Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:25 PM EDT

PDB ID	:	1JB0
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 (i) 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 (1)) were used in the production of this report:

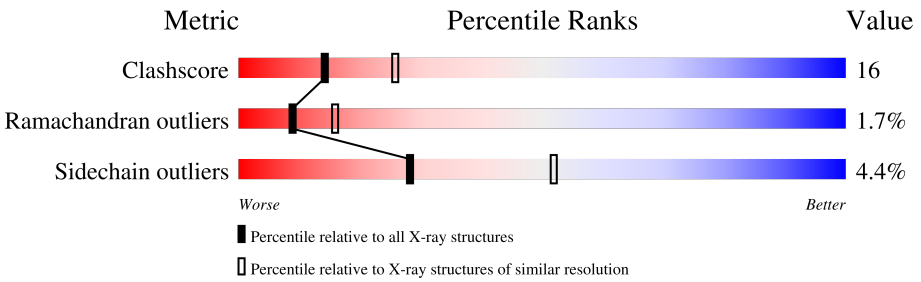
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	755	71% 24% • •
2	B	740	71% 26% •
3	C	80	74% 25% •
4	D	138	67% 28% •
5	E	75	72% 16% • 8%
6	F	164	57% 28% • 14%
7	I	38	74% 21% 5%
8	J	41	54% 41% 5%

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Mol	Chain	Length	Quality of chain
9	K	83	42% 12% 45%
10	L	154	79% 16%
11	M	31	74% 19%
12	X	35	54% 26% 17%

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
			Total	C	N	O	S			
1	A	740	5784	3794	988	976	26	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

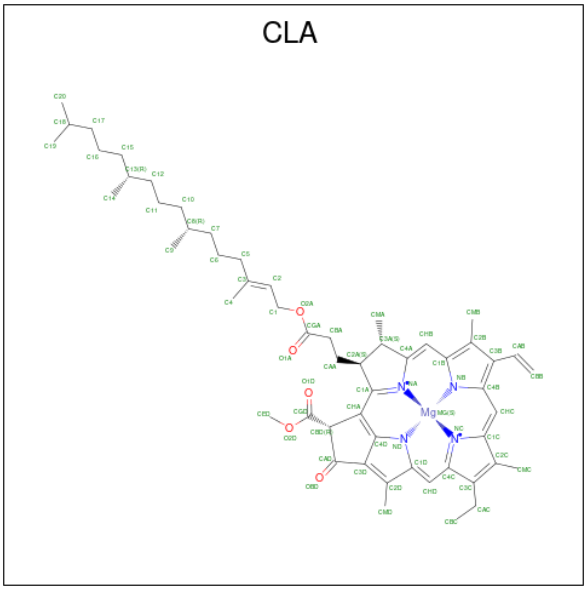
- Molecule 11 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII.

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 (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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

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

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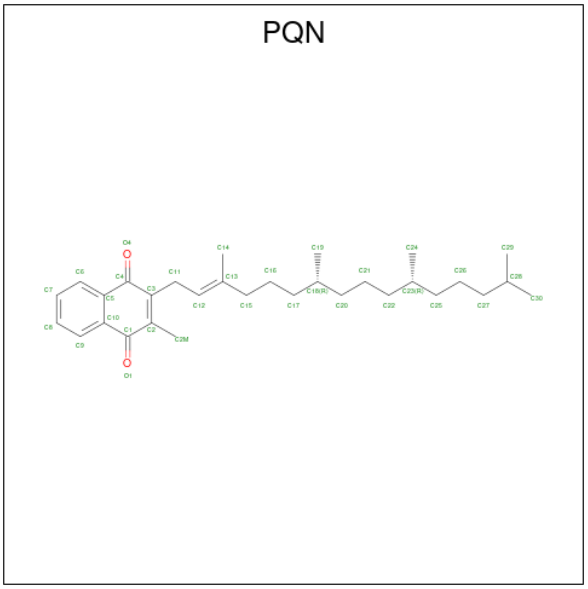
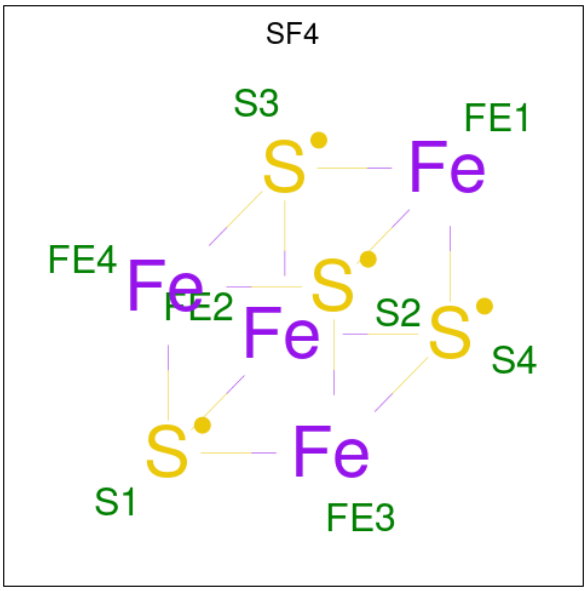
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
13	M	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
13	X	1	45	35	1	4	5	0	0

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



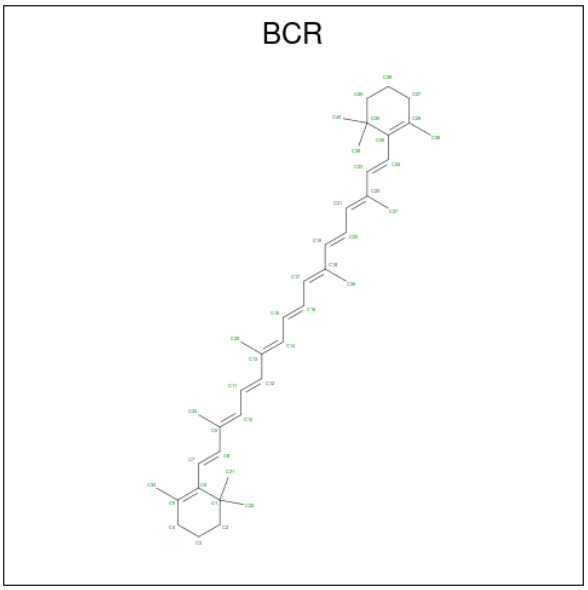
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	A	1	33	31	2	0	0
			Total	C	O		
14	B	1	33	31	2	0	0

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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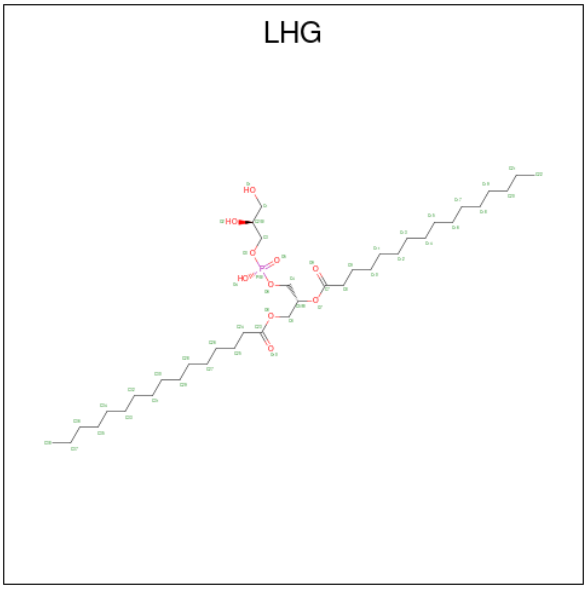
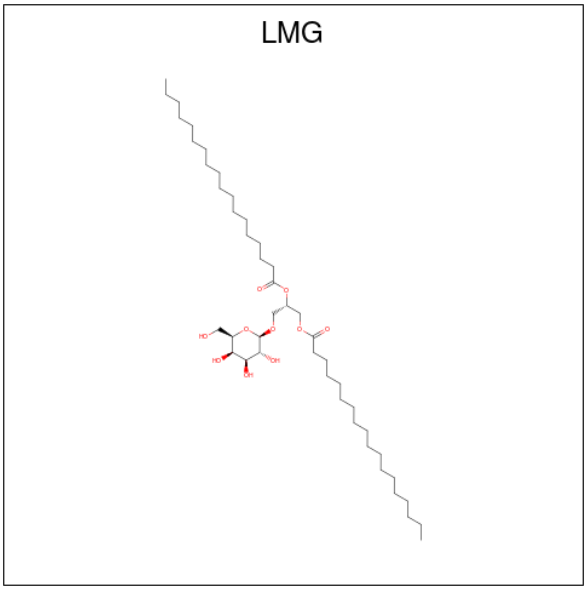
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	A	1	40	40	0	0
			Total	C		
16	B	1	40	40	0	0
			Total	C		
16	B	1	40	40	0	0
			Total	C		
16	B	1	40	40	0	0
			Total	C		
16	B	1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

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



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

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



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

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 20 is water.

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

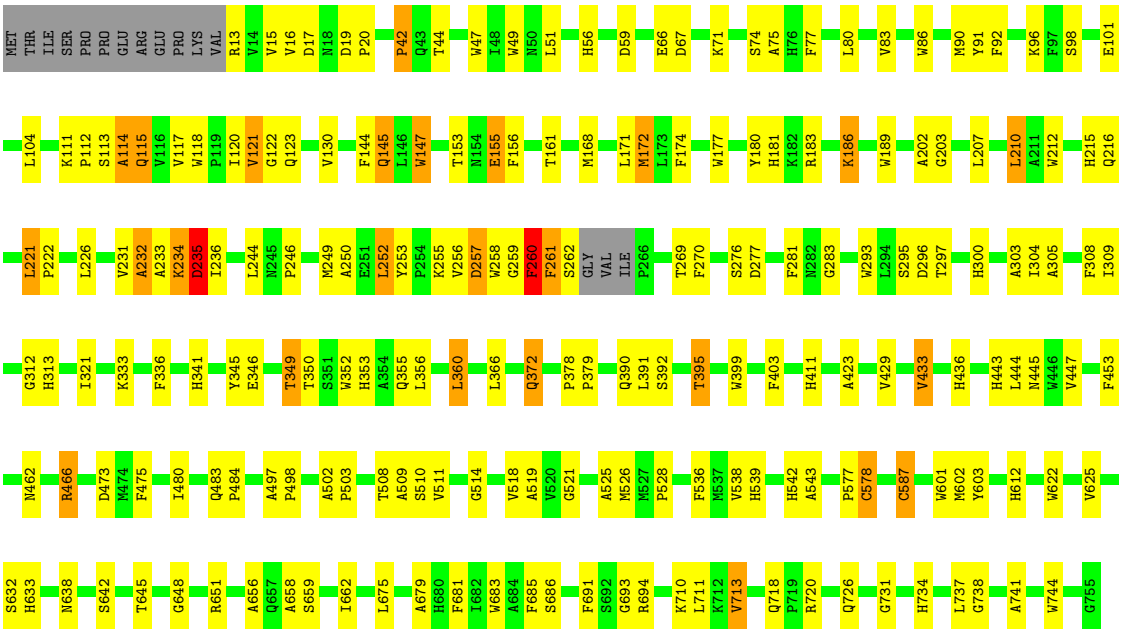
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

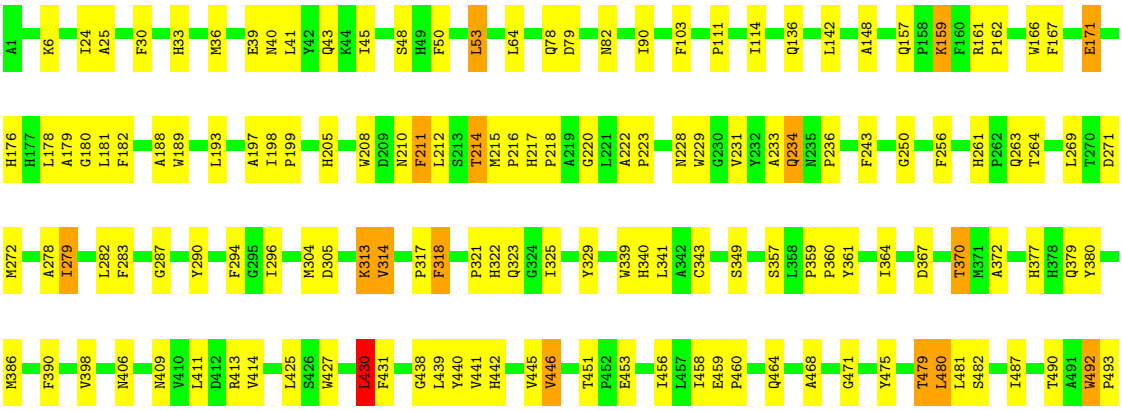
• Molecule 1: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

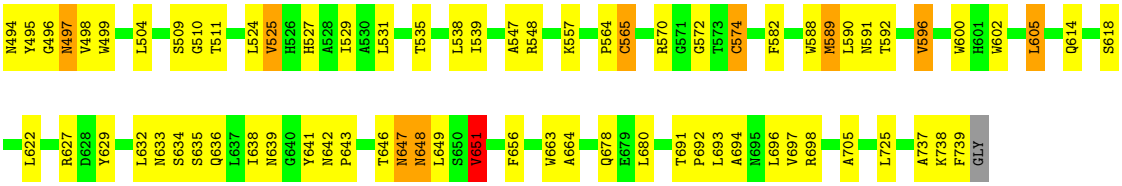
Chain A: 71% 24%



• Molecule 2: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

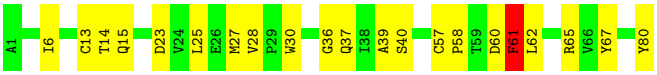
Chain B: 71% 26%





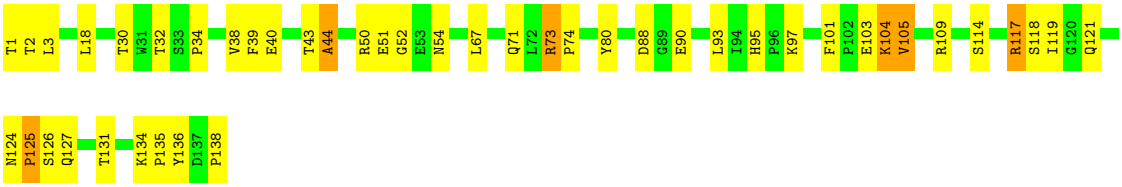
- Molecule 3: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C:



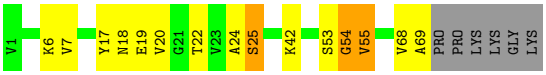
- Molecule 4: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II

Chain D:



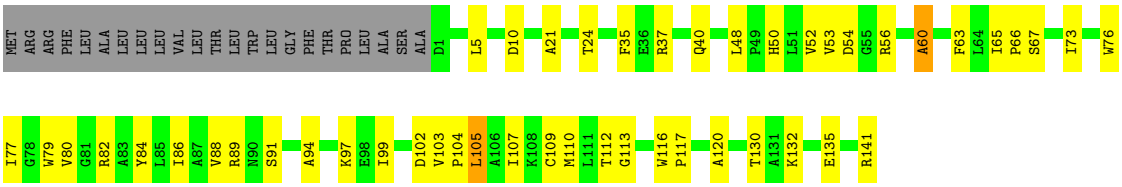
- Molecule 5: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV

Chain E:



- Molecule 6: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III

Chain F:



- Molecule 7: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII

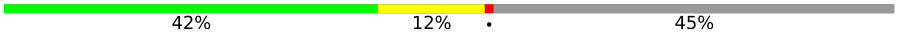
Chain I:

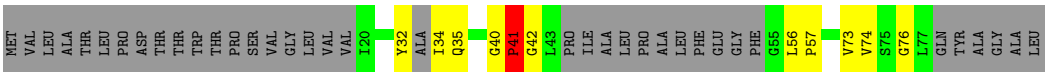
- Molecule 8: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX

Chain J:

• Molecule 9: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X

Chain K:



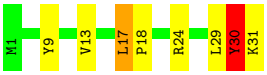


• Molecule 10: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI

Chain L:

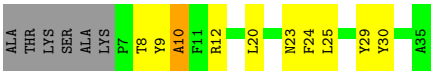
• Molecule 11: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII

Chain M:



• Molecule 12: PHOTOSYSTEM I SUBUNIT PSAX

Chain X:



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.51	0/5983	0.66	2/8158 (0.0%)
2	B	0.56	0/6096	0.67	2/8332 (0.0%)
3	C	0.74	0/608	0.96	4/824 (0.5%)
4	D	0.57	0/1101	0.81	1/1492 (0.1%)
5	E	0.57	0/551	0.84	2/750 (0.3%)
6	F	0.47	0/1087	0.66	0/1476
7	I	0.66	0/312	0.75	0/425
8	J	0.45	0/350	0.65	0/477
9	K	0.52	0/219	0.86	3/297 (1.0%)
10	L	0.67	0/1148	0.75	0/1558
11	M	0.63	0/244	0.85	1/332 (0.3%)
12	X	0.55	0/242	0.67	0/332
All	All	0.55	0/17941	0.70	15/24453 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	80	TYR	CA-C-O	9.95	140.99	120.10
11	M	30	TYR	N-CA-C	7.84	132.18	111.00
4	D	131	THR	N-CA-C	-7.83	89.86	111.00
5	E	54	GLY	N-CA-C	7.52	131.91	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	521	GLY	N-CA-C	-6.39	97.13	113.10
3	C	60	ASP	CA-C-N	-6.29	103.37	117.20
9	K	57	PRO	N-CA-CB	6.14	110.67	103.30
3	C	60	ASP	C-N-CA	5.89	136.41	121.70
1	A	114	ALA	N-CA-C	-5.87	95.16	111.00
3	C	61	PHE	N-CA-CB	5.85	121.14	110.60
9	K	41	PRO	N-CA-CB	5.78	110.24	103.30
9	K	35	GLN	N-CA-C	5.35	125.45	111.00
2	B	430	LEU	CA-CB-CG	5.12	127.08	115.30
2	B	651	VAL	CB-CA-C	-5.10	101.72	111.40
5	E	55	VAL	N-CA-C	5.01	124.53	111.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	215	0
2	B	5879	0	5632	238	0
3	C	598	0	580	16	0
4	D	1075	0	1077	40	0
5	E	539	0	528	10	0
6	F	1065	0	1079	42	0
7	I	301	0	306	7	0
8	J	338	0	347	23	0
9	K	222	0	110	4	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	143	0
13	B	2349	0	2304	152	0
13	F	45	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	11	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	22	0
16	B	265	0	369	17	0
16	F	40	0	56	2	0
16	I	80	0	112	3	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
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	743	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 16.

All (743) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.12	0.80
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
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: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:367:ASP:CG	2:B:370:THR:HG23	2.07	0.75
2:B:647:ASN:HD22	2:B:649:LEU:H	1.35	0.75
13:B:1215:CLA:HMB1	13:B:1215:CLA:HBB1	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:36:MET:HE3	2:B:40:ASN:HB2	1.72	0.71
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
1:A:341:HIS:HE1	17:A:5003:LHG:HC11	1.56	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
2:B:589:MET:HE1	2:B:590:LEU:HA	1.75	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:318:PHE:HB2	13:B:1220:CLA:HMA1	1.78	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
6:F:63:PHE:C	6:F:66:PRO:HD2	2.17	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
13:A:1237:CLA:H191	13:L:1502:CLA:HBB1	1.78	0.65
6:F:54:ASP:OD2	12:X:30:TYR:CE2	2.50	0.64
13:B:1226:CLA:HBB1	13:B:1226:CLA:HMB1	1.78	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
13:B:1203:CLA:H162	13:B:1225:CLA:HBB2	1.80	0.64
6:F:103:VAL:HB	6:F:104:PRO:HD3	1.79	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
1:A:177:TRP:HB2	13:A:1109:CLA:HMC3	1.80	0.62
2:B:166:TRP:CZ2	13:B:1208:CLA:HMA1	2.33	0.62
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:480:LEU:C	2:B:482:SER:H	2.02	0.62
1:A:356:LEU:O	1:A:360:LEU:HB2	2.00	0.62
1:A:353:HIS:CD2	1:A:411:HIS:HD1	2.11	0.61
13:A:1237:CLA:HMA1	2:B:694:ALA:CB	2.29	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
1:A:543:ALA:HB1	13:A:1136:CLA:HMB3	1.83	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:90:MET:HE3	13:A:1106:CLA:HED2	1.82	0.61
13:B:1234:CLA:HMB2	13:B:1236:CLA:HED1	1.81	0.61
1:A:453:PHE:O	13:A:1132:CLA:CBB	2.48	0.61
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
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
13:A:1013:CLA:H71	13:A:1140:CLA:HMC3	1.83	0.59
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
4:D:40:GLU:H	4:D:71:GLN:NE2	2.01	0.59
1:A:257:ASP:CG	1:A:258:TRP:N	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:7:ALA:HB1	7:I:10:LEU:HD22	1.83	0.59
2:B:591:ASN:HB2	13:B:1012:CLA:HBC2	1.83	0.58
7:I:37:GLU:C	7:I:38:ALA:OXT	2.41	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
10:L:36:ALA:HB2	13:L:1502:CLA:HMD1	1.84	0.58
1:A:86:TRP:HA	13:A:1105:CLA:CBB	2.33	0.58
13:A:1121:CLA:HMA1	13:A:1801:CLA:HAC2	1.85	0.58
2:B:589:MET:HE2	2:B:589:MET:O	2.02	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
13:A:1106:CLA:HMC2	13:A:1126:CLA:H142	1.84	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
1:A:392:SER:HB3	13:A:1126:CLA:HMA1	1.87	0.57
2:B:414:VAL:HG11	16:B:4009:BCR:H401	1.85	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
1:A:189:TRP:CZ2	13:A:1108:CLA:HMA1	2.40	0.56
2:B:282:LEU:HD12	13:B:1216:CLA:HMC1	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:20:LEU:HD11	12:X:24:PHE:HE1	1.71	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: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
13:A:1102:CLA:HMC3	13:A:1104:CLA:HED2	1.86	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
2:B:589:MET:HE1	2:B:590:LEU:CA	2.36	0.55
9:K:40:GLY:O	9:K:41:PRO:C	2.44	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
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:A:1237:CLA:HMA1	2:B:694:ALA:HB1	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
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:157:GLN:O	2:B:161:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:B:1216:CLA:HMB2	13:B:1221:CLA:HMA3	1.89	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:589:MET:HE2	2:B:589:MET:C	2.29	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
13:A:1022:CLA:OBD	13:B:1021:CLA:HMB3	2.08	0.53
2:B:212:LEU:HD21	16:B:4006:BCR:H341	1.90	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:1125:CLA:HBB1	13:A:1133:CLA:HMA2	1.89	0.53
13:A:1011:CLA:HMB3	13:B:1012:CLA:OBD	2.09	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
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
8:J:19:MET:HA	8:J:19:MET:CE	2.38	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:168:MET:HE1	1:A:171:LEU:HD23	1.91	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
13:A:1119:CLA:HMB2	13:A:1123:CLA:HMA3	1.92	0.52
2:B:406:ASN:HD22	2:B:409:ASN:ND2	1.84	0.52
1:A:244:LEU:C	1:A:246:PRO:HD3	2.30	0.52
1:A:296:ASP:HB3	13:A:1116:CLA:HMA1	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:MET:CE	13:A:1106:CLA:HED2	2.39	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:36:MET:HE2	2:B:41:LEU:N	2.25	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
13:A:1133:CLA:HMD2	13:A:1134:CLA:HBB1	1.92	0.52
8:J:28:GLU:OE1	8:J:28:GLU:HA	2.09	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
2:B:294:PHE:HE1	13:B:1209:CLA:HMA1	1.75	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
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
1:A:259:GLY:C	1:A:261:PHE:H	2.14	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
13:A:1125:CLA:HMB3	13:A:1133:CLA:H12	1.93	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
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
1:A:453:PHE:C	13:A:1132:CLA:HBB2	2.31	0.51
2:B:379:GLN:HA	2:B:379:GLN:OE1	2.11	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
13:B:1216:CLA:HMD1	13:B:1218:CLA:HBB1	1.93	0.50
4:D:117:ARG:HG2	4:D:118:SER:N	2.26	0.50
7:I:30:LEU:O	7:I:34:ILE:HG12	2.11	0.50
1:A:16:VAL:CG1	1:A:17:ASP:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:588:TRP:HH2	13:B:1012:CLA:HBB1	1.77	0.50
13:B:1220:CLA:HBB1	13:B:1227:CLA:HMD2	1.94	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
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
2:B:548:ARG:HH22	4:D:124:ASN:CG	2.15	0.49
2:B:664:ALA:C	13:B:1023:CLA:HBB1	2.31	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
13:A:1117:CLA:HMB1	13:A:1117:CLA:HBB1	1.93	0.49
2:B:114:ILE:O	13:B:1205:CLA:HMD3	2.13	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
13:B:1021:CLA:H72	13:B:1012:CLA:CED	2.41	0.49
13:B:1216:CLA:CMB	13:B:1221:CLA:HMA3	2.42	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
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
2:B:487:ILE:HG12	13:B:1232:CLA:HMD3	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1203:CLA:H143	13:B:1225:CLA:HBB2	1.95	0.48
1:A:120:ILE:C	1:A:122:GLY:H	2.16	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
13:A:1013:CLA:H71	13:A:1140:CLA:CMC	2.42	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: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:A:1107:CLA:HMA1	8:J:27:ILE:HD13	1.95	0.48
2:B:271:ASP:HB3	13:B:1214:CLA:HMA1	1.96	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:360:LEU:CD1	13:A:1128:CLA:HBB1	2.44	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
9:K:74:VAL:C	9:K:76:GLY:H	2.16	0.48
1:A:203:GLY:O	1:A:207:LEU:HB2	2.14	0.47
1:A:577:PRO:O	1:A:578:CYS:HB3	2.14	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
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
13:B:1205:CLA:H142	13:B:1205:CLA:HMB2	1.96	0.47
1:A:121:VAL:HB	13:B:1230:CLA:HMD1	1.96	0.47
13:A:1112:CLA:HBA2	13:A:1114:CLA:HMB3	1.96	0.47
1:A:56:HIS:CG	13:A:1103:CLA:HAB	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:HD2	13:A:1108:CLA:CBC	2.28	0.47
1:A:399:TRP:HB3	13:A:1126:CLA:HMC3	1.96	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
13:A:1103:CLA:HMC3	13:A:1128:CLA:HMA1	1.97	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
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: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
13:A:1119:CLA:CMB	13:A:1123:CLA:HMA3	2.46	0.46
4:D:34:PRO:O	4:D:51:GLU:HG3	2.16	0.46
2:B:386:MET:HE1	16:B:4010:BCR:H361	1.98	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:90:MET:HE1	13:A:1106:CLA:HAA2	1.98	0.46
1:A:656:ALA:O	1:A:659:SER:HB2	2.16	0.46
13:A:1118:CLA:HMC1	13:A:1118:CLA:HBC2	1.97	0.46
2:B:361:TYR:O	2:B:364:ILE:HG22	2.15	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:THR:H	2:B:482:SER:HB3	1.79	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
16:A:4011:BCR:H381	13:B:1229:CLA:HMA1	1.97	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:257:ASP:OD2	1:A:262:SER:C	2.55	0.45
1:A:539:HIS:CG	13:A:1136:CLA:HED2	2.51	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:36:MET:CE	2:B:40:ASN:HB2	2.45	0.45
2:B:339:TRP:CZ3	16:B:4009:BCR:H372	2.51	0.45
2:B:509:SER:O	2:B:509:SER:OG	2.25	0.45
2:B:589:MET:HE1	2:B:590:LEU:HD23	1.97	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
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
2:B:220:GLY:HA3	13:B:1212:CLA:HMD1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:39:PHE:HB2	4:D:71:GLN:HE21	1.81	0.45
1:A:168:MET:HE2	1:A:171:LEU:HD23	1.97	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
13:B:1229:CLA:HBB1	13:B:1230:CLA:HMB2	1.98	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
1:A:90:MET:HE2	13:A:1126:CLA:HED1	1.99	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
8:J:1:MET:HE2	8:J:1:MET:O	2.17	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
1:A:737:LEU:HD22	13:A:1140:CLA:HMA1	1.99	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
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
2:B:370:THR:HG21	20:B:5026:HOH:O	2.16	0.44
2:B:480:LEU:C	2:B:482:SER:N	2.70	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
13:B:1232:CLA:HMB1	16:B:4010:BCR:HC31	1.98	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:125:PRO:HG3	4:D:135:PRO:HG3	2.00	0.44
13:A:1103:CLA:H71	16:A:4003:BCR:H402	2.00	0.44
3:C:65:ARG:HD2	4:D:119:ILE:CD1	2.48	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
2:B:181:LEU:HD13	13:B:1210:CLA:HHB	2.00	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
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
13:B:1232:CLA:HBA2	13:B:1233:CLA:HMB3	2.00	0.43
2:B:439:LEU:HD11	16:J:4015:BCR:H342	2.00	0.43
2:B:529:ILE:HG21	13:B:1234:CLA:HAB	1.99	0.43
8:J:1:MET:HE2	8:J:5:LEU:HG	2.01	0.43
10:L:7:PRO:HB3	10:L:12:PRO:HA	2.00	0.43
2:B:36:MET:HE1	2:B:41:LEU:N	2.33	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: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
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
13:A:1117:CLA:HMB1	13:A:1117:CLA:CBB	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:HIS:CD2	13:A:1129:CLA:HMB1	2.53	0.43
2:B:231:VAL:C	2:B:234:GLN:HG2	2.36	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
16:J:4015:BCR:H20C	16:J:4015:BCR:H361	1.89	0.43
1:A:231:VAL:HG11	1:A:236:ILE:HG12	1.99	0.43
2:B:24:ILE:HA	13:B:1201:CLA:HMD3	2.01	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:36:MET:HE1	2:B:40:ASN:C	2.39	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
13:A:1117:CLA:O1A	13:A:1127:CLA:HMD1	2.20	0.42
2:B:360:PRO:HG3	13:B:1215:CLA:HBA1	2.00	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:215:HIS:CD2	1:A:215:HIS:C	2.92	0.42
1:A:403:PHE:CB	13:A:1104:CLA:H112	2.49	0.42
1:A:683:TRP:CE3	13:A:1011:CLA:HMA1	2.54	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
2:B:357:SER:C	2:B:359:PRO:HD3	2.39	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: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
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
13:B:1226:CLA:HMB1	13:B:1226:CLA:CBB	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:458:ILE:CD1	2:B:458:ILE:N	2.82	0.42
2:B:492:TRP:CZ3	13:B:1233:CLA:HMD3	2.54	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
1:A:145:GLN:H	1:A:145:GLN:CD	2.22	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
2:B:589:MET:HE1	2:B:590:LEU:N	2.35	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
8:J:19:MET:HA	8:J:19:MET:HE2	2.00	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:663:TRP:CE3	13:B:1021:CLA:HMA1	2.56	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:202:ALA:C	13:A:1118:CLA:HBC3	2.41	0.41
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.83	0.41
13:A:1134:CLA:H3A	13:A:1134:CLA:HBA2	1.73	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
1:A:49:TRP:HZ3	17:A:5001:LHG:H121	1.86	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
1:A:161:THR:HG22	16:A:4002:BCR:HC32	2.01	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:A:1119:CLA:HMD1	13:A:1120:CLA:HBB1	2.02	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
1:A:260:PHE:O	1:A:261:PHE:HB2	2.21	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
2:B:30:PHE:CD1	2:B:45:ILE:HD13	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1211:CLA:HMA2	16:B:4006:BCR:H282	2.03	0.40
13:B:1214:CLA:O1D	13:B:1215:CLA:HMA1	2.21	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
1:A:713:VAL:HG11	13:A:1138:CLA:HMB3	2.03	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
5:E:19:GLU:OE1	5:E:42:LYS:NZ	2.52	0.40
1:A:212:TRP:O	1:A:216:GLN:HG3	2.22	0.40
13:A:1122:CLA:HHB	13:A:1801:CLA:HBB1	2.02	0.40
13:A:1126:CLA:H62	13:A:1126:CLA:H41	1.75	0.40
13:A:1130:CLA:HMC2	13:A:1136:CLA:H203	2.03	0.40
2:B:176:HIS:CG	13:B:1210:CLA:HMC2	2.56	0.40
2:B:193:LEU:HA	2:B:197:ALA:HB3	2.03	0.40
2:B:269:LEU:HD23	2:B:272:MET:HE3	2.02	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
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:1107:CLA:CBB	13:B:1230:CLA:HMD2	2.51	0.40
2:B:36:MET:HE3	2:B:40:ASN:CB	2.47	0.40
2:B:496:GLY:O	2:B:497:ASN:C	2.59	0.40
13:B:1220:CLA:CBB	13:B:1227:CLA:HMD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	11	20
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	13	24
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	12	21
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	6	10
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	1	1
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	6	10
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	1
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	12	21
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	3	5
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	3	4
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	9	16

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
9	K	56	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	565 (96%)	24 (4%)	30	55
2	B	595/597 (100%)	567 (95%)	28 (5%)	26	49
3	C	67/67 (100%)	66 (98%)	1 (2%)	65	85
4	D	115/115 (100%)	107 (93%)	8 (7%)	15	29
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	107 (98%)	2 (2%)	59	81
7	I	32/32 (100%)	30 (94%)	2 (6%)	18	34
8	J	36/36 (100%)	34 (94%)	2 (6%)	21	40
10	L	117/119 (98%)	109 (93%)	8 (7%)	16	30
11	M	26/26 (100%)	25 (96%)	1 (4%)	33	58
12	X	20/24 (83%)	18 (90%)	2 (10%)	7	15
All	All	1765/1811 (98%)	1687 (96%)	78 (4%)	28	52

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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
1	A	253	TYR
1	A	257	ASP
1	A	260	PHE
1	A	281	PHE
1	A	349	THR
1	A	360	LEU
1	A	372	GLN
1	A	395	THR
1	A	433	VAL
1	A	466	ARG
1	A	538	VAL

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Mol	Chain	Res	Type
1	A	587	CYS
1	A	632	SER
1	A	675	LEU
1	A	713	VAL
2	B	53	LEU
2	B	142	LEU
2	B	159	LYS
2	B	171	GLU
2	B	211	PHE
2	B	214	THR
2	B	256	PHE
2	B	279	ILE
2	B	318	PHE
2	B	349	SER
2	B	370	THR
2	B	411	LEU
2	B	430	LEU
2	B	446	VAL
2	B	479	THR
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
2	B	647	ASN
2	B	648	ASN
2	B	651	VAL
2	B	697	VAL
2	B	698	ARG
3	C	61	PHE
4	D	1	THR
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

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Mol	Chain	Res	Type
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	69	ARG
10	L	85	LEU
10	L	134	VAL
11	M	17	LEU
12	X	8	THR
12	X	23	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	50	ASN
1	A	145	GLN
1	A	353	HIS
1	A	359	ASN
1	A	372	GLN
1	A	390	GLN
1	A	426	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	40	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

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Mol	Chain	Res	Type
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	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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
13	CLA	M	1601	20	45,53,73	1.59	7 (15%)	52,89,113	2.21	8 (15%)
13	CLA	A	1114	20	49,57,73	1.48	7 (14%)	55,93,113	2.06	10 (18%)
16	BCR	A	4001	-	41,41,41	1.37	5 (12%)	56,56,56	1.88	16 (28%)
16	BCR	J	4013	-	41,41,41	1.28	4 (9%)	56,56,56	1.83	19 (33%)
13	CLA	B	1238	20	65,73,73	1.31	8 (12%)	76,113,113	1.65	12 (15%)
13	CLA	B	1210	-	65,73,73	1.43	7 (10%)	76,113,113	1.70	11 (14%)
13	CLA	A	1117	-	65,73,73	1.40	12 (18%)	76,113,113	1.89	14 (18%)
13	CLA	B	1216	20	65,73,73	1.36	7 (10%)	76,113,113	1.73	11 (14%)
13	CLA	A	1128	-	65,73,73	1.57	11 (16%)	76,113,113	1.69	9 (11%)
16	BCR	B	4009	-	25,25,41	1.36	4 (16%)	33,33,56	1.86	11 (33%)
13	CLA	J	1302	8	45,53,73	1.64	7 (15%)	52,89,113	2.15	10 (19%)
13	CLA	A	1022	20	65,73,73	1.41	11 (16%)	76,113,113	1.62	8 (10%)
13	CLA	B	1226	-	65,73,73	1.41	10 (15%)	76,113,113	1.79	12 (15%)
13	CLA	B	1211	-	65,73,73	1.34	8 (12%)	76,113,113	1.80	10 (13%)
13	CLA	B	1225	-	65,73,73	1.55	13 (20%)	76,113,113	1.70	13 (17%)
13	CLA	A	1131	-	65,73,73	1.20	5 (7%)	76,113,113	1.70	14 (18%)
13	CLA	A	1138	-	65,73,73	1.35	7 (10%)	76,113,113	1.74	10 (13%)
13	CLA	A	1108	-	45,53,73	1.59	7 (15%)	52,89,113	1.97	10 (19%)
16	BCR	B	4017	-	41,41,41	1.28	4 (9%)	56,56,56	1.74	17 (30%)
13	CLA	X	1701	12	45,53,73	1.60	5 (11%)	52,89,113	2.12	11 (21%)
13	CLA	A	1121	-	51,59,73	1.57	10 (19%)	59,96,113	1.94	11 (18%)
13	CLA	B	1239	-	65,73,73	1.17	9 (13%)	76,113,113	1.73	10 (13%)
13	CLA	B	1214	-	59,67,73	1.45	8 (13%)	68,105,113	1.84	13 (19%)
15	SF4	C	3003	3	0,12,12	-	-	-		
13	CLA	B	1203	-	65,73,73	1.29	6 (9%)	76,113,113	1.64	10 (13%)
13	CLA	A	1103	-	65,73,73	1.20	4 (6%)	76,113,113	1.81	15 (19%)
13	CLA	B	1208	-	45,53,73	1.54	8 (17%)	52,89,113	2.00	10 (19%)
13	CLA	A	1136	-	65,73,73	1.36	8 (12%)	76,113,113	1.66	8 (10%)
13	CLA	A	1119	20	65,73,73	1.33	8 (12%)	76,113,113	1.82	12 (15%)
16	BCR	J	4012	-	41,41,41	1.29	5 (12%)	56,56,56	1.91	16 (28%)
13	CLA	B	1230	-	58,66,73	1.45	11 (18%)	67,104,113	1.98	12 (17%)
13	CLA	A	1104	-	65,73,73	1.39	8 (12%)	76,113,113	1.90	14 (18%)
13	CLA	B	1217	-	47,55,73	1.53	8 (17%)	54,91,113	2.22	11 (20%)
13	CLA	A	1120	-	49,57,73	1.47	6 (12%)	55,93,113	2.12	12 (21%)
13	CLA	A	1237	20	65,73,73	1.34	10 (15%)	76,113,113	1.67	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	CLA	B	1232	20	45,53,73	1.70	8 (17%)	52,89,113	1.99	12 (23%)
13	CLA	A	1115	-	54,62,73	1.57	10 (18%)	62,99,113	1.81	9 (14%)
13	CLA	B	1228	-	49,57,73	1.53	7 (14%)	55,93,113	1.99	7 (12%)
16	BCR	B	4010	-	41,41,41	1.25	5 (12%)	56,56,56	1.88	18 (32%)
13	CLA	A	1105	-	51,59,73	1.62	10 (19%)	59,96,113	1.97	10 (16%)
16	BCR	B	4014	-	41,41,41	1.23	5 (12%)	56,56,56	1.99	20 (35%)
16	BCR	J	4015	-	41,41,41	1.40	5 (12%)	56,56,56	1.88	14 (25%)
13	CLA	J	1303	-	38,45,73	1.79	7 (18%)	43,78,113	2.16	8 (18%)
13	CLA	A	1402	-	42,49,73	1.67	9 (21%)	48,83,113	1.99	7 (14%)
18	LMG	B	5002	-	55,55,55	0.88	2 (3%)	63,63,63	1.30	3 (4%)
16	BCR	F	4016	-	41,41,41	1.27	4 (9%)	56,56,56	1.81	17 (30%)
13	CLA	A	1110	-	54,62,73	1.48	9 (16%)	62,99,113	2.02	11 (17%)
13	CLA	B	1023	-	65,73,73	1.50	9 (13%)	76,113,113	1.65	7 (9%)
13	CLA	B	1234	-	60,68,73	1.48	8 (13%)	70,107,113	1.76	11 (15%)
13	CLA	A	1132	-	65,73,73	1.37	9 (13%)	76,113,113	1.71	11 (14%)
13	CLA	A	1111	-	60,68,73	1.32	7 (11%)	70,107,113	1.88	14 (20%)
13	CLA	A	1101	-	65,73,73	1.32	6 (9%)	76,113,113	1.75	9 (11%)
13	CLA	A	1126	-	65,73,73	1.28	7 (10%)	76,113,113	1.65	11 (14%)
14	PQN	B	2002	-	34,34,34	3.46	16 (47%)	42,45,45	2.10	4 (9%)
16	BCR	A	4008	-	41,41,41	1.26	8 (19%)	56,56,56	1.90	18 (32%)
13	CLA	A	1139	20	51,59,73	1.47	7 (13%)	59,96,113	1.91	10 (16%)
13	CLA	B	1235	-	65,73,73	1.31	8 (12%)	76,113,113	1.81	13 (17%)
15	SF4	A	3001	2,1	0,12,12	-	-	-		
13	CLA	B	1236	-	47,55,73	1.55	8 (17%)	54,91,113	1.86	10 (18%)
13	CLA	A	1113	-	45,53,73	1.50	6 (13%)	52,89,113	2.24	14 (26%)
13	CLA	B	1222	20	46,54,73	1.43	8 (17%)	53,90,113	2.13	12 (22%)
16	BCR	L	4019	-	41,41,41	1.43	8 (19%)	56,56,56	1.81	15 (26%)
16	BCR	L	4022	-	41,41,41	1.60	7 (17%)	56,56,56	1.72	12 (21%)
13	CLA	A	1106	1	65,73,73	1.35	7 (10%)	76,113,113	1.80	9 (11%)
13	CLA	K	1401	-	45,53,73	1.62	8 (17%)	52,89,113	1.95	7 (13%)
13	CLA	A	1118	-	61,69,73	1.46	9 (14%)	71,108,113	1.95	11 (15%)
13	CLA	B	1219	20	55,63,73	1.47	7 (12%)	64,101,113	1.95	9 (14%)
13	CLA	B	1218	-	45,53,73	1.61	8 (17%)	52,89,113	2.19	12 (23%)
13	CLA	B	1209	-	45,53,73	1.55	6 (13%)	52,89,113	2.16	10 (19%)
13	CLA	A	1122	-	59,67,73	1.36	7 (11%)	68,105,113	1.79	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	CLA	B	1224	-	65,73,73	1.54	9 (13%)	76,113,113	1.81	13 (17%)
13	CLA	A	1013	-	65,73,73	1.36	9 (13%)	76,113,113	1.80	14 (18%)
16	BCR	A	4007	-	41,41,41	1.37	6 (14%)	56,56,56	1.78	14 (25%)
16	BCR	B	4005	-	41,41,41	1.57	7 (17%)	56,56,56	2.09	19 (33%)
17	LHG	B	5004	-	22,22,48	2.80	5 (22%)	25,28,54	1.13	1 (4%)
13	CLA	B	1227	-	45,53,73	1.55	8 (17%)	52,89,113	2.16	11 (21%)
13	CLA	L	1501	10	65,73,73	1.51	9 (13%)	76,113,113	1.74	10 (13%)
13	CLA	A	1107	1	65,73,73	1.38	8 (12%)	76,113,113	1.84	14 (18%)
14	PQN	A	2001	-	34,34,34	3.54	17 (50%)	42,45,45	2.21	3 (7%)
13	CLA	A	1134	1	45,53,73	1.50	8 (17%)	52,89,113	2.15	10 (19%)
13	CLA	B	1229	-	65,73,73	1.36	7 (10%)	76,113,113	1.75	8 (10%)
16	BCR	B	4006	-	41,41,41	1.26	5 (12%)	56,56,56	2.01	20 (35%)
13	CLA	A	1123	20	65,73,73	1.42	7 (10%)	76,113,113	1.70	12 (15%)
13	CLA	A	1137	-	47,55,73	1.64	6 (12%)	54,91,113	1.94	10 (18%)
13	CLA	B	1220	-	45,53,73	1.58	5 (11%)	52,89,113	1.97	9 (17%)
13	CLA	B	1021	-	65,73,73	1.40	6 (9%)	76,113,113	1.71	9 (11%)
13	CLA	B	1012	20	65,73,73	1.46	6 (9%)	76,113,113	1.71	11 (14%)
13	CLA	A	1112	-	45,53,73	1.65	9 (20%)	52,89,113	2.02	10 (19%)
13	CLA	B	1213	-	55,63,73	1.58	11 (20%)	64,101,113	1.84	9 (14%)
13	CLA	B	1204	-	65,73,73	1.25	8 (12%)	76,113,113	1.78	9 (11%)
13	CLA	L	1502	-	65,73,73	1.43	8 (12%)	76,113,113	1.76	10 (13%)
13	CLA	B	1215	-	60,68,73	1.44	9 (15%)	70,107,113	1.96	11 (15%)
16	BCR	A	4011	-	41,41,41	1.39	6 (14%)	56,56,56	2.03	19 (33%)
13	CLA	A	1102	13	59,67,73	1.41	7 (11%)	68,105,113	1.89	12 (17%)
13	CLA	A	1109	13	65,73,73	1.30	8 (12%)	76,113,113	1.78	10 (13%)
13	CLA	A	1133	-	54,62,73	1.40	10 (18%)	62,99,113	2.00	11 (17%)
13	CLA	A	1129	-	50,58,73	1.53	7 (14%)	58,95,113	2.08	14 (24%)
13	CLA	B	1207	2	65,73,73	1.43	9 (13%)	76,113,113	1.79	14 (18%)
13	CLA	A	1135	-	51,59,73	1.34	4 (7%)	59,96,113	2.08	13 (22%)
16	BCR	I	4020	-	41,41,41	1.28	7 (17%)	56,56,56	1.82	17 (30%)
13	CLA	L	1503	20	65,73,73	1.44	8 (12%)	76,113,113	1.68	9 (11%)
13	CLA	A	1125	-	65,73,73	1.39	6 (9%)	76,113,113	1.77	11 (14%)
16	BCR	I	4018	-	41,41,41	1.30	7 (17%)	56,56,56	1.79	15 (26%)
13	CLA	B	1202	-	65,73,73	1.33	7 (10%)	76,113,113	1.68	10 (13%)
16	BCR	M	4021	-	41,41,41	1.34	6 (14%)	56,56,56	1.79	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	CLA	B	1231	-	45,53,73	1.56	9 (20%)	52,89,113	2.07	12 (23%)
13	CLA	A	1140	-	65,73,73	1.38	8 (12%)	76,113,113	1.81	14 (18%)
13	CLA	A	1130	-	65,73,73	1.23	7 (10%)	76,113,113	1.90	10 (13%)
13	CLA	A	1801	17	52,60,73	1.61	11 (21%)	60,97,113	2.15	13 (21%)
13	CLA	B	1223	-	65,73,73	1.44	7 (10%)	76,113,113	1.80	11 (14%)
13	CLA	B	1205	-	65,73,73	1.33	7 (10%)	76,113,113	1.71	11 (14%)
13	CLA	B	1206	2	65,73,73	1.36	5 (7%)	76,113,113	1.71	10 (13%)
13	CLA	B	1212	-	45,53,73	1.57	10 (22%)	52,89,113	2.06	9 (17%)
13	CLA	B	1221	2	54,62,73	1.74	12 (22%)	62,99,113	1.91	10 (16%)
13	CLA	A	1124	20	65,73,73	1.25	7 (10%)	76,113,113	1.76	10 (13%)
16	BCR	A	4002	-	41,41,41	1.27	4 (9%)	56,56,56	1.77	17 (30%)
16	BCR	A	4003	-	41,41,41	1.41	6 (14%)	56,56,56	1.93	17 (30%)
13	CLA	A	1116	-	54,62,73	1.57	10 (18%)	62,99,113	1.90	11 (17%)
13	CLA	B	1233	20	45,53,73	1.52	6 (13%)	52,89,113	2.09	10 (19%)
13	CLA	A	1127	-	65,73,73	1.43	7 (10%)	76,113,113	1.73	7 (9%)
13	CLA	F	1301	20	45,53,73	1.64	7 (15%)	52,89,113	2.06	7 (13%)
17	LHG	A	5003	13	26,26,48	2.32	5 (19%)	29,32,54	1.59	5 (17%)
15	SF4	C	3002	3	0,12,12	-	-	-		
16	BCR	B	4004	-	41,41,41	1.52	5 (12%)	56,56,56	2.02	16 (28%)
17	LHG	A	5001	-	48,48,48	1.76	6 (12%)	51,54,54	1.30	3 (5%)
13	CLA	B	1201	-	54,62,73	1.47	8 (14%)	62,99,113	2.02	12 (19%)
13	CLA	A	1011	-	65,73,73	1.42	7 (10%)	76,113,113	2.04	17 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	M	1601	20	1/1/11/20	9/13/91/115	-
13	CLA	A	1114	20	1/1/11/20	9/18/96/115	-
16	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
16	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1238	20	1/1/15/20	2/37/115/115	-
13	CLA	B	1210	-	1/1/15/20	13/37/115/115	-
13	CLA	A	1117	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1216	20	1/1/15/20	4/37/115/115	-
13	CLA	A	1128	-	1/1/15/20	6/37/115/115	-
16	BCR	B	4009	-	-	6/18/35/63	0/1/1/2
13	CLA	J	1302	8	1/1/11/20	11/13/91/115	-
13	CLA	A	1022	20	1/1/15/20	4/37/115/115	-
13	CLA	B	1226	-	1/1/15/20	9/37/115/115	-
13	CLA	B	1211	-	1/1/15/20	11/37/115/115	-
13	CLA	B	1225	-	-	10/37/115/115	-
13	CLA	A	1131	-	-	5/37/115/115	-
13	CLA	A	1138	-	1/1/15/20	7/37/115/115	-
13	CLA	A	1108	-	-	9/13/91/115	-
16	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	X	1701	12	1/1/11/20	5/13/91/115	-
13	CLA	A	1121	-	1/1/12/20	10/21/99/115	-
13	CLA	B	1239	-	-	8/37/115/115	-
13	CLA	B	1214	-	1/1/13/20	7/30/108/115	-
15	SF4	C	3003	3	-	-	0/6/5/5
13	CLA	B	1203	-	1/1/15/20	15/37/115/115	-
13	CLA	A	1103	-	1/1/15/20	16/37/115/115	-
13	CLA	B	1208	-	1/1/11/20	3/13/91/115	-
13	CLA	A	1136	-	1/1/15/20	8/37/115/115	-
13	CLA	A	1119	20	1/1/15/20	6/37/115/115	-
16	BCR	J	4012	-	-	3/29/63/63	0/2/2/2
13	CLA	B	1230	-	1/1/13/20	6/29/107/115	-
13	CLA	A	1104	-	1/1/15/20	14/37/115/115	-
13	CLA	B	1217	-	1/1/11/20	6/16/94/115	-
13	CLA	A	1120	-	1/1/11/20	10/18/96/115	-
13	CLA	A	1237	20	1/1/15/20	10/37/115/115	-
13	CLA	B	1232	20	1/1/11/20	0/13/91/115	-
13	CLA	A	1115	-	-	1/24/102/115	-
13	CLA	B	1228	-	1/1/11/20	9/18/96/115	-
16	BCR	B	4010	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1105	-	1/1/12/20	6/21/99/115	-
16	BCR	B	4014	-	-	1/29/63/63	0/2/2/2
16	BCR	J	4015	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	J	1303	-	1/1/8/20	0/2/76/115	-
13	CLA	A	1402	-	1/1/9/20	3/7/81/115	-
18	LMG	B	5002	-	-	8/50/70/70	0/1/1/1
16	BCR	F	4016	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1110	-	1/1/12/20	8/24/102/115	-
13	CLA	B	1023	-	-	2/37/115/115	-
13	CLA	B	1234	-	1/1/14/20	9/31/109/115	-
13	CLA	A	1132	-	1/1/15/20	8/37/115/115	-
13	CLA	A	1111	-	1/1/14/20	11/31/109/115	-
13	CLA	A	1101	-	1/1/15/20	6/37/115/115	-
13	CLA	A	1126	-	1/1/15/20	8/37/115/115	-
14	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
16	BCR	A	4008	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1139	20	1/1/12/20	8/21/99/115	-
13	CLA	B	1235	-	1/1/15/20	0/37/115/115	-
15	SF4	A	3001	2,1	-	-	0/6/5/5
13	CLA	B	1236	-	-	4/16/94/115	-
13	CLA	A	1113	-	1/1/11/20	4/13/91/115	-
13	CLA	B	1222	20	1/1/11/20	6/15/93/115	-
16	BCR	L	4019	-	-	1/29/63/63	0/2/2/2
16	BCR	L	4022	-	-	1/29/63/63	0/2/2/2
13	CLA	A	1106	1	1/1/15/20	16/37/115/115	-
13	CLA	K	1401	-	-	6/13/91/115	-
13	CLA	A	1118	-	1/1/14/20	14/33/111/115	-
13	CLA	B	1219	20	1/1/13/20	8/25/103/115	-
13	CLA	B	1218	-	1/1/11/20	5/13/91/115	-
13	CLA	B	1209	-	1/1/11/20	3/13/91/115	-
13	CLA	A	1122	-	1/1/13/20	12/30/108/115	-
13	CLA	B	1224	-	1/1/15/20	14/37/115/115	-
13	CLA	A	1013	-	1/1/15/20	10/37/115/115	-
16	BCR	A	4007	-	-	2/29/63/63	0/2/2/2
16	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
17	LHG	B	5004	-	-	7/26/26/53	-
13	CLA	B	1227	-	1/1/11/20	8/13/91/115	-
13	CLA	L	1501	10	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1107	1	1/1/15/20	13/37/115/115	-
14	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
13	CLA	A	1134	1	1/1/11/20	5/13/91/115	-
13	CLA	B	1229	-	1/1/15/20	16/37/115/115	-
16	BCR	B	4006	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1123	20	1/1/15/20	11/37/115/115	-
13	CLA	A	1137	-	1/1/11/20	5/16/94/115	-
13	CLA	B	1220	-	1/1/11/20	3/13/91/115	-
13	CLA	B	1021	-	1/1/15/20	10/37/115/115	-
13	CLA	B	1012	20	1/1/15/20	7/37/115/115	-
13	CLA	A	1112	-	1/1/11/20	1/13/91/115	-
13	CLA	B	1213	-	1/1/13/20	8/25/103/115	-
13	CLA	B	1204	-	1/1/15/20	2/37/115/115	-
13	CLA	L	1502	-	-	7/37/115/115	-
13	CLA	B	1215	-	1/1/14/20	10/31/109/115	-
16	BCR	A	4011	-	-	8/29/63/63	0/2/2/2
13	CLA	A	1102	13	1/1/13/20	12/30/108/115	-
13	CLA	A	1109	13	1/1/15/20	12/37/115/115	-
13	CLA	A	1133	-	1/1/12/20	6/24/102/115	-
13	CLA	A	1129	-	1/1/12/20	4/19/97/115	-
13	CLA	B	1207	2	1/1/15/20	7/37/115/115	-
13	CLA	A	1135	-	1/1/12/20	6/21/99/115	-
16	BCR	I	4020	-	-	4/29/63/63	0/2/2/2
13	CLA	L	1503	20	1/1/15/20	8/37/115/115	-
13	CLA	A	1125	-	1/1/15/20	7/37/115/115	-
16	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
13	CLA	B	1202	-	1/1/15/20	13/37/115/115	-
16	BCR	M	4021	-	-	4/29/63/63	0/2/2/2
13	CLA	B	1231	-	1/1/11/20	4/13/91/115	-
13	CLA	A	1140	-	1/1/15/20	8/37/115/115	-
13	CLA	A	1130	-	1/1/15/20	7/37/115/115	-
13	CLA	A	1801	17	1/1/12/20	15/22/100/115	-
13	CLA	B	1223	-	1/1/15/20	12/37/115/115	-
13	CLA	B	1205	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1206	2	1/1/15/20	14/37/115/115	-
13	CLA	B	1212	-	-	8/13/91/115	-
13	CLA	B	1221	2	1/1/12/20	7/24/102/115	-
13	CLA	A	1124	20	1/1/15/20	12/37/115/115	-
16	BCR	A	4002	-	-	4/29/63/63	0/2/2/2
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	A	1116	-	1/1/12/20	9/24/102/115	-
13	CLA	B	1233	20	1/1/11/20	4/13/91/115	-
13	CLA	A	1127	-	1/1/15/20	9/37/115/115	-
13	CLA	F	1301	20	1/1/11/20	4/13/91/115	-
17	LHG	A	5003	13	1/1/5/5	10/31/31/53	-
15	SF4	C	3002	3	-	-	0/6/5/5
16	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
17	LHG	A	5001	-	-	19/53/53/53	-
13	CLA	B	1201	-	1/1/12/20	4/24/102/115	-
13	CLA	A	1011	-	1/1/15/20	1/37/115/115	-

All (932) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	2001	PQN	O4-C4	9.27	1.42	1.23
14	B	2002	PQN	O4-C4	8.95	1.42	1.23
14	A	2001	PQN	O1-C1	8.92	1.42	1.23
17	B	5004	LHG	P-O5	8.61	1.81	1.50
14	B	2002	PQN	O1-C1	8.42	1.41	1.23
14	A	2001	PQN	C12-C13	8.26	1.52	1.33
14	B	2002	PQN	C12-C13	8.26	1.52	1.33
17	A	5001	LHG	P-O5	8.18	1.79	1.50
17	A	5003	LHG	P-O5	7.67	1.78	1.50
14	A	2001	PQN	C2M-C2	-6.77	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
13	B	1210	CLA	MG-NA	6.51	2.21	2.06
13	A	1137	CLA	MG-NA	6.46	2.21	2.06
13	B	1207	CLA	MG-NA	6.43	2.21	2.06
14	B	2002	PQN	C2M-C2	-6.42	1.37	1.50
14	A	2001	PQN	C3-C2	6.38	1.46	1.35
14	B	2002	PQN	C3-C2	6.34	1.46	1.35
13	B	1225	CLA	MG-NA	6.30	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
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
17	B	5004	LHG	P-O6	5.90	1.83	1.59
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	1128	CLA	C4B-NB	5.57	1.40	1.35
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
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
13	A	1125	CLA	MG-NA	5.39	2.19	2.06
13	A	1107	CLA	MG-NA	5.36	2.19	2.06
13	A	1138	CLA	C4B-NB	5.35	1.40	1.35
13	A	1109	CLA	MG-NA	5.33	2.18	2.06
13	B	1201	CLA	MG-NA	5.33	2.18	2.06
17	B	5004	LHG	P-O3	5.30	1.80	1.59
13	B	1206	CLA	C4B-NB	5.28	1.39	1.35
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	A	1127	CLA	C4B-NB	5.22	1.39	1.35
17	A	5001	LHG	P-O3	5.21	1.80	1.59
13	B	1222	CLA	MG-NA	5.20	2.18	2.06
13	A	1122	CLA	MG-NA	5.20	2.18	2.06
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	1011	CLA	C4B-NB	5.11	1.39	1.35
13	A	1119	CLA	MG-NA	5.11	2.18	2.06
13	B	1224	CLA	C4B-NB	5.10	1.39	1.35
13	A	1022	CLA	MG-NA	5.09	2.18	2.06
13	A	1133	CLA	MG-NA	5.09	2.18	2.06
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	L	1501	CLA	C4B-NB	5.00	1.39	1.35
13	B	1214	CLA	MG-NA	5.00	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1221	CLA	C4B-NB	4.99	1.39	1.35
13	B	1205	CLA	MG-NA	4.98	2.18	2.06
13	B	1023	CLA	MG-NA	4.98	2.18	2.06
16	L	4022	BCR	C1-C6	4.96	1.60	1.53
13	A	1013	CLA	MG-NA	4.95	2.18	2.06
13	F	1301	CLA	C4B-NB	4.94	1.39	1.35
17	A	5003	LHG	P-O6	4.93	1.79	1.59
13	A	1138	CLA	MG-NA	4.88	2.17	2.06
16	B	4005	BCR	C1-C6	4.82	1.60	1.53
16	L	4019	BCR	C30-C25	4.75	1.60	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
16	B	4004	BCR	C30-C25	4.71	1.60	1.53
13	A	1140	CLA	MG-NA	4.69	2.17	2.06
14	B	2002	PQN	C16-C15	-4.69	1.34	1.52
13	B	1012	CLA	C4B-NB	4.66	1.39	1.35
13	A	1132	CLA	MG-NA	4.63	2.17	2.06
13	B	1023	CLA	C4B-NB	4.62	1.39	1.35
13	A	1124	CLA	MG-NA	4.61	2.17	2.06
16	L	4022	BCR	C30-C25	4.59	1.60	1.53
13	X	1701	CLA	C4B-NB	4.57	1.39	1.35
13	B	1231	CLA	MG-NA	4.57	2.17	2.06
14	A	2001	PQN	C16-C15	-4.57	1.35	1.52
13	B	1210	CLA	C4B-NB	4.50	1.39	1.35
13	A	1130	CLA	MG-NA	4.49	2.16	2.06
16	A	4007	BCR	C30-C25	4.47	1.59	1.53
13	A	1125	CLA	C4B-NB	4.47	1.39	1.35
13	A	1022	CLA	C4B-NB	4.46	1.39	1.35
17	A	5003	LHG	P-O3	4.46	1.77	1.59
13	B	1223	CLA	C4B-NB	4.45	1.39	1.35
13	A	1103	CLA	MG-NA	4.42	2.16	2.06
13	J	1303	CLA	C4B-NB	4.41	1.39	1.35
13	B	1232	CLA	C4B-NB	4.40	1.39	1.35
13	B	1239	CLA	MG-NA	4.34	2.16	2.06
13	B	1229	CLA	C4B-NB	4.34	1.39	1.35
13	A	1237	CLA	MG-NA	4.34	2.16	2.06
13	B	1021	CLA	C4B-NB	4.31	1.39	1.35
13	A	1107	CLA	C4B-NB	4.29	1.39	1.35
13	A	1115	CLA	C4B-NB	4.28	1.39	1.35
13	B	1228	CLA	C4B-NB	4.28	1.39	1.35
13	B	1231	CLA	C4B-NB	4.25	1.39	1.35
13	B	1218	CLA	C4B-NB	4.23	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	5001	LHG	P-O6	4.12	1.76	1.59
13	B	1205	CLA	C4B-NB	4.06	1.38	1.35
13	A	1801	CLA	C4B-NB	4.04	1.38	1.35
13	B	1235	CLA	CHC-C1C	4.04	1.45	1.35
13	K	1401	CLA	C4B-NB	4.04	1.38	1.35
13	A	1105	CLA	C4B-NB	4.01	1.38	1.35
13	B	1204	CLA	MG-NA	4.00	2.15	2.06
13	M	1601	CLA	C4B-NB	3.97	1.38	1.35
13	L	1501	CLA	CHC-C1C	3.96	1.45	1.35
13	A	1132	CLA	C4B-NB	3.95	1.38	1.35
13	L	1503	CLA	C4B-NB	3.91	1.38	1.35
13	B	1023	CLA	CHC-C1C	3.88	1.44	1.35
13	A	1137	CLA	C4B-NB	3.88	1.38	1.35
13	B	1218	CLA	CHC-C1C	3.83	1.44	1.35
13	A	1112	CLA	C4B-NB	3.82	1.38	1.35
13	B	1217	CLA	C4B-NB	3.81	1.38	1.35
13	A	1108	CLA	C4B-NB	3.81	1.38	1.35
17	A	5003	LHG	O7-C7	3.81	1.45	1.34
13	A	1110	CLA	C4B-NB	3.80	1.38	1.35
13	J	1302	CLA	C4B-NB	3.80	1.38	1.35
13	A	1101	CLA	C4B-NB	3.79	1.38	1.35
13	A	1128	CLA	CHC-C1C	3.76	1.44	1.35
13	B	1214	CLA	C4B-NB	3.76	1.38	1.35
13	A	1111	CLA	C4B-NB	3.75	1.38	1.35
16	J	4013	BCR	C29-C30	3.75	1.62	1.54
13	A	1138	CLA	CHC-C1C	3.74	1.44	1.35
13	B	1233	CLA	C4B-NB	3.73	1.38	1.35
13	B	1224	CLA	CHC-C1C	3.73	1.44	1.35
13	L	1502	CLA	CHC-C1C	3.73	1.44	1.35
13	B	1221	CLA	CHC-C1C	3.72	1.44	1.35
13	A	1801	CLA	CHC-C1C	3.72	1.44	1.35
13	A	1106	CLA	CHC-C1C	3.72	1.44	1.35
13	B	1225	CLA	C4B-NB	3.70	1.38	1.35
13	A	1129	CLA	C4B-NB	3.70	1.38	1.35
13	A	1116	CLA	C4B-NB	3.70	1.38	1.35
16	A	4003	BCR	C1-C6	3.70	1.58	1.53
13	B	1231	CLA	CHC-C1C	3.69	1.44	1.35
13	A	1134	CLA	C4B-NB	3.69	1.38	1.35
13	A	1125	CLA	CHC-C1C	3.69	1.44	1.35
14	B	2002	PQN	C10-C5	3.69	1.46	1.40
13	X	1701	CLA	CHC-C1C	3.67	1.44	1.35
16	A	4003	BCR	C30-C25	3.66	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1112	CLA	CHC-C1C	3.66	1.44	1.35
13	B	1201	CLA	C4B-NB	3.65	1.38	1.35
13	B	1220	CLA	CHC-C1C	3.64	1.44	1.35
13	B	1207	CLA	C1B-NB	3.64	1.38	1.35
13	B	1209	CLA	C4B-NB	3.64	1.38	1.35
13	B	1208	CLA	C4B-NB	3.63	1.38	1.35
13	B	1219	CLA	C4B-NB	3.63	1.38	1.35
13	B	1212	CLA	CHC-C1C	3.62	1.44	1.35
16	J	4015	BCR	C30-C25	3.62	1.58	1.53
13	A	1118	CLA	CHC-C1C	3.62	1.44	1.35
16	J	4013	BCR	C2-C1	3.62	1.62	1.54
13	B	1220	CLA	C4B-NB	3.61	1.38	1.35
13	A	1402	CLA	C4B-NB	3.60	1.38	1.35
13	B	1232	CLA	CHC-C1C	3.60	1.44	1.35
13	A	1119	CLA	CHC-C1C	3.59	1.44	1.35
13	L	1503	CLA	C1B-NB	3.59	1.38	1.35
16	A	4001	BCR	C30-C25	3.59	1.58	1.53
17	B	5004	LHG	O7-C7	3.59	1.44	1.34
13	A	1123	CLA	CHC-C1C	3.58	1.44	1.35
13	A	1120	CLA	CHC-C1C	3.58	1.44	1.35
13	B	1204	CLA	C3B-C2B	-3.57	1.35	1.40
13	B	1234	CLA	CHC-C1C	3.57	1.44	1.35
13	A	1129	CLA	C1D-ND	-3.55	1.33	1.37
13	B	1224	CLA	MG-NC	3.55	2.14	2.06
13	B	1235	CLA	C4B-NB	3.54	1.38	1.35
13	A	1129	CLA	CHC-C1C	3.54	1.44	1.35
16	F	4016	BCR	C2-C1	3.52	1.62	1.54
13	A	1122	CLA	C4B-NB	3.52	1.38	1.35
16	A	4001	BCR	C1-C6	3.52	1.58	1.53
13	L	1503	CLA	CHC-C1C	3.52	1.44	1.35
13	B	1012	CLA	CHC-C1C	3.52	1.44	1.35
13	J	1302	CLA	CHC-C1C	3.51	1.44	1.35
14	B	2002	PQN	C11-C12	3.51	1.55	1.50
13	A	1140	CLA	C4B-NB	3.50	1.38	1.35
16	A	4011	BCR	C30-C25	3.49	1.58	1.53
13	F	1301	CLA	CHC-C1C	3.48	1.43	1.35
13	A	1132	CLA	C3B-C2B	-3.47	1.35	1.40
13	A	1102	CLA	CHC-C1C	3.46	1.43	1.35
13	A	1123	CLA	C4B-NB	3.46	1.38	1.35
13	A	1103	CLA	C4B-NB	3.46	1.38	1.35
13	A	1137	CLA	CHC-C1C	3.45	1.43	1.35
13	A	1136	CLA	CHC-C1C	3.44	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1207	CLA	MG-NC	3.44	2.14	2.06
16	A	4002	BCR	C30-C25	3.44	1.58	1.53
13	B	1211	CLA	C4B-NB	3.43	1.38	1.35
13	A	1140	CLA	C1D-ND	-3.43	1.33	1.37
13	B	1227	CLA	C3B-C2B	-3.43	1.35	1.40
13	A	1114	CLA	C4B-NB	3.42	1.38	1.35
13	B	1223	CLA	CHC-C1C	3.41	1.43	1.35
13	B	1215	CLA	C1D-ND	-3.41	1.33	1.37
13	B	1201	CLA	CHC-C1C	3.41	1.43	1.35
13	B	1216	CLA	C4B-NB	3.41	1.38	1.35
13	A	1140	CLA	CHC-C1C	3.40	1.43	1.35
13	A	1120	CLA	C4B-NB	3.40	1.38	1.35
13	B	1228	CLA	CHC-C1C	3.39	1.43	1.35
13	B	1202	CLA	C4B-NB	3.38	1.38	1.35
16	M	4021	BCR	C1-C6	3.38	1.58	1.53
13	A	1118	CLA	C4B-NB	3.37	1.38	1.35
16	L	4022	BCR	C2-C1	3.36	1.61	1.54
13	M	1601	CLA	CHC-C1C	3.36	1.43	1.35
13	A	1102	CLA	C4B-NB	3.36	1.38	1.35
13	A	1116	CLA	CHC-C1C	3.35	1.43	1.35
13	B	1214	CLA	CHC-C1C	3.35	1.43	1.35
13	B	1230	CLA	C4B-NB	3.34	1.38	1.35
13	B	1215	CLA	C4B-NB	3.33	1.38	1.35
13	A	1117	CLA	C4B-NB	3.32	1.38	1.35
13	B	1213	CLA	C4B-NB	3.32	1.38	1.35
13	A	1105	CLA	CHC-C1C	3.32	1.43	1.35
13	A	1103	CLA	CHC-C1C	3.32	1.43	1.35
16	B	4004	BCR	C1-C6	3.30	1.58	1.53
13	B	1212	CLA	C4B-NB	3.29	1.38	1.35
16	A	4011	BCR	C1-C6	3.29	1.58	1.53
13	B	1236	CLA	C4B-NB	3.29	1.38	1.35
13	A	1237	CLA	C1B-NB	3.28	1.38	1.35
13	B	1217	CLA	CHC-C1C	3.28	1.43	1.35
13	B	1219	CLA	CHC-C1C	3.28	1.43	1.35
13	J	1303	CLA	CHC-C1C	3.27	1.43	1.35
13	A	1118	CLA	C1D-ND	-3.27	1.33	1.37
13	L	1502	CLA	C1B-NB	3.27	1.38	1.35
13	B	1227	CLA	CHC-C1C	3.27	1.43	1.35
13	A	1134	CLA	CHC-C1C	3.26	1.43	1.35
13	B	1229	CLA	CHC-C1C	3.26	1.43	1.35
16	I	4020	BCR	C30-C25	3.26	1.58	1.53
16	J	4015	BCR	C1-C6	3.25	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	4008	BCR	C1-C6	3.25	1.58	1.53
13	A	1115	CLA	CHC-C1C	3.24	1.43	1.35
13	A	1113	CLA	C4B-NB	3.24	1.38	1.35
13	L	1501	CLA	C1B-NB	3.24	1.38	1.35
16	B	4004	BCR	C2-C1	3.23	1.61	1.54
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	A	1104	CLA	CHC-C1C	3.23	1.43	1.35
13	A	1119	CLA	C1D-ND	-3.23	1.33	1.37
13	B	1226	CLA	C4B-NB	3.23	1.38	1.35
13	B	1012	CLA	MG-NC	3.22	2.13	2.06
16	B	4004	BCR	C26-C25	3.22	1.40	1.34
13	B	1239	CLA	C1D-ND	-3.21	1.33	1.37
14	A	2001	PQN	C10-C5	3.21	1.46	1.40
13	A	1122	CLA	CHC-C1C	3.21	1.43	1.35
13	B	1209	CLA	CHC-C1C	3.20	1.43	1.35
13	A	1022	CLA	CHC-C1C	3.19	1.43	1.35
13	A	1109	CLA	C4B-NB	3.18	1.38	1.35
13	B	1206	CLA	MG-NC	3.18	2.13	2.06
13	B	1211	CLA	CHC-C1C	3.18	1.43	1.35
13	B	1210	CLA	MG-NC	3.18	2.13	2.06
13	B	1236	CLA	CHC-C1C	3.17	1.43	1.35
13	B	1225	CLA	C2-C3	3.17	1.40	1.33
13	A	1136	CLA	C4B-NB	3.17	1.38	1.35
16	J	4013	BCR	C30-C25	3.17	1.58	1.53
16	B	4010	BCR	C30-C25	3.16	1.58	1.53
13	A	1107	CLA	C1D-ND	-3.16	1.33	1.37
13	B	1235	CLA	C3B-C2B	-3.16	1.36	1.40
13	K	1401	CLA	CHC-C1C	3.16	1.43	1.35
13	B	1213	CLA	CHC-C1C	3.15	1.43	1.35
13	A	1104	CLA	C4B-NB	3.14	1.38	1.35
13	F	1301	CLA	MG-NC	3.14	2.13	2.06
16	A	4007	BCR	C29-C30	3.14	1.61	1.54
16	J	4012	BCR	C29-C30	3.14	1.61	1.54
16	B	4017	BCR	C2-C1	3.13	1.61	1.54
13	B	1216	CLA	CHC-C1C	3.13	1.43	1.35
13	A	1107	CLA	CHC-C1C	3.12	1.43	1.35
13	A	1013	CLA	C4B-NB	3.12	1.38	1.35
13	B	1208	CLA	CHC-C1C	3.12	1.43	1.35
13	A	1135	CLA	MG-NC	3.12	2.13	2.06
16	J	4015	BCR	C2-C1	3.11	1.61	1.54
14	B	2002	PQN	C6-C5	3.10	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	1502	CLA	C4B-NB	3.10	1.38	1.35
16	A	4002	BCR	C2-C1	3.09	1.61	1.54
16	A	4011	BCR	C2-C1	3.09	1.61	1.54
16	F	4016	BCR	C30-C25	3.08	1.58	1.53
13	A	1011	CLA	CHC-C1C	3.08	1.42	1.35
13	A	1113	CLA	CHC-C1C	3.07	1.42	1.35
13	A	1022	CLA	MG-NC	3.07	2.13	2.06
13	B	1233	CLA	CHC-C1C	3.07	1.42	1.35
13	A	1125	CLA	C5-C3	3.07	1.57	1.51
13	B	1210	CLA	CHC-C1C	3.06	1.42	1.35
13	A	1101	CLA	CHC-C1C	3.06	1.42	1.35
13	B	1234	CLA	C3B-C2B	-3.05	1.36	1.40
13	A	1106	CLA	CAA-C2A	3.05	1.59	1.54
14	A	2001	PQN	C6-C5	3.04	1.44	1.39
13	B	1205	CLA	CHC-C1C	3.04	1.42	1.35
13	B	1228	CLA	C3B-C2B	-3.03	1.36	1.40
13	A	1133	CLA	CHC-C1C	3.03	1.42	1.35
13	B	1230	CLA	CHC-C1C	3.03	1.42	1.35
16	A	4003	BCR	C2-C1	3.02	1.61	1.54
16	B	4014	BCR	C29-C30	3.02	1.61	1.54
16	A	4002	BCR	C29-C30	3.02	1.61	1.54
13	A	1013	CLA	CHC-C1C	3.02	1.42	1.35
13	A	1114	CLA	CHC-C1C	3.01	1.42	1.35
13	A	1121	CLA	CHC-C1C	3.01	1.42	1.35
13	B	1234	CLA	C4B-NB	3.00	1.37	1.35
13	A	1111	CLA	CHC-C1C	3.00	1.42	1.35
13	A	1127	CLA	MG-NC	2.99	2.13	2.06
16	M	4021	BCR	C2-C1	2.99	1.61	1.54
13	B	1229	CLA	C3B-C2B	-2.98	1.36	1.40
13	A	1108	CLA	MG-NC	2.98	2.13	2.06
16	B	4005	BCR	C30-C25	2.98	1.57	1.53
16	M	4021	BCR	C29-C30	2.97	1.61	1.54
13	A	1116	CLA	CAA-C2A	2.97	1.59	1.54
13	A	1119	CLA	C4B-NB	2.96	1.37	1.35
13	A	1116	CLA	C3B-C2B	-2.95	1.36	1.40
13	B	1222	CLA	C4B-NB	2.95	1.37	1.35
13	B	1222	CLA	CHC-C1C	2.95	1.42	1.35
13	A	1109	CLA	CHC-C1C	2.95	1.42	1.35
13	B	1213	CLA	C5-C3	2.94	1.57	1.51
16	B	4005	BCR	C2-C1	2.94	1.60	1.54
16	B	4009	BCR	C29-C30	2.94	1.60	1.54
13	A	1124	CLA	C1D-ND	-2.94	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	4012	BCR	C1-C6	2.93	1.57	1.53
16	B	4017	BCR	C29-C30	2.93	1.60	1.54
16	F	4016	BCR	C29-C30	2.93	1.60	1.54
13	B	1021	CLA	MG-NC	2.93	2.13	2.06
16	B	4006	BCR	C2-C1	2.93	1.60	1.54
13	B	1205	CLA	C1B-CHB	-2.92	1.32	1.41
13	A	1402	CLA	CHC-C1C	2.92	1.42	1.35
13	B	1219	CLA	CAA-C2A	2.92	1.59	1.54
13	B	1221	CLA	C5-C3	2.91	1.57	1.51
16	B	4010	BCR	C2-C1	2.90	1.60	1.54
16	A	4001	BCR	C29-C30	2.90	1.60	1.54
13	A	1127	CLA	CHC-C1C	2.90	1.42	1.35
13	B	1228	CLA	C1B-CHB	-2.89	1.32	1.41
16	J	4015	BCR	C29-C30	2.89	1.60	1.54
13	A	1137	CLA	CAA-C2A	2.89	1.59	1.54
13	A	1129	CLA	C3B-C2B	-2.88	1.36	1.40
16	B	4006	BCR	C29-C30	2.88	1.60	1.54
17	A	5003	LHG	O8-C23	2.87	1.41	1.33
13	A	1237	CLA	CMD-C2D	2.87	1.56	1.50
13	A	1108	CLA	CHC-C1C	2.86	1.42	1.35
16	B	4004	BCR	C29-C30	2.86	1.60	1.54
16	B	4017	BCR	C30-C25	2.86	1.57	1.53
13	A	1130	CLA	MG-NC	2.86	2.13	2.06
13	B	1213	CLA	CAA-C2A	2.85	1.59	1.54
13	B	1209	CLA	C1D-ND	-2.85	1.34	1.37
13	A	1801	CLA	CAA-C2A	2.85	1.59	1.54
13	A	1110	CLA	CHC-C1C	2.85	1.42	1.35
13	A	1013	CLA	C1B-CHB	-2.84	1.33	1.41
13	A	1133	CLA	C4B-NB	2.84	1.37	1.35
16	B	4006	BCR	C1-C6	2.84	1.57	1.53
16	I	4020	BCR	C2-C1	2.84	1.60	1.54
16	B	4006	BCR	C30-C25	2.84	1.57	1.53
16	A	4011	BCR	C29-C30	2.84	1.60	1.54
13	A	1121	CLA	C4B-NB	2.84	1.37	1.35
13	B	1227	CLA	C4B-NB	2.84	1.37	1.35
16	J	4012	BCR	C30-C25	2.84	1.57	1.53
16	B	4005	BCR	C26-C25	2.83	1.39	1.34
13	B	1232	CLA	CAA-C2A	2.83	1.59	1.54
13	A	1237	CLA	C1D-ND	-2.83	1.34	1.37
13	B	1224	CLA	CAA-C2A	2.83	1.59	1.54
13	B	1205	CLA	MG-NC	2.82	2.13	2.06
13	B	1225	CLA	CHC-C1C	2.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1023	CLA	CHD-C1D	2.82	1.43	1.38
13	A	1105	CLA	MG-NC	2.81	2.13	2.06
16	J	4012	BCR	C2-C1	2.80	1.60	1.54
13	A	1129	CLA	C1B-CHB	-2.80	1.33	1.41
13	A	1119	CLA	C1B-CHB	-2.80	1.33	1.41
13	A	1119	CLA	CAA-C2A	2.79	1.59	1.54
13	B	1023	CLA	C3B-C2B	-2.79	1.36	1.40
13	A	1123	CLA	C3B-C2B	-2.79	1.36	1.40
13	B	1226	CLA	CAA-C2A	2.79	1.59	1.54
16	L	4019	BCR	C29-C30	2.79	1.60	1.54
13	J	1302	CLA	MG-NC	2.79	2.12	2.06
13	B	1225	CLA	MG-NC	2.78	2.12	2.06
16	B	4009	BCR	C30-C25	2.77	1.57	1.53
13	M	1601	CLA	C1D-ND	-2.77	1.34	1.37
13	B	1023	CLA	C1B-CHB	-2.77	1.33	1.41
13	B	1212	CLA	MG-NC	2.77	2.12	2.06
14	A	2001	PQN	C11-C12	2.76	1.54	1.50
18	B	5002	LMG	O8-C28	2.76	1.41	1.33
16	M	4021	BCR	C30-C25	2.76	1.57	1.53
13	A	1136	CLA	C3B-C2B	-2.75	1.36	1.40
13	B	1226	CLA	CHC-C1C	2.75	1.42	1.35
13	A	1106	CLA	C3B-C2B	-2.75	1.36	1.40
13	B	1204	CLA	CHD-C1D	2.75	1.43	1.38
16	I	4018	BCR	C29-C30	2.75	1.60	1.54
17	A	5001	LHG	O8-C23	2.74	1.41	1.33
13	B	1204	CLA	C1B-CHB	-2.74	1.33	1.41
13	A	1104	CLA	MG-ND	-2.74	2.00	2.05
13	A	1140	CLA	C1B-NB	2.74	1.37	1.35
13	B	1214	CLA	C1D-ND	-2.74	1.34	1.37
13	A	1135	CLA	C4B-NB	2.73	1.37	1.35
14	B	2002	PQN	C11-C3	2.73	1.55	1.51
13	B	1208	CLA	C3B-C2B	-2.73	1.36	1.40
13	B	1230	CLA	C5-C3	2.73	1.57	1.51
13	B	1214	CLA	CAA-C2A	2.72	1.59	1.54
14	A	2001	PQN	C15-C13	2.72	1.56	1.51
16	A	4002	BCR	C1-C6	2.72	1.57	1.53
13	A	1128	CLA	C3B-C2B	-2.72	1.36	1.40
16	A	4001	BCR	C2-C1	2.71	1.60	1.54
16	A	4007	BCR	C1-C6	2.71	1.57	1.53
13	J	1303	CLA	CHD-C1D	2.71	1.43	1.38
13	A	1013	CLA	C1D-ND	-2.70	1.34	1.37
13	A	1137	CLA	MG-NC	2.70	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1203	CLA	C4B-NB	2.70	1.37	1.35
13	B	1203	CLA	MG-NC	2.69	2.12	2.06
13	A	1124	CLA	C1B-CHB	-2.69	1.33	1.41
16	A	4008	BCR	C30-C25	2.69	1.57	1.53
16	I	4020	BCR	C29-C30	2.69	1.60	1.54
13	A	1126	CLA	MG-NC	2.69	2.12	2.06
13	B	1239	CLA	CHC-C1C	2.68	1.41	1.35
13	B	1021	CLA	C1B-CHB	-2.68	1.33	1.41
13	A	1106	CLA	C1D-ND	-2.68	1.34	1.37
13	B	1012	CLA	C1D-ND	-2.68	1.34	1.37
13	L	1502	CLA	C1B-CHB	-2.68	1.33	1.41
13	B	1021	CLA	C1B-NB	2.68	1.37	1.35
13	B	1223	CLA	C1D-C2D	-2.67	1.40	1.45
13	L	1501	CLA	MG-NC	2.67	2.12	2.06
13	B	1223	CLA	C1B-NB	2.67	1.37	1.35
16	L	4022	BCR	C29-C30	2.67	1.60	1.54
13	B	1205	CLA	C3B-C2B	-2.66	1.36	1.40
13	B	1214	CLA	C1B-CHB	-2.66	1.33	1.41
13	B	1236	CLA	C1B-CHB	-2.66	1.33	1.41
13	A	1106	CLA	C1B-CHB	-2.66	1.33	1.41
13	B	1208	CLA	C1B-CHB	-2.66	1.33	1.41
13	B	1215	CLA	CAA-C2A	2.66	1.59	1.54
14	A	2001	PQN	C10-C1	-2.66	1.43	1.48
13	A	1109	CLA	C1D-ND	-2.65	1.34	1.37
13	B	1234	CLA	C1D-ND	-2.65	1.34	1.37
13	A	1105	CLA	C3B-C2B	-2.65	1.36	1.40
17	A	5001	LHG	O7-C7	2.65	1.41	1.34
13	A	1107	CLA	MG-NC	2.64	2.12	2.06
13	B	1225	CLA	C5-C3	2.64	1.56	1.51
13	B	1202	CLA	CHC-C1C	2.64	1.41	1.35
16	B	4010	BCR	C1-C6	2.63	1.57	1.53
13	A	1140	CLA	C1-C2	2.63	1.57	1.49
16	A	4007	BCR	C2-C1	2.63	1.60	1.54
16	B	4014	BCR	C2-C1	2.63	1.60	1.54
13	A	1138	CLA	C1B-CHB	-2.63	1.33	1.41
13	B	1215	CLA	CHC-C1C	2.63	1.41	1.35
13	B	1221	CLA	C1B-CHB	-2.63	1.33	1.41
13	B	1202	CLA	C1D-ND	-2.62	1.34	1.37
13	B	1236	CLA	C3B-C2B	-2.62	1.36	1.40
16	A	4011	BCR	C23-C22	-2.62	1.40	1.45
13	A	1108	CLA	C3B-C2B	-2.61	1.36	1.40
13	B	1203	CLA	CHD-C1D	2.61	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1231	CLA	C3B-C2B	-2.60	1.36	1.40
13	B	1021	CLA	CHC-C1C	2.60	1.41	1.35
13	B	1203	CLA	CHC-C1C	2.60	1.41	1.35
13	A	1106	CLA	C4B-NB	2.60	1.37	1.35
13	A	1237	CLA	CAA-C2A	2.60	1.58	1.54
13	B	1216	CLA	MG-NC	2.60	2.12	2.06
13	A	1104	CLA	MG-NC	2.59	2.12	2.06
13	B	1232	CLA	C3B-C2B	-2.59	1.36	1.40
13	L	1502	CLA	CMD-C2D	2.59	1.56	1.50
13	A	1101	CLA	C1D-ND	-2.59	1.34	1.37
13	A	1139	CLA	CHC-C1C	2.58	1.41	1.35
13	A	1102	CLA	CAA-C2A	2.58	1.58	1.54
13	A	1121	CLA	CHD-C1D	2.58	1.43	1.38
13	A	1121	CLA	C3B-C2B	-2.58	1.36	1.40
13	A	1112	CLA	C1B-CHB	-2.57	1.33	1.41
13	A	1101	CLA	C1B-CHB	-2.57	1.33	1.41
13	A	1132	CLA	CHC-C1C	2.57	1.41	1.35
13	B	1235	CLA	C1B-CHB	-2.57	1.33	1.41
13	B	1217	CLA	C1D-ND	-2.57	1.34	1.37
13	A	1132	CLA	C1B-CHB	-2.57	1.33	1.41
13	A	1130	CLA	C4B-NB	2.56	1.37	1.35
13	B	1236	CLA	MG-NC	2.56	2.12	2.06
13	A	1011	CLA	C4D-CHA	2.56	1.47	1.38
13	A	1115	CLA	C1D-ND	-2.55	1.34	1.37
13	A	1116	CLA	C5-C3	2.55	1.56	1.51
16	A	4008	BCR	C29-C30	2.54	1.60	1.54
13	A	1136	CLA	C1B-CHB	-2.54	1.33	1.41
13	B	1216	CLA	C3B-C2B	-2.54	1.36	1.40
13	A	1124	CLA	CHC-C1C	2.54	1.41	1.35
13	A	1110	CLA	CHD-C1D	2.53	1.43	1.38
13	A	1111	CLA	C1B-CHB	-2.53	1.33	1.41
13	B	1209	CLA	CHD-C1D	2.53	1.43	1.38
13	A	1126	CLA	CHC-C1C	2.53	1.41	1.35
13	A	1103	CLA	C1B-CHB	-2.53	1.34	1.41
13	B	1210	CLA	C1B-CHB	-2.53	1.34	1.41
13	B	1232	CLA	C1B-CHB	-2.53	1.34	1.41
13	A	1133	CLA	C5-C3	2.53	1.56	1.51
13	B	1225	CLA	C3B-C2B	-2.53	1.36	1.40
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	1128	CLA	C1B-NB	2.52	1.37	1.35
13	A	1402	CLA	CBD-CAD	2.52	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	4015	BCR	C5-C6	2.52	1.38	1.34
13	A	1115	CLA	C1B-CHB	-2.52	1.34	1.41
13	A	1128	CLA	C5-C3	2.52	1.56	1.51
13	A	1109	CLA	C1B-CHB	-2.52	1.34	1.41
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	1238	CLA	C3B-C2B	-2.51	1.36	1.40
13	B	1202	CLA	CMD-C2D	2.51	1.56	1.50
13	A	1126	CLA	C4B-NB	2.51	1.37	1.35
13	A	1132	CLA	C1D-ND	-2.51	1.34	1.37
13	A	1122	CLA	C1B-CHB	-2.51	1.34	1.41
13	A	1013	CLA	CAA-C2A	2.51	1.58	1.54
13	B	1216	CLA	C1B-CHB	-2.50	1.34	1.41
13	M	1601	CLA	CAA-C2A	2.50	1.58	1.54
16	A	4011	BCR	C14-C13	2.50	1.39	1.35
13	B	1229	CLA	C1D-ND	-2.50	1.34	1.37
13	A	1118	CLA	C5-C3	2.50	1.56	1.51
13	B	1207	CLA	MG-ND	-2.50	2.00	2.05
18	B	5002	LMG	O7-C8	-2.50	1.40	1.46
13	B	1217	CLA	CAA-C2A	2.49	1.58	1.54
13	B	1206	CLA	C1D-ND	-2.49	1.34	1.37
13	B	1231	CLA	C1B-CHB	-2.49	1.34	1.41
13	A	1139	CLA	MG-NC	2.49	2.12	2.06
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
13	A	1128	CLA	C1D-ND	-2.48	1.34	1.37
13	B	1227	CLA	C1B-CHB	-2.48	1.34	1.41
13	A	1117	CLA	C1-C2	2.48	1.56	1.49
13	A	1117	CLA	C2-C3	2.48	1.38	1.33
16	L	4019	BCR	C2-C1	2.48	1.59	1.54
13	A	1139	CLA	C4B-NB	2.48	1.37	1.35
14	B	2002	PQN	C9-C10	2.48	1.43	1.39
16	I	4018	BCR	C2-C1	2.47	1.59	1.54
16	B	4005	BCR	C29-C30	2.47	1.59	1.54
13	B	1207	CLA	C3B-C2B	-2.47	1.36	1.40
13	B	1023	CLA	MG-NC	2.47	2.12	2.06
13	B	1211	CLA	C1B-CHB	-2.47	1.34	1.41
13	B	1232	CLA	C1D-ND	-2.47	1.34	1.37
14	A	2001	PQN	C11-C3	2.47	1.55	1.51
13	A	1124	CLA	MG-NC	2.47	2.12	2.06
13	A	1123	CLA	MG-NC	2.46	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1227	CLA	C1D-ND	-2.45	1.34	1.37
13	A	1108	CLA	CAA-C2A	2.45	1.58	1.54
16	M	4021	BCR	C23-C22	-2.45	1.40	1.45
13	A	1128	CLA	MG-NC	2.45	2.12	2.06
13	B	1216	CLA	C1D-ND	-2.45	1.34	1.37
13	K	1401	CLA	C1B-CHB	-2.45	1.34	1.41
13	A	1102	CLA	C1D-ND	-2.44	1.34	1.37
13	L	1502	CLA	CAA-C2A	2.44	1.58	1.54
13	A	1117	CLA	CHC-C1C	2.44	1.41	1.35
13	A	1117	CLA	CAA-C2A	2.44	1.58	1.54
13	A	1115	CLA	C1B-NB	2.44	1.37	1.35
13	J	1302	CLA	CHD-C1D	2.44	1.43	1.38
16	L	4019	BCR	C19-C18	-2.44	1.40	1.45
13	B	1221	CLA	CHD-C1D	2.43	1.43	1.38
13	A	1121	CLA	CAA-C2A	2.43	1.58	1.54
16	B	4010	BCR	C29-C30	2.43	1.59	1.54
13	A	1022	CLA	C1B-CHB	-2.43	1.34	1.41
13	A	1126	CLA	C1B-CHB	-2.43	1.34	1.41
13	B	1238	CLA	CHC-C1C	2.43	1.41	1.35
13	A	1120	CLA	C3B-C2B	-2.43	1.37	1.40
13	B	1231	CLA	CHD-C1D	2.42	1.43	1.38
13	B	1214	CLA	C3B-C2B	-2.42	1.37	1.40
13	B	1225	CLA	CAA-C2A	2.42	1.58	1.54
13	B	1224	CLA	C1D-ND	-2.42	1.34	1.37
13	A	1112	CLA	C3B-C2B	-2.42	1.37	1.40
13	A	1115	CLA	MG-NC	2.42	2.12	2.06
13	A	1127	CLA	CHD-C1D	2.42	1.43	1.38
13	A	1237	CLA	C1B-CHB	-2.42	1.34	1.41
13	A	1105	CLA	C1D-ND	-2.42	1.34	1.37
13	K	1401	CLA	MG-NC	2.42	2.12	2.06
16	L	4022	BCR	C38-C26	2.41	1.54	1.50
16	B	4005	BCR	C38-C26	2.41	1.54	1.50
13	B	1212	CLA	C1B-CHB	-2.41	1.34	1.41
13	A	1801	CLA	C1B-CHB	-2.41	1.34	1.41
13	A	1137	CLA	C3B-C2B	-2.41	1.37	1.40
13	X	1701	CLA	MG-NC	2.41	2.12	2.06
16	A	4001	BCR	C26-C25	2.41	1.38	1.34
13	A	1013	CLA	CMD-C2D	2.41	1.55	1.50
13	A	1237	CLA	C3B-C2B	-2.41	1.37	1.40
16	A	4003	BCR	C29-C30	2.40	1.59	1.54
16	I	4018	BCR	C30-C25	2.40	1.57	1.53
13	A	1139	CLA	C5-C3	2.40	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1210	CLA	CMD-C2D	2.39	1.55	1.50
13	A	1123	CLA	CHD-C1D	2.39	1.43	1.38
13	B	1204	CLA	CAA-C2A	2.39	1.58	1.54
13	B	1206	CLA	CHC-C1C	2.39	1.41	1.35
13	A	1110	CLA	CAA-C2A	2.39	1.58	1.54
13	B	1226	CLA	C1B-NB	2.39	1.37	1.35
13	A	1131	CLA	MG-NC	2.38	2.11	2.06
13	A	1118	CLA	CAA-C2A	2.38	1.58	1.54
13	B	1212	CLA	C3B-C2B	-2.37	1.37	1.40
13	L	1501	CLA	CMD-C2D	2.37	1.55	1.50
13	A	1121	CLA	MG-NC	2.37	2.11	2.06
13	B	1221	CLA	C3B-C2B	-2.36	1.37	1.40
13	A	1114	CLA	C1B-CHB	-2.36	1.34	1.41
13	L	1501	CLA	CAA-C2A	2.36	1.58	1.54
16	L	4022	BCR	C26-C25	2.36	1.38	1.34
13	B	1225	CLA	C1-C2	2.36	1.56	1.49
13	A	1124	CLA	C4B-NB	2.36	1.37	1.35
13	A	1801	CLA	C3B-C2B	-2.36	1.37	1.40
14	B	2002	PQN	C5-C4	-2.35	1.43	1.48
13	A	1130	CLA	CHC-C1C	2.35	1.41	1.35
13	A	1109	CLA	MG-NC	2.35	2.11	2.06
13	A	1121	CLA	C1B-CHB	-2.35	1.34	1.41
13	A	1022	CLA	C3B-C2B	-2.35	1.37	1.40
13	B	1222	CLA	MG-NC	2.35	2.11	2.06
16	B	4009	BCR	C23-C22	-2.35	1.40	1.45
16	B	4017	BCR	C23-C22	-2.35	1.40	1.45
13	J	1303	CLA	CBD-CAD	2.34	1.57	1.51
16	I	4018	BCR	C33-C5	2.34	1.54	1.50
13	A	1114	CLA	C1D-ND	-2.34	1.34	1.37
13	B	1230	CLA	CAA-C2A	2.34	1.58	1.54
16	B	4014	BCR	C23-C22	-2.34	1.40	1.45
13	B	1224	CLA	CMD-C2D	2.34	1.55	1.50
13	B	1229	CLA	C1B-CHB	-2.34	1.34	1.41
13	A	1120	CLA	C1B-CHB	-2.33	1.34	1.41
13	B	1213	CLA	C1B-CHB	-2.33	1.34	1.41
13	A	1801	CLA	C5-C3	2.33	1.56	1.51
13	A	1120	CLA	CHD-C1D	2.33	1.42	1.38
13	A	1132	CLA	MG-ND	-2.33	2.01	2.05
13	L	1503	CLA	CMD-C2D	2.33	1.55	1.50
13	A	1112	CLA	C1D-ND	-2.33	1.34	1.37
13	B	1225	CLA	C1B-CHB	-2.33	1.34	1.41
13	A	1237	CLA	CHC-C1C	2.33	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1211	CLA	C5-C3	2.32	1.56	1.51
13	A	1134	CLA	C1D-ND	-2.32	1.34	1.37
14	A	2001	PQN	C9-C10	2.32	1.43	1.39
13	A	1110	CLA	C1B-CHB	-2.32	1.34	1.41
13	B	1231	CLA	C1D-ND	-2.32	1.34	1.37
13	B	1215	CLA	C3B-CAB	2.32	1.52	1.47
13	A	1109	CLA	C3B-C2B	-2.32	1.37	1.40
13	A	1108	CLA	C1B-CHB	-2.31	1.34	1.41
13	A	1117	CLA	C1B-CHB	-2.31	1.34	1.41
13	A	1136	CLA	CHD-C1D	2.31	1.42	1.38
13	B	1213	CLA	C3B-C2B	-2.31	1.37	1.40
13	B	1222	CLA	CHD-C1D	2.31	1.42	1.38
13	A	1117	CLA	C1D-ND	-2.31	1.34	1.37
13	A	1130	CLA	CMD-C2D	2.30	1.55	1.50
13	B	1238	CLA	CAA-C2A	2.30	1.58	1.54
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	1116	CLA	C1D-ND	-2.30	1.35	1.37
13	B	1224	CLA	OBD-CAD	2.30	1.26	1.22
13	A	1237	CLA	C4-C3	2.29	1.56	1.50
13	B	1235	CLA	MG-NC	2.29	2.11	2.06
13	B	1208	CLA	CAA-C2A	2.29	1.58	1.54
13	A	1107	CLA	C1B-CHB	-2.29	1.34	1.41
13	A	1402	CLA	MG-NC	2.29	2.11	2.06
13	A	1110	CLA	C3B-C2B	-2.29	1.37	1.40
13	A	1113	CLA	CHD-C1D	2.29	1.42	1.38
13	A	1119	CLA	CHD-C1D	2.29	1.42	1.38
13	A	1101	CLA	C3B-C2B	-2.28	1.37	1.40
13	B	1207	CLA	C1B-CHB	-2.28	1.34	1.41
13	A	1022	CLA	CHD-C1D	2.28	1.42	1.38
13	B	1211	CLA	MG-NC	2.28	2.11	2.06
13	A	1118	CLA	C3B-C2B	-2.28	1.37	1.40
13	A	1125	CLA	MG-NC	2.27	2.11	2.06
16	L	4019	BCR	C38-C26	2.27	1.54	1.50
16	I	4020	BCR	C19-C18	-2.27	1.41	1.45
13	B	1210	CLA	CHD-C1D	2.27	1.42	1.38
13	B	1207	CLA	CMD-C2D	2.27	1.55	1.50
13	A	1111	CLA	MG-NC	2.27	2.11	2.06
16	B	4014	BCR	C5-C6	2.27	1.38	1.34
13	K	1401	CLA	CMD-C2D	2.27	1.55	1.50
13	B	1225	CLA	C1D-ND	-2.26	1.35	1.37
16	B	4005	BCR	C29-C28	-2.26	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	4018	BCR	C2-C3	-2.25	1.47	1.52
16	I	4020	BCR	C33-C5	2.25	1.54	1.50
13	A	1138	CLA	CAA-C2A	2.25	1.58	1.54
13	A	1124	CLA	CAA-C2A	2.25	1.58	1.54
14	A	2001	PQN	C8-C7	2.25	1.44	1.38
13	B	1239	CLA	C1C-NC	-2.25	1.34	1.37
13	B	1204	CLA	C4B-NB	2.25	1.37	1.35
13	A	1114	CLA	MG-NC	2.25	2.11	2.06
13	A	1135	CLA	CHC-C1C	2.25	1.40	1.35
13	B	1219	CLA	MG-NC	2.25	2.11	2.06
13	B	1226	CLA	CHD-C1D	2.25	1.42	1.38
13	A	1011	CLA	MG-ND	-2.24	2.01	2.05
13	A	1138	CLA	C1D-ND	-2.24	1.35	1.37
13	A	1130	CLA	C1D-ND	-2.24	1.35	1.37
16	A	4008	BCR	C2-C1	2.24	1.59	1.54
13	B	1012	CLA	CMD-C2D	2.24	1.55	1.50
13	A	1801	CLA	MG-NC	2.23	2.11	2.06
13	B	1202	CLA	C5-C3	2.23	1.55	1.51
13	B	1201	CLA	C1B-CHB	-2.23	1.34	1.41
14	A	2001	PQN	C5-C4	-2.23	1.43	1.48
13	A	1116	CLA	C1B-CHB	-2.23	1.34	1.41
13	B	1238	CLA	C1B-CHB	-2.23	1.34	1.41
13	B	1218	CLA	CHD-C1D	2.23	1.42	1.38
14	A	2001	PQN	C8-C9	2.23	1.43	1.38
13	A	1136	CLA	MG-NC	2.23	2.11	2.06
13	K	1401	CLA	CHD-C1D	2.22	1.42	1.38
13	B	1219	CLA	C1B-CHB	-2.22	1.34	1.41
13	B	1228	CLA	MG-ND	-2.22	2.01	2.05
13	K	1401	CLA	C3B-C2B	-2.22	1.37	1.40
13	B	1207	CLA	C1D-C2D	-2.22	1.40	1.45
13	F	1301	CLA	C1B-CHB	-2.22	1.34	1.41
13	B	1225	CLA	C1B-NB	2.21	1.37	1.35
13	B	1215	CLA	C1B-CHB	-2.21	1.34	1.41
13	B	1230	CLA	C1D-ND	-2.21	1.35	1.37
16	L	4022	BCR	C23-C22	-2.21	1.41	1.45
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	B	1239	CLA	CAA-CBA	-2.21	1.45	1.52
13	A	1133	CLA	C1-C2	2.21	1.55	1.49
13	A	1134	CLA	CAA-C2A	2.21	1.58	1.54
13	A	1105	CLA	C1-C2	2.21	1.55	1.49
13	B	1201	CLA	C1D-ND	-2.20	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	B	1227	CLA	CHD-C1D	2.20	1.42	1.38
13	B	1238	CLA	CMD-C2D	2.20	1.55	1.50
13	A	1133	CLA	C1D-ND	-2.20	1.35	1.37
13	B	1220	CLA	C1B-CHB	-2.20	1.34	1.41
13	A	1133	CLA	MG-NC	2.20	2.11	2.06
13	A	1139	CLA	C3B-C2B	-2.20	1.37	1.40
13	B	1234	CLA	MG-NC	2.20	2.11	2.06
14	B	2002	PQN	C8-C9	2.19	1.43	1.38
14	B	2002	PQN	C10-C1	-2.19	1.44	1.48
13	B	1226	CLA	C1D-ND	-2.19	1.35	1.37
13	B	1223	CLA	C3B-CAB	2.19	1.52	1.47
13	B	1233	CLA	C1D-ND	-2.19	1.35	1.37
13	B	1213	CLA	C1-C2	2.19	1.55	1.49
16	I	4018	BCR	C19-C18	-2.19	1.41	1.45
13	B	1213	CLA	C4-C3	2.19	1.56	1.50
13	J	1302	CLA	CAA-C2A	2.19	1.58	1.54
13	A	1119	CLA	C1-C2	2.18	1.55	1.49
13	A	1122	CLA	C1D-ND	-2.18	1.35	1.37
13	B	1221	CLA	C1-C2	2.18	1.55	1.49
13	L	1502	CLA	C1D-ND	-2.18	1.35	1.37
13	A	1128	CLA	C1B-CHB	-2.18	1.34	1.41
16	A	4008	BCR	C33-C5	2.18	1.54	1.50
13	B	1239	CLA	C1B-CHB	-2.18	1.34	1.41
16	J	4012	BCR	C26-C25	2.18	1.38	1.34
13	A	1132	CLA	MG-NC	2.18	2.11	2.06
13	B	1211	CLA	CHD-C1D	2.18	1.42	1.38
13	A	1140	CLA	C1B-CHB	-2.18	1.34	1.41
16	L	4019	BCR	C26-C25	2.18	1.38	1.34
13	A	1133	CLA	C3B-C2B	-2.17	1.37	1.40
13	B	1224	CLA	C1B-NB	2.17	1.37	1.35
13	B	1023	CLA	CMD-C2D	2.17	1.55	1.50
13	A	1126	CLA	C1D-ND	-2.17	1.35	1.37
13	B	1234	CLA	C5-C3	2.17	1.55	1.51
13	A	1140	CLA	C5-C3	2.17	1.55	1.51
13	A	1109	CLA	CAA-C2A	2.17	1.58	1.54
13	B	1204	CLA	C5-C3	2.16	1.55	1.51
13	B	1218	CLA	C1D-ND	-2.16	1.35	1.37
13	A	1011	CLA	MG-NC	2.16	2.11	2.06
13	B	1233	CLA	C1B-CHB	-2.16	1.35	1.41
16	B	4006	BCR	C5-C6	2.16	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1227	CLA	CAA-C2A	2.16	1.58	1.54
13	A	1113	CLA	MG-NC	2.16	2.11	2.06
13	B	1208	CLA	MG-NC	2.16	2.11	2.06
13	B	1222	CLA	CAA-C2A	2.16	1.58	1.54
13	B	1239	CLA	CMD-C2D	2.16	1.55	1.50
13	B	1231	CLA	CAA-C2A	2.16	1.58	1.54
16	A	4003	BCR	C29-C28	-2.16	1.47	1.52
13	X	1701	CLA	C1B-NB	2.16	1.37	1.35
13	L	1501	CLA	C1B-CHB	-2.16	1.35	1.41
13	B	1222	CLA	C1D-ND	-2.16	1.35	1.37
13	A	1122	CLA	CHD-C1D	2.15	1.42	1.38
13	A	1117	CLA	CMD-C2D	2.15	1.55	1.50
13	A	1138	CLA	CMD-C2D	2.15	1.55	1.50
16	L	4019	BCR	C29-C28	-2.15	1.47	1.52
13	B	1230	CLA	CMD-C2D	2.15	1.55	1.50
13	A	1128	CLA	CAA-C2A	2.15	1.58	1.54
16	M	4021	BCR	C2-C3	-2.15	1.47	1.52
13	A	1110	CLA	C5-C3	2.15	1.55	1.51
16	I	4020	BCR	C26-C25	2.14	1.38	1.34
13	B	1205	CLA	C1B-NB	2.14	1.37	1.35
13	B	1207	CLA	C4B-NB	2.14	1.37	1.35
13	A	1022	CLA	C1D-ND	-2.14	1.35	1.37
13	A	1118	CLA	MG-ND	-2.14	2.01	2.05
16	A	4003	BCR	C26-C25	2.14	1.38	1.34
14	B	2002	PQN	C8-C7	2.14	1.43	1.38
13	B	1208	CLA	CHD-C1D	2.14	1.42	1.38
13	A	1136	CLA	CAA-C2A	2.14	1.58	1.54
13	A	1402	CLA	CAA-C2A	2.14	1.58	1.54
13	L	1503	CLA	C1B-CHB	-2.14	1.35	1.41
13	B	1209	CLA	C1B-NB	2.13	1.37	1.35
13	B	1201	CLA	CAA-C2A	2.13	1.58	1.54
13	A	1013	CLA	MG-NC	2.13	2.11	2.06
13	A	1104	CLA	C1B-CHB	-2.13	1.35	1.41
13	A	1104	CLA	CHD-C1D	2.13	1.42	1.38
16	A	4008	BCR	C19-C18	-2.12	1.41	1.45
14	B	2002	PQN	C15-C13	2.12	1.55	1.51
13	A	1112	CLA	CAA-C2A	2.12	1.58	1.54
13	A	1011	CLA	C1B-CHB	-2.12	1.35	1.41
13	B	1231	CLA	CMD-C2D	2.12	1.55	1.50
13	A	1127	CLA	C1D-C2D	-2.12	1.41	1.45
13	A	1117	CLA	MG-NC	2.12	2.11	2.06
16	B	4014	BCR	C29-C28	-2.11	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1235	CLA	C1D-ND	-2.11	1.35	1.37
13	B	1201	CLA	C1-C2	2.11	1.55	1.49
13	A	1402	CLA	C1B-CHB	-2.11	1.35	1.41
13	A	1104	CLA	CAA-CBA	-2.11	1.46	1.52
13	A	1123	CLA	C1B-CHB	-2.10	1.35	1.41
13	A	1115	CLA	C3B-C2B	-2.10	1.37	1.40
13	A	1402	CLA	C1D-ND	-2.10	1.35	1.37
13	B	1221	CLA	C1D-ND	-2.10	1.35	1.37
13	A	1127	CLA	C5-C3	2.10	1.55	1.51
13	A	1118	CLA	C1B-CHB	-2.10	1.35	1.41
13	B	1235	CLA	CHD-C1D	2.10	1.42	1.38
13	A	1013	CLA	CHD-C1D	2.10	1.42	1.38
13	A	1105	CLA	C1D-C2D	-2.10	1.41	1.45
13	B	1211	CLA	C3B-C2B	-2.09	1.37	1.40
13	B	1225	CLA	CHD-C1D	2.09	1.42	1.38
13	A	1112	CLA	CHD-C1D	2.09	1.42	1.38
13	A	1131	CLA	CHC-C1C	2.09	1.40	1.35
13	A	1132	CLA	C1-C2	2.09	1.55	1.49
13	A	1801	CLA	C4-C3	2.09	1.56	1.50
13	A	1237	CLA	C5-C3	2.09	1.55	1.51
13	F	1301	CLA	C1D-C2D	-2.09	1.41	1.45
14	A	2001	PQN	C7-C6	2.08	1.43	1.38
13	A	1131	CLA	CHD-C1D	2.08	1.42	1.38
13	A	1102	CLA	C1B-CHB	-2.08	1.35	1.41
13	A	1133	CLA	C1B-CHB	-2.08	1.35	1.41
13	A	1105	CLA	C1B-CHB	-2.08	1.35	1.41
13	B	1228	CLA	CHD-C1D	2.08	1.42	1.38
13	A	1126	CLA	C4-C3	2.08	1.56	1.50
13	B	1218	CLA	C1B-CHB	-2.08	1.35	1.41
13	B	1233	CLA	C3B-C2B	-2.08	1.37	1.40
13	A	1134	CLA	CMD-C2D	2.08	1.55	1.50
13	A	1114	CLA	C3B-C2B	-2.07	1.37	1.40
13	A	1131	CLA	C4B-NB	2.07	1.37	1.35
13	A	1121	CLA	C1-C2	2.07	1.55	1.49
16	J	4013	BCR	C1-C6	2.07	1.56	1.53
13	B	1203	CLA	CAA-C2A	2.07	1.57	1.54
13	M	1601	CLA	MG-NC	2.07	2.11	2.06
13	B	1023	CLA	C4-C3	2.07	1.56	1.50
16	A	4008	BCR	C29-C28	-2.07	1.47	1.52
13	A	1022	CLA	C1D-C2D	-2.07	1.41	1.45
13	B	1230	CLA	CHD-C1D	2.07	1.42	1.38
13	B	1218	CLA	CAA-C2A	2.07	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1217	CLA	CHD-C1D	2.07	1.42	1.38
13	A	1134	CLA	C1B-CHB	-2.07	1.35	1.41
13	J	1302	CLA	C1B-CHB	-2.07	1.35	1.41
13	B	1220	CLA	C3B-C2B	-2.07	1.37	1.40
13	B	1239	CLA	C3B-C2B	-2.06	1.37	1.40
13	B	1221	CLA	CMD-C2D	2.06	1.55	1.50
13	A	1115	CLA	CAA-C2A	2.06	1.57	1.54
13	A	1402	CLA	CHD-C1D	2.06	1.42	1.38
13	A	1801	CLA	CHD-C1D	2.06	1.42	1.38
13	B	1212	CLA	C1D-ND	-2.06	1.35	1.37
13	M	1601	CLA	C1B-CHB	-2.06	1.35	1.41
13	A	1117	CLA	CHD-C1D	2.06	1.42	1.38
16	B	4009	BCR	C14-C13	2.06	1.40	1.35
16	I	4018	BCR	C26-C25	2.06	1.38	1.34
13	B	1238	CLA	C1-C2	2.06	1.55	1.49
13	A	1122	CLA	C5-C3	2.06	1.55	1.51
13	A	1111	CLA	CMD-C2D	2.06	1.55	1.50
16	B	4010	BCR	C5-C6	2.06	1.38	1.34
13	B	1213	CLA	MG-NC	2.05	2.11	2.06
13	B	1217	CLA	C1B-CHB	-2.05	1.35	1.41
13	F	1301	CLA	CHD-C1D	2.05	1.42	1.38
13	B	1214	CLA	MG-NC	2.05	2.11	2.06
16	L	4019	BCR	C2-C3	-2.05	1.47	1.52
13	B	1222	CLA	C1B-CHB	-2.05	1.35	1.41
13	A	1130	CLA	CHD-C1D	2.05	1.42	1.38
13	B	1213	CLA	CMD-C2D	2.04	1.55	1.50
13	B	1215	CLA	CMD-C2D	2.04	1.55	1.50
13	B	1221	CLA	CAA-C2A	2.04	1.57	1.54
13	A	1129	CLA	CMD-C2D	2.04	1.55	1.50
16	A	4007	BCR	C14-C13	2.04	1.38	1.35
13	B	1236	CLA	C3D-C4D	-2.04	1.39	1.44
13	B	1201	CLA	MG-NC	2.04	2.11	2.06
13	J	1303	CLA	C1D-ND	-2.04	1.35	1.37
17	B	5004	LHG	O8-C23	2.04	1.43	1.33
13	A	1125	CLA	C1B-CHB	-2.04	1.35	1.41
16	A	4007	BCR	C2-C3	-2.03	1.47	1.52
17	A	5001	LHG	O7-C5	-2.03	1.41	1.46
13	B	1230	CLA	C4-C3	2.03	1.55	1.50
13	B	1218	CLA	MG-NC	2.03	2.11	2.06
13	A	1105	CLA	CMD-C2D	2.03	1.55	1.50
13	A	1117	CLA	C3B-CAB	2.03	1.52	1.47
16	I	4020	BCR	C14-C13	2.03	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1139	CLA	C1B-CHB	-2.03	1.35	1.41
13	B	1232	CLA	MG-NC	2.02	2.11	2.06
13	A	1022	CLA	C3D-C4D	-2.02	1.39	1.44
13	B	1212	CLA	CMD-C2D	2.02	1.55	1.50
13	L	1501	CLA	C1C-C2C	2.02	1.48	1.44
16	A	4008	BCR	C26-C25	2.02	1.37	1.34
13	A	1110	CLA	C4-C3	2.02	1.55	1.50
13	B	1212	CLA	C1D-C2D	-2.02	1.41	1.45
13	B	1234	CLA	C4-C3	2.02	1.55	1.50
16	F	4016	BCR	C23-C22	-2.02	1.41	1.45
13	B	1226	CLA	MG-ND	-2.02	2.01	2.05
13	B	1226	CLA	C3B-CAB	2.02	1.52	1.47
13	B	1204	CLA	CHC-C1C	2.02	1.40	1.35
13	A	1107	CLA	CHD-C1D	2.02	1.42	1.38
13	B	1212	CLA	CAA-C2A	2.02	1.57	1.54
13	B	1236	CLA	C1D-C2D	-2.01	1.41	1.45
13	A	1121	CLA	C1D-ND	-2.01	1.35	1.37
13	B	1230	CLA	C1-C2	2.01	1.55	1.49
13	B	1215	CLA	C5-C3	2.01	1.55	1.51
13	A	1113	CLA	C1B-NB	2.01	1.37	1.35
13	L	1503	CLA	CBA-CGA	-2.01	1.44	1.50
13	B	1217	CLA	MG-NC	2.01	2.11	2.06
13	A	1112	CLA	CMD-C2D	2.00	1.55	1.50
13	A	1128	CLA	CHD-C1D	2.00	1.42	1.38
13	A	1134	CLA	CHD-C1D	2.00	1.42	1.38
13	A	1115	CLA	C1-C2	2.00	1.55	1.49
13	B	1219	CLA	C1-C2	2.00	1.55	1.49
13	A	1111	CLA	C1D-ND	-2.00	1.35	1.37
13	A	1801	CLA	CMD-C2D	2.00	1.55	1.50
13	A	1133	CLA	CAA-C2A	2.00	1.57	1.54

All (1417) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1217	CLA	C4A-NA-C1A	12.31	112.24	106.71
13	A	1130	CLA	C4A-NA-C1A	12.24	112.21	106.71
13	M	1601	CLA	C4A-NA-C1A	12.18	112.18	106.71
13	A	1113	CLA	C4A-NA-C1A	12.01	112.10	106.71
13	A	1118	CLA	C4A-NA-C1A	11.91	112.06	106.71
13	B	1209	CLA	C4A-NA-C1A	11.86	112.04	106.71
13	A	1110	CLA	C4A-NA-C1A	11.86	112.04	106.71
13	B	1218	CLA	C4A-NA-C1A	11.83	112.03	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	J	1302	CLA	C4A-NA-C1A	11.76	112.00	106.71
13	A	1801	CLA	C4A-NA-C1A	11.70	111.96	106.71
13	X	1701	CLA	C4A-NA-C1A	11.70	111.96	106.71
13	B	1233	CLA	C4A-NA-C1A	11.68	111.96	106.71
13	A	1134	CLA	C4A-NA-C1A	11.64	111.94	106.71
13	B	1227	CLA	C4A-NA-C1A	11.51	111.88	106.71
13	F	1301	CLA	C4A-NA-C1A	11.45	111.85	106.71
13	A	1114	CLA	C4A-NA-C1A	11.37	111.82	106.71
13	A	1109	CLA	C4A-NA-C1A	11.37	111.82	106.71
13	J	1303	CLA	C4A-NA-C1A	11.34	111.80	106.71
13	B	1230	CLA	C4A-NA-C1A	11.32	111.79	106.71
13	B	1215	CLA	C4A-NA-C1A	11.28	111.78	106.71
13	A	1120	CLA	C4A-NA-C1A	11.27	111.77	106.71
13	B	1219	CLA	C4A-NA-C1A	11.21	111.74	106.71
13	A	1107	CLA	C4A-NA-C1A	11.18	111.73	106.71
13	A	1133	CLA	C4A-NA-C1A	11.15	111.72	106.71
13	B	1204	CLA	C4A-NA-C1A	11.14	111.72	106.71
13	A	1117	CLA	C4A-NA-C1A	11.10	111.70	106.71
13	A	1129	CLA	C4A-NA-C1A	11.10	111.70	106.71
13	A	1111	CLA	C4A-NA-C1A	11.08	111.69	106.71
13	B	1207	CLA	C4A-NA-C1A	11.07	111.68	106.71
13	B	1222	CLA	C4A-NA-C1A	11.05	111.67	106.71
13	B	1201	CLA	C4A-NA-C1A	11.03	111.67	106.71
13	A	1135	CLA	C4A-NA-C1A	10.96	111.63	106.71
13	B	1223	CLA	C4A-NA-C1A	10.95	111.63	106.71
13	A	1105	CLA	C4A-NA-C1A	10.95	111.63	106.71
13	B	1235	CLA	C4A-NA-C1A	10.95	111.63	106.71
13	A	1106	CLA	C4A-NA-C1A	10.91	111.61	106.71
13	A	1402	CLA	C4A-NA-C1A	10.91	111.61	106.71
13	A	1102	CLA	C4A-NA-C1A	10.86	111.59	106.71
13	A	1125	CLA	C4A-NA-C1A	10.85	111.58	106.71
13	A	1138	CLA	C4A-NA-C1A	10.80	111.56	106.71
13	B	1239	CLA	C4A-NA-C1A	10.78	111.55	106.71
13	B	1216	CLA	C4A-NA-C1A	10.74	111.53	106.71
13	B	1228	CLA	C4A-NA-C1A	10.71	111.52	106.71
13	A	1116	CLA	C4A-NA-C1A	10.68	111.51	106.71
13	B	1212	CLA	C4A-NA-C1A	10.67	111.50	106.71
13	B	1231	CLA	C4A-NA-C1A	10.67	111.50	106.71
13	A	1124	CLA	C4A-NA-C1A	10.65	111.50	106.71
13	B	1214	CLA	C4A-NA-C1A	10.60	111.47	106.71
13	B	1211	CLA	C4A-NA-C1A	10.59	111.47	106.71
13	B	1021	CLA	C4A-NA-C1A	10.55	111.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1101	CLA	C4A-NA-C1A	10.53	111.44	106.71
13	B	1220	CLA	C4A-NA-C1A	10.44	111.40	106.71
13	B	1229	CLA	C4A-NA-C1A	10.43	111.40	106.71
13	A	1122	CLA	C4A-NA-C1A	10.43	111.39	106.71
13	A	1112	CLA	C4A-NA-C1A	10.40	111.38	106.71
13	L	1502	CLA	C4A-NA-C1A	10.39	111.38	106.71
13	A	1119	CLA	C4A-NA-C1A	10.37	111.37	106.71
13	A	1140	CLA	C4A-NA-C1A	10.37	111.37	106.71
13	A	1139	CLA	C4A-NA-C1A	10.36	111.36	106.71
13	B	1221	CLA	C4A-NA-C1A	10.35	111.36	106.71
13	B	1232	CLA	C4A-NA-C1A	10.33	111.35	106.71
13	B	1208	CLA	C4A-NA-C1A	10.29	111.33	106.71
13	A	1127	CLA	C4A-NA-C1A	10.29	111.33	106.71
13	B	1206	CLA	C4A-NA-C1A	10.26	111.32	106.71
13	L	1501	CLA	C4A-NA-C1A	10.21	111.30	106.71
13	A	1136	CLA	C4A-NA-C1A	10.21	111.30	106.71
13	A	1108	CLA	C4A-NA-C1A	10.18	111.28	106.71
13	A	1123	CLA	C4A-NA-C1A	10.17	111.28	106.71
13	K	1401	CLA	C4A-NA-C1A	10.13	111.26	106.71
13	B	1224	CLA	C4A-NA-C1A	10.13	111.26	106.71
13	B	1213	CLA	C4A-NA-C1A	10.10	111.25	106.71
13	A	1104	CLA	C4A-NA-C1A	10.05	111.22	106.71
13	A	1121	CLA	C4A-NA-C1A	10.03	111.22	106.71
13	B	1234	CLA	C4A-NA-C1A	9.98	111.19	106.71
13	L	1503	CLA	C4A-NA-C1A	9.94	111.17	106.71
13	B	1226	CLA	C4A-NA-C1A	9.88	111.15	106.71
13	A	1131	CLA	C4A-NA-C1A	9.84	111.13	106.71
13	A	1115	CLA	C4A-NA-C1A	9.83	111.12	106.71
13	B	1238	CLA	C4A-NA-C1A	9.81	111.12	106.71
13	A	1103	CLA	C4A-NA-C1A	9.80	111.11	106.71
13	B	1023	CLA	C4A-NA-C1A	9.78	111.10	106.71
13	A	1128	CLA	C4A-NA-C1A	9.74	111.09	106.71
13	B	1236	CLA	C4A-NA-C1A	9.60	111.02	106.71
13	A	1132	CLA	C4A-NA-C1A	9.57	111.01	106.71
13	A	1013	CLA	C4A-NA-C1A	9.56	111.00	106.71
13	B	1203	CLA	C4A-NA-C1A	9.55	111.00	106.71
13	B	1012	CLA	C4A-NA-C1A	9.54	111.00	106.71
13	A	1137	CLA	C4A-NA-C1A	9.54	110.99	106.71
13	A	1126	CLA	C4A-NA-C1A	9.51	110.98	106.71
13	A	1237	CLA	C4A-NA-C1A	9.46	110.96	106.71
13	B	1210	CLA	C4A-NA-C1A	9.39	110.93	106.71
13	B	1202	CLA	C4A-NA-C1A	9.20	110.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1011	CLA	C4A-NA-C1A	9.12	110.81	106.71
13	A	1022	CLA	C4A-NA-C1A	9.06	110.78	106.71
13	B	1225	CLA	C4A-NA-C1A	8.85	110.69	106.71
13	B	1205	CLA	C4A-NA-C1A	8.77	110.65	106.71
13	A	1011	CLA	O2D-CGD-CBD	8.55	126.47	111.27
14	B	2002	PQN	C11-C12-C13	-8.20	113.14	126.79
14	A	2001	PQN	C11-C12-C13	-8.08	113.34	126.79
14	A	2001	PQN	C14-C13-C15	7.42	127.76	115.27
14	A	2001	PQN	C15-C13-C12	-7.27	106.41	121.12
14	B	2002	PQN	C14-C13-C15	6.38	126.01	115.27
17	A	5001	LHG	C25-C24-C23	6.20	136.18	113.62
14	B	2002	PQN	C15-C13-C12	-6.18	108.62	121.12
18	B	5002	LMG	C30-C29-C28	6.15	135.97	113.62
16	B	4004	BCR	C38-C26-C25	5.95	131.22	124.53
16	B	4005	BCR	C38-C26-C25	5.75	130.99	124.53
16	A	4008	BCR	C38-C26-C25	5.48	130.68	124.53
13	A	1011	CLA	O1D-CGD-CBD	-5.30	113.64	124.48
16	L	4022	BCR	C33-C5-C6	5.14	130.31	124.53
16	A	4001	BCR	C38-C26-C25	5.12	130.28	124.53
16	B	4014	BCR	C33-C5-C6	5.07	130.22	124.53
16	J	4012	BCR	C38-C26-C25	5.05	130.20	124.53
16	L	4019	BCR	C33-C5-C6	4.89	130.02	124.53
13	B	1012	CLA	O2D-CGD-CBD	4.88	119.94	111.27
13	A	1132	CLA	O2D-CGD-CBD	4.86	119.91	111.27
13	B	1226	CLA	O2D-CGD-CBD	4.86	119.90	111.27
17	A	5003	LHG	C25-C24-C23	4.84	137.56	114.15
16	J	4015	BCR	C33-C5-C6	4.77	129.88	124.53
13	B	1201	CLA	O2D-CGD-CBD	4.74	119.70	111.27
16	B	4006	BCR	C33-C5-C6	4.74	129.85	124.53
13	A	1104	CLA	CAA-C2A-C3A	-4.72	99.84	112.78
16	B	4010	BCR	C33-C5-C6	4.67	129.78	124.53
13	L	1501	CLA	O2D-CGD-CBD	4.66	119.55	111.27
16	I	4018	BCR	C33-C5-C6	4.65	129.75	124.53
13	A	1104	CLA	O2A-CGA-CBA	4.64	126.48	111.91
16	B	4004	BCR	C33-C5-C6	4.64	129.74	124.53
16	J	4015	BCR	C38-C26-C25	4.60	129.69	124.53
13	A	1102	CLA	O2D-CGD-CBD	4.57	119.38	111.27
16	A	4003	BCR	C38-C26-C25	4.56	129.65	124.53
13	B	1205	CLA	O2D-CGD-CBD	4.53	119.31	111.27
13	B	1230	CLA	O2D-CGD-CBD	4.51	119.29	111.27
16	L	4022	BCR	C38-C26-C25	4.49	129.57	124.53
13	A	1801	CLA	O2D-CGD-CBD	4.48	119.22	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1119	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
16	F	4016	BCR	C38-C26-C25	4.47	129.55	124.53
13	B	1211	CLA	O2D-CGD-CBD	4.46	119.20	111.27
16	A	4002	BCR	C38-C26-C25	4.44	129.51	124.53
16	B	4006	BCR	C7-C8-C9	4.43	132.93	126.23
13	A	1117	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
16	I	4018	BCR	C38-C26-C25	4.42	129.49	124.53
13	B	1215	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
16	B	4014	BCR	C38-C26-C25	4.40	129.46	124.53
13	B	1224	CLA	O2A-CGA-CBA	4.38	125.66	111.91
16	M	4021	BCR	C38-C26-C25	4.37	129.43	124.53
13	B	1212	CLA	O2D-CGD-CBD	4.33	118.96	111.27
16	B	4006	BCR	C29-C30-C25	4.31	117.11	110.48
16	A	4001	BCR	C33-C5-C6	4.30	129.36	124.53
16	A	4003	BCR	C33-C5-C6	4.29	129.35	124.53
16	A	4007	BCR	C38-C26-C25	4.29	129.34	124.53
16	A	4011	BCR	C7-C8-C9	4.26	132.68	126.23
13	A	1123	CLA	O2D-CGD-CBD	4.25	118.82	111.27
16	B	4006	BCR	C38-C26-C25	4.25	129.30	124.53
13	A	1113	CLA	O2D-CGD-CBD	4.24	118.81	111.27
13	A	1125	CLA	O2D-CGD-CBD	4.23	118.78	111.27
13	B	1222	CLA	O2D-CGD-CBD	4.22	118.77	111.27
16	L	4019	BCR	C38-C26-C25	4.21	129.25	124.53
13	A	1101	CLA	O2D-CGD-CBD	4.17	118.69	111.27
13	A	1106	CLA	O2D-CGD-CBD	4.15	118.64	111.27
16	B	4009	BCR	C38-C26-C25	4.14	129.18	124.53
16	B	4005	BCR	C33-C5-C6	4.12	129.16	124.53
13	A	1128	CLA	O2D-CGD-CBD	4.11	118.57	111.27
16	I	4018	BCR	C2-C1-C6	4.11	116.81	110.48
16	A	4011	BCR	C33-C5-C6	4.10	129.13	124.53
13	M	1601	CLA	O2D-CGD-CBD	4.09	118.54	111.27
13	B	1217	CLA	O2D-CGD-CBD	4.07	118.50	111.27
13	A	1129	CLA	O2D-CGD-CBD	4.06	118.48	111.27
13	B	1226	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
16	I	4020	BCR	C38-C26-C25	4.05	129.08	124.53
13	A	1135	CLA	O2A-CGA-CBA	4.05	124.62	111.91
16	J	4012	BCR	C33-C5-C6	4.05	129.08	124.53
13	B	1229	CLA	O2D-CGD-CBD	4.04	118.44	111.27
13	A	1013	CLA	O2A-CGA-CBA	4.03	124.56	111.91
13	B	1227	CLA	O2D-CGD-CBD	4.03	118.43	111.27
13	A	1127	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
16	J	4015	BCR	C8-C7-C6	4.02	138.50	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1137	CLA	O2A-CGA-CBA	4.02	124.53	111.91
16	A	4008	BCR	C38-C26-C27	-3.99	105.95	113.62
13	B	1234	CLA	O2D-CGD-CBD	3.99	118.35	111.27
16	I	4020	BCR	C24-C23-C22	3.99	132.26	126.23
13	B	1218	CLA	O2D-CGD-CBD	3.96	118.31	111.27
16	F	4016	BCR	C33-C5-C6	3.96	128.98	124.53
13	A	1121	CLA	O2D-CGD-CBD	3.96	118.30	111.27
13	B	1225	CLA	O2A-CGA-CBA	3.95	124.32	111.91
13	J	1302	CLA	O2D-CGD-CBD	3.95	118.29	111.27
16	A	4011	BCR	C38-C26-C25	3.94	128.95	124.53
16	A	4002	BCR	C33-C5-C6	3.93	128.95	124.53
16	B	4010	BCR	C38-C26-C25	3.93	128.94	124.53
13	B	1210	CLA	O2D-CGD-CBD	3.91	118.21	111.27
13	B	1202	CLA	O2D-CGD-CBD	3.90	118.20	111.27
16	B	4004	BCR	C38-C26-C27	-3.89	106.14	113.62
16	B	4005	BCR	C7-C8-C9	3.89	132.12	126.23
16	B	4017	BCR	C33-C5-C6	3.89	128.89	124.53
16	B	4017	BCR	C38-C26-C25	3.88	128.89	124.53
13	B	1223	CLA	O2D-CGD-CBD	3.87	118.14	111.27
16	A	4007	BCR	C33-C5-C6	3.86	128.86	124.53
13	K	1401	CLA	O2D-CGD-CBD	3.85	118.11	111.27
13	A	1103	CLA	O2D-CGD-CBD	3.85	118.11	111.27
13	A	1120	CLA	O2D-CGD-CBD	3.84	118.08	111.27
13	A	1140	CLA	O2A-CGA-CBA	3.83	123.93	111.91
13	A	1107	CLA	O2A-CGA-CBA	3.82	123.91	111.91
16	A	4011	BCR	C24-C23-C22	3.82	132.01	126.23
13	B	1224	CLA	CBA-CAA-C2A	3.82	125.12	113.86
13	B	1221	CLA	O2D-CGD-CBD	3.81	118.05	111.27
13	B	1205	CLA	O2A-CGA-CBA	3.81	123.86	111.91
13	A	1120	CLA	O2A-CGA-CBA	3.79	123.81	111.91
13	B	1228	CLA	O2D-CGD-CBD	3.79	118.00	111.27
16	B	4014	BCR	C7-C8-C9	3.79	131.96	126.23
13	A	1117	CLA	O2A-CGA-CBA	3.79	123.80	111.91
16	J	4015	BCR	C2-C1-C6	3.79	116.31	110.48
13	B	1215	CLA	O2A-CGA-CBA	3.78	123.78	111.91
13	A	1237	CLA	O2A-CGA-CBA	3.78	123.76	111.91
16	M	4021	BCR	C24-C23-C22	3.77	131.93	126.23
13	B	1211	CLA	C1-C2-C3	3.77	132.56	126.04
13	A	1118	CLA	O2A-CGA-CBA	3.76	123.71	111.91
13	A	1801	CLA	O2A-CGA-CBA	3.76	123.71	111.91
13	A	1111	CLA	O2D-CGD-CBD	3.76	117.94	111.27
16	A	4011	BCR	C2-C1-C6	3.75	116.26	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1801	CLA	C1-C2-C3	3.75	132.53	126.04
16	A	4011	BCR	C40-C30-C25	3.75	116.39	110.30
13	B	1231	CLA	O2D-CGD-CBD	3.74	117.91	111.27
16	J	4012	BCR	C29-C30-C25	3.74	116.24	110.48
13	B	1223	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
16	B	4004	BCR	C2-C1-C6	3.74	116.23	110.48
13	A	1139	CLA	O2A-CGA-CBA	3.72	123.57	111.91
16	A	4003	BCR	C29-C30-C25	3.69	116.17	110.48
13	A	1104	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
13	A	1121	CLA	O2A-CGA-CBA	3.67	123.42	111.91
16	B	4005	BCR	C24-C23-C22	3.66	131.77	126.23
13	A	1127	CLA	O2A-CGA-CBA	3.65	123.37	111.91
16	B	4014	BCR	C33-C5-C4	-3.65	106.61	113.62
16	M	4021	BCR	C33-C5-C6	3.65	128.62	124.53
13	B	1217	CLA	O2A-CGA-CBA	3.64	123.34	111.91
16	B	4005	BCR	C30-C25-C26	-3.64	117.49	122.61
16	J	4013	BCR	C33-C5-C6	3.64	128.61	124.53
16	B	4005	BCR	C38-C26-C27	-3.63	106.64	113.62
16	B	4010	BCR	C7-C8-C9	3.62	131.71	126.23
13	A	1127	CLA	O2D-CGD-CBD	3.61	117.68	111.27
13	B	1204	CLA	O2D-CGD-CBD	3.61	117.68	111.27
13	B	1214	CLA	O2A-CGA-CBA	3.60	123.21	111.91
16	I	4020	BCR	C33-C5-C6	3.59	128.56	124.53
16	A	4007	BCR	C24-C23-C22	3.59	131.66	126.23
13	A	1114	CLA	O2D-CGD-CBD	3.59	117.64	111.27
16	A	4003	BCR	C38-C26-C27	-3.58	106.74	113.62
13	A	1116	CLA	O2A-CGA-CBA	3.58	123.13	111.91
13	A	1137	CLA	O2D-CGD-CBD	3.57	117.62	111.27
16	J	4013	BCR	C2-C1-C6	3.57	115.98	110.48
13	A	1110	CLA	O2A-CGA-CBA	3.57	123.12	111.91
13	A	1130	CLA	O2D-CGD-CBD	3.56	117.60	111.27
16	A	4008	BCR	C33-C5-C6	3.56	128.53	124.53
16	J	4013	BCR	C29-C30-C25	3.56	115.95	110.48
13	B	1209	CLA	O2D-CGD-CBD	3.55	117.58	111.27
16	A	4001	BCR	C38-C26-C27	-3.55	106.80	113.62
16	A	4003	BCR	C24-C23-C22	3.55	131.60	126.23
13	B	1206	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
13	B	1232	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
16	J	4012	BCR	C38-C26-C27	-3.54	106.81	113.62
13	L	1503	CLA	O2D-CGD-CBD	3.54	117.55	111.27
16	J	4015	BCR	C24-C23-C22	3.52	131.56	126.23
13	X	1701	CLA	O2D-CGD-CBD	3.52	117.52	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1105	CLA	O2A-CGA-CBA	3.52	122.95	111.91
13	B	1213	CLA	O2D-CGD-CBD	3.52	117.52	111.27
16	B	4006	BCR	C38-C26-C27	-3.52	106.86	113.62
13	A	1106	CLA	O2A-CGA-CBA	3.52	122.95	111.91
13	A	1118	CLA	O2D-CGD-CBD	3.51	117.51	111.27
17	A	5003	LHG	O8-C23-C24	3.51	120.59	111.38
13	B	1201	CLA	O2A-CGA-CBA	3.51	122.92	111.91
13	B	1210	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
13	A	1130	CLA	C1-C2-C3	3.49	132.08	126.04
13	A	1124	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
13	A	1119	CLA	CMB-C2B-C3B	3.49	131.20	124.68
13	A	1131	CLA	O2D-CGD-CBD	3.48	117.46	111.27
13	B	1224	CLA	O2D-CGD-CBD	3.47	117.44	111.27
13	B	1213	CLA	O2A-CGA-CBA	3.47	122.79	111.91
13	A	1112	CLA	O2D-CGD-CBD	3.46	117.42	111.27
13	L	1502	CLA	O2D-CGD-CBD	3.46	117.42	111.27
16	B	4005	BCR	C29-C30-C25	3.46	115.81	110.48
13	A	1103	CLA	CHD-C1D-ND	-3.46	121.28	124.45
13	A	1124	CLA	O2D-CGD-CBD	3.45	117.39	111.27
16	I	4020	BCR	C33-C5-C4	-3.44	107.00	113.62
13	A	1011	CLA	C4D-CHA-C1A	-3.44	117.06	121.25
16	I	4020	BCR	C38-C26-C27	-3.44	107.01	113.62
13	B	1239	CLA	O2D-CGD-CBD	3.44	117.38	111.27
16	A	4002	BCR	C38-C26-C27	-3.43	107.02	113.62
13	B	1235	CLA	O2D-CGD-CBD	3.43	117.36	111.27
16	J	4012	BCR	C2-C1-C6	3.42	115.75	110.48
13	A	1139	CLA	O2D-CGD-CBD	3.42	117.34	111.27
16	F	4016	BCR	C15-C14-C13	3.41	132.18	127.31
13	A	1125	CLA	O2A-CGA-CBA	3.41	122.62	111.91
13	B	1222	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
13	A	1133	CLA	C1-C2-C3	3.41	131.93	126.04
16	B	4009	BCR	C20-C21-C22	3.41	132.17	127.31
13	B	1220	CLA	O2D-CGD-CBD	3.40	117.31	111.27
13	A	1135	CLA	O2D-CGD-CBD	3.40	117.31	111.27
16	L	4019	BCR	C33-C5-C4	-3.40	107.09	113.62
13	B	1215	CLA	O2D-CGD-CBD	3.39	117.29	111.27
16	A	4011	BCR	C29-C30-C25	3.38	115.69	110.48
16	A	4008	BCR	C24-C23-C22	3.38	131.34	126.23
13	A	1109	CLA	O2A-CGA-CBA	3.37	122.50	111.91
13	A	1022	CLA	O2D-CGD-CBD	3.37	117.26	111.27
16	A	4002	BCR	C2-C1-C6	3.36	115.66	110.48
16	B	4010	BCR	C33-C5-C4	-3.36	107.16	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	4006	BCR	C33-C5-C4	-3.36	107.17	113.62
16	B	4014	BCR	C2-C1-C6	3.35	115.64	110.48
16	B	4014	BCR	C29-C30-C25	3.35	115.64	110.48
13	A	1013	CLA	CHD-C1D-ND	-3.35	121.38	124.45
16	J	4015	BCR	C33-C5-C4	-3.35	107.19	113.62
16	J	4012	BCR	C23-C24-C25	3.35	136.60	127.20
13	B	1226	CLA	CMB-C2B-C3B	3.34	130.94	124.68
16	A	4001	BCR	C29-C30-C25	3.34	115.62	110.48
13	A	1113	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
13	B	1202	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
13	A	1107	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
16	B	4009	BCR	C38-C26-C27	-3.32	107.24	113.62
16	B	4017	BCR	C2-C1-C6	3.32	115.59	110.48
16	M	4021	BCR	C2-C1-C6	3.32	115.59	110.48
13	A	1102	CLA	O2A-CGA-CBA	3.32	122.31	111.91
16	I	4018	BCR	C38-C26-C27	-3.31	107.25	113.62
13	B	1234	CLA	C1-C2-C3	3.31	131.78	126.04
16	B	4006	BCR	C2-C1-C6	3.31	115.58	110.48
13	L	1501	CLA	O2A-CGA-CBA	3.31	122.30	111.91
16	J	4015	BCR	C38-C26-C27	-3.31	107.26	113.62
13	A	1135	CLA	C1-C2-C3	3.31	131.76	126.04
16	B	4004	BCR	C23-C24-C25	3.31	136.49	127.20
16	B	4010	BCR	C2-C1-C6	3.30	115.57	110.48
13	A	1110	CLA	O2D-CGD-CBD	3.30	117.13	111.27
16	J	4015	BCR	C29-C30-C25	3.30	115.56	110.48
13	B	1235	CLA	O2A-CGA-CBA	3.30	122.26	111.91
13	B	1219	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
13	A	1134	CLA	O2D-CGD-CBD	3.29	117.12	111.27
13	A	1115	CLA	O2D-CGD-CBD	3.29	117.12	111.27
13	B	1219	CLA	C1-C2-C3	3.29	131.73	126.04
13	A	1105	CLA	O2D-CGD-CBD	3.29	117.11	111.27
16	B	4014	BCR	C38-C26-C27	-3.27	107.33	113.62
13	B	1238	CLA	C1-C2-C3	3.27	131.70	126.04
16	L	4022	BCR	C2-C1-C6	3.27	115.52	110.48
16	F	4016	BCR	C2-C1-C6	3.26	115.51	110.48
13	A	1101	CLA	O2A-CGA-CBA	3.26	122.14	111.91
13	A	1114	CLA	O2A-CGA-CBA	3.26	122.14	111.91
13	B	1202	CLA	C1-C2-C3	3.26	131.67	126.04
13	A	1129	CLA	O2A-CGA-CBA	3.26	122.12	111.91
13	A	1126	CLA	O2A-CGA-CBA	3.25	122.11	111.91
13	A	1133	CLA	O2D-CGD-CBD	3.25	117.04	111.27
13	A	1103	CLA	CMB-C2B-C1B	-3.24	123.48	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	4004	BCR	C24-C23-C22	3.24	131.13	126.23
13	B	1207	CLA	O2A-CGA-CBA	3.24	122.06	111.91
16	B	4004	BCR	C33-C5-C4	-3.24	107.40	113.62
16	A	4008	BCR	C29-C30-C25	3.23	115.46	110.48
16	L	4022	BCR	C33-C5-C4	-3.23	107.41	113.62
13	B	1204	CLA	O2A-CGA-CBA	3.23	122.05	111.91
13	B	1215	CLA	CMB-C2B-C3B	3.23	130.72	124.68
17	A	5001	LHG	O8-C23-C24	3.23	122.04	111.91
13	A	1138	CLA	O2A-CGA-CBA	3.23	122.04	111.91
13	A	1011	CLA	O2A-CGA-CBA	3.22	122.02	111.91
16	B	4004	BCR	C30-C25-C26	-3.22	118.08	122.61
13	A	1126	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
16	A	4007	BCR	C38-C26-C27	-3.22	107.44	113.62
13	A	1130	CLA	O2A-CGA-CBA	3.21	121.99	111.91
16	J	4013	BCR	C38-C26-C25	3.21	128.13	124.53
13	A	1237	CLA	O2A-CGA-O1A	-3.21	115.50	123.59
16	M	4021	BCR	C29-C30-C25	3.20	115.41	110.48
16	F	4016	BCR	C33-C5-C4	-3.20	107.47	113.62
16	F	4016	BCR	C29-C30-C25	3.19	115.40	110.48
13	A	1133	CLA	O2A-CGA-CBA	3.19	121.92	111.91
13	A	1102	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
13	A	1131	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
16	L	4019	BCR	C38-C26-C27	-3.18	107.50	113.62
13	B	1238	CLA	CED-O2D-CGD	3.18	123.13	115.94
13	B	1223	CLA	O2A-CGA-CBA	3.18	121.88	111.91
16	F	4016	BCR	C38-C26-C27	-3.18	107.51	113.62
13	A	1114	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
13	A	1111	CLA	O2A-CGA-CBA	3.17	121.86	111.91
16	J	4013	BCR	C7-C8-C9	3.17	131.02	126.23
13	A	1119	CLA	CED-O2D-CGD	3.16	123.09	115.94
13	A	1103	CLA	O2A-CGA-CBA	3.16	121.84	111.91
13	A	1013	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
13	A	1136	CLA	O2A-CGA-CBA	3.16	121.82	111.91
16	A	4003	BCR	C33-C5-C4	-3.16	107.55	113.62
13	B	1233	CLA	O2D-CGD-CBD	3.15	116.87	111.27
16	A	4001	BCR	C30-C25-C26	-3.15	118.17	122.61
16	A	4011	BCR	C33-C5-C4	-3.15	107.56	113.62
16	A	4001	BCR	C33-C5-C4	-3.15	107.56	113.62
16	A	4007	BCR	C29-C30-C25	3.15	115.33	110.48
16	B	4004	BCR	C29-C30-C25	3.15	115.33	110.48
13	B	1229	CLA	O2A-CGA-CBA	3.15	121.78	111.91
13	A	1022	CLA	C1-C2-C3	3.14	131.48	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	1502	CLA	CHD-C1D-ND	-3.14	121.56	124.45
13	B	1202	CLA	O2A-CGA-CBA	3.14	121.77	111.91
13	B	1210	CLA	O2A-CGA-CBA	3.14	121.77	111.91
13	A	1107	CLA	O2D-CGD-CBD	3.14	116.85	111.27
13	A	1011	CLA	C2D-C1D-ND	3.14	112.42	110.10
13	B	1206	CLA	O2D-CGD-CBD	3.14	116.85	111.27
13	A	1136	CLA	CHD-C1D-ND	-3.14	121.57	124.45
13	A	1138	CLA	CED-O2D-CGD	3.14	123.03	115.94
13	A	1108	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
13	B	1230	CLA	C1-C2-C3	3.12	131.44	126.04
13	B	1012	CLA	O2A-CGA-CBA	3.12	121.70	111.91
13	A	1121	CLA	C1-C2-C3	3.12	131.43	126.04
16	A	4003	BCR	C2-C1-C6	3.11	115.27	110.48
16	J	4012	BCR	C30-C25-C26	-3.11	118.23	122.61
13	F	1301	CLA	O2D-CGD-CBD	3.10	116.78	111.27
13	A	1013	CLA	O2A-CGA-O1A	-3.10	115.76	123.59
16	B	4005	BCR	C33-C5-C4	-3.10	107.66	113.62
13	B	1021	CLA	C7-C6-C5	-3.10	104.94	113.36
13	B	1236	CLA	O2A-CGA-CBA	3.09	121.61	111.91
16	A	4007	BCR	C2-C1-C6	3.09	115.24	110.48
18	B	5002	LMG	O8-C28-C29	3.09	121.60	111.91
16	A	4008	BCR	C30-C25-C26	-3.08	118.27	122.61
13	B	1207	CLA	O2D-CGD-CBD	3.08	116.74	111.27
13	A	1118	CLA	C1-C2-C3	3.08	131.37	126.04
13	A	1122	CLA	O2D-CGD-CBD	3.07	116.73	111.27
13	B	1205	CLA	O1D-CGD-CBD	-3.07	118.20	124.48
13	B	1023	CLA	O2A-CGA-CBA	3.07	121.53	111.91
13	B	1227	CLA	CHD-C1D-ND	-3.06	121.64	124.45
16	B	4010	BCR	C38-C26-C27	-3.06	107.73	113.62
13	B	1216	CLA	O2D-CGD-CBD	3.06	116.71	111.27
16	M	4021	BCR	C38-C26-C27	-3.06	107.73	113.62
13	A	1013	CLA	CED-O2D-CGD	3.06	122.85	115.94
13	A	1140	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
13	A	1129	CLA	CHD-C1D-ND	-3.06	121.65	124.45
13	A	1135	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
13	A	1111	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
16	L	4019	BCR	C24-C23-C22	3.05	130.84	126.23
13	B	1226	CLA	O2A-CGA-CBA	3.04	121.45	111.91
13	J	1303	CLA	CAA-C2A-C3A	-3.04	109.01	116.10
16	B	4017	BCR	C38-C26-C27	-3.04	107.78	113.62
16	A	4001	BCR	C2-C1-C6	3.04	115.16	110.48
16	A	4002	BCR	C33-C5-C4	-3.04	107.78	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1127	CLA	CMB-C2B-C3B	3.04	130.36	124.68
13	A	1123	CLA	O2A-CGA-CBA	3.03	121.43	111.91
13	A	1011	CLA	C4D-C3D-CAD	-3.03	104.52	108.10
16	B	4005	BCR	C2-C1-C6	3.03	115.14	110.48
13	B	1224	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
13	B	1021	CLA	O2A-CGA-CBA	3.03	121.40	111.91
16	J	4015	BCR	C1-C6-C5	-3.02	118.35	122.61
13	B	1219	CLA	O2D-CGD-CBD	3.02	116.64	111.27
16	B	4017	BCR	C7-C8-C9	3.02	130.80	126.23
16	A	4011	BCR	C38-C26-C27	-3.02	107.81	113.62
16	B	4004	BCR	C7-C8-C9	3.02	130.80	126.23
13	B	1221	CLA	O2A-CGA-CBA	3.02	121.38	111.91
13	A	1114	CLA	CED-O2D-CGD	3.02	122.77	115.94
13	A	1116	CLA	O2D-CGD-CBD	3.02	116.63	111.27
13	A	1103	CLA	CAA-C2A-C3A	-3.01	104.53	112.78
13	B	1229	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
13	B	1230	CLA	CHD-C1D-ND	-3.01	121.69	124.45
13	B	1203	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
17	B	5004	LHG	O7-C7-C8	3.00	117.98	111.50
13	B	1216	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
13	M	1601	CLA	CED-O2D-CGD	3.00	122.73	115.94
13	A	1120	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
13	B	1216	CLA	O2A-CGA-CBA	3.00	121.31	111.91
13	B	1219	CLA	O2A-CGA-CBA	3.00	121.31	111.91
13	B	1218	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
13	A	1135	CLA	O2A-CGA-O1A	-2.99	116.04	123.59
16	B	4009	BCR	C29-C30-C25	2.99	115.08	110.48
13	A	1108	CLA	O2D-CGD-CBD	2.99	116.58	111.27
13	A	1115	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
13	A	1104	CLA	CED-O2D-CGD	2.98	122.69	115.94
16	B	4014	BCR	C8-C9-C10	-2.98	114.36	118.94
13	B	1231	CLA	CHD-C1D-ND	-2.98	121.72	124.45
13	B	1214	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
16	B	4009	BCR	C24-C23-C22	2.97	130.73	126.23
13	B	1235	CLA	CED-O2D-CGD	2.97	122.66	115.94
13	B	1239	CLA	O2A-CGA-CBA	2.97	121.23	111.91
16	B	4005	BCR	C1-C6-C5	-2.96	118.45	122.61
13	A	1134	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
16	B	4010	BCR	C24-C23-C22	2.95	130.70	126.23
13	B	1228	CLA	O2A-CGA-CBA	2.95	121.18	111.91
13	A	1128	CLA	CMB-C2B-C1B	-2.95	123.92	128.46
16	J	4013	BCR	C33-C5-C4	-2.95	107.94	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1104	CLA	C2A-C3A-C4A	2.95	106.64	101.87
16	B	4004	BCR	C1-C6-C5	-2.95	118.46	122.61
13	A	1122	CLA	O2A-CGA-CBA	2.95	121.17	111.91
17	A	5001	LHG	O7-C7-C8	2.95	117.86	111.50
13	B	1236	CLA	O2D-CGD-CBD	2.95	116.51	111.27
13	B	1201	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
13	A	1101	CLA	CMB-C2B-C1B	-2.95	123.94	128.46
13	A	1119	CLA	C1-C2-C3	2.95	131.14	126.04
16	A	4011	BCR	C16-C17-C18	2.95	131.51	127.31
16	L	4019	BCR	C2-C1-C6	2.95	115.02	110.48
13	B	1206	CLA	O2A-CGA-CBA	2.94	121.15	111.91
13	B	1230	CLA	O2A-CGA-CBA	2.94	121.14	111.91
13	A	1104	CLA	CMB-C2B-C3B	2.94	130.18	124.68
13	A	1133	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
13	M	1601	CLA	O2A-CGA-CBA	2.94	123.48	114.03
13	B	1212	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
13	A	1135	CLA	C4-C3-C5	-2.94	112.62	115.98
13	B	1023	CLA	CED-O2D-CGD	2.94	122.58	115.94
16	B	4006	BCR	C24-C23-C22	2.94	130.67	126.23
13	A	1120	CLA	CHD-C1D-ND	-2.94	121.75	124.45
13	X	1701	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
13	B	1208	CLA	CED-O2D-CGD	2.93	122.57	115.94
13	B	1205	CLA	CAA-C2A-C3A	-2.93	104.75	112.78
13	A	1115	CLA	O2A-CGA-CBA	2.92	121.09	111.91
13	A	1121	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
16	L	4019	BCR	C30-C25-C24	2.92	124.05	115.78
13	B	1220	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
13	L	1502	CLA	O2A-CGA-CBA	2.92	121.08	111.91
16	A	4003	BCR	C40-C30-C25	2.92	115.04	110.30
16	B	4005	BCR	C23-C24-C25	2.92	135.40	127.20
13	A	1801	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
16	A	4007	BCR	C30-C25-C26	-2.92	118.50	122.61
13	B	1213	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
16	I	4018	BCR	C7-C8-C9	2.92	130.64	126.23
13	B	1226	CLA	C1-C2-C3	2.92	131.09	126.04
16	A	4007	BCR	C33-C5-C4	-2.91	108.02	113.62
13	A	1124	CLA	CMB-C2B-C3B	2.91	130.13	124.68
13	A	1117	CLA	CMB-C2B-C3B	2.91	130.12	124.68
13	A	1140	CLA	O2D-CGD-CBD	2.91	116.44	111.27
13	L	1503	CLA	O2A-CGA-CBA	2.91	121.04	111.91
13	A	1110	CLA	C1-C2-C3	2.91	131.07	126.04
16	B	4017	BCR	C29-C30-C25	2.91	114.95	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	4017	BCR	C33-C5-C4	-2.91	108.03	113.62
13	B	1221	CLA	CED-O2D-CGD	2.91	122.51	115.94
13	A	1137	CLA	O2A-CGA-O1A	-2.90	116.26	123.59
16	A	4002	BCR	C29-C30-C25	2.90	114.95	110.48
13	B	1203	CLA	O2D-CGD-CBD	2.90	116.43	111.27
13	B	1209	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
13	J	1302	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
13	B	1012	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
13	B	1217	CLA	CED-O2D-CGD	2.89	122.48	115.94
13	B	1208	CLA	O2D-CGD-CBD	2.89	116.41	111.27
16	B	4014	BCR	C12-C13-C14	-2.89	114.50	118.94
13	A	1134	CLA	CHD-C1D-ND	-2.89	121.80	124.45
16	J	4012	BCR	C8-C7-C6	2.89	135.31	127.20
13	L	1503	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
16	J	4012	BCR	C33-C5-C4	-2.89	108.07	113.62
13	B	1214	CLA	O2D-CGD-CBD	2.88	116.38	111.27
13	B	1225	CLA	CMB-C2B-C1B	-2.88	124.05	128.46
13	B	1211	CLA	O2A-CGA-CBA	2.87	120.93	111.91
17	A	5003	LHG	O7-C7-C8	2.87	117.69	111.50
13	B	1230	CLA	CED-O2D-CGD	2.87	122.44	115.94
13	B	1210	CLA	C1-C2-C3	2.87	131.01	126.04
13	A	1117	CLA	O2D-CGD-CBD	2.87	116.37	111.27
16	A	4001	BCR	C23-C24-C25	2.87	135.26	127.20
13	B	1217	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
16	M	4021	BCR	C1-C6-C7	2.87	123.89	115.78
16	M	4021	BCR	C1-C6-C5	-2.86	118.58	122.61
13	B	1231	CLA	CED-O2D-CGD	2.86	122.41	115.94
16	A	4003	BCR	C7-C8-C9	2.86	130.56	126.23
13	B	1222	CLA	CMB-C2B-C3B	2.86	130.03	124.68
13	A	1104	CLA	C1-C2-C3	2.86	130.99	126.04
16	F	4016	BCR	C24-C23-C22	2.86	130.56	126.23
13	B	1223	CLA	CMB-C2B-C3B	2.86	130.03	124.68
16	J	4012	BCR	C36-C18-C19	2.86	122.58	118.08
13	B	1225	CLA	C4-C3-C5	-2.86	110.47	115.27
13	A	1116	CLA	CMB-C2B-C1B	-2.86	124.08	128.46
13	A	1124	CLA	O2A-CGA-CBA	2.85	120.87	111.91
16	B	4006	BCR	C1-C6-C5	-2.85	118.59	122.61
13	B	1207	CLA	C4D-CHA-C1A	2.85	124.72	121.25
16	J	4013	BCR	C30-C25-C24	2.85	123.85	115.78
13	B	1219	CLA	CED-O2D-CGD	2.85	122.38	115.94
13	B	1213	CLA	C1-C2-C3	2.85	130.97	126.04
16	B	4006	BCR	C30-C25-C26	-2.85	118.60	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1104	CLA	CBA-CAA-C2A	2.85	122.26	113.86
16	M	4021	BCR	C33-C5-C4	-2.84	108.15	113.62
16	A	4008	BCR	C2-C1-C6	2.84	114.86	110.48
13	B	1236	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
13	B	1218	CLA	CED-O2D-CGD	2.83	122.35	115.94
13	B	1210	CLA	CMB-C2B-C3B	2.83	129.98	124.68
13	A	1131	CLA	O2A-CGA-CBA	2.83	120.80	111.91
13	J	1302	CLA	CED-O2D-CGD	2.83	122.34	115.94
17	A	5003	LHG	C6-C5-C4	-2.83	105.09	111.79
13	A	1022	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
16	I	4018	BCR	C33-C5-C4	-2.83	108.18	113.62
13	B	1229	CLA	CHD-C1D-ND	-2.83	121.86	124.45
16	A	4001	BCR	C24-C23-C22	2.83	130.51	126.23
13	B	1209	CLA	O2A-CGA-CBA	2.83	123.11	114.03
13	A	1117	CLA	CED-O2D-CGD	2.83	122.33	115.94
13	B	1239	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
13	B	1205	CLA	O2A-CGA-O1A	-2.82	116.48	123.59
13	A	1126	CLA	O2D-CGD-CBD	2.82	116.27	111.27
13	B	1225	CLA	C5-C3-C2	2.81	126.81	121.12
13	A	1138	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
16	L	4022	BCR	C38-C26-C27	-2.81	108.21	113.62
13	A	1109	CLA	C2D-C1D-ND	2.81	112.17	110.10
13	A	1112	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
13	B	1021	CLA	CED-O2D-CGD	2.80	122.28	115.94
13	B	1232	CLA	CED-O2D-CGD	2.80	122.28	115.94
16	A	4007	BCR	C30-C25-C24	2.80	123.70	115.78
13	K	1401	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
13	B	1211	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
16	B	4014	BCR	C15-C14-C13	2.80	131.30	127.31
13	A	1122	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
13	B	1225	CLA	O2D-CGD-CBD	2.80	116.24	111.27
13	A	1130	CLA	CED-O2D-CGD	2.79	122.25	115.94
16	J	4013	BCR	C38-C26-C27	-2.79	108.25	113.62
16	A	4001	BCR	C1-C6-C5	-2.79	118.69	122.61
13	A	1109	CLA	CHD-C1D-ND	-2.79	121.89	124.45
16	A	4002	BCR	C30-C25-C26	-2.79	118.69	122.61
13	A	1103	CLA	CED-O2D-CGD	2.78	122.23	115.94
13	B	1205	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
13	B	1212	CLA	C2D-C1D-ND	2.78	112.16	110.10
13	A	1237	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
16	I	4020	BCR	C7-C8-C9	2.78	130.44	126.23
16	B	4009	BCR	C40-C30-C25	2.78	114.81	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1228	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
13	A	1140	CLA	CED-O2D-CGD	2.78	122.21	115.94
13	A	1109	CLA	CED-O2D-CGD	2.77	122.21	115.94
16	I	4020	BCR	C32-C1-C6	2.77	114.80	110.30
18	B	5002	LMG	C7-O1-C1	2.77	119.15	113.74
13	L	1503	CLA	CHD-C1D-ND	-2.77	121.91	124.45
16	L	4022	BCR	C8-C7-C6	2.77	134.97	127.20
16	B	4005	BCR	C1-C6-C7	2.77	123.60	115.78
13	A	1119	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
16	A	4011	BCR	C32-C1-C6	2.76	114.78	110.30
16	B	4009	BCR	C35-C13-C12	2.76	120.71	114.60
13	A	1116	CLA	CED-O2D-CGD	2.76	122.19	115.94
13	A	1112	CLA	CED-O2D-CGD	2.76	122.18	115.94
13	B	1202	CLA	CHD-C1D-ND	-2.76	121.92	124.45
16	A	4003	BCR	C1-C6-C5	-2.75	118.74	122.61
13	A	1108	CLA	O2A-CGA-CBA	2.75	122.87	114.03
13	A	1125	CLA	C1-C2-C3	2.75	130.80	126.04
16	L	4022	BCR	C29-C30-C25	2.75	114.72	110.48
13	A	1132	CLA	O2A-CGA-CBA	2.75	120.54	111.91
16	I	4020	BCR	C30-C25-C26	-2.75	118.74	122.61
13	B	1230	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
13	M	1601	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
13	B	1208	CLA	CHD-C1D-ND	-2.75	121.93	124.45
13	B	1221	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
16	J	4015	BCR	C30-C25-C26	-2.75	118.75	122.61
16	I	4018	BCR	C36-C18-C19	2.74	122.40	118.08
13	A	1124	CLA	CHD-C1D-ND	-2.74	121.94	124.45
16	B	4005	BCR	C20-C21-C22	2.74	131.22	127.31
13	A	1237	CLA	O2D-CGD-CBD	2.74	116.13	111.27
13	B	1209	CLA	CHD-C1D-ND	-2.74	121.94	124.45
16	A	4008	BCR	C23-C24-C25	2.73	134.87	127.20
13	A	1130	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
13	B	1203	CLA	O2A-CGA-CBA	2.73	120.47	111.91
13	A	1133	CLA	CED-O2D-CGD	2.73	122.10	115.94
16	L	4019	BCR	C30-C25-C26	-2.73	118.78	122.61
13	B	1210	CLA	O1D-CGD-CBD	-2.72	118.91	124.48
16	A	4001	BCR	C8-C7-C6	2.72	134.85	127.20
16	B	4010	BCR	C29-C30-C25	2.72	114.67	110.48
13	A	1115	CLA	CHD-C1D-ND	-2.72	121.95	124.45
13	A	1108	CLA	CED-O2D-CGD	2.72	122.08	115.94
13	B	1233	CLA	O2A-CGA-CBA	2.72	122.75	114.03
13	B	1214	CLA	CED-O2D-CGD	2.72	122.08	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	L	4019	BCR	C8-C7-C6	2.72	134.83	127.20
13	B	1225	CLA	CHD-C1D-ND	-2.71	121.96	124.45
13	A	1113	CLA	CHD-C1D-ND	-2.71	121.96	124.45
13	B	1207	CLA	C2A-C1A-CHA	2.71	128.60	123.86
16	I	4018	BCR	C23-C24-C25	2.70	134.79	127.20
13	A	1113	CLA	CMB-C2B-C3B	2.70	129.73	124.68
13	A	1011	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
13	B	1203	CLA	C1-C2-C3	2.70	130.72	126.04
13	A	1104	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
16	A	4011	BCR	C30-C25-C24	2.70	123.42	115.78
13	B	1201	CLA	CHD-C1D-ND	-2.70	121.98	124.45
13	F	1301	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
13	B	1225	CLA	O2A-C1-C2	2.70	115.72	108.64
13	A	1131	CLA	CMB-C2B-C3B	2.69	129.72	124.68
13	B	1234	CLA	O2A-CGA-CBA	2.69	120.36	111.91
13	B	1202	CLA	C2D-C1D-ND	2.69	112.09	110.10
13	B	1208	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
13	A	1131	CLA	CHD-C1D-ND	-2.69	121.98	124.45
16	L	4019	BCR	C40-C30-C25	2.69	114.66	110.30
13	A	1126	CLA	CHD-C1D-ND	-2.69	121.98	124.45
13	B	1228	CLA	CHD-C1D-ND	-2.68	121.99	124.45
13	J	1303	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
13	X	1701	CLA	O2A-CGA-CBA	2.68	122.64	114.03
13	A	1115	CLA	CED-O2D-CGD	2.68	122.00	115.94
13	B	1206	CLA	CED-O2D-CGD	2.68	122.00	115.94
13	A	1108	CLA	CHD-C1D-ND	-2.68	121.99	124.45
13	A	1109	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
13	B	1216	CLA	CED-O2D-CGD	2.67	121.99	115.94
13	A	1110	CLA	CMB-C2B-C1B	-2.67	124.35	128.46
13	B	1023	CLA	CHD-C1D-ND	-2.67	122.00	124.45
13	A	1112	CLA	O2A-CGA-CBA	2.67	122.62	114.03
13	F	1301	CLA	O2A-CGA-CBA	2.67	122.62	114.03
16	B	4014	BCR	C32-C1-C6	2.67	114.63	110.30
13	A	1402	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
13	B	1222	CLA	CHD-C1D-ND	-2.67	122.00	124.45
16	B	4010	BCR	C36-C18-C19	2.67	122.28	118.08
16	F	4016	BCR	C1-C6-C5	-2.67	118.85	122.61
16	A	4003	BCR	C30-C25-C26	-2.67	118.86	122.61
13	A	1106	CLA	CHD-C1D-ND	-2.67	122.00	124.45
13	B	1021	CLA	C1-C2-C3	2.67	130.66	126.04
13	A	1125	CLA	CMB-C2B-C1B	-2.67	124.37	128.46
16	B	4010	BCR	C30-C25-C26	-2.67	118.86	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1801	CLA	CED-O2D-CGD	2.67	121.97	115.94
13	A	1134	CLA	CED-O2D-CGD	2.66	121.96	115.94
13	A	1105	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
13	B	1221	CLA	C1-C2-C3	2.66	130.65	126.04
13	A	1124	CLA	C2D-C1D-ND	2.66	112.07	110.10
13	A	1801	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
16	I	4020	BCR	C37-C22-C23	2.66	122.27	118.08
13	B	1230	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
13	A	1237	CLA	CHD-C1D-ND	-2.66	122.01	124.45
13	A	1109	CLA	O2D-CGD-CBD	2.65	115.98	111.27
13	B	1225	CLA	CED-O2D-CGD	2.65	121.94	115.94
13	A	1128	CLA	O2A-CGA-CBA	2.65	120.23	111.91
13	A	1107	CLA	C2A-C1A-CHA	2.65	128.50	123.86
16	L	4022	BCR	C30-C25-C26	-2.65	118.88	122.61
13	B	1238	CLA	O2D-CGD-CBD	2.65	115.98	111.27
13	A	1013	CLA	CMB-C2B-C3B	2.65	129.63	124.68
13	A	1102	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
16	B	4014	BCR	C30-C25-C26	-2.65	118.88	122.61
16	I	4018	BCR	C29-C30-C25	2.65	114.56	110.48
13	A	1128	CLA	C2D-C1D-ND	2.65	112.05	110.10
13	A	1237	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
13	B	1204	CLA	CHD-C1D-ND	-2.64	122.03	124.45
16	J	4012	BCR	C1-C6-C7	2.64	123.24	115.78
13	A	1140	CLA	O2A-C1-C2	2.64	115.56	108.64
16	F	4016	BCR	C30-C25-C26	-2.63	118.90	122.61
13	B	1210	CLA	CED-O2D-CGD	2.63	121.89	115.94
13	B	1213	CLA	CHD-C1D-ND	-2.63	122.03	124.45
13	B	1220	CLA	CHD-C1D-ND	-2.63	122.04	124.45
13	A	1106	CLA	C2D-C1D-ND	2.63	112.04	110.10
13	A	1103	CLA	CMB-C2B-C3B	2.63	129.59	124.68
16	J	4013	BCR	C23-C24-C25	2.63	134.57	127.20
13	A	1123	CLA	O1D-CGD-CBD	-2.62	119.11	124.48
13	A	1111	CLA	O1D-CGD-CBD	-2.62	119.11	124.48
16	A	4008	BCR	C11-C10-C9	2.62	131.05	127.31
13	A	1136	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
13	A	1129	CLA	CED-O2D-CGD	2.62	121.86	115.94
13	B	1238	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
13	B	1208	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
13	B	1219	CLA	CHD-C1D-ND	-2.62	122.05	124.45
13	B	1211	CLA	O1D-CGD-CBD	-2.62	119.13	124.48
13	B	1227	CLA	O1D-CGD-CBD	-2.61	119.13	124.48
13	A	1112	CLA	CHD-C1D-ND	-2.61	122.05	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1202	CLA	CMB-C2B-C3B	2.61	129.57	124.68
13	B	1235	CLA	C1-C2-C3	2.61	130.56	126.04
13	A	1113	CLA	O2A-CGA-CBA	2.61	122.42	114.03
13	A	1124	CLA	C1-C2-C3	2.61	130.56	126.04
13	B	1207	CLA	CED-O2D-CGD	2.61	121.84	115.94
16	B	4017	BCR	C8-C9-C10	-2.61	114.94	118.94
16	J	4012	BCR	C1-C6-C5	-2.61	118.94	122.61
16	B	4010	BCR	C30-C25-C24	2.61	123.15	115.78
13	L	1501	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
16	B	4014	BCR	C34-C9-C8	2.60	122.18	118.08
13	B	1211	CLA	CHD-C1D-ND	-2.60	122.06	124.45
13	A	1105	CLA	CED-O2D-CGD	2.60	121.82	115.94
13	B	1235	CLA	CHD-C1D-ND	-2.60	122.06	124.45
13	B	1203	CLA	CMB-C2B-C3B	2.60	129.54	124.68
13	A	1111	CLA	CHD-C1D-ND	-2.60	122.07	124.45
13	K	1401	CLA	CHD-C1D-ND	-2.60	122.07	124.45
13	B	1023	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
16	J	4013	BCR	C30-C25-C26	-2.60	118.96	122.61
13	A	1139	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
13	B	1220	CLA	O2A-CGA-CBA	2.59	122.36	114.03
16	L	4019	BCR	C29-C30-C25	2.59	114.47	110.48
13	B	1209	CLA	CED-O2D-CGD	2.59	121.80	115.94
13	A	1132	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
13	B	1223	CLA	C1-C2-C3	2.59	130.52	126.04
13	A	1111	CLA	CED-O2D-CGD	2.59	121.79	115.94
13	B	1233	CLA	CMB-C2B-C1B	-2.58	124.49	128.46
13	A	1106	CLA	O1D-CGD-CBD	-2.58	119.19	124.48
13	A	1126	CLA	CMB-C2B-C3B	2.58	129.51	124.68
13	B	1238	CLA	O2A-CGA-CBA	2.58	120.02	111.91
13	A	1117	CLA	CHD-C1D-ND	-2.58	122.08	124.45
13	A	1022	CLA	C4D-CHA-C1A	2.58	124.39	121.25
16	A	4011	BCR	C30-C25-C26	-2.58	118.98	122.61
13	A	1129	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
13	A	1118	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
16	B	4010	BCR	C16-C17-C18	2.57	130.98	127.31
13	B	1228	CLA	CED-O2D-CGD	2.57	121.76	115.94
13	B	1219	CLA	CMB-C2B-C3B	2.57	129.49	124.68
13	B	1218	CLA	O2A-CGA-CBA	2.57	122.30	114.03
13	B	1216	CLA	C1-C2-C3	2.57	130.49	126.04
13	J	1302	CLA	O2A-CGA-CBA	2.57	122.29	114.03
13	A	1119	CLA	O2D-CGD-CBD	2.57	115.84	111.27
13	B	1224	CLA	C1-C2-C3	2.57	130.49	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1123	CLA	CMB-C2B-C1B	-2.57	124.51	128.46
16	A	4008	BCR	C33-C5-C4	-2.57	108.68	113.62
13	B	1212	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
16	L	4022	BCR	C1-C6-C5	-2.57	119.00	122.61
13	A	1132	CLA	CHD-C1D-ND	-2.57	122.09	124.45
13	B	1216	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
13	A	1135	CLA	C2D-C1D-ND	2.57	112.00	110.10
13	A	1115	CLA	C2D-C1D-ND	2.56	111.99	110.10
13	A	1011	CLA	OBD-CAD-C3D	2.56	134.69	128.52
16	M	4021	BCR	C30-C25-C26	-2.56	119.00	122.61
13	L	1502	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
13	B	1012	CLA	C4D-CHA-C1A	2.56	124.37	121.25
13	A	1119	CLA	CAA-CBA-CGA	2.56	120.74	113.25
13	A	1120	CLA	CED-O2D-CGD	2.56	121.73	115.94
13	A	1129	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
13	A	1137	CLA	CMB-C2B-C1B	-2.56	124.54	128.46
13	B	1215	CLA	CHD-C1D-ND	-2.55	122.11	124.45
13	A	1126	CLA	C2D-C1D-ND	2.55	111.98	110.10
16	J	4013	BCR	C1-C6-C5	-2.55	119.02	122.61
16	A	4011	BCR	C15-C14-C13	2.55	130.95	127.31
16	B	4006	BCR	C35-C13-C12	2.55	122.09	118.08
13	A	1133	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
13	A	1101	CLA	CHD-C1D-ND	-2.55	122.11	124.45
16	A	4002	BCR	C1-C6-C5	-2.54	119.03	122.61
13	A	1011	CLA	C1-C2-C3	2.54	130.44	126.04
13	A	1127	CLA	C2D-C1D-ND	2.54	111.98	110.10
13	B	1227	CLA	O2A-CGA-CBA	2.54	122.19	114.03
13	A	1113	CLA	CED-O2D-CGD	2.54	121.67	115.94
16	M	4021	BCR	C8-C7-C6	2.54	134.33	127.20
13	B	1216	CLA	CHD-C1D-ND	-2.54	122.12	124.45
13	L	1502	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
13	A	1128	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
13	B	1215	CLA	CED-O2D-CGD	2.53	121.66	115.94
16	I	4018	BCR	C1-C6-C5	-2.53	119.05	122.61
13	B	1218	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
13	A	1111	CLA	C1-C2-C3	2.53	130.41	126.04
13	A	1402	CLA	O2A-CGA-CBA	2.53	122.15	114.03
16	J	4013	BCR	C36-C18-C19	2.52	122.05	118.08
13	B	1208	CLA	O2A-CGA-CBA	2.52	122.14	114.03
13	A	1105	CLA	C1-C2-C3	2.52	130.41	126.04
13	B	1212	CLA	O2A-CGA-CBA	2.52	122.13	114.03
13	L	1501	CLA	CHD-C1D-ND	-2.52	122.14	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1118	CLA	CHD-C1D-ND	-2.52	122.14	124.45
13	B	1226	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
16	B	4006	BCR	C23-C24-C25	2.52	134.27	127.20
13	A	1237	CLA	C2D-C1D-ND	2.52	111.96	110.10
13	A	1137	CLA	CED-O2D-CGD	2.51	121.62	115.94
16	B	4014	BCR	C23-C24-C25	2.51	134.26	127.20
13	A	1128	CLA	CHD-C1D-ND	-2.51	122.15	124.45
13	A	1132	CLA	CED-O2D-CGD	2.51	121.60	115.94
13	B	1229	CLA	C1-C2-C3	2.50	130.38	126.04
13	B	1235	CLA	CMB-C2B-C1B	-2.50	124.61	128.46
13	A	1134	CLA	O2A-CGA-CBA	2.50	122.08	114.03
13	A	1138	CLA	CHD-C1D-ND	-2.50	122.15	124.45
13	B	1012	CLA	C2A-C1A-CHA	2.50	128.24	123.86
13	A	1138	CLA	O2D-CGD-CBD	2.50	115.72	111.27
16	B	4010	BCR	C32-C1-C6	2.50	114.36	110.30
13	A	1111	CLA	C4D-CHA-C1A	2.50	124.29	121.25
13	A	1125	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
13	A	1013	CLA	C1-O2A-CGA	2.50	123.00	116.44
16	B	4014	BCR	C35-C13-C12	2.50	122.01	118.08
16	B	4017	BCR	C34-C9-C8	2.50	122.01	118.08
13	B	1234	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
16	B	4005	BCR	C32-C1-C6	2.50	114.35	110.30
13	A	1117	CLA	C4D-CHA-C1A	2.49	124.28	121.25
13	B	1213	CLA	CED-O2D-CGD	2.49	121.58	115.94
13	J	1303	CLA	CHD-C1D-ND	-2.49	122.16	124.45
13	B	1227	CLA	CMB-C2B-C1B	-2.49	124.63	128.46
13	A	1139	CLA	C1-C2-C3	2.49	130.36	126.04
16	A	4011	BCR	C1-C6-C7	2.49	122.83	115.78
13	B	1238	CLA	C4D-CHA-C1A	2.49	124.28	121.25
13	A	1140	CLA	C1-C2-C3	2.49	130.35	126.04
13	B	1202	CLA	CED-O2D-CGD	2.49	121.57	115.94
13	L	1501	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
13	A	1129	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
13	B	1222	CLA	C2A-C3A-C4A	2.49	105.89	101.87
13	B	1211	CLA	CED-O2D-CGD	2.49	121.56	115.94
13	A	1130	CLA	CMB-C2B-C3B	2.49	129.33	124.68
13	B	1207	CLA	C2D-C1D-ND	2.48	111.93	110.10
13	B	1236	CLA	CED-O2D-CGD	2.48	121.54	115.94
13	B	1210	CLA	CHD-C1D-ND	-2.48	122.18	124.45
13	A	1117	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
13	K	1401	CLA	CED-O2D-CGD	2.48	121.54	115.94
13	B	1207	CLA	C1-C2-C3	2.48	130.32	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	I	4020	BCR	C36-C18-C19	2.48	121.98	118.08
13	B	1227	CLA	C3C-C4C-NC	-2.47	107.80	110.57
16	A	4011	BCR	C23-C22-C21	-2.47	115.15	118.94
13	A	1022	CLA	O2A-CGA-CBA	2.47	119.66	111.91
13	B	1214	CLA	C1-C2-C3	2.47	130.31	126.04
13	A	1104	CLA	C2A-C1A-CHA	2.47	128.18	123.86
13	A	1140	CLA	C1-O2A-CGA	2.47	122.92	116.44
16	A	4008	BCR	C1-C6-C7	2.47	122.76	115.78
13	B	1221	CLA	CHD-C1D-ND	-2.47	122.19	124.45
13	A	1126	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
13	B	1203	CLA	CHD-C1D-ND	-2.47	122.19	124.45
13	J	1303	CLA	C2A-C3A-C4A	2.46	104.93	101.78
13	B	1213	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
13	A	1135	CLA	CMB-C2B-C3B	2.46	129.29	124.68
13	B	1236	CLA	CHD-C1D-ND	-2.46	122.19	124.45
13	B	1232	CLA	O2D-CGD-CBD	2.46	115.64	111.27
13	B	1212	CLA	CHD-C1D-ND	-2.46	122.19	124.45
13	B	1214	CLA	CHD-C1D-ND	-2.46	122.19	124.45
16	A	4003	BCR	C1-C6-C7	2.46	122.73	115.78
13	A	1801	CLA	CHD-C1D-ND	-2.45	122.20	124.45
13	A	1123	CLA	CED-O2D-CGD	2.45	121.49	115.94
13	B	1012	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
13	A	1126	CLA	CED-O2D-CGD	2.45	121.49	115.94
13	A	1106	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
16	A	4002	BCR	C7-C8-C9	2.45	129.94	126.23
13	A	1119	CLA	O2A-CGA-CBA	2.45	119.61	111.91
13	F	1301	CLA	CED-O2D-CGD	2.45	121.48	115.94
13	A	1119	CLA	C12-C11-C10	-2.45	101.97	113.24
13	A	1106	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
13	A	1801	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
16	J	4012	BCR	C35-C13-C12	2.45	121.94	118.08
13	B	1226	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
13	A	1126	CLA	CAA-C2A-C3A	-2.44	106.08	112.78
16	A	4002	BCR	C30-C25-C24	2.44	122.69	115.78
16	I	4020	BCR	C30-C25-C24	2.44	122.69	115.78
13	A	1013	CLA	C2D-C1D-ND	2.44	111.90	110.10
13	A	1133	CLA	CHD-C1D-ND	-2.44	122.21	124.45
16	A	4003	BCR	C30-C25-C24	2.44	122.68	115.78
13	B	1231	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
13	A	1132	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
13	A	1113	CLA	O1D-CGD-CBD	-2.44	119.50	124.48
13	B	1201	CLA	CMD-C2D-C1D	2.44	129.01	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	4009	BCR	C30-C25-C26	-2.44	119.18	122.61
13	A	1122	CLA	CHD-C1D-ND	-2.44	122.22	124.45
16	A	4008	BCR	C37-C22-C23	2.43	121.91	118.08
16	A	4002	BCR	C24-C23-C22	2.43	129.91	126.23
13	B	1204	CLA	CED-O2D-CGD	2.43	121.44	115.94
13	B	1232	CLA	O2A-CGA-O1A	-2.43	117.24	123.30
13	A	1013	CLA	C1-C2-C3	2.43	130.24	126.04
13	A	1114	CLA	CHD-C1D-ND	-2.43	122.22	124.45
13	A	1402	CLA	CHD-C1D-ND	-2.43	122.22	124.45
13	B	1204	CLA	C3C-C4C-NC	-2.43	107.85	110.57
13	A	1118	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
13	B	1211	CLA	CMD-C2D-C1D	2.42	128.98	124.71
13	B	1201	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
16	L	4019	BCR	C36-C18-C19	2.42	121.89	118.08
13	B	1233	CLA	CED-O2D-CGD	2.42	121.40	115.94
13	A	1140	CLA	C2D-C1D-ND	2.41	111.88	110.10
13	B	1215	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
13	A	1127	CLA	CED-O2D-CGD	2.41	121.39	115.94
13	A	1137	CLA	CHD-C1D-ND	-2.41	122.24	124.45
16	A	4007	BCR	C32-C1-C6	2.41	114.20	110.30
13	A	1135	CLA	CHD-C1D-ND	-2.41	122.24	124.45
13	A	1128	CLA	CED-O2D-CGD	2.41	121.38	115.94
13	A	1111	CLA	CMB-C2B-C3B	2.41	129.18	124.68
16	A	4011	BCR	C1-C6-C5	-2.41	119.22	122.61
13	A	1237	CLA	CED-O2D-CGD	2.40	121.38	115.94
13	B	1205	CLA	C7-C6-C5	-2.40	106.83	113.36
13	B	1232	CLA	O2A-CGA-CBA	2.40	121.75	114.03
16	I	4018	BCR	C30-C25-C26	-2.40	119.23	122.61
16	B	4010	BCR	C1-C6-C5	-2.40	119.23	122.61
13	A	1103	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
13	B	1203	CLA	CED-O2D-CGD	2.40	121.36	115.94
13	B	1222	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
16	B	4014	BCR	C36-C18-C19	2.39	121.85	118.08
13	A	1109	CLA	C1-C2-C3	2.39	130.18	126.04
13	A	1137	CLA	CMD-C2D-C1D	2.39	128.93	124.71
13	B	1206	CLA	C12-C11-C10	-2.39	102.26	113.24
13	B	1210	CLA	C2D-C1D-ND	2.39	111.86	110.10
13	A	1135	CLA	C4D-CHA-C1A	2.39	124.15	121.25
13	B	1233	CLA	CHD-C1D-ND	-2.38	122.26	124.45
13	B	1223	CLA	C2D-C1D-ND	2.38	111.86	110.10
13	K	1401	CLA	O2A-CGA-CBA	2.38	121.67	114.03
13	B	1217	CLA	O1D-CGD-CBD	-2.38	119.62	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1139	CLA	C2D-C1D-ND	2.38	111.86	110.10
13	B	1227	CLA	CED-O2D-CGD	2.38	121.31	115.94
16	I	4020	BCR	C29-C30-C25	2.38	114.14	110.48
13	A	1103	CLA	C1-C2-C3	2.37	130.15	126.04
13	A	1103	CLA	C2A-C3A-C4A	2.37	105.70	101.87
13	B	1231	CLA	C2A-C3A-C4A	2.37	105.69	101.87
13	L	1502	CLA	C4D-CHA-C1A	2.37	124.13	121.25
13	A	1102	CLA	CMB-C2B-C3B	2.37	129.10	124.68
13	B	1221	CLA	C2A-C1A-CHA	2.37	128.00	123.86
13	A	1125	CLA	CHD-C1D-ND	-2.36	122.28	124.45
13	B	1239	CLA	C2D-C1D-ND	2.36	111.85	110.10
16	F	4016	BCR	C7-C8-C9	2.36	129.81	126.23
13	L	1502	CLA	C3C-C4C-NC	-2.36	107.92	110.57
13	B	1239	CLA	CHD-C1D-ND	-2.36	122.28	124.45
16	A	4008	BCR	C8-C9-C10	-2.36	115.32	118.94
13	A	1110	CLA	CHD-C1D-ND	-2.36	122.28	124.45
16	J	4012	BCR	C24-C23-C22	2.36	129.80	126.23
13	A	1136	CLA	C3C-C4C-NC	-2.36	107.92	110.57
16	B	4006	BCR	C28-C27-C26	2.36	118.29	114.08
16	A	4008	BCR	C34-C9-C8	2.36	121.79	118.08
16	I	4020	BCR	C1-C6-C5	-2.36	119.29	122.61
13	A	1103	CLA	CMD-C2D-C1D	2.36	128.87	124.71
13	B	1218	CLA	C4D-CHA-C1A	2.36	124.12	121.25
13	A	1136	CLA	O2D-CGD-CBD	2.36	115.46	111.27
13	A	1129	CLA	C2D-C1D-ND	2.36	111.84	110.10
13	B	1201	CLA	C2D-C1D-ND	2.36	111.84	110.10
13	X	1701	CLA	CHD-C1D-ND	-2.35	122.29	124.45
13	B	1239	CLA	CMB-C2B-C3B	2.35	129.08	124.68
13	A	1136	CLA	CED-O2D-CGD	2.35	121.26	115.94
13	A	1011	CLA	C2A-C3A-C4A	2.35	105.67	101.87
13	B	1218	CLA	CHD-C1D-ND	-2.35	122.29	124.45
13	B	1227	CLA	CMD-C2D-C1D	2.35	128.85	124.71
13	L	1501	CLA	C4D-CHA-C1A	2.35	124.10	121.25
13	B	1021	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
13	B	1229	CLA	C12-C11-C10	-2.34	102.47	113.24
13	A	1121	CLA	CHD-C1D-ND	-2.34	122.30	124.45
13	B	1231	CLA	O2A-CGA-CBA	2.34	121.55	114.03
13	B	1208	CLA	O2A-CGA-O1A	-2.34	117.46	123.30
16	A	4007	BCR	C1-C6-C7	2.34	122.40	115.78
13	A	1107	CLA	CHD-C1D-ND	-2.34	122.30	124.45
13	A	1117	CLA	C4-C3-C5	-2.34	111.34	115.27
13	B	1234	CLA	CED-O2D-CGD	2.34	121.22	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1801	CLA	C2A-C1A-CHA	2.33	127.94	123.86
13	B	1204	CLA	CMB-C2B-C1B	-2.33	124.88	128.46
13	A	1112	CLA	O2A-CGA-O1A	-2.33	117.49	123.30
13	A	1119	CLA	CHD-C1D-ND	-2.33	122.31	124.45
13	B	1224	CLA	C2D-C1D-ND	2.33	111.82	110.10
13	A	1402	CLA	O2A-CGA-O1A	-2.33	117.49	123.30
16	A	4001	BCR	C1-C6-C7	2.33	122.37	115.78
16	A	4007	BCR	C1-C6-C5	-2.33	119.34	122.61
13	B	1225	CLA	CBA-CAA-C2A	2.33	120.73	113.86
13	A	1011	CLA	CHD-C1D-ND	-2.33	122.32	124.45
13	B	1234	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
13	A	1132	CLA	C2D-C1D-ND	2.32	111.82	110.10
16	A	4007	BCR	C40-C30-C25	2.32	114.06	110.30
16	A	4002	BCR	C23-C24-C25	2.32	133.72	127.20
13	B	1222	CLA	CED-O2D-CGD	2.32	121.19	115.94
13	A	1110	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
13	B	1201	CLA	C1-C2-C3	2.32	130.06	126.04
13	A	1129	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
16	J	4015	BCR	C30-C25-C24	2.32	122.34	115.78
13	A	1123	CLA	CHD-C1D-ND	-2.32	122.33	124.45
13	B	1232	CLA	CHD-C1D-ND	-2.31	122.33	124.45
13	F	1301	CLA	C2A-C1A-CHA	2.31	127.90	123.86
13	M	1601	CLA	O2A-CGA-O1A	-2.31	117.53	123.30
13	A	1130	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
13	J	1302	CLA	C2A-C1A-CHA	2.31	127.89	123.86
13	A	1118	CLA	CED-O2D-CGD	2.31	121.15	115.94
13	B	1219	CLA	C3C-C4C-NC	-2.30	107.99	110.57
13	A	1101	CLA	C1-C2-C3	2.30	130.03	126.04
16	A	4007	BCR	C23-C24-C25	2.30	133.67	127.20
13	A	1130	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
13	B	1205	CLA	CHD-C1D-ND	-2.30	122.34	124.45
13	A	1134	CLA	O2A-CGA-O1A	-2.30	117.57	123.30
13	B	1231	CLA	C3C-C4C-NC	-2.30	107.99	110.57
13	B	1238	CLA	C3C-C4C-NC	-2.30	108.00	110.57
13	A	1122	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
13	A	1132	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
13	B	1230	CLA	CMD-C2D-C1D	2.29	128.75	124.71
16	B	4017	BCR	C30-C25-C26	-2.29	119.39	122.61
13	B	1217	CLA	C2A-C1A-CHA	2.29	127.86	123.86
16	L	4019	BCR	C1-C6-C5	-2.29	119.39	122.61
16	B	4017	BCR	C24-C23-C22	2.29	129.69	126.23
13	B	1234	CLA	C4D-CHA-C1A	2.29	124.03	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1128	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
16	A	4002	BCR	C1-C6-C7	2.28	122.23	115.78
16	B	4005	BCR	C35-C13-C12	2.28	121.67	118.08
13	A	1011	CLA	CHA-C4D-ND	2.28	137.27	132.50
13	A	1013	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
13	B	1224	CLA	CHD-C1D-ND	-2.28	122.36	124.45
13	A	1103	CLA	C3C-C4C-NC	-2.28	108.02	110.57
13	B	1023	CLA	C12-C11-C10	-2.27	102.81	113.24
13	B	1234	CLA	CHD-C1D-ND	-2.27	122.37	124.45
16	B	4004	BCR	C8-C7-C6	2.27	133.57	127.20
16	I	4020	BCR	C3-C4-C5	2.27	118.13	114.08
13	B	1218	CLA	C2A-C1A-CHA	2.27	127.83	123.86
13	A	1139	CLA	CED-O2D-CGD	2.27	121.07	115.94
16	J	4013	BCR	C40-C30-C25	2.27	113.98	110.30
13	B	1226	CLA	CED-O2D-CGD	2.27	121.06	115.94
13	A	1125	CLA	C4D-CHA-C1A	2.26	124.00	121.25
13	X	1701	CLA	CED-O2D-CGD	2.26	121.06	115.94
13	A	1117	CLA	C1-C2-C3	2.26	129.96	126.04
13	A	1121	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
13	A	1125	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
13	B	1207	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
13	A	1120	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
16	B	4005	BCR	C34-C9-C8	2.26	121.64	118.08
16	A	4008	BCR	C23-C22-C21	-2.26	115.47	118.94
13	A	1129	CLA	C1-C2-C3	2.26	130.40	126.75
13	B	1230	CLA	C4D-CHA-C1A	2.26	124.00	121.25
13	A	1118	CLA	C4D-CHA-C1A	2.25	123.99	121.25
13	A	1116	CLA	C1-C2-C3	2.25	129.94	126.04
16	B	4017	BCR	C23-C24-C25	2.25	133.53	127.20
13	A	1105	CLA	C2D-C1D-ND	2.25	111.77	110.10
13	A	1011	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
13	A	1013	CLA	O2A-C1-C2	-2.25	102.71	108.64
13	L	1503	CLA	C2D-C1D-ND	2.25	111.76	110.10
13	A	1102	CLA	CED-O2D-CGD	2.25	121.03	115.94
13	B	1224	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
16	B	4005	BCR	C36-C18-C19	2.25	121.62	118.08
13	B	1232	CLA	C2A-C1A-CHA	2.25	127.79	123.86
13	A	1122	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
13	A	1104	CLA	CAA-CBA-CGA	2.25	119.81	113.25
13	L	1502	CLA	O2A-CGA-O1A	-2.25	117.93	123.59
13	B	1226	CLA	C2D-C1D-ND	2.24	111.76	110.10
13	B	1211	CLA	CAA-C2A-C3A	-2.24	106.63	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	4008	BCR	C1-C6-C5	-2.24	119.45	122.61
13	A	1139	CLA	CHD-C1D-ND	-2.24	122.39	124.45
13	B	1217	CLA	CHD-C1D-ND	-2.24	122.39	124.45
13	A	1105	CLA	C4-C3-C5	-2.24	113.42	115.98
16	I	4020	BCR	C1-C6-C7	2.24	122.12	115.78
13	A	1103	CLA	C2D-C1D-ND	2.24	111.75	110.10
13	A	1117	CLA	C3C-C4C-NC	-2.24	108.06	110.57
16	I	4018	BCR	C34-C9-C8	2.24	121.60	118.08
13	B	1221	CLA	O1D-CGD-CBD	-2.23	119.91	124.48
13	B	1021	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
13	A	1120	CLA	C3C-C4C-NC	-2.23	108.07	110.57
13	A	1801	CLA	C2D-C1D-ND	2.23	111.75	110.10
13	A	1129	CLA	C2C-C1C-NC	-2.23	107.88	109.97
13	A	1118	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
13	B	1236	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
16	A	4001	BCR	C37-C22-C23	2.23	121.59	118.08
16	A	4001	BCR	C35-C13-C12	2.23	121.59	118.08
13	A	1107	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
16	B	4017	BCR	C23-C22-C21	-2.23	115.52	118.94
13	B	1227	CLA	C4D-CHA-C1A	2.23	123.96	121.25
13	A	1013	CLA	O2D-CGD-CBD	2.23	115.23	111.27
16	I	4018	BCR	C19-C18-C17	-2.23	115.52	118.94
13	A	1138	CLA	C4D-CHA-C1A	2.23	123.96	121.25
16	L	4022	BCR	C30-C25-C24	2.22	122.07	115.78
16	B	4006	BCR	C34-C9-C8	2.22	121.58	118.08
13	A	1140	CLA	CMB-C2B-C3B	2.22	128.84	124.68
13	B	1021	CLA	C2D-C1D-ND	2.22	111.74	110.10
13	A	1123	CLA	C4D-CHA-C1A	2.22	123.95	121.25
16	J	4013	BCR	C24-C23-C22	2.22	129.59	126.23
13	B	1222	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
13	A	1110	CLA	CED-O2D-CGD	2.22	120.96	115.94
16	B	4006	BCR	C36-C18-C19	2.22	121.58	118.08
14	B	2002	PQN	C17-C16-C15	-2.22	107.33	113.36
13	B	1234	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
16	A	4011	BCR	C34-C9-C8	2.22	121.57	118.08
16	B	4009	BCR	C36-C18-C19	2.22	121.57	118.08
13	A	1120	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
16	I	4020	BCR	C19-C18-C17	-2.22	115.54	118.94
13	A	1110	CLA	C3C-C4C-NC	-2.22	108.08	110.57
13	A	1122	CLA	C4D-CHA-C1A	2.22	123.95	121.25
16	F	4016	BCR	C30-C25-C24	2.21	122.04	115.78
13	A	1112	CLA	O1D-CGD-CBD	-2.21	119.95	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1221	CLA	C4D-CHA-C1A	2.21	123.94	121.25
13	A	1110	CLA	C4D-CHA-C1A	2.21	123.94	121.25
13	B	1222	CLA	O2A-CGA-CBA	2.21	120.97	112.23
13	B	1217	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
13	B	1214	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
13	J	1303	CLA	CMA-C3A-C2A	-2.21	110.94	116.10
16	J	4012	BCR	C37-C22-C23	2.21	121.56	118.08
16	B	4014	BCR	C1-C6-C5	-2.21	119.50	122.61
13	A	1113	CLA	C4D-CHA-C1A	2.21	123.94	121.25
13	A	1237	CLA	CMA-C3A-C2A	-2.21	104.92	113.83
16	B	4017	BCR	C1-C6-C5	-2.21	119.51	122.61
16	B	4004	BCR	C1-C6-C7	2.21	122.02	115.78
13	B	1235	CLA	C3C-C4C-NC	-2.20	108.10	110.57
16	B	4009	BCR	C30-C25-C24	2.20	122.01	115.78
13	A	1114	CLA	CMB-C2B-C3B	2.20	128.80	124.68
13	B	1238	CLA	CHD-C1D-ND	-2.20	122.43	124.45
13	A	1126	CLA	CMD-C2D-C1D	2.20	128.59	124.71
13	A	1116	CLA	CBA-CAA-C2A	2.20	120.36	113.86
16	A	4003	BCR	C8-C7-C6	2.20	133.38	127.20
13	B	1023	CLA	C2D-C1D-ND	2.20	111.72	110.10
13	F	1301	CLA	O2A-CGA-O1A	-2.20	117.82	123.30
13	A	1110	CLA	C2D-C1D-ND	2.20	111.72	110.10
16	J	4013	BCR	C35-C13-C12	2.19	121.53	118.08
16	J	4013	BCR	C34-C9-C8	2.19	121.53	118.08
13	A	1104	CLA	C3C-C4C-NC	-2.19	108.11	110.57
16	B	4006	BCR	C30-C25-C24	2.19	121.98	115.78
13	A	1139	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
13	B	1205	CLA	CMB-C2B-C3B	2.19	128.78	124.68
13	B	1223	CLA	CED-O2D-CGD	2.19	120.89	115.94
13	L	1501	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
13	B	1205	CLA	CED-O2D-CGD	2.19	120.89	115.94
13	A	1133	CLA	C3C-C4C-NC	-2.19	108.12	110.57
16	J	4013	BCR	C1-C6-C7	2.18	121.95	115.78
13	B	1239	CLA	CED-O2D-CGD	2.18	120.87	115.94
13	A	1118	CLA	C2A-C1A-CHA	2.18	127.67	123.86
13	B	1206	CLA	C1-C2-C3	2.18	129.81	126.04
13	B	1207	CLA	CAA-C2A-C1A	2.18	119.11	111.97
13	B	1239	CLA	CBA-CAA-C2A	2.18	120.29	113.86
16	A	4001	BCR	C32-C1-C6	2.18	113.83	110.30
16	L	4019	BCR	C23-C24-C25	2.17	133.31	127.20
13	B	1233	CLA	C2A-C1A-CHA	2.17	127.66	123.86
16	I	4018	BCR	C1-C6-C7	2.17	121.92	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	4008	BCR	C7-C8-C9	2.17	129.52	126.23
13	B	1232	CLA	CMB-C2B-C3B	2.17	128.74	124.68
13	A	1123	CLA	C1-C2-C3	2.17	129.80	126.04
13	B	1235	CLA	C4D-CHA-C1A	2.17	123.89	121.25
13	A	1107	CLA	CMB-C2B-C3B	2.17	128.74	124.68
13	A	1022	CLA	CED-O2D-CGD	2.17	120.84	115.94
16	L	4019	BCR	C37-C22-C23	2.17	121.49	118.08
13	A	1133	CLA	CMB-C2B-C3B	2.17	128.73	124.68
13	A	1106	CLA	CED-O2D-CGD	2.16	120.83	115.94
16	B	4014	BCR	C24-C23-C22	2.16	129.50	126.23
13	X	1701	CLA	O2A-CGA-O1A	-2.16	117.91	123.30
13	A	1102	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
13	A	1109	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
13	A	1113	CLA	C2D-C1D-ND	2.16	111.70	110.10
13	B	1207	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
13	B	1223	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
13	A	1108	CLA	CMB-C2B-C3B	2.16	128.72	124.68
13	B	1233	CLA	O2A-CGA-O1A	-2.16	117.92	123.30
13	B	1224	CLA	CAA-CBA-CGA	2.16	119.55	113.25
16	A	4011	BCR	C37-C22-C23	2.16	121.47	118.08
16	A	4003	BCR	C35-C13-C12	2.15	121.47	118.08
13	B	1204	CLA	C1-C2-C3	2.15	129.77	126.04
13	B	1209	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
13	M	1601	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	B	1228	CLA	C2D-C1D-ND	2.15	111.69	110.10
13	A	1133	CLA	C4D-CHA-C1A	2.15	123.87	121.25
13	A	1108	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
13	A	1131	CLA	CED-O2D-CGD	2.15	120.80	115.94
13	B	1238	CLA	CMB-C2B-C3B	2.15	128.70	124.68
13	B	1202	CLA	C2A-C3A-C4A	2.15	105.34	101.87
13	A	1136	CLA	CMD-C2D-C1D	2.15	128.50	124.71
13	J	1303	CLA	C3C-C4C-NC	-2.15	108.16	110.57
13	B	1213	CLA	CMB-C2B-C3B	2.15	128.70	124.68
13	A	1140	CLA	CHD-C1D-ND	-2.15	122.48	124.45
16	B	4010	BCR	C1-C6-C7	2.15	121.86	115.78
13	A	1131	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
16	M	4021	BCR	C35-C13-C12	2.15	121.46	118.08
13	B	1229	CLA	C2D-C1D-ND	2.15	111.69	110.10
13	B	1220	CLA	C4D-CHA-C1A	2.14	123.86	121.25
13	A	1130	CLA	C2A-C3A-C4A	2.14	105.33	101.87
13	B	1238	CLA	CMD-C2D-C1D	2.14	128.49	124.71
13	M	1601	CLA	C2A-C1A-CHA	2.14	127.60	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	4002	BCR	C40-C30-C25	2.14	113.77	110.30
16	B	4006	BCR	C1-C6-C7	2.14	121.83	115.78
13	B	1012	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
13	B	1234	CLA	C2D-C1D-ND	2.14	111.68	110.10
13	A	1131	CLA	CMD-C2D-C1D	2.14	128.48	124.71
13	B	1224	CLA	CED-O2D-CGD	2.14	120.77	115.94
13	A	1135	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
13	B	1227	CLA	O2A-CGA-O1A	-2.14	117.98	123.30
13	A	1116	CLA	CHD-C1D-ND	-2.13	122.49	124.45
13	B	1236	CLA	CMB-C2B-C3B	2.13	128.67	124.68
13	A	1135	CLA	C2A-C1A-CHA	2.13	127.59	123.86
13	B	1214	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
13	A	1105	CLA	CHD-C1D-ND	-2.13	122.50	124.45
13	L	1501	CLA	C12-C11-C10	-2.13	103.46	113.24
13	X	1701	CLA	CMB-C2B-C3B	2.13	128.66	124.68
13	A	1116	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
13	A	1134	CLA	C2A-C1A-CHA	2.13	127.58	123.86
13	A	1121	CLA	C4-C3-C5	-2.13	113.55	115.98
13	A	1122	CLA	CED-O2D-CGD	2.13	120.75	115.94
13	B	1209	CLA	C3C-C4C-NC	-2.12	108.19	110.57
13	A	1102	CLA	C12-C11-C10	-2.12	106.11	113.62
13	A	1117	CLA	CBA-CAA-C2A	2.12	120.13	113.86
16	B	4010	BCR	C34-C9-C8	2.12	121.42	118.08
13	A	1801	CLA	CMB-C2B-C3B	2.12	128.64	124.68
13	A	1122	CLA	C1-C2-C3	2.12	129.71	126.04
13	B	1209	CLA	C4D-CHA-C1A	2.12	123.83	121.25
16	A	4008	BCR	C8-C7-C6	2.12	133.15	127.20
13	A	1121	CLA	CMB-C2B-C3B	2.12	128.64	124.68
13	L	1503	CLA	CMB-C2B-C3B	2.12	128.64	124.68
13	A	1111	CLA	C2A-C1A-CHA	2.12	127.56	123.86
13	A	1140	CLA	C12-C11-C10	-2.12	103.52	113.24
13	A	1112	CLA	C2A-C1A-CHA	2.11	127.56	123.86
13	A	1120	CLA	C2A-C3A-C4A	2.11	105.28	101.87
13	A	1112	CLA	C4D-CHA-C1A	2.11	123.82	121.25
13	B	1236	CLA	C2D-C1D-ND	2.11	111.66	110.10
13	J	1302	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
13	A	1138	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
13	B	1206	CLA	C2D-C1D-ND	2.11	111.66	110.10
13	B	1210	CLA	C2A-C1A-CHA	2.11	127.55	123.86
13	B	1201	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
16	J	4013	BCR	C19-C18-C17	-2.11	115.70	118.94
16	B	4017	BCR	C15-C14-C13	2.11	130.32	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1137	CLA	C4D-CHA-C1A	2.11	123.82	121.25
13	A	1107	CLA	C2D-C1D-ND	2.11	111.66	110.10
13	A	1107	CLA	CMD-C2D-C1D	2.11	128.43	124.71
13	A	1140	CLA	CMD-C2D-C1D	2.11	128.43	124.71
13	A	1131	CLA	C3C-C4C-NC	-2.11	108.21	110.57
13	B	1214	CLA	CMB-C2B-C3B	2.11	128.62	124.68
13	A	1107	CLA	C1-C2-C3	2.11	129.69	126.04
13	B	1223	CLA	C4D-CHA-C1A	2.11	123.81	121.25
16	F	4016	BCR	C1-C6-C7	2.11	121.74	115.78
13	B	1203	CLA	CMD-C2D-C1D	2.11	128.42	124.71
13	B	1218	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
16	B	4004	BCR	C34-C9-C8	2.10	121.39	118.08
16	B	4010	BCR	C19-C18-C17	-2.10	115.71	118.94
13	B	1207	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
13	A	1113	CLA	C3C-C4C-NC	-2.10	108.22	110.57
13	B	1230	CLA	CBA-CAA-C2A	2.10	120.06	113.86
13	A	1131	CLA	C2D-C1D-ND	2.10	111.65	110.10
13	A	1124	CLA	CED-O2D-CGD	2.10	120.69	115.94
13	A	1122	CLA	CMD-C2D-C1D	2.10	128.41	124.71
13	B	1222	CLA	CMD-C2D-C1D	2.10	128.41	124.71
13	A	1402	CLA	C2A-C3A-C4A	2.10	105.26	101.87
13	A	1105	CLA	C4D-CHA-C1A	2.10	123.80	121.25
16	B	4006	BCR	C40-C30-C25	2.10	113.70	110.30
13	B	1231	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
13	A	1102	CLA	C2A-C1A-CHA	2.10	127.53	123.86
13	A	1113	CLA	O2A-CGA-O1A	-2.10	118.08	123.30
13	A	1123	CLA	C2A-C1A-CHA	2.10	127.52	123.86
13	A	1134	CLA	C2D-C1D-ND	2.10	111.65	110.10
16	B	4017	BCR	C11-C10-C9	2.09	130.30	127.31
13	B	1217	CLA	C3C-C4C-NC	-2.09	108.22	110.57
13	B	1212	CLA	CMB-C2B-C3B	2.09	128.59	124.68
13	B	1231	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
13	A	1102	CLA	C1-C2-C3	2.09	129.66	126.04
13	A	1119	CLA	C3C-C4C-NC	-2.09	108.22	110.57
13	B	1235	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
13	A	1022	CLA	C6-C5-C3	-2.09	107.97	113.45
13	B	1222	CLA	C3C-C4C-NC	-2.09	108.23	110.57
13	J	1302	CLA	CHD-C1D-ND	-2.09	122.53	124.45
16	F	4016	BCR	C36-C18-C19	2.09	121.36	118.08
16	B	4004	BCR	C37-C22-C23	2.09	121.36	118.08
13	B	1201	CLA	CMB-C2B-C3B	2.09	128.58	124.68
13	A	1120	CLA	CMB-C2B-C3B	2.08	128.58	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	J	1303	CLA	OBD-CAD-CBD	-2.08	121.71	125.97
13	B	1238	CLA	C12-C11-C10	-2.08	103.67	113.24
13	K	1401	CLA	C2D-C1D-ND	2.08	111.64	110.10
13	B	1224	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
16	M	4021	BCR	C37-C22-C23	2.08	121.36	118.08
13	A	1120	CLA	C2A-C1A-CHA	2.08	127.50	123.86
13	A	1013	CLA	C2A-C3A-C4A	2.08	105.23	101.87
13	A	1140	CLA	CBA-CAA-C2A	2.08	120.01	113.86
13	A	1107	CLA	CBA-CAA-C2A	2.08	120.00	113.86
13	A	1132	CLA	CMD-C2D-C1D	2.08	128.38	124.71
13	A	1107	CLA	C4D-CHA-C1A	2.08	123.78	121.25
13	L	1502	CLA	C2D-C1D-ND	2.08	111.64	110.10
13	L	1501	CLA	CMD-C2D-C1D	2.08	128.37	124.71
13	A	1011	CLA	CGD-CBD-CAD	2.08	117.46	110.73
16	J	4013	BCR	C15-C14-C13	2.08	130.27	127.31
13	A	1121	CLA	CMD-C2D-C1D	2.08	128.37	124.71
13	B	1206	CLA	CMB-C2B-C3B	2.07	128.56	124.68
13	B	1201	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
16	L	4022	BCR	C23-C24-C25	2.07	133.03	127.20
16	A	4002	BCR	C35-C13-C12	2.07	121.34	118.08
13	A	1131	CLA	C4D-CHA-C1A	2.07	123.77	121.25
16	F	4016	BCR	C8-C7-C6	2.07	133.02	127.20
16	B	4014	BCR	C40-C30-C25	2.07	113.66	110.30
13	A	1131	CLA	C2A-C3A-C4A	2.07	105.21	101.87
16	L	4022	BCR	C32-C1-C6	2.07	113.65	110.30
13	A	1123	CLA	C7-C6-C5	-2.07	107.74	113.36
13	B	1225	CLA	C2D-C1D-ND	2.07	111.63	110.10
13	A	1109	CLA	CMB-C2B-C3B	2.07	128.55	124.68
13	B	1232	CLA	C4D-CHA-C1A	2.07	123.77	121.25
16	I	4020	BCR	C35-C13-C12	2.07	121.33	118.08
13	B	1218	CLA	C3C-C4C-NC	-2.07	108.25	110.57
16	M	4021	BCR	C30-C25-C24	2.07	121.62	115.78
13	A	1137	CLA	C3C-C4C-NC	-2.06	108.26	110.57
16	B	4004	BCR	C20-C21-C22	2.06	130.25	127.31
13	B	1203	CLA	C3C-C4C-NC	-2.06	108.26	110.57
16	A	4002	BCR	C15-C14-C13	2.06	130.25	127.31
13	B	1212	CLA	C2A-C1A-CHA	2.06	127.46	123.86
13	B	1021	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	B	1233	CLA	C2D-C1D-ND	2.06	111.62	110.10
16	J	4015	BCR	C16-C17-C18	2.06	130.25	127.31
16	I	4018	BCR	C32-C1-C6	2.06	113.64	110.30
16	B	4006	BCR	C20-C21-C22	2.06	130.24	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1217	CLA	CMB-C2B-C3B	2.06	128.52	124.68
13	X	1701	CLA	C2A-C1A-CHA	2.05	127.45	123.86
13	A	1101	CLA	CMD-C2D-C1D	2.05	128.33	124.71
13	A	1117	CLA	C2A-C1A-CHA	2.05	127.45	123.86
13	B	1206	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
16	J	4015	BCR	C37-C22-C23	2.05	121.31	118.08
13	A	1138	CLA	C3C-C4C-NC	-2.05	108.27	110.57
13	B	1207	CLA	C3A-C2A-C1A	2.05	104.41	101.34
13	A	1125	CLA	CMD-C2D-C1D	2.05	128.33	124.71
13	B	1208	CLA	CMD-C2D-C1D	2.05	128.33	124.71
13	A	1132	CLA	C1-C2-C3	2.05	129.59	126.04
16	A	4001	BCR	C30-C25-C24	2.05	121.58	115.78
13	B	1226	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	J	1302	CLA	CMB-C2B-C3B	2.05	128.51	124.68
13	B	1232	CLA	C2D-C1D-ND	2.05	111.61	110.10
16	B	4005	BCR	C15-C14-C13	2.05	130.23	127.31
13	A	1114	CLA	C2A-C1A-CHA	2.05	127.44	123.86
13	A	1104	CLA	O2D-CGD-CBD	2.05	114.91	111.27
16	J	4012	BCR	C19-C18-C17	-2.05	115.80	118.94
13	A	1125	CLA	C2A-C3A-C4A	2.05	105.17	101.87
13	A	1108	CLA	C2D-C1D-ND	2.04	111.61	110.10
13	B	1216	CLA	C4D-CHA-C1A	2.04	123.73	121.25
13	A	1134	CLA	CMB-C2B-C3B	2.04	128.49	124.68
13	A	1113	CLA	C2A-C1A-CHA	2.04	127.42	123.86
16	B	4010	BCR	C23-C24-C25	2.04	132.93	127.20
13	B	1012	CLA	C1-C2-C3	2.04	129.57	126.04
13	B	1214	CLA	C2A-C1A-CHA	2.04	127.42	123.86
13	A	1111	CLA	CMD-C2D-C1D	2.04	128.30	124.71
13	J	1302	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
13	B	1235	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
13	A	1402	CLA	CMB-C2B-C3B	2.04	128.49	124.68
13	B	1216	CLA	CMB-C2B-C3B	2.04	128.49	124.68
13	A	1123	CLA	CMD-C2D-C1D	2.03	128.30	124.71
16	B	4017	BCR	C30-C25-C24	2.03	121.53	115.78
13	A	1139	CLA	C2A-C1A-CHA	2.03	127.41	123.86
13	B	1230	CLA	C2D-C1D-ND	2.03	111.60	110.10
13	A	1101	CLA	C2A-C1A-CHA	2.03	127.41	123.86
13	A	1801	CLA	C2C-C1C-NC	-2.03	108.07	109.97
13	B	1207	CLA	CMD-C2D-C1D	2.03	128.29	124.71
13	B	1220	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
13	A	1102	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	X	1701	CLA	C3C-C4C-NC	-2.03	108.29	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	1012	CLA	CHA-C1A-NA	-2.03	121.75	126.40
13	B	1239	CLA	C4D-CHA-C1A	2.03	123.72	121.25
13	A	1011	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
13	B	1235	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
13	B	1223	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
13	B	1215	CLA	C2D-C1D-ND	2.03	111.60	110.10
13	A	1131	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
13	A	1129	CLA	C3C-C4C-NC	-2.03	108.30	110.57
13	A	1113	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
13	A	1115	CLA	CMB-C2B-C3B	2.03	128.47	124.68
13	A	1103	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
16	A	4002	BCR	C32-C1-C6	2.02	113.58	110.30
13	A	1011	CLA	CMB-C2B-C3B	2.02	128.47	124.68
13	A	1116	CLA	C2A-C1A-CHA	2.02	127.40	123.86
13	B	1012	CLA	CMB-C2B-C3B	2.02	128.46	124.68
17	A	5003	LHG	P-O6-C4	-2.02	109.82	121.68
13	A	1121	CLA	CED-O2D-CGD	2.02	120.51	115.94
13	A	1111	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
16	J	4015	BCR	C40-C30-C25	2.02	113.58	110.30
16	M	4021	BCR	C32-C1-C6	2.02	113.58	110.30
16	B	4014	BCR	C11-C10-C9	2.02	130.19	127.31
16	B	4005	BCR	C8-C7-C6	2.02	132.88	127.20
13	B	1214	CLA	C2A-C3A-C4A	2.02	105.13	101.87
13	B	1224	CLA	C12-C11-C10	-2.02	103.96	113.24
13	A	1101	CLA	CMB-C2B-C3B	2.02	128.46	124.68
13	A	1122	CLA	CMB-C2B-C3B	2.02	128.46	124.68
16	F	4016	BCR	C40-C30-C25	2.02	113.58	110.30
13	B	1218	CLA	CMB-C2B-C3B	2.02	128.46	124.68
13	X	1701	CLA	C2A-C3A-C4A	2.02	105.13	101.87
13	L	1503	CLA	CED-O2D-CGD	2.02	120.50	115.94
13	B	1236	CLA	CMD-C2D-C1D	2.02	128.27	124.71
13	B	1231	CLA	CMA-C3A-C2A	-2.02	105.69	113.83
13	B	1225	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	B	1209	CLA	CMB-C2B-C3B	2.02	128.45	124.68
13	A	1122	CLA	C3C-C4C-NC	-2.02	108.31	110.57
13	B	1231	CLA	CMA-C3A-C4A	-2.01	106.36	111.77
13	A	1129	CLA	CMD-C2D-C1D	2.01	128.26	124.71
13	A	1138	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
13	B	1215	CLA	C1-C2-C3	2.01	129.53	126.04
13	B	1220	CLA	CMB-C2B-C3B	2.01	128.44	124.68
13	A	1114	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
16	F	4016	BCR	C35-C13-C14	-2.01	120.10	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	1116	CLA	CMB-C2B-C3B	2.01	128.44	124.68
13	B	1214	CLA	C3C-C4C-NC	-2.01	108.32	110.57
13	A	1108	CLA	CMD-C2D-C1D	2.01	128.26	124.71
13	B	1215	CLA	CMD-C2D-C1D	2.01	128.26	124.71
13	B	1232	CLA	C2A-C3A-C4A	2.01	105.12	101.87
13	A	1115	CLA	CMD-C2D-C1D	2.01	128.25	124.71
16	A	4003	BCR	C37-C22-C23	2.01	121.24	118.08
13	L	1503	CLA	C4D-CHA-C1A	2.01	123.69	121.25
13	B	1235	CLA	CMD-C2D-C1D	2.01	128.25	124.71
13	B	1208	CLA	C2D-C1D-ND	2.00	111.58	110.10
16	A	4003	BCR	C15-C14-C13	2.00	130.17	127.31
13	B	1204	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
13	B	1233	CLA	C4D-CHA-C1A	2.00	123.69	121.25
13	B	1226	CLA	C2A-C3A-C4A	2.00	105.10	101.87
13	A	1124	CLA	C4D-CHA-C1A	2.00	123.69	121.25
13	A	1111	CLA	C2A-C3A-C4A	2.00	105.10	101.87
16	B	4006	BCR	C32-C1-C6	2.00	113.55	110.30
13	B	1220	CLA	C3C-C4C-NC	-2.00	108.33	110.57
16	B	4009	BCR	C19-C18-C17	-2.00	115.87	118.94
13	A	1107	CLA	CED-O2D-CGD	2.00	120.46	115.94
13	B	1225	CLA	C3A-C2A-C1A	2.00	104.33	101.34
13	B	1216	CLA	C2D-C1D-ND	2.00	111.58	110.10
13	A	1114	CLA	C4D-CHA-C1A	2.00	123.68	121.25

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

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Mol	Chain	Res	Type	Atom
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
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

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

All (864) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1013	CLA	O2A-C1-C2-C3
13	A	1102	CLA	C3A-C2A-CAA-CBA
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	CHA-CBD-CGD-O1D
13	A	1103	CLA	CHA-CBD-CGD-O2D
13	A	1103	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	A	1103	CLA	O2A-C1-C2-C3
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	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	C1-C2-C3-C4
13	A	1121	CLA	C4-C3-C5-C6
13	A	1126	CLA	C2-C3-C5-C6
13	A	1126	CLA	C4-C3-C5-C6
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	1134	CLA	CHA-CBD-CGD-O1D
13	A	1134	CLA	CHA-CBD-CGD-O2D
13	A	1135	CLA	C4-C3-C5-C6
13	A	1138	CLA	CHA-CBD-CGD-O1D
13	A	1138	CLA	CHA-CBD-CGD-O2D
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	1140	CLA	C4-C3-C5-C6
13	A	1237	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	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	A	1801	CLA	CHA-CBD-CGD-O2D
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	1202	CLA	C1A-C2A-CAA-CBA
13	B	1202	CLA	C3A-C2A-CAA-CBA
13	B	1203	CLA	C4-C3-C5-C6
13	B	1208	CLA	CBD-CGD-O2D-CED
13	B	1210	CLA	C1A-C2A-CAA-CBA
13	B	1212	CLA	C1A-C2A-CAA-CBA
13	B	1212	CLA	C3A-C2A-CAA-CBA
13	B	1212	CLA	C2A-CAA-CBA-CGA
13	B	1213	CLA	C1A-C2A-CAA-CBA
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	1215	CLA	C3A-C2A-CAA-CBA
13	B	1215	CLA	C2-C3-C5-C6
13	B	1215	CLA	C4-C3-C5-C6
13	B	1217	CLA	C3A-C2A-CAA-CBA
13	B	1218	CLA	CBD-CGD-O2D-CED
13	B	1219	CLA	CBD-CGD-O2D-CED
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	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	CBD-CGD-O2D-CED
13	B	1229	CLA	C1A-C2A-CAA-CBA
13	B	1229	CLA	C3A-C2A-CAA-CBA
13	B	1229	CLA	O2A-C1-C2-C3
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

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Mol	Chain	Res	Type	Atoms
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
13	L	1501	CLA	C3A-C2A-CAA-CBA
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
14	A	2001	PQN	C14-C13-C15-C16
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	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	1104	CLA	CBD-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	1228	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	1801	CLA	O1D-CGD-O2D-CED
13	B	1208	CLA	O1D-CGD-O2D-CED
13	B	1219	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	K	1401	CLA	O1D-CGD-O2D-CED
13	A	1133	CLA	CBA-CGA-O2A-C1
13	A	1237	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	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	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	A	1122	CLA	CBD-CGD-O2D-CED
13	A	1127	CLA	CBD-CGD-O2D-CED
13	B	1218	CLA	O1D-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
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	A	1140	CLA	C2-C3-C5-C6
13	B	1203	CLA	C2-C3-C5-C6
13	A	1121	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	B	1236	CLA	CBD-CGD-O2D-CED
13	A	1127	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	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	B	1201	CLA	O1D-CGD-O2D-CED
13	B	1203	CLA	CBD-CGD-O2D-CED
13	A	1108	CLA	O1D-CGD-O2D-CED
13	A	1109	CLA	O1D-CGD-O2D-CED
13	F	1301	CLA	O1D-CGD-O2D-CED
17	B	5004	LHG	O9-C7-O7-C5
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
18	B	5002	LMG	O6-C5-C6-O5
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	1123	CLA	C3-C5-C6-C7
13	A	1106	CLA	CBA-CGA-O2A-C1
13	A	1129	CLA	CBA-CGA-O2A-C1
13	L	1502	CLA	CBA-CGA-O2A-C1
13	A	1117	CLA	O1A-CGA-O2A-C1
13	A	1137	CLA	O1A-CGA-O2A-C1
13	A	1113	CLA	O1D-CGD-O2D-CED
13	B	1212	CLA	O1D-CGD-O2D-CED
13	B	1228	CLA	O1D-CGD-O2D-CED
17	B	5004	LHG	C8-C7-O7-C5
13	A	1103	CLA	CBD-CGD-O2D-CED
13	A	1107	CLA	O1D-CGD-O2D-CED
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	CBA-CGA-O2A-C1
13	B	1213	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
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	A	1133	CLA	C4-C3-C5-C6
13	B	1012	CLA	C4-C3-C5-C6
13	B	1213	CLA	C4-C3-C5-C6
13	B	1221	CLA	C4-C3-C5-C6
13	A	1133	CLA	C2-C3-C5-C6
13	A	1237	CLA	C2-C3-C5-C6
13	B	1012	CLA	C2-C3-C5-C6
13	B	1213	CLA	C2-C3-C5-C6
13	B	1221	CLA	C2-C3-C5-C6
14	A	2001	PQN	C12-C13-C15-C16
13	B	1239	CLA	CBD-CGD-O2D-CED
13	A	1104	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	A	1120	CLA	O1D-CGD-O2D-CED
13	A	1132	CLA	O1D-CGD-O2D-CED
13	A	1140	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	O1A-CGA-O2A-C1
13	A	1102	CLA	O1D-CGD-O2D-CED
13	A	1105	CLA	O1D-CGD-O2D-CED
13	B	1230	CLA	O1D-CGD-O2D-CED
17	B	5004	LHG	O10-C23-O8-C6
17	A	5003	LHG	C1-C2-C3-O3
13	B	1215	CLA	O1A-CGA-O2A-C1
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	B	1202	CLA	CBD-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
17	A	5003	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
13	A	1120	CLA	O1A-CGA-O2A-C1
13	B	1210	CLA	O1A-CGA-O2A-C1
13	L	1503	CLA	O1D-CGD-O2D-CED
13	L	1503	CLA	C5-C6-C7-C8
13	X	1701	CLA	O1D-CGD-O2D-CED
13	A	1109	CLA	O1A-CGA-O2A-C1
13	A	1106	CLA	O1D-CGD-O2D-CED
13	A	1104	CLA	C15-C16-C17-C18
13	A	1136	CLA	C8-C10-C11-C12
17	B	5004	LHG	O1-C1-C2-O2
13	A	1130	CLA	CBD-CGD-O2D-CED
13	B	1207	CLA	C15-C16-C17-C18
13	A	1140	CLA	C2-C1-O2A-CGA
13	A	1116	CLA	CBD-CGD-O2D-CED
14	B	2002	PQN	C25-C26-C27-C28
13	A	1128	CLA	C11-C10-C8-C7
13	B	1021	CLA	C12-C13-C15-C16
13	B	1206	CLA	C12-C13-C15-C16
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	A	1126	CLA	O1D-CGD-O2D-CED
13	B	1226	CLA	O1A-CGA-O2A-C1
16	B	4009	BCR	C18-C19-C20-C21
18	B	5002	LMG	C4-C5-C6-O5
13	A	1107	CLA	C8-C10-C11-C12
13	B	1223	CLA	C10-C11-C12-C13
13	B	1225	CLA	C15-C16-C17-C18
13	B	1234	CLA	O1A-CGA-O2A-C1
13	A	1124	CLA	C5-C6-C7-C8
13	B	1205	CLA	C13-C15-C16-C17
13	B	1225	CLA	C5-C6-C7-C8
13	B	1234	CLA	C8-C10-C11-C12
13	A	1107	CLA	C13-C15-C16-C17
13	A	1109	CLA	C15-C16-C17-C18
17	A	5001	LHG	C4-O6-P-O3
14	A	2001	PQN	C13-C15-C16-C17
13	A	1128	CLA	CBA-CGA-O2A-C1
13	A	1139	CLA	CBA-CGA-O2A-C1
13	B	1236	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	1127	CLA	O1D-CGD-O2D-CED
13	B	1226	CLA	C13-C15-C16-C17
13	B	1229	CLA	C10-C11-C12-C13
13	L	1502	CLA	C8-C10-C11-C12
13	A	1122	CLA	O1D-CGD-O2D-CED
13	B	1202	CLA	CBA-CGA-O2A-C1
13	A	1106	CLA	C5-C6-C7-C8
17	A	5001	LHG	C24-C25-C26-C27
16	B	4009	BCR	C16-C17-C18-C36
16	B	4009	BCR	C20-C21-C22-C37
13	A	1121	CLA	O1D-CGD-O2D-CED
13	B	1203	CLA	O1D-CGD-O2D-CED
13	B	1236	CLA	O1D-CGD-O2D-CED
14	B	2002	PQN	C26-C27-C28-C29
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	1130	CLA	C8-C10-C11-C12
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	B	1219	CLA	C6-C7-C8-C9
14	B	2002	PQN	C26-C27-C28-C30
13	A	1123	CLA	C4-C3-C5-C6
13	A	1123	CLA	C2-C3-C5-C6
13	A	1118	CLA	C6-C7-C8-C9
13	B	1021	CLA	C14-C13-C15-C16
13	A	1107	CLA	C2A-CAA-CBA-CGA
13	A	1120	CLA	C2A-CAA-CBA-CGA
13	A	1103	CLA	C10-C11-C12-C13
13	B	1229	CLA	C15-C16-C17-C18
17	A	5001	LHG	C28-C29-C30-C31
17	A	5003	LHG	C9-C10-C11-C12
13	B	1219	CLA	C6-C7-C8-C10
13	B	1202	CLA	C13-C15-C16-C17
13	A	1101	CLA	CBD-CGD-O2D-CED
13	B	1205	CLA	O1D-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
13	B	1210	CLA	C3A-C2A-CAA-CBA
13	B	1221	CLA	O2A-C1-C2-C3
13	B	1012	CLA	C3-C5-C6-C7
13	A	1131	CLA	C4-C3-C5-C6
13	A	1131	CLA	C2-C3-C5-C6
13	B	1207	CLA	O1D-CGD-O2D-CED
13	B	1202	CLA	O1A-CGA-O2A-C1
13	B	1234	CLA	C5-C6-C7-C8
13	A	1118	CLA	C4C-C3C-CAC-CBC
13	B	1215	CLA	C3-C5-C6-C7
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	4008	BCR	C5-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	B	4017	BCR	C1-C6-C7-C8
16	I	4020	BCR	C23-C24-C25-C26
16	I	4020	BCR	C23-C24-C25-C30
16	J	4013	BCR	C1-C6-C7-C8
16	J	4013	BCR	C5-C6-C7-C8
16	M	4021	BCR	C1-C6-C7-C8
16	M	4021	BCR	C5-C6-C7-C8
13	A	1103	CLA	C8-C10-C11-C12
13	B	1021	CLA	C13-C15-C16-C17
13	A	1103	CLA	O1D-CGD-O2D-CED
13	A	1104	CLA	C11-C12-C13-C15
13	A	1117	CLA	C11-C12-C13-C15
13	A	1118	CLA	C6-C7-C8-C10
13	A	1124	CLA	C12-C13-C15-C16
13	A	1131	CLA	C12-C13-C15-C16
13	B	1223	CLA	C6-C7-C8-C10
13	B	1229	CLA	C2-C3-C5-C6
13	L	1502	CLA	C11-C10-C8-C7
14	A	2001	PQN	C16-C17-C18-C20
13	B	1239	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	B	1216	CLA	C10-C11-C12-C13
13	B	1229	CLA	O1D-CGD-O2D-CED
13	B	1202	CLA	O1D-CGD-O2D-CED
13	B	1224	CLA	CBD-CGD-O2D-CED
17	A	5001	LHG	C10-C11-C12-C13
13	A	1111	CLA	C3-C5-C6-C7
13	A	1140	CLA	C5-C6-C7-C8
13	B	1229	CLA	C4-C3-C5-C6
13	A	1801	CLA	C2-C3-C5-C6
13	A	1104	CLA	C11-C12-C13-C14
13	A	1117	CLA	C11-C12-C13-C14
13	A	1124	CLA	C14-C13-C15-C16
13	A	1128	CLA	C11-C10-C8-C9
13	A	1131	CLA	C14-C13-C15-C16
13	B	1206	CLA	C14-C13-C15-C16
13	B	1223	CLA	C6-C7-C8-C9
13	B	1223	CLA	C11-C12-C13-C14
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	A	1022	CLA	C15-C16-C17-C18
13	B	1224	CLA	C10-C11-C12-C13
13	B	1210	CLA	C8-C10-C11-C12
13	A	1130	CLA	O1D-CGD-O2D-CED
13	B	1213	CLA	C3-C5-C6-C7
13	A	1138	CLA	C5-C6-C7-C8
13	A	1801	CLA	C4-C3-C5-C6
13	B	1230	CLA	C4-C3-C5-C6
13	A	1134	CLA	C2A-CAA-CBA-CGA
13	A	1237	CLA	C3-C5-C6-C7
18	B	5002	LMG	C30-C31-C32-C33
13	B	1222	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	I	4020	BCR	C20-C21-C22-C37
13	B	1214	CLA	CBA-CGA-O2A-C1
13	B	1228	CLA	CBA-CGA-O2A-C1
13	B	1223	CLA	CBD-CGD-O2D-CED
13	A	1114	CLA	C1-C2-C3-C4
13	A	1109	CLA	C2A-CAA-CBA-CGA
17	A	5001	LHG	C24-C23-O8-C6
13	A	1136	CLA	C5-C6-C7-C8
16	B	4014	BCR	C11-C10-C9-C8
13	A	1116	CLA	CAA-CBA-CGA-O2A
13	A	1123	CLA	C8-C10-C11-C12
17	A	5003	LHG	C11-C10-C9-C8
13	A	1127	CLA	C4-C3-C5-C6
13	B	1211	CLA	C4-C3-C5-C6
13	B	1225	CLA	C4-C3-C5-C6
13	A	1106	CLA	C11-C10-C8-C7
13	B	1202	CLA	C12-C13-C15-C16
13	B	1211	CLA	C2-C3-C5-C6
13	B	1223	CLA	C11-C12-C13-C15
13	B	1225	CLA	C2-C3-C5-C6
13	A	1106	CLA	C11-C10-C8-C9
13	A	1117	CLA	C11-C10-C8-C9
13	A	1127	CLA	C14-C13-C15-C16
13	L	1502	CLA	C11-C10-C8-C9
14	A	2001	PQN	C16-C17-C18-C19
13	A	1125	CLA	CBA-CGA-O2A-C1
13	B	1206	CLA	C16-C17-C18-C20
13	A	1130	CLA	C3-C5-C6-C7
13	A	1101	CLA	O1D-CGD-O2D-CED
13	A	1013	CLA	C15-C16-C17-C18
13	A	1111	CLA	C8-C10-C11-C12
13	A	1124	CLA	C15-C16-C17-C18
13	A	1116	CLA	O1D-CGD-O2D-CED
13	A	1127	CLA	C5-C6-C7-C8
13	A	1123	CLA	C13-C15-C16-C17
13	B	1203	CLA	C15-C16-C17-C18
13	A	1127	CLA	C2-C3-C5-C6
13	A	1106	CLA	C8-C10-C11-C12
13	A	1106	CLA	C15-C16-C17-C18
13	B	1215	CLA	C5-C6-C7-C8
13	L	1501	CLA	C13-C15-C16-C17
13	A	1119	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	1402	CLA	C3A-C2A-CAA-CBA
13	A	1801	CLA	C3A-C2A-CAA-CBA
13	B	1222	CLA	C3A-C2A-CAA-CBA
13	B	1228	CLA	C3A-C2A-CAA-CBA
13	A	1123	CLA	CBA-CGA-O2A-C1
13	A	1124	CLA	CBA-CGA-O2A-C1
13	A	1124	CLA	C8-C10-C11-C12
13	B	1228	CLA	O1A-CGA-O2A-C1
13	A	1104	CLA	C16-C17-C18-C19
13	B	1206	CLA	C16-C17-C18-C19
13	B	1230	CLA	C2-C3-C5-C6
13	A	1125	CLA	O1A-CGA-O2A-C1
13	B	1021	CLA	C5-C6-C7-C8
13	B	1214	CLA	O1A-CGA-O2A-C1
17	A	5001	LHG	O10-C23-O8-C6
13	A	1111	CLA	C2-C1-O2A-CGA
13	B	1012	CLA	C14-C13-C15-C16
13	A	1105	CLA	C4-C3-C5-C6
13	A	1013	CLA	C2A-CAA-CBA-CGA
13	A	1108	CLA	C2A-CAA-CBA-CGA
13	B	1229	CLA	C2A-CAA-CBA-CGA
13	A	1114	CLA	O2A-C1-C2-C3
16	B	4005	BCR	C23-C24-C25-C30
16	B	4017	BCR	C5-C6-C7-C8
16	F	4016	BCR	C23-C24-C25-C26
16	F	4016	BCR	C23-C24-C25-C30
16	M	4021	BCR	C23-C24-C25-C26
16	M	4021	BCR	C23-C24-C25-C30
13	A	1124	CLA	O1A-CGA-O2A-C1
14	A	2001	PQN	C15-C16-C17-C18
13	A	1127	CLA	C12-C13-C15-C16
13	A	1132	CLA	C12-C13-C15-C16
13	A	1138	CLA	C11-C10-C8-C7
13	B	1012	CLA	C12-C13-C15-C16
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	A	1104	CLA	C16-C17-C18-C20
13	B	1225	CLA	C2A-CAA-CBA-CGA
16	F	4016	BCR	C20-C21-C22-C37
16	J	4012	BCR	C35-C13-C14-C15
16	L	4022	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
13	A	1011	CLA	CAD-CBD-CGD-O2D
13	A	1113	CLA	CAD-CBD-CGD-O2D
13	A	1120	CLA	CAD-CBD-CGD-O2D
13	A	1124	CLA	CAD-CBD-CGD-O2D
13	B	1012	CLA	CAD-CBD-CGD-O2D
13	B	1218	CLA	CAD-CBD-CGD-O2D
16	L	4019	BCR	C22-C23-C24-C25
13	B	1211	CLA	CBA-CGA-O2A-C1
13	A	1120	CLA	O2A-C1-C2-C3
13	A	1106	CLA	CHA-CBD-CGD-O1D
13	A	1106	CLA	CHA-CBD-CGD-O2D
13	A	1128	CLA	CHA-CBD-CGD-O1D
13	A	1128	CLA	CHA-CBD-CGD-O2D
13	B	1202	CLA	CHA-CBD-CGD-O1D
13	B	1202	CLA	CHA-CBD-CGD-O2D
13	B	1205	CLA	CHA-CBD-CGD-O1D
13	B	1205	CLA	CHA-CBD-CGD-O2D
13	B	1216	CLA	CHA-CBD-CGD-O1D
13	B	1216	CLA	CHA-CBD-CGD-O2D
13	B	1221	CLA	CHA-CBD-CGD-O1D
13	B	1231	CLA	CHA-CBD-CGD-O2D
13	A	1119	CLA	O1A-CGA-O2A-C1
13	A	1123	CLA	O1A-CGA-O2A-C1
13	A	1117	CLA	C16-C17-C18-C20
13	B	1234	CLA	C4-C3-C5-C6
13	L	1503	CLA	C4-C3-C5-C6
13	B	1234	CLA	C2-C3-C5-C6
13	A	1107	CLA	C11-C12-C13-C14
13	L	1501	CLA	C11-C10-C8-C9
18	B	5002	LMG	C41-C42-C43-C44
13	A	1107	CLA	C1A-C2A-CAA-CBA
13	A	1119	CLA	C1A-C2A-CAA-CBA
13	A	1122	CLA	C1A-C2A-CAA-CBA
13	A	1237	CLA	C1A-C2A-CAA-CBA
13	A	1402	CLA	C1A-C2A-CAA-CBA
13	A	1237	CLA	O1D-CGD-O2D-CED
13	B	1203	CLA	C5-C6-C7-C8
13	B	1211	CLA	C3-C5-C6-C7
13	L	1503	CLA	C2-C3-C5-C6
17	A	5001	LHG	C4-O6-P-O4
13	B	1228	CLA	O2A-C1-C2-C3
13	B	1211	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	1121	CLA	C2-C3-C5-C6
13	A	1135	CLA	C2-C3-C5-C6
13	B	1202	CLA	CAD-CBD-CGD-O1D
13	A	1140	CLA	C3-C5-C6-C7
13	L	1501	CLA	C3-C5-C6-C7
13	B	1223	CLA	O1D-CGD-O2D-CED
13	B	1234	CLA	CBD-CGD-O2D-CED
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
13	L	1501	CLA	C11-C10-C8-C7
17	A	5001	LHG	C27-C28-C29-C30
13	B	1226	CLA	C10-C11-C12-C13
13	B	1209	CLA	C2A-CAA-CBA-CGA
13	B	1217	CLA	C2A-CAA-CBA-CGA
13	B	1229	CLA	C16-C17-C18-C20
13	A	1102	CLA	C4-C3-C5-C6
13	A	1116	CLA	CBA-CGA-O2A-C1
13	A	1132	CLA	C14-C13-C15-C16
13	A	1138	CLA	C11-C10-C8-C9
13	B	1203	CLA	C14-C13-C15-C16
13	B	1210	CLA	C11-C10-C8-C9
13	B	1239	CLA	C14-C13-C15-C16
16	B	4006	BCR	C22-C23-C24-C25
13	A	1117	CLA	C16-C17-C18-C19
13	B	1228	CLA	C1-C2-C3-C4
17	A	5001	LHG	C1-C2-C3-O3
13	A	1132	CLA	C2A-CAA-CBA-CGA
13	B	1206	CLA	C2-C1-O2A-CGA
13	B	1211	CLA	C2-C1-O2A-CGA
13	B	1225	CLA	C2-C1-O2A-CGA
13	B	1239	CLA	C2-C1-O2A-CGA
13	B	1023	CLA	C10-C11-C12-C13
13	A	1116	CLA	O1A-CGA-O2A-C1
13	A	1104	CLA	CAA-CBA-CGA-O2A
13	B	1210	CLA	C4-C3-C5-C6
13	B	1224	CLA	C4-C3-C5-C6
13	B	1222	CLA	O1A-CGA-O2A-C1
16	J	4015	BCR	C23-C24-C25-C30
18	B	5002	LMG	C34-C35-C36-C37
13	A	1114	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	B	4006	BCR	C20-C21-C22-C23
17	A	5001	LHG	C3-O3-P-O6
17	A	5003	LHG	C3-O3-P-O6
17	B	5004	LHG	C3-O3-P-O6
13	B	1207	CLA	C13-C15-C16-C17
13	B	1207	CLA	C4-C3-C5-C6
13	L	1501	CLA	C4-C3-C5-C6
13	A	1107	CLA	C11-C12-C13-C15
13	A	1117	CLA	C11-C10-C8-C7
13	B	1239	CLA	C12-C13-C15-C16
13	L	1502	CLA	C12-C13-C15-C16
13	A	1103	CLA	C11-C10-C8-C9
13	B	1202	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	1237	CLA	C5-C6-C7-C8
13	B	1012	CLA	C13-C15-C16-C17
13	L	1503	CLA	C3-C5-C6-C7
13	B	1202	CLA	C15-C16-C17-C18
13	A	1136	CLA	C4-C3-C5-C6
13	B	1229	CLA	C16-C17-C18-C19
17	A	5001	LHG	C26-C27-C28-C29
13	A	1109	CLA	C10-C11-C12-C13
13	B	1224	CLA	O1D-CGD-O2D-CED
13	B	1224	CLA	C2-C1-O2A-CGA
13	A	1106	CLA	C2A-CAA-CBA-CGA
13	M	1601	CLA	C2A-CAA-CBA-CGA
13	A	1121	CLA	C3A-C2A-CAA-CBA
13	A	1133	CLA	C3A-C2A-CAA-CBA
13	M	1601	CLA	CAA-CBA-CGA-O1A
18	B	5002	LMG	C15-C16-C17-C18
13	B	1227	CLA	CAA-CBA-CGA-O2A
13	J	1302	CLA	CAA-CBA-CGA-O1A
13	A	1122	CLA	C6-C7-C8-C9
13	B	1211	CLA	C11-C12-C13-C14
13	B	1227	CLA	CAA-CBA-CGA-O1A
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	B	1220	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	A	1107	CLA	C10-C11-C12-C13
13	X	1701	CLA	CAA-CBA-CGA-O1A
13	X	1701	CLA	CAA-CBA-CGA-O2A
13	A	1117	CLA	C4-C3-C5-C6
13	A	1124	CLA	C1A-C2A-CAA-CBA
17	A	5001	LHG	O9-C7-O7-C5
13	A	1111	CLA	C11-C10-C8-C7
17	A	5001	LHG	C19-C20-C21-C22
13	B	1218	CLA	CAA-CBA-CGA-O2A
13	M	1601	CLA	CAA-CBA-CGA-O2A
18	B	5002	LMG	C31-C32-C33-C34
13	B	1218	CLA	CAA-CBA-CGA-O1A
13	B	1220	CLA	CAA-CBA-CGA-O1A
13	J	1302	CLA	CAA-CBA-CGA-O2A
13	A	1124	CLA	O1D-CGD-O2D-CED
13	A	1125	CLA	C4-C3-C5-C6
13	A	1102	CLA	C2-C3-C5-C6
13	B	1214	CLA	C8-C10-C11-C12
14	B	2002	PQN	C23-C25-C26-C27
16	A	4011	BCR	C11-C10-C9-C8
16	A	4011	BCR	C16-C17-C18-C19
16	F	4016	BCR	C12-C13-C14-C15
13	B	1233	CLA	CAA-CBA-CGA-O1A
13	A	1013	CLA	C8-C10-C11-C12
13	A	1138	CLA	C3-C5-C6-C7
13	A	1022	CLA	C4-C3-C5-C6
13	A	1111	CLA	C4-C3-C5-C6
13	B	1205	CLA	C4-C3-C5-C6
13	A	1102	CLA	C2-C1-O2A-CGA
13	A	1107	CLA	C2-C1-O2A-CGA
13	A	1119	CLA	C2-C1-O2A-CGA
13	A	1135	CLA	C2-C1-O2A-CGA
13	B	1210	CLA	C2-C3-C5-C6
13	L	1501	CLA	C2-C3-C5-C6
13	A	1136	CLA	C11-C12-C13-C14
13	B	1205	CLA	C14-C13-C15-C16
13	B	1233	CLA	CAA-CBA-CGA-O2A
13	J	1302	CLA	C2A-CAA-CBA-CGA
16	B	4006	BCR	C23-C24-C25-C30
16	B	4009	BCR	C23-C24-C25-C30
13	B	1219	CLA	C5-C6-C7-C8
13	B	1223	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	B	1207	CLA	C2-C3-C5-C6
13	B	1224	CLA	C2-C3-C5-C6
13	A	1131	CLA	C13-C15-C16-C17
13	B	1207	CLA	C10-C11-C12-C13
13	A	1106	CLA	C4-C3-C5-C6
13	A	1116	CLA	CAA-CBA-CGA-O1A
13	A	1117	CLA	C2-C3-C5-C6
13	A	1136	CLA	C2-C3-C5-C6
13	B	1203	CLA	C12-C13-C15-C16
13	A	1108	CLA	CAA-CBA-CGA-O1A
13	A	1237	CLA	CBD-CGD-O2D-CED
13	F	1301	CLA	CAA-CBA-CGA-O2A
13	A	1125	CLA	C3-C5-C6-C7
17	A	5001	LHG	C11-C10-C9-C8
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	A	1107	CLA	C4-C3-C5-C6
13	A	1109	CLA	C4-C3-C5-C6
13	A	1122	CLA	C4-C3-C5-C6
13	B	1206	CLA	C4-C3-C5-C6
13	B	1226	CLA	C4-C3-C5-C6
13	A	1118	CLA	C8-C10-C11-C12
13	A	1125	CLA	C2-C3-C5-C6
13	B	1206	CLA	C6-C7-C8-C9
13	A	1124	CLA	C3A-C2A-CAA-CBA
13	A	1102	CLA	CAD-CBD-CGD-O2D
13	A	1103	CLA	CAD-CBD-CGD-O2D
13	A	1110	CLA	CAD-CBD-CGD-O2D
13	A	1125	CLA	CAD-CBD-CGD-O2D
13	A	1129	CLA	CAD-CBD-CGD-O2D
13	B	1201	CLA	CAD-CBD-CGD-O2D
13	B	1212	CLA	CAD-CBD-CGD-O2D
13	B	1217	CLA	CAD-CBD-CGD-O2D
13	A	1801	CLA	C2-C1-O2A-CGA
13	A	1123	CLA	CAA-CBA-CGA-O2A
13	A	1126	CLA	CAA-CBA-CGA-O2A
17	A	5003	LHG	O7-C7-C8-C9
13	A	1013	CLA	C4-C3-C5-C6
13	A	1116	CLA	C4-C3-C5-C6
13	K	1401	CLA	CAA-CBA-CGA-O2A
13	A	1107	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	B	1206	CLA	C2-C3-C5-C6
13	A	1102	CLA	CAA-CBA-CGA-O2A
13	A	1013	CLA	CAA-CBA-CGA-O2A
13	B	1203	CLA	CAA-CBA-CGA-O2A
13	F	1301	CLA	CAA-CBA-CGA-O1A
13	A	1110	CLA	O2A-C1-C2-C3
13	A	1123	CLA	O2A-C1-C2-C3
13	A	1130	CLA	O2A-C1-C2-C3
13	B	1214	CLA	O2A-C1-C2-C3
13	B	1213	CLA	C2A-CAA-CBA-CGA
13	B	1224	CLA	C2A-CAA-CBA-CGA
13	X	1701	CLA	C2A-CAA-CBA-CGA
13	A	1122	CLA	C11-C12-C13-C14
13	B	1219	CLA	CAA-CBA-CGA-O2A
13	K	1401	CLA	CAA-CBA-CGA-O1A
17	A	5001	LHG	C11-C12-C13-C14
13	A	1101	CLA	CHA-CBD-CGD-O1D
13	A	1101	CLA	CHA-CBD-CGD-O2D
13	A	1108	CLA	CHA-CBD-CGD-O1D
13	A	1108	CLA	CHA-CBD-CGD-O2D
13	A	1117	CLA	CHA-CBD-CGD-O1D
13	A	1117	CLA	CHA-CBD-CGD-O2D
13	A	1118	CLA	CHA-CBD-CGD-O2D
13	A	1122	CLA	CHA-CBD-CGD-O1D
13	A	1122	CLA	CHA-CBD-CGD-O2D
13	A	1123	CLA	CHA-CBD-CGD-O1D
13	A	1137	CLA	CHA-CBD-CGD-O1D
13	A	1137	CLA	CHA-CBD-CGD-O2D
13	B	1021	CLA	CHA-CBD-CGD-O1D
13	B	1021	CLA	CHA-CBD-CGD-O2D
13	B	1204	CLA	CHA-CBD-CGD-O2D
13	B	1206	CLA	CHA-CBD-CGD-O1D
13	B	1206	CLA	CHA-CBD-CGD-O2D
13	B	1211	CLA	CHA-CBD-CGD-O1D
13	B	1211	CLA	CHA-CBD-CGD-O2D
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	J	1302	CLA	CHA-CBD-CGD-O1D
13	J	1302	CLA	CHA-CBD-CGD-O2D
13	K	1401	CLA	CHA-CBD-CGD-O2D
13	B	1219	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	1109	CLA	CAA-CBA-CGA-O2A
13	B	1229	CLA	CAA-CBA-CGA-O2A
13	B	1226	CLA	C2-C3-C5-C6
17	A	5001	LHG	C13-C14-C15-C16
16	B	4006	BCR	C11-C10-C9-C8
13	B	1210	CLA	CAA-CBA-CGA-O2A
13	B	1221	CLA	C6-C7-C8-C9
13	A	1105	CLA	C2A-CAA-CBA-CGA
13	B	1203	CLA	C16-C17-C18-C20
13	A	1105	CLA	CAA-CBA-CGA-O2A
13	A	1119	CLA	C4-C3-C5-C6
13	A	1111	CLA	O1A-CGA-O2A-C1
13	A	1111	CLA	C2-C3-C5-C6
13	A	1136	CLA	C11-C12-C13-C15
13	B	1210	CLA	C6-C7-C8-C10
13	A	1801	CLA	CAA-CBA-CGA-O2A
13	A	1111	CLA	C11-C10-C8-C9
13	A	1136	CLA	C14-C13-C15-C16
13	B	1210	CLA	C6-C7-C8-C9
13	B	1215	CLA	C11-C10-C8-C9
13	B	1224	CLA	C11-C12-C13-C14
13	L	1502	CLA	C14-C13-C15-C16
13	A	1108	CLA	CAA-CBA-CGA-O2A
17	A	5001	LHG	C8-C7-O7-C5
13	A	1104	CLA	C2A-CAA-CBA-CGA
13	A	1122	CLA	C2A-CAA-CBA-CGA
17	A	5001	LHG	C25-C26-C27-C28
13	B	1212	CLA	CAA-CBA-CGA-O2A
13	A	1124	CLA	C4-C3-C5-C6
17	A	5003	LHG	O10-C23-O8-C6
13	A	1022	CLA	C2-C3-C5-C6
13	B	1205	CLA	C2-C3-C5-C6
13	A	1111	CLA	CBA-CGA-O2A-C1
13	A	1119	CLA	C13-C15-C16-C17
13	A	1111	CLA	C1A-C2A-CAA-CBA
13	A	1121	CLA	C1A-C2A-CAA-CBA
13	A	1133	CLA	C1A-C2A-CAA-CBA
13	A	1135	CLA	C1A-C2A-CAA-CBA
13	B	1220	CLA	C1A-C2A-CAA-CBA
13	B	1234	CLA	C1A-C2A-CAA-CBA
13	L	1503	CLA	C1A-C2A-CAA-CBA
13	B	1021	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
17	A	5003	LHG	C24-C23-O8-C6
13	A	1102	CLA	CAA-CBA-CGA-O1A
13	A	1022	CLA	C2A-CAA-CBA-CGA
13	L	1503	CLA	C2A-CAA-CBA-CGA
13	B	1203	CLA	C16-C17-C18-C19
13	A	1132	CLA	C13-C15-C16-C17
17	A	5001	LHG	C4-O6-P-O5
13	A	1013	CLA	CAA-CBA-CGA-O1A
13	A	1126	CLA	CAA-CBA-CGA-O1A
13	B	1203	CLA	CAA-CBA-CGA-O1A
16	B	4009	BCR	C23-C24-C25-C26
13	B	1226	CLA	C8-C10-C11-C12
13	A	1105	CLA	CAA-CBA-CGA-O1A
13	A	1109	CLA	CAA-CBA-CGA-O1A
13	A	1123	CLA	CAA-CBA-CGA-O1A
13	B	1219	CLA	CAA-CBA-CGA-O1A
13	B	1211	CLA	CAA-CBA-CGA-O2A
13	B	1209	CLA	CAA-CBA-CGA-O1A
13	B	1212	CLA	CAA-CBA-CGA-O1A
13	B	1229	CLA	CAA-CBA-CGA-O1A
13	A	1118	CLA	C4-C3-C5-C6
13	A	1112	CLA	O1D-CGD-O2D-CED
13	A	1013	CLA	C2-C3-C5-C6
13	A	1111	CLA	CAD-CBD-CGD-O1D
13	A	1122	CLA	CAD-CBD-CGD-O1D
13	B	1206	CLA	CAD-CBD-CGD-O1D
13	B	1215	CLA	CAD-CBD-CGD-O1D
13	B	1223	CLA	CAD-CBD-CGD-O1D
13	B	1227	CLA	CAD-CBD-CGD-O1D
13	B	1234	CLA	CAD-CBD-CGD-O1D
17	A	5003	LHG	O9-C7-C8-C9
13	L	1501	CLA	C8-C10-C11-C12
13	B	1021	CLA	C11-C10-C8-C9
13	B	1206	CLA	C11-C10-C8-C9
13	B	1224	CLA	C5-C6-C7-C8
13	A	1118	CLA	CAA-CBA-CGA-O2A
13	A	1237	CLA	CAA-CBA-CGA-O2A
13	B	1209	CLA	CAA-CBA-CGA-O2A
13	A	1127	CLA	C13-C15-C16-C17
13	A	1110	CLA	CAA-CBA-CGA-O2A
13	A	1115	CLA	CAA-CBA-CGA-O2A
13	B	1239	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	A	1136	CLA	C12-C13-C15-C16
13	B	1211	CLA	C11-C12-C13-C15
13	A	1118	CLA	CAA-CBA-CGA-O1A
13	A	1121	CLA	CAA-CBA-CGA-O2A
13	B	1023	CLA	CAA-CBA-CGA-O2A
17	A	5003	LHG	O8-C23-C24-C25
13	B	1210	CLA	CAA-CBA-CGA-O1A
18	B	5002	LMG	C16-C17-C18-C19
13	A	1138	CLA	CAA-CBA-CGA-O2A
13	B	1204	CLA	CAA-CBA-CGA-O2A
13	A	1121	CLA	CAA-CBA-CGA-O1A
13	A	1801	CLA	CAA-CBA-CGA-O1A
13	A	1129	CLA	C2A-CAA-CBA-CGA
13	B	1214	CLA	C2A-CAA-CBA-CGA
13	B	1223	CLA	CAA-CBA-CGA-O2A
13	A	1113	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

114 monomers are involved in 339 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1601	CLA	1	0
13	A	1114	CLA	2	0
16	A	4001	BCR	2	0
16	J	4013	BCR	7	0
13	B	1238	CLA	3	0
13	B	1210	CLA	6	0
13	A	1117	CLA	6	0
13	B	1216	CLA	5	0
13	A	1128	CLA	7	0
16	B	4009	BCR	5	0
13	J	1302	CLA	1	0
13	A	1022	CLA	3	0
13	B	1226	CLA	7	0
13	B	1211	CLA	6	0
13	B	1225	CLA	8	0
13	A	1138	CLA	2	0
13	A	1108	CLA	4	0
16	B	4017	BCR	1	0
13	X	1701	CLA	1	0
13	A	1121	CLA	1	0
13	B	1214	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1203	CLA	6	0
13	A	1103	CLA	6	0
13	B	1208	CLA	1	0
13	A	1136	CLA	7	0
13	A	1119	CLA	4	0
16	J	4012	BCR	4	0
13	B	1230	CLA	7	0
13	A	1104	CLA	4	0
13	B	1217	CLA	2	0
13	A	1120	CLA	2	0
13	A	1237	CLA	5	0
13	B	1232	CLA	3	0
13	B	1228	CLA	2	0
16	B	4010	BCR	3	0
13	A	1105	CLA	2	0
16	B	4014	BCR	1	0
16	J	4015	BCR	5	0
13	A	1402	CLA	1	0
18	B	5002	LMG	5	0
16	F	4016	BCR	2	0
13	B	1023	CLA	4	0
13	B	1234	CLA	3	0
13	A	1132	CLA	4	0
13	A	1111	CLA	1	0
13	A	1101	CLA	2	0
13	A	1126	CLA	14	0
14	B	2002	PQN	1	0
16	A	4008	BCR	1	0
13	B	1235	CLA	2	0
13	B	1236	CLA	4	0
13	B	1222	CLA	2	0
16	L	4022	BCR	1	0
13	A	1106	CLA	6	0
13	K	1401	CLA	1	0
13	A	1118	CLA	5	0
13	B	1219	CLA	4	0
13	B	1218	CLA	1	0
13	B	1209	CLA	1	0
13	A	1122	CLA	2	0
13	B	1224	CLA	5	0
13	A	1013	CLA	10	0
16	A	4007	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	4005	BCR	1	0
17	B	5004	LHG	1	0
13	B	1227	CLA	5	0
13	L	1501	CLA	2	0
13	A	1107	CLA	4	0
14	A	2001	PQN	1	0
13	A	1134	CLA	2	0
13	B	1229	CLA	6	0
16	B	4006	BCR	5	0
13	A	1123	CLA	4	0
13	A	1137	CLA	3	0
13	B	1220	CLA	3	0
13	B	1021	CLA	8	0
13	B	1012	CLA	17	0
13	A	1112	CLA	5	0
13	B	1213	CLA	3	0
13	B	1204	CLA	1	0
13	L	1502	CLA	8	0
13	B	1215	CLA	6	0
16	A	4011	BCR	13	0
13	A	1102	CLA	1	0
13	A	1109	CLA	1	0
13	A	1133	CLA	4	0
13	A	1129	CLA	1	0
13	B	1207	CLA	5	0
13	A	1135	CLA	2	0
13	L	1503	CLA	2	0
13	A	1125	CLA	3	0
16	I	4018	BCR	3	0
13	B	1202	CLA	3	0
16	M	4021	BCR	2	0
13	A	1140	CLA	8	0
13	A	1130	CLA	2	0
13	A	1801	CLA	5	0
13	B	1223	CLA	3	0
13	B	1205	CLA	3	0
13	B	1206	CLA	2	0
13	B	1212	CLA	2	0
13	B	1221	CLA	10	0
13	A	1124	CLA	5	0
16	A	4002	BCR	2	0
16	A	4003	BCR	1	0

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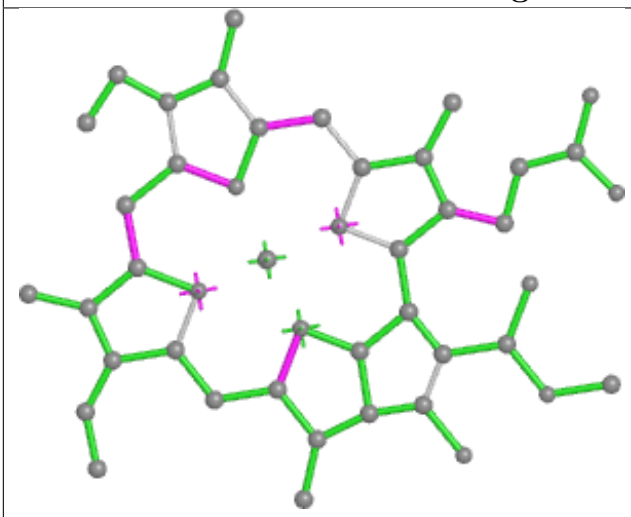
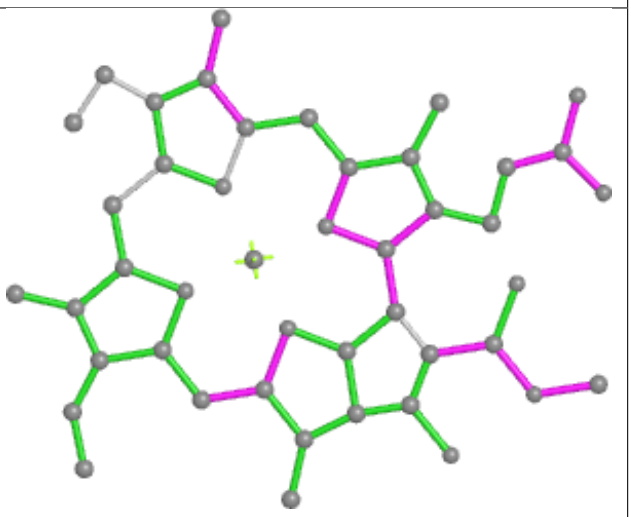
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1116	CLA	5	0
13	B	1233	CLA	2	0
13	A	1127	CLA	1	0
13	F	1301	CLA	1	0
17	A	5003	LHG	2	0
16	B	4004	BCR	1	0
17	A	5001	LHG	4	0
13	B	1201	CLA	2	0
13	A	1011	CLA	9	0

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 then 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.

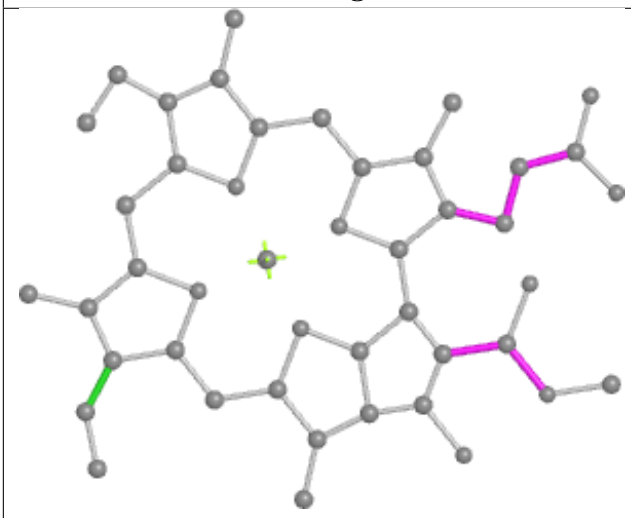
Ligand CLA M 1601



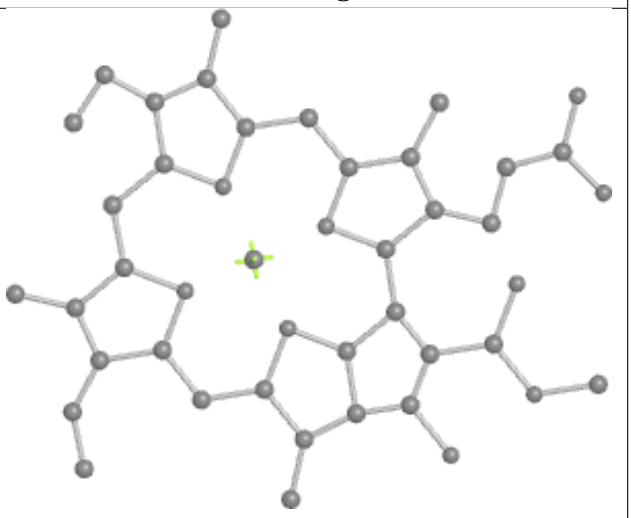
Bond lengths



Bond angles

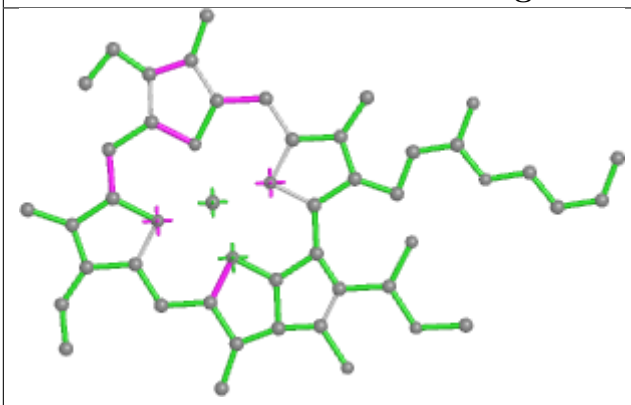


Torsions

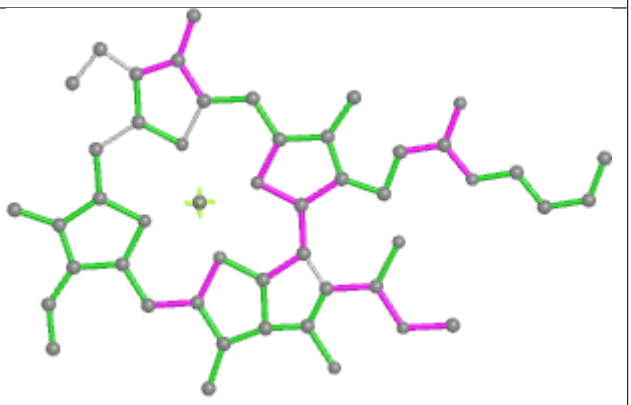


Rings

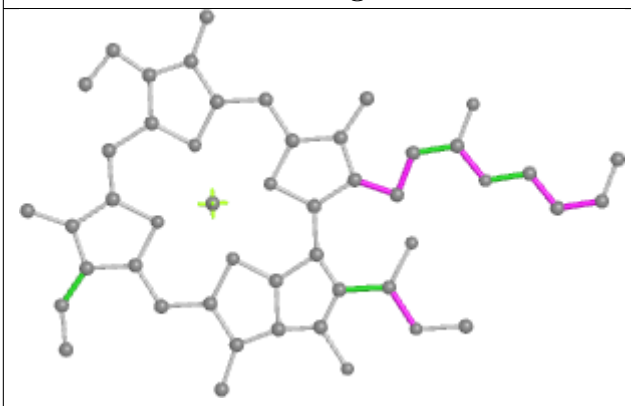
Ligand CLA A 1114



Bond lengths



Bond angles



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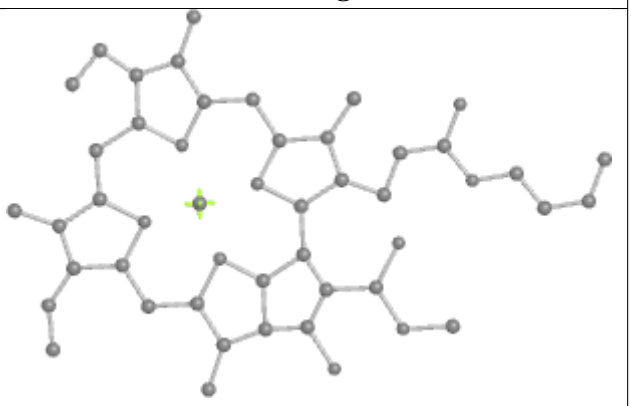
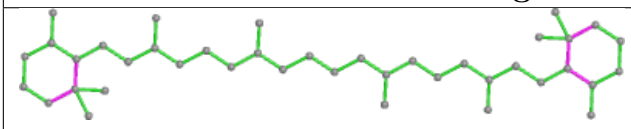
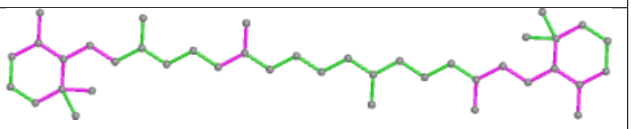


Rings

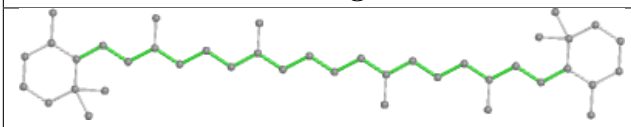
Ligand BCR A 4001



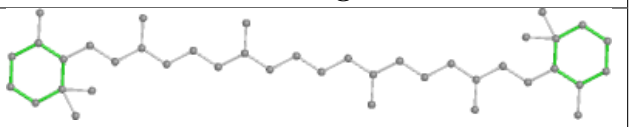
Bond lengths



Bond angles

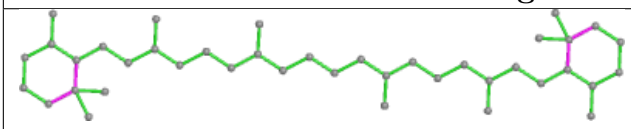


Torsions

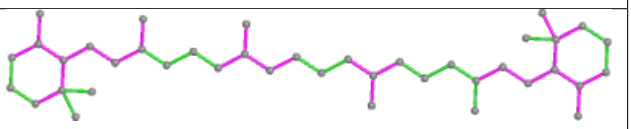


Rings

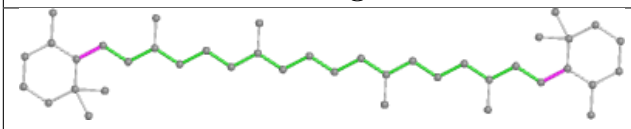
Ligand BCR J 4013



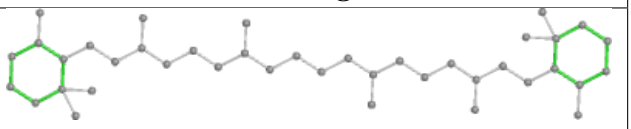
Bond lengths



Bond angles

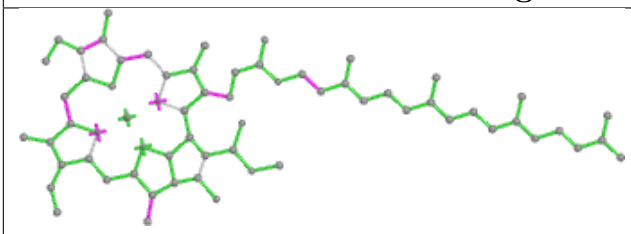


Torsions

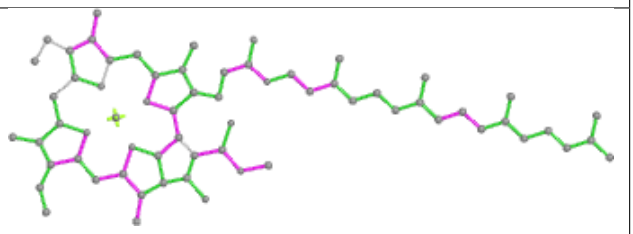


Rings

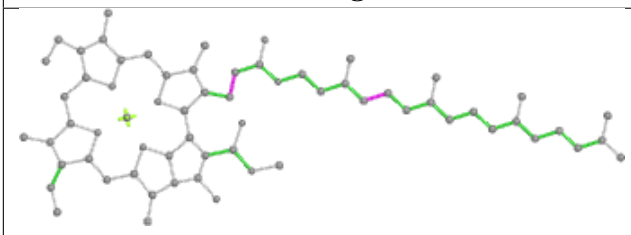
Ligand CLA B 1238



Bond lengths



Bond angles



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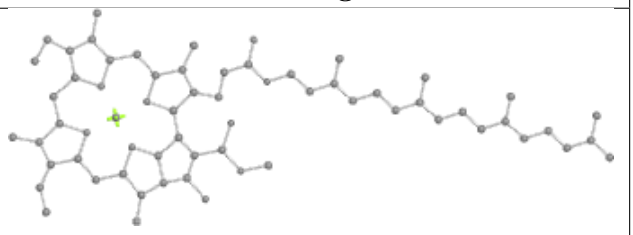
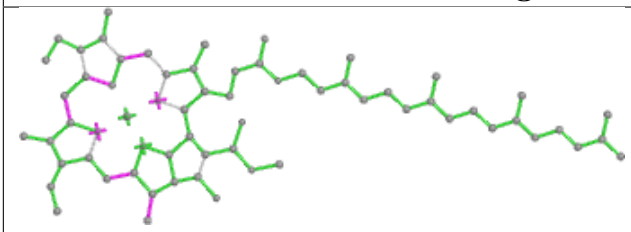
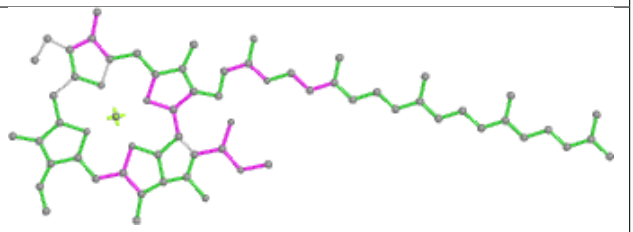


Rings

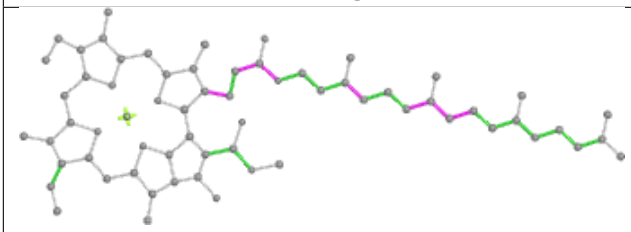
Ligand CLA B 1210



Bond lengths



Bond angles



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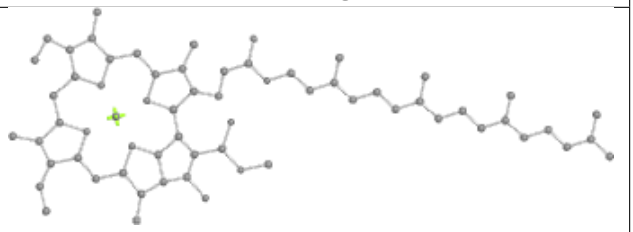
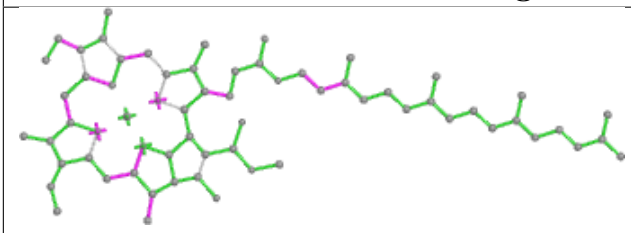
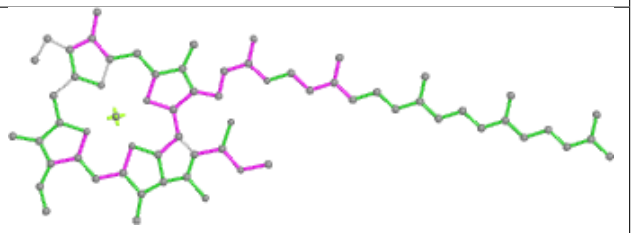


Rings

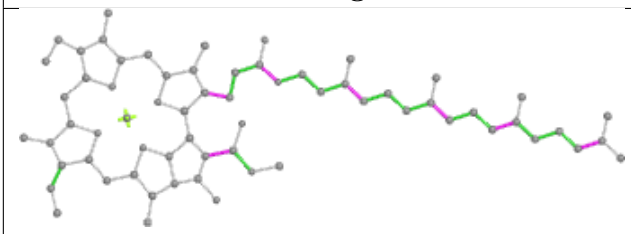
Ligand CLA A 1117



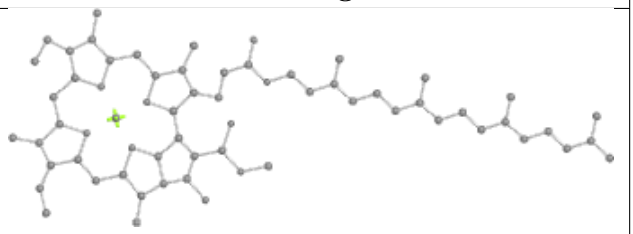
Bond lengths



Bond angles

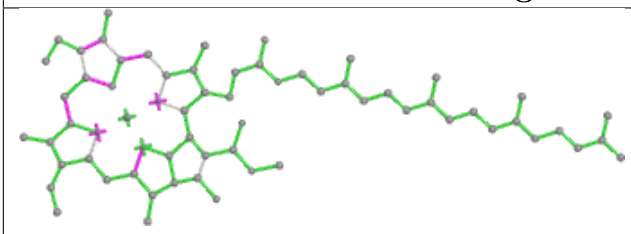


Torsions

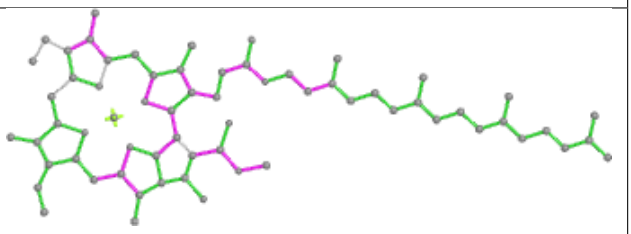


Rings

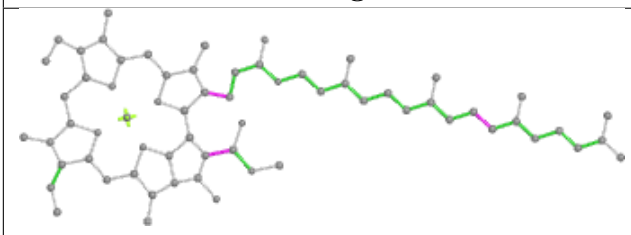
Ligand CLA B 1216



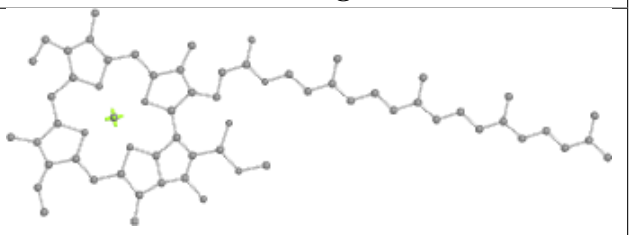
Bond lengths



Bond angles

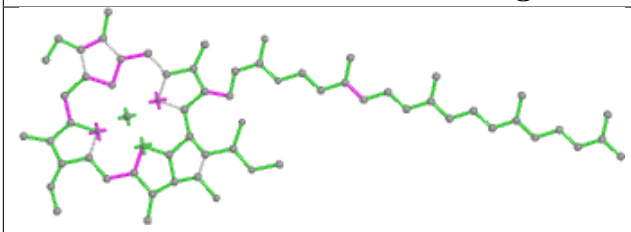


Torsions



Rings

Ligand CLA A 1128



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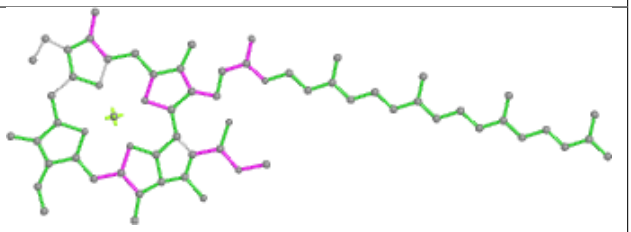
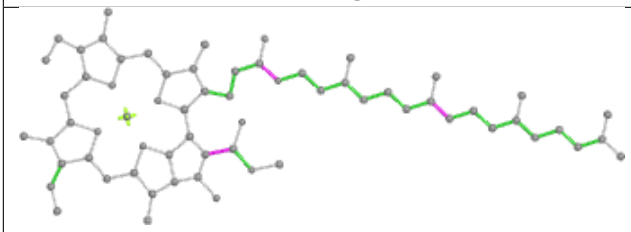


Bond angles



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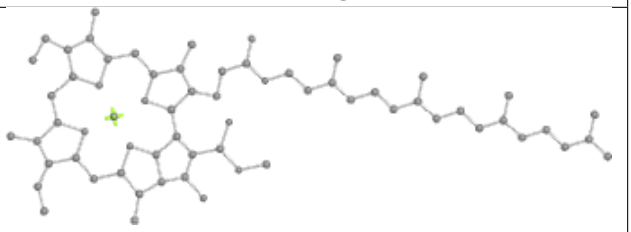
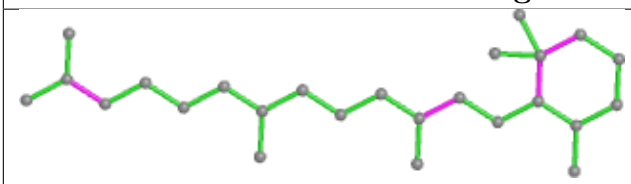


Rings

Ligand BCR B 4009



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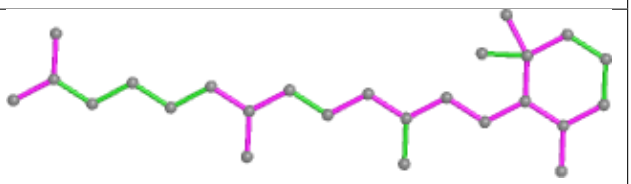
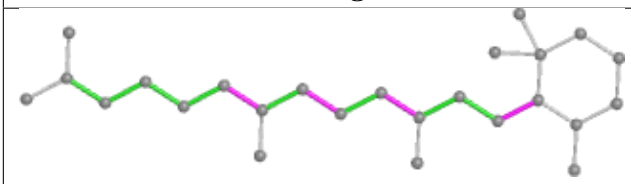


Bond angles



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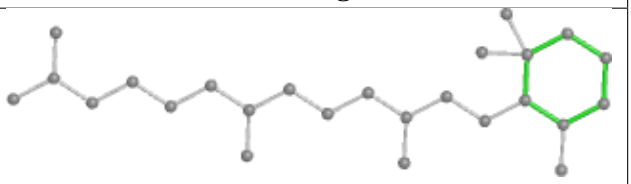
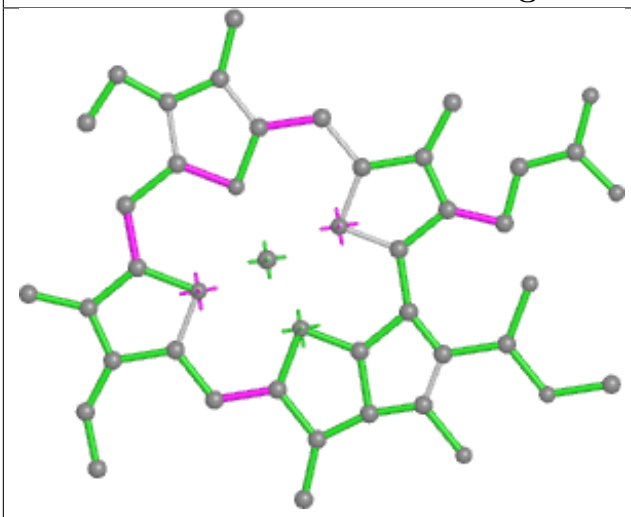


Rings

Ligand CLA J 1302



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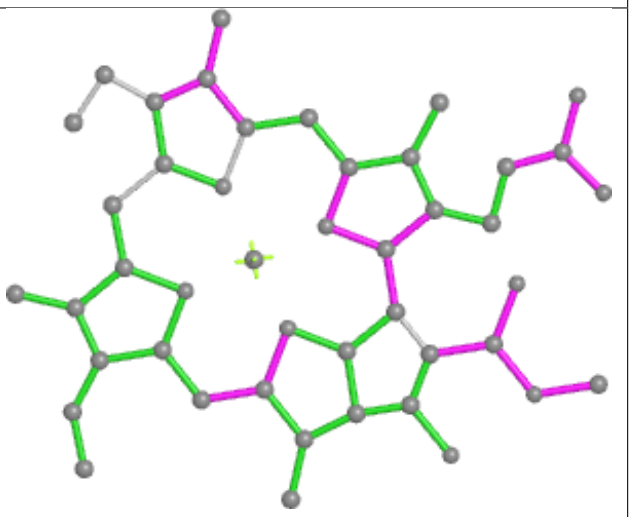
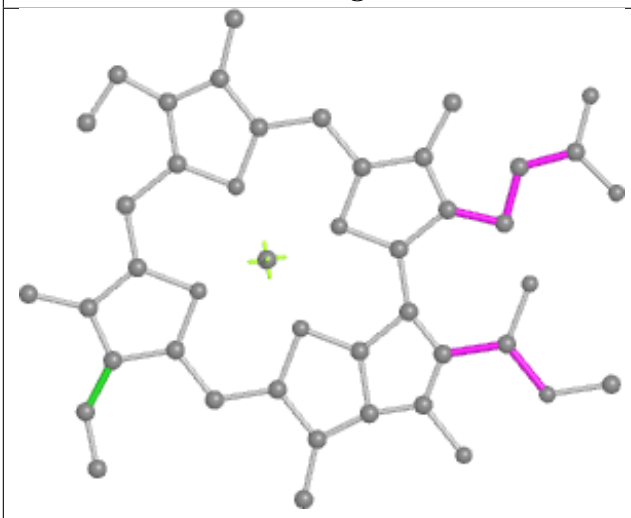


Bond angles



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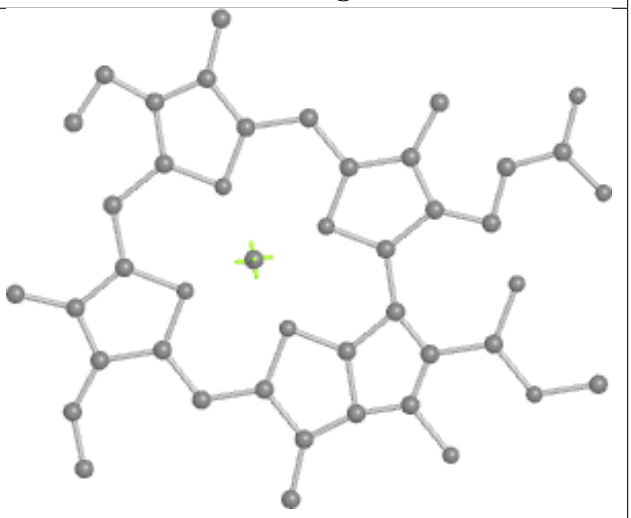
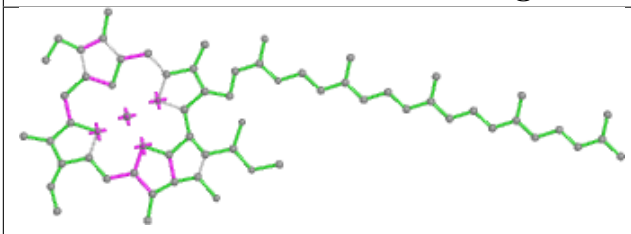


Rings

Ligand CLA A 1022



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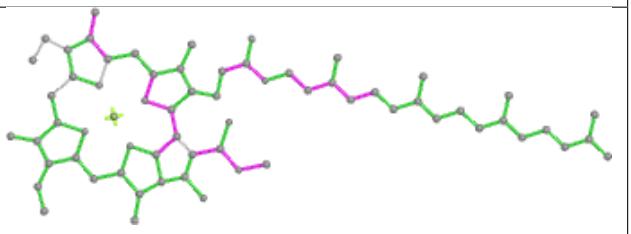
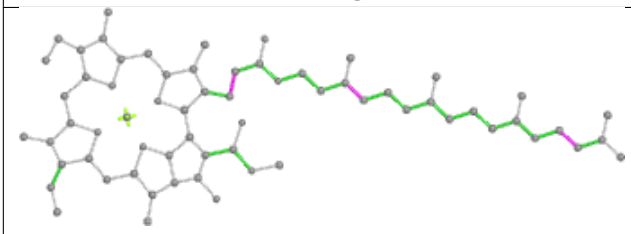


Bond angles



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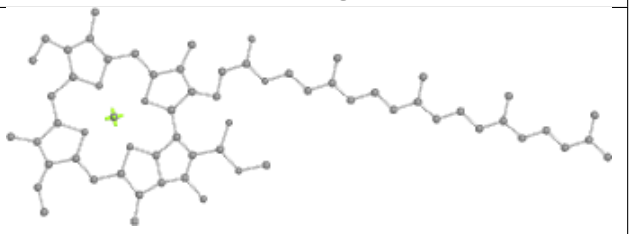
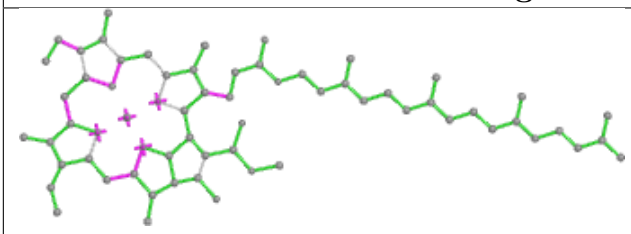


Rings

Ligand CLA B 1226



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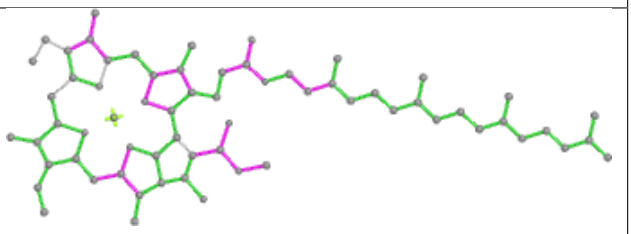
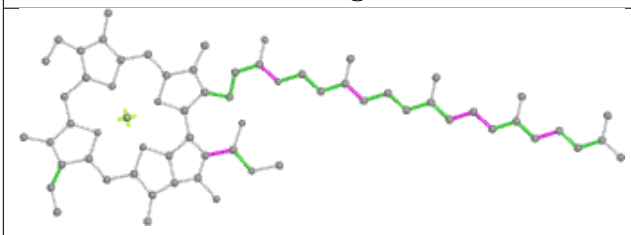


Bond angles



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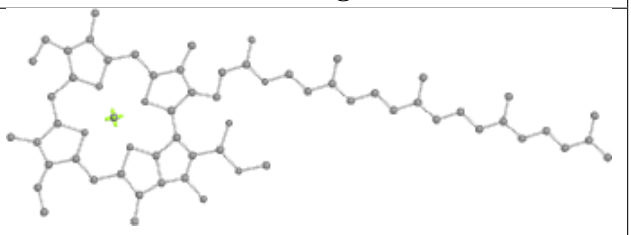
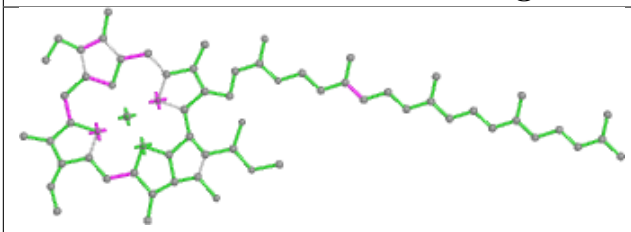


Rings

Ligand CLA B 1211



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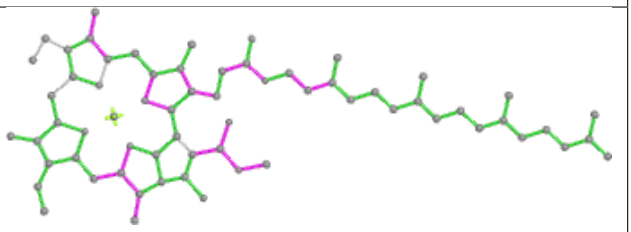
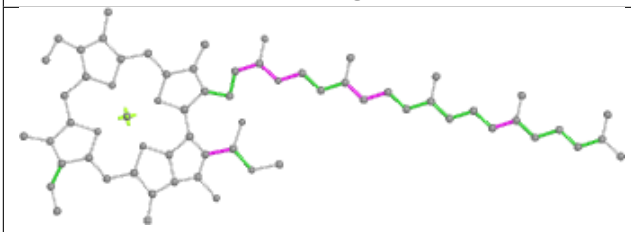


Bond angles



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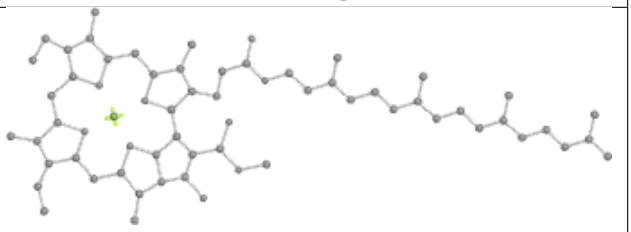
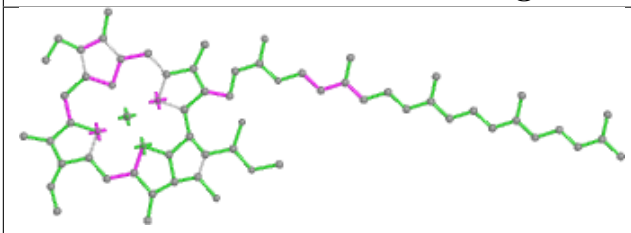


Rings

Ligand CLA B 1225



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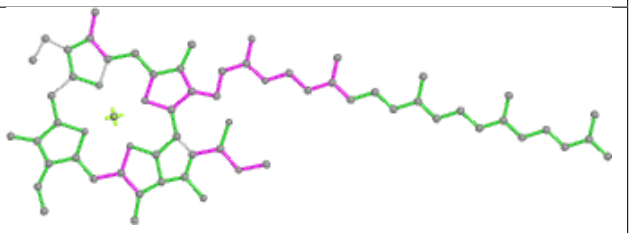
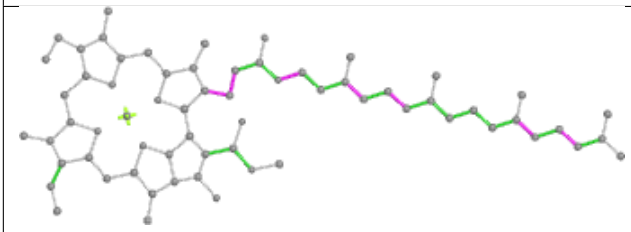


Bond angles



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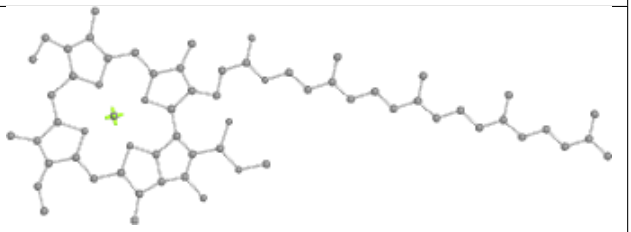
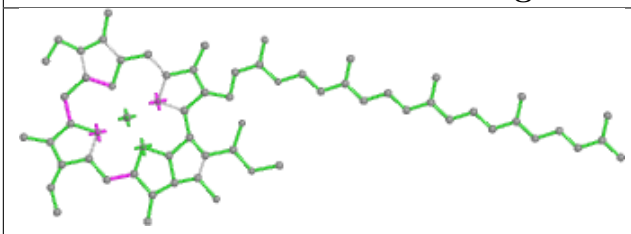
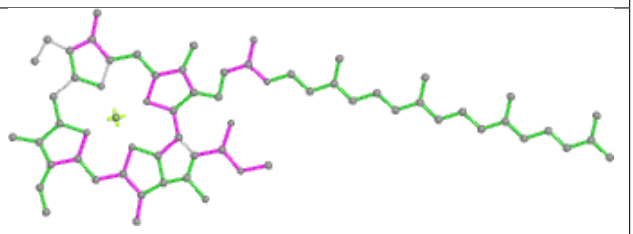
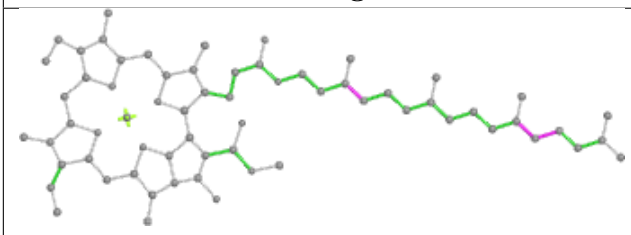
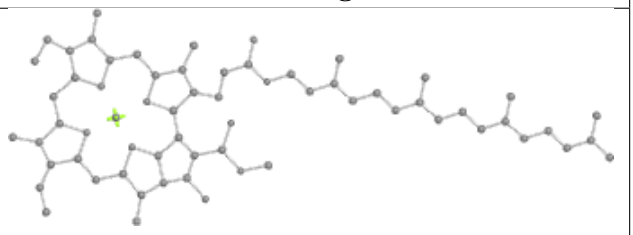
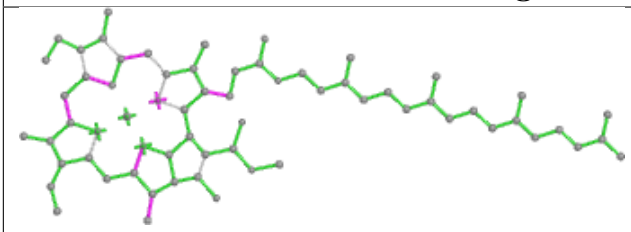
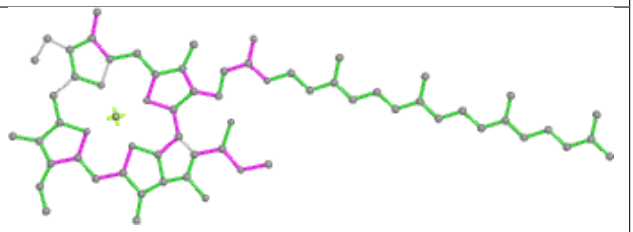
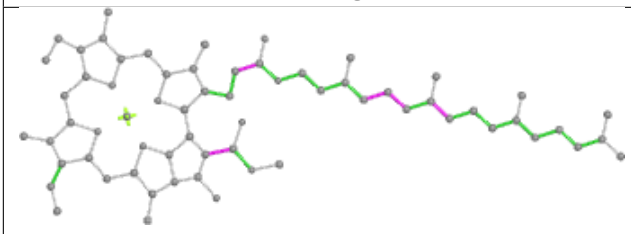
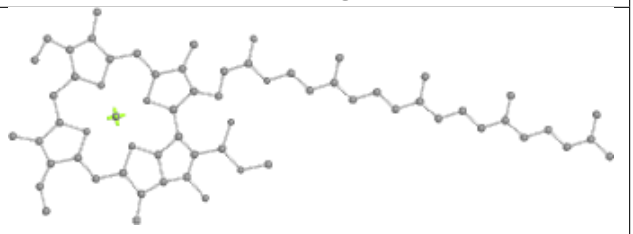
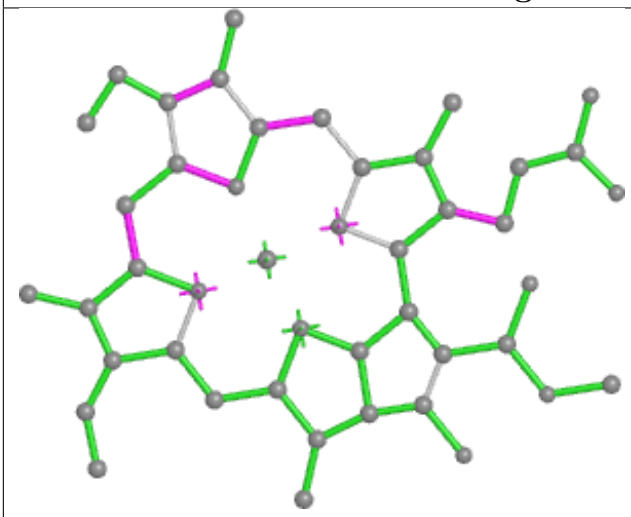


Rings

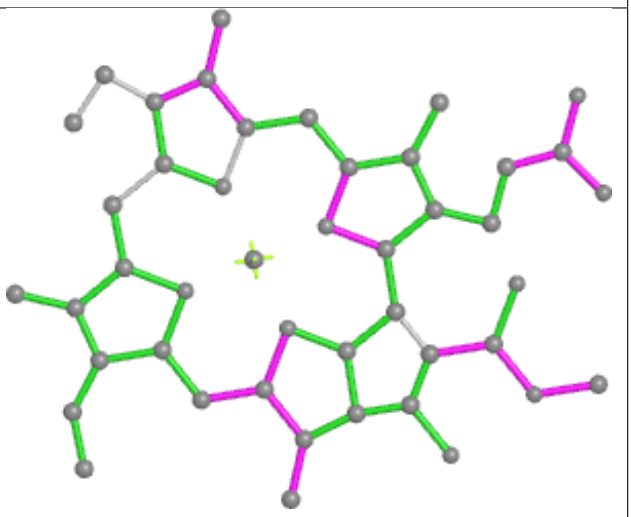
Ligand CLA A 1131	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1138	
 Bond lengths	 Bond angles
 Torsions	 Rings

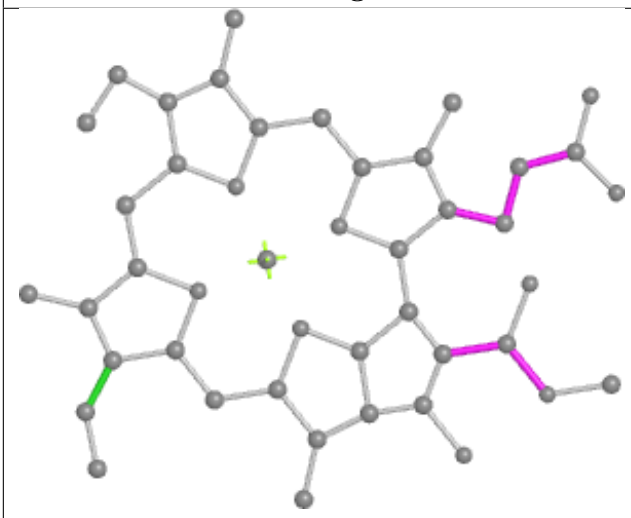
Ligand CLA A 1108



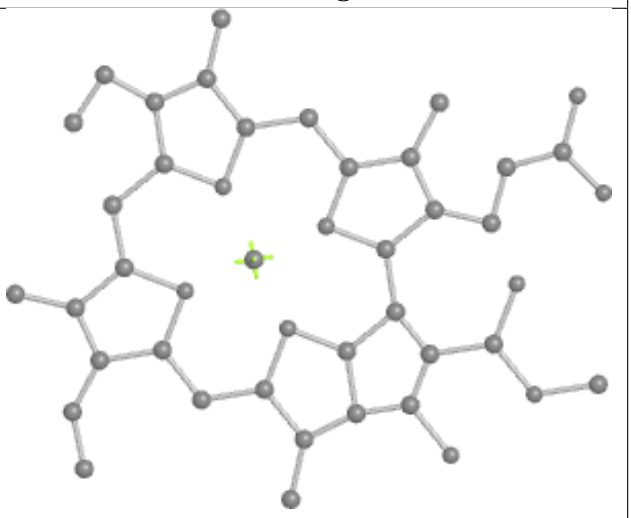
Bond lengths



Bond angles

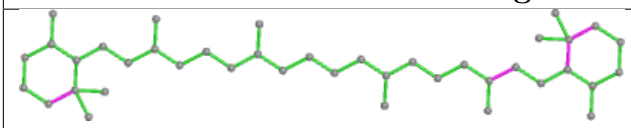


Torsions



Rings

Ligand BCR B 4017



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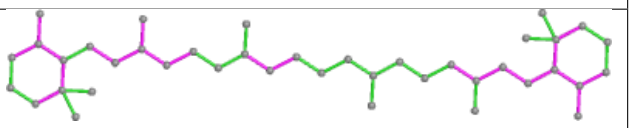
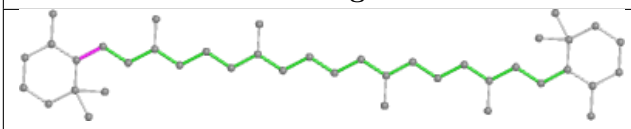


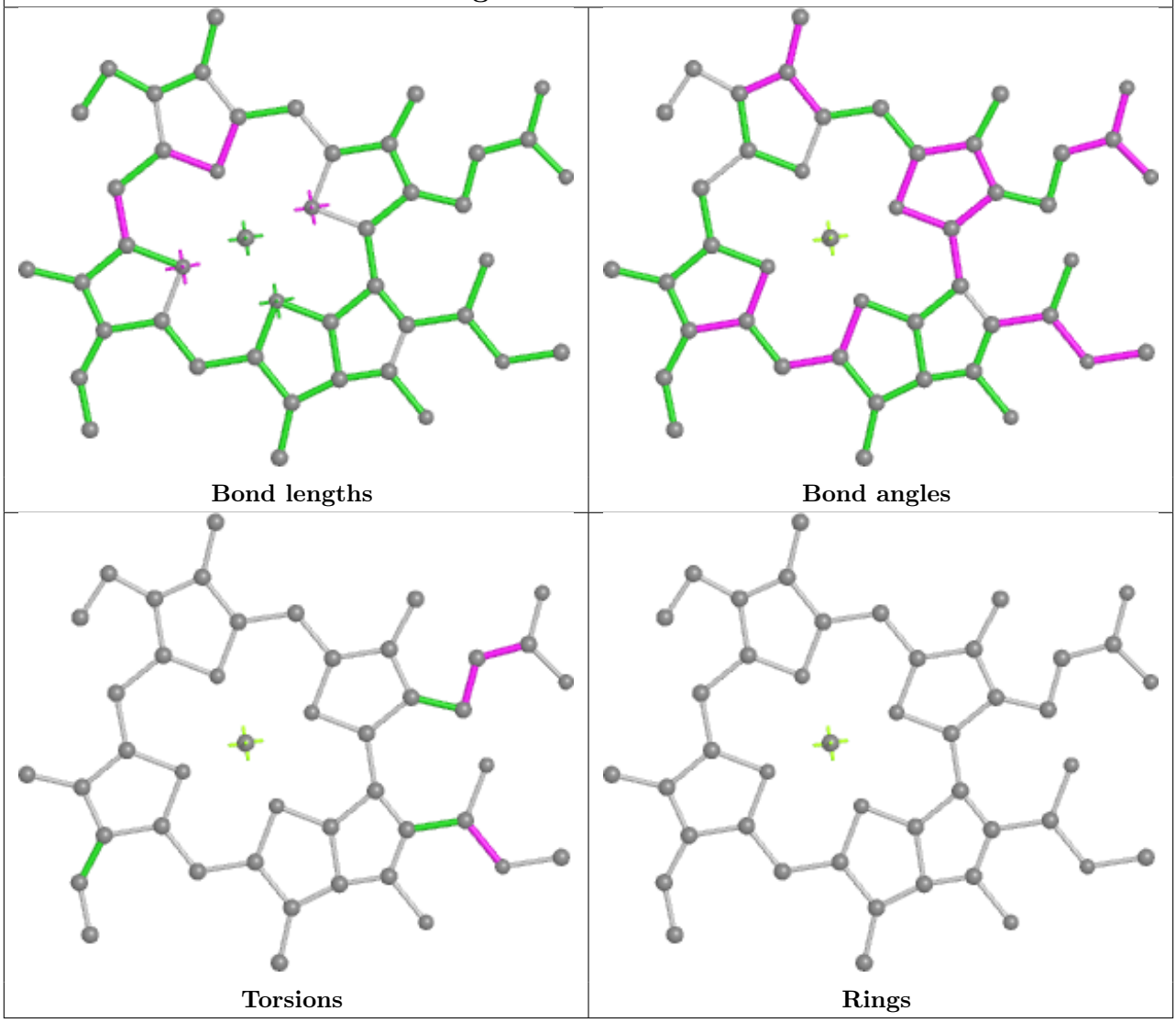
Bond angles

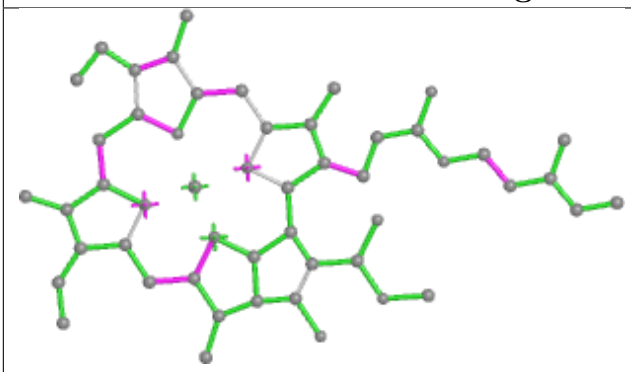
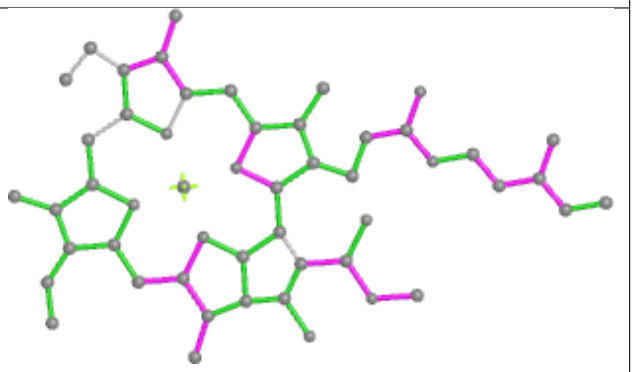
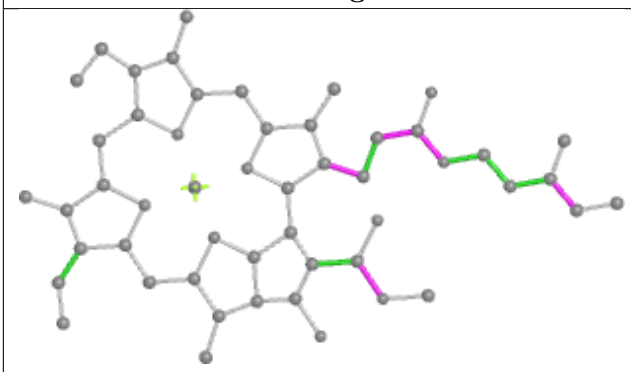
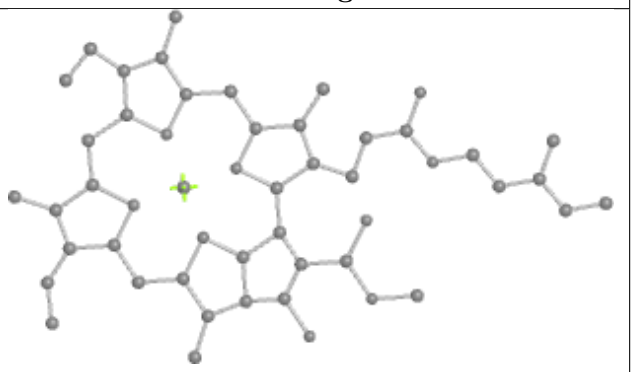


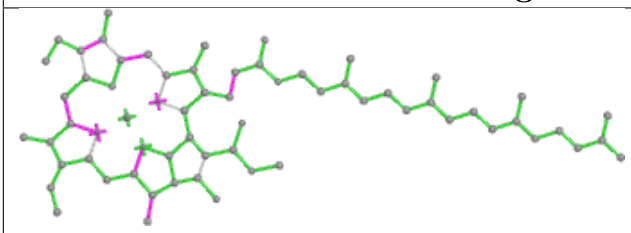
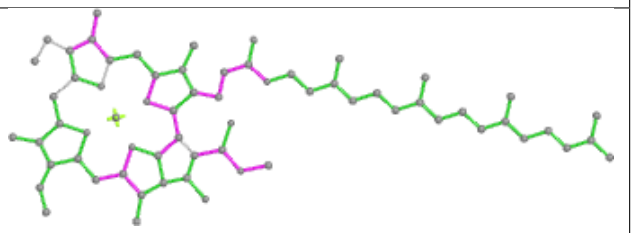
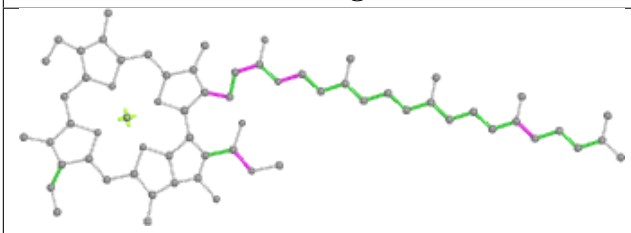
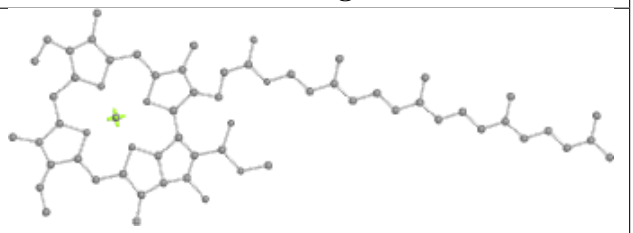
Torsions

Rings

Ligand CLA X 1701



Ligand CLA A 1121	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1239	
 Bond lengths	 Bond angles
 Torsions	 Rings

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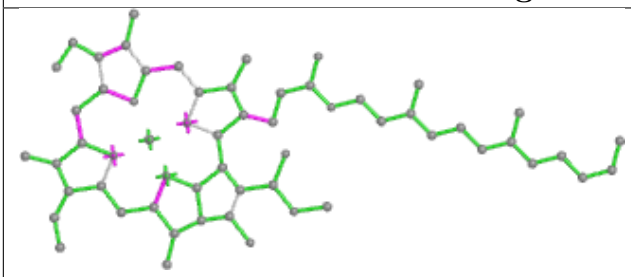
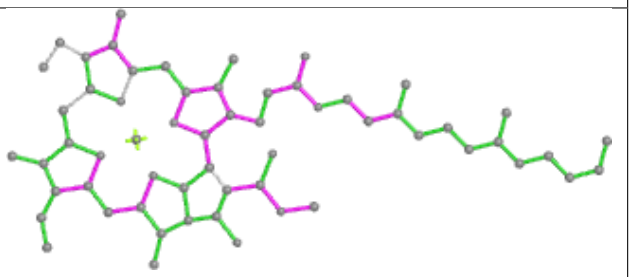
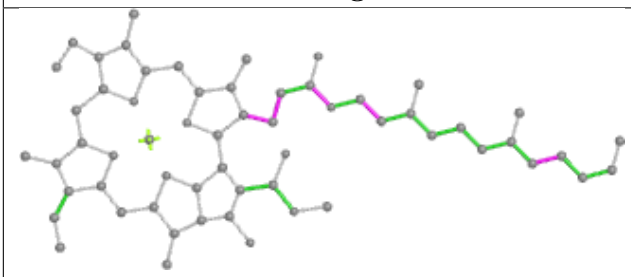
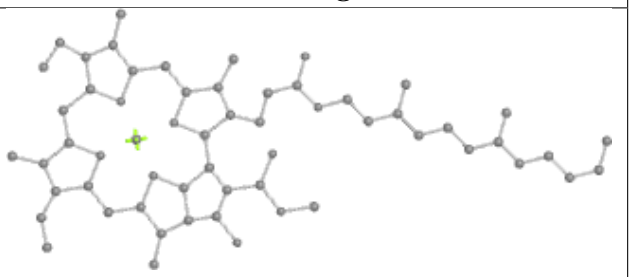
 Bond lengths	 Bond angles
 Torsions	 Rings

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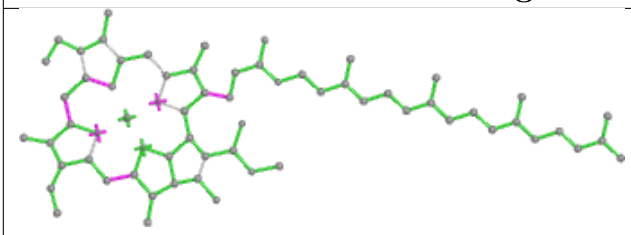
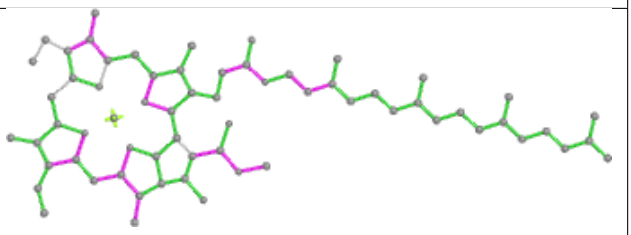
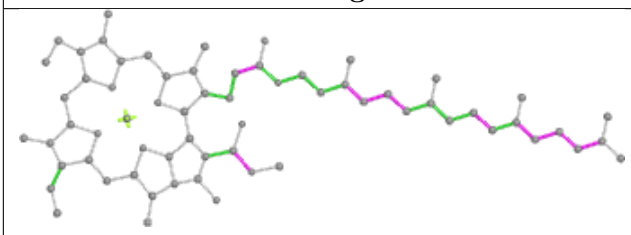
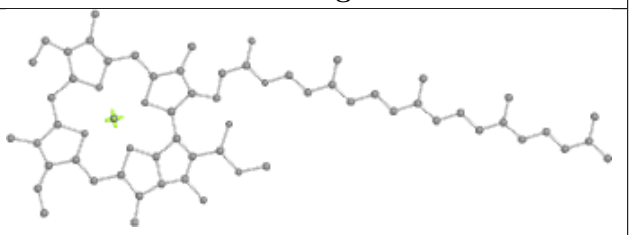
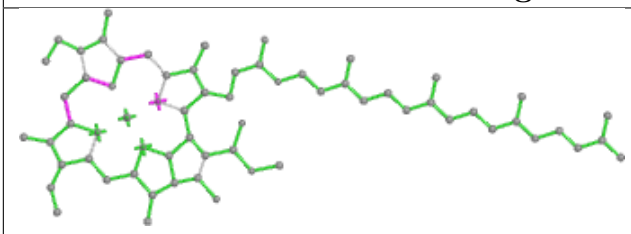
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1103



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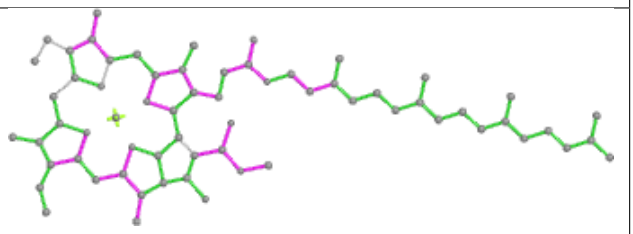
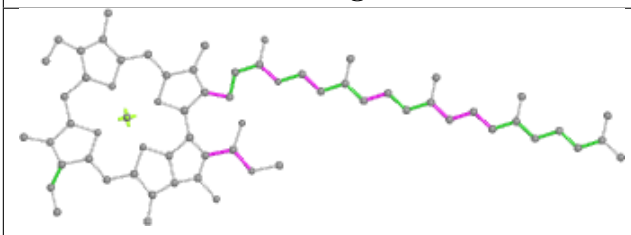


Bond angles



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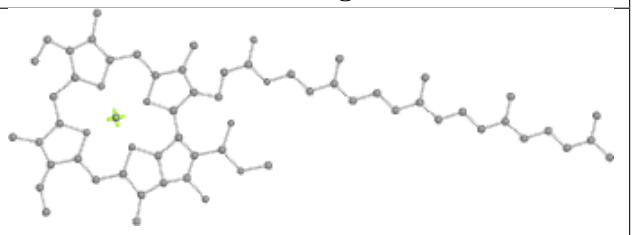
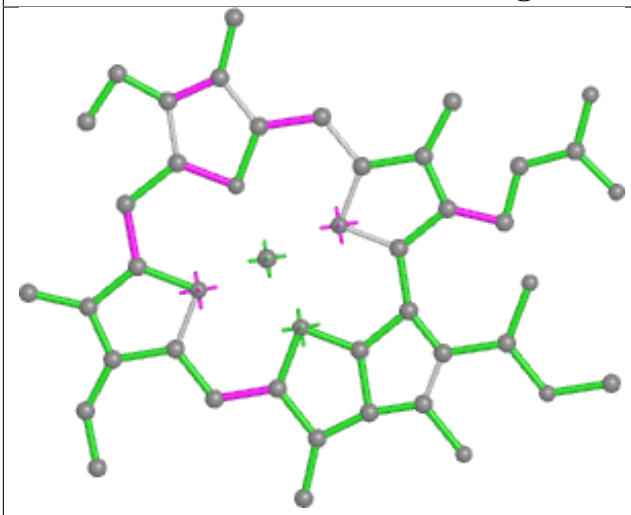


Rings

Ligand CLA B 1208



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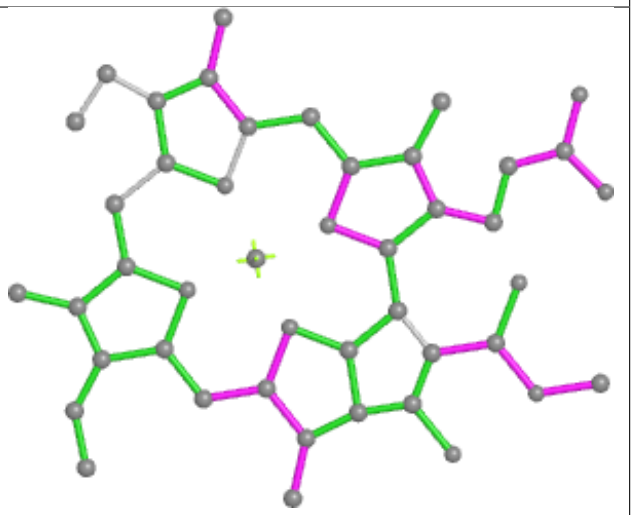
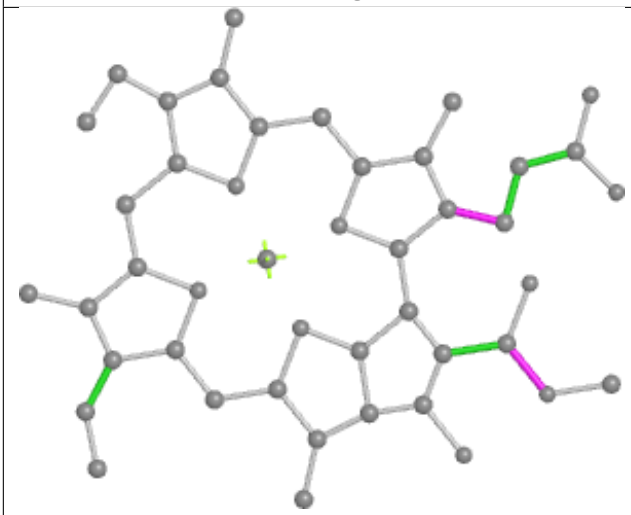


Bond angles



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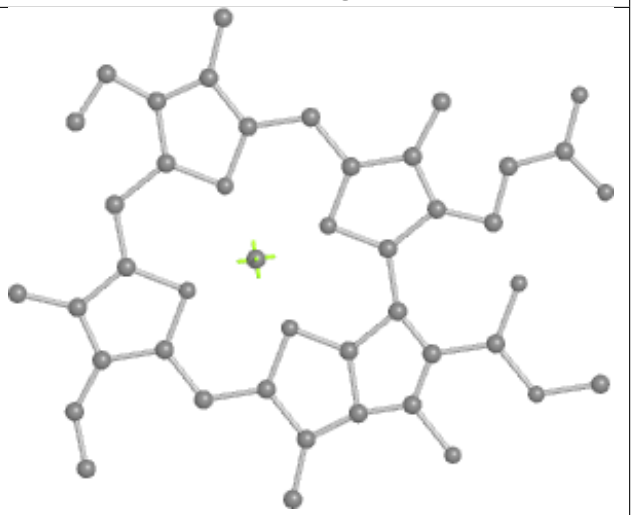
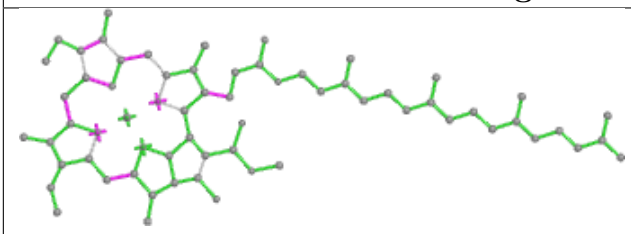


Rings

Ligand CLA A 1136



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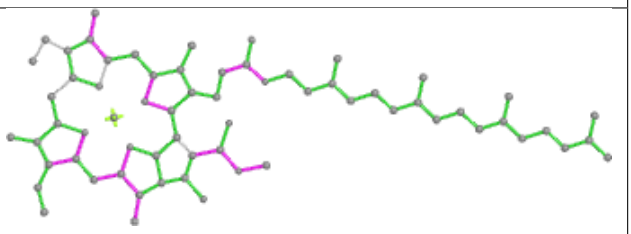

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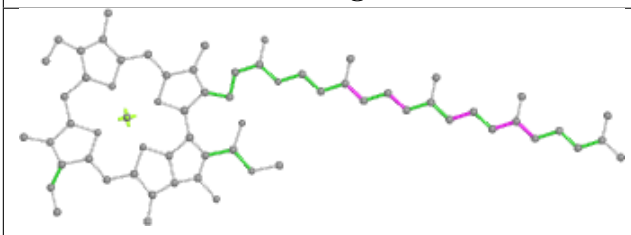

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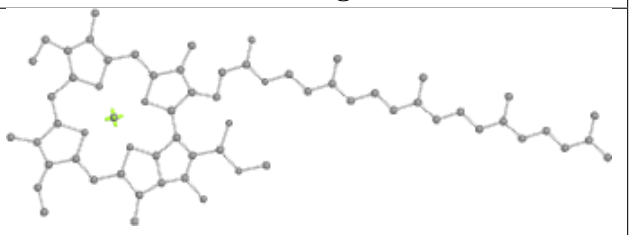
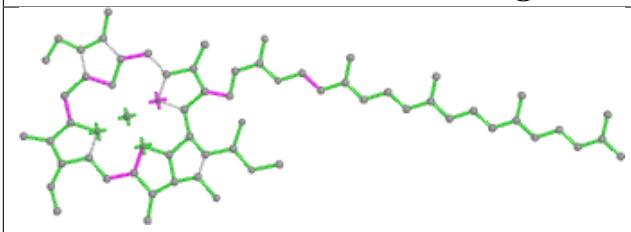


Rings

Ligand CLA A 1119



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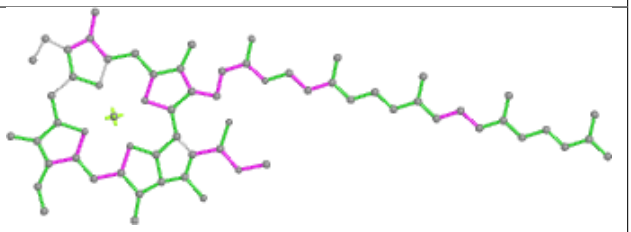
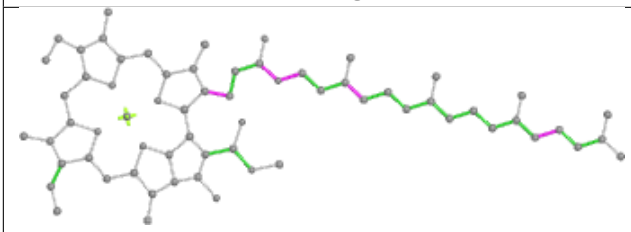


Bond angles



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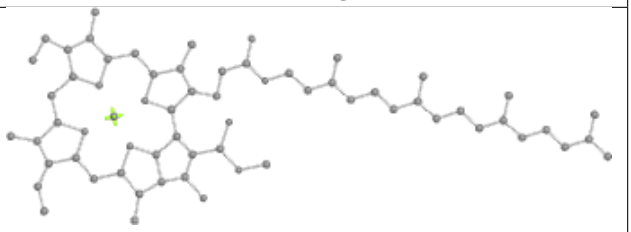
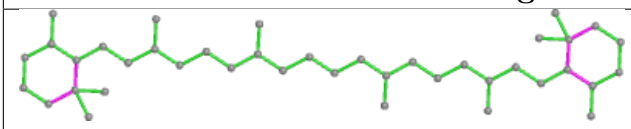


Rings

Ligand BCR J 4012



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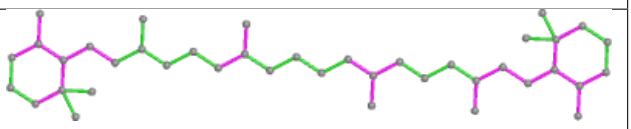
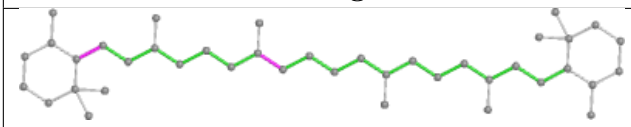
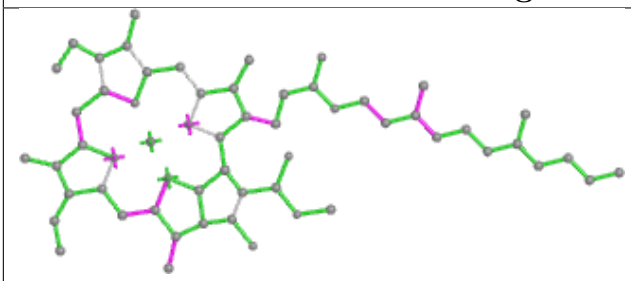
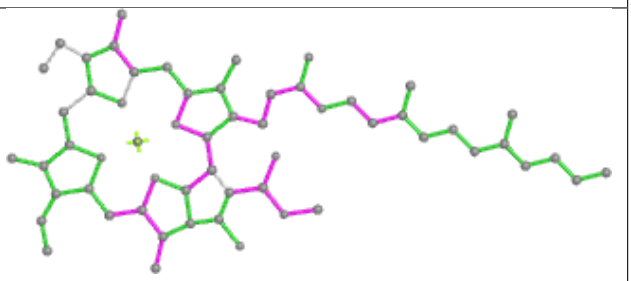
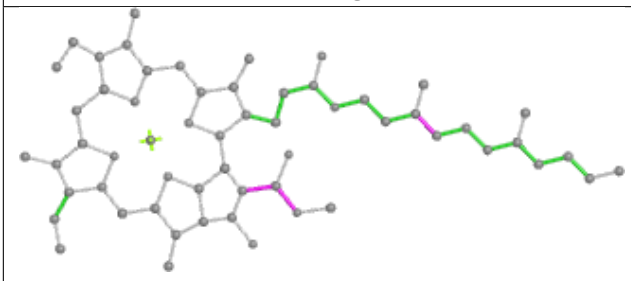
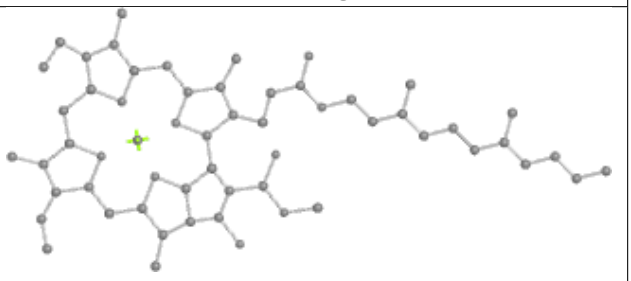


Bond angles



Torsions

Rings

Ligand CLA B 1230	
 Bond lengths	 Bond angles
 Torsions	 Rings

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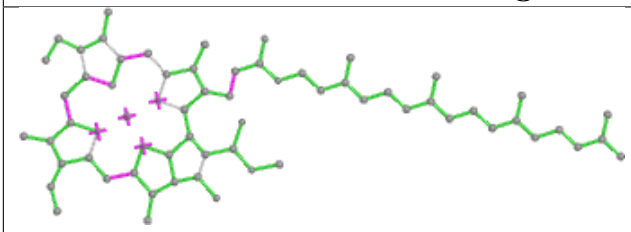
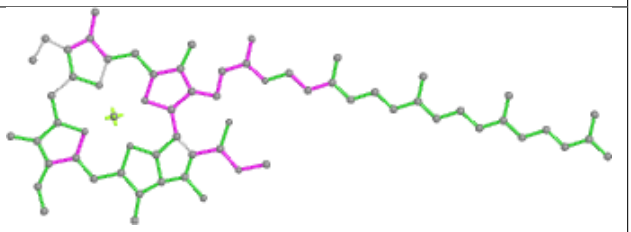
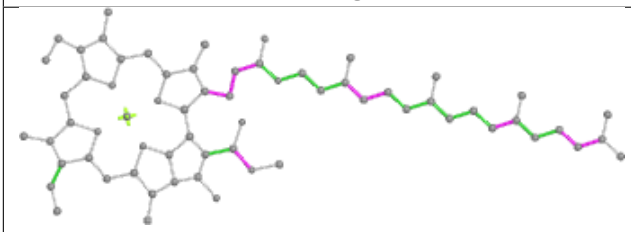
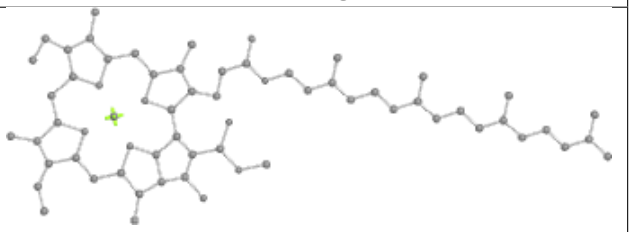
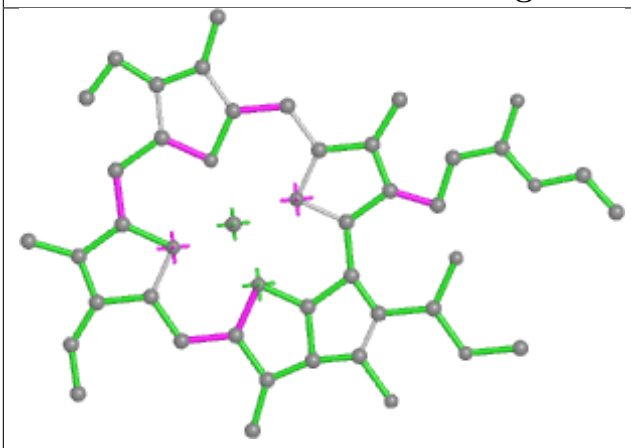
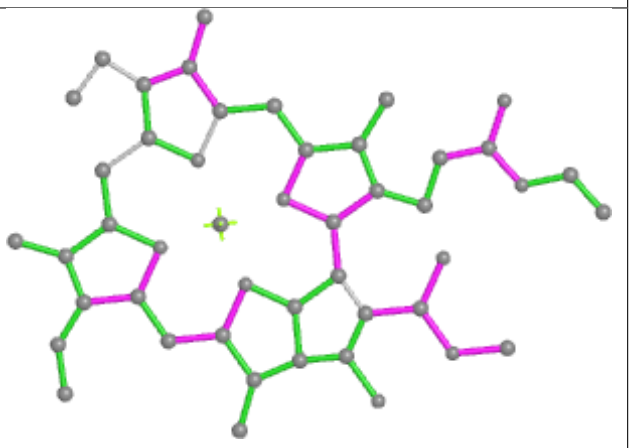
 Bond lengths	 Bond angles
 Torsions	 Rings

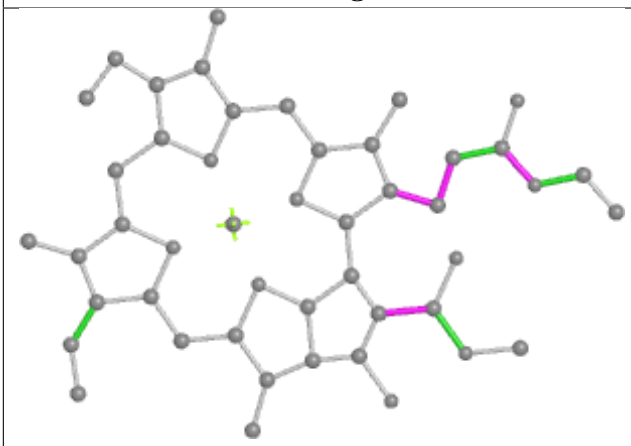
Ligand CLA B 1217



Bond lengths



Bond angles



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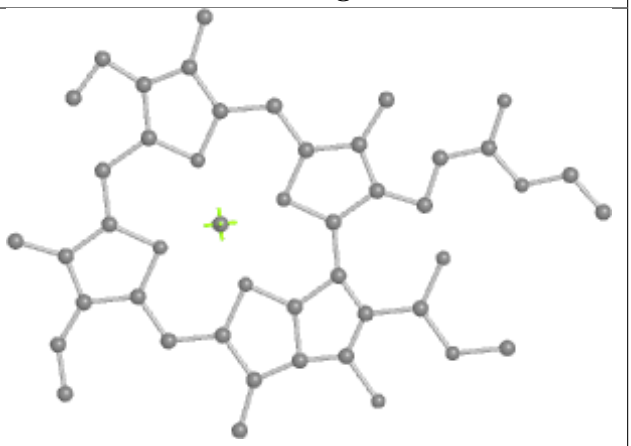
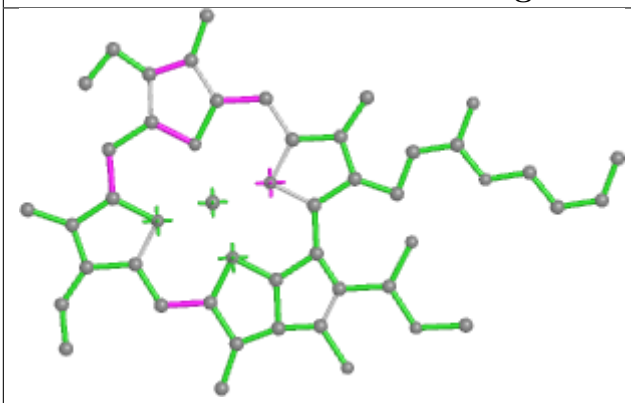


Rings

Ligand CLA A 1120



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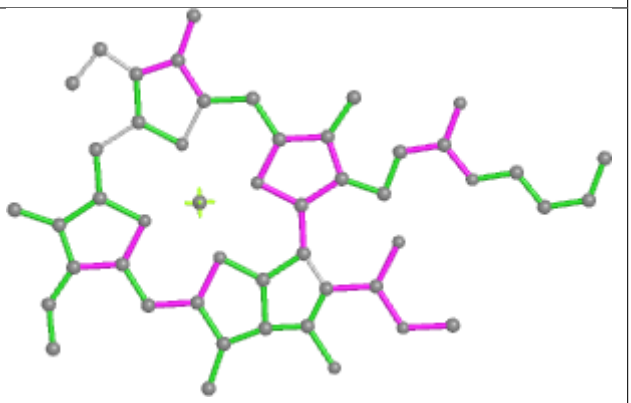
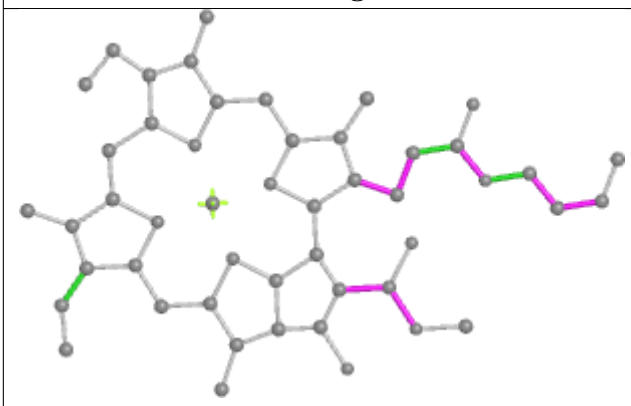


Bond angles



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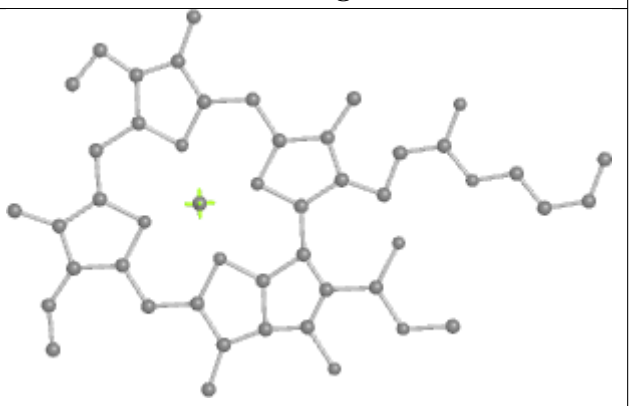

Rings

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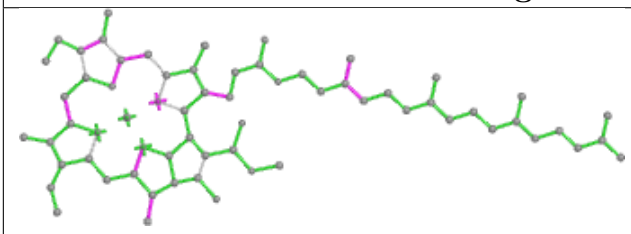

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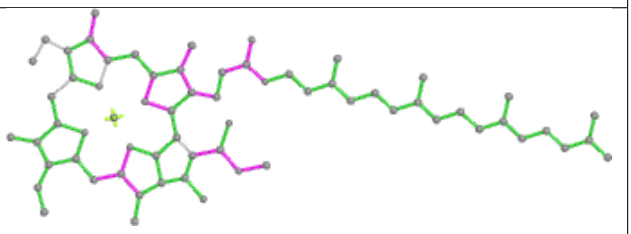
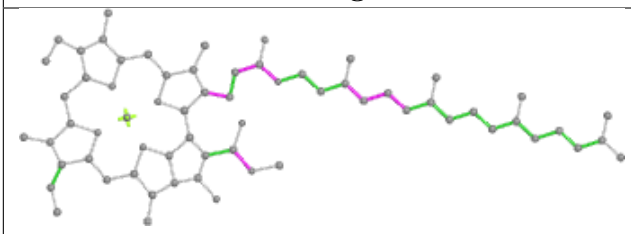


Bond angles



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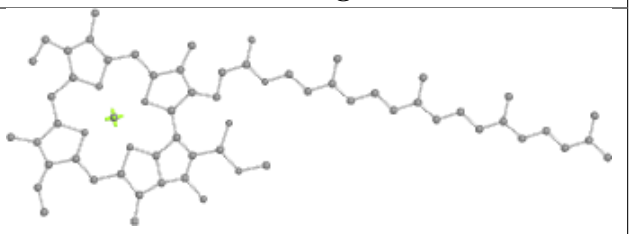
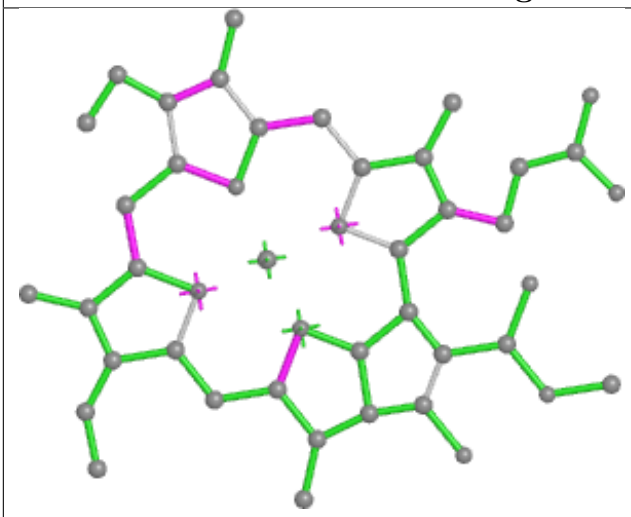
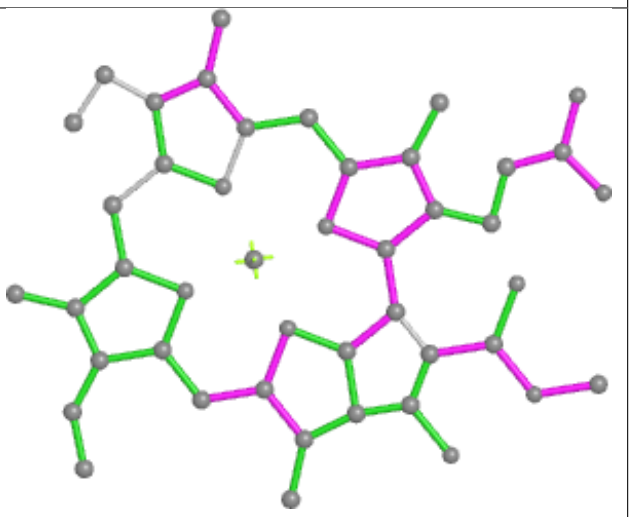


Rings

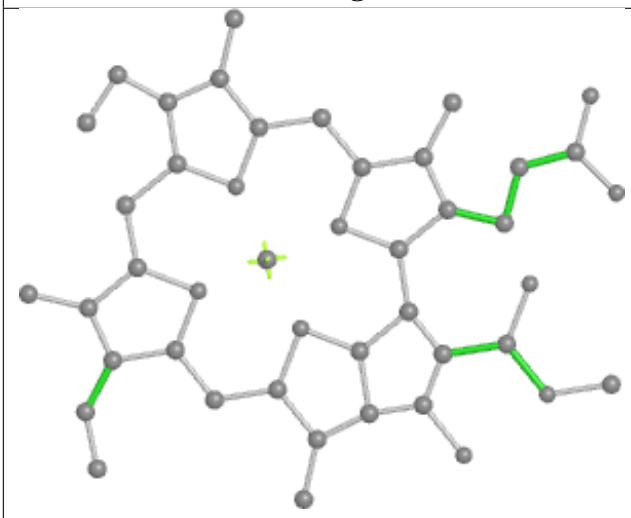
Ligand CLA B 1232



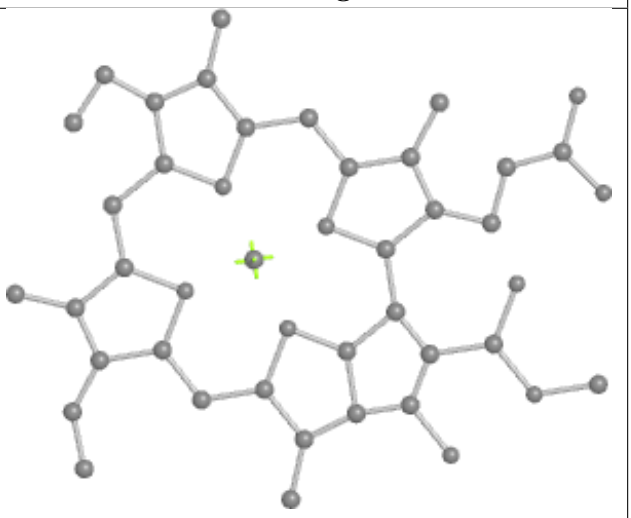
Bond lengths



Bond angles

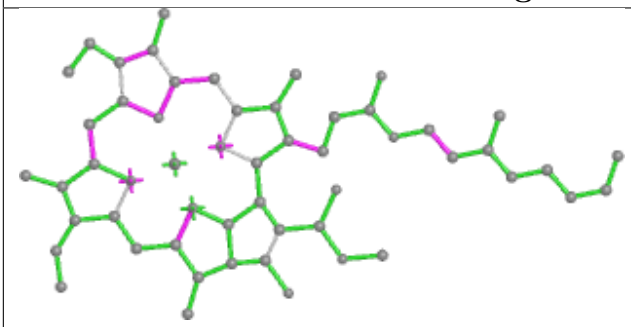


Torsions



Rings

Ligand CLA A 1115



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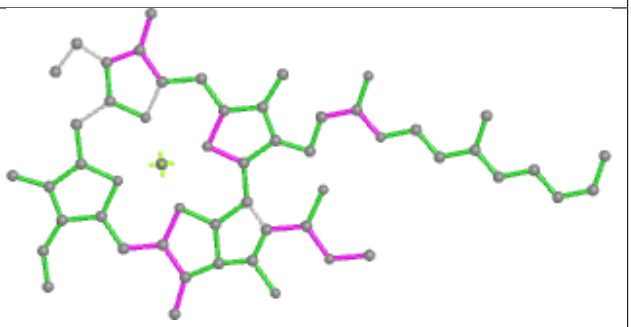
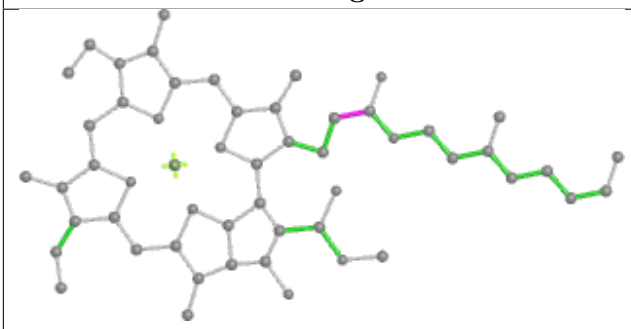


Bond angles



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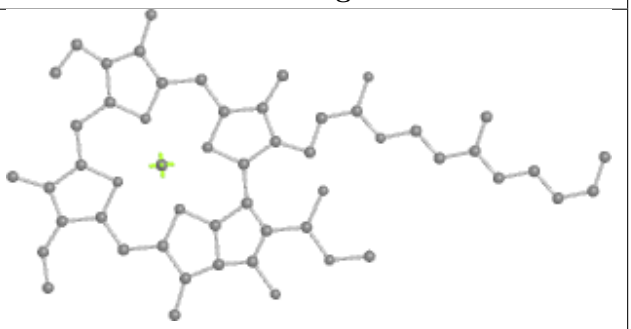
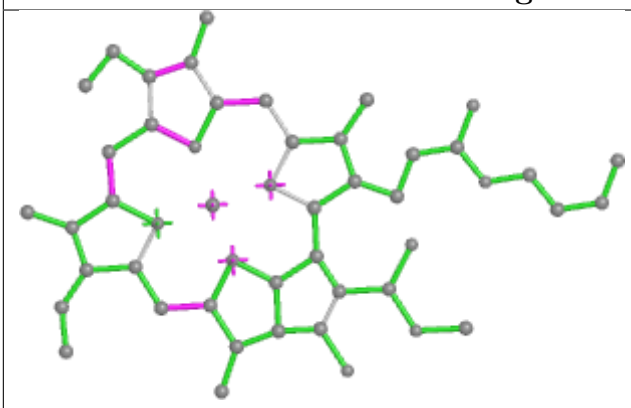


Rings

Ligand CLA B 1228



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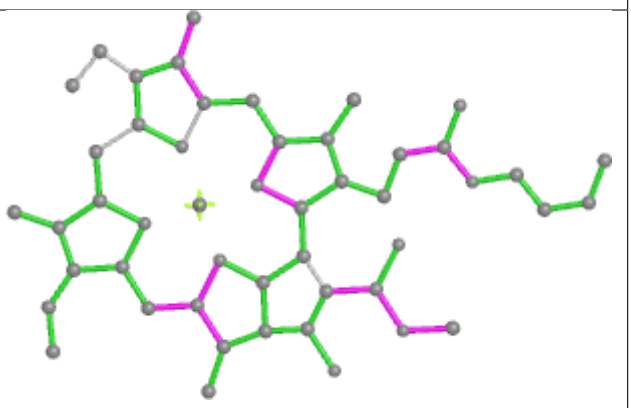
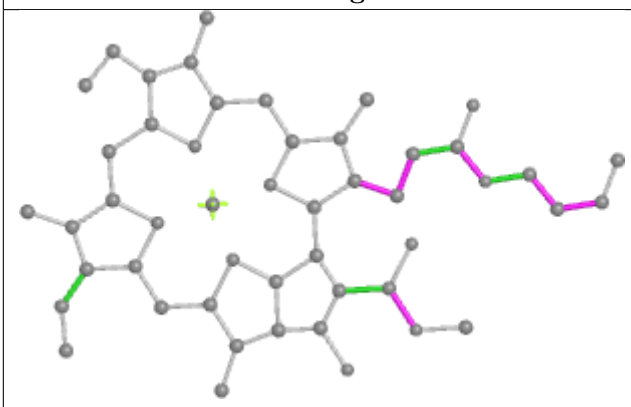


Bond angles



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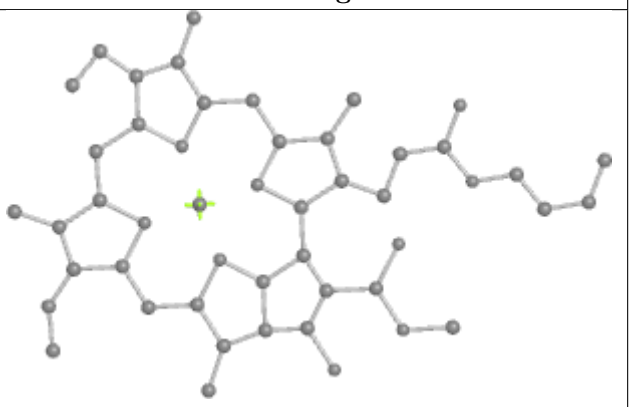
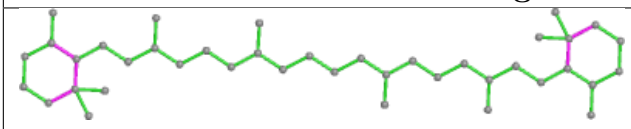


Rings

Ligand BCR B 4010



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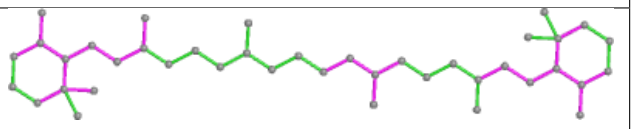
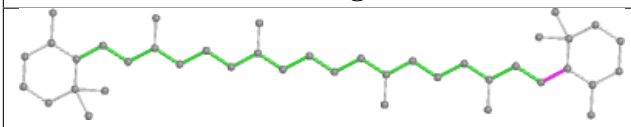


Bond angles



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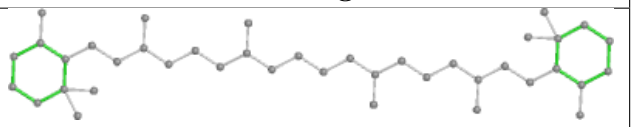
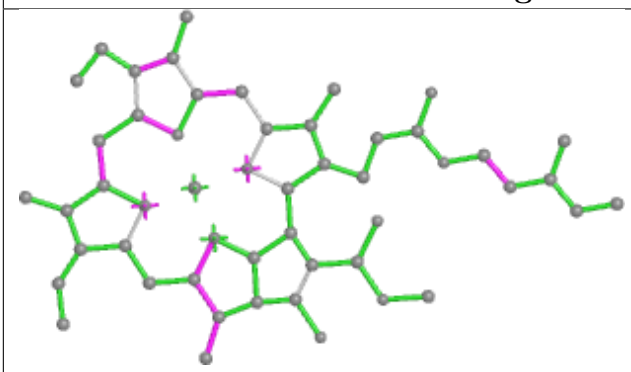


Rings

Ligand CLA A 1105



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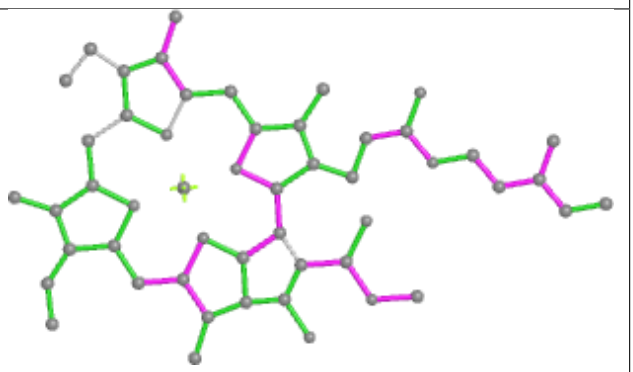
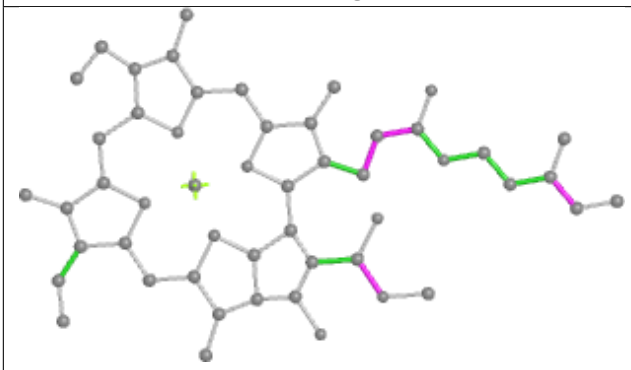


Bond angles



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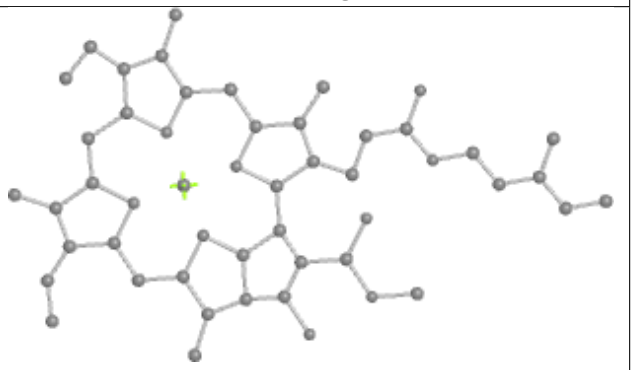
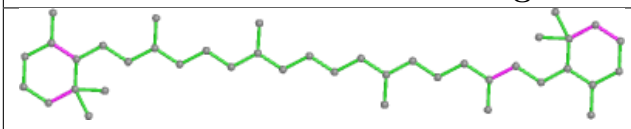


Rings

Ligand BCR B 4014



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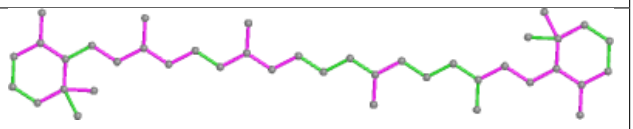
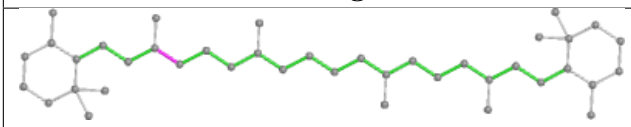
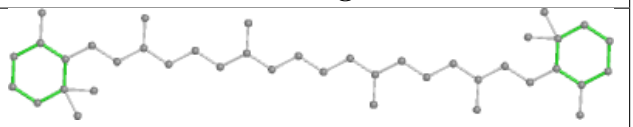


Bond angles

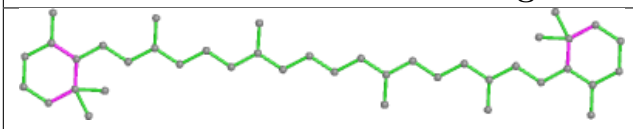


Torsions



Rings

Ligand BCR J 4015



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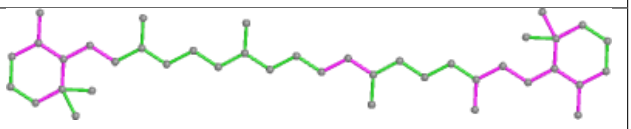
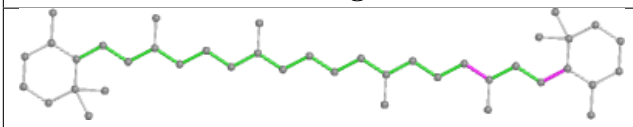


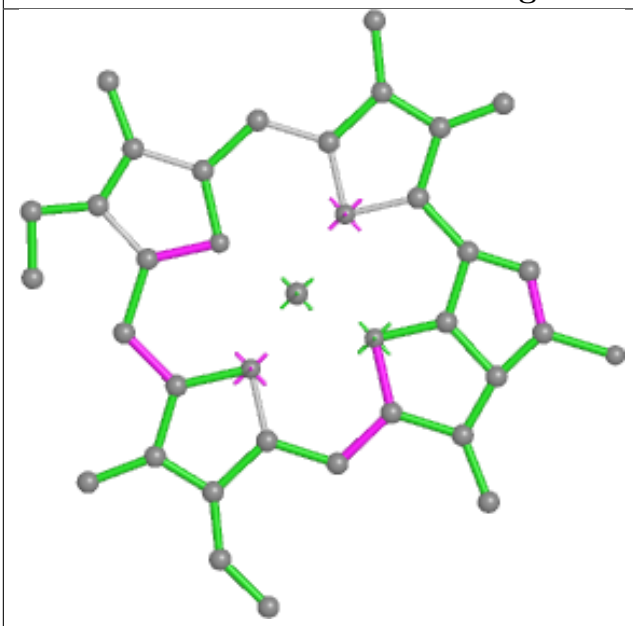
Bond angles



Torsions

Rings

Ligand CLA J 1303



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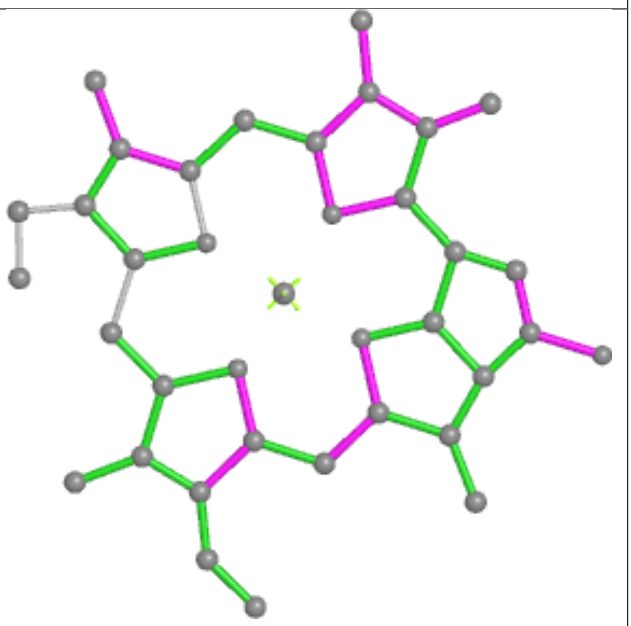
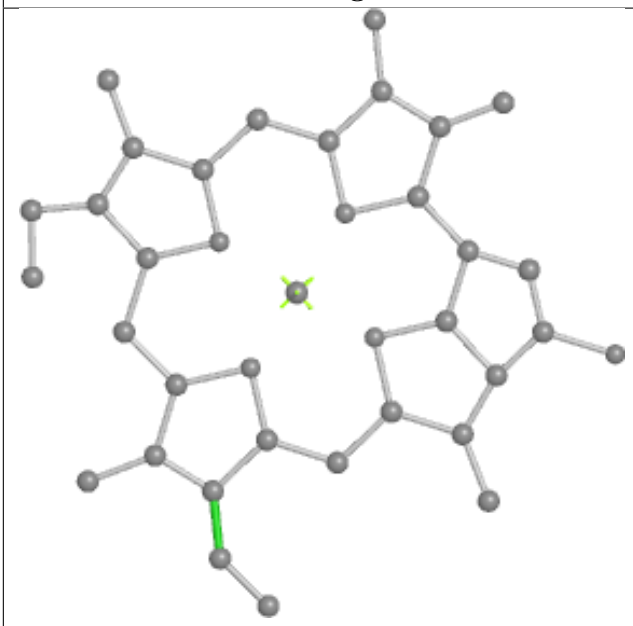
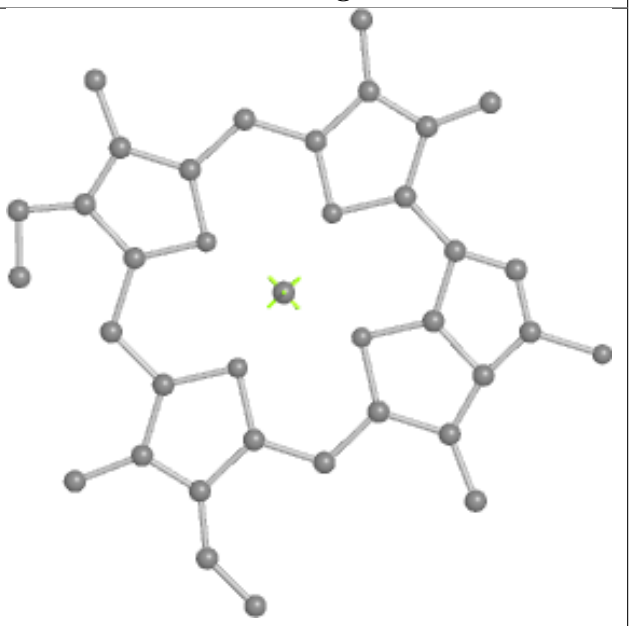


Bond angles

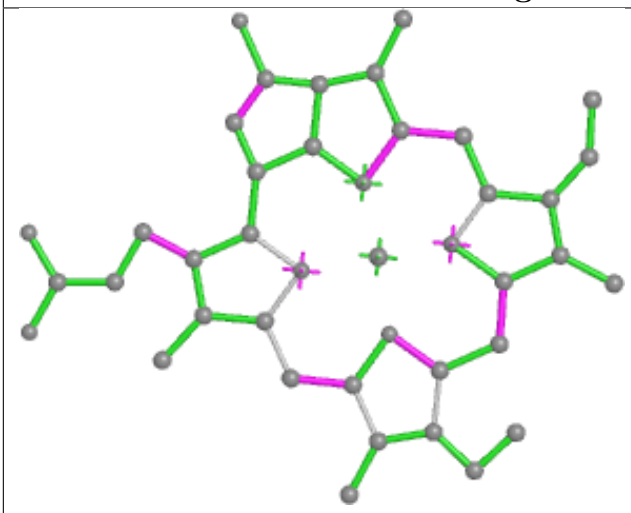


Torsions



Rings

Ligand CLA A 1402



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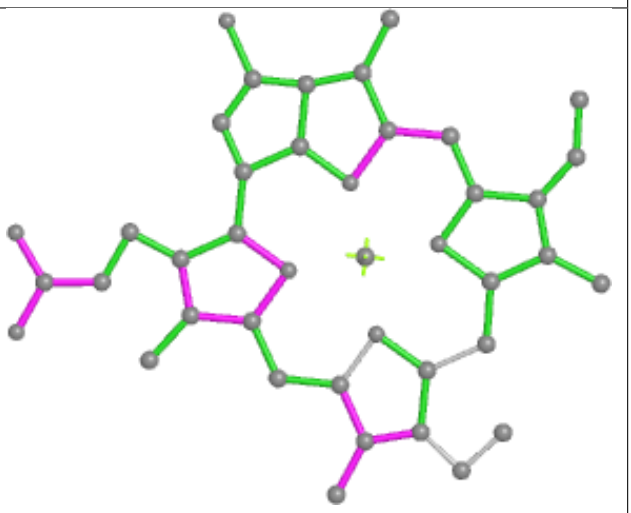
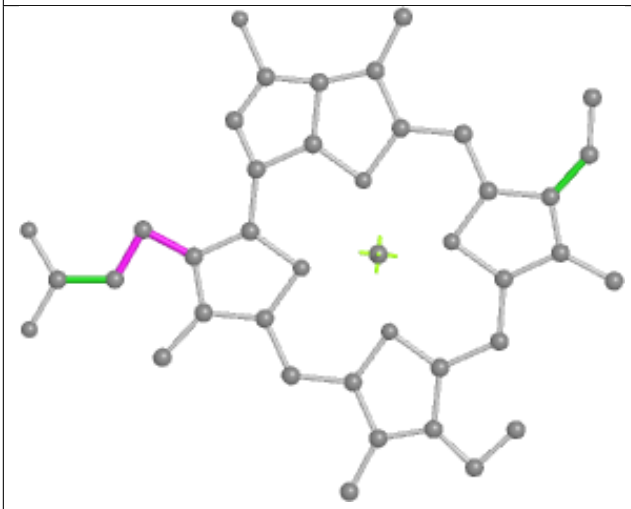


Bond angles



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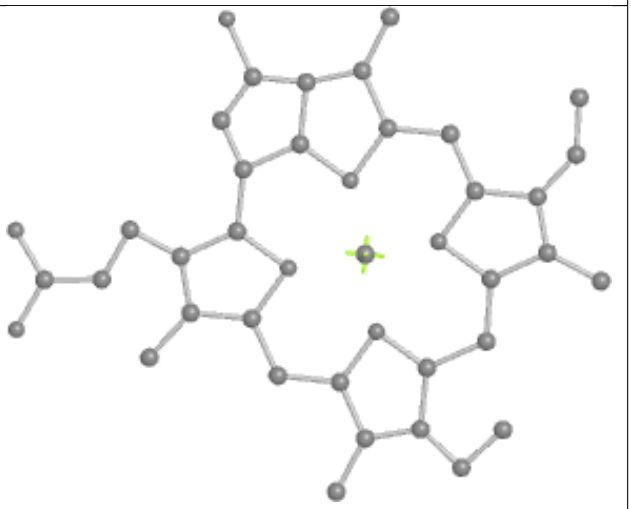
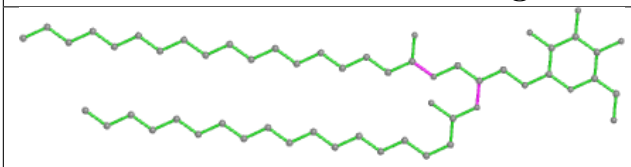


Rings

Ligand LMG B 5002



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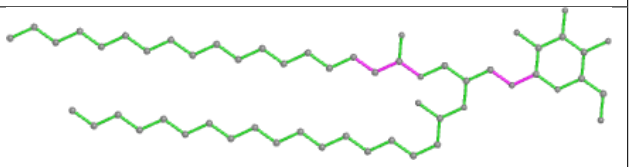
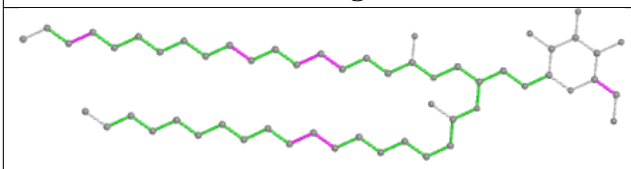


Bond angles



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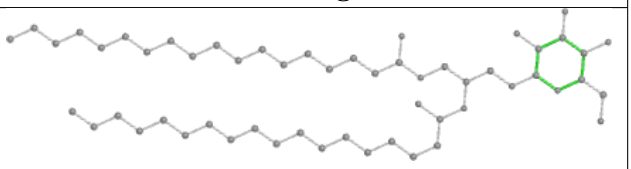
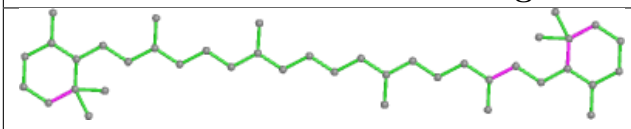


Rings

Ligand BCR F 4016



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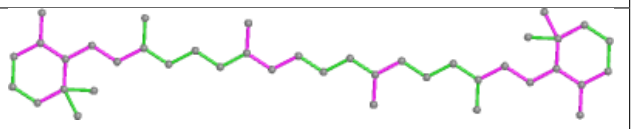
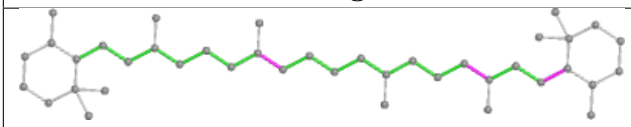


Bond angles



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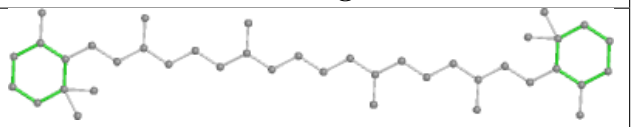
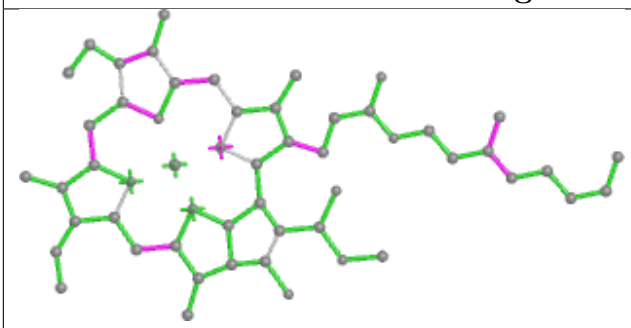


Rings

Ligand CLA A 1110



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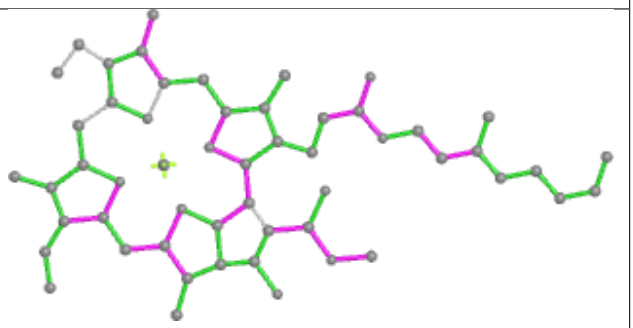
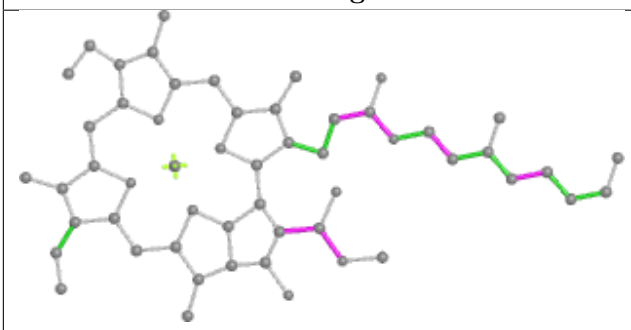


Bond angles



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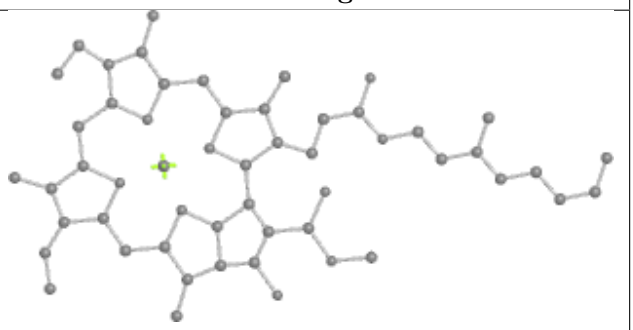
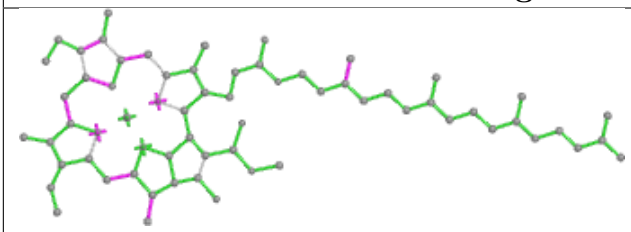


Rings

Ligand CLA B 1023



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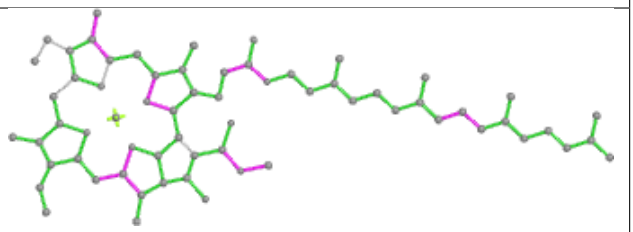
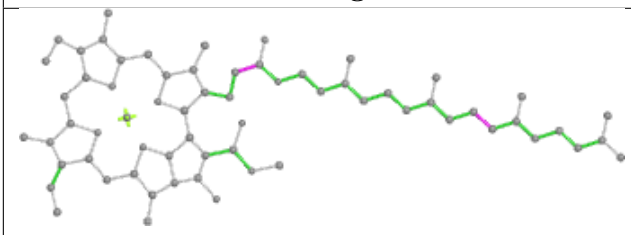


Bond angles



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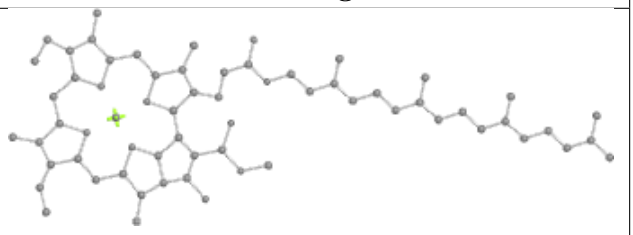
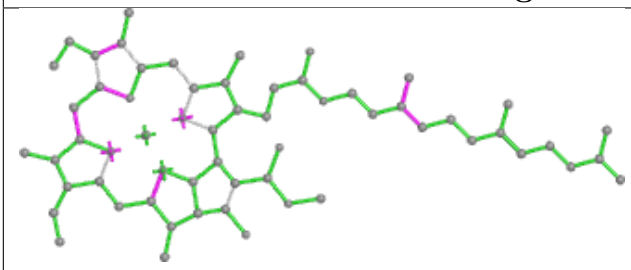
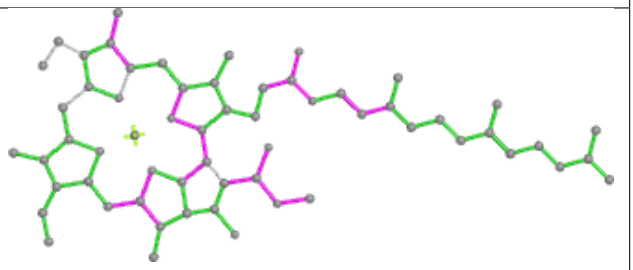
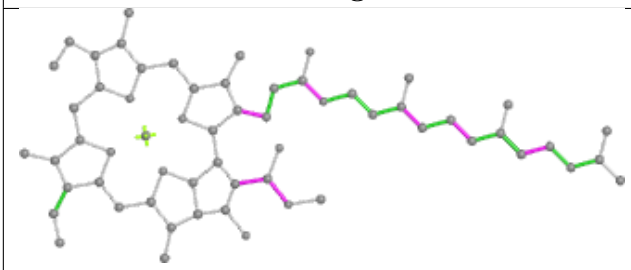
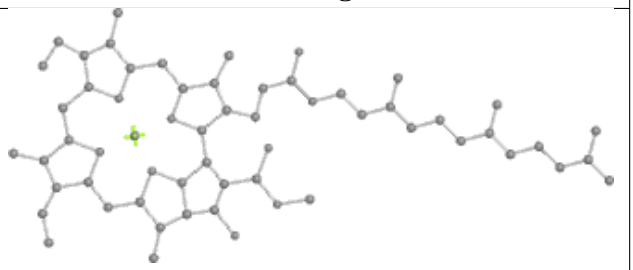
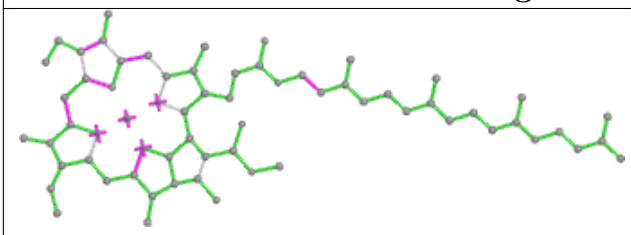
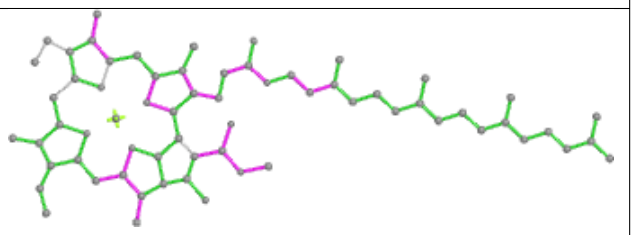
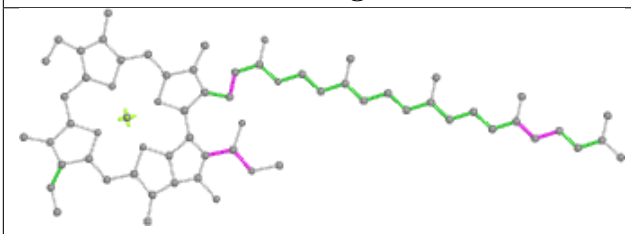
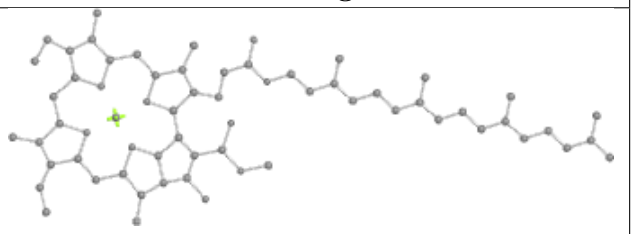
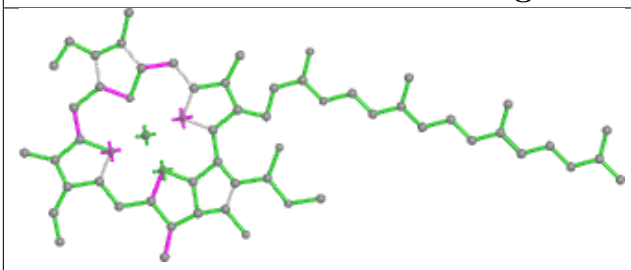
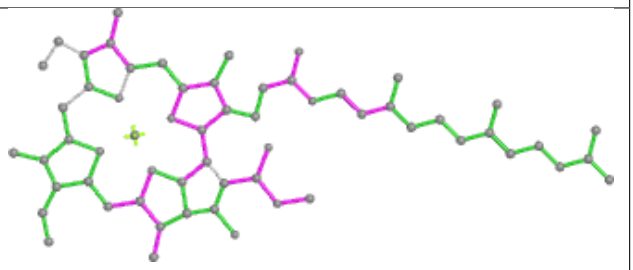
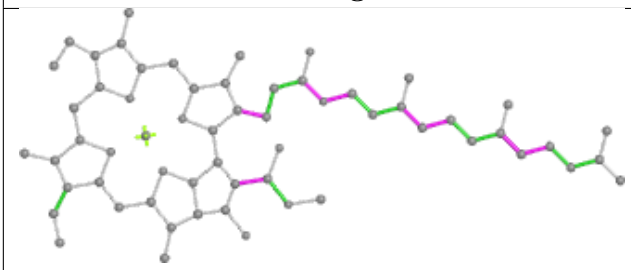
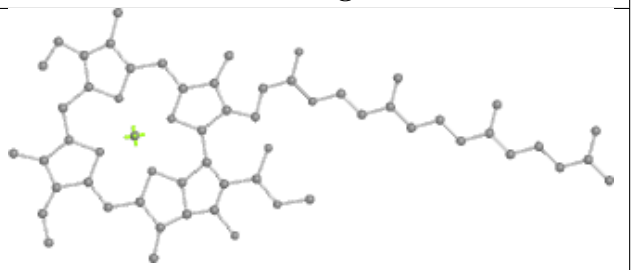


Rings

Ligand CLA B 1234	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1132	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1111	
 Bond lengths	 Bond angles
 Torsions	 Rings

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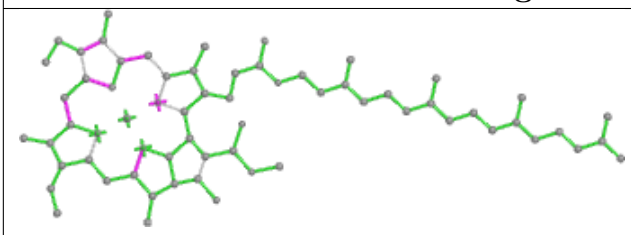
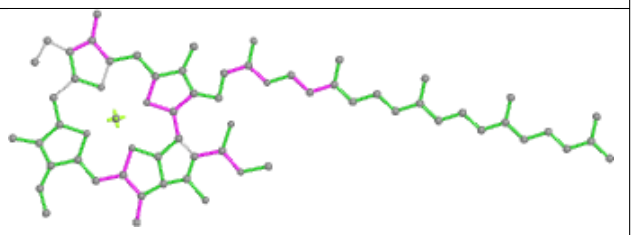
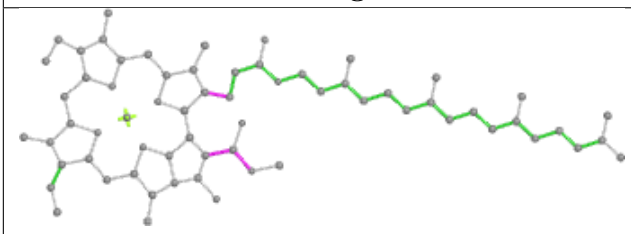
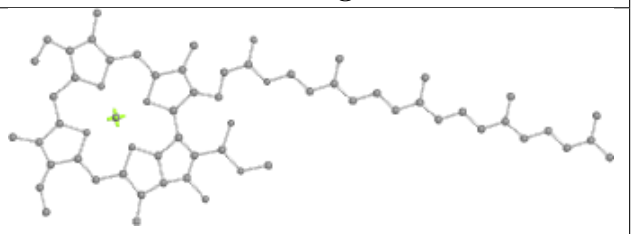
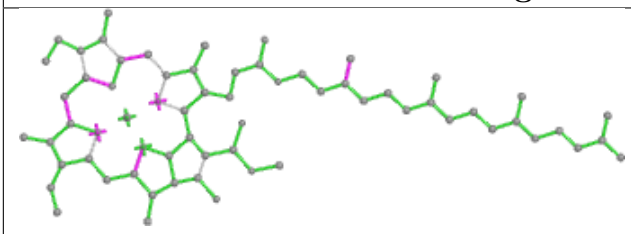
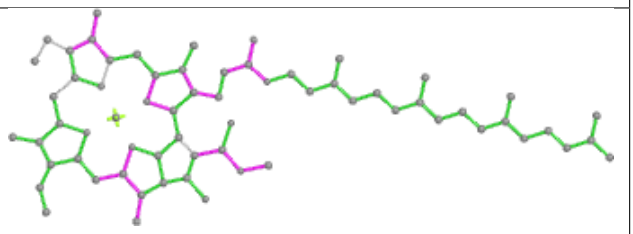
 Bond lengths	 Bond angles
 Torsions	 Rings

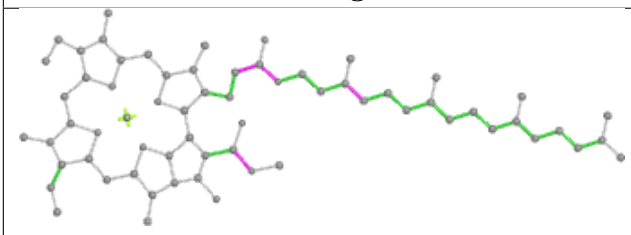
Ligand CLA A 1126



Bond lengths



Bond angles



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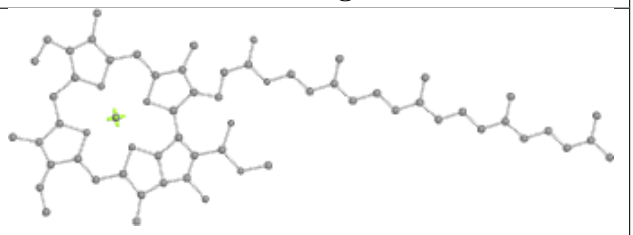
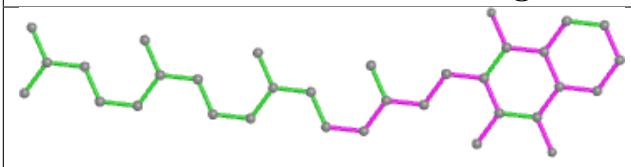


Rings

Ligand PQN B 2002



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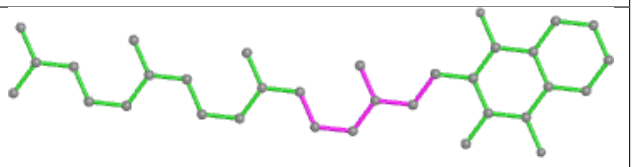
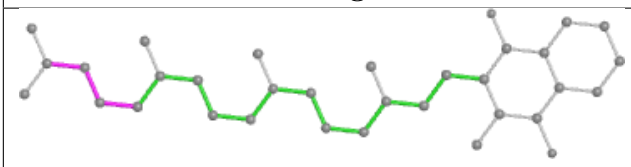


Bond angles



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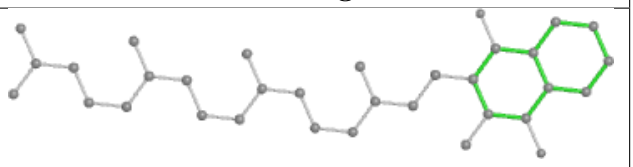
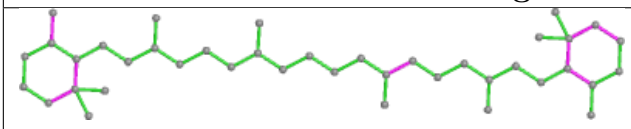


Rings

Ligand BCR A 4008



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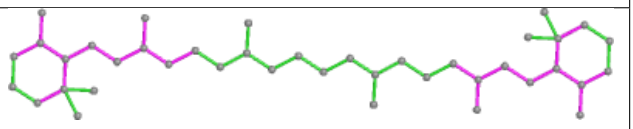

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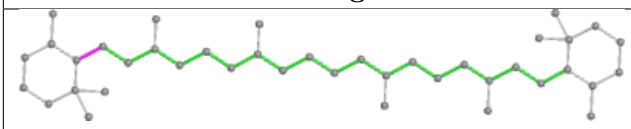

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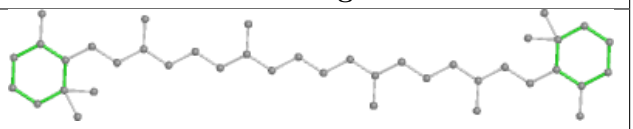
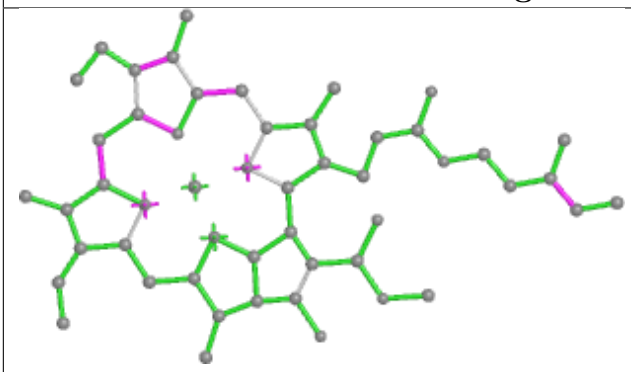


Rings

Ligand CLA A 1139



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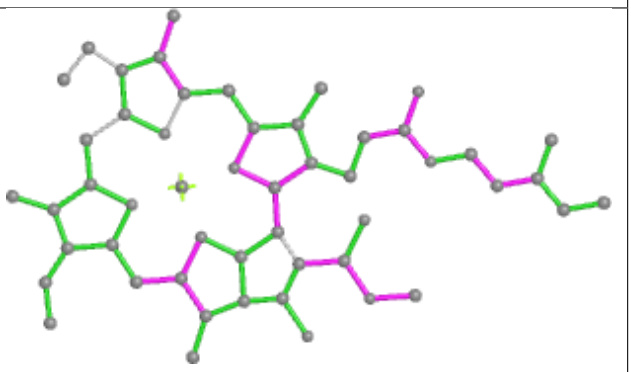
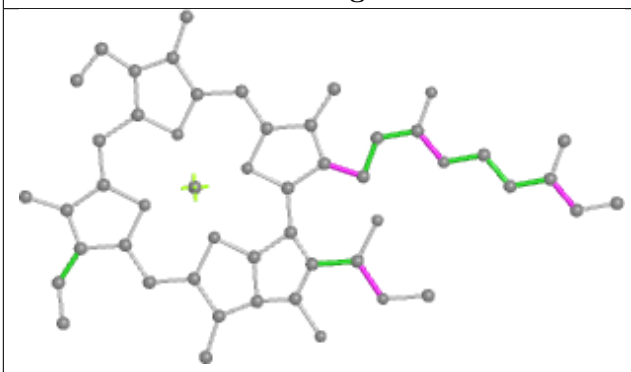


Bond angles



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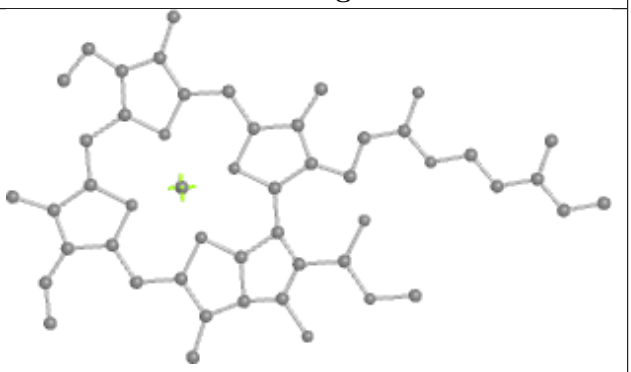
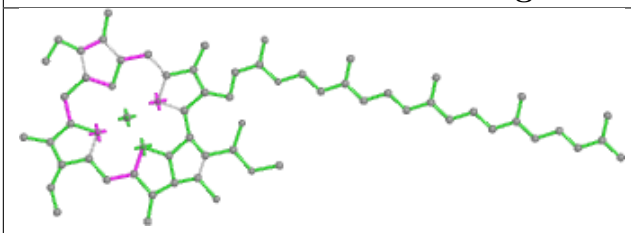


Rings

Ligand CLA B 1235



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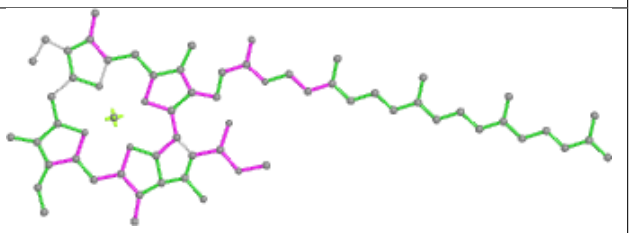

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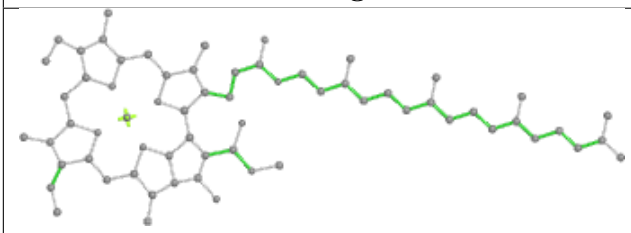

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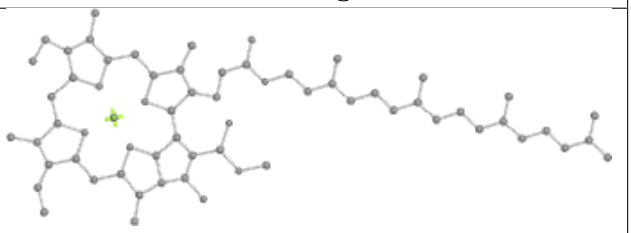
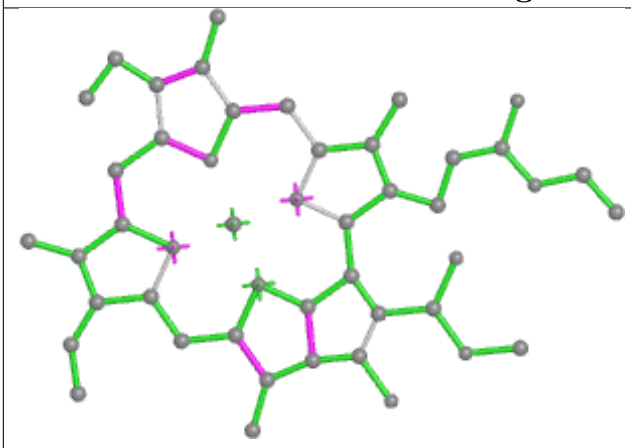


Rings

Ligand CLA B 1236



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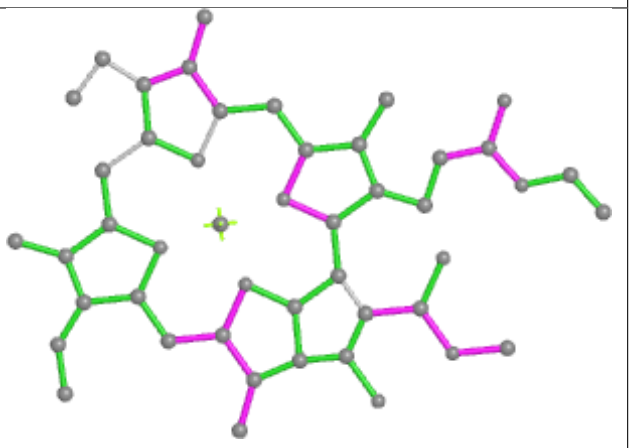
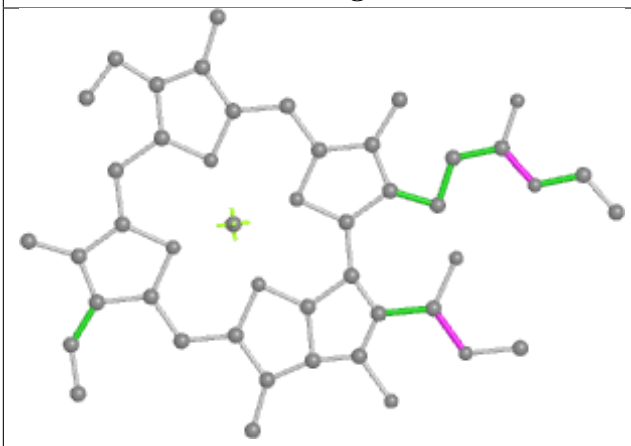


Bond angles



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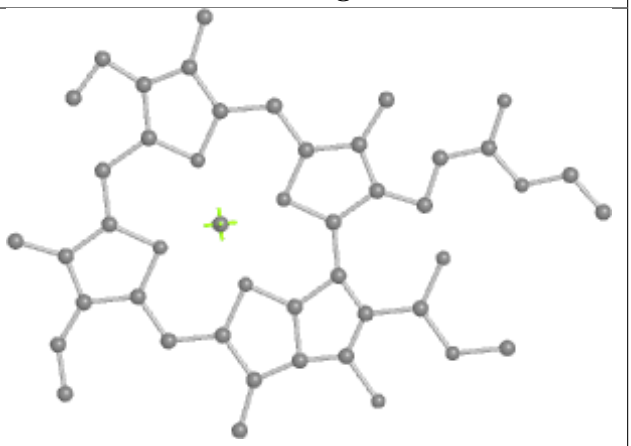
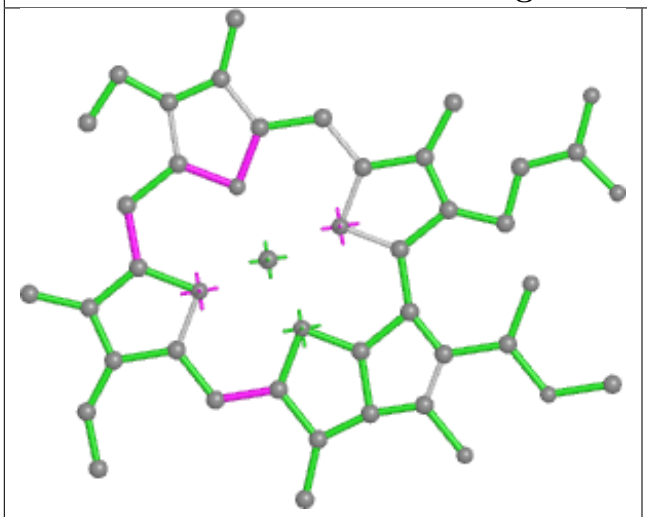


Rings

Ligand CLA A 1113



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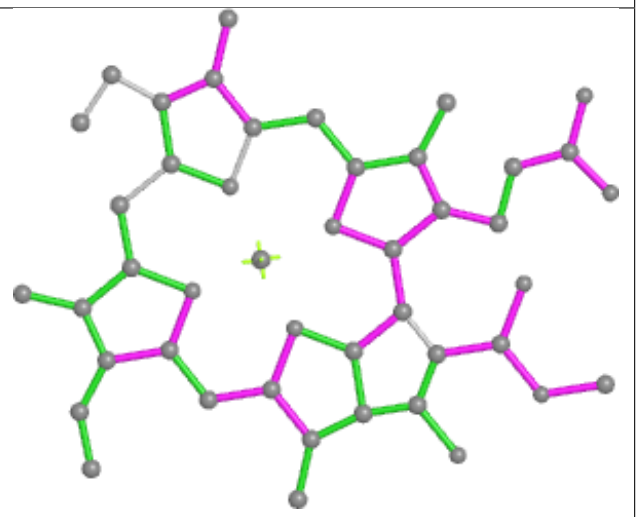
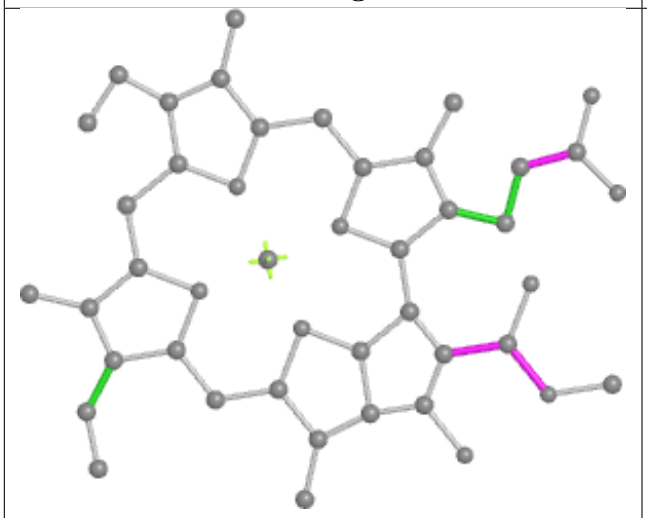


Bond angles



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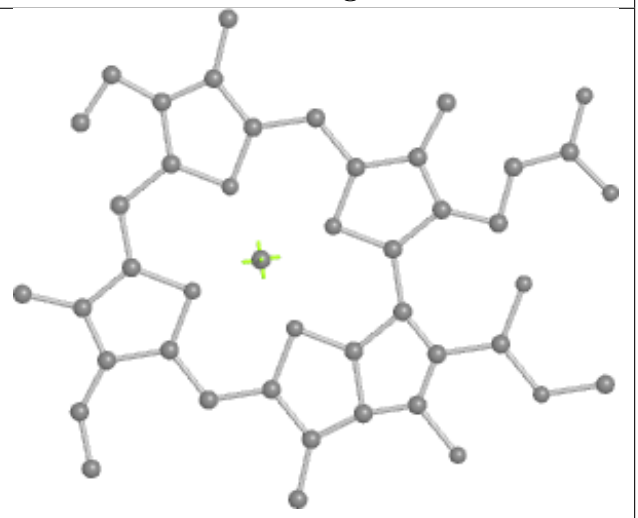
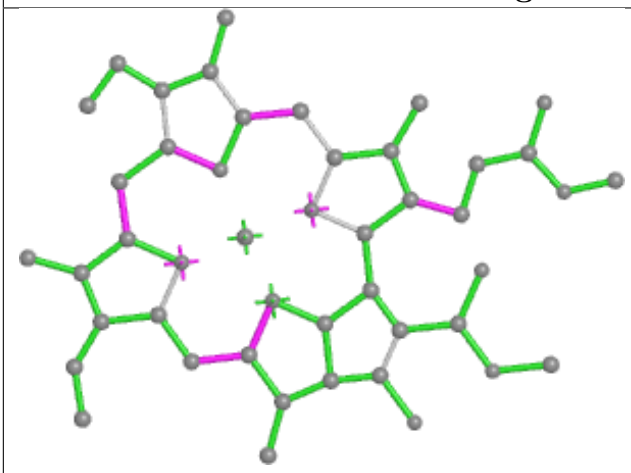
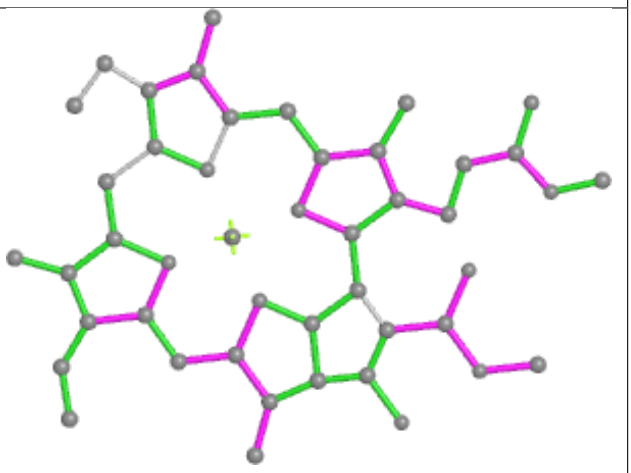


Rings

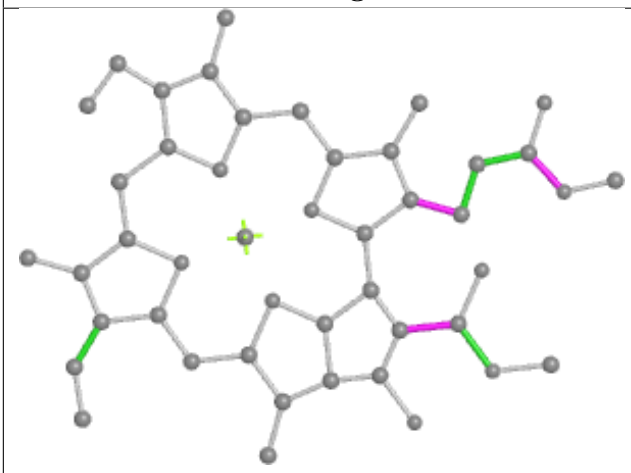
Ligand CLA B 1222



Bond lengths



Bond angles



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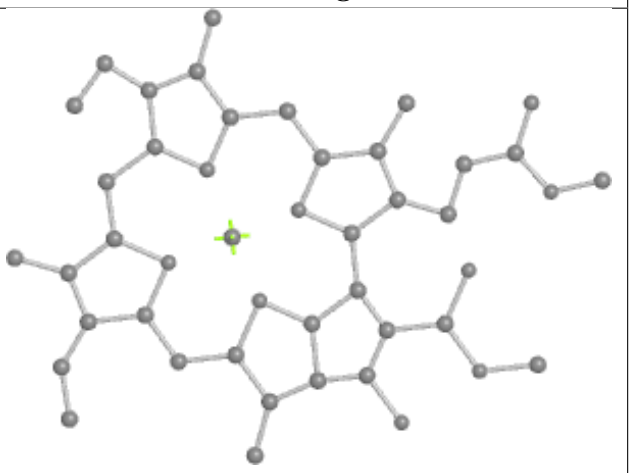
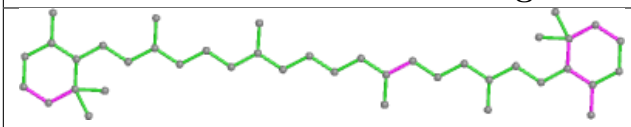
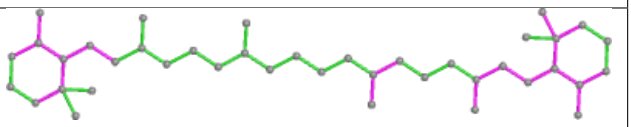


Rings

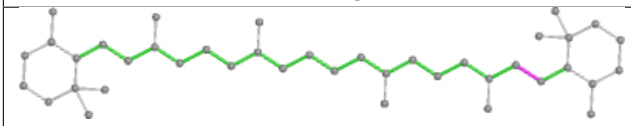
Ligand BCR L 4019



Bond lengths

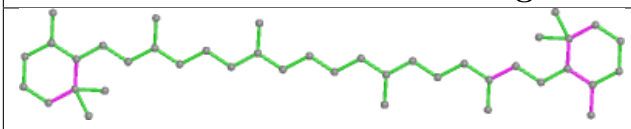
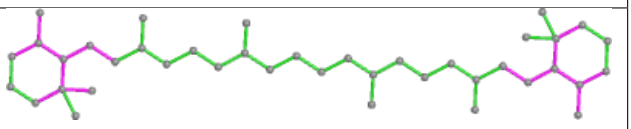
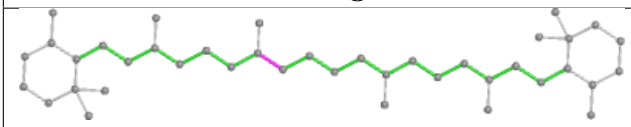


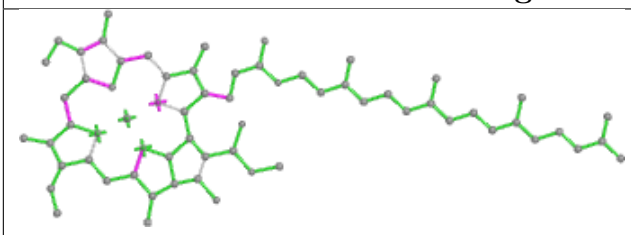
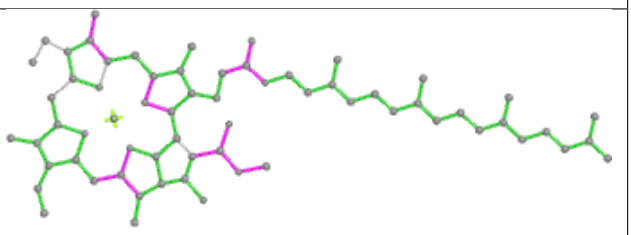
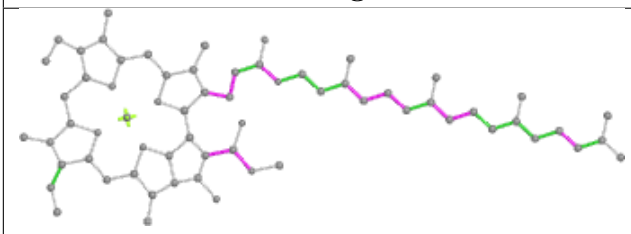
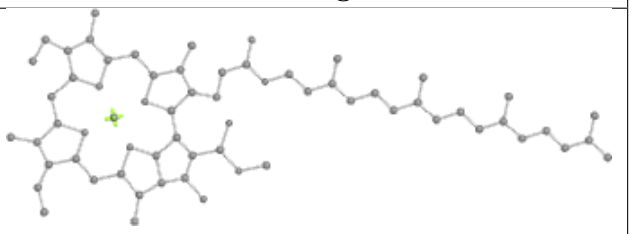
Bond angles



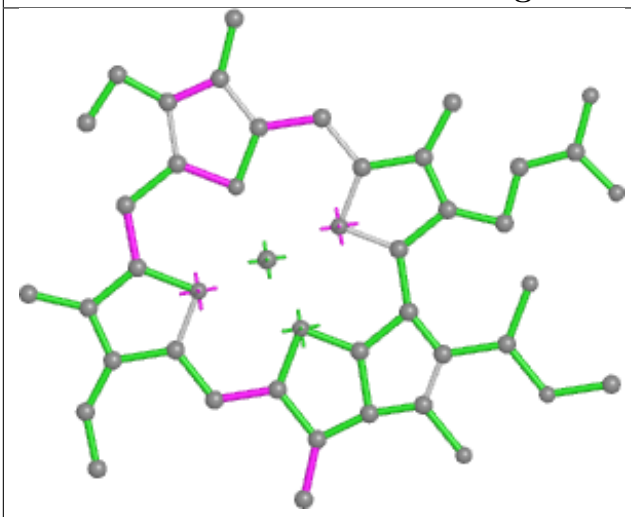
Torsions

Rings

Ligand BCR L 4022	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA A 1106	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 1401



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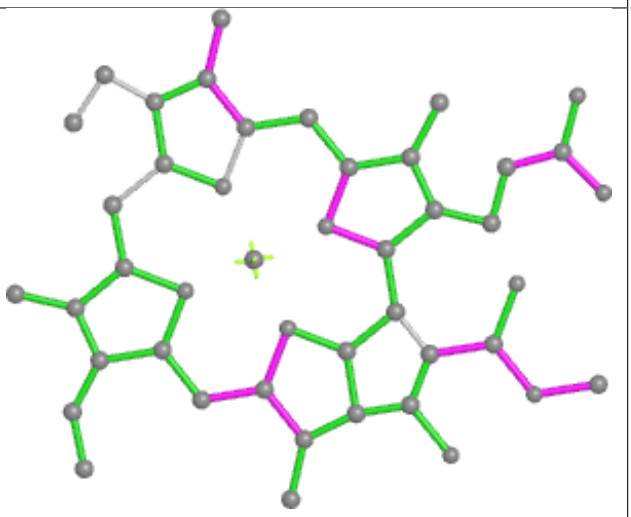

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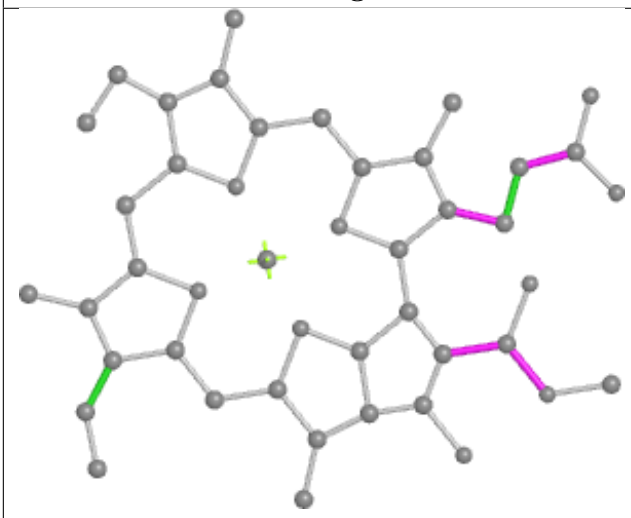

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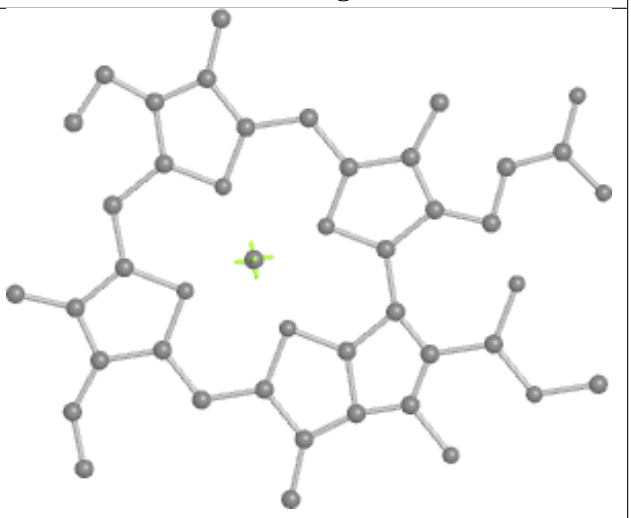
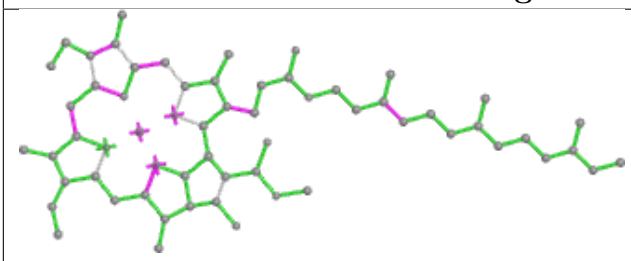


Rings

Ligand CLA A 1118



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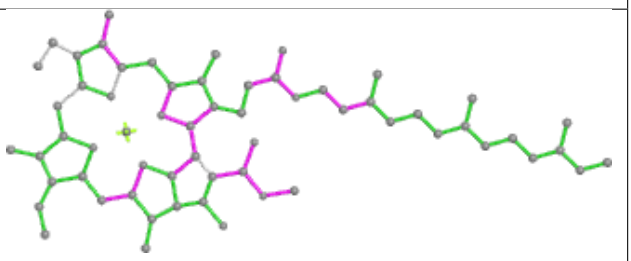

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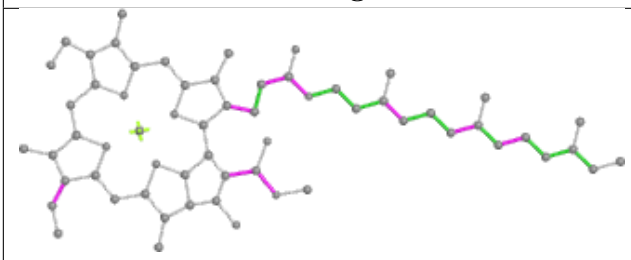

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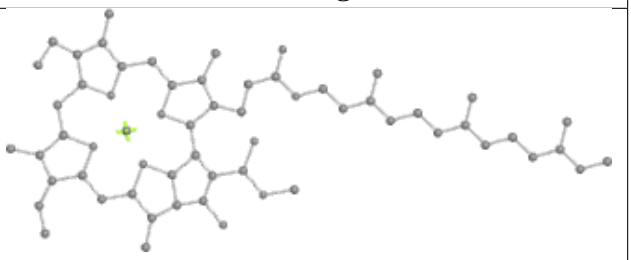
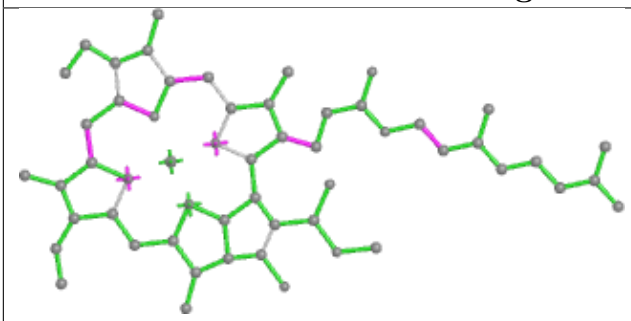


Rings

Ligand CLA B 1219



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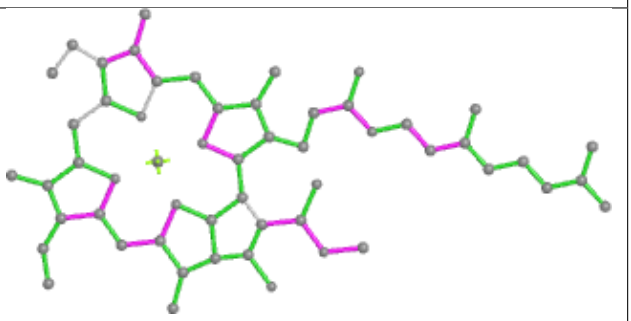

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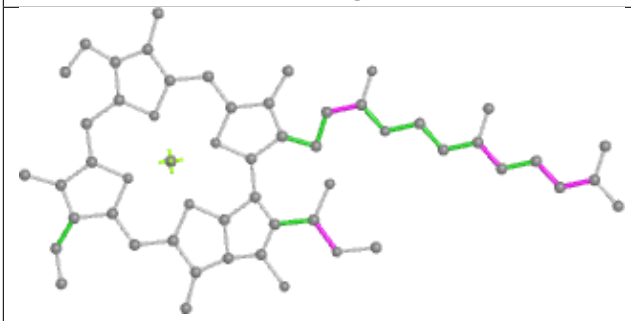

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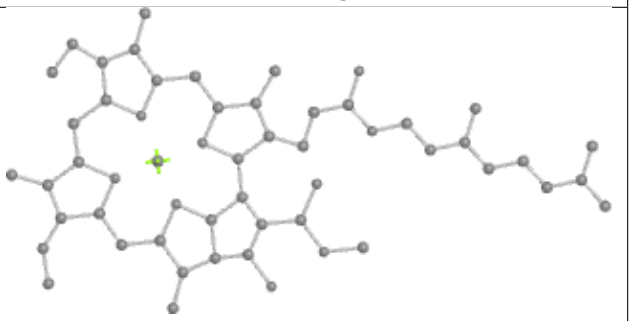
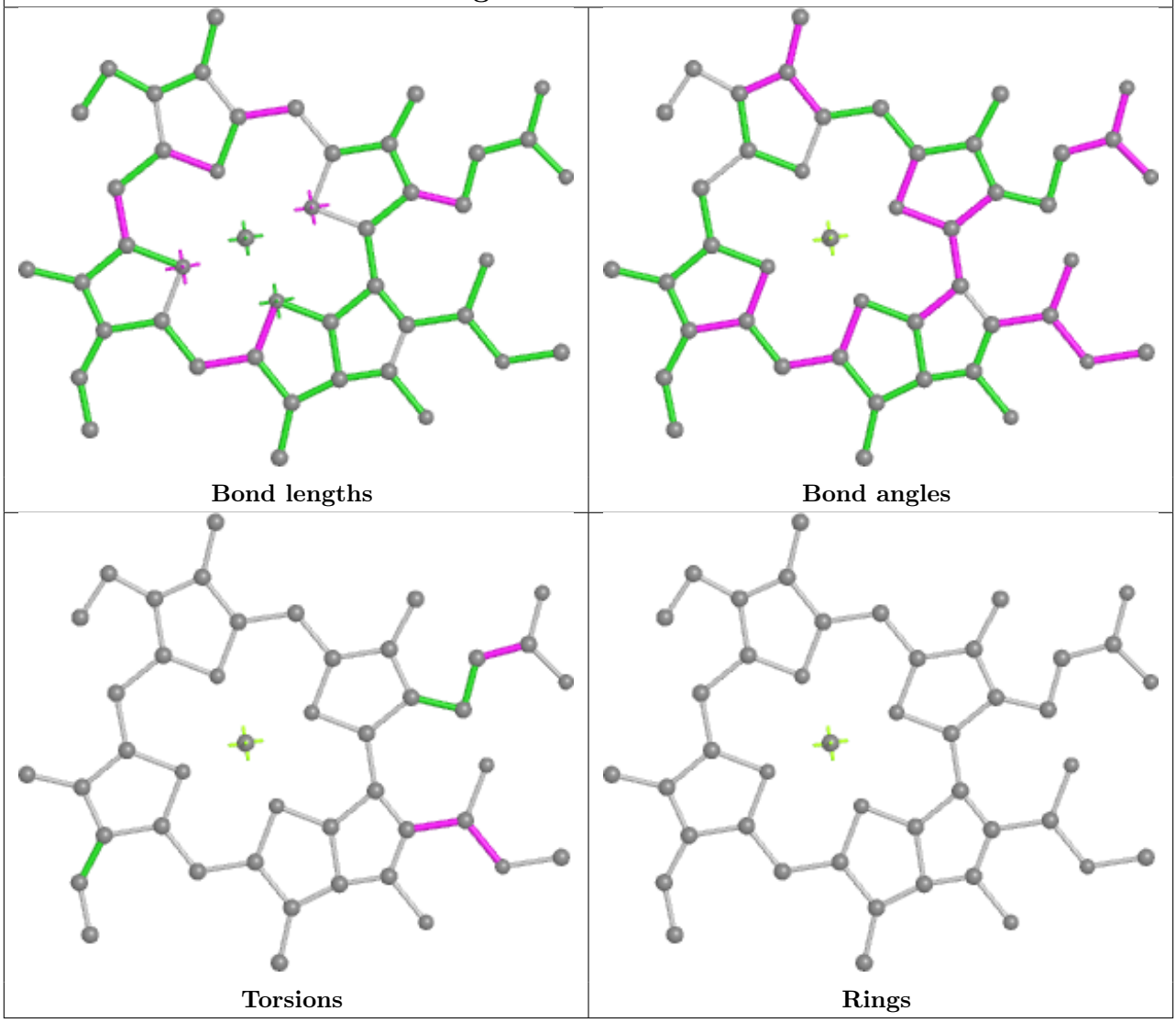
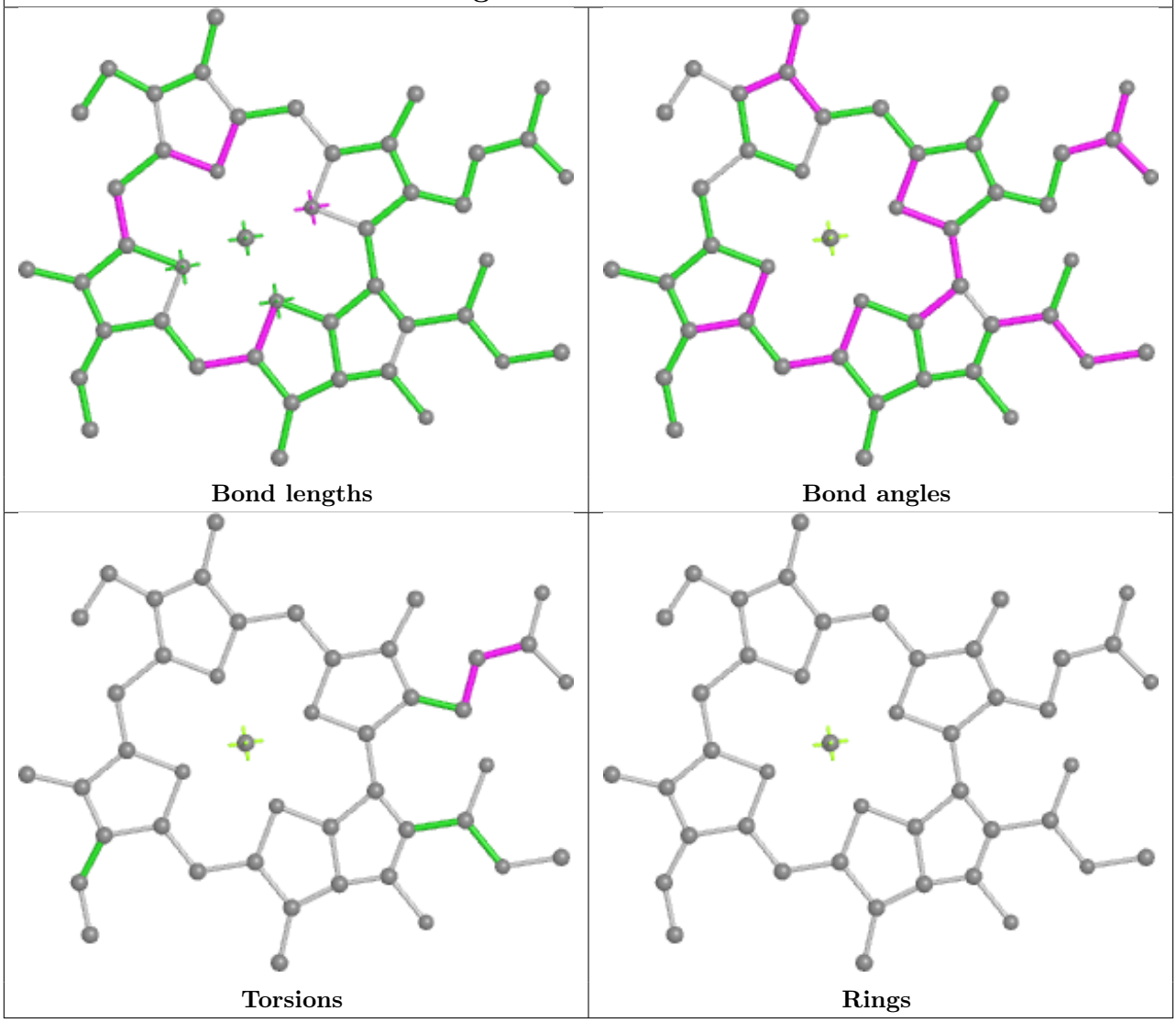


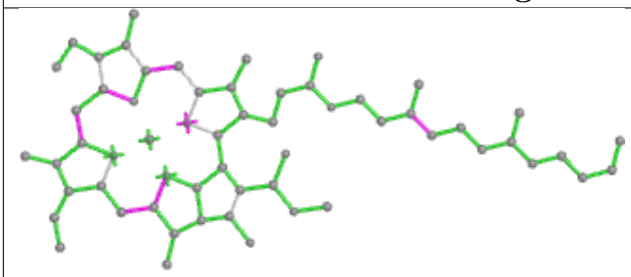
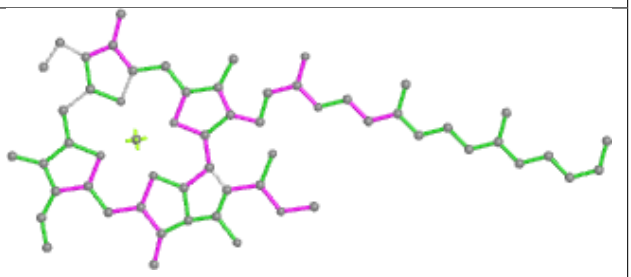
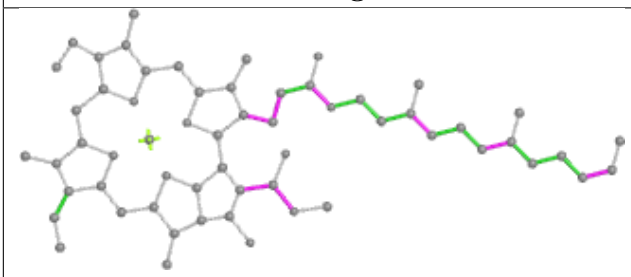
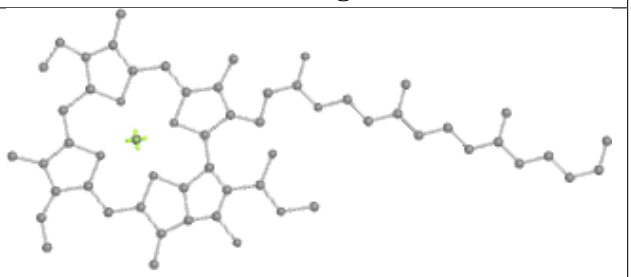
Rings

Ligand CLA B 1218



Ligand CLA B 1209



Ligand CLA A 1122	
 Bond lengths	 Bond angles
 Torsions	 Rings

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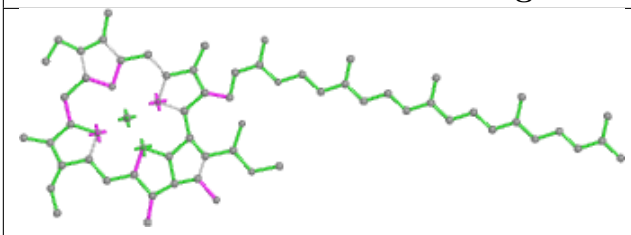
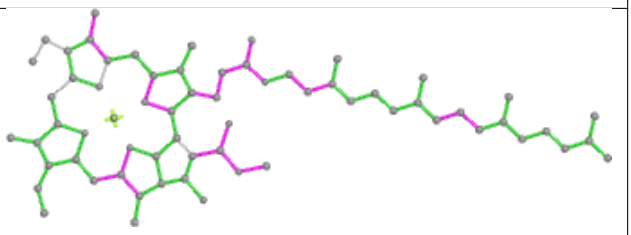
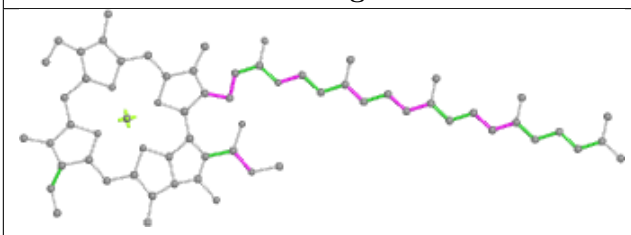
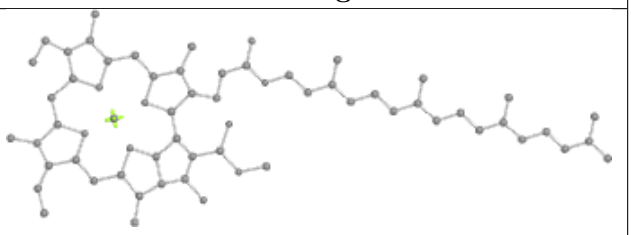
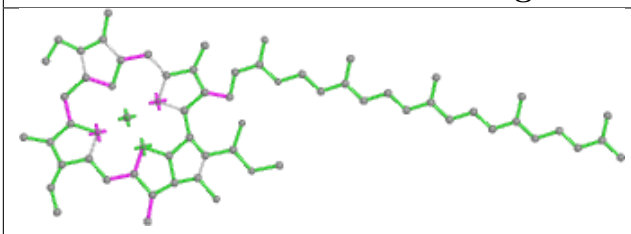
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1013



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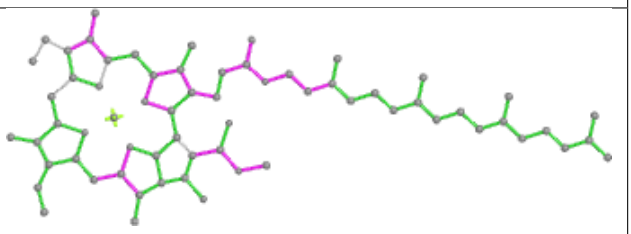
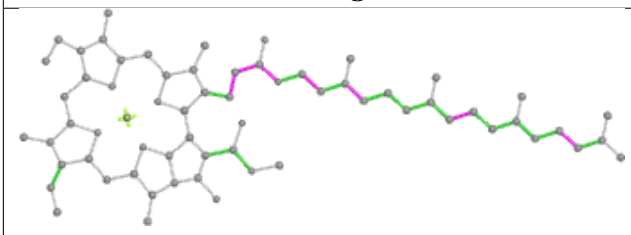


Bond angles



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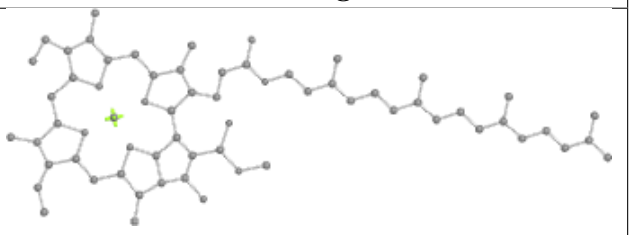
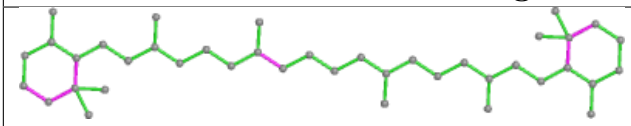


Rings

Ligand BCR A 4007



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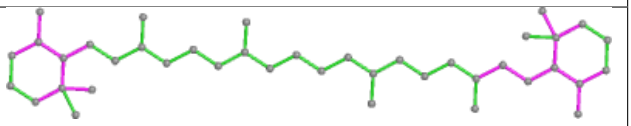
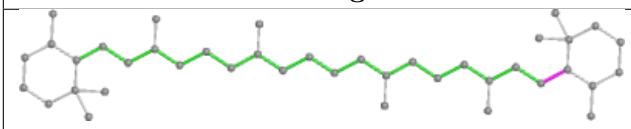


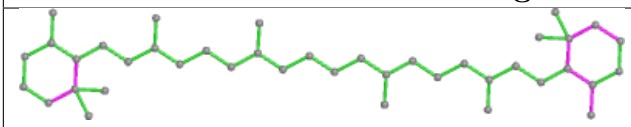
Bond angles



Torsions

Rings

Ligand BCR B 4005



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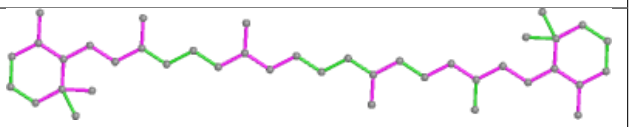

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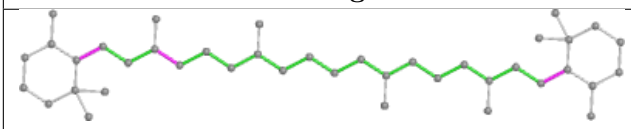
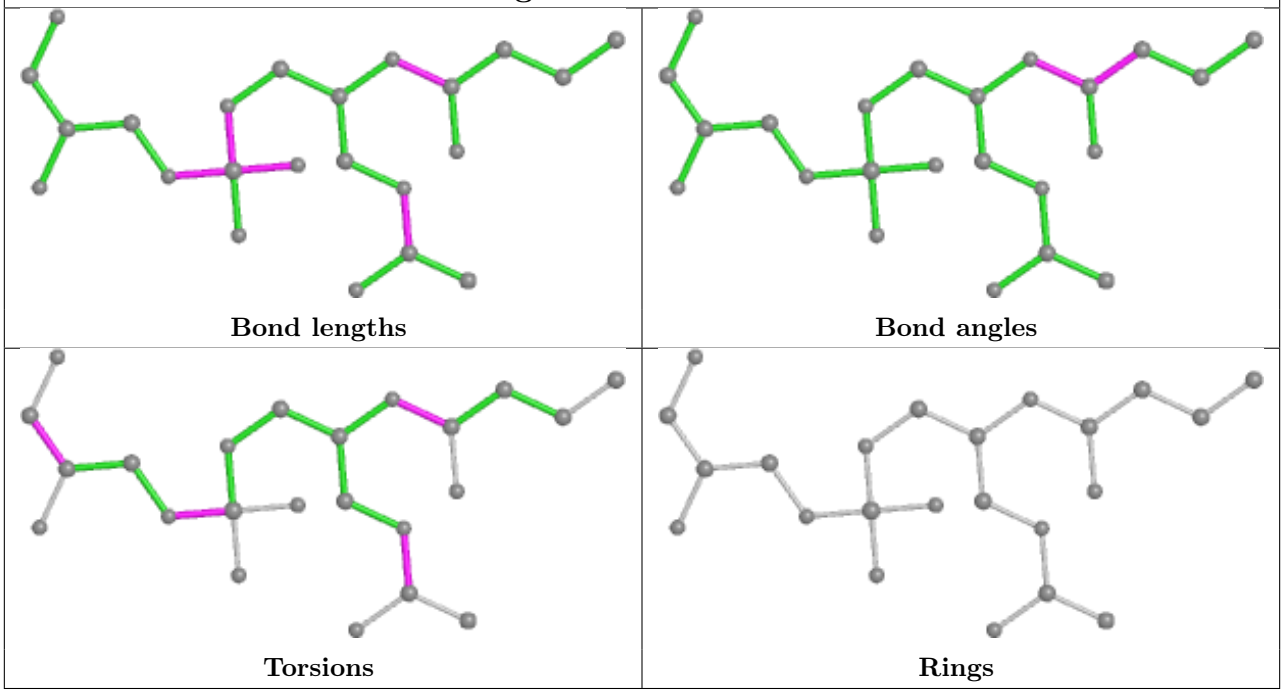


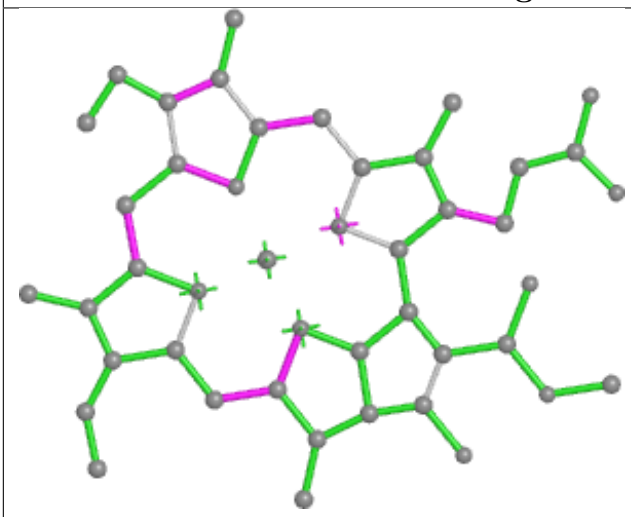
Torsions

Rings

Ligand LHG B 5004



Ligand CLA B 1227



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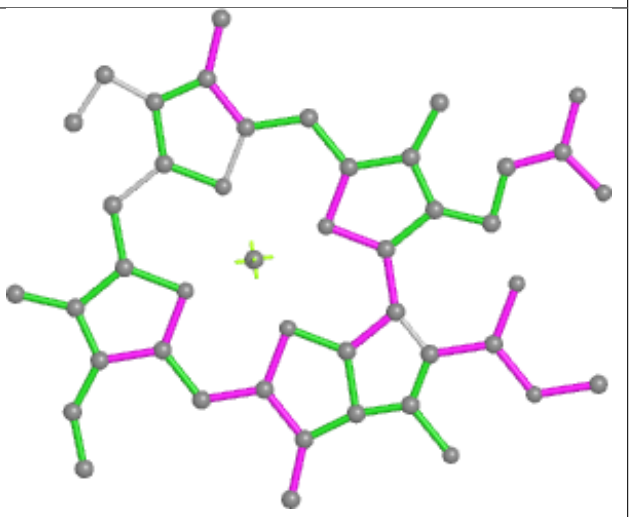
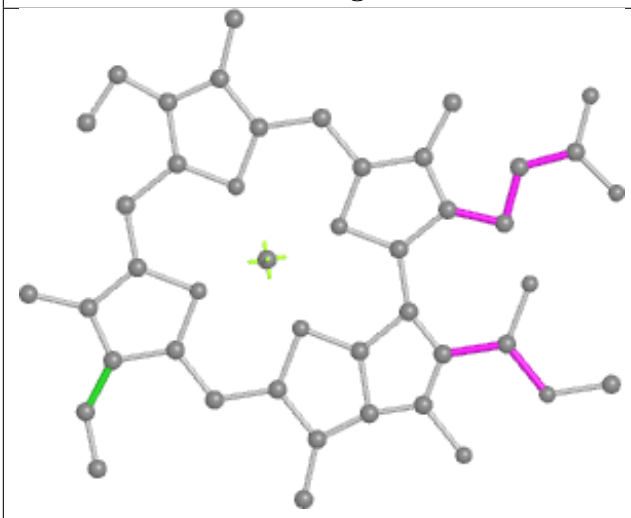
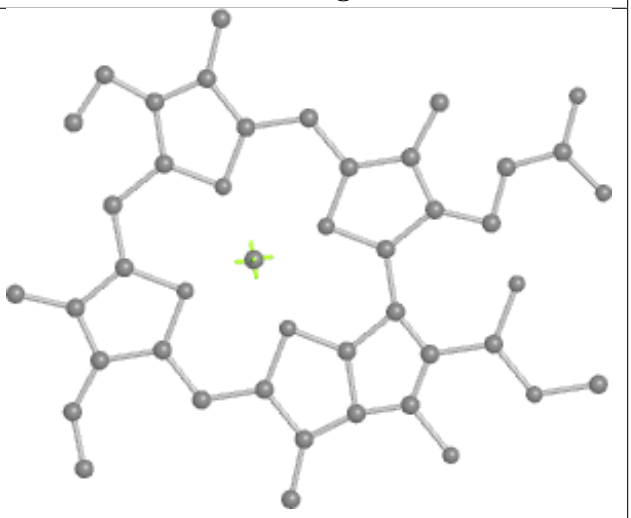


Bond angles

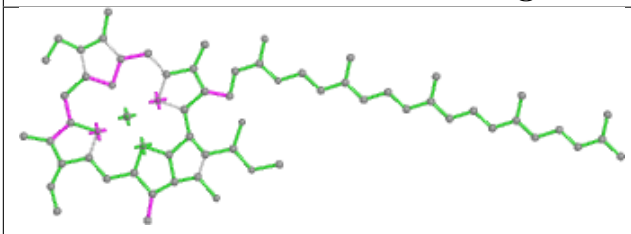


Torsions



Rings

Ligand CLA L 1501



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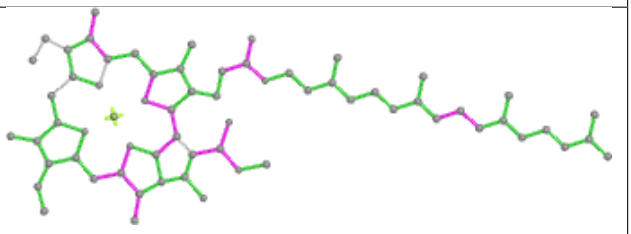
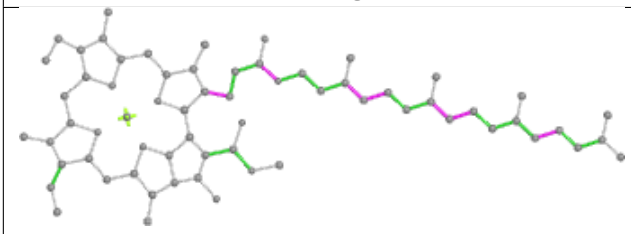


Bond angles



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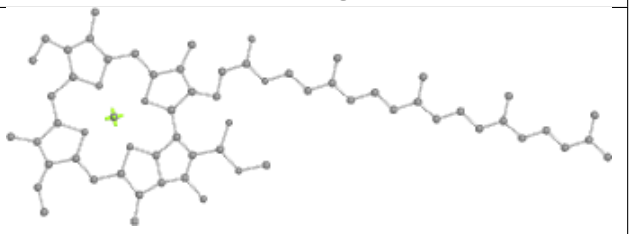
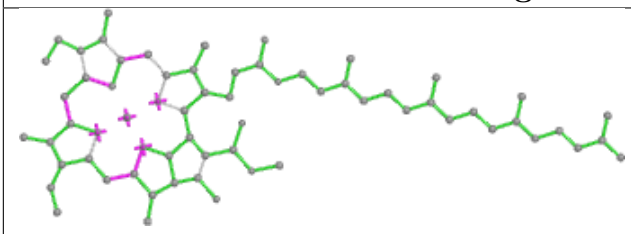
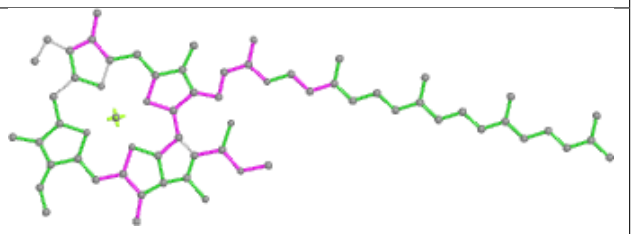
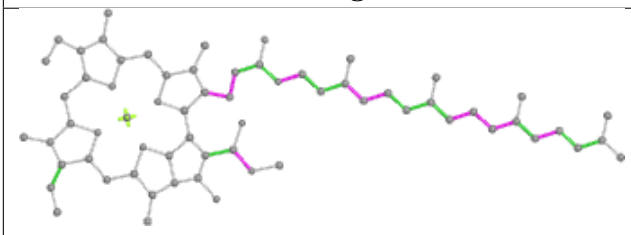
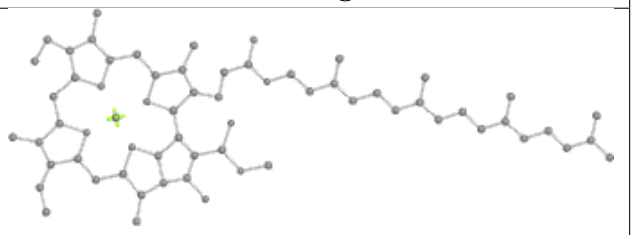


Rings

Ligand CLA A 1107	
 Bond lengths	 Bond angles
 Torsions	 Rings

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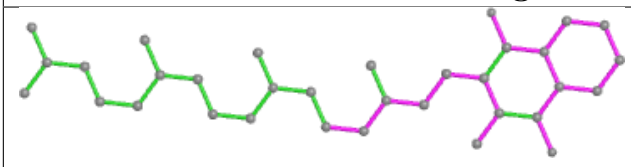
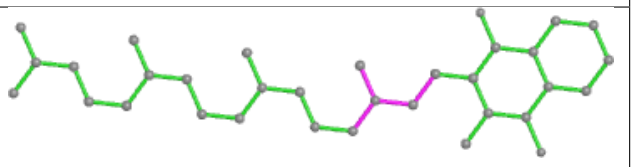
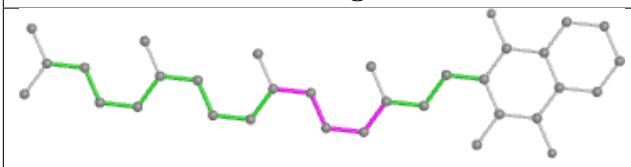
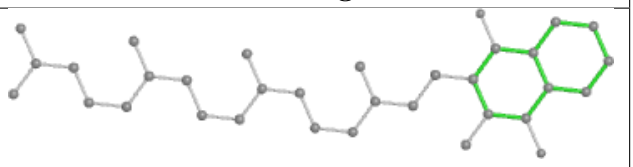
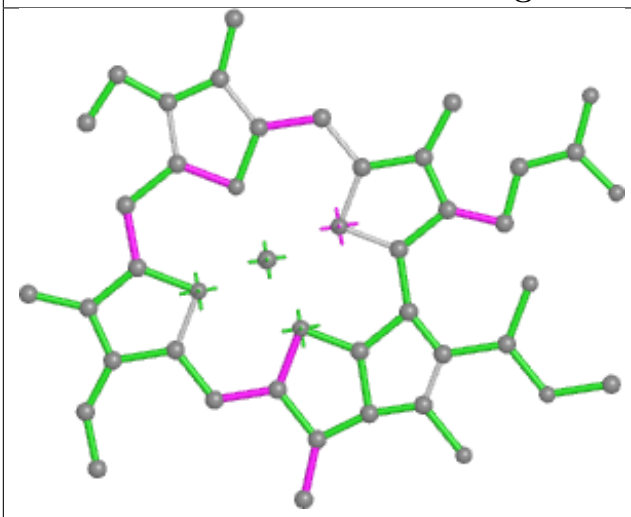
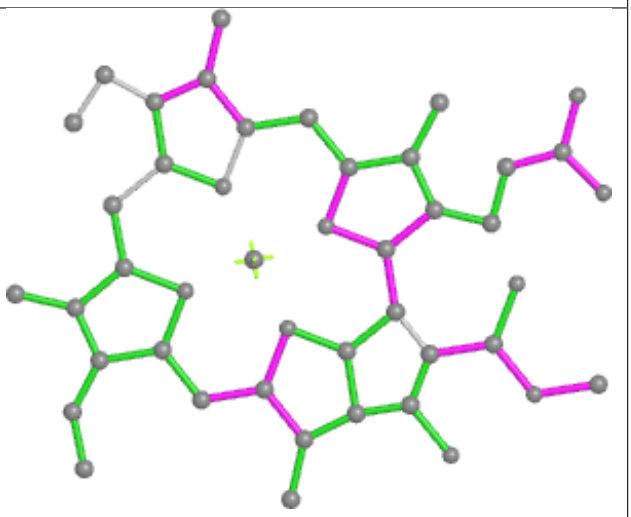
 Bond lengths	 Bond angles
 Torsions	 Rings

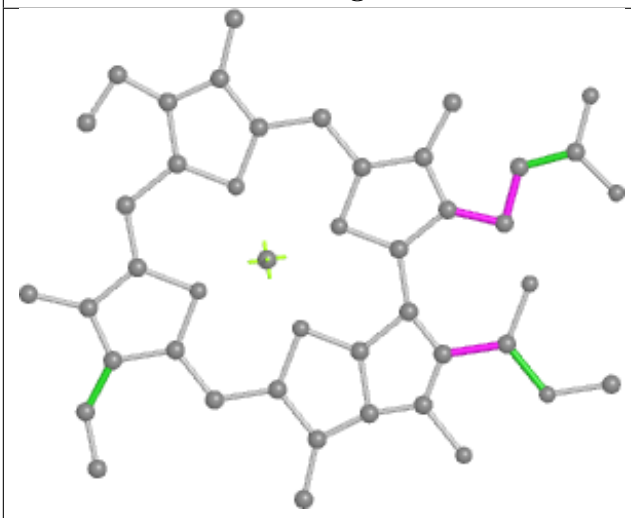
Ligand CLA A 1134



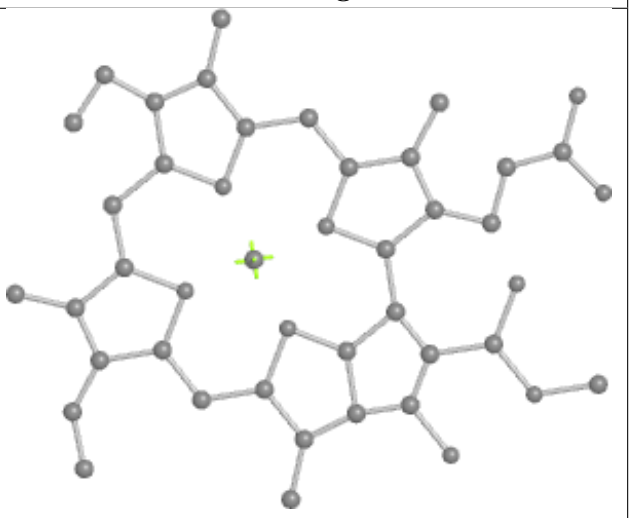
Bond lengths



Bond angles

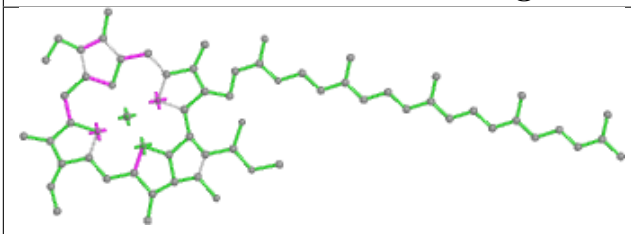


Torsions

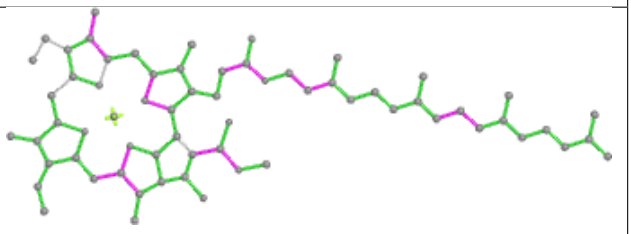


Rings

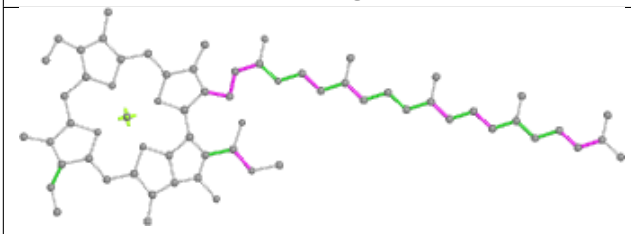
Ligand CLA B 1229



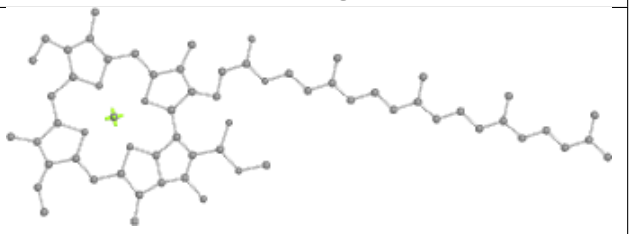
Bond lengths



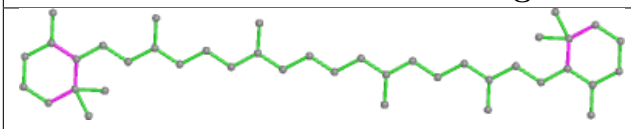
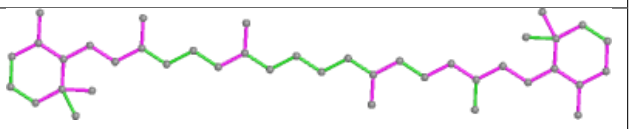
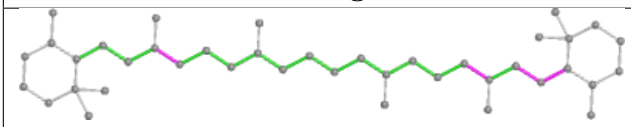
Bond angles

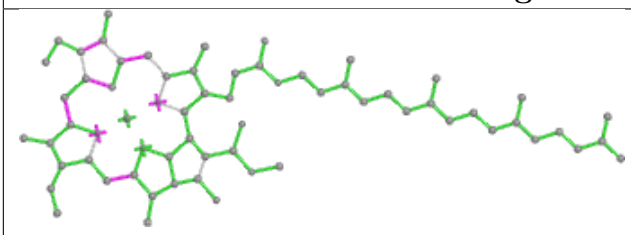
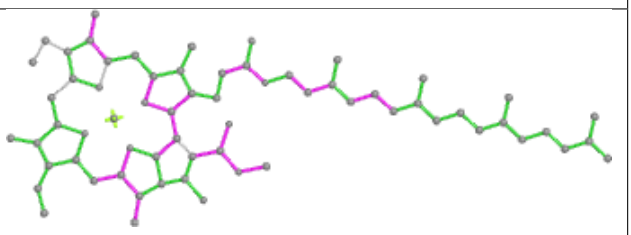
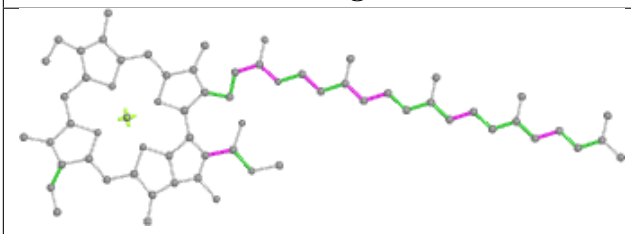
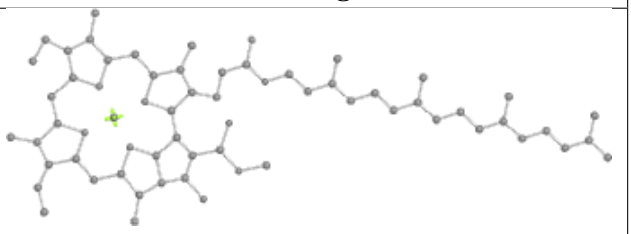


Torsions

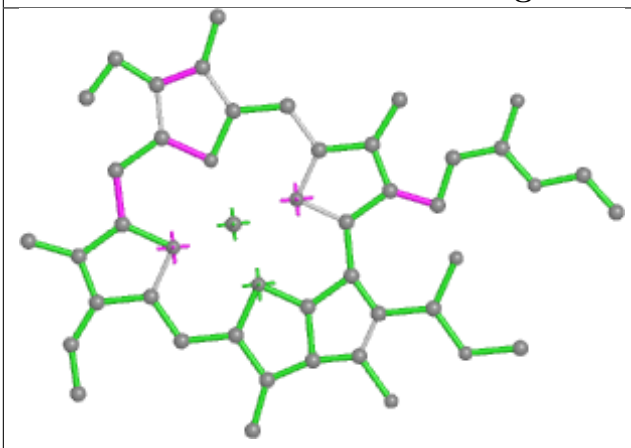


Rings

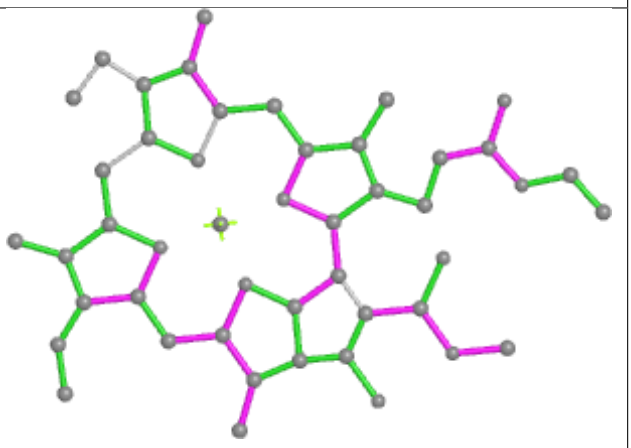
Ligand BCR B 4006	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA A 1123	
 Bond lengths	 Bond angles
 Torsions	 Rings

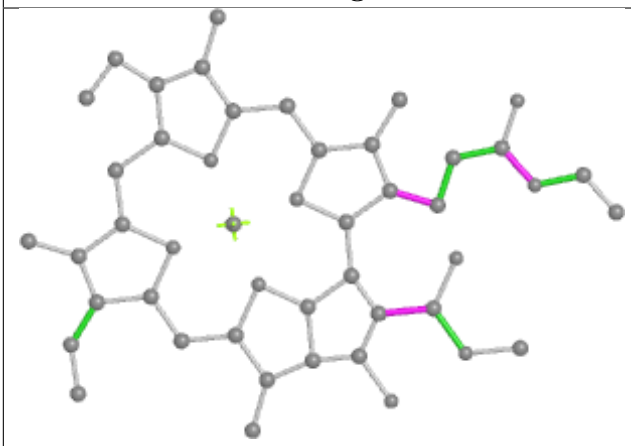
Ligand CLA A 1137



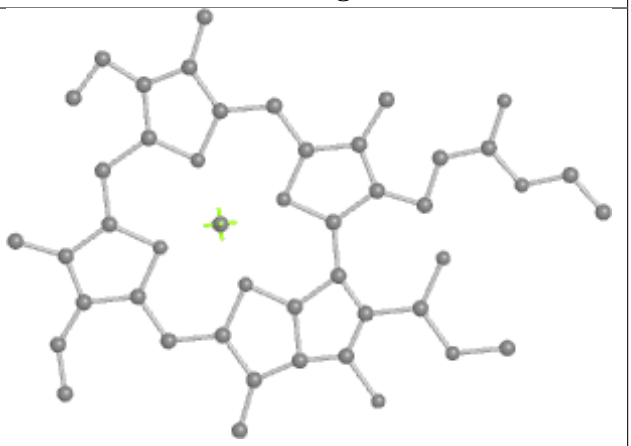
Bond lengths



Bond angles

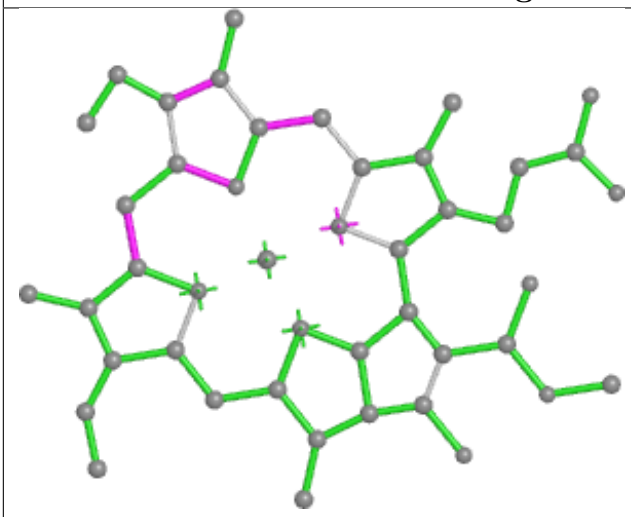


Torsions



Rings

Ligand CLA B 1220



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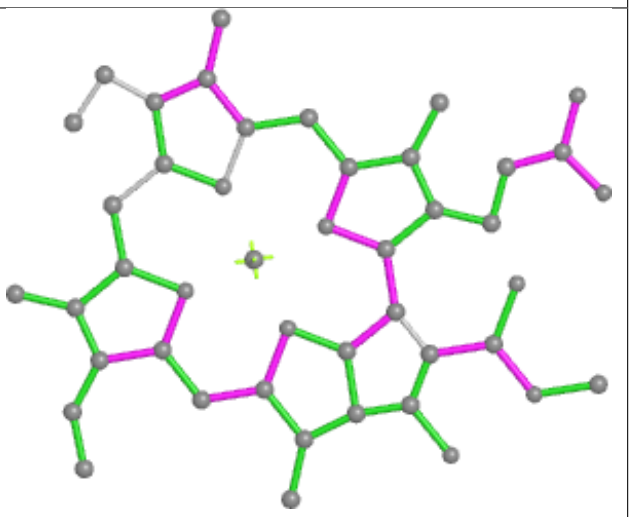
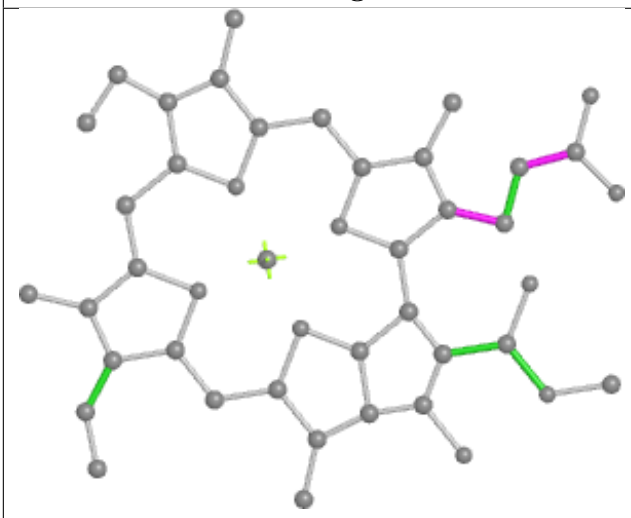


Bond angles



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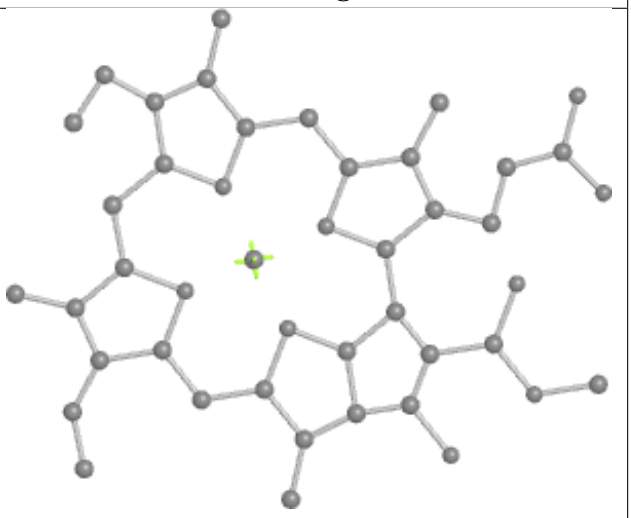
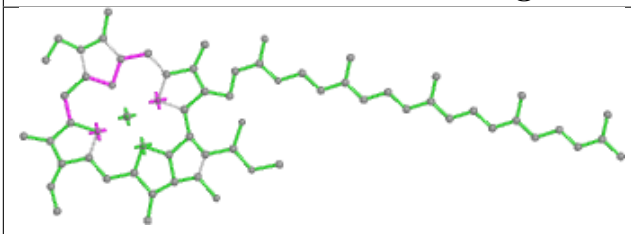


Rings

Ligand CLA B 1021



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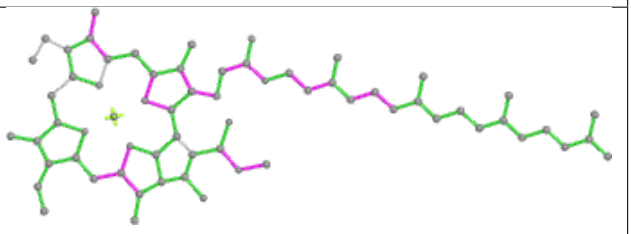
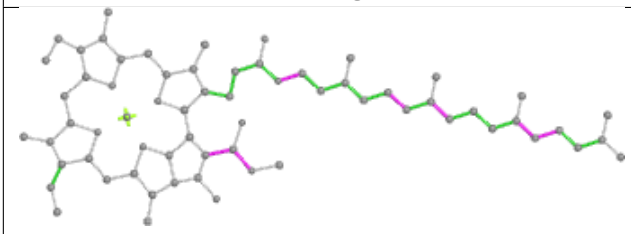


Bond angles



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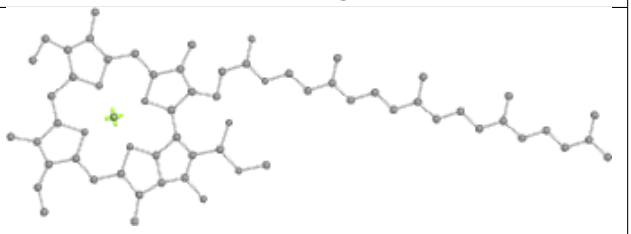
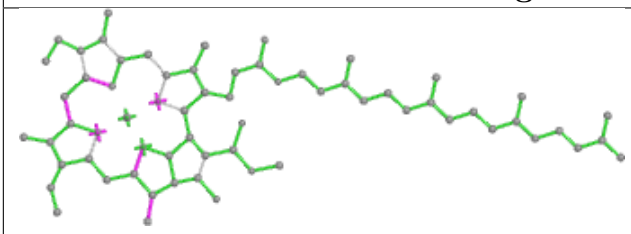


Rings

Ligand CLA B 1012



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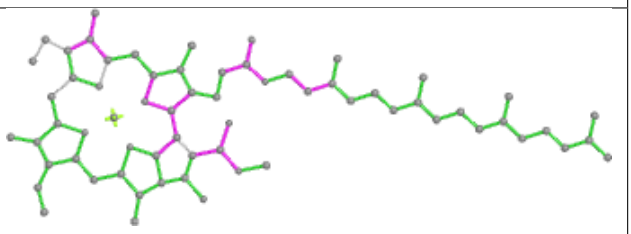
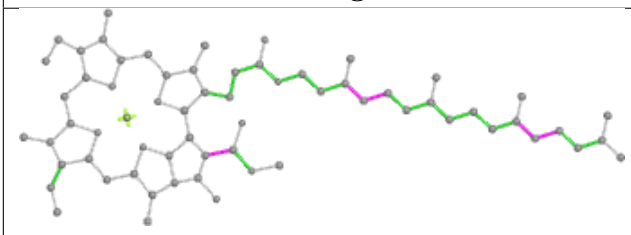


Bond angles



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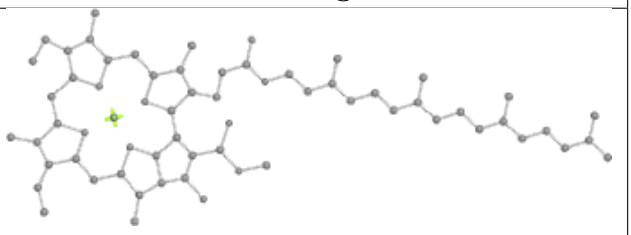
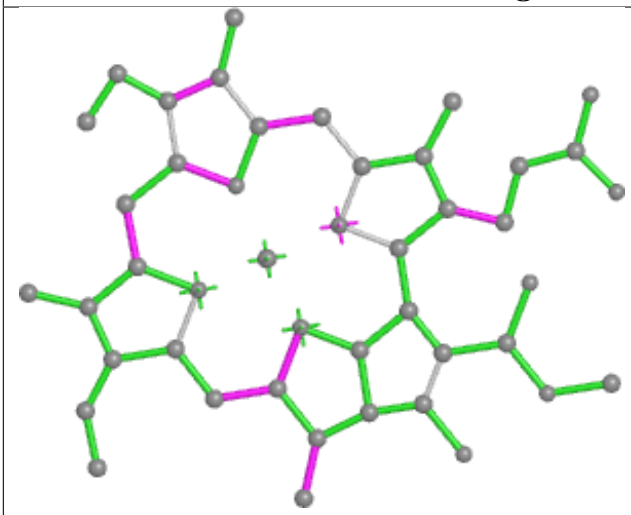


Rings

Ligand CLA A 1112



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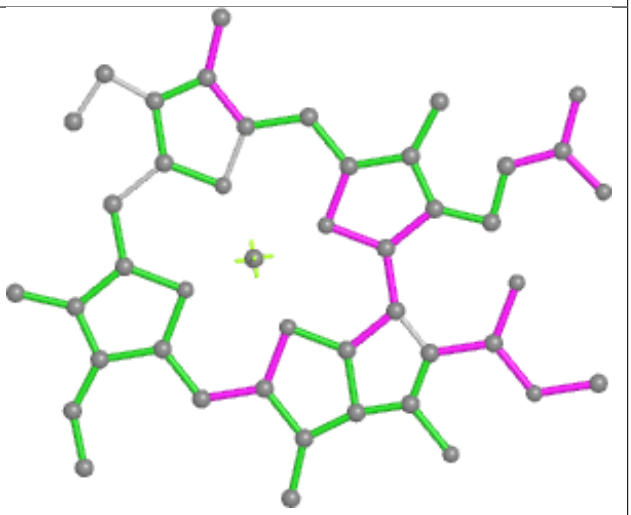

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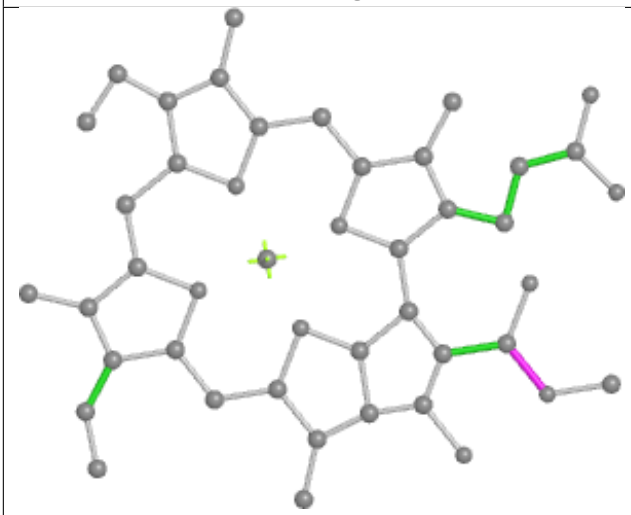

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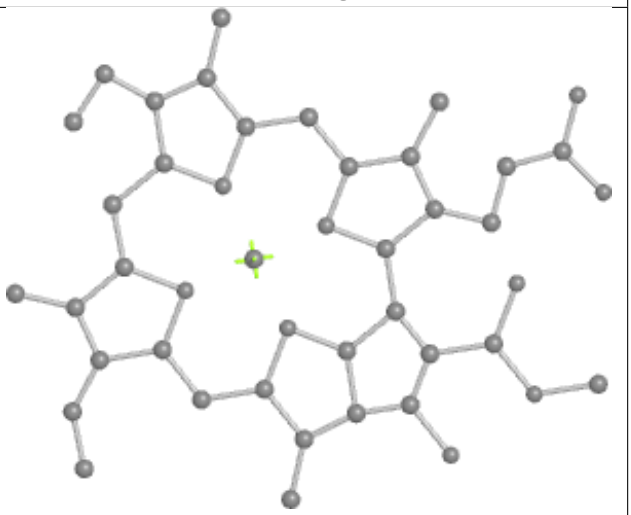
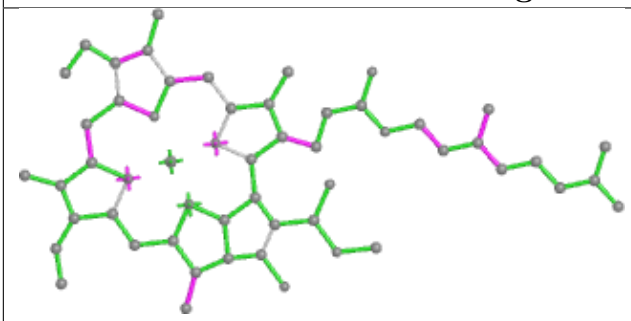


Rings

Ligand CLA B 1213



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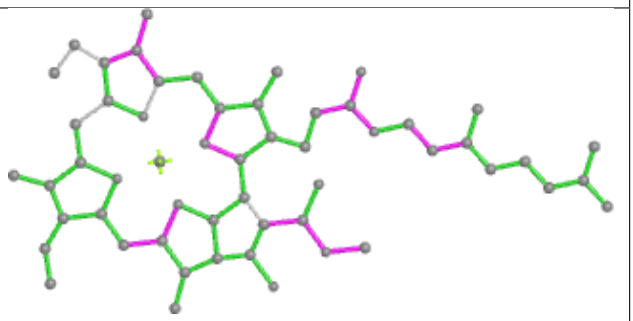
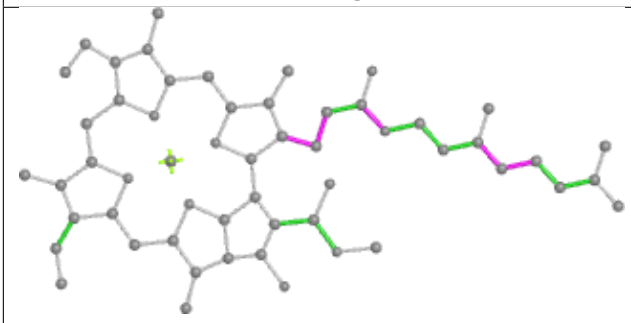


Bond angles



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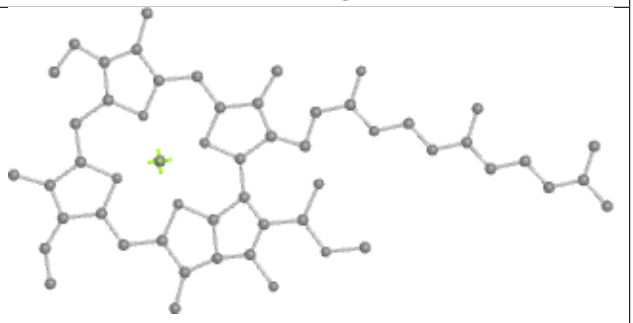
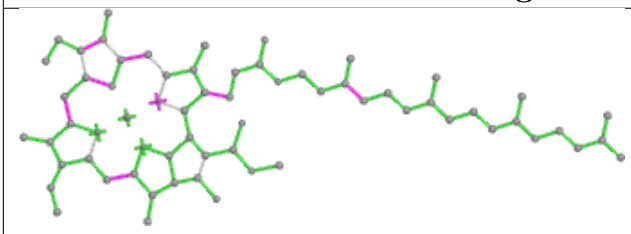


Rings

Ligand CLA B 1204



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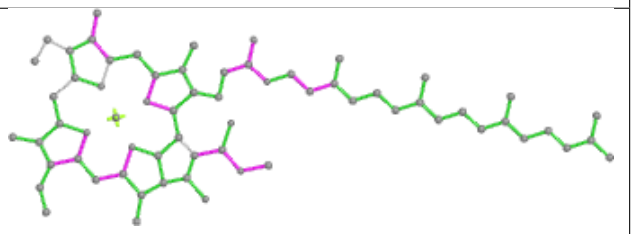
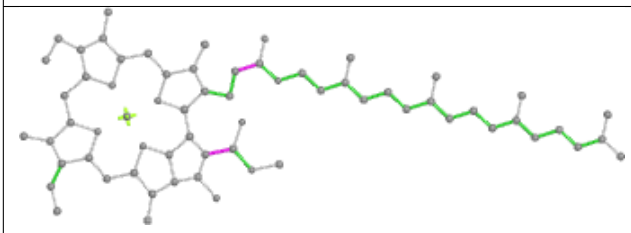


Bond angles



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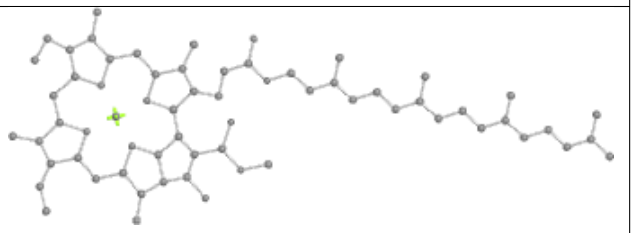
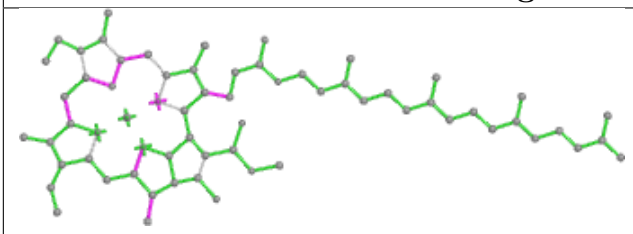


Rings

Ligand CLA L 1502



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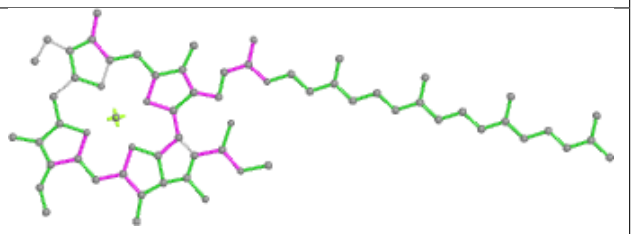
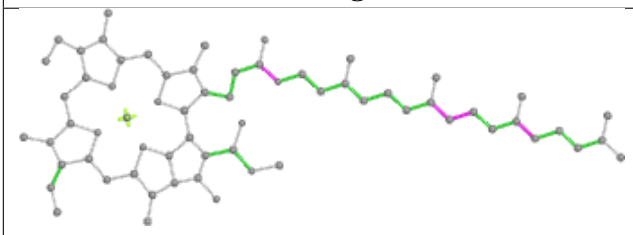


Bond angles



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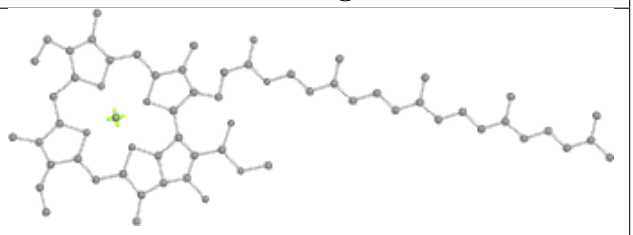
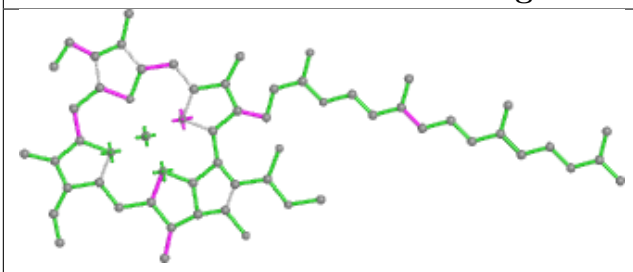


Rings

Ligand CLA B 1215



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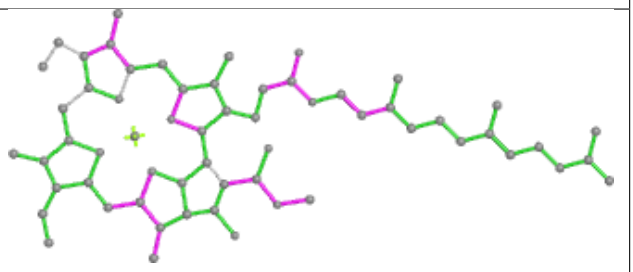
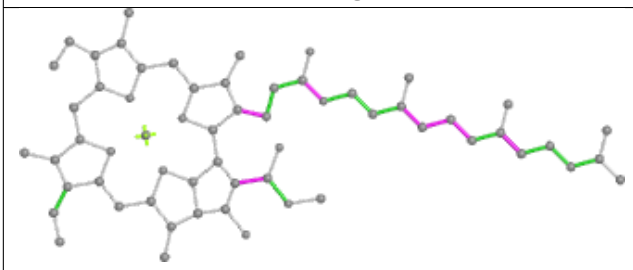


Bond angles



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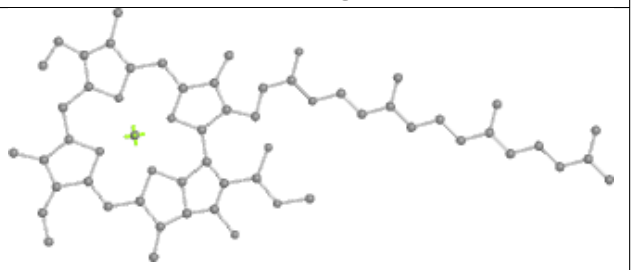
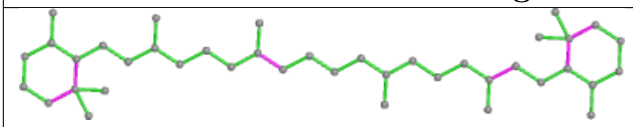
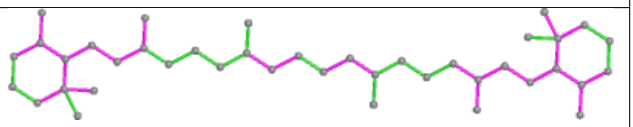


Rings

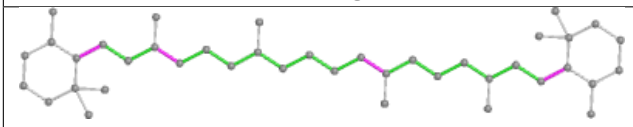
Ligand BCR A 4011



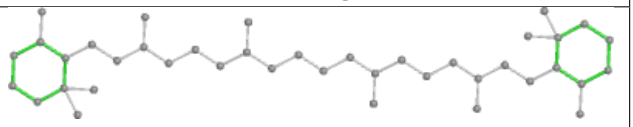
Bond lengths



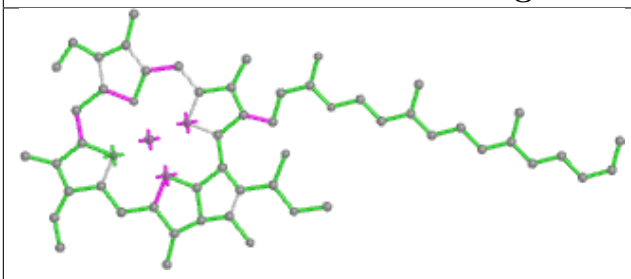
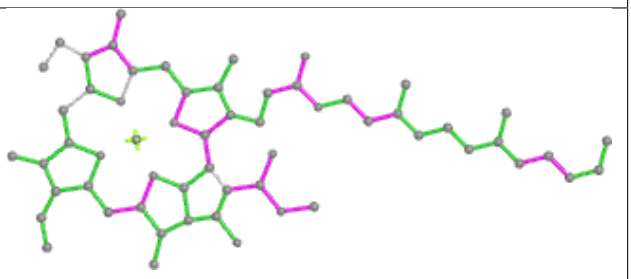
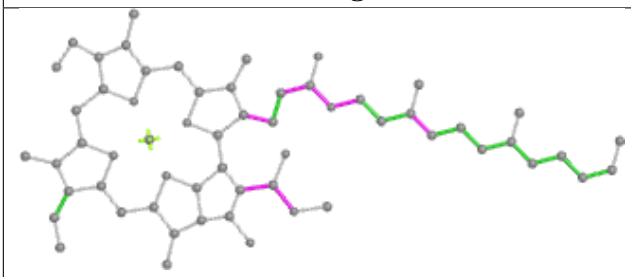
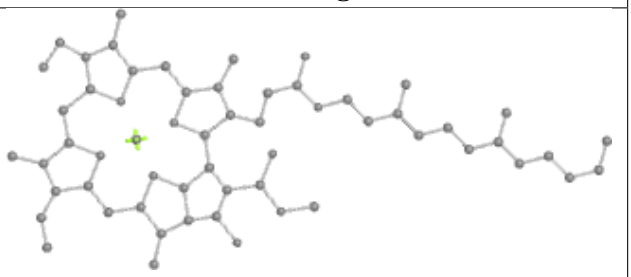
Bond angles

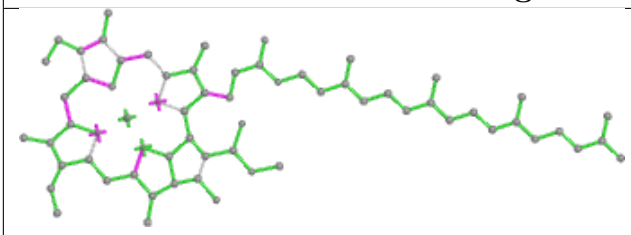
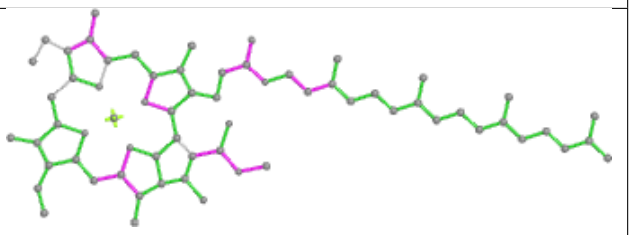
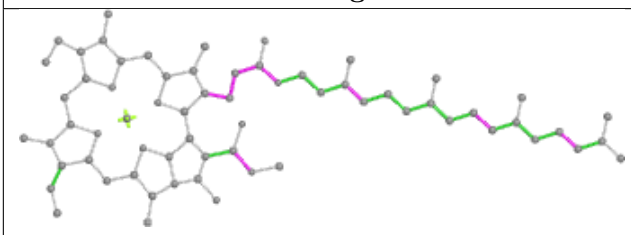
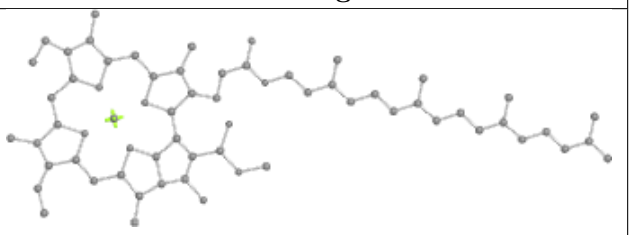


Torsions

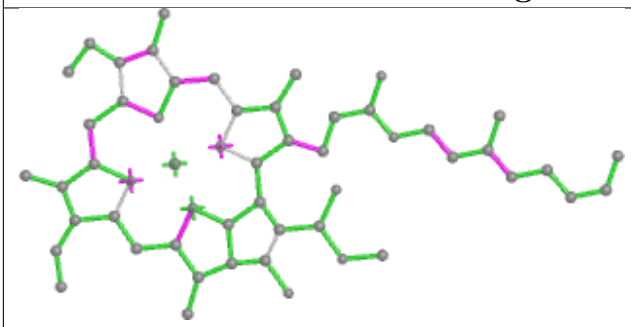


Rings

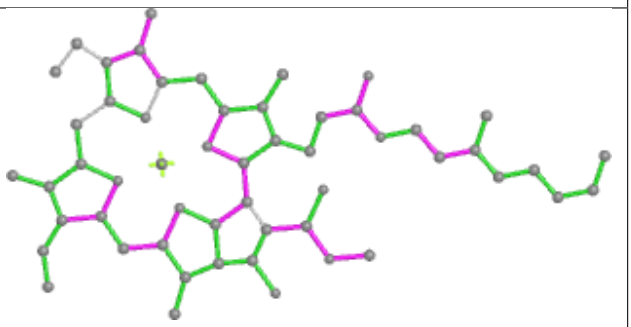
Ligand CLA A 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1109	
 Bond lengths	 Bond angles
 Torsions	 Rings

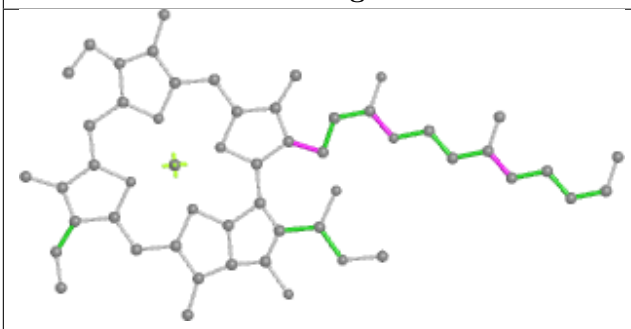
Ligand CLA A 1133



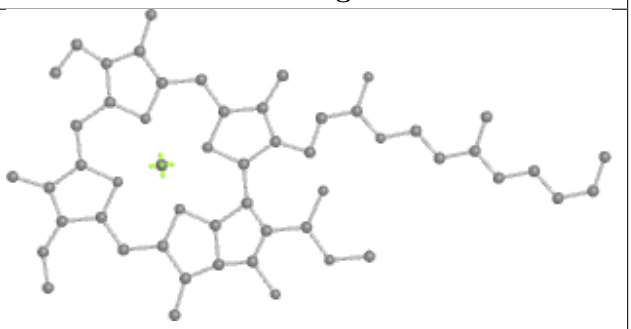
Bond lengths



Bond angles

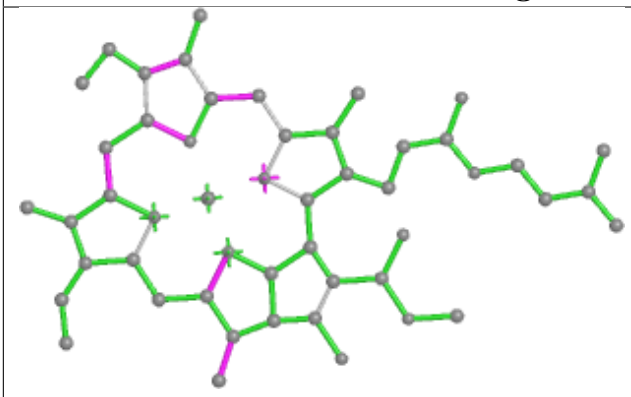


Torsions

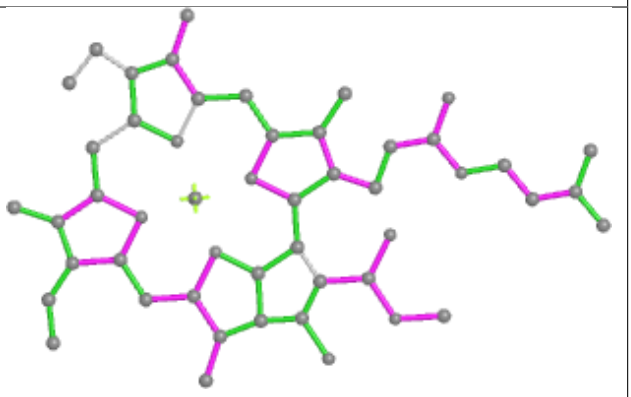


Rings

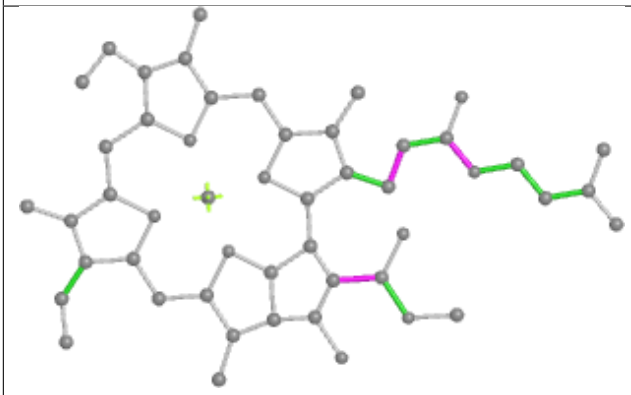
Ligand CLA A 1129



Bond lengths



Bond angles



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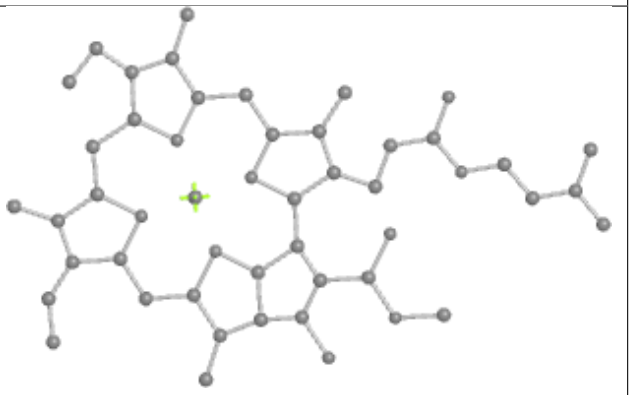
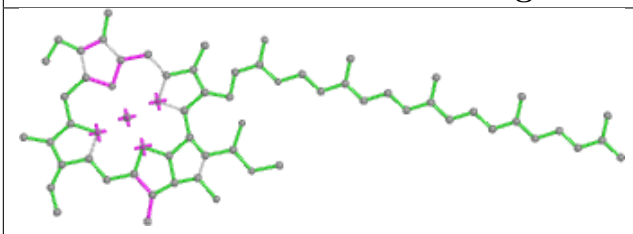
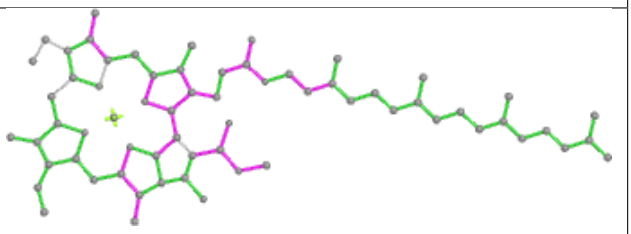


Rings

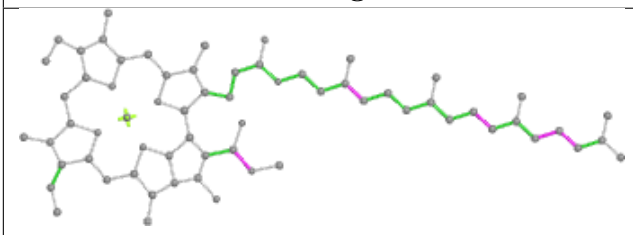
Ligand CLA B 1207



Bond lengths



Bond angles



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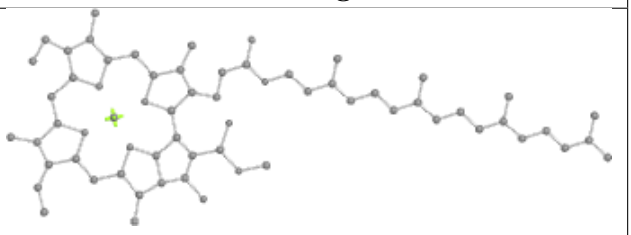
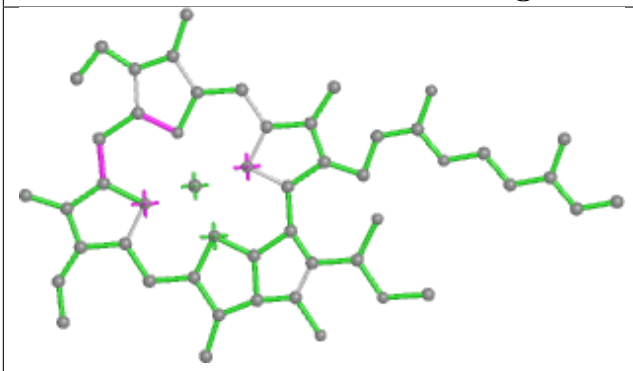
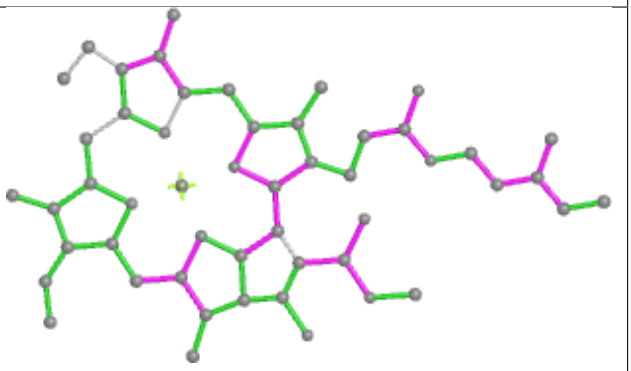


Rings

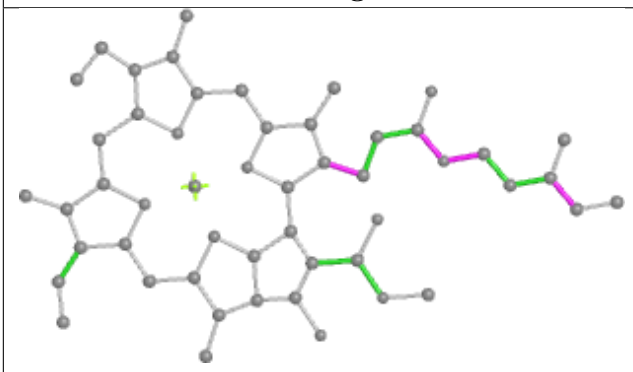
Ligand CLA A 1135



Bond lengths



Bond angles



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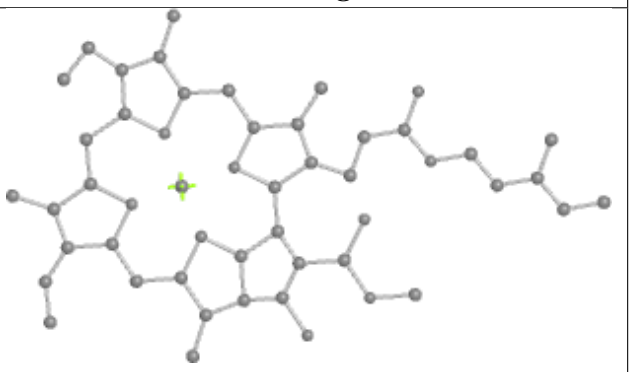
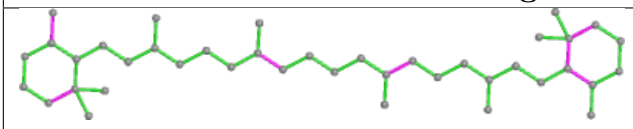


Rings

Ligand BCR I 4020



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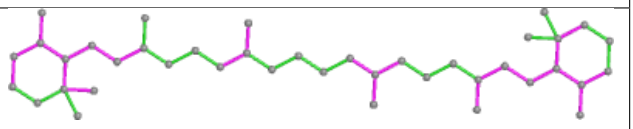
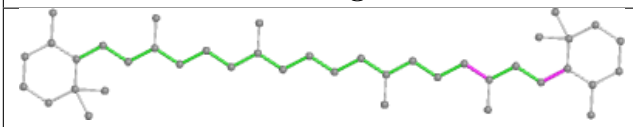
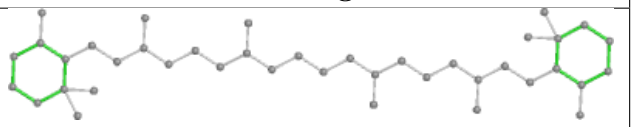


Bond angles

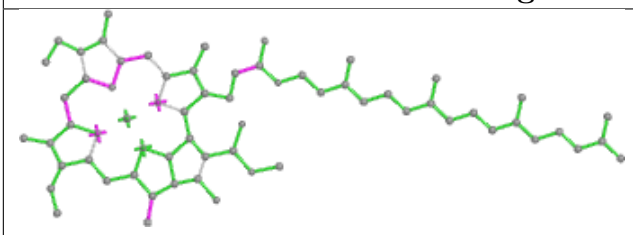


Torsions



Rings

Ligand CLA L 1503



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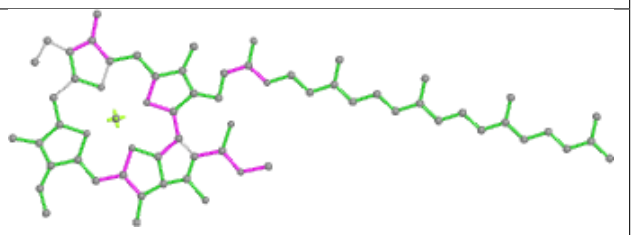
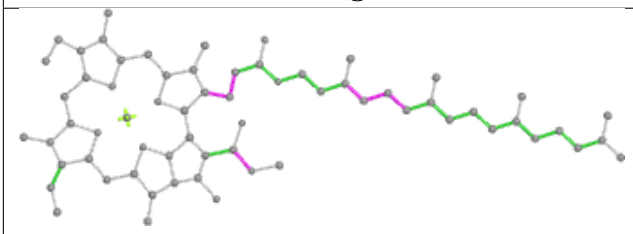
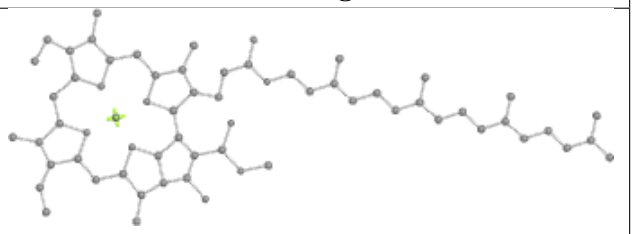


Bond angles

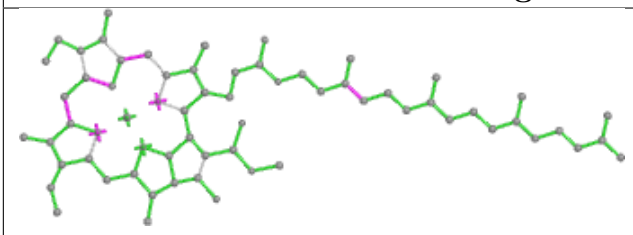


Torsions



Rings

Ligand CLA A 1125



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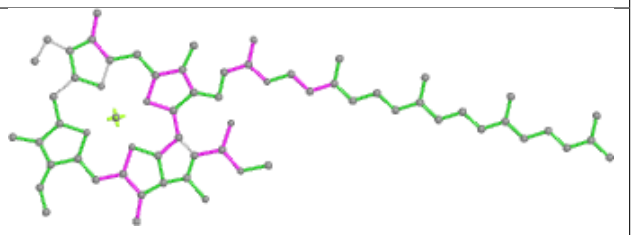
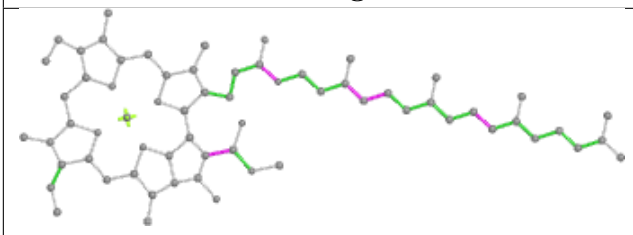


Bond angles



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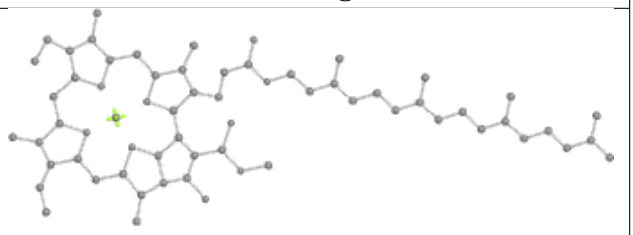
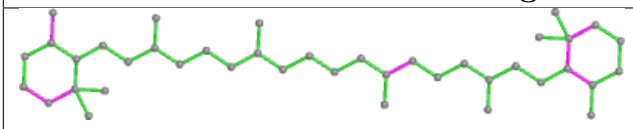


Rings

Ligand BCR I 4018



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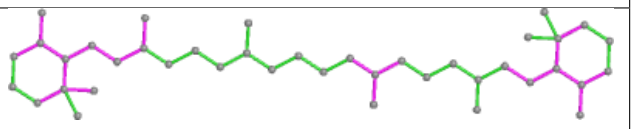
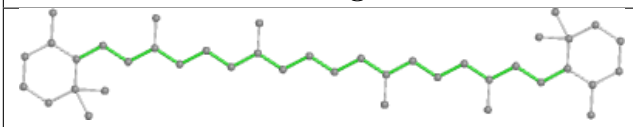


Bond angles



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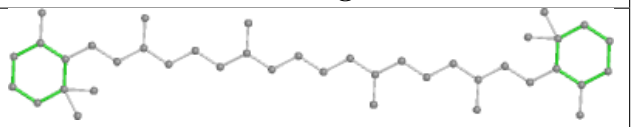
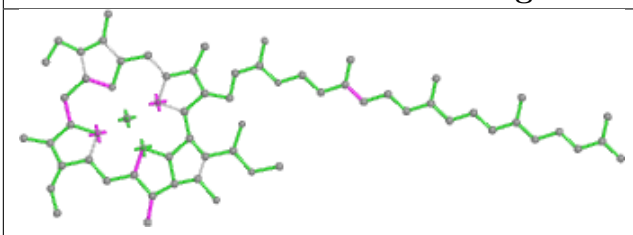
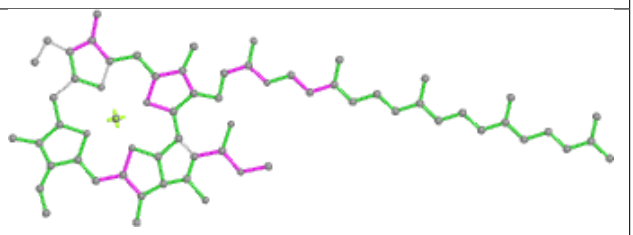


Rings

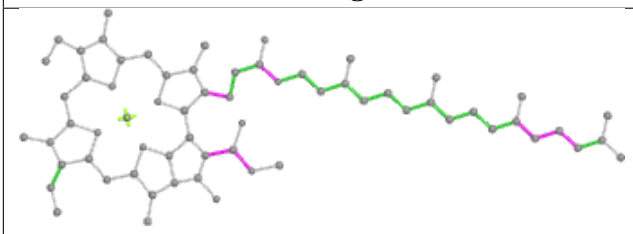
Ligand CLA B 1202



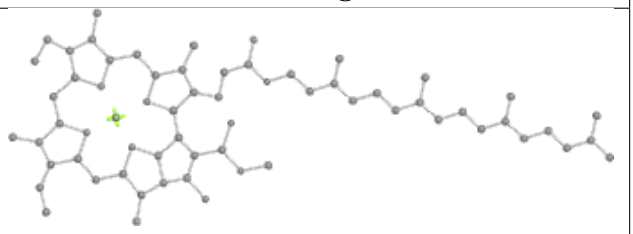
Bond lengths



Bond angles

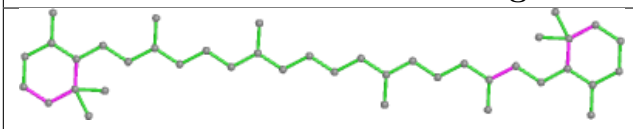


Torsions



Rings

Ligand BCR M 4021



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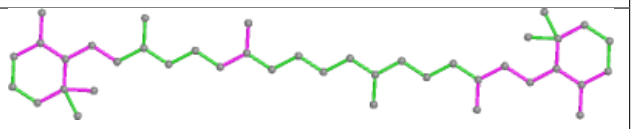
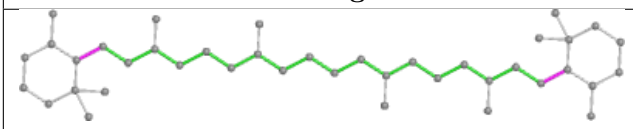


Bond angles



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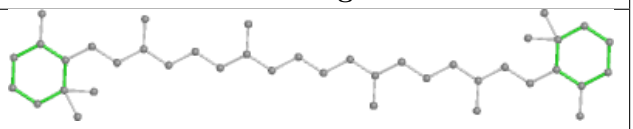
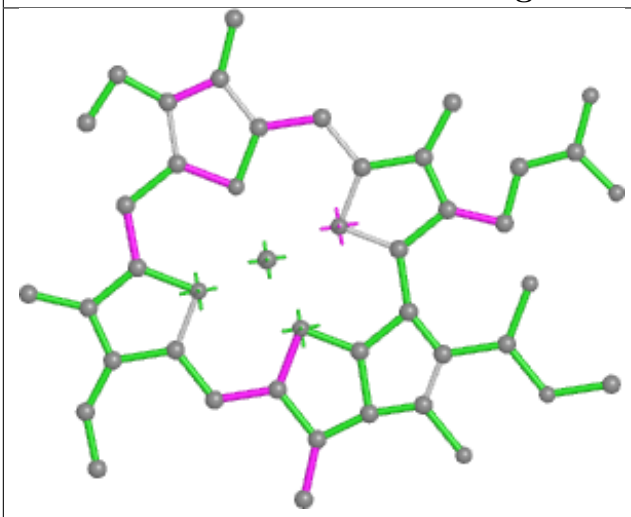
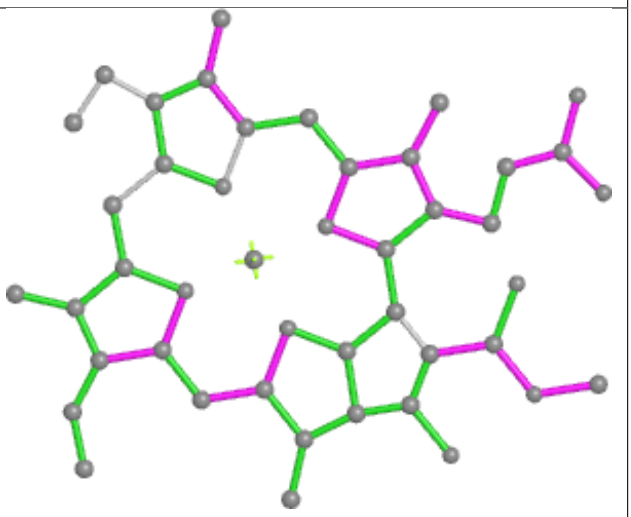


Rings

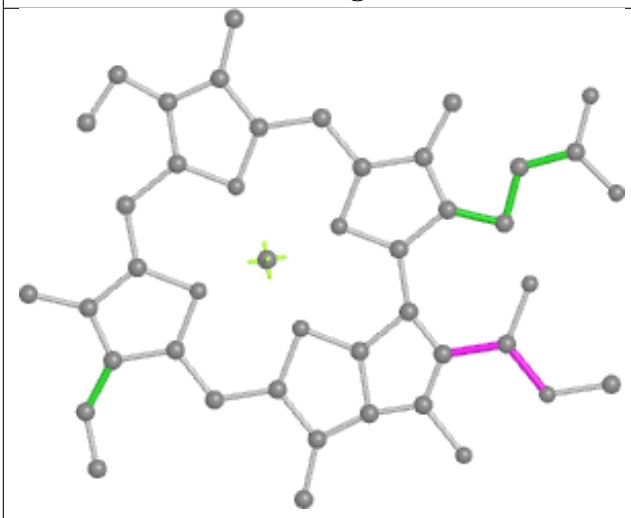
Ligand CLA B 1231



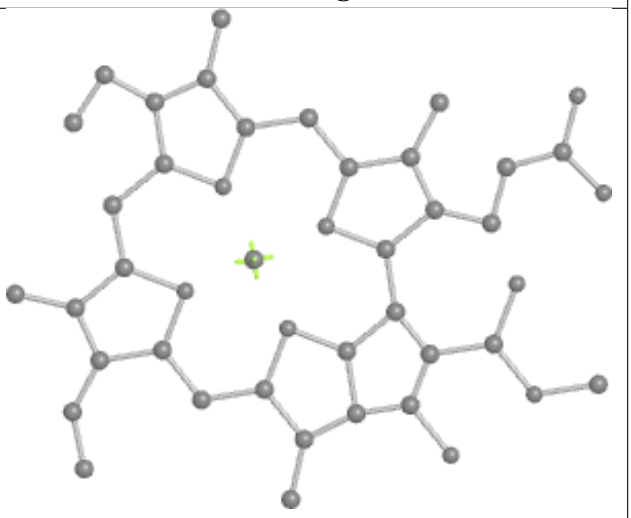
Bond lengths



Bond angles

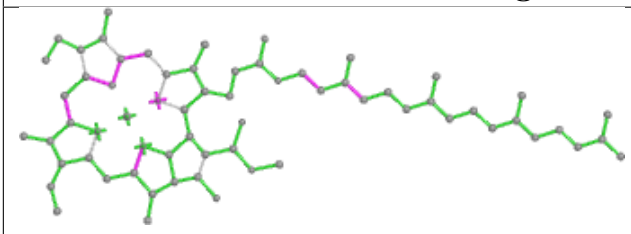


Torsions

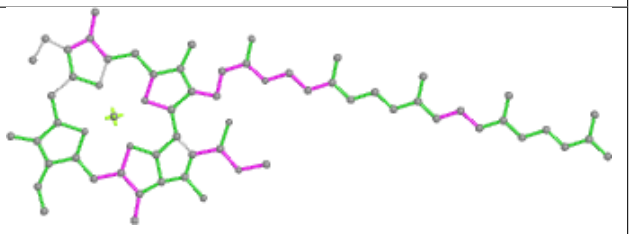


Rings

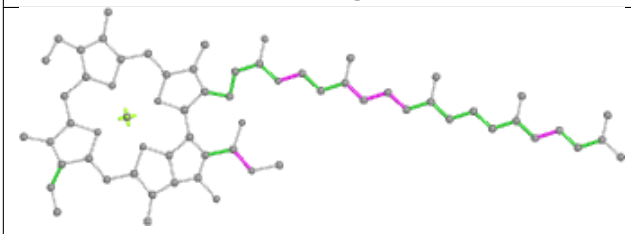
Ligand CLA A 1140



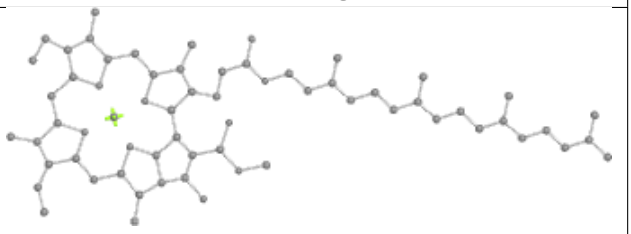
Bond lengths



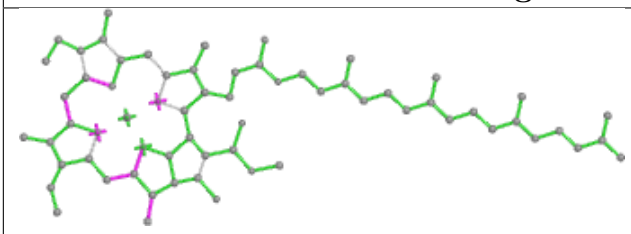
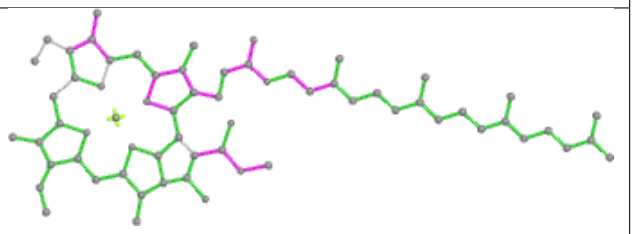
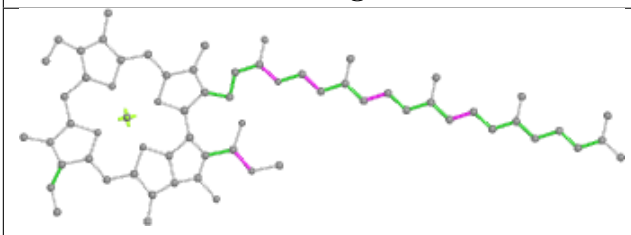
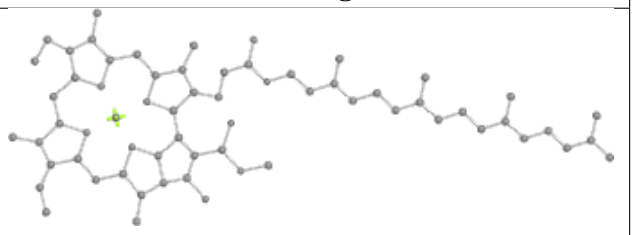
Bond angles

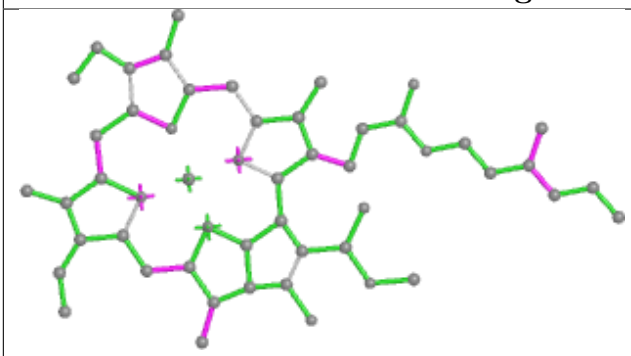
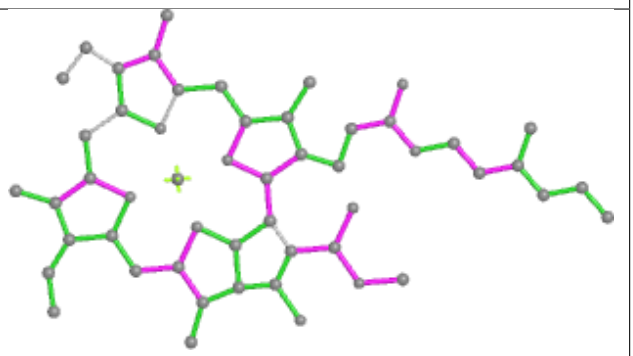
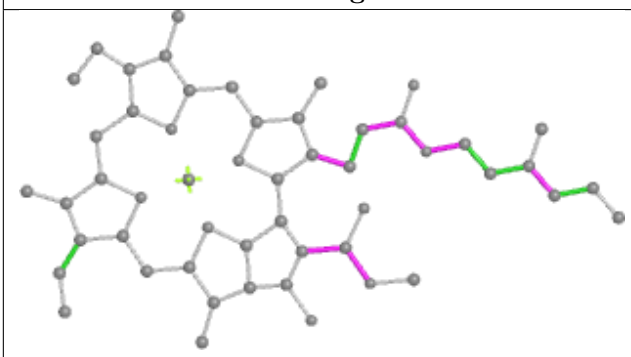
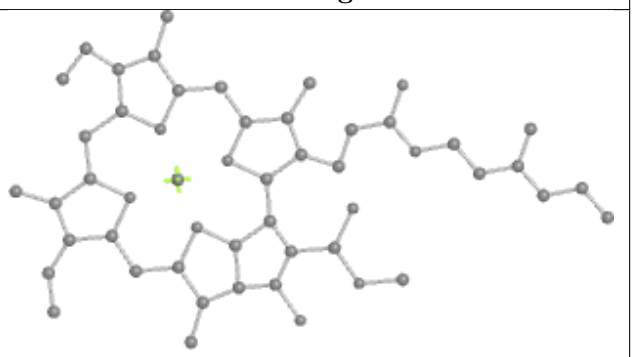


Torsions

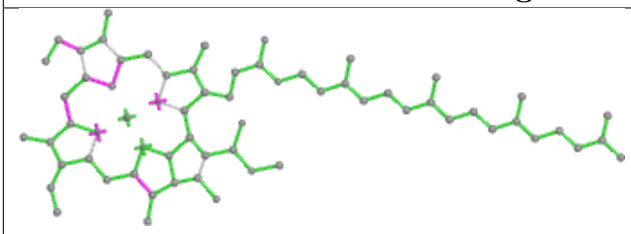


Rings

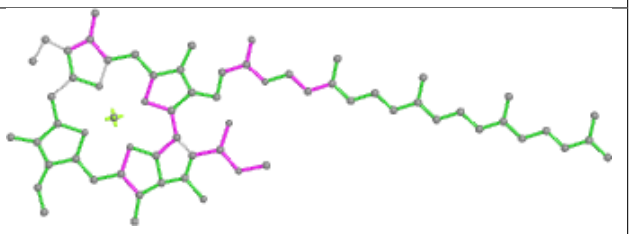
Ligand CLA A 1130	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1801	
 Bond lengths	 Bond angles
 Torsions	 Rings

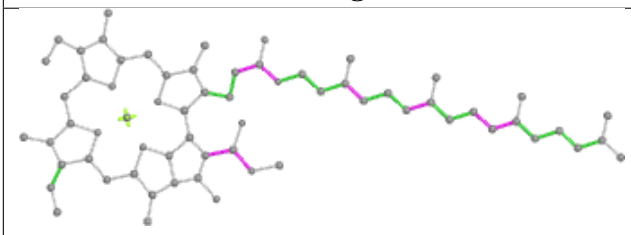
Ligand CLA B 1223



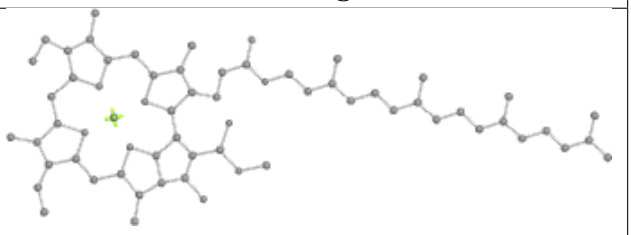
Bond lengths



Bond angles

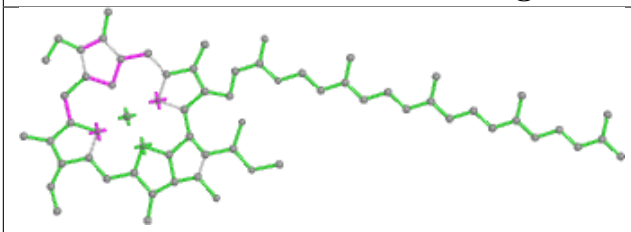


Torsions



Rings

Ligand CLA B 1205



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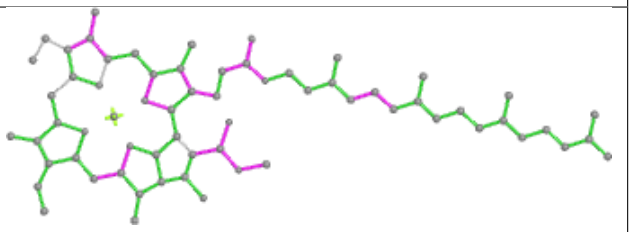
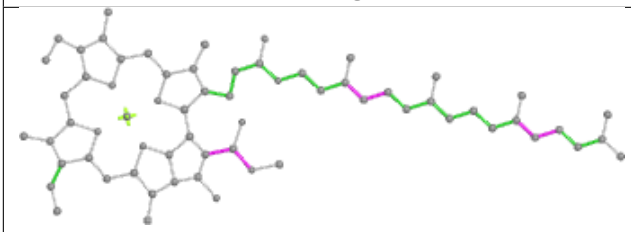


Bond angles



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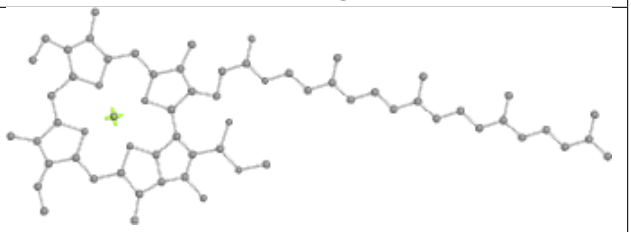
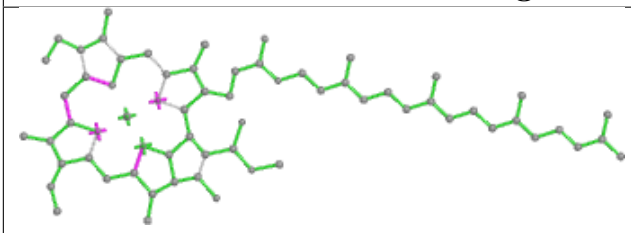


Rings

Ligand CLA B 1206



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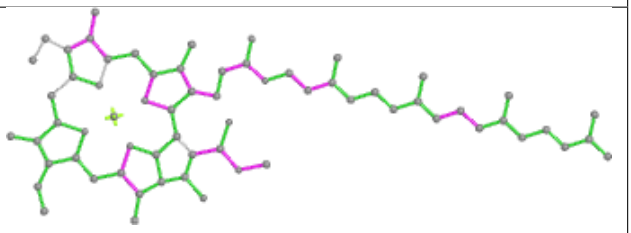
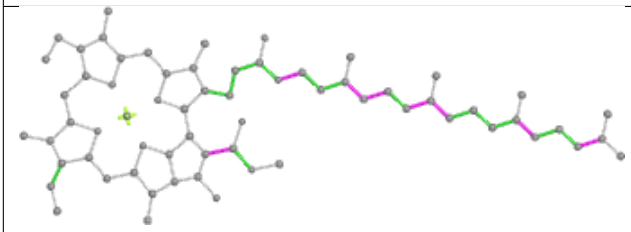


Bond angles



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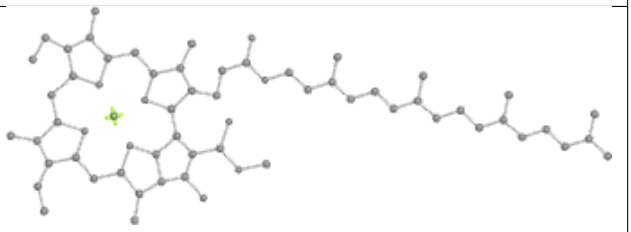
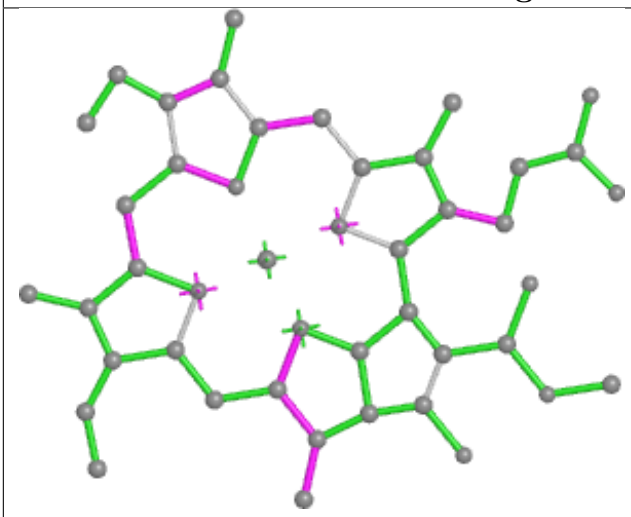


Rings

Ligand CLA B 1212



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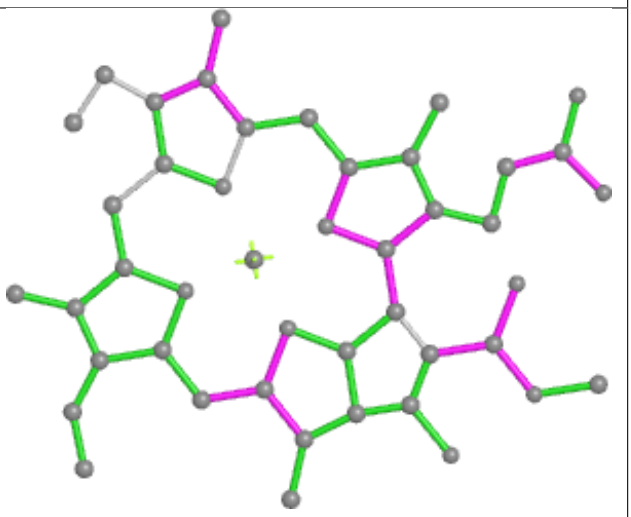

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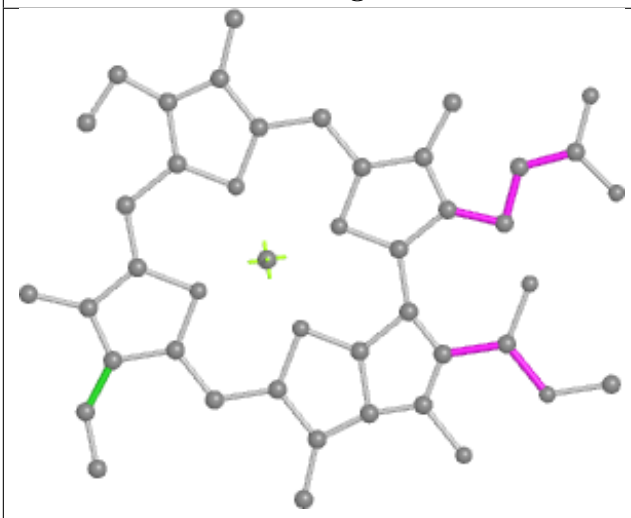

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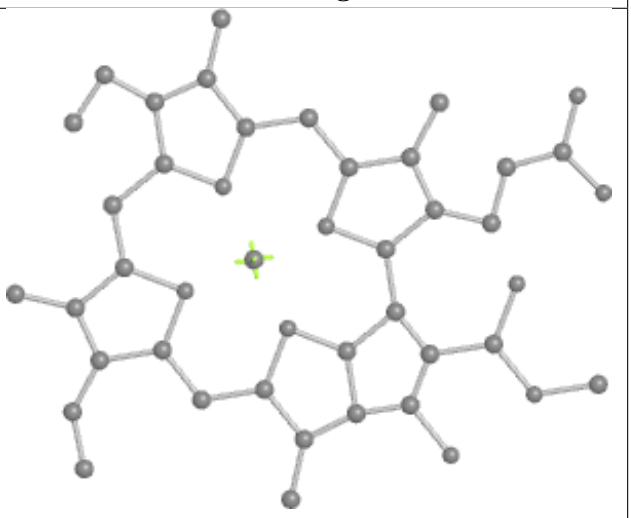
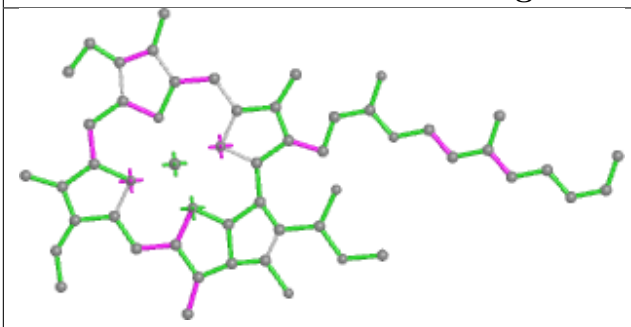


Rings

Ligand CLA B 1221



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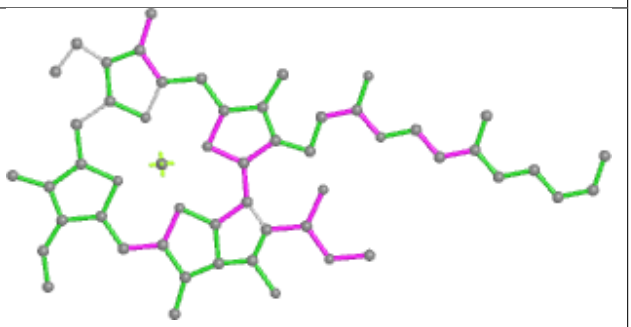
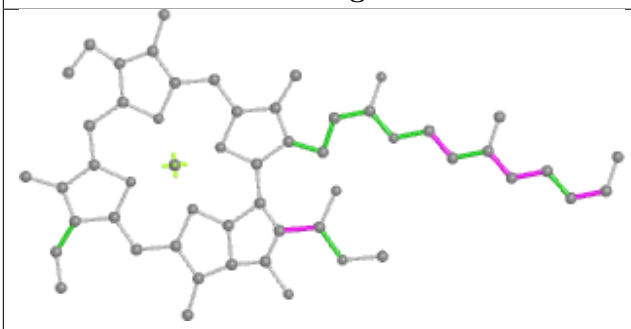


Bond angles



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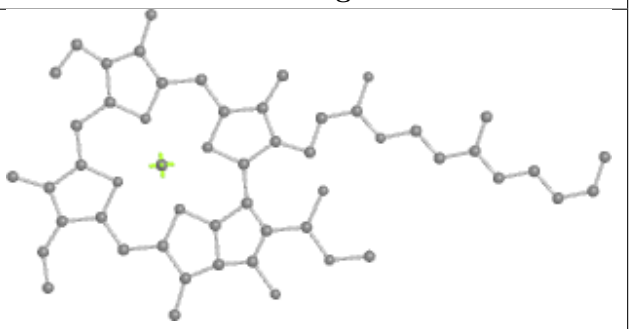
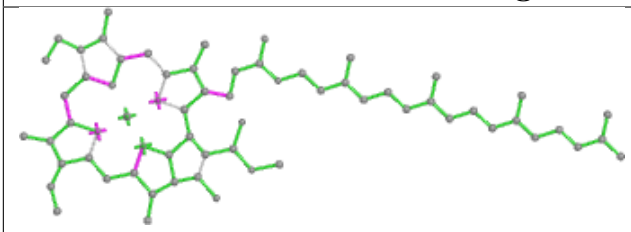


Rings

Ligand CLA A 1124



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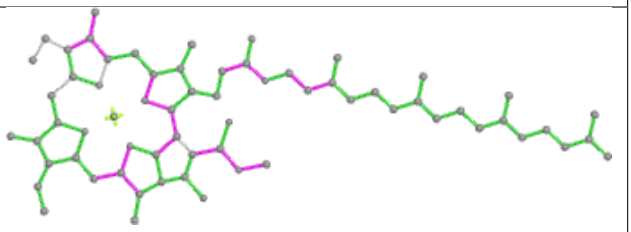
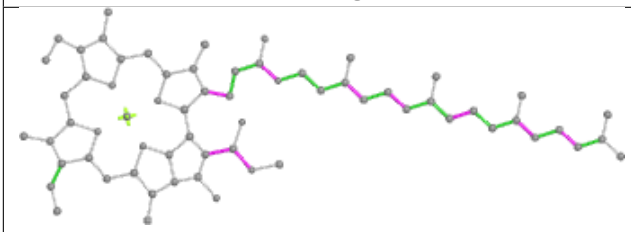


Bond angles



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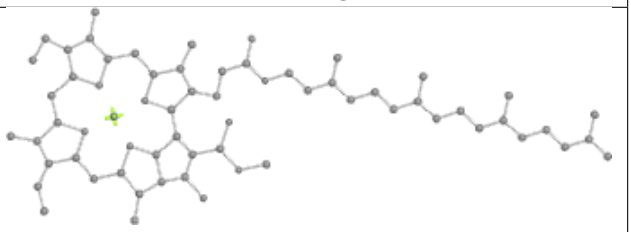
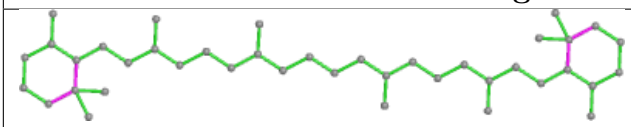


Rings

Ligand BCR A 4002



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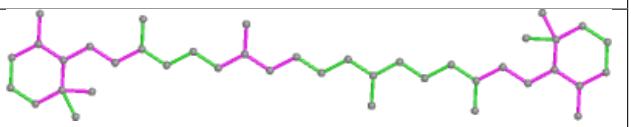
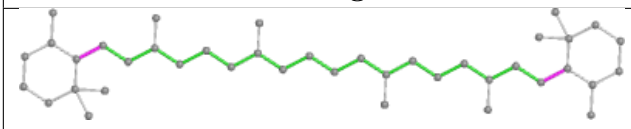


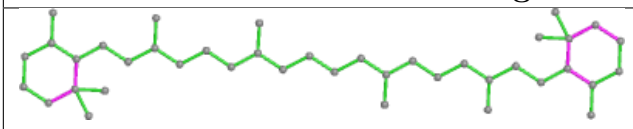
Bond angles



Torsions

Rings

Ligand BCR A 4003



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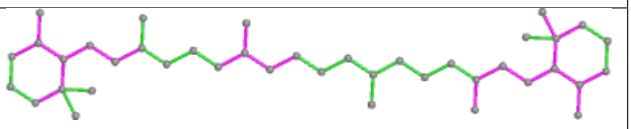
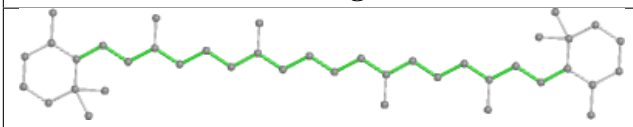


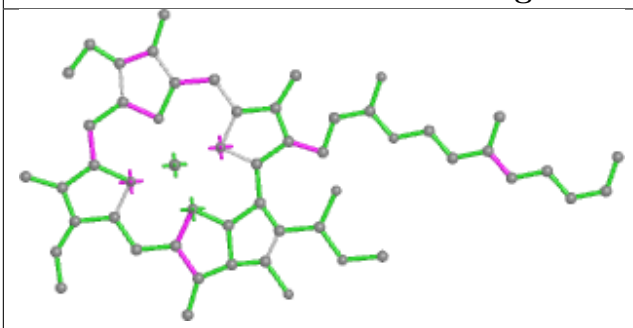
Bond angles



Torsions

Rings

Ligand CLA A 1116



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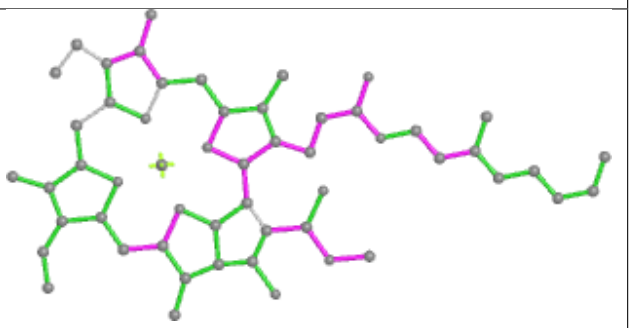
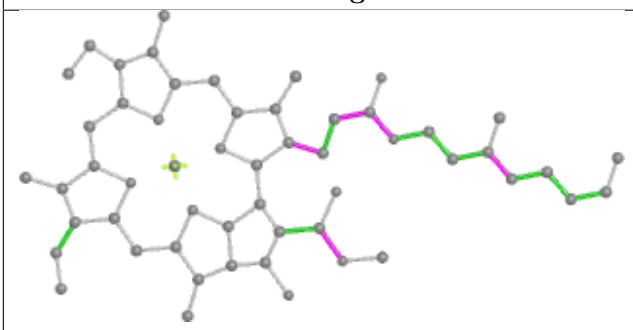
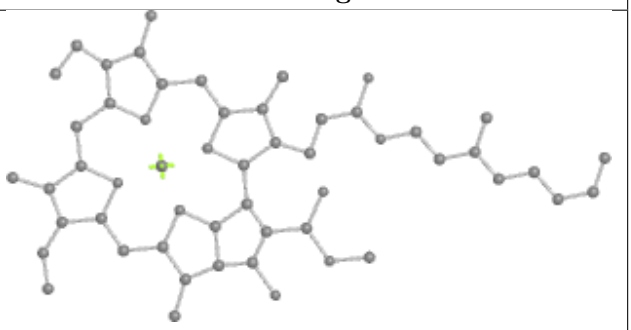


Bond angles

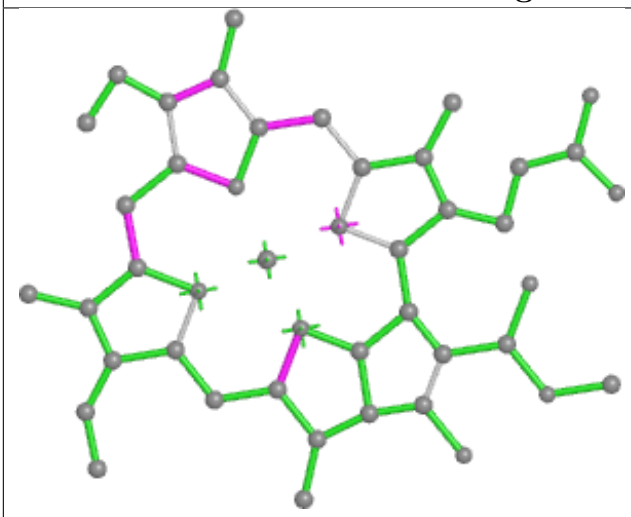


Torsions



Rings

Ligand CLA B 1233



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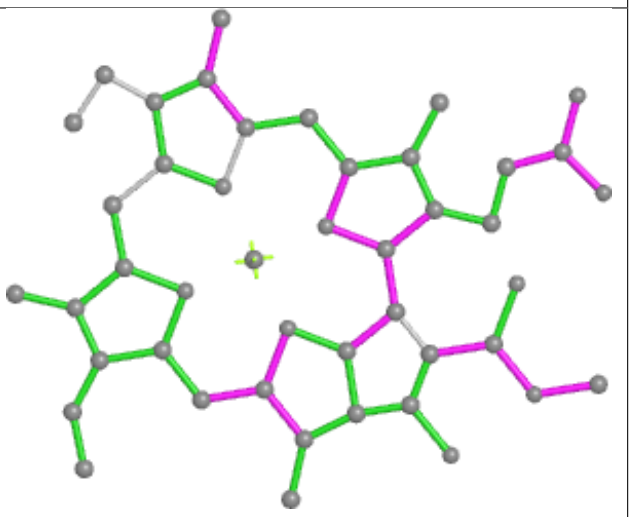
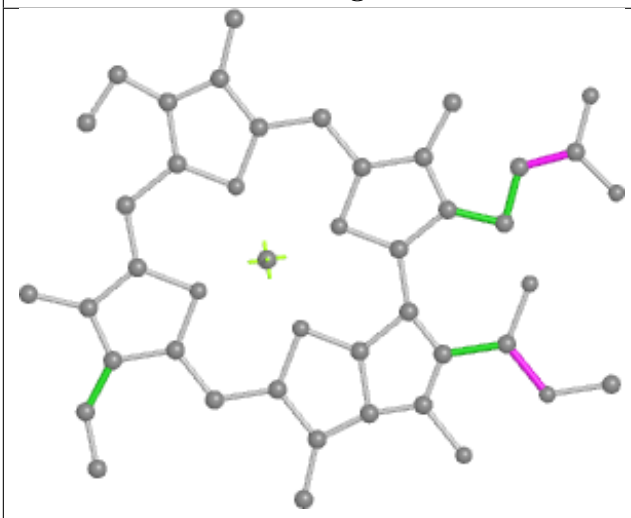
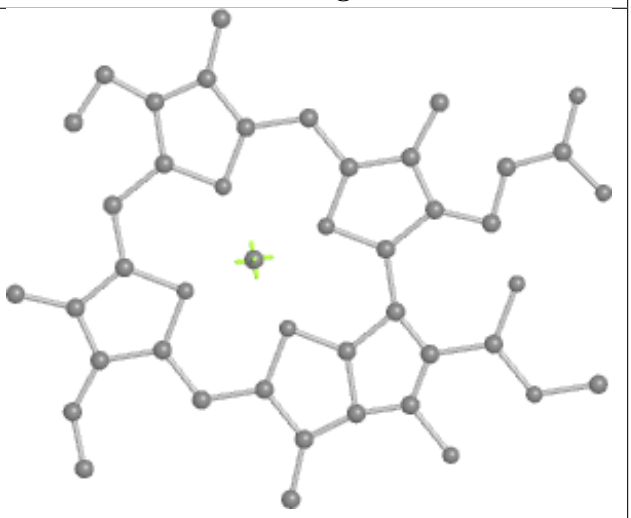


Bond angles

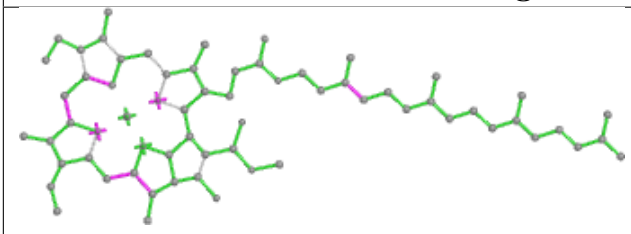


Torsions

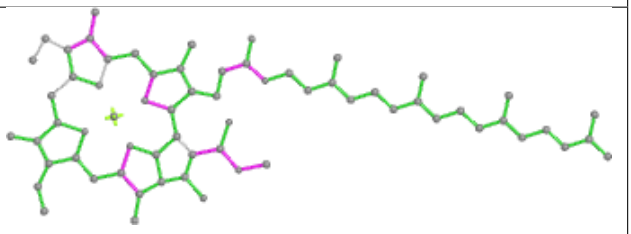


Rings

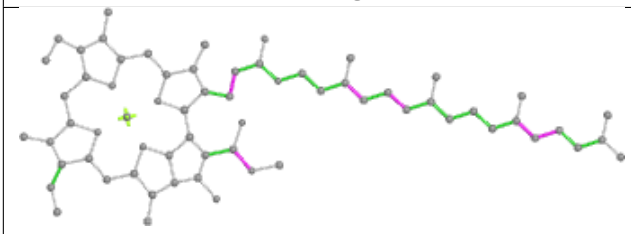
Ligand CLA A 1127



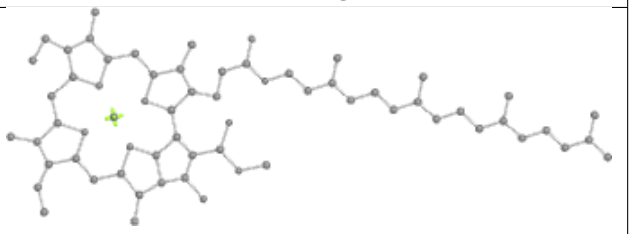
Bond lengths



Bond angles

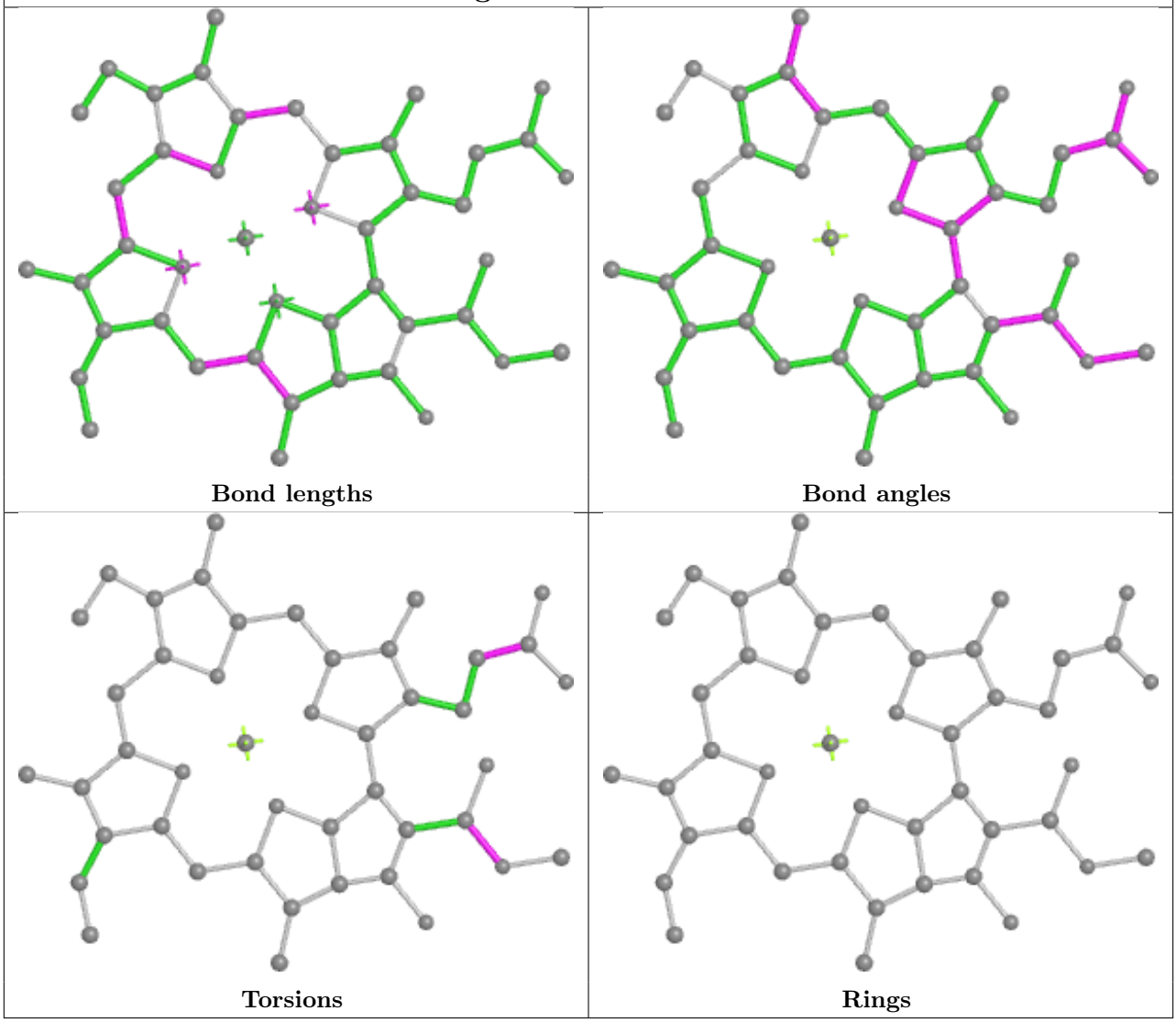


Torsions

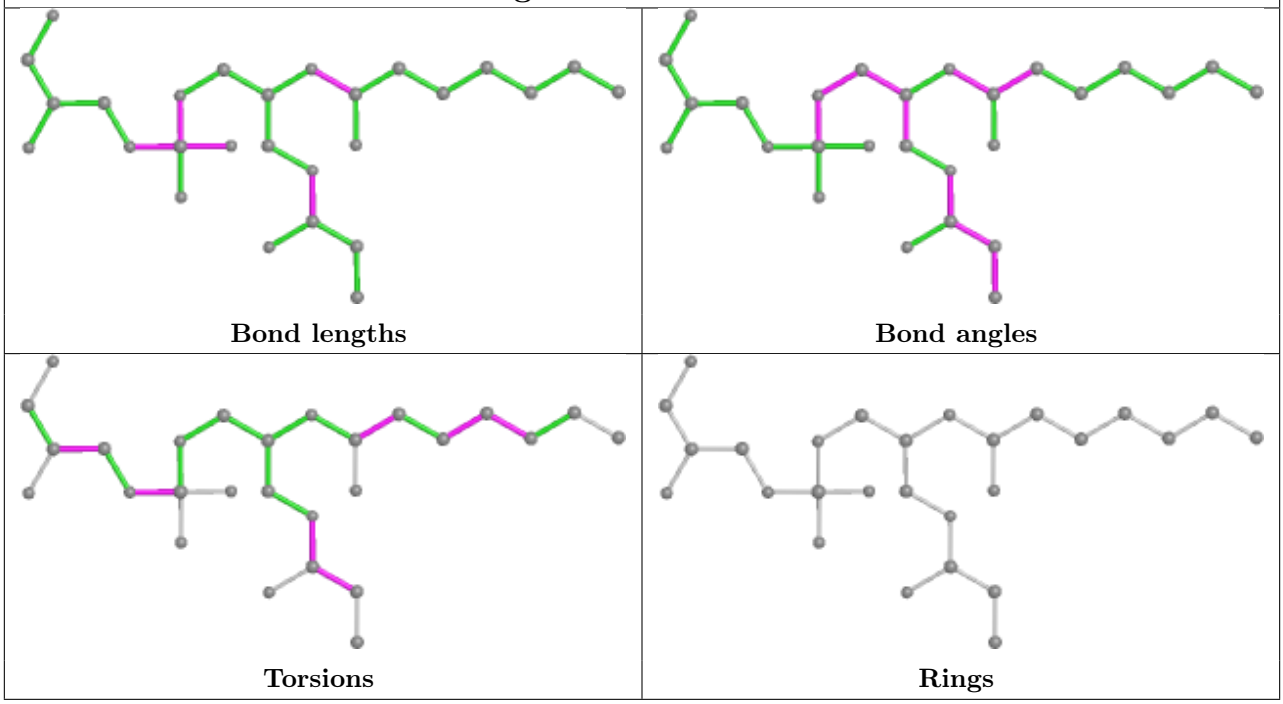


Rings

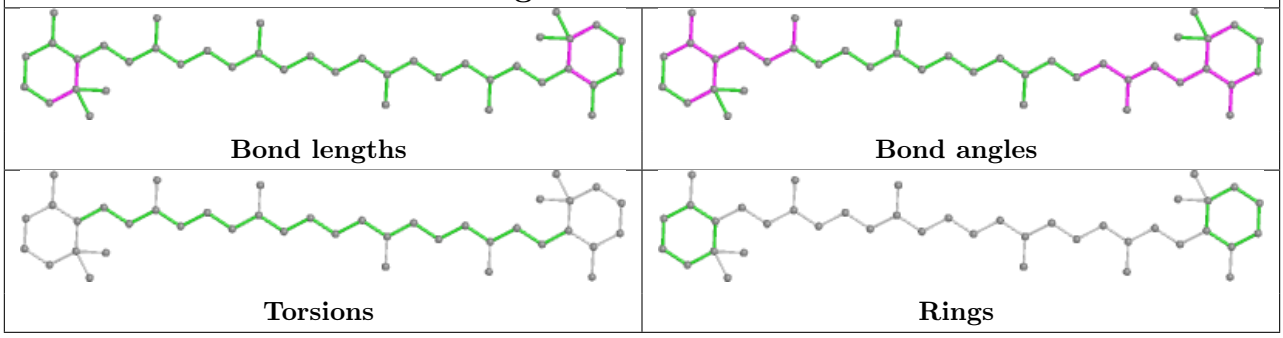
Ligand CLA F 1301



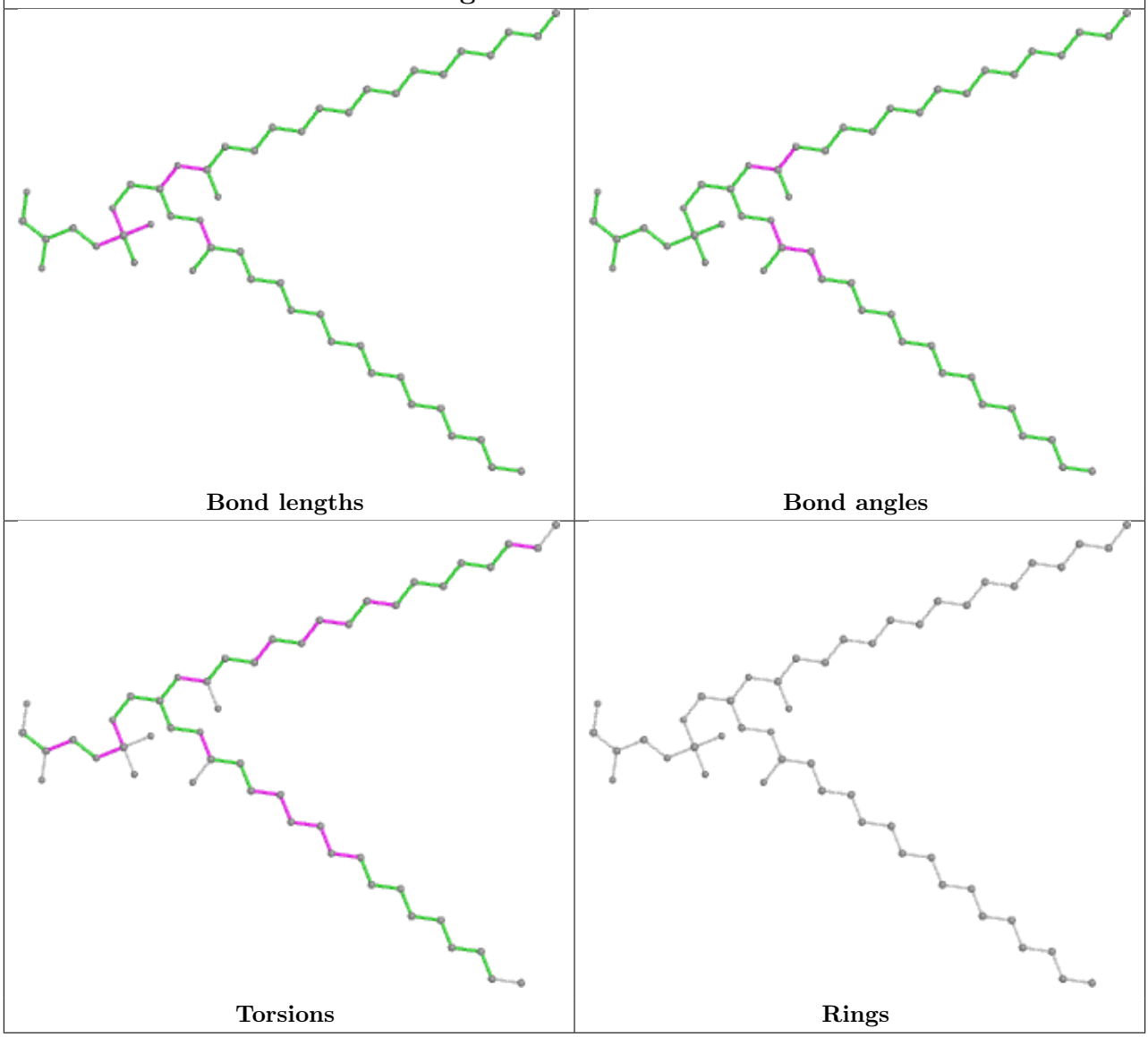
Ligand LHG A 5003



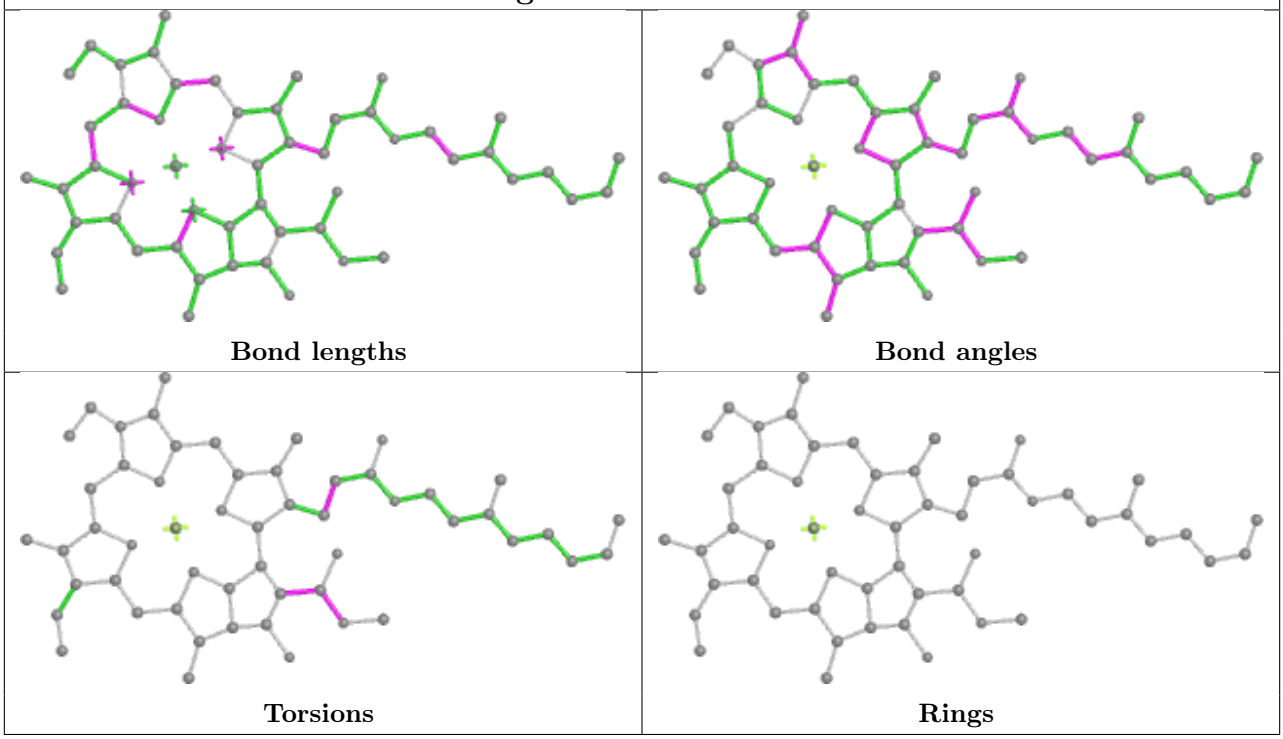
Ligand BCR B 4004



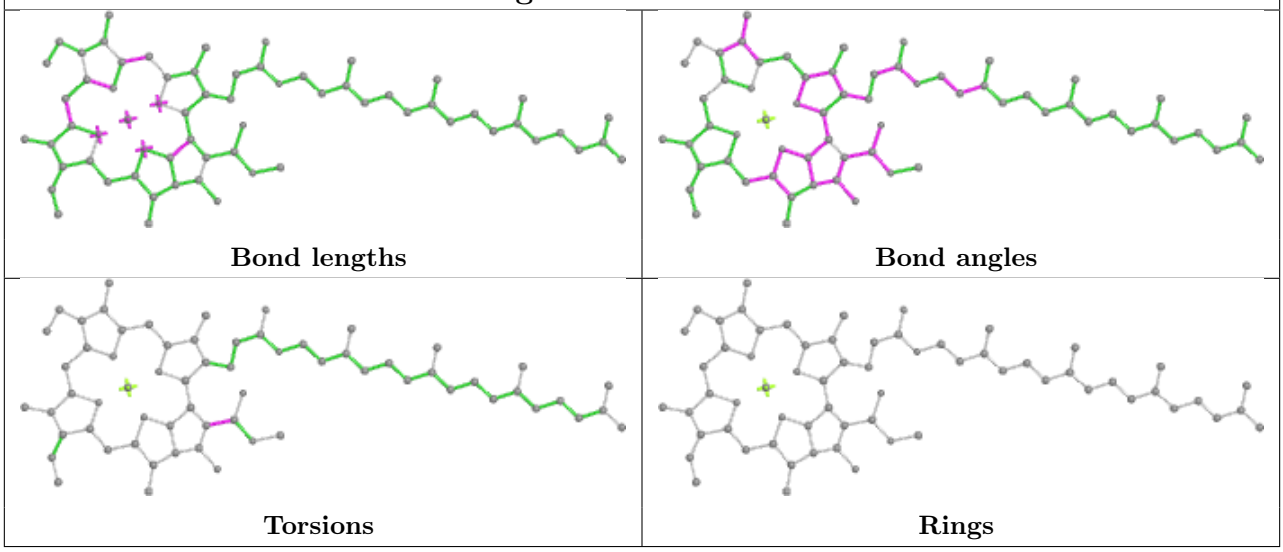
Ligand LHG A 5001



Ligand CLA B 1201



Ligand CLA A 1011



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.