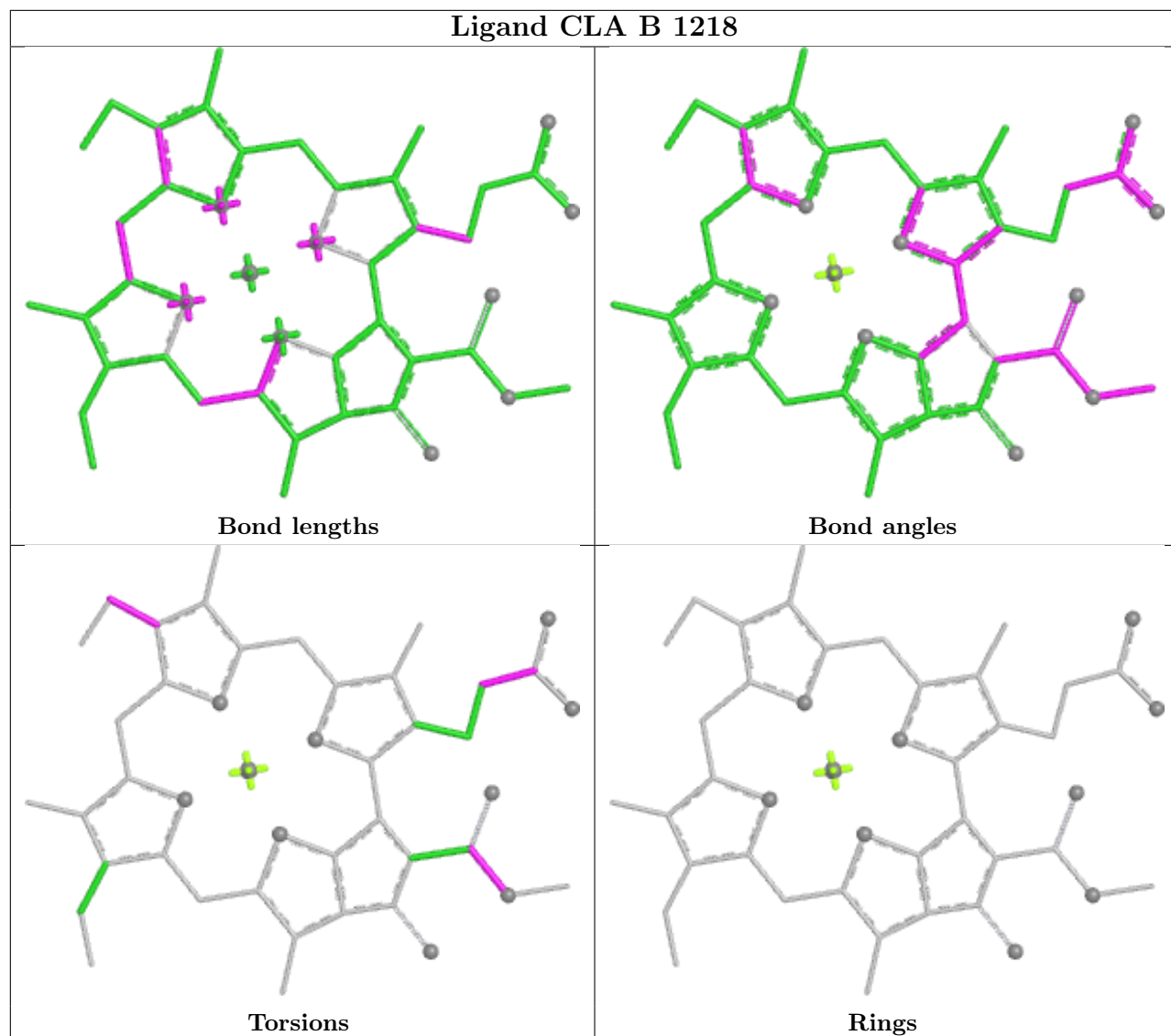




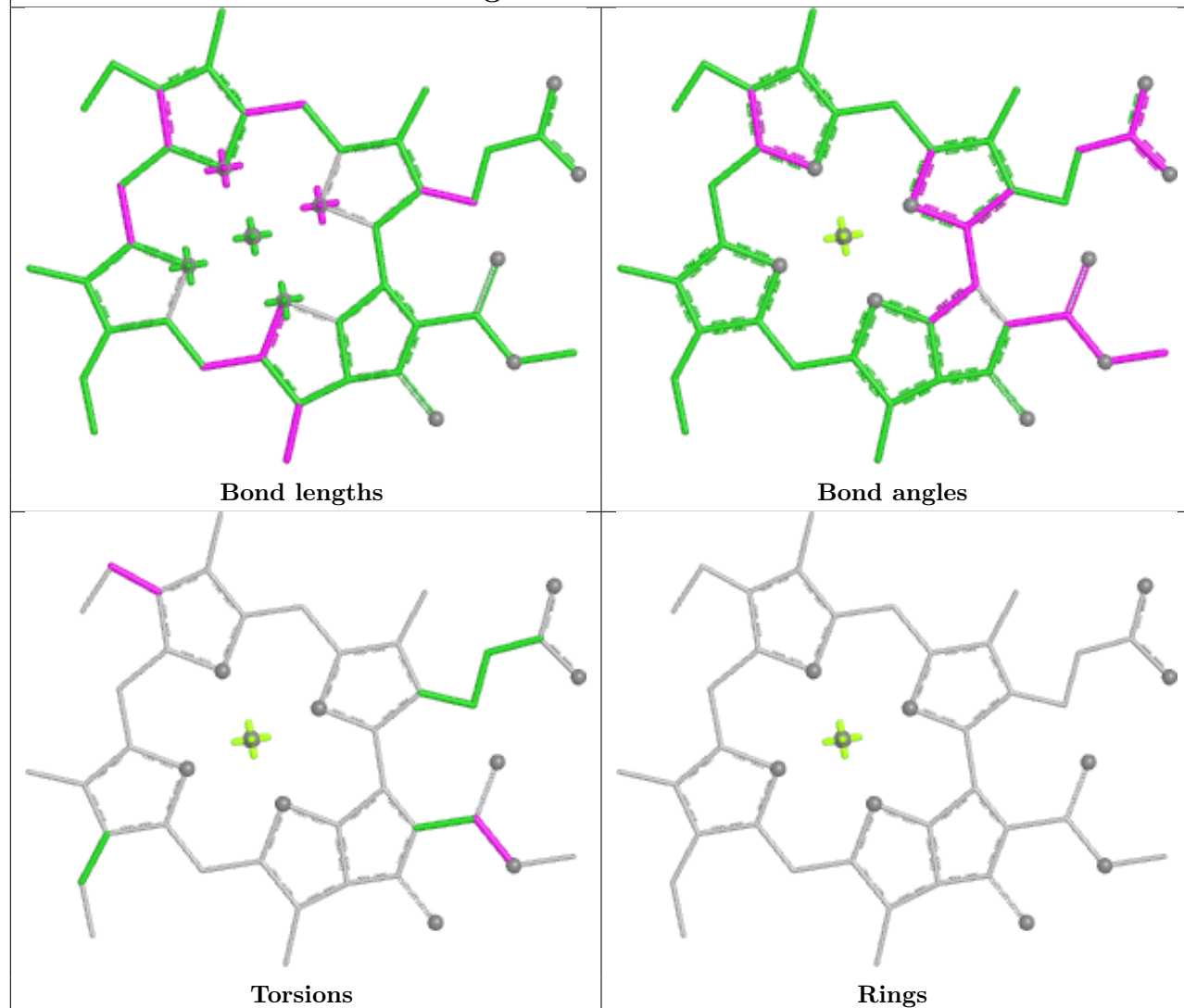
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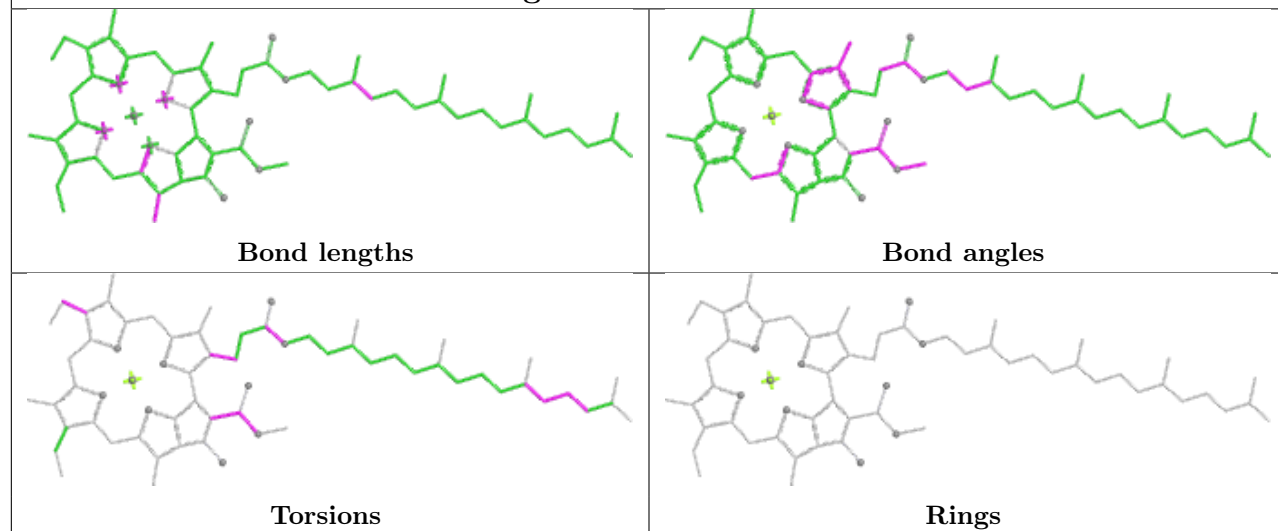
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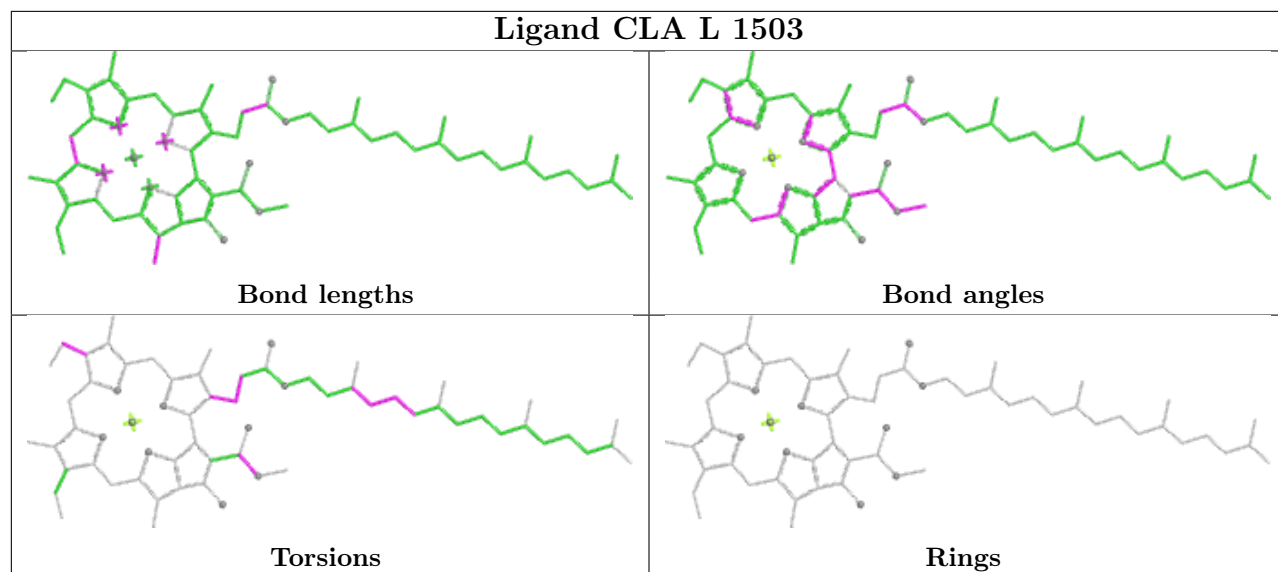
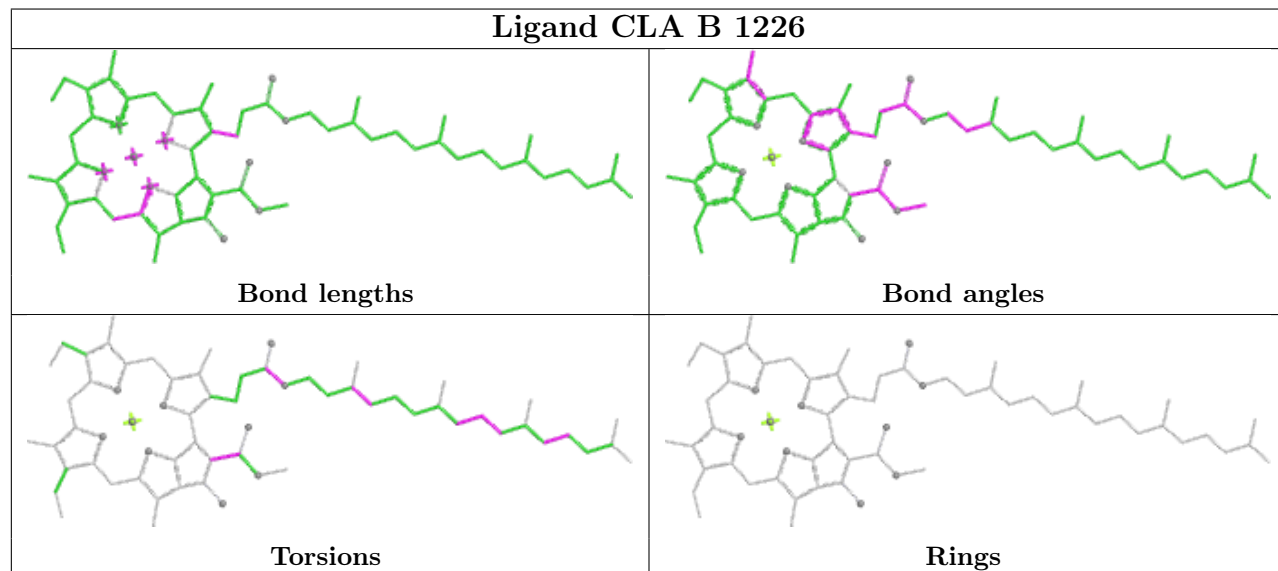


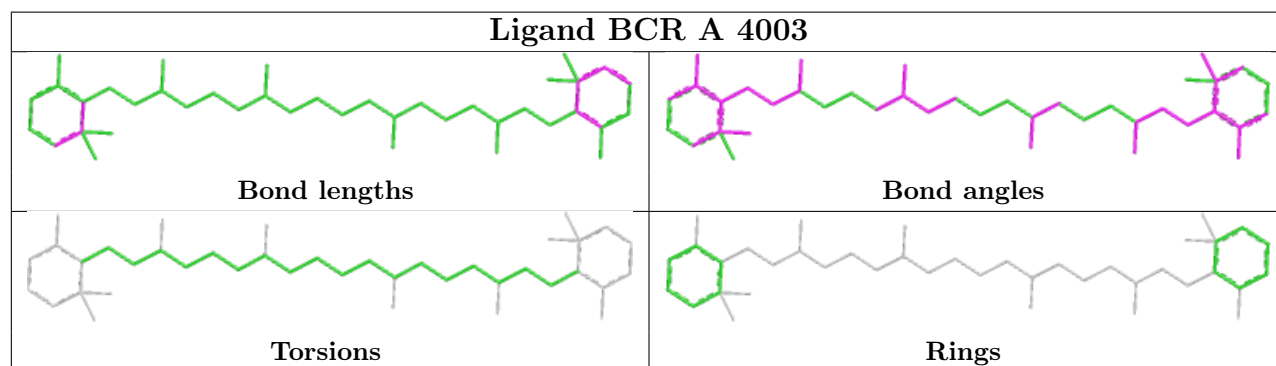
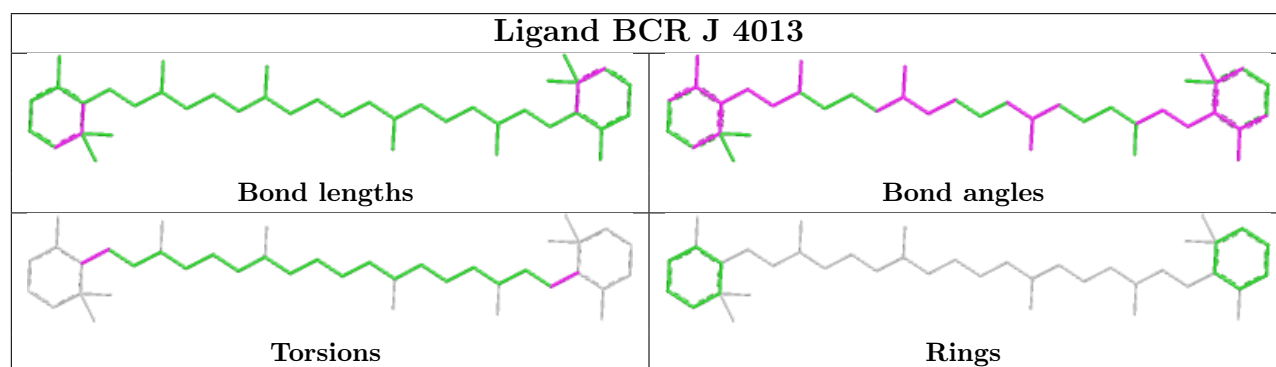
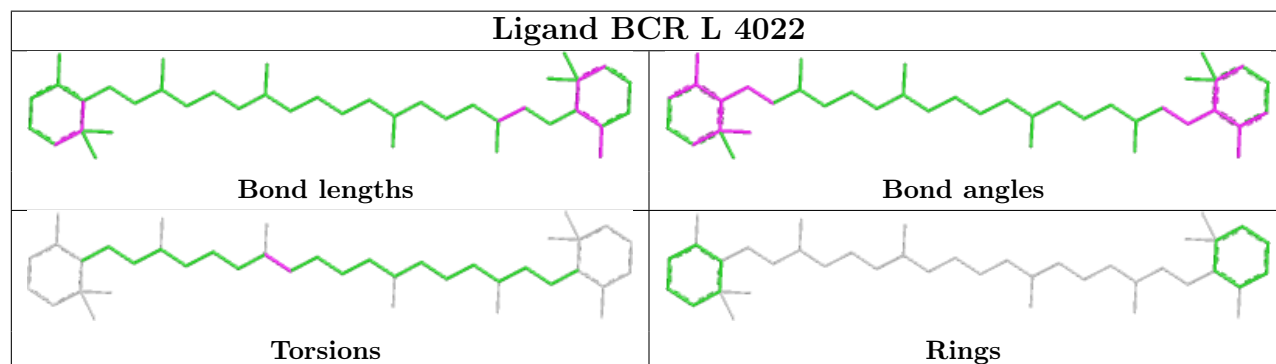
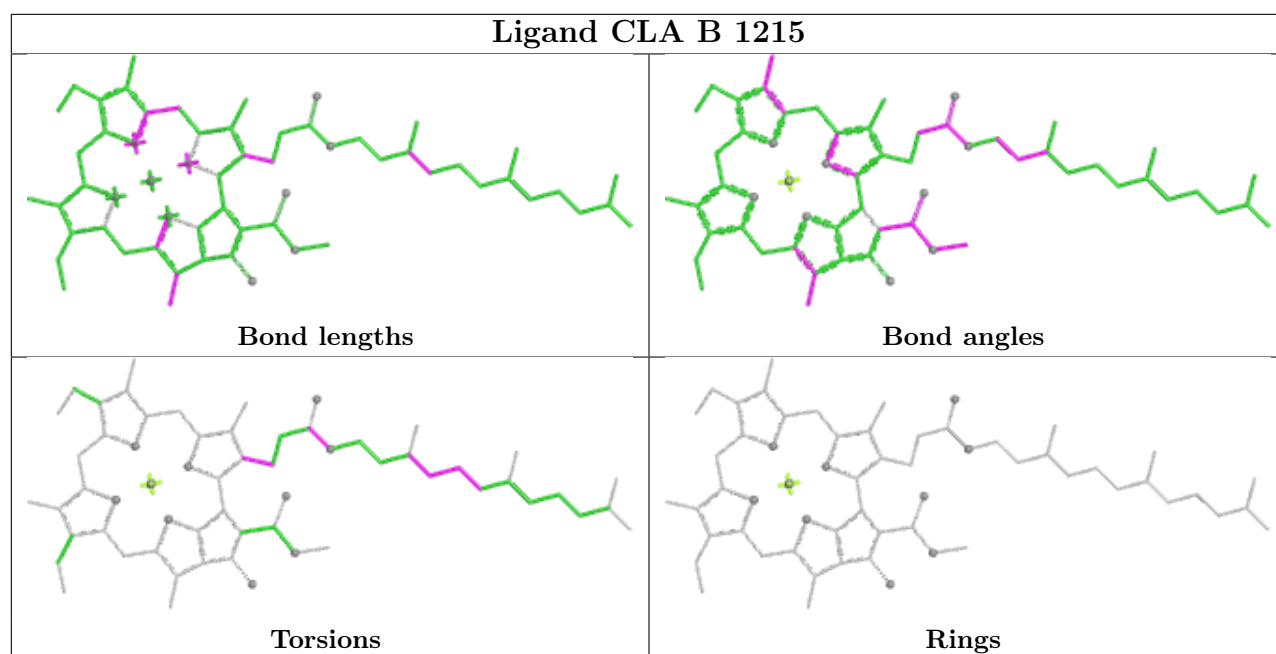
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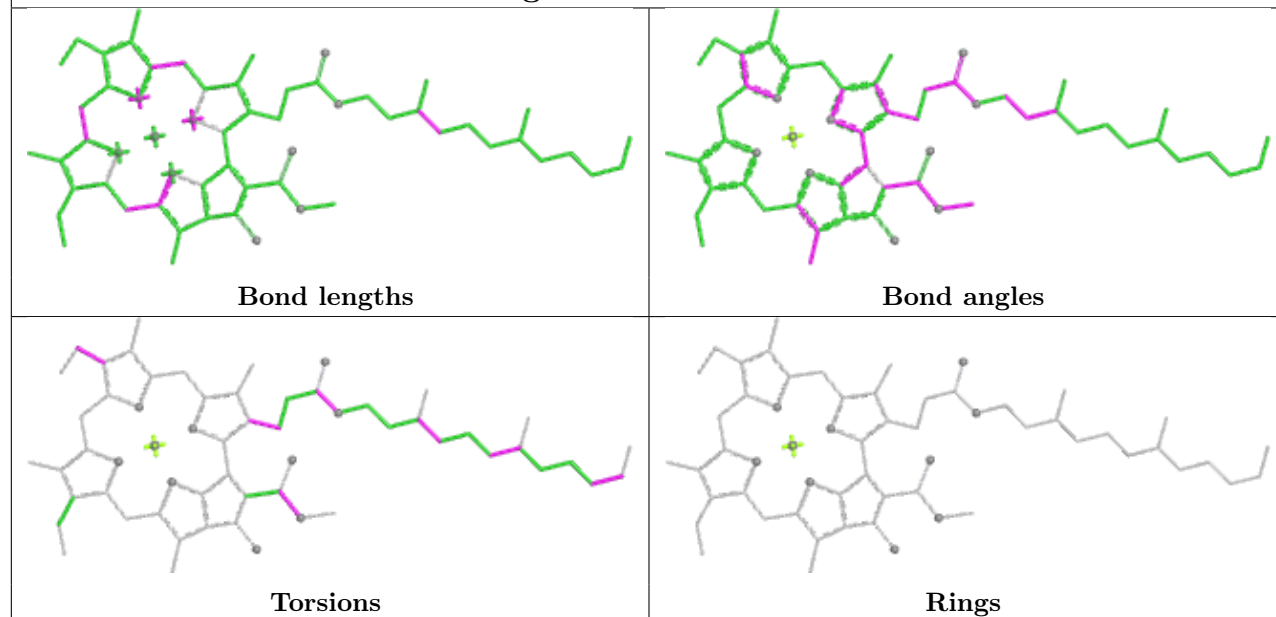
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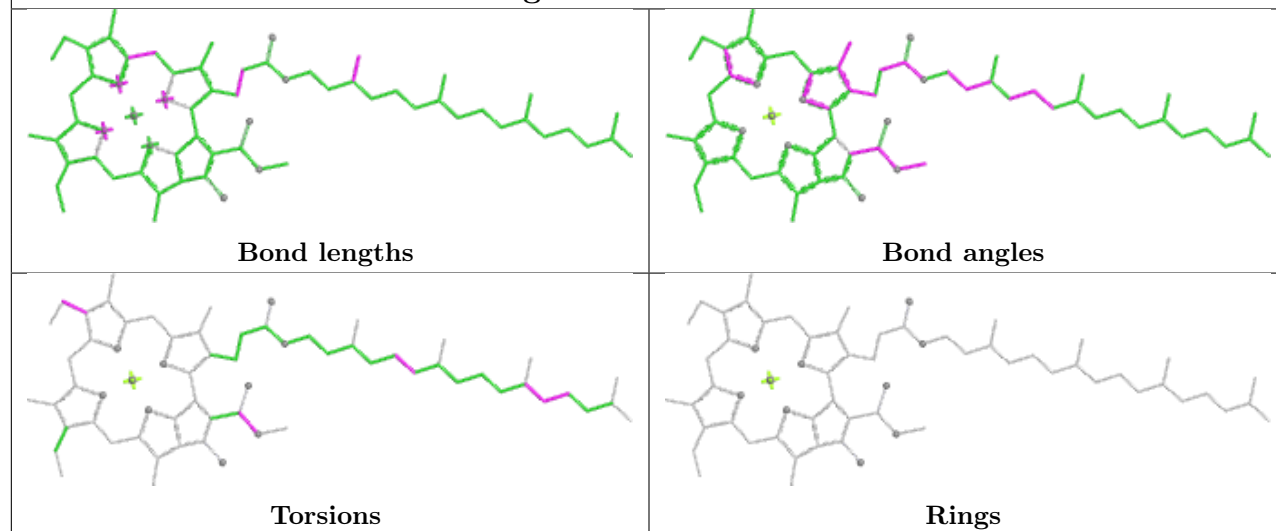
Ligand CLA L 1503**Ligand CLA B 1226**

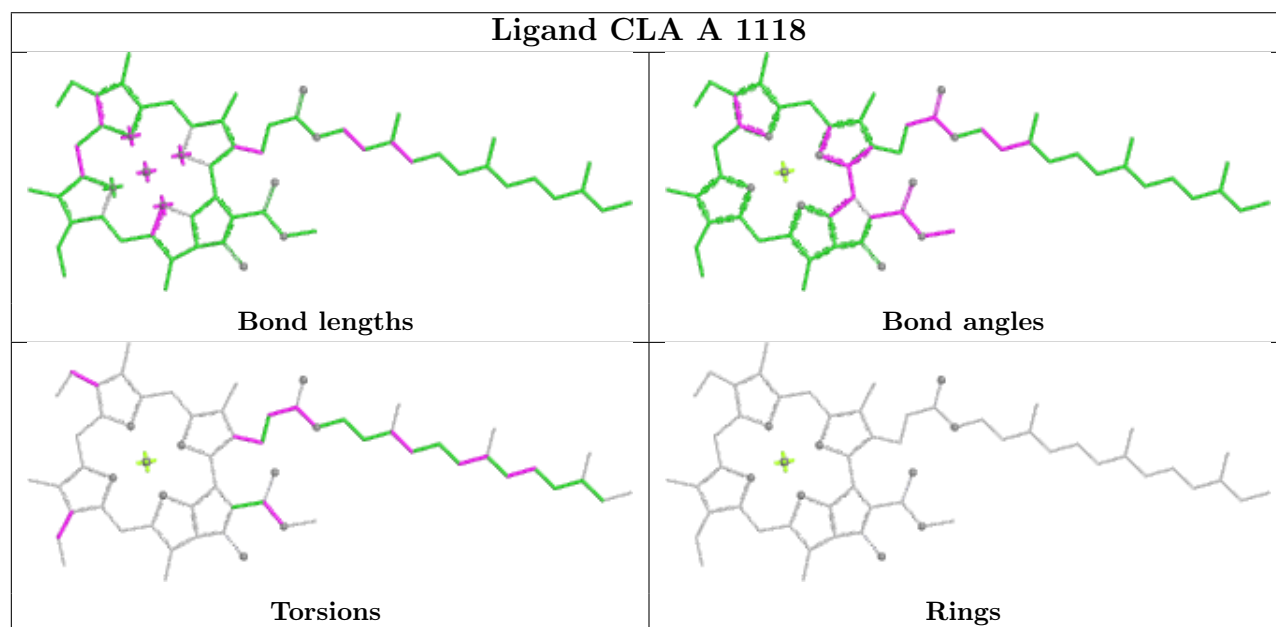
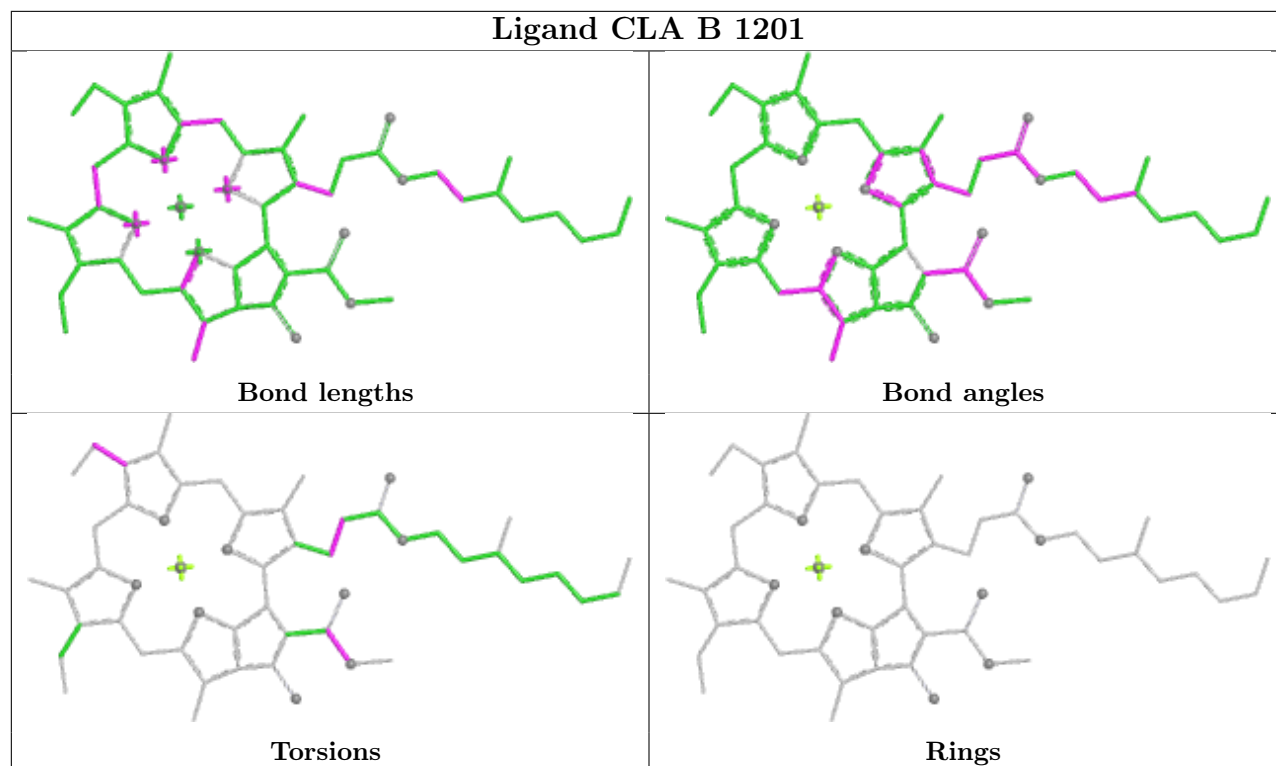


Ligand CLA A 1122

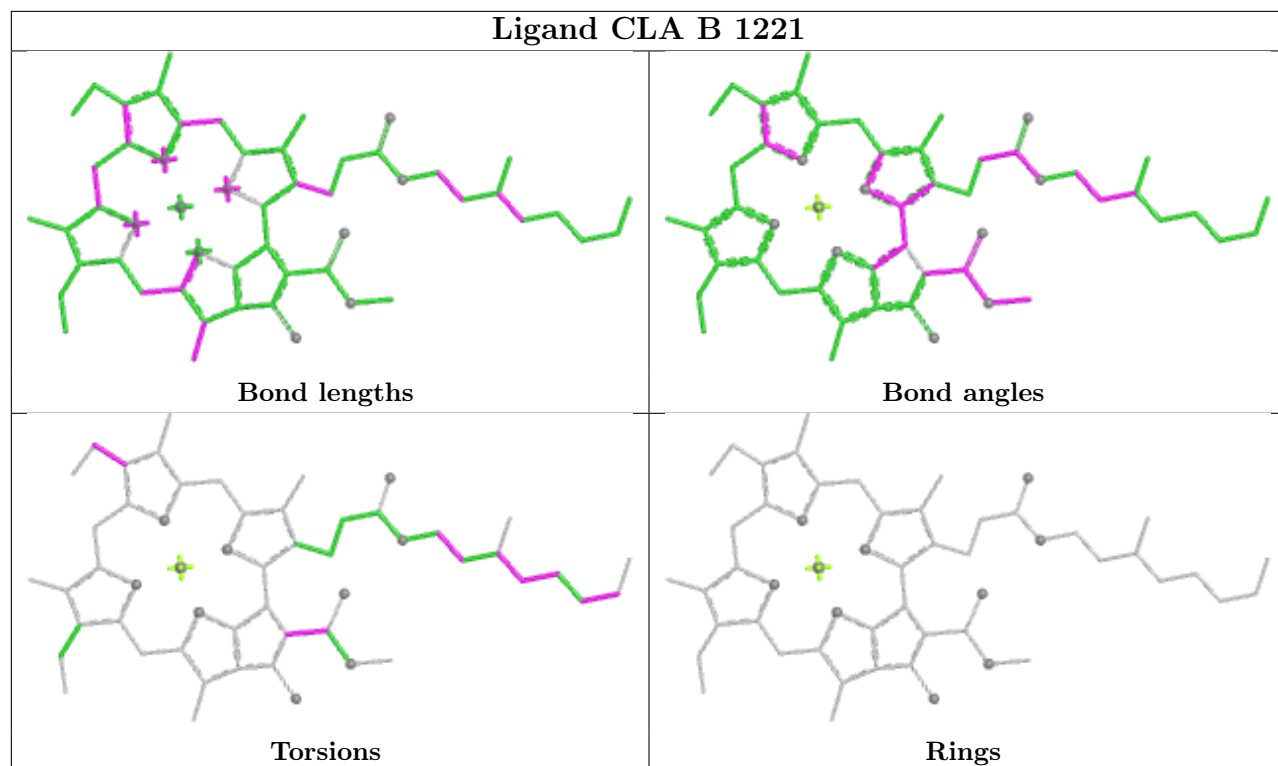


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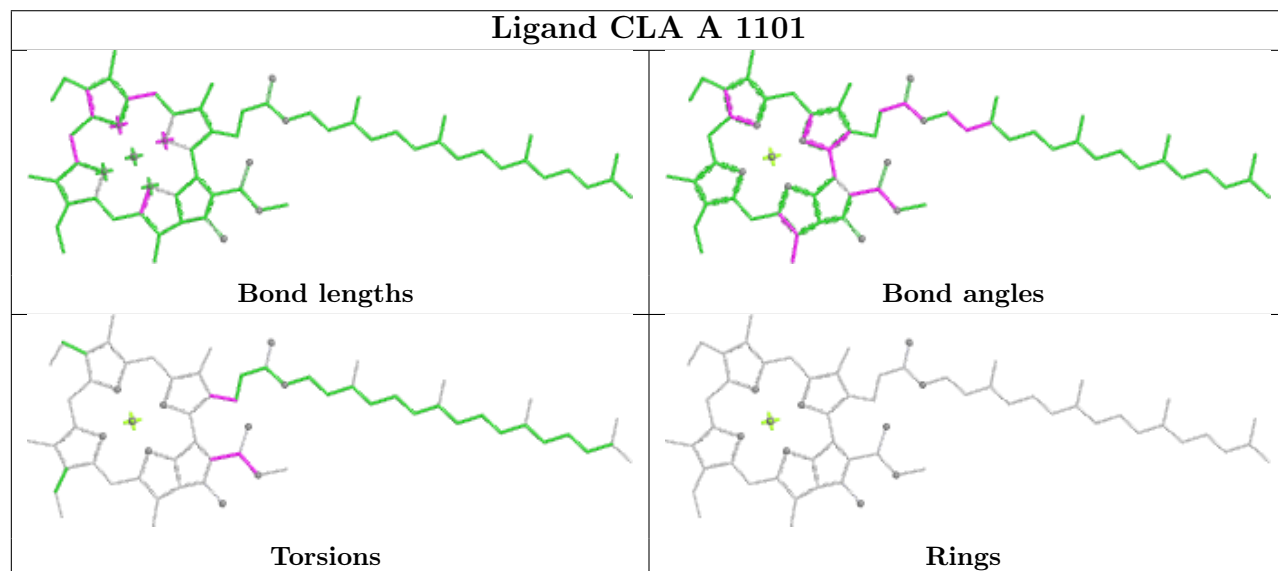




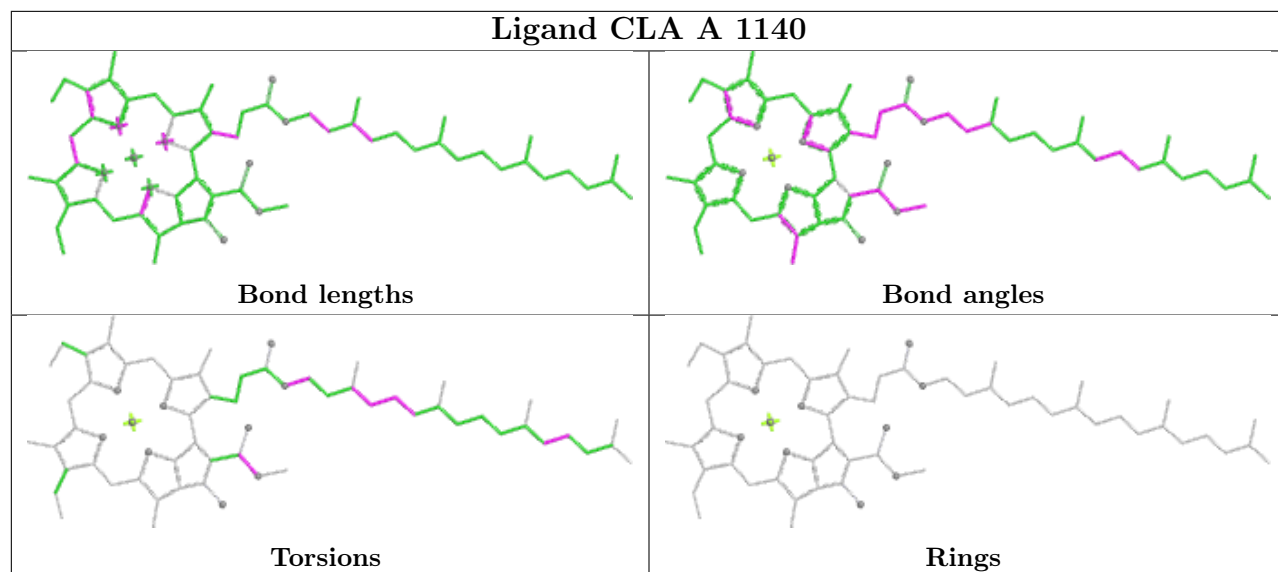
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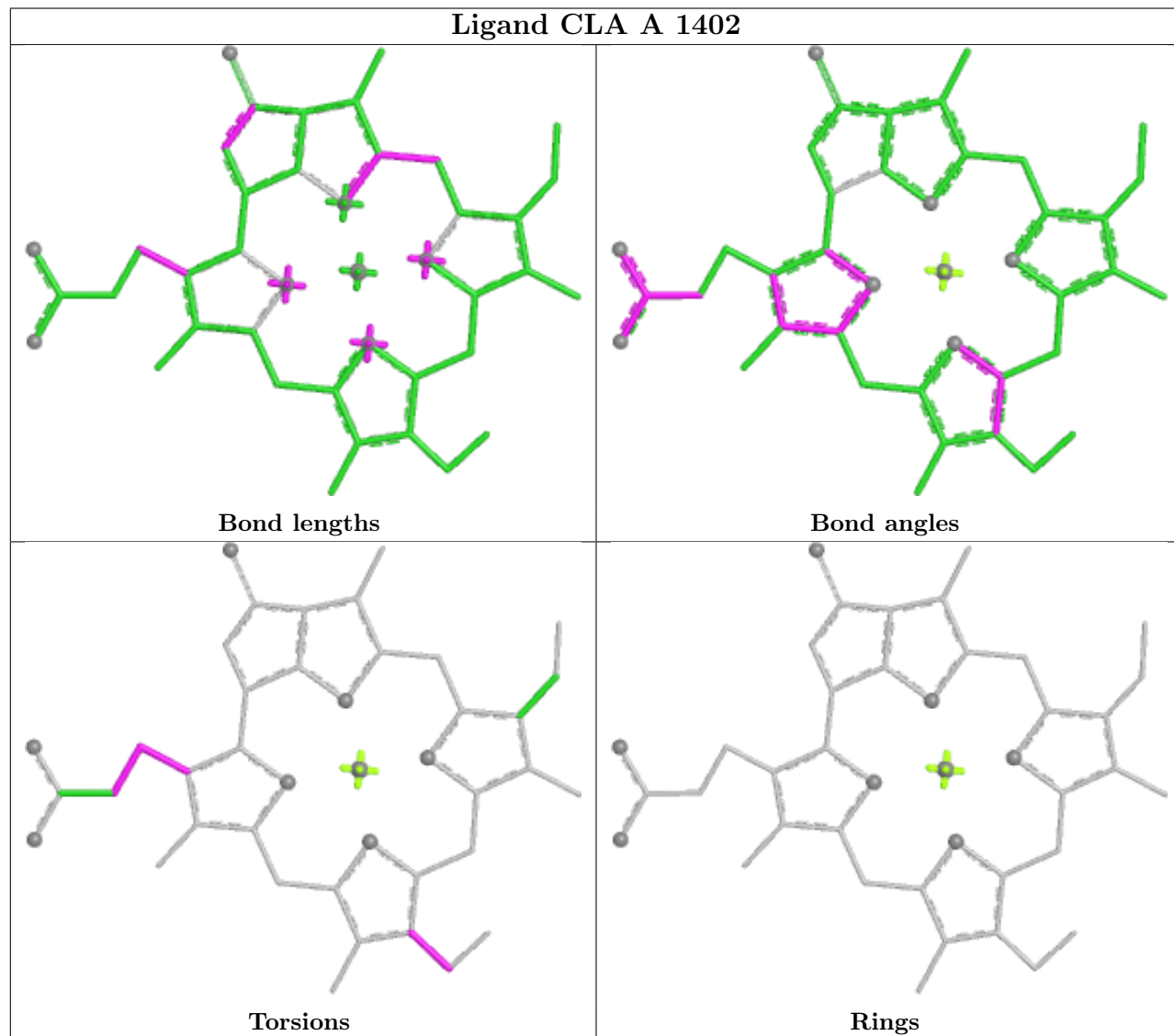
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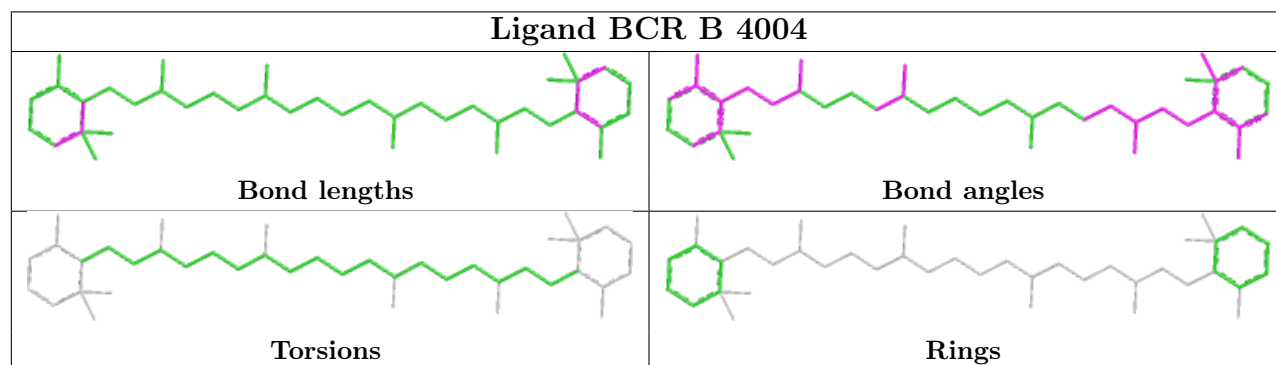
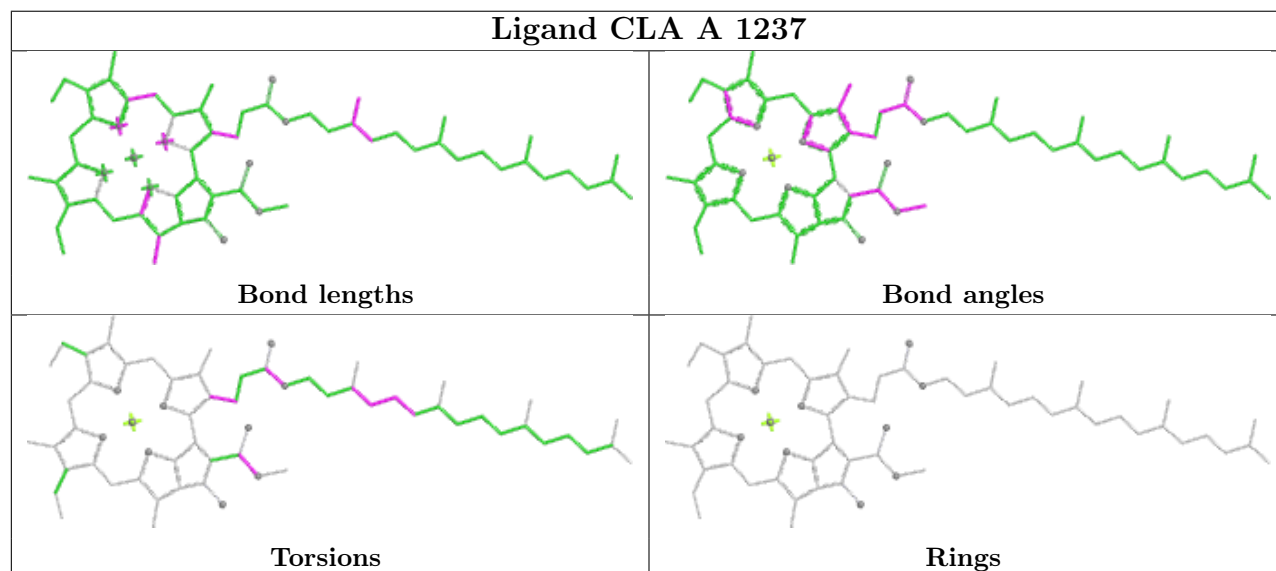
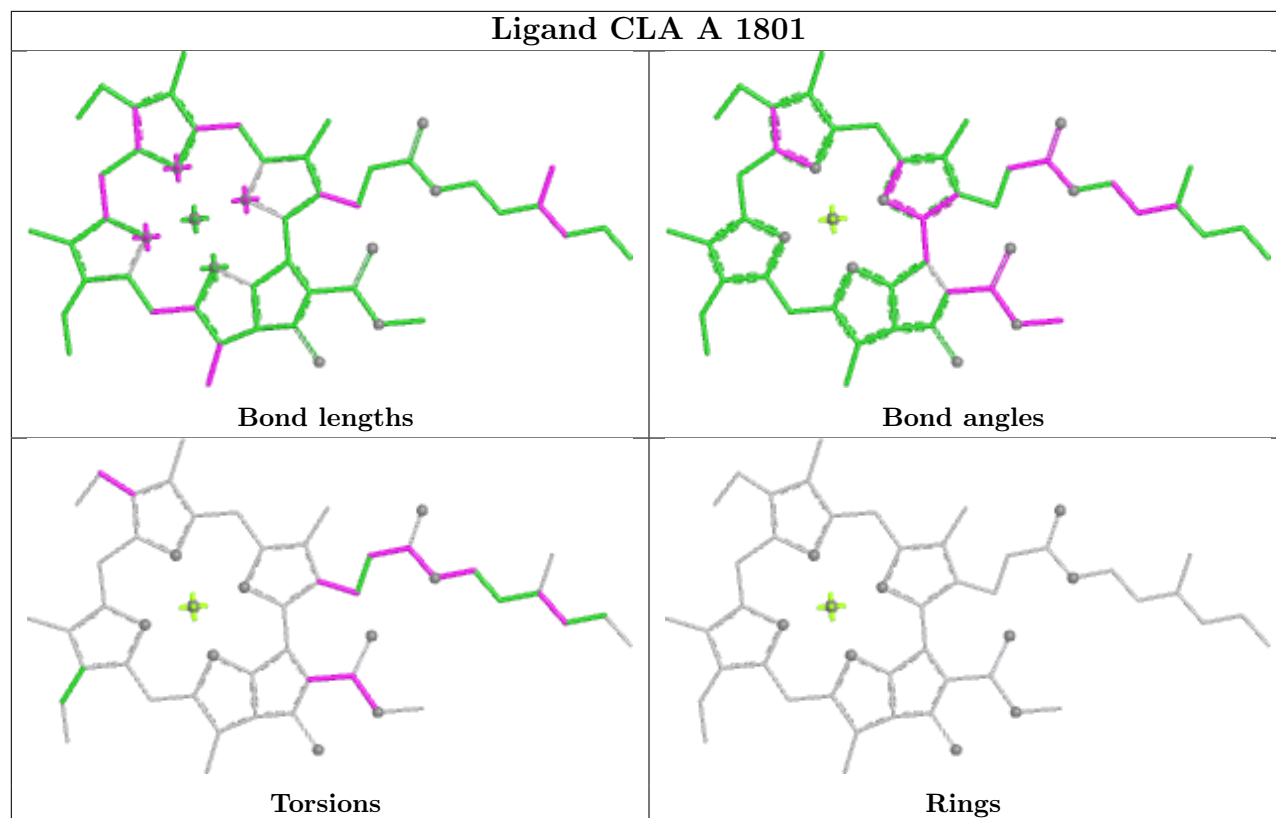


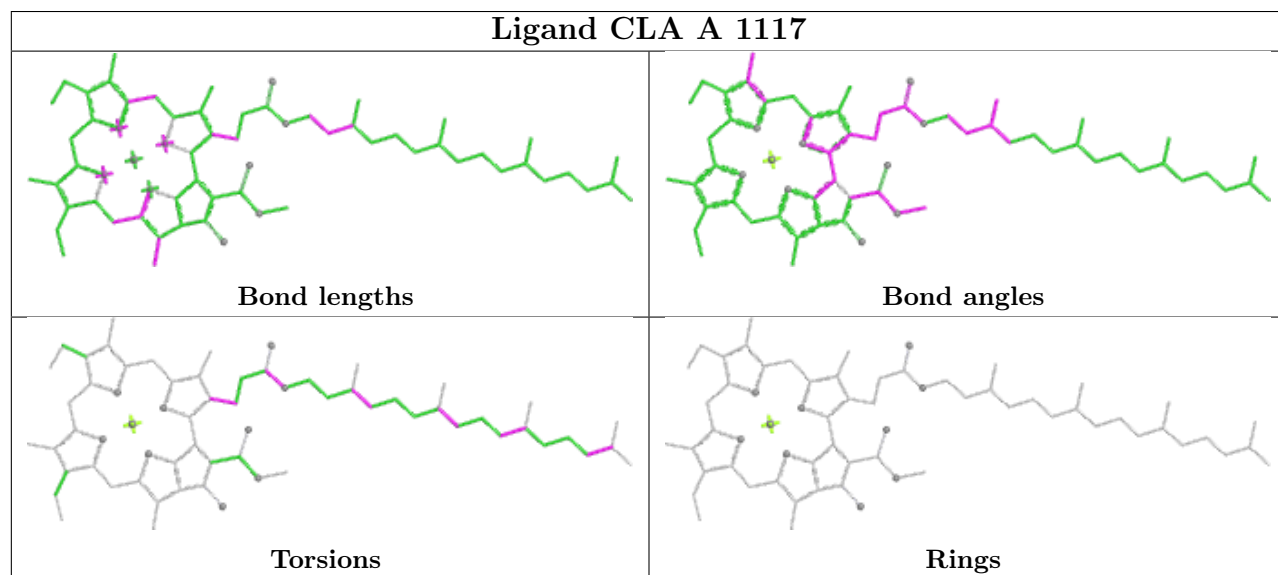
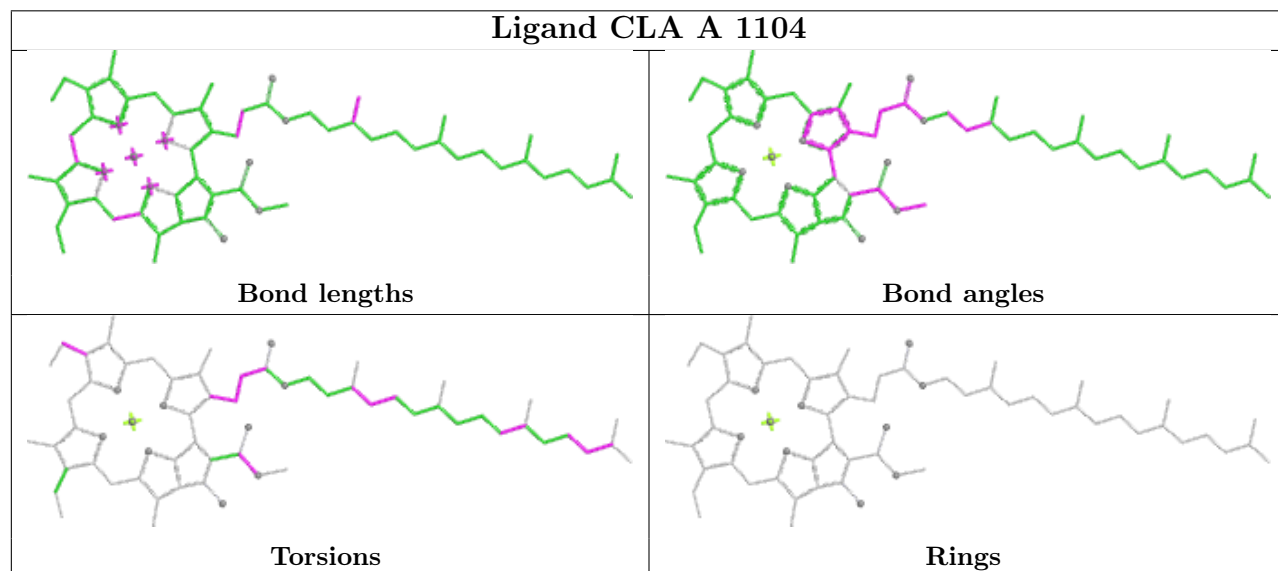
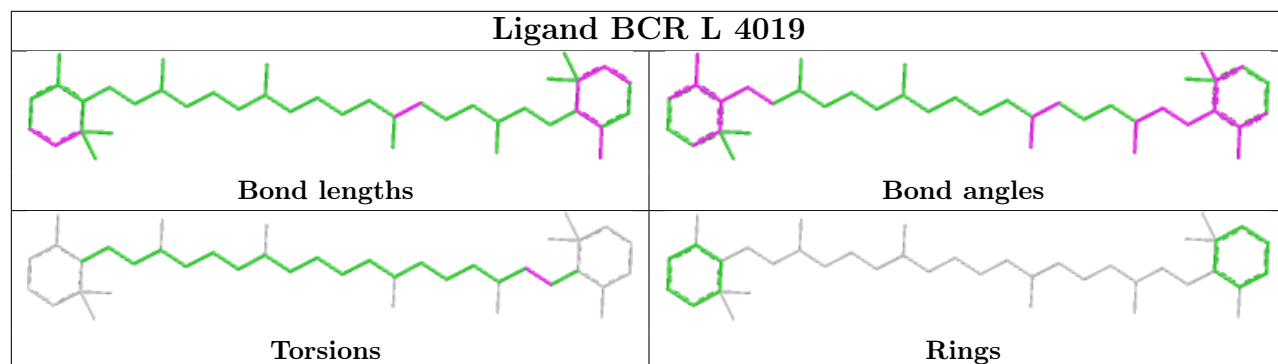
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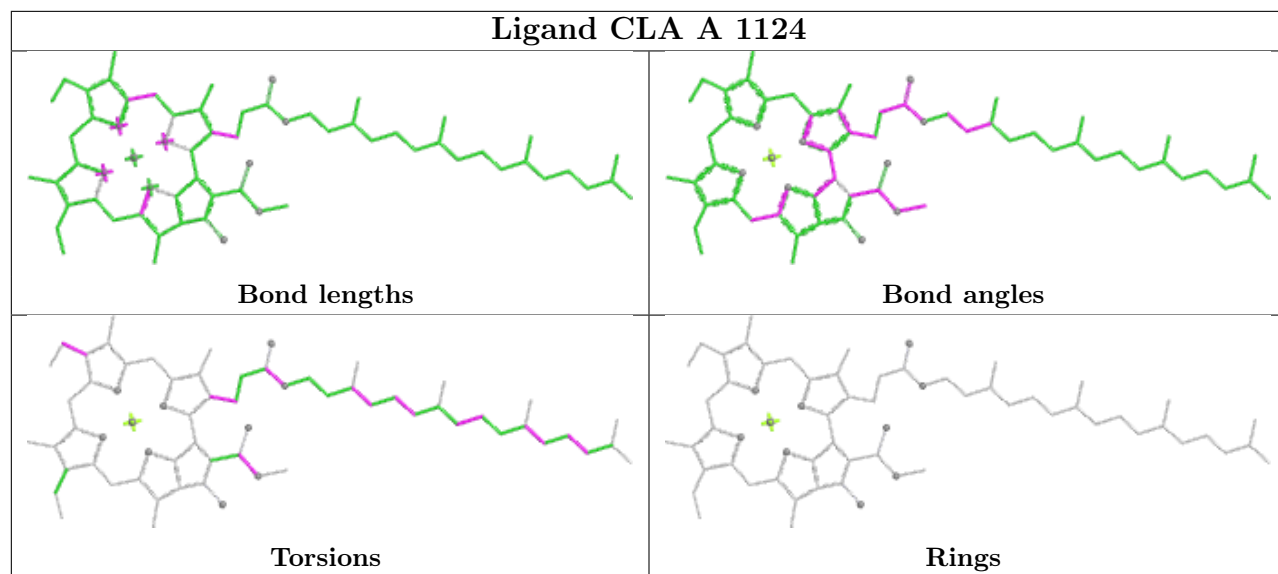
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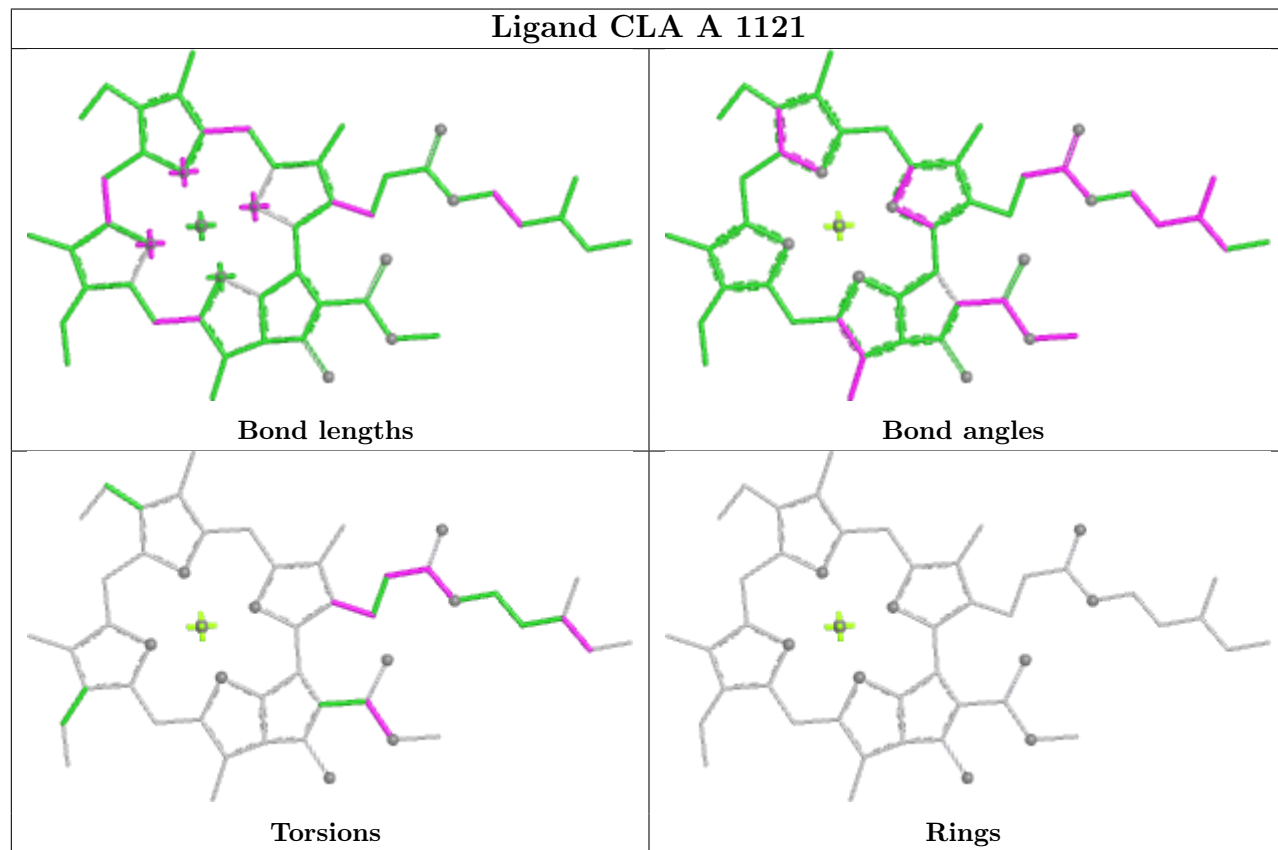




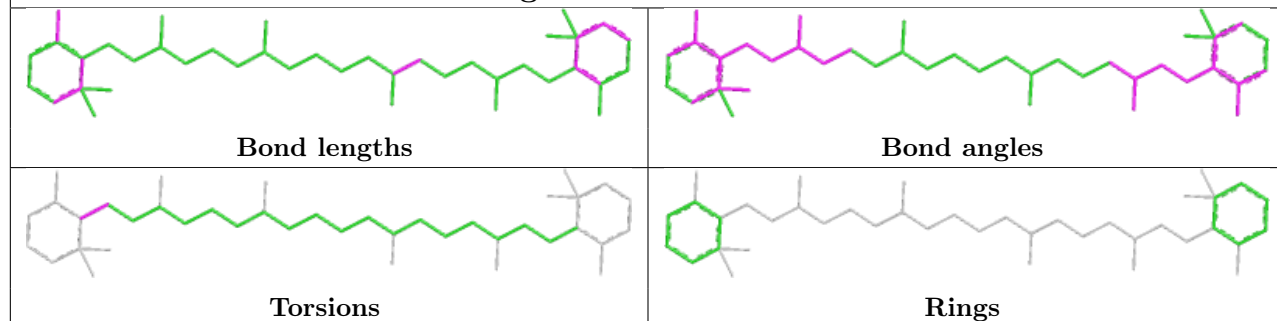
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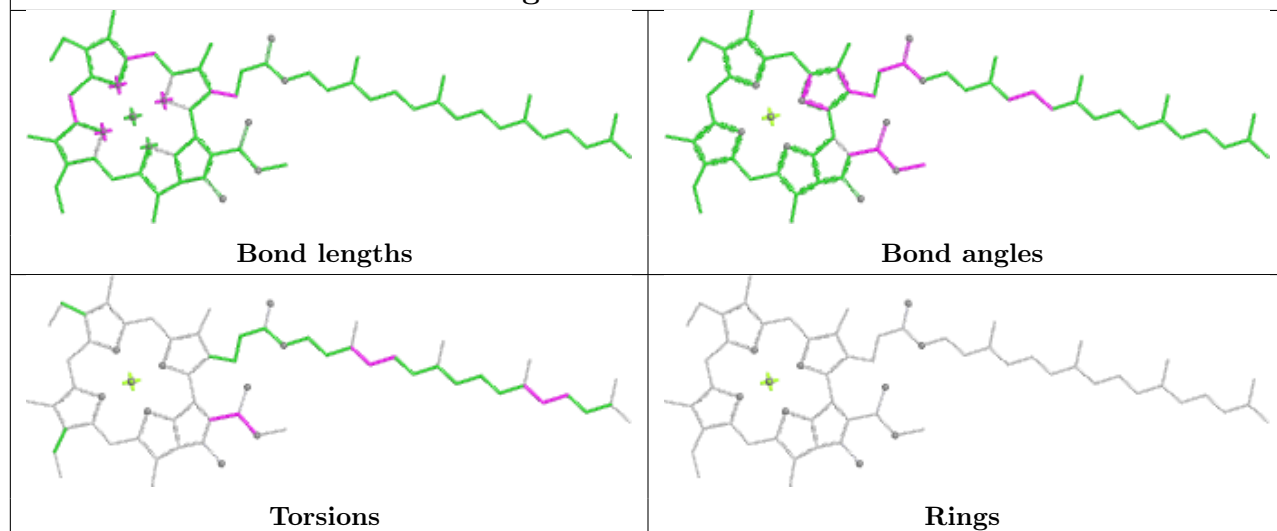
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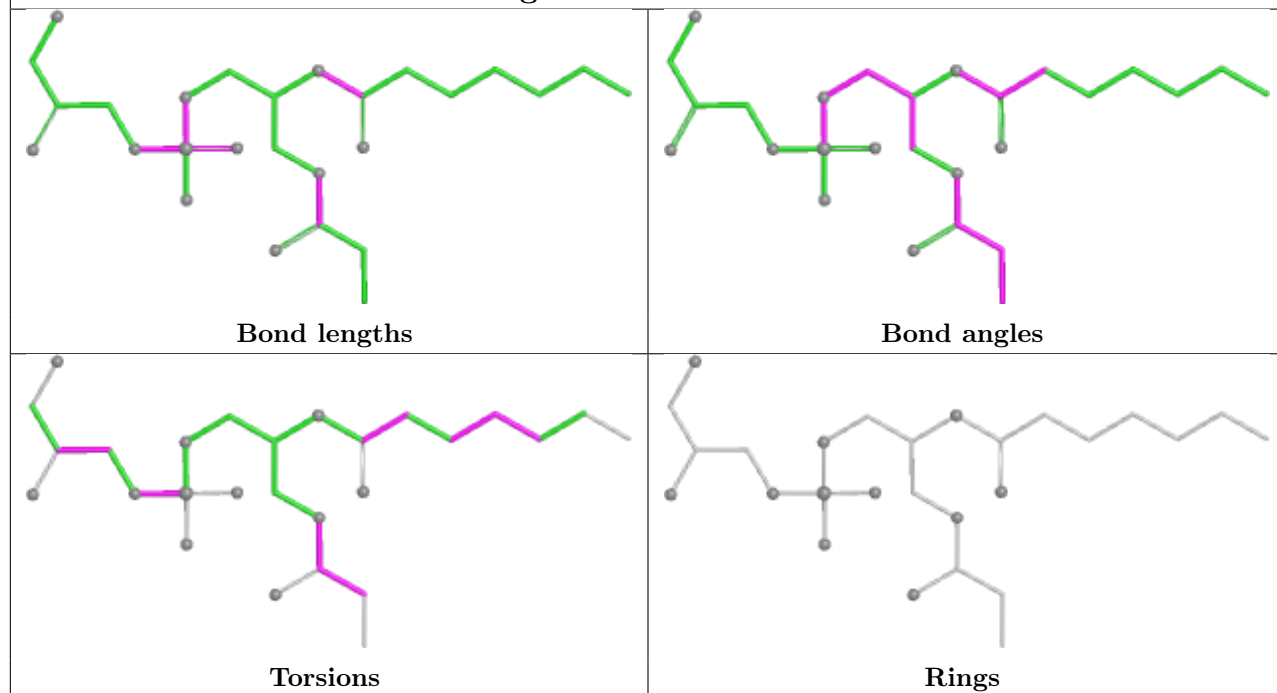
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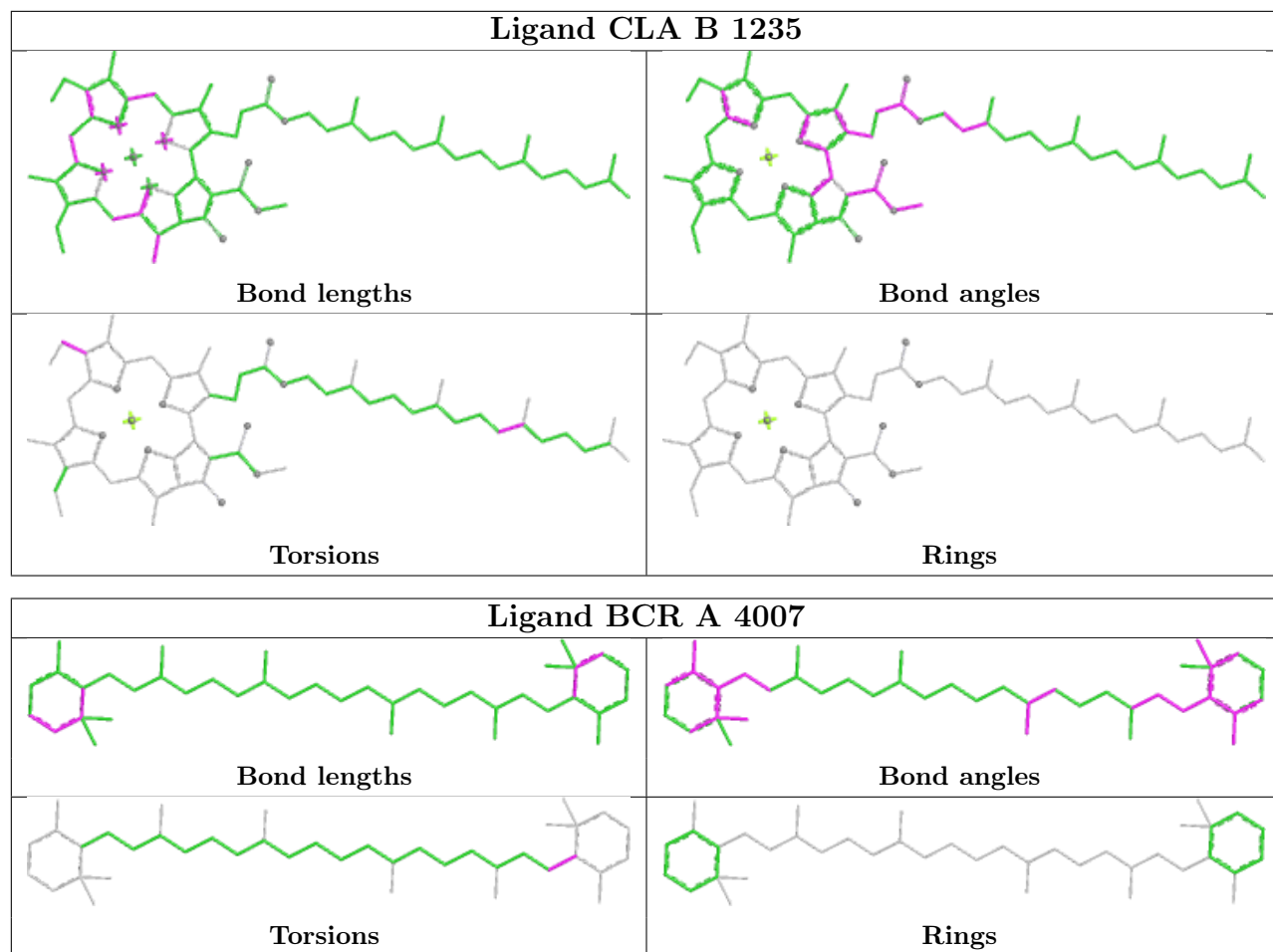


Ligand CLA B 1205

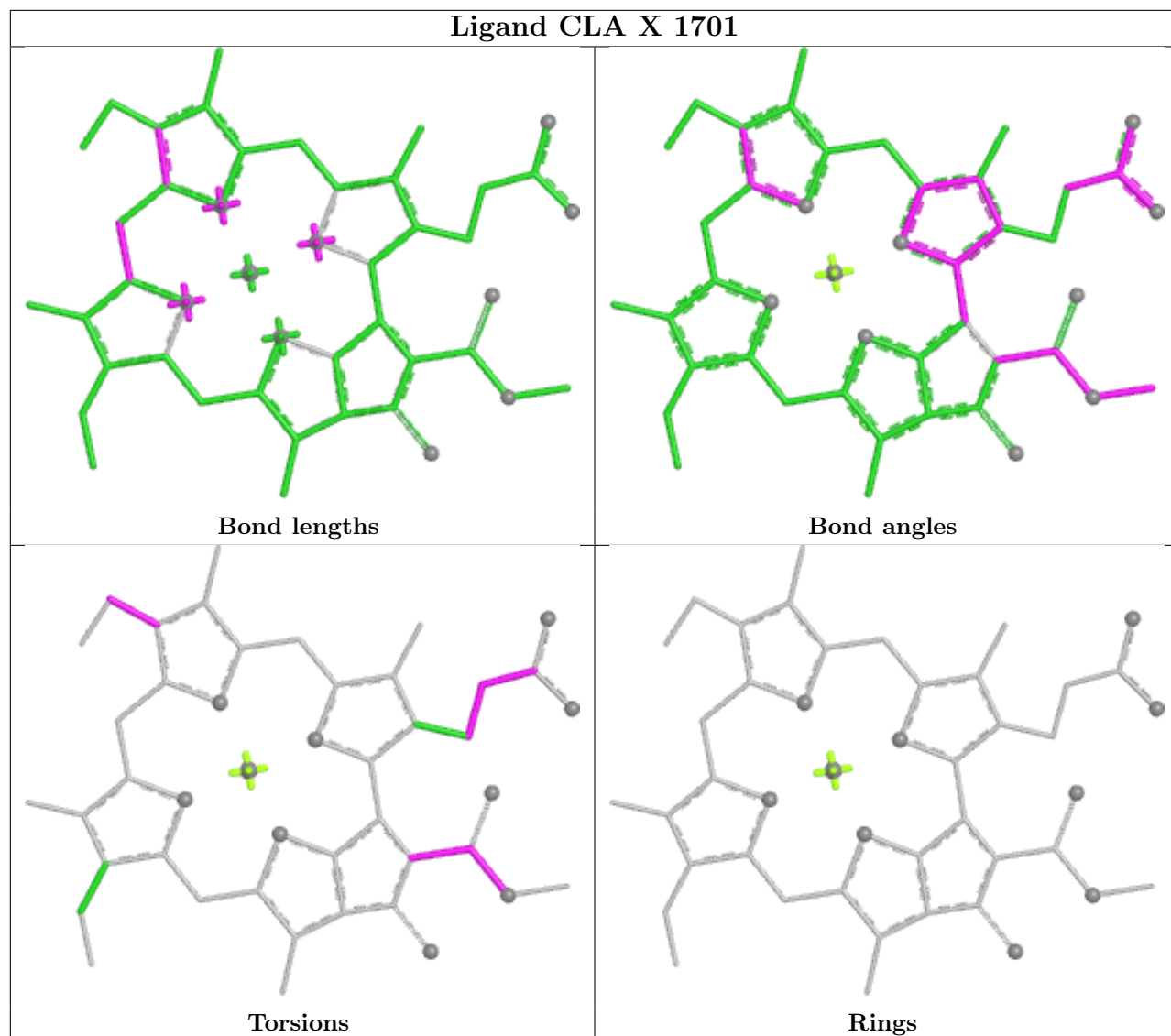


Ligand LHG A 5003

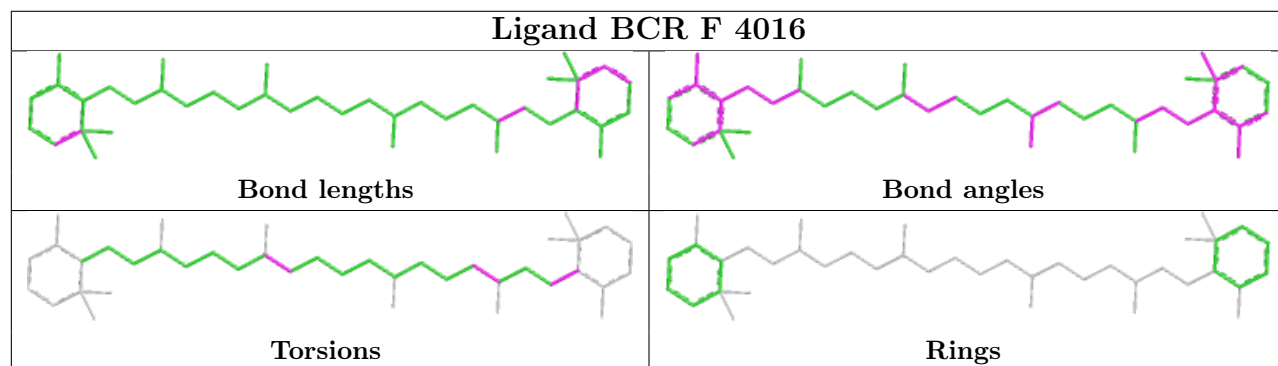


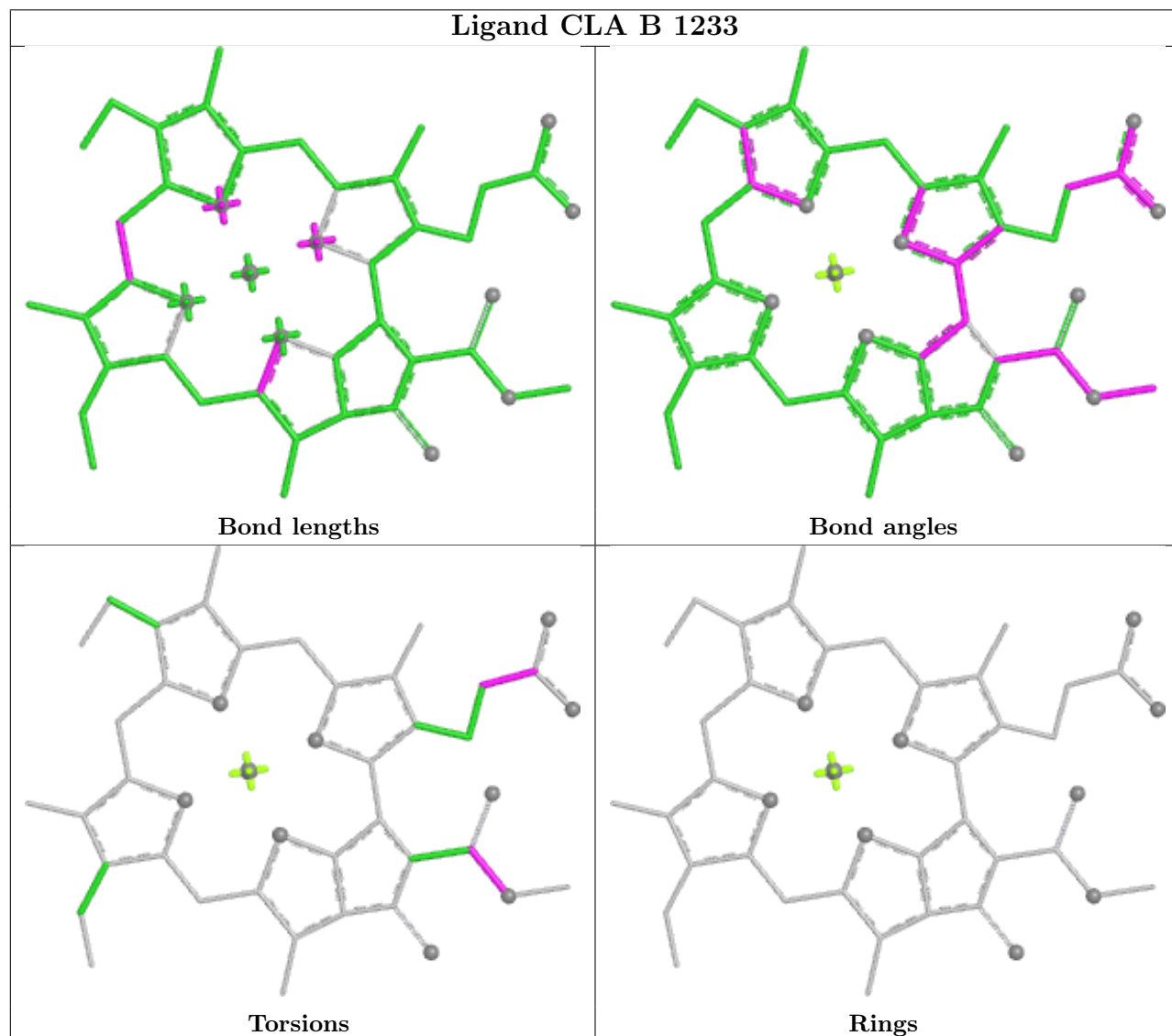
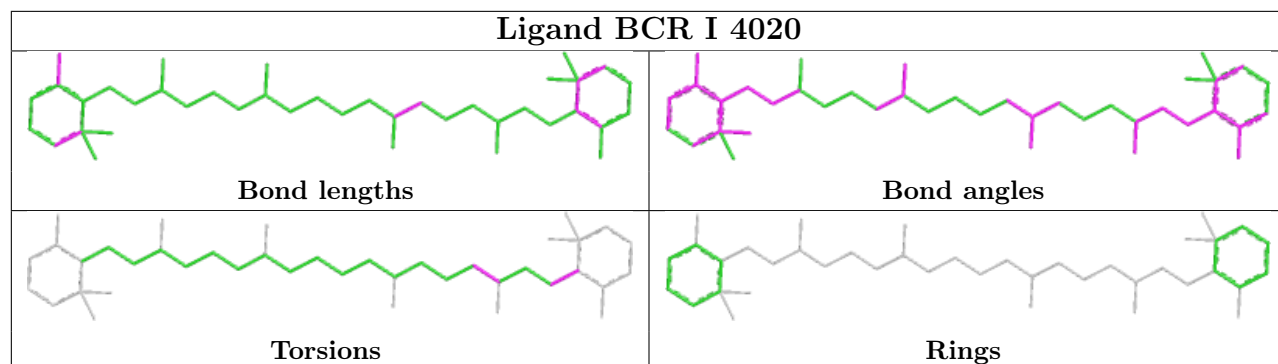


Ligand CLA X 1701

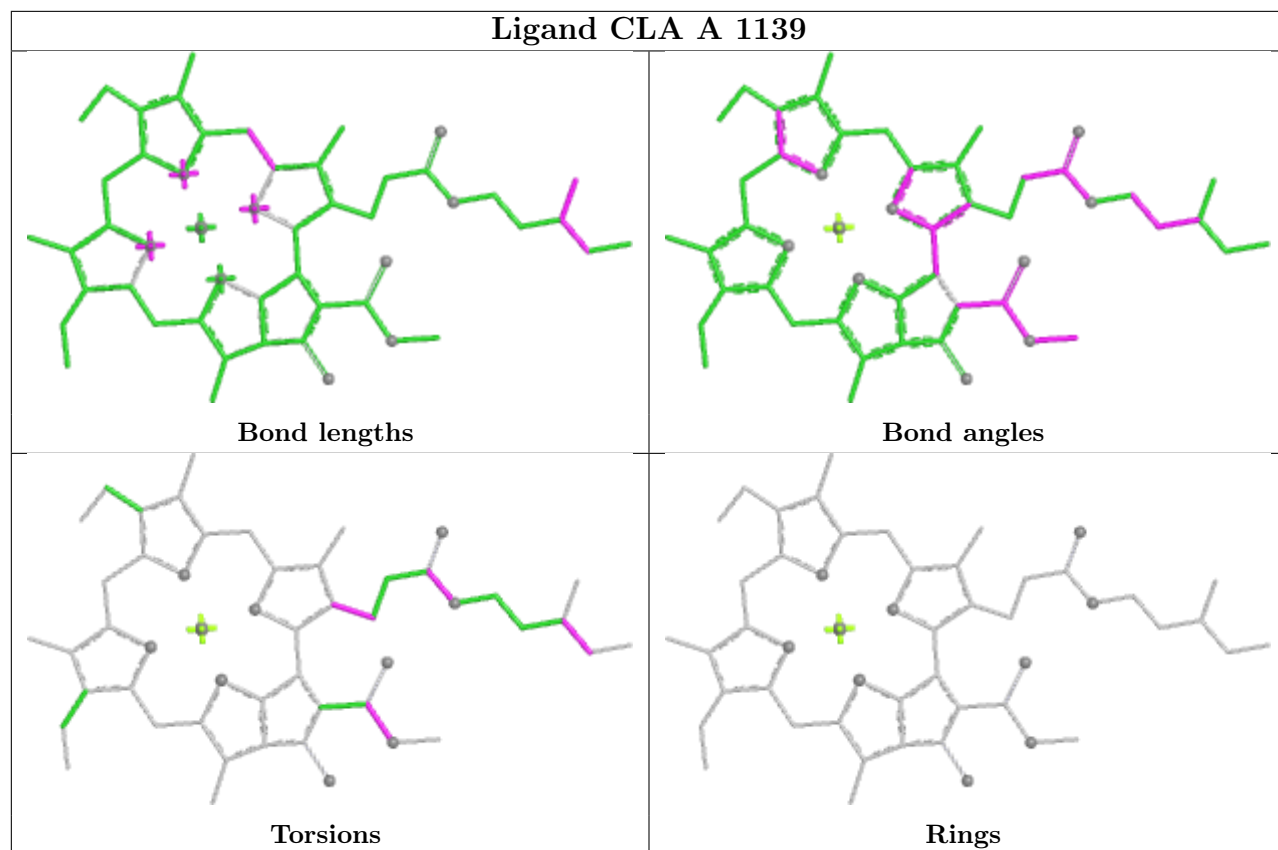


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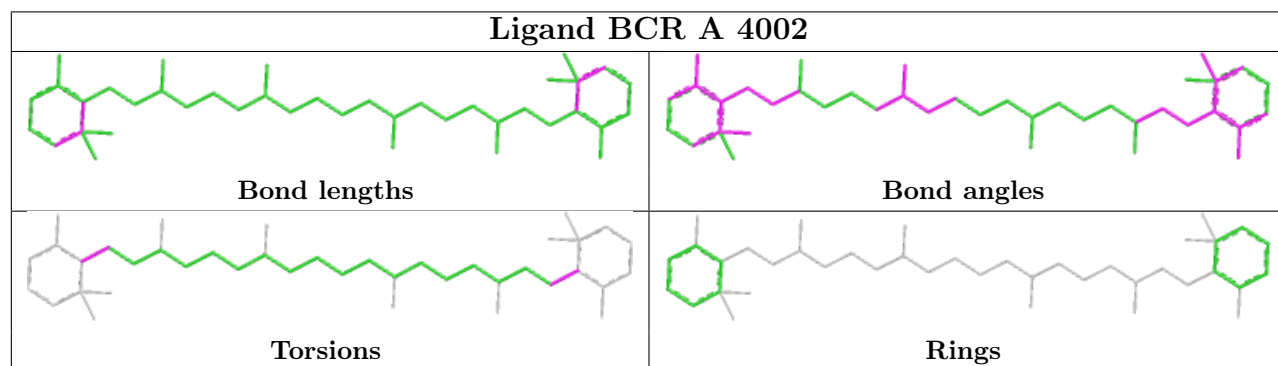


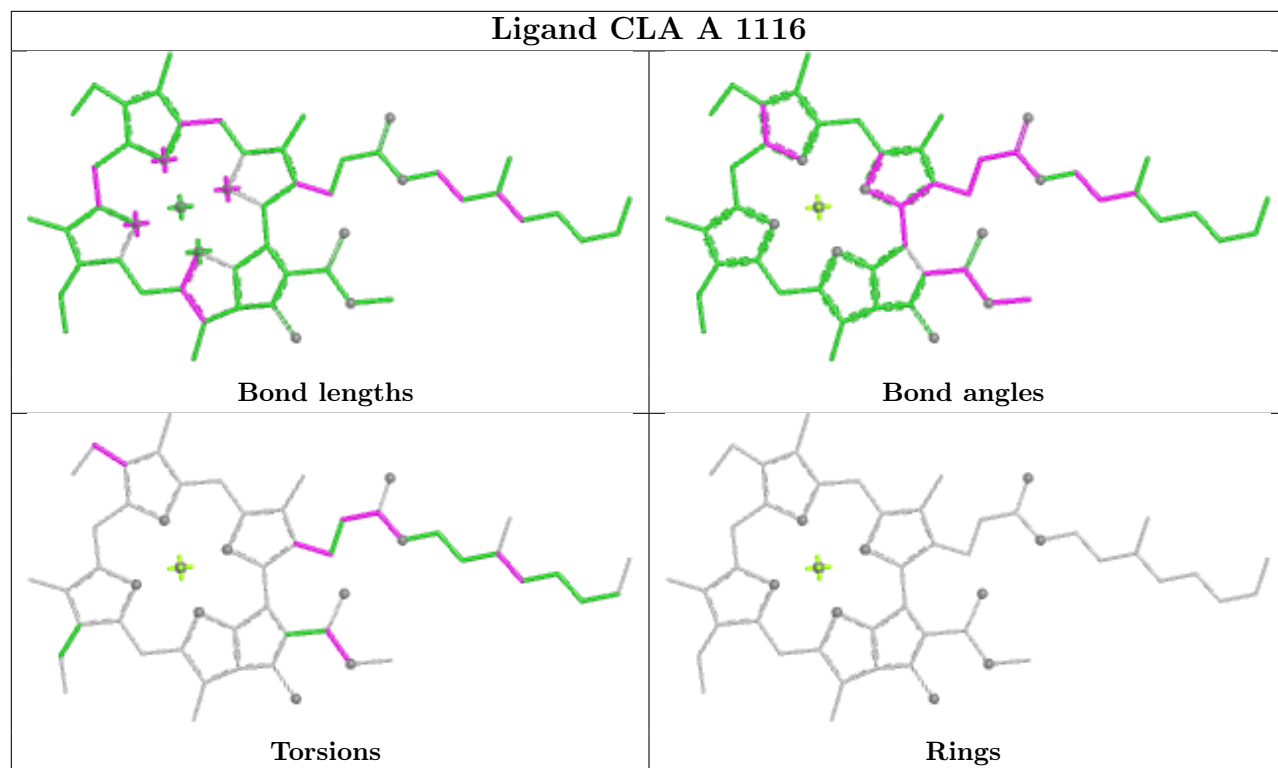


Ligand CLA A 1139

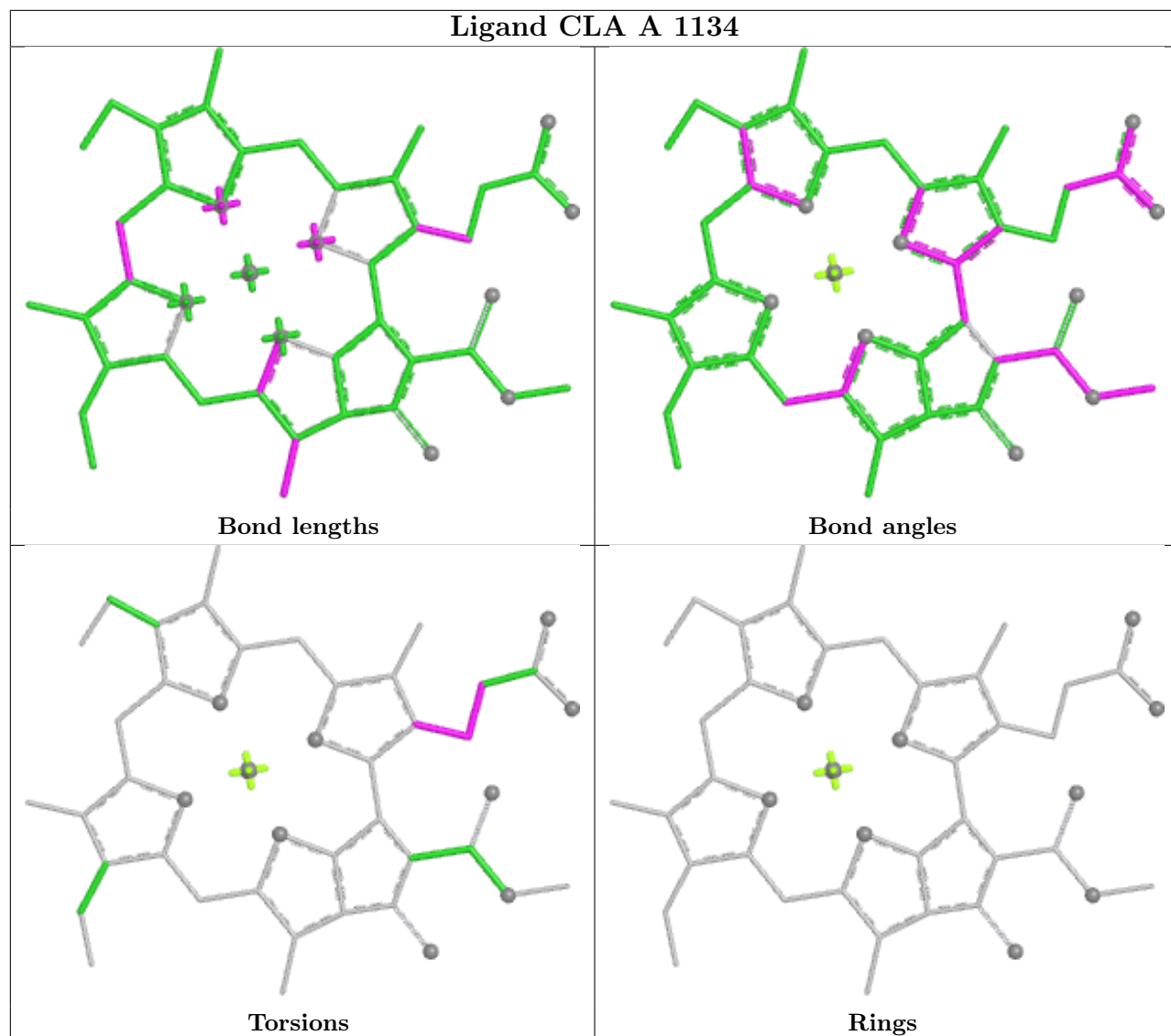


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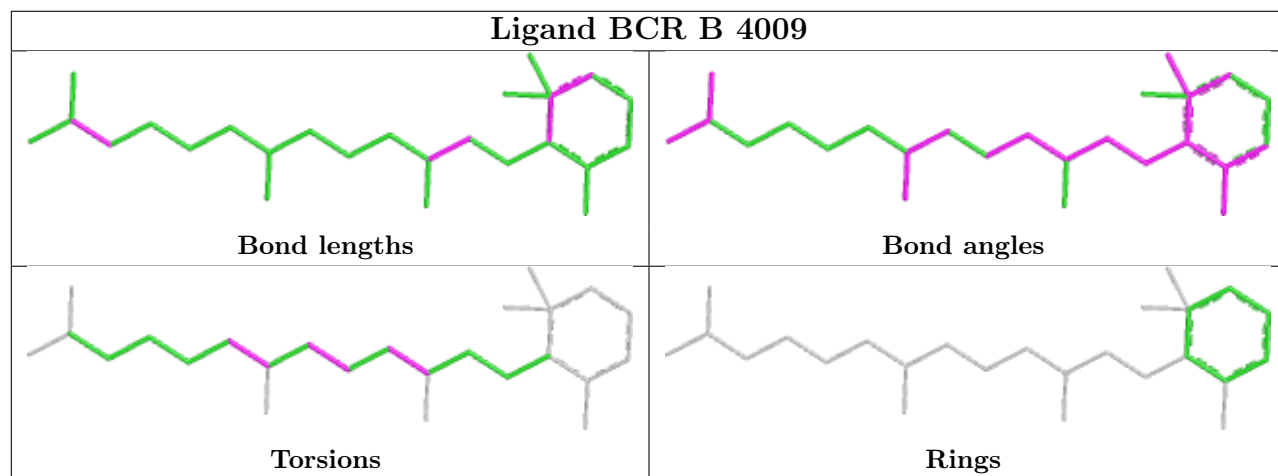




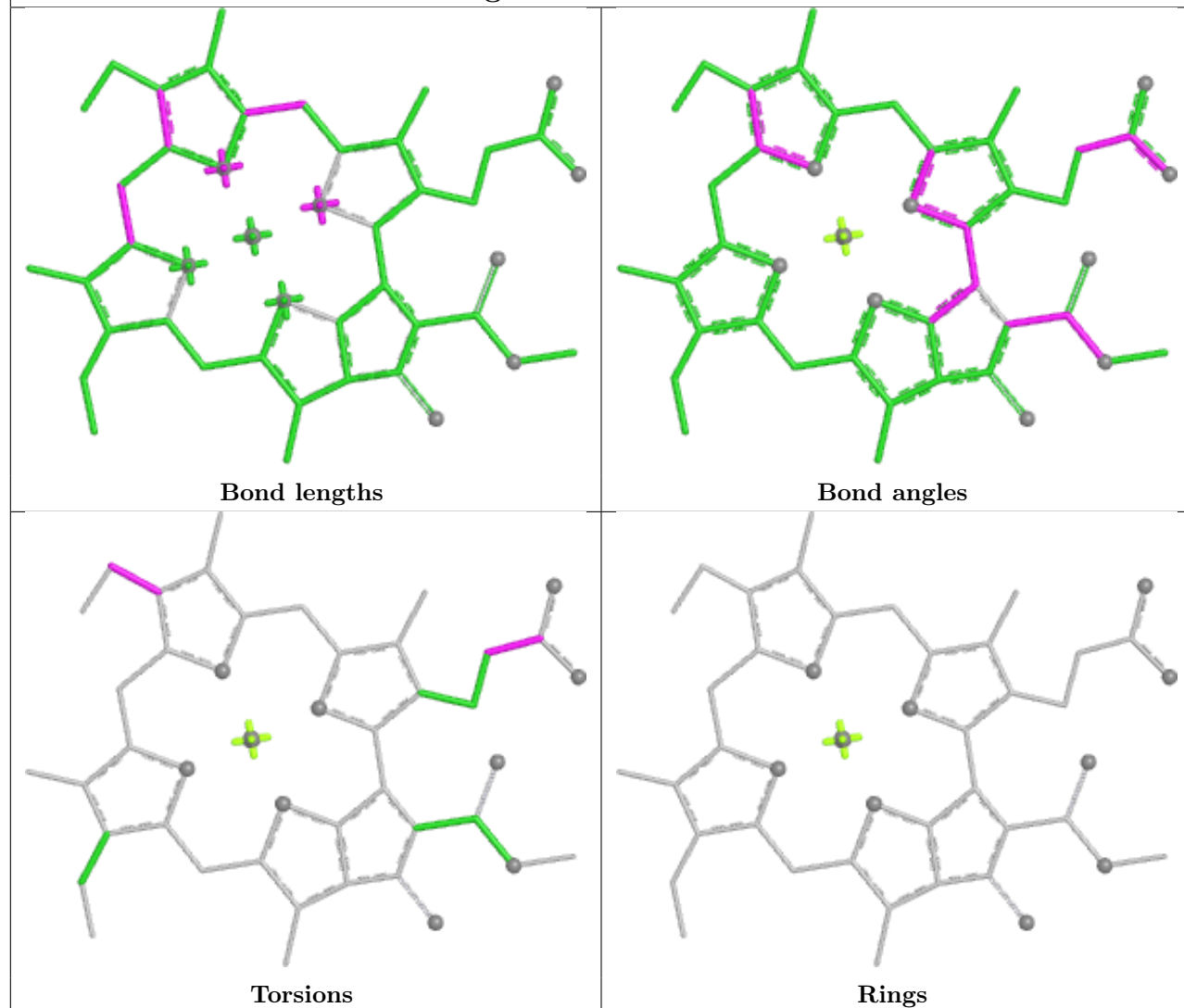
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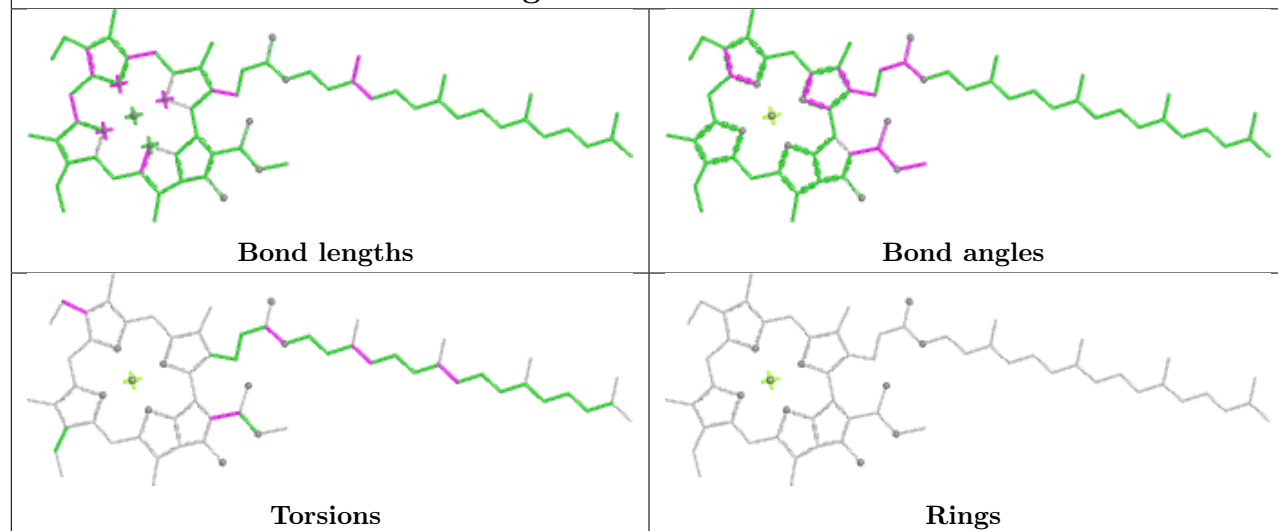
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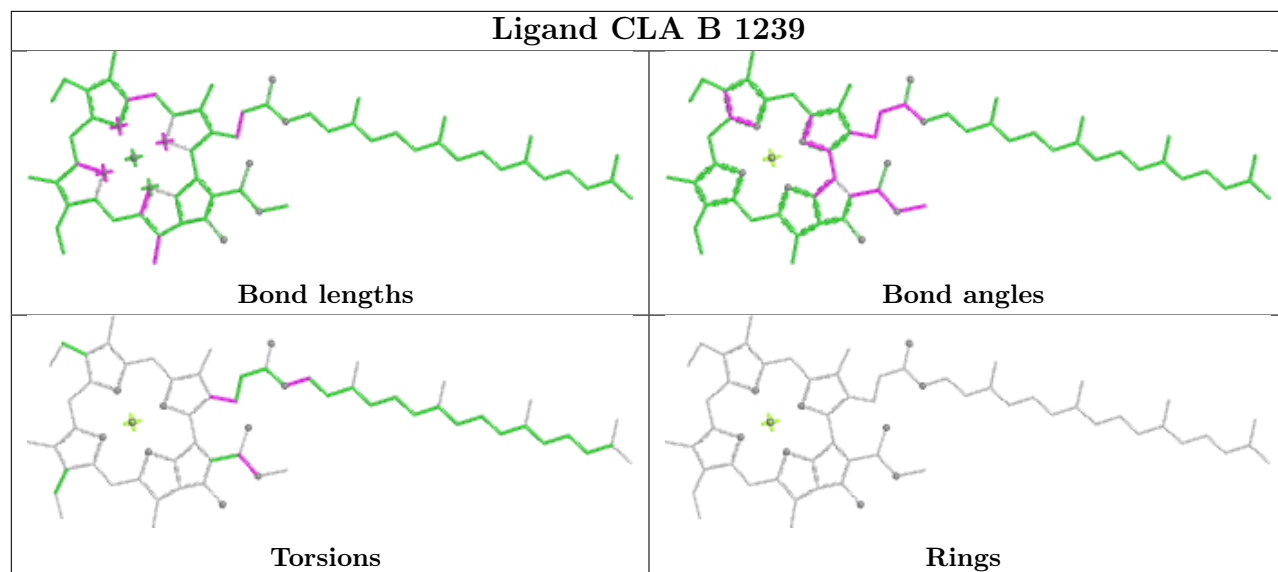
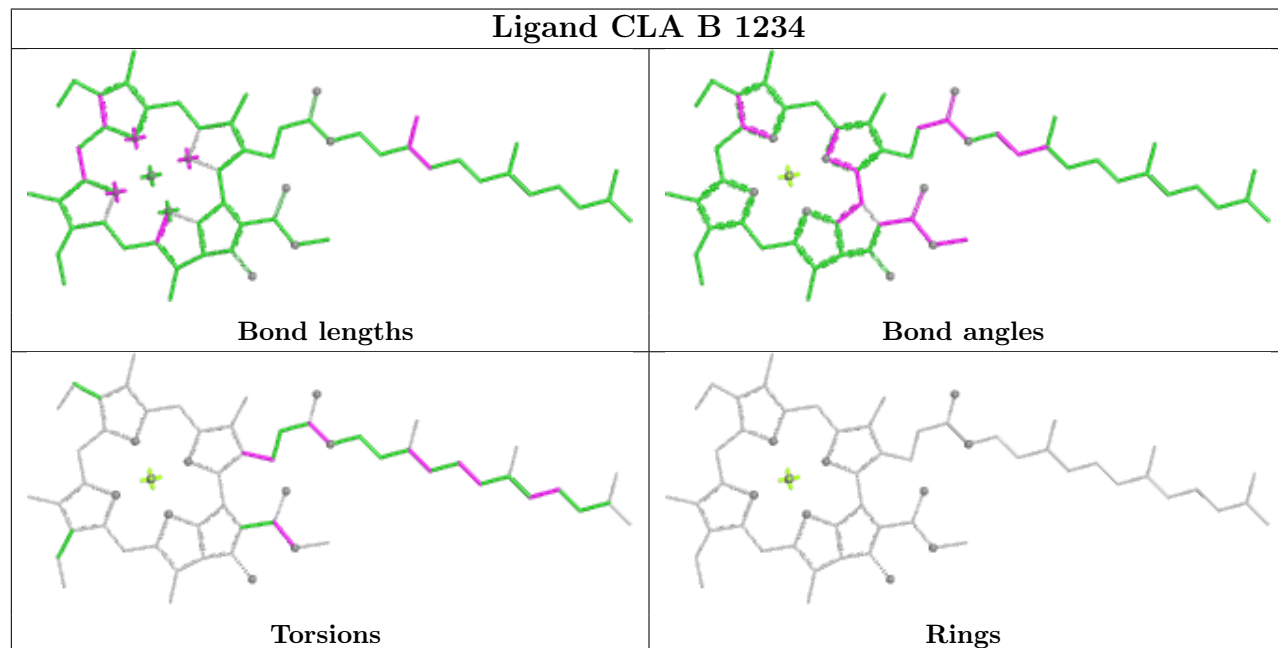


Ligand CLA B 1220

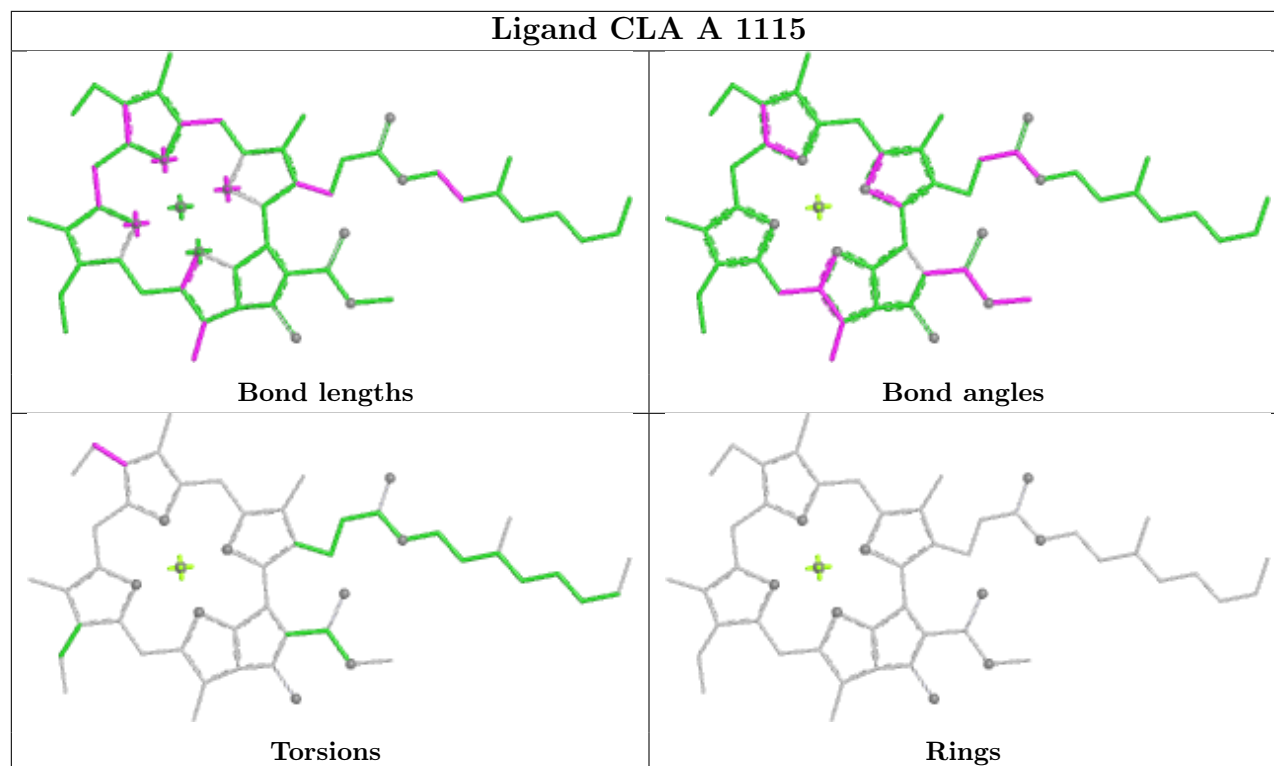


Ligand CLA A 1128

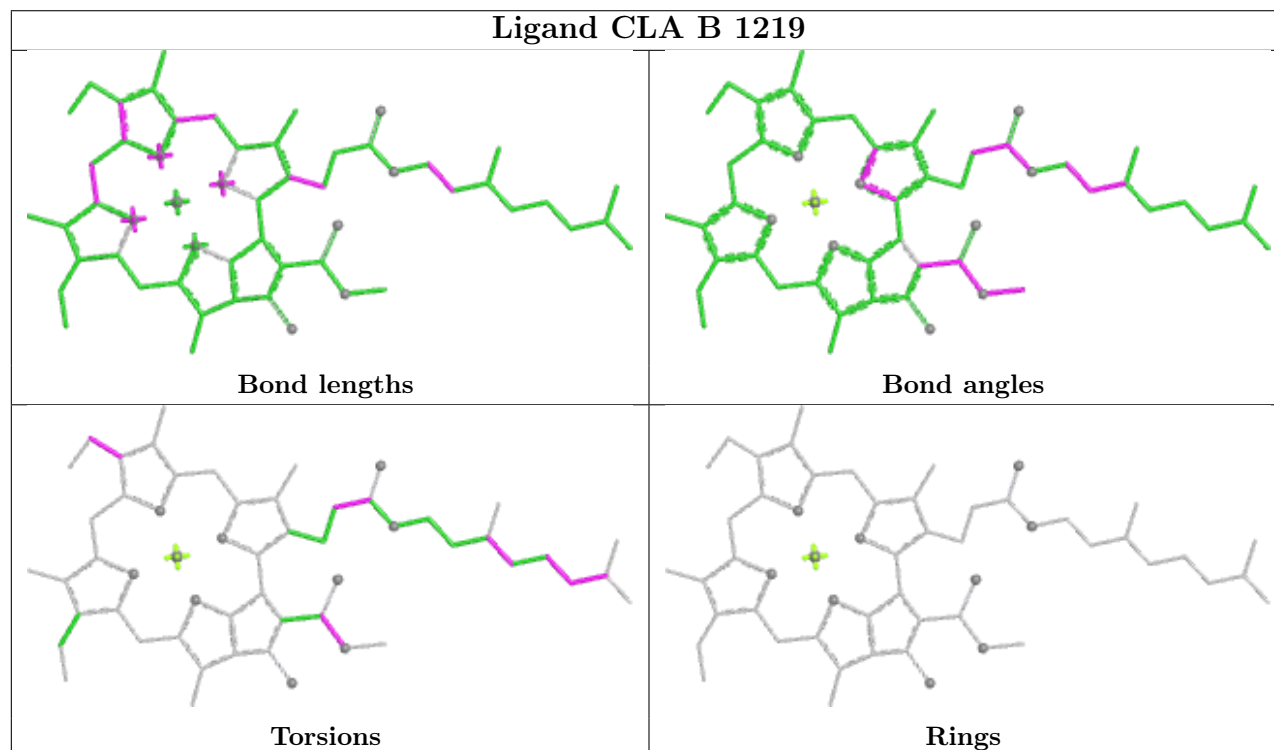


Ligand CLA B 1239**Ligand CLA B 1234**

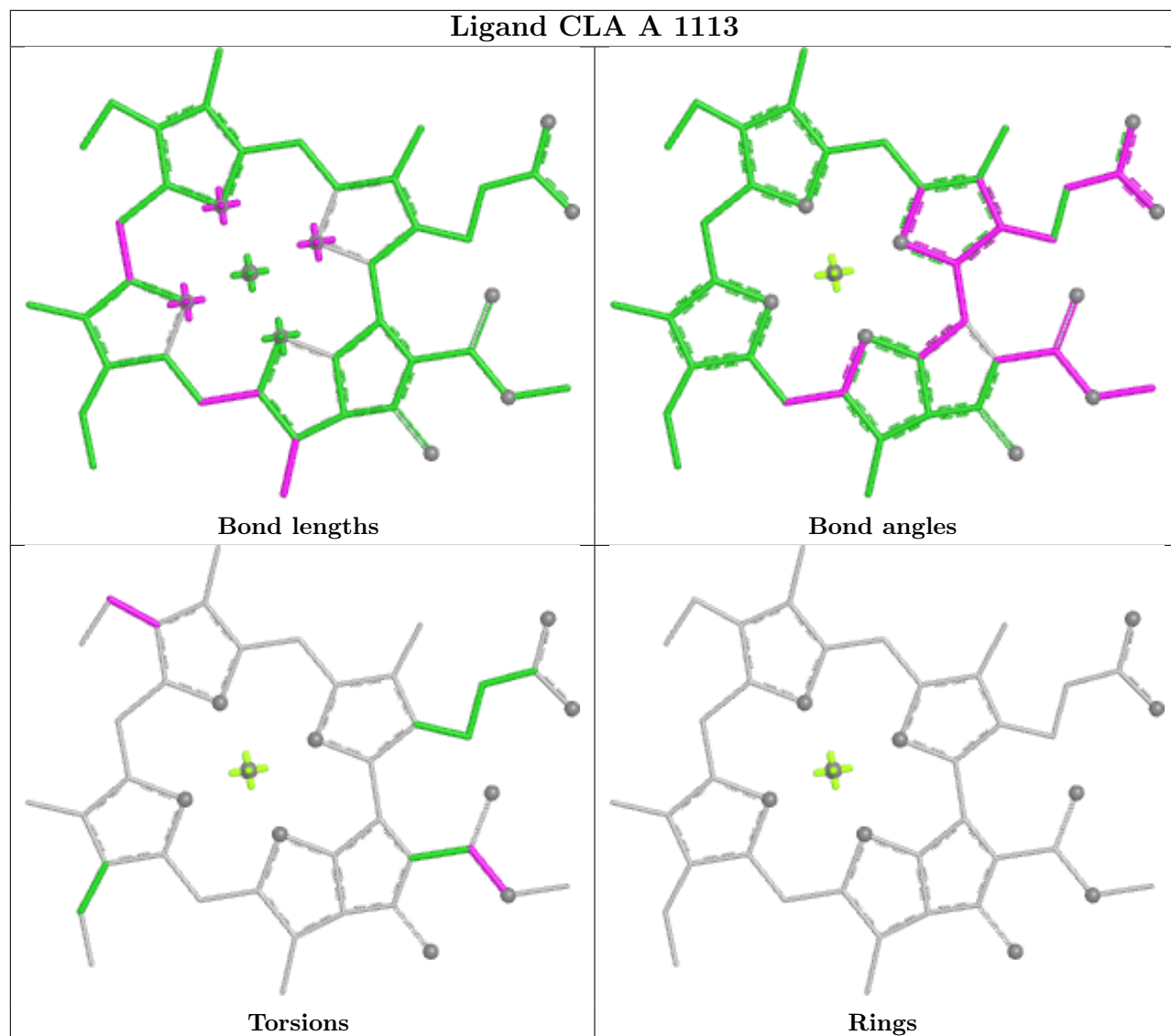
Ligand CLA A 1115



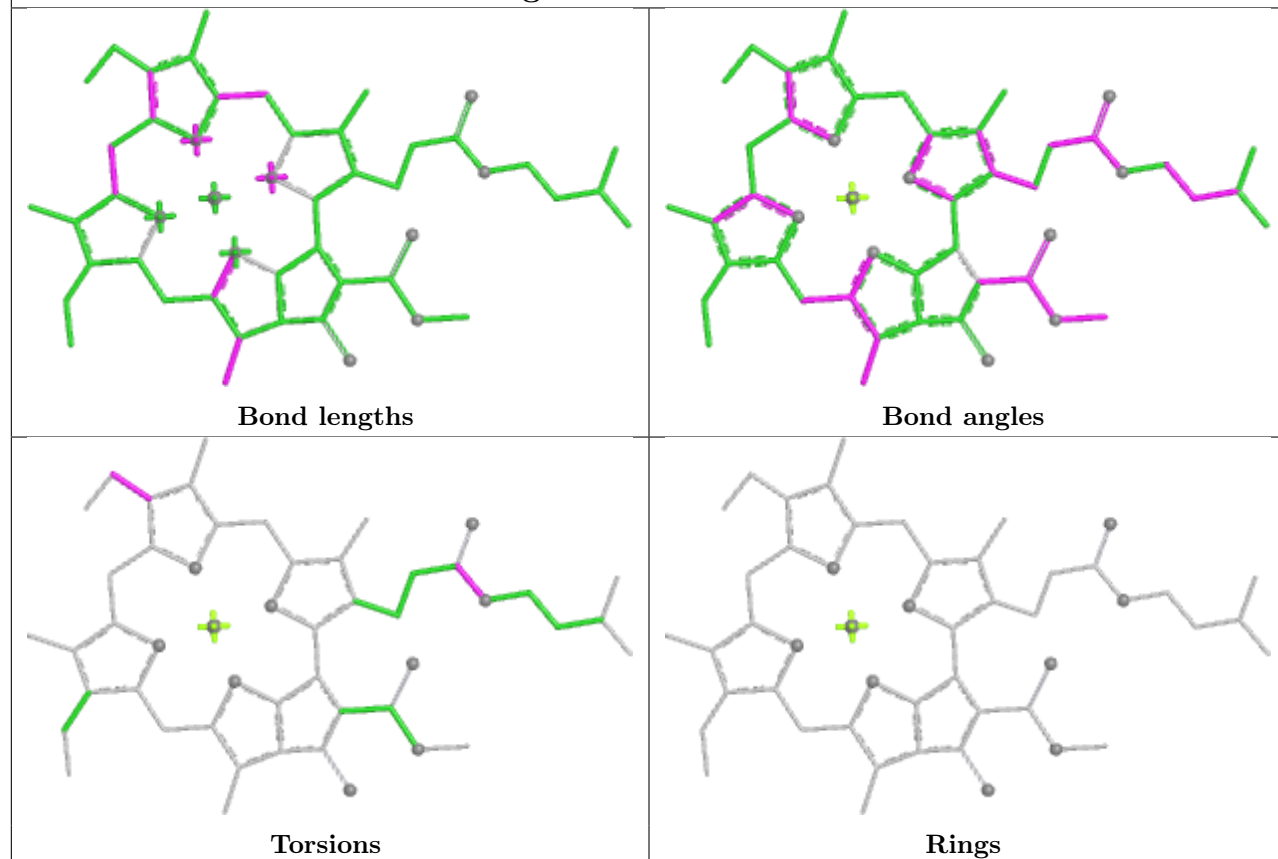
Ligand CLA B 1219



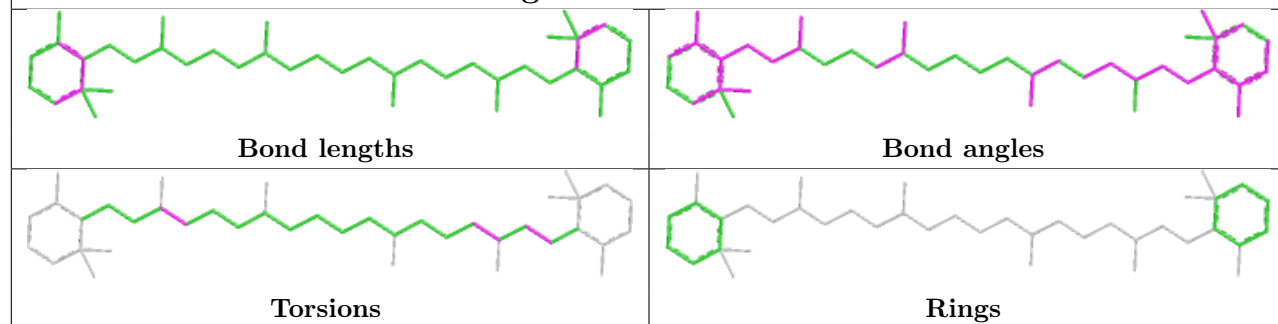
Ligand CLA A 1113



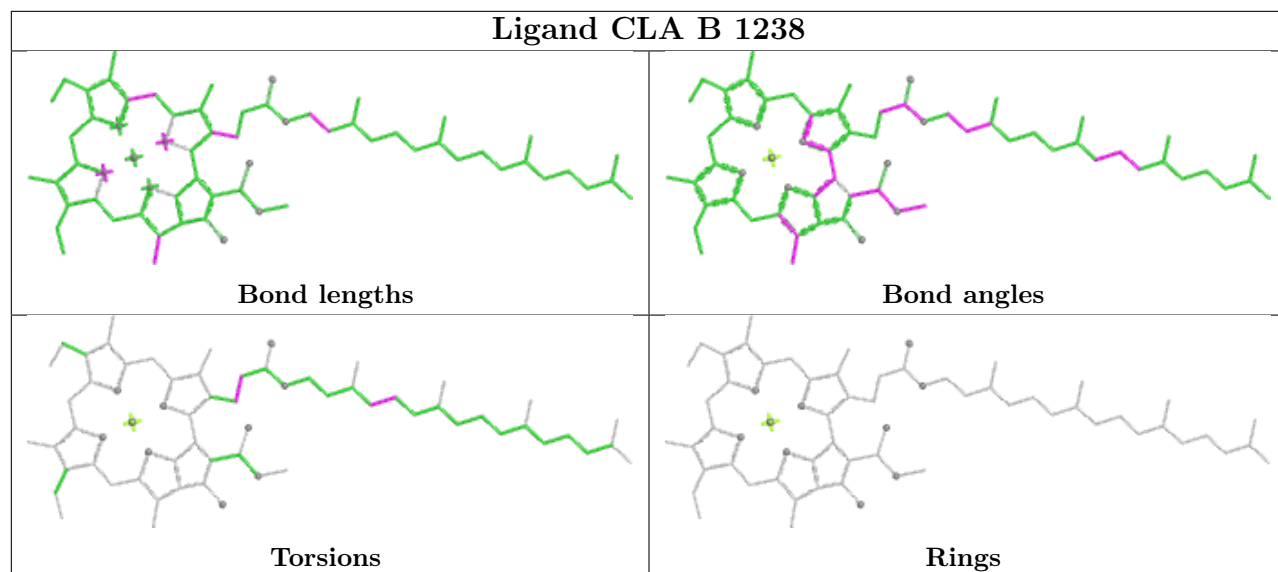
Ligand CLA A 1129



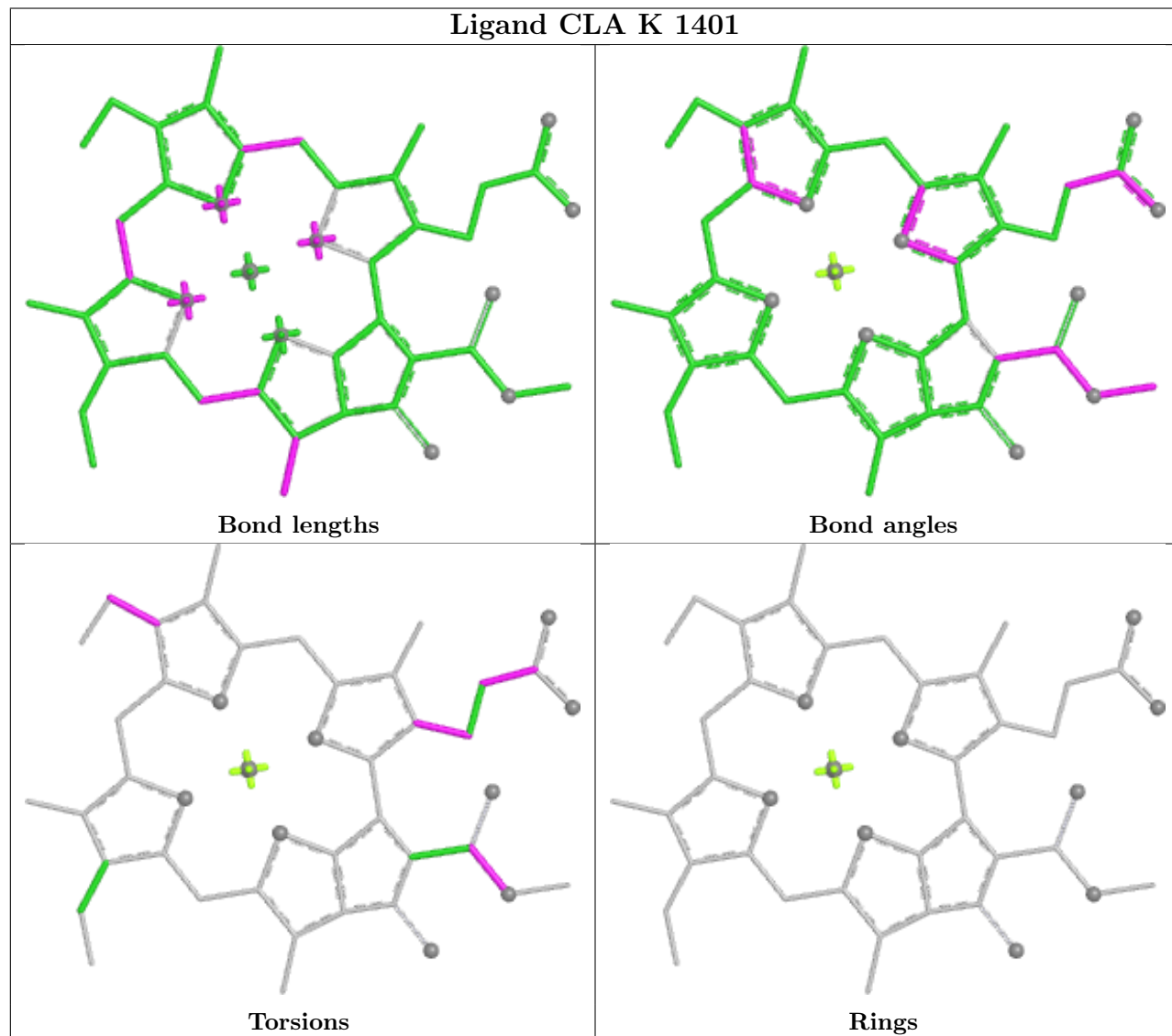
Ligand BCR B 4006



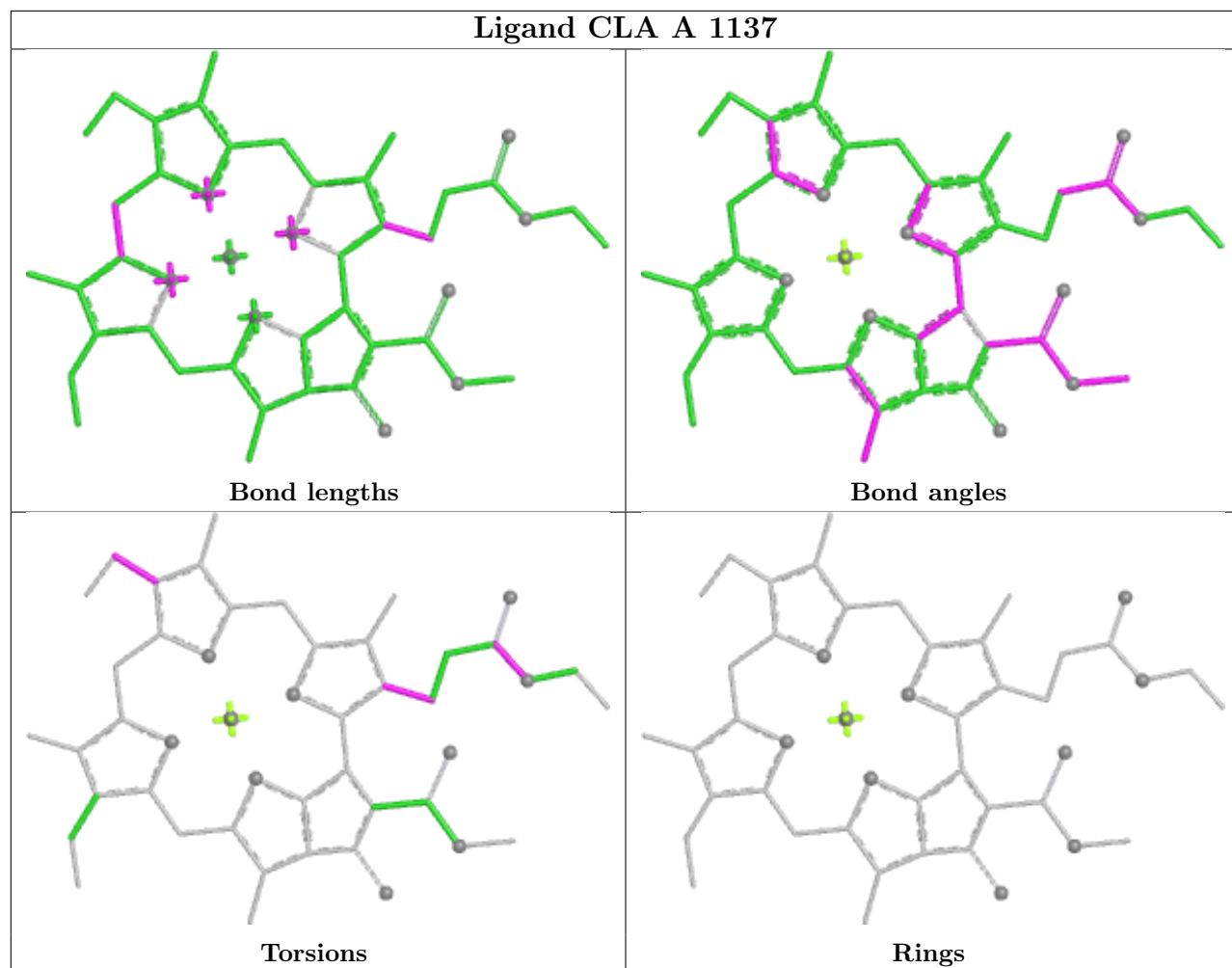
Ligand CLA B 1238



Ligand CLA K 1401



Ligand CLA A 1137



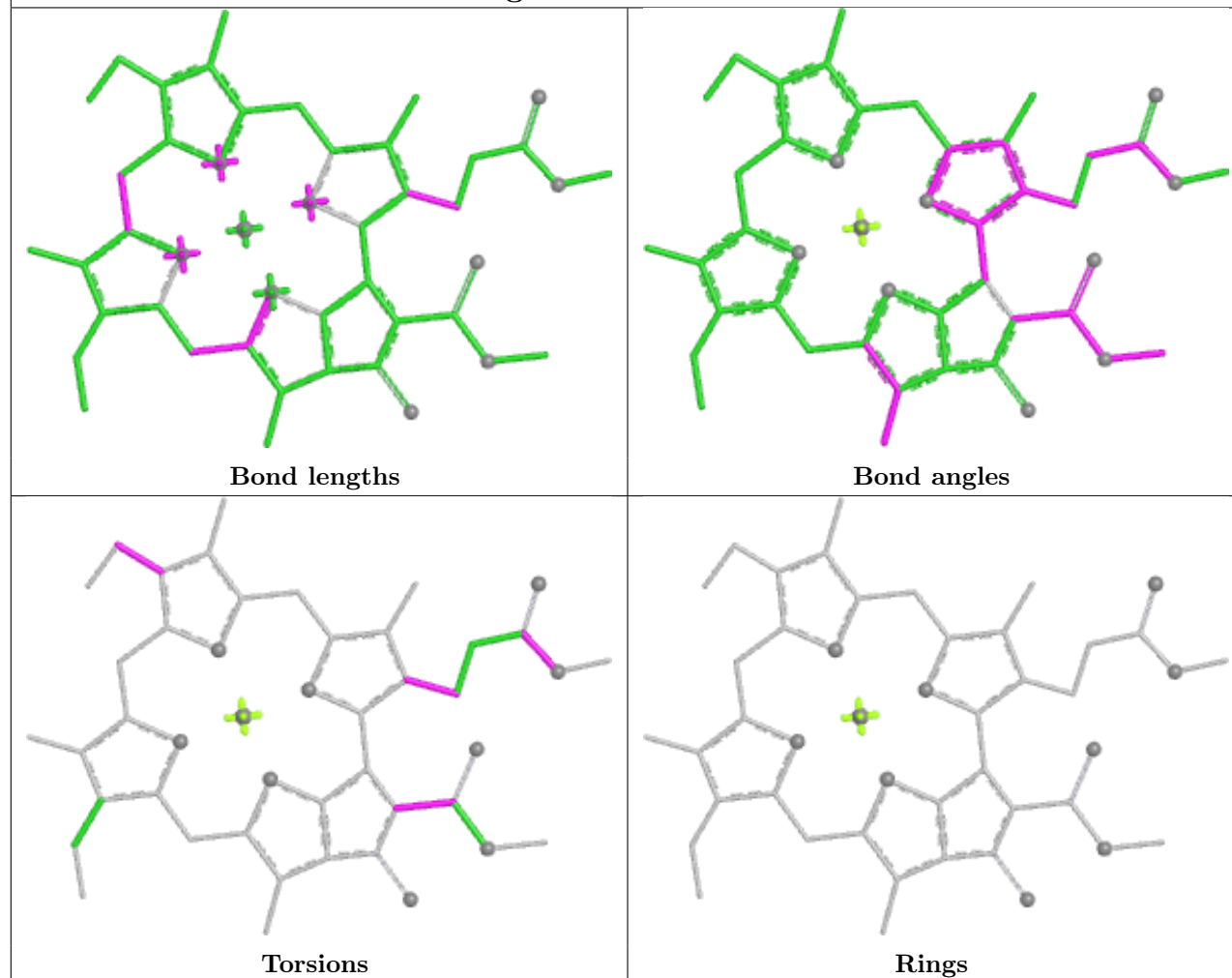
Bond lengths

Bond angles

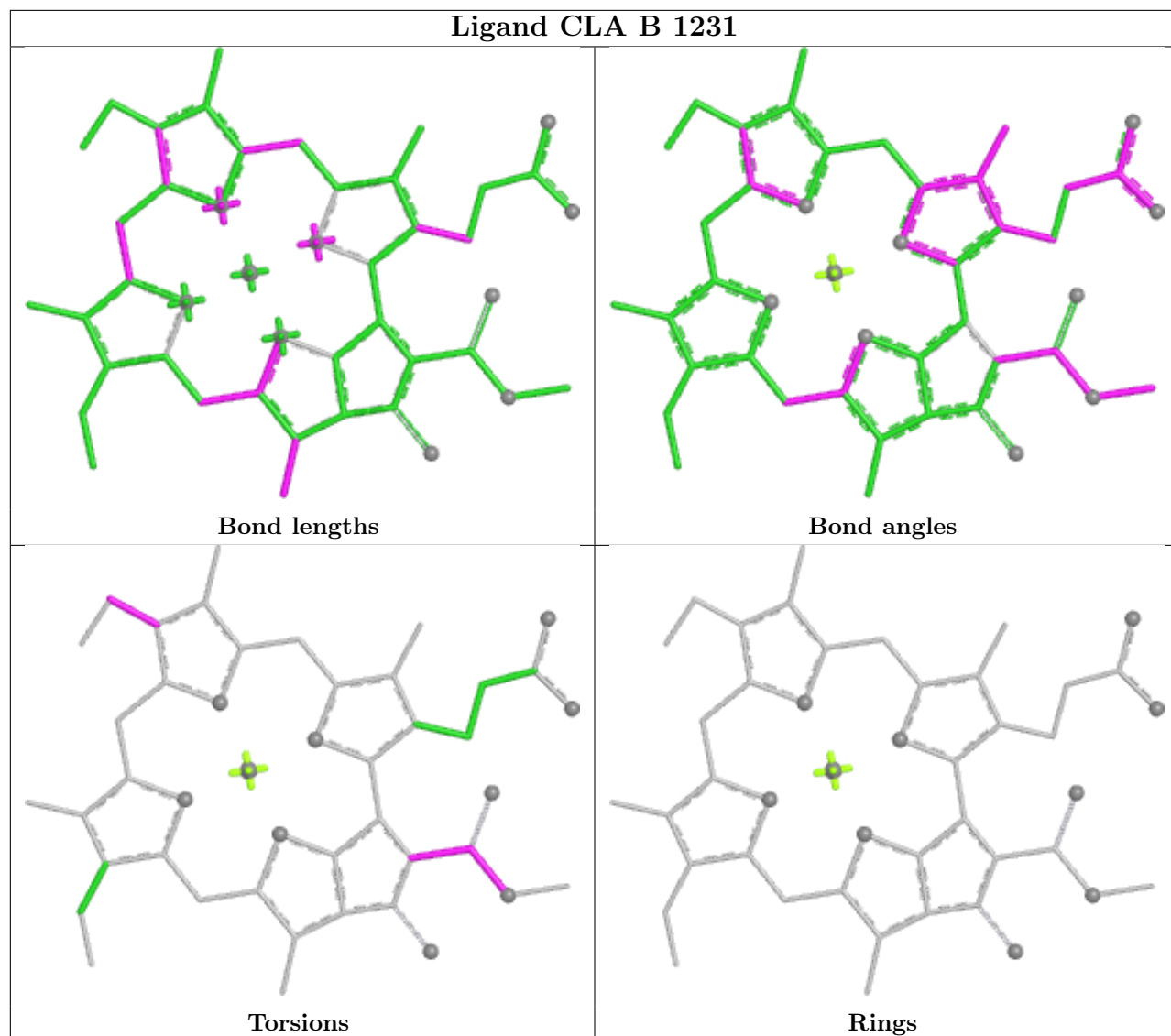
Torsions

Rings

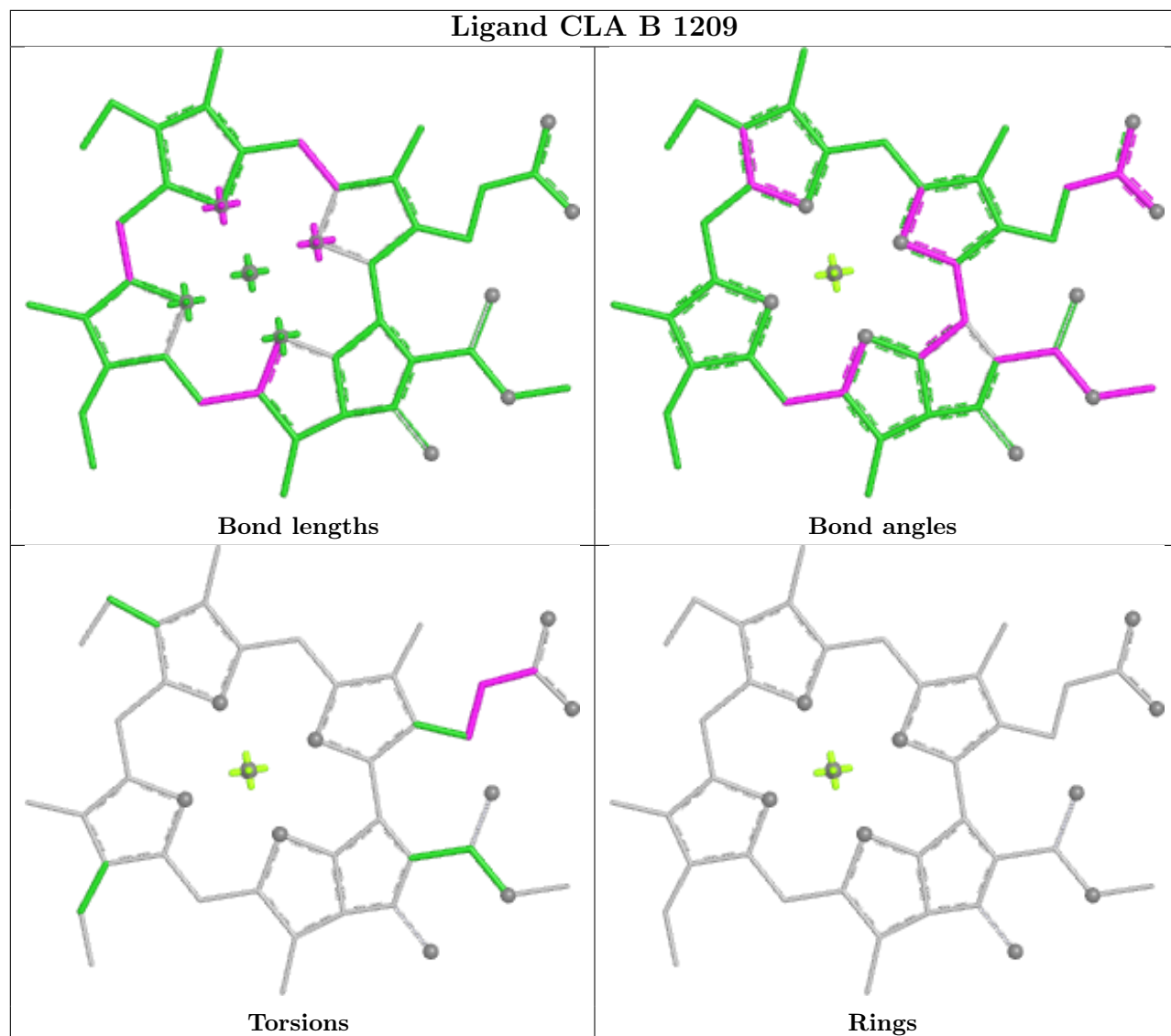
Ligand CLA B 1222



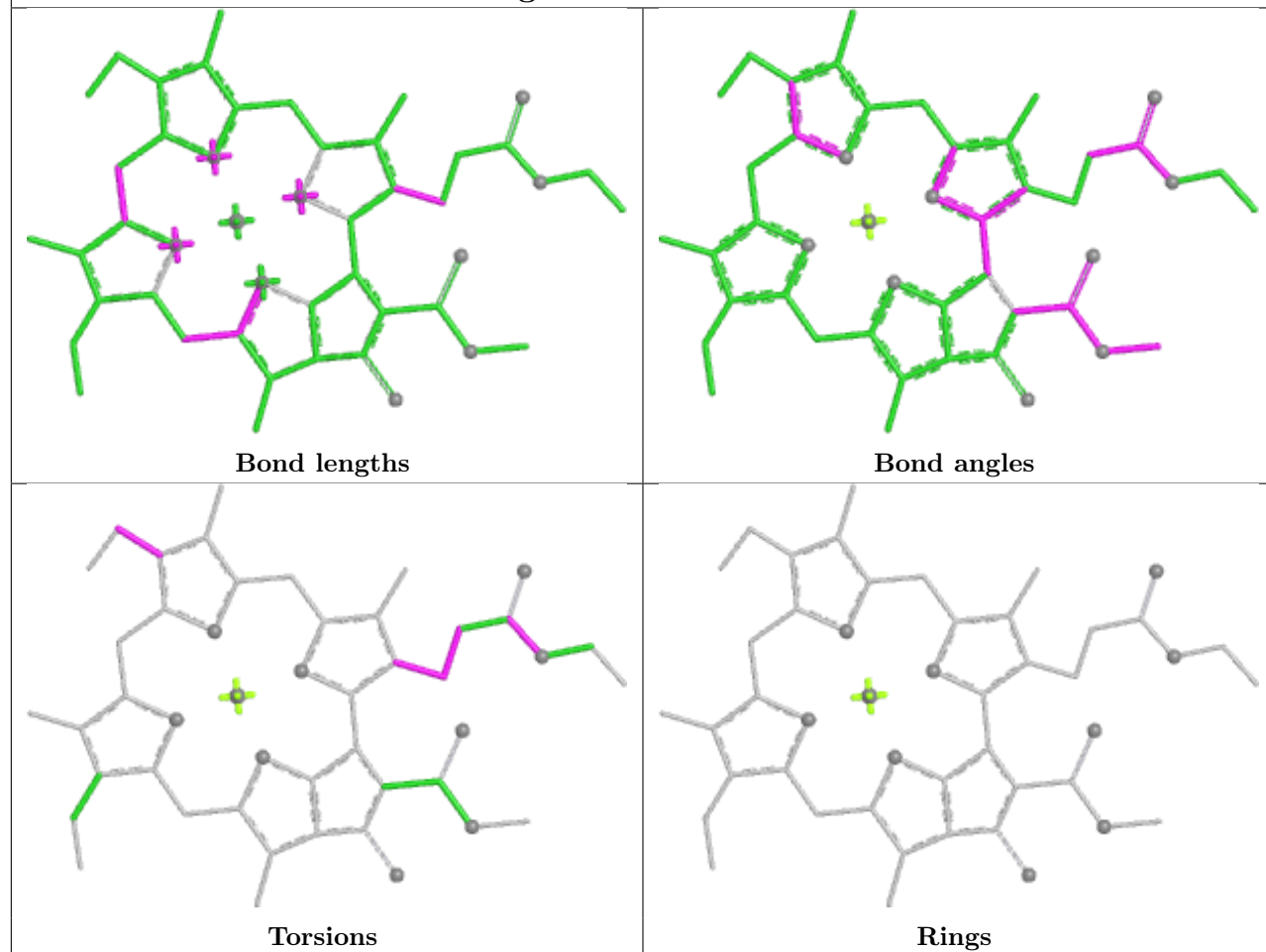
Ligand CLA B 1231



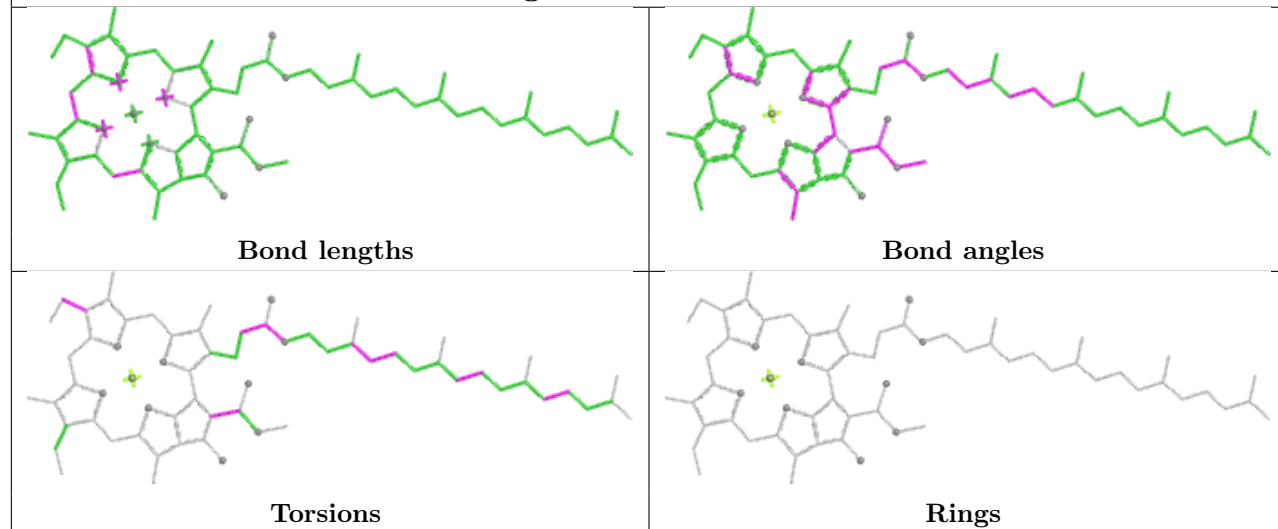
Ligand CLA B 1209

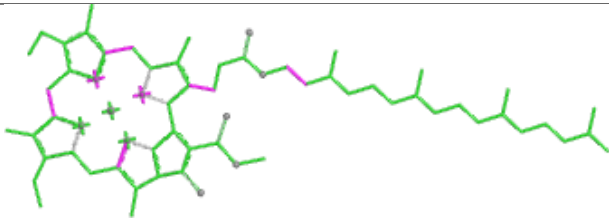
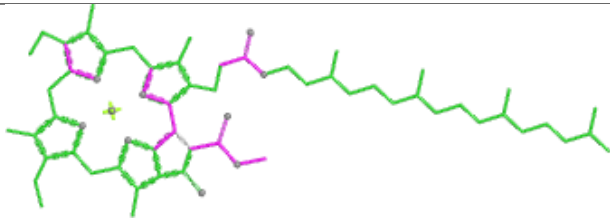
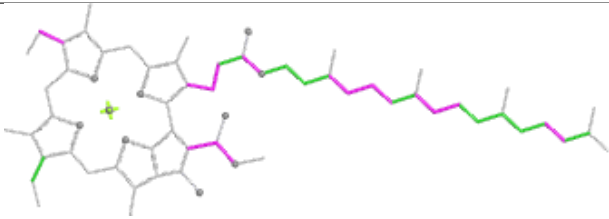
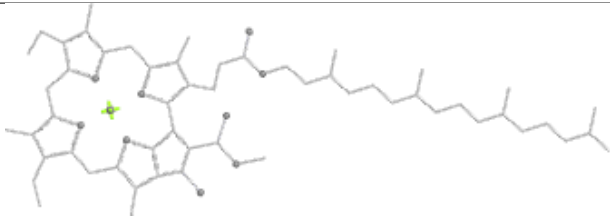


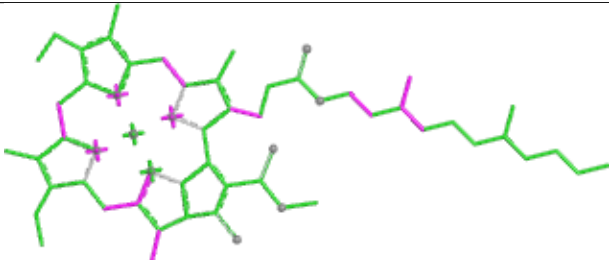
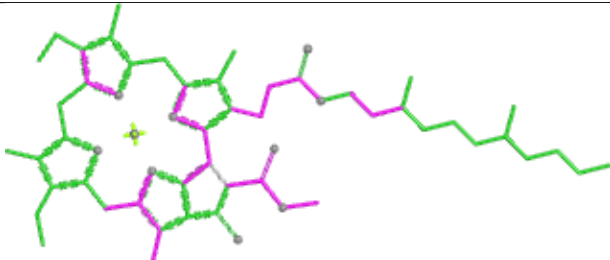
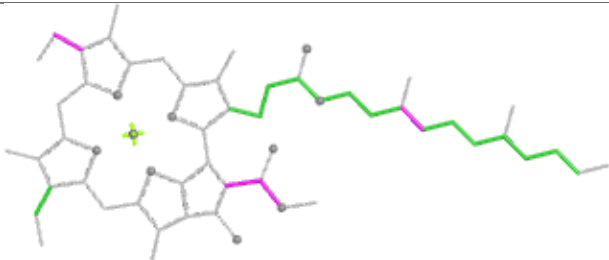
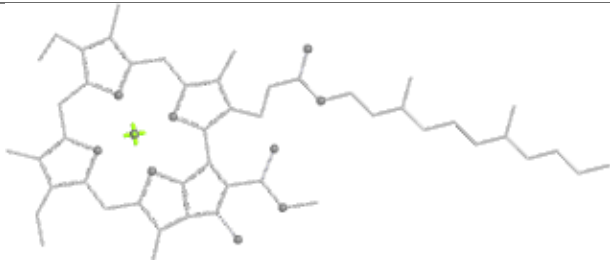
Ligand CLA B 1217

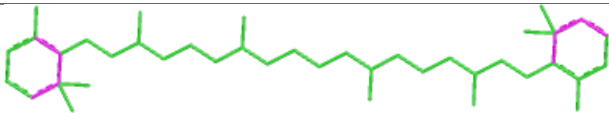
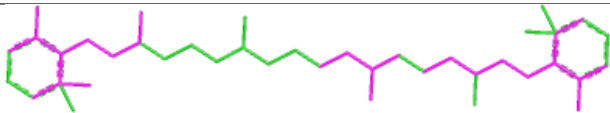
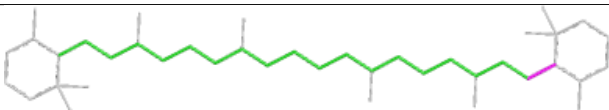
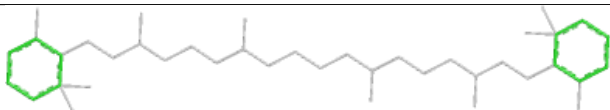


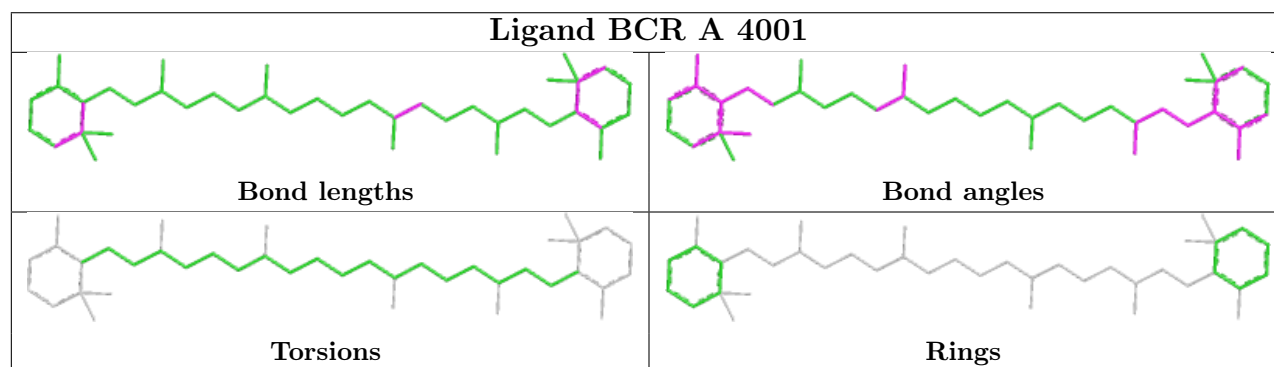
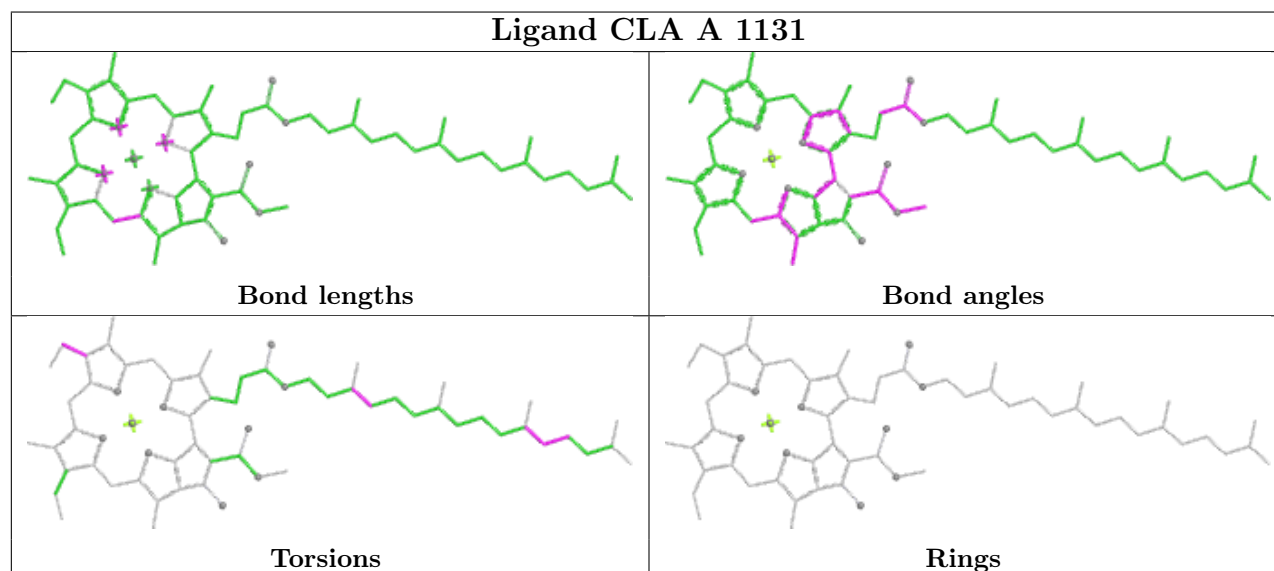
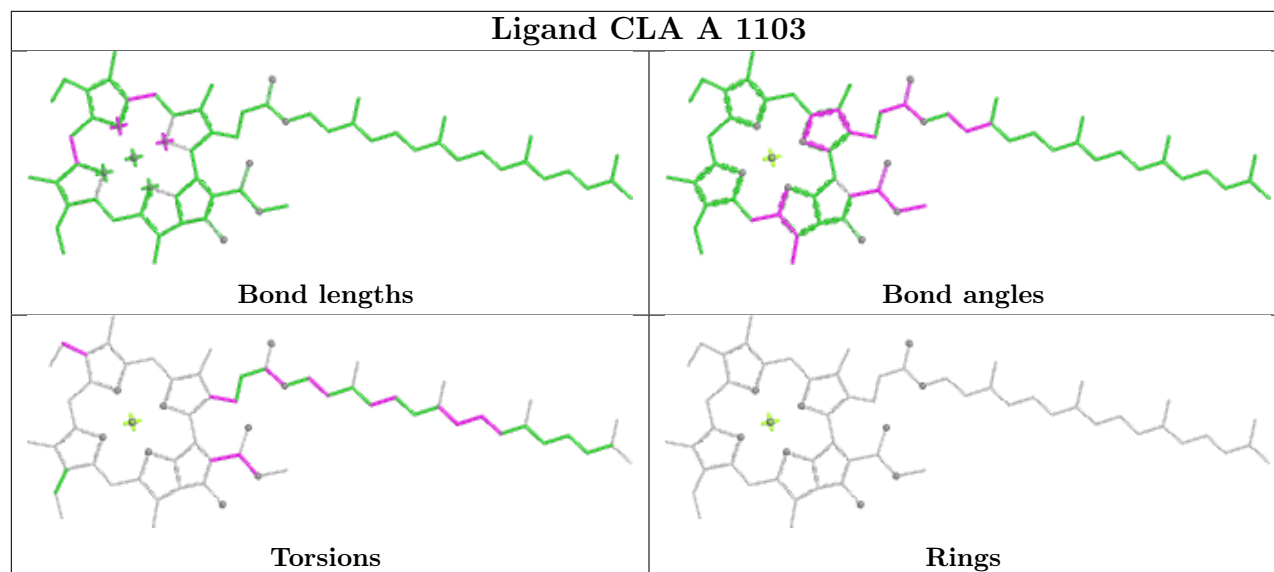
Ligand CLA A 1123

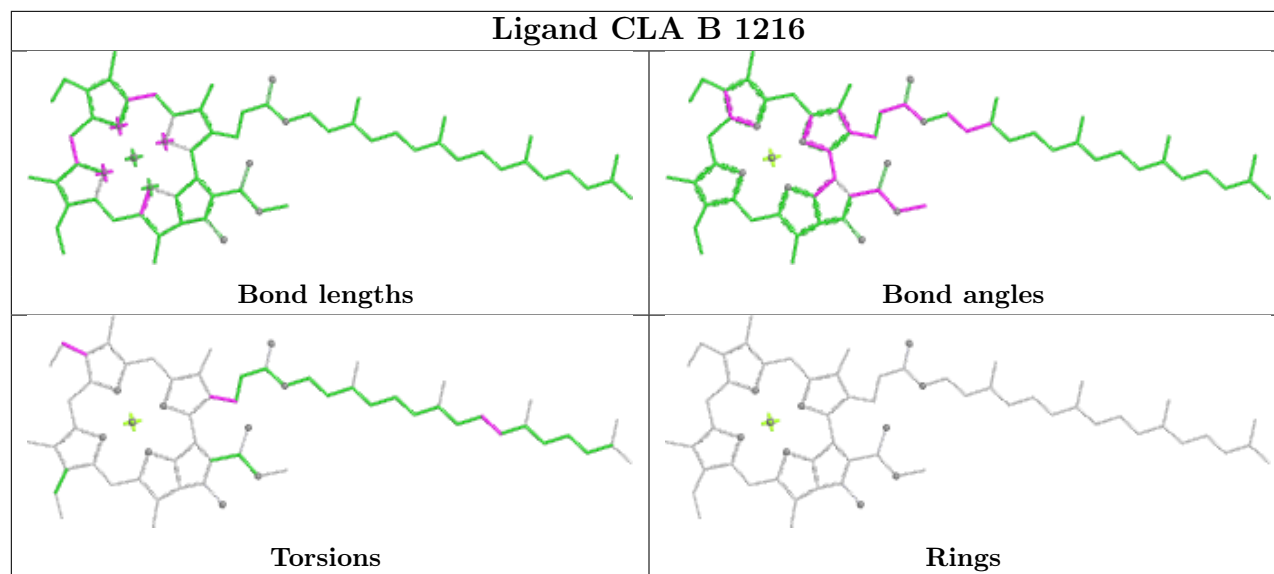


Ligand CLA A 1106	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1230	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 4010	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.