



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:03 am BST

PDB ID : 2O01
Title : The Structure of a plant photosystem I supercomplex at 3.4 Angstrom resolution
Authors : Amunts, A.; Drory, O.; Nelson, N.
Deposited on : 2006-11-27
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

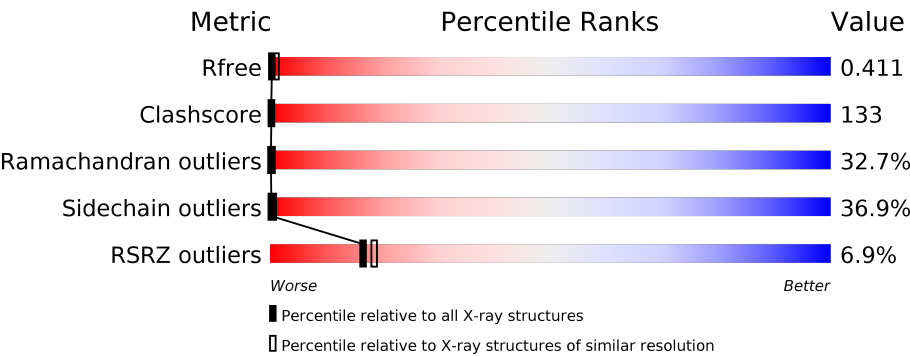
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	754	<div><div>8%</div><div>6%</div><div>39%</div><div>41%</div><div>11%</div><div></div></div>
2	B	732	<div><div>5%</div><div>5%</div><div>46%</div><div>38%</div><div>11%</div></div>
3	C	80	<div><div>14%</div><div></div><div>35%</div><div>41%</div><div>20%</div></div>
4	D	138	<div><div>4%</div><div>5%</div><div>35%</div><div>43%</div><div>17%</div></div>
5	E	62	<div><div>2%</div><div>10%</div><div>39%</div><div>39%</div><div>13%</div></div>
6	F	154	<div><div>8%</div><div>5%</div><div>43%</div><div>37%</div><div>16%</div></div>

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Mol	Chain	Length	Quality of chain
7	G	95	
8	H	75	
9	I	30	
10	J	42	
11	K	38	
12	L	164	
13	N	85	
14	1	187	
15	2	186	
16	3	165	
17	4	165	

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
18	CLA	1	1001	X	-	-	-
18	CLA	1	1002	X	-	-	-
18	CLA	1	1003	X	-	-	-
18	CLA	1	1004	X	-	-	-
18	CLA	1	1005	X	-	-	-
18	CLA	1	1006	X	-	-	-
18	CLA	1	1007	X	-	-	-
18	CLA	1	1008	X	-	-	-
18	CLA	1	1010	X	-	-	-
18	CLA	1	1011	X	-	-	-
18	CLA	1	1012	X	-	-	-
18	CLA	1	1013	X	-	-	-
18	CLA	1	1014	X	-	-	-
18	CLA	2	2001	X	-	-	-
18	CLA	2	2002	X	-	-	-
18	CLA	2	2003	X	-	-	-
18	CLA	2	2004	X	-	-	-
18	CLA	2	2005	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	2006	X	-	-	-
18	CLA	2	2007	X	-	-	-
18	CLA	2	2008	X	-	-	-
18	CLA	2	2010	X	-	-	-
18	CLA	2	2011	X	-	-	X
18	CLA	2	2012	X	-	-	-
18	CLA	2	2013	X	-	-	-
18	CLA	2	2015	X	-	-	-
18	CLA	3	2009	X	-	-	-
18	CLA	3	3001	X	-	-	X
18	CLA	3	3002	X	-	-	-
18	CLA	3	3003	X	-	-	-
18	CLA	3	3004	X	-	-	-
18	CLA	3	3005	X	-	-	-
18	CLA	3	3006	X	-	-	-
18	CLA	3	3007	X	-	-	-
18	CLA	3	3008	X	-	-	-
18	CLA	3	3009	X	-	-	-
18	CLA	3	3010	X	-	-	-
18	CLA	3	3011	X	-	-	-
18	CLA	3	3012	X	-	-	-
18	CLA	3	3013	X	-	-	-
18	CLA	3	3015	X	-	-	-
18	CLA	4	1009	X	-	-	-
18	CLA	4	1304	X	-	-	-
18	CLA	4	4001	X	-	-	X
18	CLA	4	4002	X	-	-	-
18	CLA	4	4003	X	-	-	-
18	CLA	4	4004	X	-	-	-
18	CLA	4	4005	X	-	-	-
18	CLA	4	4006	X	-	-	-
18	CLA	4	4007	X	-	-	-
18	CLA	4	4008	X	-	-	-
18	CLA	4	4009	X	-	-	-
18	CLA	4	4010	X	-	-	-
18	CLA	4	4011	X	-	-	-
18	CLA	4	4012	X	-	-	-
18	CLA	4	4013	X	-	-	-
18	CLA	A	1101	X	-	-	-
18	CLA	A	1102	X	-	-	-
18	CLA	A	1103	X	-	-	-
18	CLA	A	1104	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	1105	X	-	-	-
18	CLA	A	1106	X	-	-	-
18	CLA	A	1107	X	-	-	-
18	CLA	A	1108	X	-	-	-
18	CLA	A	1109	X	-	-	-
18	CLA	A	1110	X	-	-	-
18	CLA	A	1111	X	-	-	-
18	CLA	A	1113	X	-	-	-
18	CLA	A	1115	X	-	-	-
18	CLA	A	1116	X	-	-	-
18	CLA	A	1117	X	-	-	-
18	CLA	A	1118	X	-	-	-
18	CLA	A	1119	X	-	-	-
18	CLA	A	1120	X	-	-	-
18	CLA	A	1122	X	-	-	-
18	CLA	A	1123	X	-	X	-
18	CLA	A	1124	X	-	-	-
18	CLA	A	1126	X	-	X	-
18	CLA	A	1127	X	-	-	-
18	CLA	A	1128	X	-	-	-
18	CLA	A	1129	X	-	-	-
18	CLA	A	1131	X	-	-	-
18	CLA	A	1132	X	-	-	-
18	CLA	A	1133	X	-	-	-
18	CLA	A	1134	X	-	-	-
18	CLA	A	1135	X	-	-	X
18	CLA	A	1136	X	-	X	-
18	CLA	A	1137	X	-	-	-
18	CLA	A	1140	X	-	X	-
18	CLA	A	1142	X	-	-	-
18	CLA	A	1143	X	-	-	-
18	CLA	A	1144	X	-	-	-
18	CLA	A	1146	X	-	-	-
18	CLA	A	1147	X	-	-	-
18	CLA	A	1148	X	-	-	-
18	CLA	A	1151	X	-	-	-
18	CLA	A	1152	X	-	-	-
18	CLA	A	1309	X	-	-	-
18	CLA	A	9011	X	-	X	-
18	CLA	A	9013	X	-	-	-
18	CLA	B	1138	X	-	X	-
18	CLA	B	1201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	1202	X	-	X	-
18	CLA	B	1203	X	-	-	-
18	CLA	B	1205	X	-	-	-
18	CLA	B	1206	X	-	-	-
18	CLA	B	1207	X	-	-	-
18	CLA	B	1208	X	-	-	-
18	CLA	B	1209	X	-	X	-
18	CLA	B	1210	X	-	-	-
18	CLA	B	1211	X	-	-	-
18	CLA	B	1212	X	-	-	X
18	CLA	B	1213	X	-	-	-
18	CLA	B	1214	X	-	X	-
18	CLA	B	1215	X	-	X	-
18	CLA	B	1216	X	-	X	-
18	CLA	B	1217	X	-	-	-
18	CLA	B	1218	X	-	X	-
18	CLA	B	1219	X	-	-	-
18	CLA	B	1220	X	-	X	-
18	CLA	B	1221	X	-	X	-
18	CLA	B	1222	X	-	-	-
18	CLA	B	1223	X	-	-	-
18	CLA	B	1224	X	-	-	-
18	CLA	B	1225	X	-	X	-
18	CLA	B	1226	X	-	-	-
18	CLA	B	1227	X	-	X	-
18	CLA	B	1228	X	-	X	-
18	CLA	B	1229	X	-	-	-
18	CLA	B	1230	X	-	-	-
18	CLA	B	1231	X	-	-	-
18	CLA	B	1232	X	-	-	-
18	CLA	B	1234	X	-	X	-
18	CLA	B	1235	X	-	-	-
18	CLA	B	1236	X	-	-	-
18	CLA	B	1237	X	-	-	-
18	CLA	B	1238	X	-	X	-
18	CLA	B	1239	X	-	X	-
18	CLA	B	1241	X	-	-	-
18	CLA	B	1242	X	-	-	-
18	CLA	B	1301	X	-	-	-
18	CLA	B	9010	X	-	X	-
18	CLA	B	9012	X	-	-	-
18	CLA	B	9022	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	9023	X	-	-	-
18	CLA	F	1139	X	-	X	-
18	CLA	F	1240	X	-	-	-
18	CLA	F	1302	X	-	-	-
18	CLA	F	1303	X	-	-	-
18	CLA	F	1305	X	-	-	-
18	CLA	F	1306	X	-	-	-
18	CLA	F	4015	X	-	-	-
18	CLA	G	1233	X	-	-	-
18	CLA	G	1248	X	-	-	-
18	CLA	H	1501	X	-	-	-
18	CLA	H	1505	X	-	-	-
18	CLA	I	1204	X	-	-	-
18	CLA	J	1307	X	-	-	-
18	CLA	J	1308	X	-	-	-
18	CLA	J	2107	X	-	-	-
18	CLA	K	1141	X	-	-	-
18	CLA	K	1150	X	-	-	-
18	CLA	K	1153	X	-	-	-
18	CLA	L	1125	X	-	-	-
18	CLA	L	1130	X	-	X	-
18	CLA	L	1502	X	-	-	-
18	CLA	L	1503	X	-	X	-
18	CLA	L	1504	X	-	-	-
19	PQN	A	5001	X	-	X	-
19	PQN	B	5002	X	-	-	X
20	BCR	B	6017	-	-	-	X
21	SF4	B	3101	-	-	X	-
21	SF4	C	3102	-	-	X	-
21	SF4	C	3103	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 29846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5732	3758	975	981	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLY	ARG	CONFLICT	UNP P05310

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	732	Total	C	N	O	S	0	0	0
			5844	3841	996	994	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	ALA	PHE	CONFLICT	UNP P05311

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	62	Total	C	N	O	0	0	0
			503	321	90	92			

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	S	0	0	0
			744	484	121	137	2			

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplast.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	0	0	0
			577	379	96	102			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			344	236	51	56	1			

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplast.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	37	Total	C	N	O	0	0	0
			185	111	37	37			

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	164	Total	C	N	O	S	0	0	0
			1235	815	197	218	5			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 14 is a protein called AT3g54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	175	Total	C	N	O	S	0	0	0
			1187	755	211	217	4			

- Molecule 15 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	166	Total	C	N	O	S	0	0	0
			1268	828	207	230	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	17	GLU	PRO	CONFLICT	UNP Q41038
2	35	SER	GLY	CONFLICT	UNP Q41038

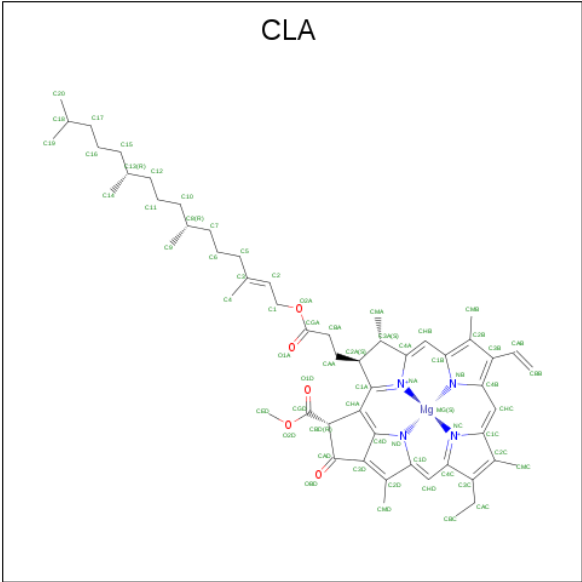
- Molecule 16 is a protein called PSI type III chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	115	Total	C	N	O	S	0	0	0
			857	559	141	153	4			

- Molecule 17 is a protein called PSI light-harvesting antenna chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	165	Total	C	N	O	S	0	0	0
			1282	839	214	226	3			

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
18	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N		0	0
			24	19	1	4			
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			44	34	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total 25	C 20	Mg 1	N 4	0	0
18	A	1	Total 25	C 20	Mg 1	N 4	0	0
18	A	1	Total 25	C 20	Mg 1	N 4	0	0
18	A	1	Total 25	C 20	Mg 1	N 4	0	0
18	A	1	Total 25	C 20	Mg 1	N 4	0	0
18	A	1	Total 25	C 20	Mg 1	N 4	0	0
18	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	A	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	A	1	Total 25	C 20	Mg 1	N 4	0	0
18	B	1	Total 56	C 46	Mg 1	N 4 O 5	0	0
18	B	1	Total 47	C 37	Mg 1	N 4 O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	B	1	Total 54	C 44	Mg 1	N 4 O 5	0	0
18	B	1	Total 47	C 37	Mg 1	N 4 O 5	0	0
18	B	1	Total 25	C 20	Mg 1	N 4	0	0
18	B	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	B	1	Total 48	C 38	Mg 1	N 4 O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	B	1	Total 25	C 20	Mg 1	N 4	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	B	1	Total 25	C 20	Mg 1	N 4	0	0
18	B	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	B	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	B	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	B	1	Total 51	C 41	Mg 1	N 4 O 5	0	0
18	B	1	Total 54	C 44	Mg 1	N 4 O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	B	1	Total 25	C 20	Mg 1	N 4	0	0
18	B	1	Total 47	C 37	Mg 1	N 4 O 5	0	0
18	B	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 44	C 35	Mg 1	N 4 O 4	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	G	1	Total 51	C 41	Mg 1	N 4 O 5	0	0
18	G	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	H	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	I	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	J	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	J	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
18	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	L	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0

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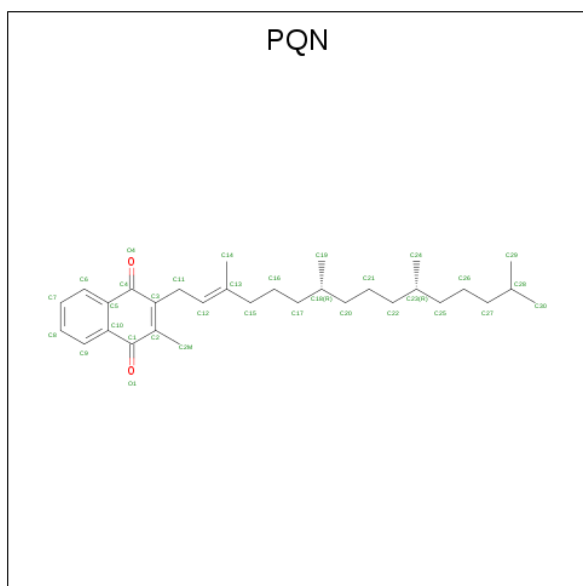
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0

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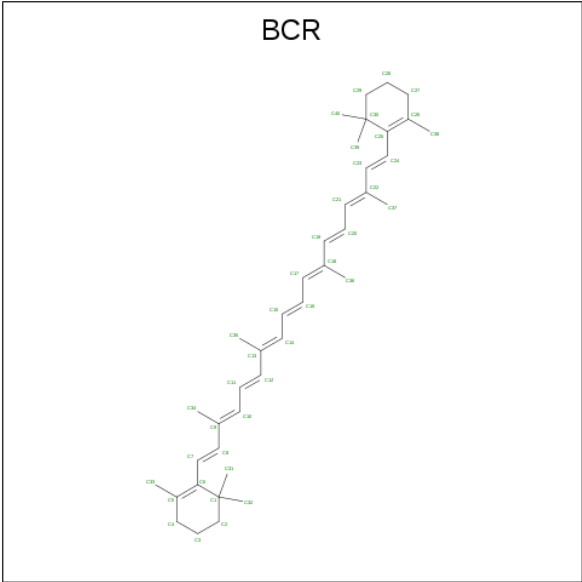
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



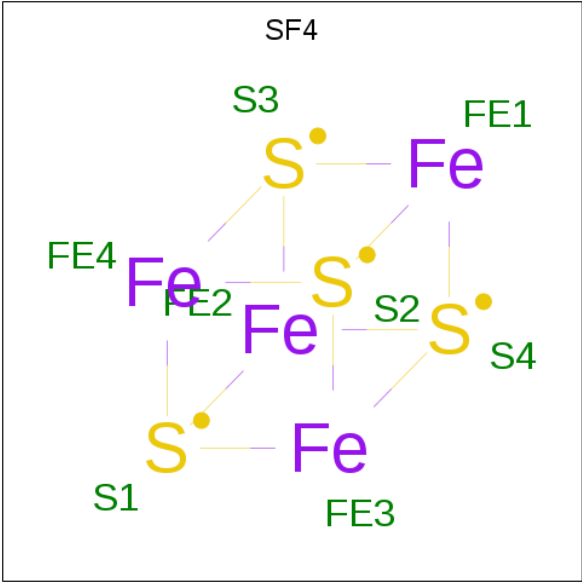
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			33	31	2		
19	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	F	1	Total C 40 40	0	0
20	I	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

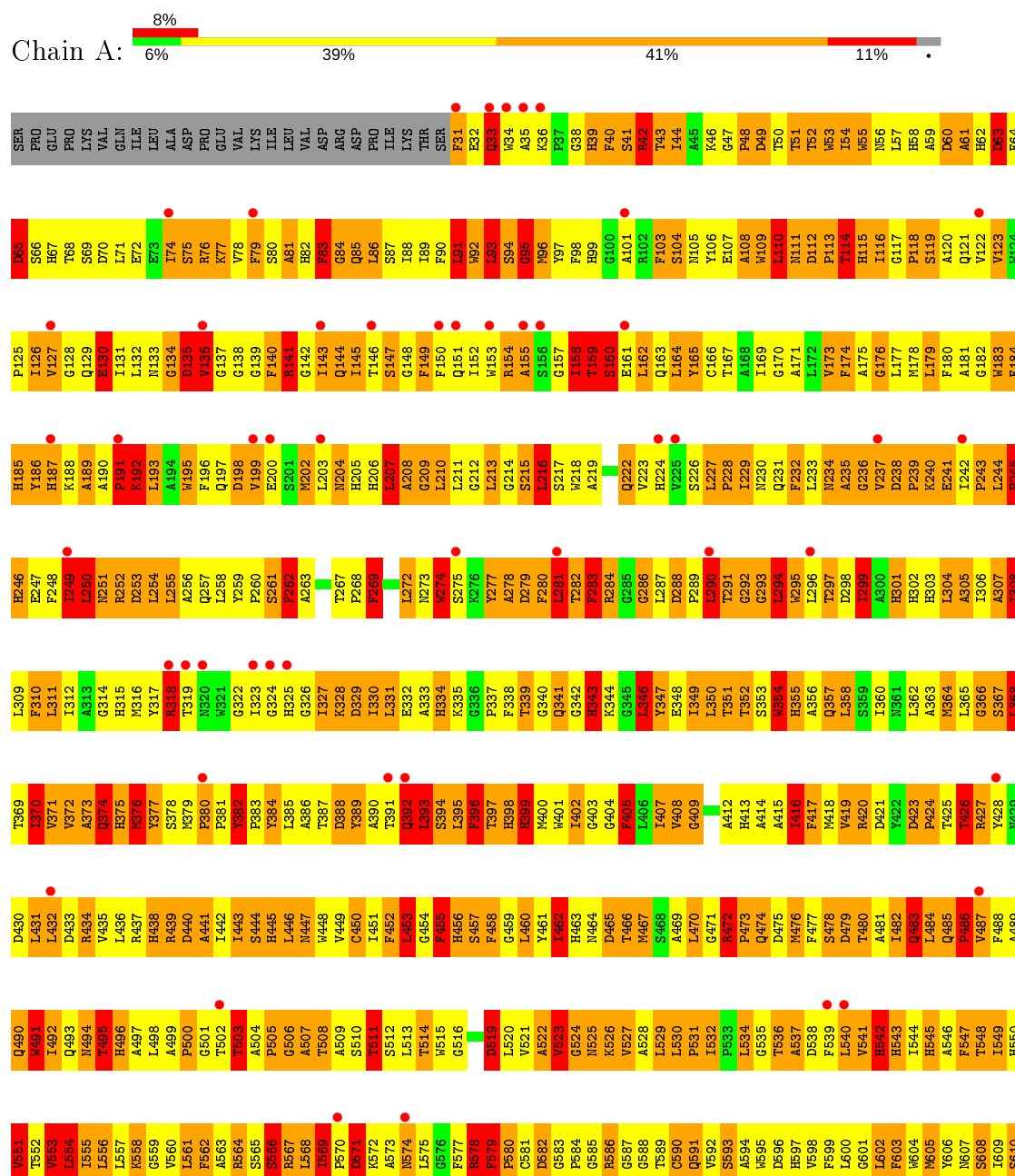


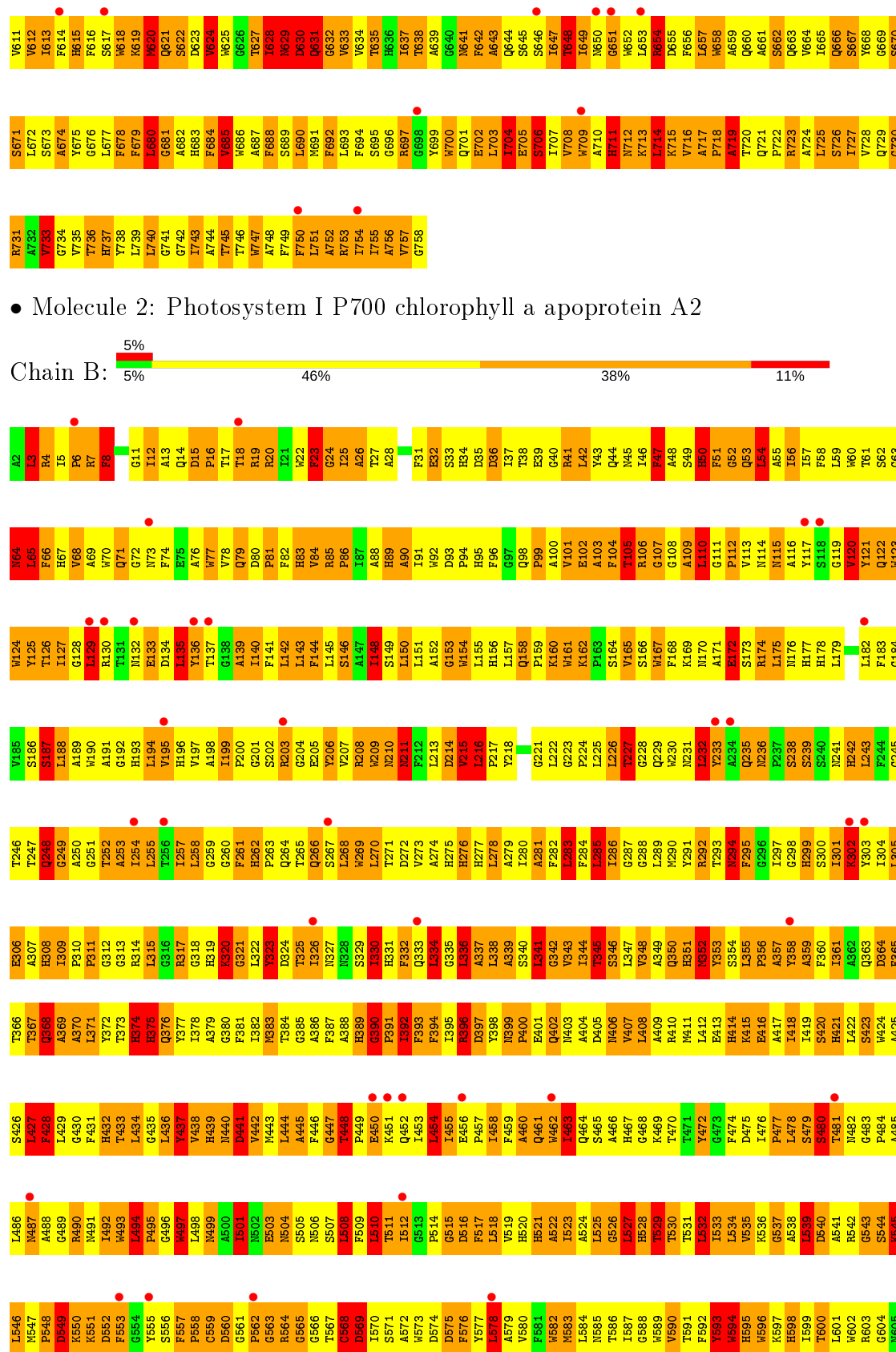
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total 8	Fe 4	S 4	0	0
21	C	1	Total 8	Fe 4	S 4	0	0
21	C	1	Total 8	Fe 4	S 4	0	0

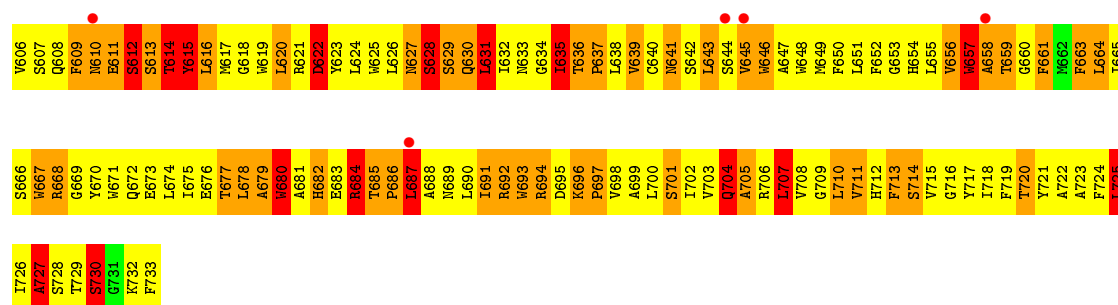
3 Residue-property plots

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

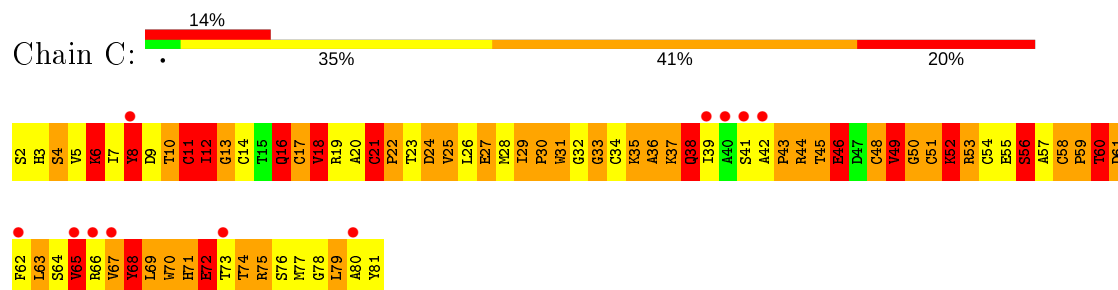
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



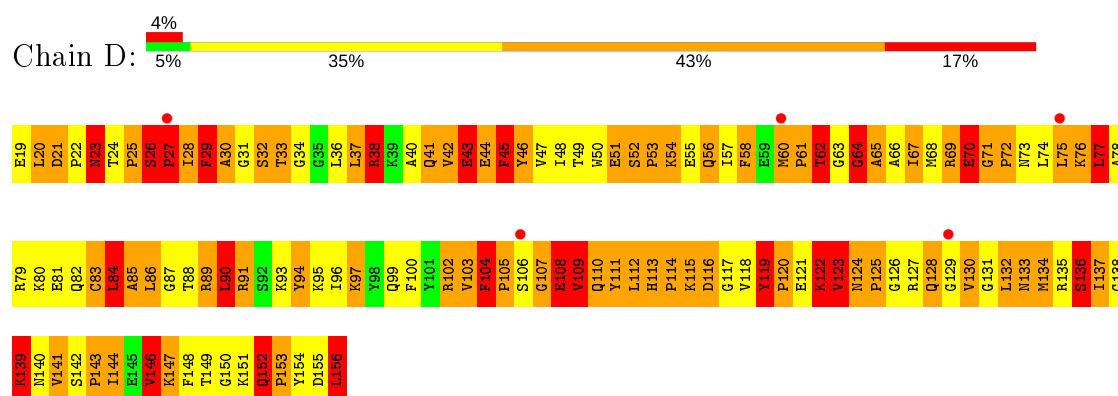




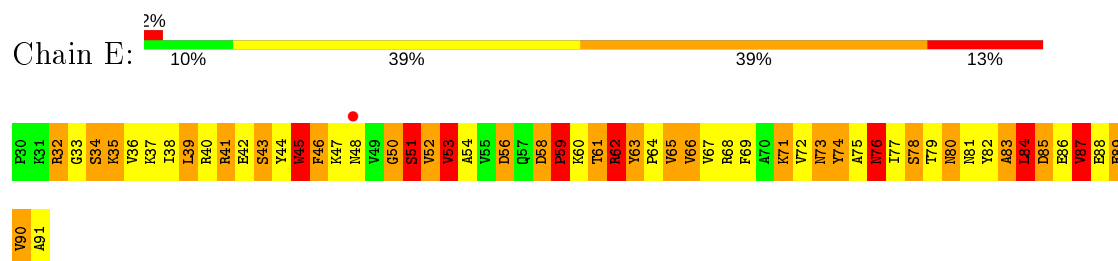
- Molecule 3: Photosystem I iron-sulfur center



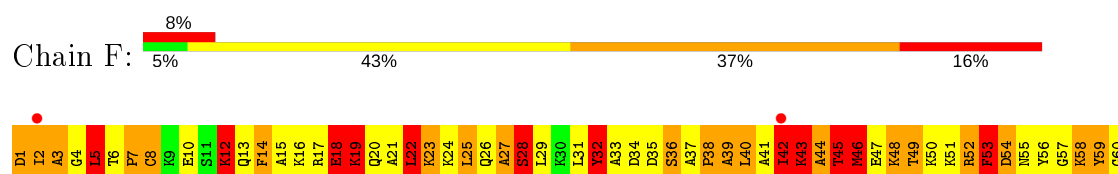
- Molecule 4: Photosystem I reaction center subunit II, chloroplast



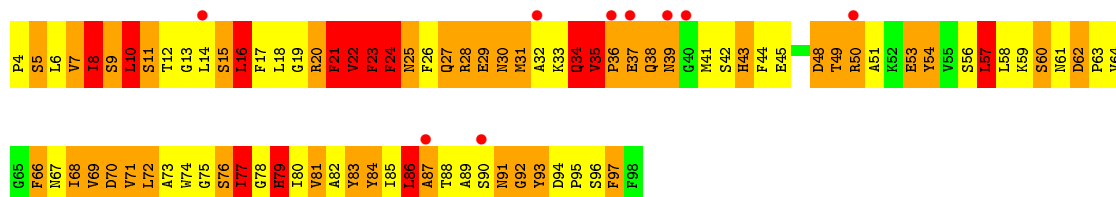
- Molecule 5: Photosystem I reaction center subunit IV A, chloroplast



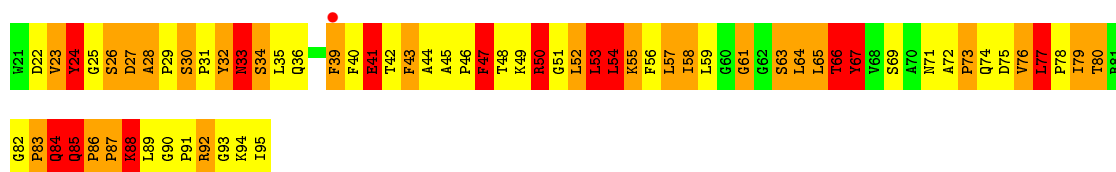
- Molecule 6: Photosystem I reaction center subunit III, chloroplast



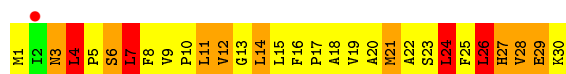
- Molecule 7: Photosystem I reaction center subunit V, chloroplast



- Molecule 8: Photosystem I reaction center subunit VI, chloroplast



- Molecule 9: Photosystem I reaction center subunit VIII



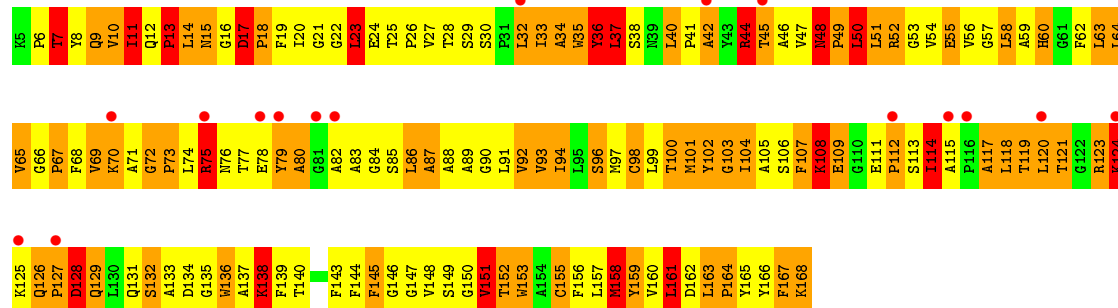
- Molecule 10: Photosystem I reaction center subunit IX



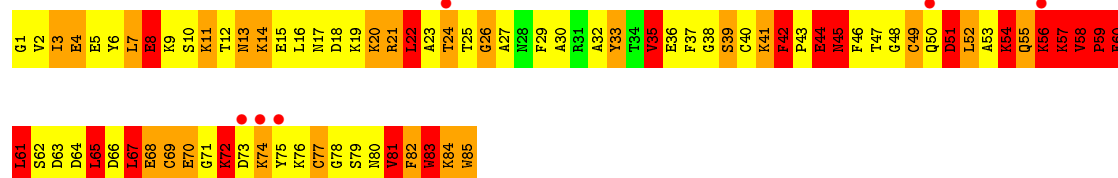
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplast



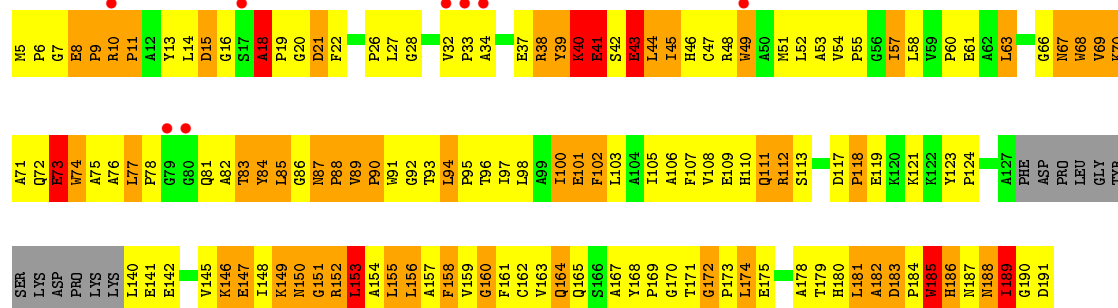
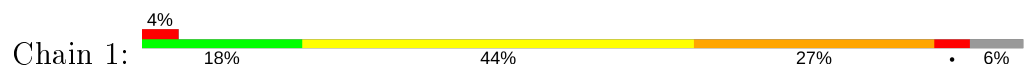
- Molecule 12: Photosystem I reaction center subunit XI, chloroplast



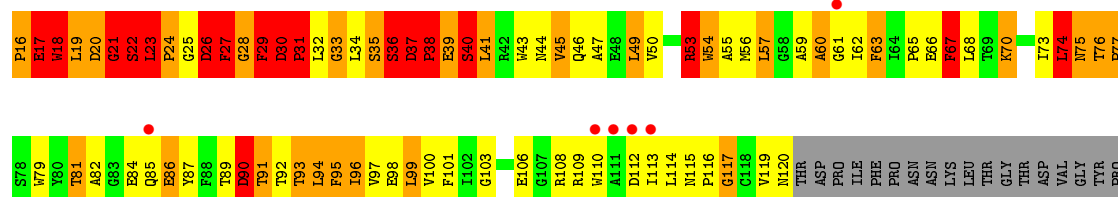
• Molecule 13: Photosystem I-N subunit

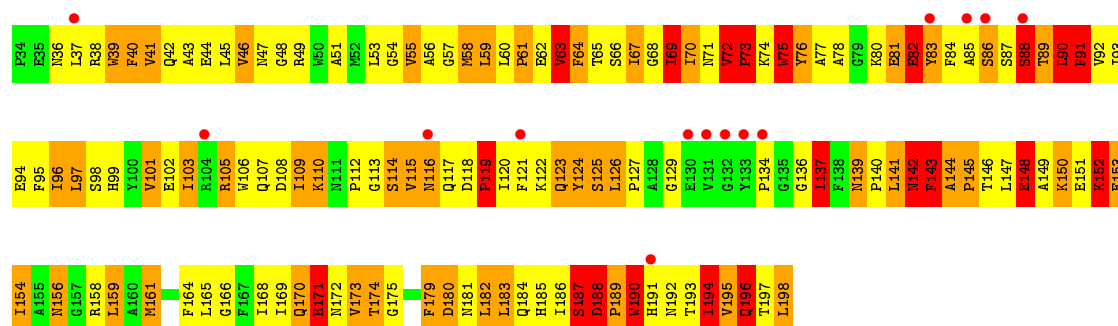


• Molecule 14: AT3g54890



• Molecule 15: Type II chlorophyll a/b binding protein from photosystem I





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.05Å 188.78Å 127.52Å 90.00° 95.19° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 50.40 – 3.01	Depositor EDS
% Data completeness (in resolution range)	90.8 (40.00-3.40) 64.2 (50.40-3.01)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.348 , 0.409 0.353 , 0.411	Depositor DCC
R_{free} test set	3517 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	96.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 500.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	29846	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.75	0/5928	1.06	14/8092 (0.2%)
2	B	0.76	0/6054	1.06	16/8273 (0.2%)
3	C	0.97	1/624 (0.2%)	1.18	2/846 (0.2%)
4	D	0.82	0/1122	1.25	5/1514 (0.3%)
5	E	0.73	0/513	1.06	1/694 (0.1%)
6	F	0.78	0/1250	1.10	6/1687 (0.4%)
7	G	0.72	0/764	1.08	3/1035 (0.3%)
8	H	0.83	0/595	1.23	5/810 (0.6%)
9	I	0.75	0/235	1.20	2/320 (0.6%)
10	J	0.78	0/356	1.15	2/484 (0.4%)
12	L	0.78	0/1272	1.10	1/1736 (0.1%)
13	N	0.63	0/699	0.96	2/936 (0.2%)
14	1	0.61	0/1215	0.87	1/1666 (0.1%)
15	2	0.73	1/1309 (0.1%)	1.03	6/1787 (0.3%)
16	3	0.60	0/879	0.95	2/1194 (0.2%)
17	4	0.72	2/1319 (0.2%)	0.88	2/1797 (0.1%)
All	All	0.75	4/24134 (0.0%)	1.06	70/32871 (0.2%)

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
1	A	0	32
2	B	0	32
3	C	0	4
4	D	0	14
5	E	0	3
6	F	0	9
7	G	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	4
9	I	0	2
12	L	0	4
13	N	3	11
14	1	0	5
15	2	3	21
16	3	1	14
17	4	0	13
All	All	7	174

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	21	CYS	CB-SG	5.62	1.91	1.82
17	4	190	TRP	CB-CG	-5.40	1.40	1.50
15	2	40	SER	C-N	-5.35	1.21	1.34
17	4	119	PRO	N-CD	5.04	1.54	1.47

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	SER	C-N-CD	-17.32	82.50	120.60
15	2	40	SER	C-N-CA	-12.47	90.53	121.70
4	D	119	TYR	C-N-CD	-10.41	97.69	120.60
12	L	72	GLY	C-N-CD	-9.86	98.90	120.60
16	3	196	LEU	CA-CB-CG	8.27	134.32	115.30
2	B	24	GLY	N-CA-C	-7.82	93.54	113.10
6	F	5	LEU	N-CA-C	-7.60	90.48	111.00
1	A	453	LEU	CA-CB-CG	7.51	132.59	115.30
1	A	530	LEU	CA-CB-CG	7.49	132.52	115.30
1	A	294	LEU	CA-CB-CG	7.46	132.47	115.30
2	B	631	LEU	CA-CB-CG	7.39	132.31	115.30
15	2	37	ASP	C-N-CD	-7.22	104.71	120.60
2	B	232	LEU	CA-CB-CG	6.89	131.16	115.30
6	F	5	LEU	CA-CB-CG	6.77	130.87	115.30
1	A	554	LEU	CA-CB-CG	6.72	130.77	115.30
9	I	24	LEU	CA-CB-CG	6.72	130.76	115.30
2	B	707	LEU	CA-CB-CG	6.62	130.53	115.30
8	H	54	LEU	CA-CB-CG	6.58	130.43	115.30
7	G	92	GLY	N-CA-C	-6.49	96.87	113.10
1	A	250	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	216	LEU	CA-CB-CG	6.42	130.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	156	LEU	CA-CB-CG	6.41	130.04	115.30
7	G	58	LEU	N-CA-C	-6.21	94.23	111.00
6	F	72	ILE	N-CA-C	6.17	127.67	111.00
7	G	84	TYR	N-CA-C	6.12	127.53	111.00
2	B	390	GLY	C-N-CD	6.12	141.25	128.40
15	2	37	ASP	C-N-CA	6.10	147.63	122.00
4	D	84	LEU	CA-CB-CG	6.07	129.27	115.30
2	B	436	LEU	CA-CB-CG	6.06	129.23	115.30
8	H	41	GLU	N-CA-C	6.05	127.35	111.00
5	E	51	SER	N-CA-C	5.90	126.92	111.00
2	B	336	LEU	CA-CB-CG	5.88	128.83	115.30
15	2	31	PRO	N-CA-C	5.86	127.33	112.10
10	J	26	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	290	LEU	CA-CB-CG	5.81	128.66	115.30
15	2	33	GLY	N-CA-C	-5.78	98.65	113.10
2	B	454	LEU	CA-CB-CG	5.75	128.52	115.30
6	F	91	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	141	ARG	NE-CZ-NH1	5.63	123.11	120.30
3	C	68	TYR	N-CA-C	5.62	126.17	111.00
9	I	4	LEU	CA-CB-CG	5.61	128.20	115.30
2	B	299	HIS	N-CA-C	5.56	126.00	111.00
2	B	129	LEU	CA-CB-CG	5.52	127.99	115.30
2	B	82	PHE	N-CA-C	5.50	125.84	111.00
8	H	85	GLN	N-CA-C	-5.45	96.30	111.00
17	4	59	LEU	CA-CB-CG	5.43	127.80	115.30
2	B	89	HIS	N-CA-C	5.42	125.64	111.00
1	A	192	LYS	N-CA-C	5.41	125.61	111.00
13	N	42	PHE	C-N-CD	-5.39	108.74	120.60
13	N	44	GLU	C-N-CA	5.38	135.16	121.70
8	H	53	LEU	CA-CB-CG	5.37	127.65	115.30
2	B	216	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	470	LEU	CA-CB-CG	5.34	127.58	115.30
3	C	8	TYR	N-CA-C	5.30	125.30	111.00
2	B	501	ILE	N-CA-C	5.25	125.19	111.00
15	2	57	LEU	CA-CB-CG	5.22	127.32	115.30
8	H	26	SER	N-CA-C	5.22	125.09	111.00
4	D	23	ASN	N-CA-C	5.21	125.08	111.00
17	4	90	LEU	CA-CB-CG	5.21	127.29	115.30
14	1	153	LEU	CA-CB-CG	5.18	127.21	115.30
2	B	3	LEU	CA-CB-CG	5.17	127.18	115.30
2	B	341	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	529	LEU	CA-CB-CG	5.14	127.12	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLY	N-CA-C	-5.12	100.30	113.10
1	A	491	TRP	C-N-CA	5.12	134.51	121.70
6	F	40	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	393	LEU	CA-CB-CG	5.06	126.95	115.30
10	J	39	PHE	N-CA-C	5.05	124.65	111.00
6	F	95	GLY	N-CA-C	5.03	125.67	113.10
16	3	130	LEU	CA-CB-CG	5.01	126.83	115.30

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	N	59	PRO	CA
13	N	61	LEU	CA
13	N	83	TRP	CA
15	2	20	ASP	CA
15	2	23	LEU	CA
15	2	27	PHE	CA
16	3	133	TRP	CA

All (174) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	1	18	ALA	Peptide
14	1	21	ASP	Peptide
14	1	83	THR	Peptide
14	1	85	LEU	Peptide
14	1	88	PRO	Peptide
15	2	144	ASP	Peptide
15	2	16	PRO	Peptide
15	2	17	GLU	Peptide
15	2	178	TRP	Peptide
15	2	187	GLY	Peptide
15	2	197	ALA	Peptide
15	2	20	ASP	Peptide
15	2	21	GLY	Peptide
15	2	22	SER	Peptide
15	2	23	LEU	Peptide
15	2	24	PRO	Peptide
15	2	26	ASP	Peptide
15	2	27	PHE	Peptide
15	2	28	GLY	Peptide
15	2	36	SER	Peptide

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Mol	Chain	Res	Type	Group
15	2	37	ASP	Peptide
15	2	38	PRO	Peptide
15	2	40	SER	Mainchain,Peptide
15	2	90	ASP	Peptide
15	2	99	LEU	Peptide
16	3	107	TYR	Peptide
16	3	132	ASP	Peptide
16	3	133	TRP	Peptide
16	3	134	TYR	Peptide
16	3	136	PRO	Peptide
16	3	137	GLY	Peptide
16	3	138	SER	Peptide
16	3	141	LYS	Peptide
16	3	198	TYR	Peptide
16	3	204	VAL	Peptide
16	3	214	LEU	Peptide
16	3	215	ASP	Peptide
16	3	82	ALA	Peptide
16	3	86	PRO	Peptide
17	4	137	ILE	Peptide
17	4	142	ASN	Peptide
17	4	143	PHE	Peptide
17	4	148	GLU	Peptide
17	4	187	SER	Peptide
17	4	188	ASP	Peptide
17	4	189	PRO	Peptide
17	4	196	GLN	Peptide
17	4	73	PRO	Peptide
17	4	76	TYR	Peptide
17	4	81	GLU	Peptide
17	4	83	TYR	Peptide
17	4	88	SER	Peptide
1	A	104	SER	Peptide
1	A	117	GLY	Peptide
1	A	187	HIS	Peptide
1	A	191	PRO	Peptide
1	A	210	LEU	Peptide
1	A	245	PRO	Peptide
1	A	269	PHE	Peptide
1	A	305	ALA	Peptide
1	A	308	ILE	Peptide
1	A	314	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	33	GLN	Peptide
1	A	343	HIS	Peptide
1	A	346	LEU	Peptide
1	A	357	GLN	Peptide
1	A	368	LEU	Peptide
1	A	392	GLN	Peptide
1	A	441	ALA	Peptide
1	A	457	SER	Peptide
1	A	47	GLY	Peptide
1	A	486	PRO	Peptide
1	A	506	GLY	Peptide
1	A	569	ILE	Peptide
1	A	610	SER	Peptide
1	A	629	ASN	Peptide
1	A	630	ASP	Peptide
1	A	632	GLY	Peptide
1	A	65	ASP	Peptide
1	A	685	VAL	Peptide
1	A	704	ILE	Peptide
1	A	719	ALA	Peptide
1	A	730	GLY	Peptide
1	A	756	ALA	Peptide
2	B	134	ASP	Peptide
2	B	208	ARG	Peptide
2	B	23	PHE	Peptide
2	B	238	SER	Peptide
2	B	283	LEU	Peptide
2	B	285	LEU	Peptide
2	B	292	ARG	Peptide
2	B	294	ASN	Peptide
2	B	298	GLY	Peptide
2	B	313	GLY	Peptide
2	B	337	ALA	Peptide
2	B	367	THR	Peptide
2	B	368	GLN	Peptide
2	B	390	GLY	Peptide
2	B	396	ARG	Peptide
2	B	405	ASP	Peptide
2	B	427	LEU	Peptide
2	B	428	PHE	Peptide
2	B	460	ALA	Peptide
2	B	484	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	B	494	LEU	Peptide
2	B	50	HIS	Peptide
2	B	515	GLY	Peptide
2	B	530	THR	Peptide
2	B	568	CYS	Peptide
2	B	569	ASP	Peptide
2	B	622	ASP	Peptide
2	B	635	ILE	Peptide
2	B	64	ASN	Peptide
2	B	679	ALA	Peptide
2	B	727	ALA	Peptide
2	B	730	SER	Peptide
3	C	21	CYS	Peptide
3	C	6	LYS	Peptide
3	C	60	THR	Peptide
3	C	67	VAL	Peptide
4	D	110	GLN	Peptide
4	D	114	PRO	Peptide
4	D	119	TYR	Peptide
4	D	122	LYS	Peptide
4	D	131	GLY	Peptide
4	D	136	SER	Peptide
4	D	152	GLN	Peptide
4	D	27	PRO	Peptide
4	D	32	SER	Peptide
4	D	52	SER	Peptide
4	D	60	MET	Peptide
4	D	64	GLY	Peptide
4	D	70	GLU	Peptide
4	D	71	GLY	Peptide
5	E	48	ASN	Peptide
5	E	50	GLY	Peptide
5	E	59	PRO	Peptide
6	F	110	ASP	Peptide
6	F	113	LYS	Peptide
6	F	116	GLN	Peptide
6	F	142	ARG	Peptide
6	F	22	LEU	Peptide
6	F	32	TYR	Peptide
6	F	36	SER	Peptide
6	F	5	LEU	Peptide
6	F	65	SER	Peptide

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Mol	Chain	Res	Type	Group
7	G	21	PHE	Peptide
7	G	22	VAL	Peptide
7	G	23	PHE	Peptide
7	G	24	PHE	Peptide
7	G	35	VAL	Peptide
7	G	57	LEU	Peptide
8	H	40	PHE	Peptide
8	H	46	PRO	Peptide
8	H	77	LEU	Peptide
8	H	84	GLN	Peptide
9	I	26	LEU	Peptide
9	I	4	LEU	Peptide
12	L	11	ILE	Peptide
12	L	128	ASP	Peptide
12	L	13	PRO	Peptide
12	L	158	MET	Peptide
13	N	42	PHE	Peptide
13	N	45	ASN	Peptide
13	N	51	ASP	Peptide
13	N	52	LEU	Peptide
13	N	55	GLN	Peptide
13	N	57	LYS	Peptide
13	N	58	VAL	Peptide
13	N	59	PRO	Peptide
13	N	67	LEU	Peptide
13	N	68	GLU	Peptide
13	N	81	VAL	Peptide

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	5732	0	5577	1855	0
2	B	5844	0	5659	1973	0
3	C	611	0	594	257	0
4	D	1095	0	1112	364	0
5	E	503	0	510	132	0
6	F	1221	0	1250	362	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	744	0	721	208	0
8	H	577	0	587	137	0
9	I	229	0	252	97	0
10	J	344	0	347	103	0
11	K	185	0	40	12	0
12	L	1235	0	1244	370	1
13	N	685	0	672	268	0
14	1	1187	0	1019	230	1
15	2	1268	0	1177	492	1
16	3	857	0	789	220	0
17	4	1282	0	1241	271	1
18	1	325	0	39	12	0
18	2	325	0	39	15	0
18	3	375	0	45	11	0
18	4	405	0	90	16	0
18	A	1601	0	870	350	0
18	B	2078	0	1535	705	0
18	F	224	0	94	43	0
18	G	76	0	43	12	0
18	H	80	0	51	13	0
18	I	55	0	48	11	0
18	J	111	0	66	8	0
18	K	75	0	9	5	0
18	L	227	0	162	107	0
19	A	33	0	46	30	0
19	B	33	0	46	20	0
20	A	40	0	54	17	0
20	B	40	0	54	20	0
20	F	40	0	54	15	0
20	I	40	0	54	13	0
20	L	40	0	54	17	0
21	B	8	0	0	4	0
21	C	16	0	0	15	0
All	All	29846	0	26244	7466	2

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 133.

All (7466) 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)
3:C:22:PRO:HG2	3:C:51:CYS:SG	1.33	1.68
15:2:192:LEU:HA	15:2:195:HIS:CE1	1.34	1.58
2:B:290:MET:CA	18:B:1218:CLA:HBC2	1.12	1.57
15:2:26:ASP:HB3	15:2:27:PHE:CB	1.34	1.56
2:B:290:MET:HA	18:B:1218:CLA:CB	1.31	1.56
2:B:289:LEU:C	18:B:1218:CLA:HBC1	1.22	1.55
18:A:1124:CLA:C3A	18:A:1135:CLA:HBB2	1.34	1.53
12:L:67:PRO:CD	18:L:1503:CLA:CAB	1.78	1.53
7:G:37:GLU:HG3	7:G:43:HIS:CE1	1.46	1.50
15:2:18:TRP:CD1	15:2:21:GLY:HA3	1.49	1.47
15:2:26:ASP:CB	15:2:27:PHE:HB3	1.40	1.47
12:L:66:GLY:HA3	18:L:1503:CLA:CAB	1.45	1.46
1:A:81:ALA:HB3	1:A:83:PHE:N	1.23	1.45
9:I:25:PHE:N	9:I:26:LEU:HB2	1.25	1.44
2:B:287:GLY:N	18:B:1218:CLA:CMC	1.83	1.42
15:2:21:GLY:HA2	15:2:25:GLY:C	1.36	1.41
2:B:287:GLY:N	18:B:1218:CLA:HMC1	1.09	1.39
12:L:67:PRO:HD3	18:L:1503:CLA:CAB	1.37	1.39
3:C:48:CYS:HB2	21:C:3102:SF4:S2	1.63	1.38
15:2:21:GLY:C	15:2:25:GLY:HA2	1.41	1.38
15:2:17:GLU:CG	15:2:18:TRP:HB2	1.52	1.38
13:N:58:VAL:HG23	13:N:59:PRO:CA	1.51	1.37
13:N:57:LYS:CD	16:3:87:ALA:HB1	1.56	1.35
5:E:66:VAL:HA	5:E:81:ASN:ND2	1.42	1.35
16:3:132:ASP:HB3	16:3:139:MET:CG	1.55	1.34
6:F:137:PRO:CA	6:F:141:TYR:HB3	1.57	1.34
16:3:54:TRP:CB	16:3:55:LEU:HA	1.54	1.34
15:2:17:GLU:HB3	15:2:18:TRP:CA	1.55	1.34
2:B:344:ILE:CD1	18:B:1225:CLA:HBC1	0.87	1.34
4:D:27:PRO:O	4:D:28:ILE:HG13	1.23	1.34
13:N:57:LYS:HD2	16:3:87:ALA:CB	1.55	1.34
18:A:1109:CLA:C1A	18:A:1109:CLA:C4D	2.05	1.33
1:A:141:ARG:CB	1:A:141:ARG:HH11	1.41	1.33
15:2:22:SER:CA	15:2:23:LEU:HG	1.57	1.32
1:A:555:ILE:N	1:A:556:LEU:HB2	1.44	1.32
2:B:334:LEU:HD12	2:B:389:HIS:CD2	1.65	1.31
15:2:18:TRP:HD1	15:2:21:GLY:CA	1.42	1.31
2:B:344:ILE:HD11	18:B:1225:CLA:CB	0.84	1.31
2:B:289:LEU:C	18:B:1218:CLA:CB	1.97	1.31
2:B:463:ILE:HG23	2:B:467:HIS:CE1	1.63	1.31
1:A:464:ASN:ND2	1:A:477:PHE:HB2	1.43	1.30
1:A:483:GLN:HG2	1:A:484:LEU:O	1.17	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:MET:CA	18:B:1218:CLA:CBC	1.92	1.30
4:D:26:SER:CA	4:D:27:PRO:O	1.80	1.30
15:2:24:PRO:CG	15:2:27:PHE:HE2	1.42	1.30
2:B:290:MET:N	18:B:1218:CLA:HBC2	1.43	1.30
12:L:164:PRO:HG3	18:L:1503:CLA:C2	1.61	1.29
18:L:1503:CLA:HBC2	18:L:1503:CLA:CHD	1.60	1.28
6:F:137:PRO:HA	6:F:141:TYR:CB	1.62	1.28
15:2:21:GLY:CA	15:2:25:GLY:HA2	1.62	1.28
6:F:49:THR:HA	6:F:56:TYR:OH	1.25	1.28
14:1:84:TYR:HB3	14:1:85:LEU:CA	1.64	1.27
1:A:302:HIS:HD2	1:A:303:HIS:CE1	1.52	1.27
7:G:60:SER:O	7:G:64:VAL:HG13	1.35	1.27
14:1:84:TYR:CB	14:1:85:LEU:HA	1.63	1.27
2:B:648:TRP:NE1	18:B:9022:CLA:H42	1.50	1.27
2:B:304:ILE:O	2:B:308:HIS:HB3	1.17	1.27
6:F:126:ALA:H	6:F:130:LEU:CD1	1.48	1.26
5:E:60:LYS:O	5:E:61:THR:HG22	1.33	1.26
1:A:96:MET:SD	1:A:96:MET:N	2.03	1.26
1:A:464:ASN:HD21	1:A:477:PHE:CB	1.46	1.26
3:C:22:PRO:CG	3:C:51:CYS:SG	2.22	1.26
15:2:17:GLU:HB3	15:2:18:TRP:C	1.53	1.26
1:A:555:ILE:H	1:A:556:LEU:CB	1.48	1.25
13:N:58:VAL:CG1	16:3:86:PRO:HA	1.66	1.25
4:D:31:GLY:CA	12:L:13:PRO:HB3	1.67	1.25
1:A:755:ILE:N	1:A:758:GLY:HA3	1.48	1.25
15:2:23:LEU:CA	15:2:25:GLY:H	1.48	1.25
1:A:147:SER:OG	18:A:1126:CLA:HMA2	1.35	1.25
16:3:133:TRP:O	16:3:137:GLY:CA	1.83	1.25
3:C:21:CYS:SG	21:C:3102:SF4:S2	2.34	1.24
15:2:17:GLU:HB3	15:2:18:TRP:CB	1.66	1.24
2:B:654:HIS:O	18:B:9022:CLA:HBD	1.38	1.23
4:D:72:PRO:CB	4:D:73:ASN:HA	1.60	1.23
16:3:134:TYR:N	16:3:136:PRO:HD2	1.54	1.23
1:A:64:PHE:CE1	18:A:1103:CLA:HMC1	1.71	1.23
4:D:72:PRO:HB2	4:D:73:ASN:CA	1.66	1.23
12:L:66:GLY:CA	18:L:1503:CLA:CAB	2.16	1.22
15:2:192:LEU:CA	15:2:195:HIS:HE1	1.51	1.21
2:B:289:LEU:O	18:B:1218:CLA:HBC1	1.39	1.21
1:A:51:THR:CG2	1:A:722:PRO:HA	1.68	1.21
1:A:302:HIS:CD2	1:A:303:HIS:HE1	1.58	1.21
3:C:55:GLU:HA	3:C:58:CYS:CB	1.70	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:GLU:CA	3:C:58:CYS:HB3	1.70	1.21
16:3:83:GLY:CA	16:3:86:PRO:HD2	1.67	1.21
18:B:1227:CLA:HHB	18:B:1228:CLA:OBD	1.35	1.21
3:C:51:CYS:SG	21:C:3102:SF4:S1	2.39	1.21
2:B:290:MET:N	18:B:1218:CLA:CBC	1.95	1.20
18:F:1302:CLA:H92	18:F:1302:CLA:CMA	1.71	1.20
6:F:136:TRP:CG	6:F:137:PRO:HD3	1.74	1.20
1:A:290:LEU:O	1:A:291:THR:HG22	1.41	1.20
6:F:33:ALA:O	6:F:43:LYS:NZ	1.73	1.20
1:A:268:PRO:HB2	1:A:273:ASN:CB	1.71	1.20
2:B:102:GLU:OE2	2:B:639:VAL:HG11	1.41	1.20
4:D:50:TRP:HD1	4:D:51:GLU:O	1.21	1.20
1:A:687:ALA:HB1	18:A:9013:CLA:CBB	1.70	1.20
15:2:28:GLY:HA3	15:2:29:PHE:CD2	1.76	1.20
1:A:342:GLY:O	1:A:431:LEU:HD23	1.41	1.19
2:B:428:PHE:HD2	2:B:432:HIS:CD2	1.59	1.19
4:D:49:THR:HA	4:D:73:ASN:O	1.38	1.19
15:2:33:GLY:H	15:2:35:SER:N	1.41	1.19
4:D:112:LEU:HG	4:D:113:HIS:CE1	1.76	1.18
15:2:19:LEU:HA	15:2:20:ASP:CG	1.62	1.18
2:B:336:LEU:HA	2:B:339:ALA:HB3	1.20	1.18
6:F:100:VAL:CG1	6:F:125:LEU:HD22	1.72	1.18
6:F:93:ILE:HA	6:F:96:TRP:CZ2	1.78	1.18
12:L:165:TYR:CD1	18:L:1503:CLA:OBD	1.95	1.18
1:A:305:ALA:HB2	18:A:1115:CLA:HMA1	1.19	1.18
1:A:625:TRP:HB2	1:A:637:ILE:HD11	1.24	1.18
2:B:422:LEU:HB2	18:B:1236:CLA:CBB	1.73	1.18
12:L:53:GLY:HA3	12:L:139:PHE:CE1	1.79	1.18
2:B:311:PRO:HD2	18:B:1220:CLA:HMA1	1.19	1.17
2:B:331:HIS:ND1	2:B:392:ILE:HG21	1.59	1.17
13:N:81:VAL:CB	13:N:82:PHE:HA	1.69	1.17
17:4:77:ALA:HB3	17:4:78:ALA:HA	1.19	1.17
2:B:547:MET:HB3	3:C:66:ARG:HH21	1.09	1.17
2:B:37:ILE:O	4:D:148:PHE:CD1	1.98	1.17
18:4:1304:CLA:HAA2	18:4:1304:CLA:C2	1.75	1.17
3:C:12:ILE:HA	3:C:13:GLY:O	1.38	1.17
7:G:37:GLU:CG	7:G:43:HIS:CE1	2.27	1.17
13:N:58:VAL:CG2	13:N:59:PRO:HA	1.75	1.17
10:J:11:ALA:CB	10:J:12:PRO:HD3	1.70	1.17
1:A:621:GLN:O	1:A:623:ASP:N	1.78	1.17
1:A:81:ALA:HB1	1:A:82:HIS:CB	1.75	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:119:THR:H	12:L:120:LEU:CA	1.55	1.17
15:2:197:ALA:H	15:2:198:ASP:HA	1.06	1.16
12:L:65:VAL:CG2	12:L:84:GLY:HA2	1.74	1.16
7:G:35:VAL:H	7:G:36:PRO:CD	1.58	1.16
12:L:119:THR:N	12:L:120:LEU:HA	1.47	1.16
1:A:553:VAL:HA	1:A:556:LEU:CD1	1.74	1.16
14:1:51:MET:O	14:1:55:PRO:HD3	1.43	1.16
2:B:304:ILE:O	2:B:308:HIS:CB	1.93	1.16
7:G:34:GLN:NE2	7:G:36:PRO:HG3	1.59	1.16
12:L:67:PRO:N	18:L:1503:CLA:CAB	2.09	1.16
1:A:450:CYS:HB3	1:A:551:VAL:HG12	1.21	1.16
13:N:48:GLY:HA2	13:N:50:GLN:H	1.11	1.15
15:2:23:LEU:HA	15:2:25:GLY:H	1.12	1.15
1:A:467:MET:HA	1:A:471:GLY:HA3	1.24	1.15
1:A:591:GLN:OE1	2:B:667:TRP:HB2	1.45	1.15
18:B:1224:CLA:H3A	18:B:1224:CLA:CGA	1.71	1.15
2:B:532:LEU:HD12	2:B:533:ILE:H	1.11	1.15
15:2:192:LEU:CA	15:2:195:HIS:CE1	2.28	1.15
1:A:606:TYR:O	1:A:610:SER:HB3	1.46	1.15
4:D:102:ARG:HD2	4:D:103:VAL:O	1.44	1.15
9:I:25:PHE:N	9:I:26:LEU:CB	2.09	1.15
15:2:24:PRO:HG2	15:2:27:PHE:HE2	1.04	1.15
16:3:54:TRP:HB2	16:3:55:LEU:CA	1.75	1.15
1:A:141:ARG:NH1	1:A:141:ARG:HB2	1.60	1.15
7:G:35:VAL:N	7:G:36:PRO:HD3	1.54	1.15
14:1:40:LYS:HG2	14:1:41:GLU:H	1.03	1.15
15:2:28:GLY:CA	15:2:29:PHE:CD2	2.30	1.15
1:A:397:THR:O	1:A:400:MET:N	1.80	1.15
1:A:483:GLN:HG2	1:A:484:LEU:C	1.67	1.15
2:B:672:GLN:HE22	2:B:698:VAL:HA	1.12	1.15
17:4:41:VAL:HG23	17:4:42:GLN:H	0.99	1.14
14:1:188:ASN:HA	14:1:189:ILE:CG1	1.77	1.14
2:B:648:TRP:HE1	18:B:9022:CLA:C4	1.60	1.14
7:G:21:PHE:HA	7:G:23:PHE:CB	1.76	1.14
15:2:191:ASN:CA	15:2:192:LEU:HB2	1.77	1.14
18:A:1132:CLA:C2B	12:L:72:GLY:HA2	1.78	1.14
15:2:24:PRO:HD2	15:2:27:PHE:CE2	1.81	1.14
15:2:24:PRO:CG	15:2:27:PHE:CE2	2.30	1.14
6:F:79:HIS:O	6:F:81:GLY:N	1.79	1.14
12:L:66:GLY:CA	18:L:1503:CLA:C2B	2.26	1.14
15:2:21:GLY:HA2	15:2:25:GLY:CA	1.78	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:HIS:CD2	1:A:303:HIS:CE1	2.34	1.13
12:L:65:VAL:HG23	12:L:84:GLY:CA	1.76	1.13
1:A:446:LEU:O	1:A:449:VAL:HG12	1.47	1.13
18:B:1227:CLA:HMB2	18:B:1228:CLA:C4D	1.78	1.13
1:A:173:VAL:O	1:A:176:GLY:N	1.82	1.13
2:B:68:VAL:HA	2:B:71:GLN:O	1.49	1.13
6:F:96:TRP:HD1	6:F:97:ILE:N	1.45	1.13
8:H:83:PRO:HB3	8:H:88:LYS:HD2	1.28	1.13
17:4:115:VAL:HG12	17:4:116:ASN:H	1.02	1.13
20:A:6011:BCR:C8	20:A:6011:BCR:H321	1.77	1.13
2:B:20:ARG:HH22	9:I:28:VAL:HG13	1.02	1.13
3:C:52:LYS:HE2	3:C:66:ARG:HA	1.24	1.13
7:G:21:PHE:HA	7:G:23:PHE:HB3	1.17	1.13
12:L:167:PHE:HB2	12:L:168:LYS:HB3	1.31	1.13
16:3:129:ARG:CD	16:3:139:MET:SD	2.36	1.12
1:A:483:GLN:CG	1:A:484:LEU:O	1.97	1.12
15:2:21:GLY:CA	15:2:23:LEU:HD22	1.78	1.12
1:A:568:LEU:O	1:A:569:ILE:HD12	1.49	1.12
6:F:126:ALA:H	6:F:130:LEU:HD11	1.09	1.12
4:D:26:SER:HA	4:D:27:PRO:C	1.61	1.12
13:N:63:ASP:CB	13:N:64:ASP:HA	1.76	1.12
1:A:477:PHE:HA	1:A:482:ILE:HB	1.25	1.12
2:B:225:LEU:HA	2:B:230:TRP:HE1	0.99	1.12
6:F:115:THR:HG23	6:F:116:GLN:H	1.11	1.12
18:A:1136:CLA:H71	18:A:1137:CLA:HAC2	1.26	1.12
17:4:190:TRP:O	17:4:191:HIS:HD2	1.32	1.12
2:B:429:LEU:HD23	2:B:524:ALA:O	1.50	1.12
2:B:667:TRP:HZ3	21:B:3101:SF4:S3	1.73	1.12
8:H:54:LEU:HD13	8:H:55:LYS:H	1.13	1.12
18:A:1124:CLA:C3A	18:A:1135:CLA:CBB	2.27	1.12
20:I:6018:BCR:H383	20:L:6020:BCR:H341	1.25	1.12
18:L:1503:CLA:HHD	18:L:1503:CLA:CBC	1.78	1.11
1:A:238:ASP:HB3	1:A:239:PRO:HD3	1.29	1.11
1:A:521:VAL:HG13	1:A:522:ALA:H	1.01	1.11
15:2:22:SER:N	15:2:23:LEU:HG	1.64	1.11
15:2:23:LEU:CB	15:2:25:GLY:H	1.63	1.11
4:D:137:ILE:HG13	4:D:140:ASN:HD21	1.12	1.11
15:2:23:LEU:HB2	15:2:25:GLY:N	1.66	1.11
1:A:268:PRO:HB2	1:A:273:ASN:HB2	1.22	1.11
15:2:189:ILE:HA	15:2:191:ASN:H	1.06	1.11
2:B:639:VAL:HG12	2:B:640:CYS:N	1.63	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:17:GLU:CG	15:2:18:TRP:CB	2.29	1.11
2:B:639:VAL:HG12	2:B:640:CYS:H	0.97	1.11
15:2:19:LEU:HG	15:2:20:ASP:OD2	1.50	1.10
16:3:212:ASN:CA	16:3:213:LEU:HB2	1.81	1.10
2:B:682:HIS:CB	18:B:1237:CLA:HMA3	1.79	1.10
15:2:23:LEU:HD22	15:2:25:GLY:C	1.69	1.10
16:3:132:ASP:OD1	16:3:139:MET:HB2	1.51	1.10
2:B:485:ALA:HA	18:B:1232:CLA:HMA3	1.11	1.10
16:3:212:ASN:HA	16:3:213:LEU:HB2	1.26	1.10
15:2:19:LEU:HA	15:2:20:ASP:OD2	1.52	1.10
15:2:24:PRO:HB3	15:2:32:LEU:HG	1.19	1.10
1:A:629:ASN:HD21	1:A:633:VAL:CG2	1.64	1.10
1:A:81:ALA:CB	1:A:83:PHE:N	2.15	1.10
7:G:37:GLU:CG	7:G:43:HIS:HE1	1.64	1.10
1:A:64:PHE:HE1	18:A:1103:CLA:CMC	1.64	1.10
2:B:527:LEU:HD23	2:B:586:THR:HG21	1.32	1.10
4:D:102:ARG:HH11	4:D:110:GLN:NE2	1.50	1.10
7:G:21:PHE:CA	7:G:23:PHE:HB3	1.81	1.10
2:B:74:PHE:HE2	2:B:130:ARG:HA	1.14	1.10
2:B:569:ASP:HB2	2:B:706:ARG:HH12	1.15	1.10
4:D:26:SER:HA	4:D:27:PRO:O	0.93	1.10
12:L:44:ARG:HH11	12:L:44:ARG:HB2	1.10	1.10
13:N:57:LYS:HB2	16:3:87:ALA:HB2	1.13	1.10
13:N:81:VAL:HB	13:N:83:TRP:HA	1.26	1.10
15:2:21:GLY:CA	15:2:25:GLY:CA	2.30	1.10
2:B:498:LEU:O	2:B:501:ILE:HG12	1.50	1.10
1:A:431:LEU:HD12	18:A:1122:CLA:HMC3	1.21	1.10
8:H:33:ASN:HD21	18:H:1501:CLA:HMD3	1.02	1.10
1:A:446:LEU:HD22	1:A:449:VAL:HG11	1.27	1.09
18:B:1216:CLA:O2A	18:B:1220:CLA:H11	1.51	1.09
18:B:1220:CLA:HHD	18:B:1220:CLA:HBC2	1.32	1.09
2:B:700:LEU:CD2	2:B:704:GLN:HE22	1.64	1.09
18:B:1138:CLA:HBB2	18:B:1138:CLA:H8	1.33	1.09
15:2:17:GLU:HG3	15:2:18:TRP:HB2	1.23	1.09
2:B:5:ILE:HG23	2:B:6:PRO:HA	1.35	1.09
2:B:629:SER:O	2:B:633:ASN:HB2	1.50	1.09
4:D:31:GLY:HA3	12:L:13:PRO:HB3	1.10	1.09
4:D:50:TRP:CD1	4:D:51:GLU:O	2.04	1.09
12:L:92:VAL:HG13	12:L:93:VAL:H	1.06	1.09
13:N:36:GLU:HB3	13:N:37:PHE:HA	1.12	1.09
14:1:152:ARG:HD2	14:1:153:LEU:HD13	1.22	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:HA	1:A:354:TRP:CZ2	1.87	1.09
18:B:1207:CLA:HBC3	20:I:6018:BCR:H21C	1.09	1.09
13:N:51:ASP:HB3	13:N:52:LEU:HG	1.31	1.09
12:L:113:SER:H	12:L:114:ILE:HB	1.02	1.09
15:2:21:GLY:HA2	15:2:23:LEU:HD22	1.13	1.09
16:3:83:GLY:HA2	16:3:86:PRO:CD	1.82	1.09
1:A:557:LEU:HA	1:A:560:VAL:HG22	1.10	1.09
2:B:133:GLU:HA	2:B:136:TYR:CE1	1.87	1.09
1:A:521:VAL:CG1	1:A:522:ALA:H	1.66	1.09
1:A:663:GLN:O	1:A:667:SER:HB2	1.53	1.09
5:E:35:LYS:HA	5:E:50:GLY:HA2	1.16	1.09
13:N:81:VAL:HB	13:N:82:PHE:CA	1.81	1.09
15:2:157:LYS:HA	15:2:160:ARG:HG2	1.21	1.08
15:2:24:PRO:CD	15:2:27:PHE:CE2	2.36	1.08
1:A:147:SER:HG	18:A:1126:CLA:HMA2	0.95	1.08
10:J:2:ARG:HB2	10:J:7:TYR:HE1	1.03	1.08
1:A:268:PRO:HD2	1:A:277:TYR:CE1	1.88	1.08
16:3:67:MET:HB2	18:3:3005:CLA:C3C	1.82	1.08
13:N:77:CYS:HB2	13:N:78:GLY:HA3	1.35	1.08
1:A:64:PHE:HA	1:A:67:HIS:HB2	1.32	1.08
1:A:483:GLN:HA	1:A:484:LEU:CB	1.83	1.08
14:1:162:CYS:HA	14:1:165:GLN:HB2	1.29	1.08
1:A:637:ILE:HD12	1:A:637:ILE:H	0.94	1.08
13:N:58:VAL:HG11	16:3:86:PRO:HA	1.35	1.08
1:A:147:SER:N	1:A:391:THR:HG21	1.69	1.08
15:2:32:LEU:HD23	15:2:32:LEU:O	1.54	1.08
1:A:553:VAL:CA	1:A:556:LEU:HD12	1.83	1.08
1:A:755:ILE:H	1:A:758:GLY:CA	1.67	1.08
15:2:17:GLU:CB	15:2:18:TRP:CB	2.30	1.08
17:4:119:PRO:HB2	18:4:4011:CLA:C3D	1.83	1.08
2:B:698:VAL:HG12	3:C:79:LEU:HD23	1.28	1.08
2:B:551:LYS:HB2	4:D:141:VAL:O	1.54	1.08
2:B:378:ILE:HG13	18:B:1225:CLA:HBB2	1.25	1.08
5:E:65:VAL:HG23	5:E:83:ALA:HB2	1.29	1.08
16:3:133:TRP:O	16:3:137:GLY:HA2	1.45	1.07
1:A:491:TRP:HA	1:A:492:ILE:HG12	1.35	1.07
5:E:66:VAL:CA	5:E:81:ASN:HD21	1.66	1.07
18:B:1217:CLA:HMA2	7:G:21:PHE:HD2	1.09	1.07
16:3:212:ASN:HB2	16:3:214:LEU:H	1.11	1.07
2:B:422:LEU:HB2	18:B:1236:CLA:HBB2	1.19	1.07
15:2:20:ASP:HB3	15:2:23:LEU:HD21	1.09	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HD11	10:J:27:ILE:CG2	1.84	1.07
2:B:57:ILE:HG21	18:B:1241:CLA:C3B	1.84	1.07
17:4:82:GLU:HG3	17:4:83:TYR:N	1.68	1.07
3:C:25:VAL:HG21	3:C:48:CYS:HB3	1.35	1.07
1:A:629:ASN:ND2	1:A:633:VAL:HG23	1.70	1.07
1:A:650:ASN:O	1:A:652:TRP:N	1.85	1.07
1:A:71:LEU:HD11	1:A:352:THR:HG22	1.36	1.07
2:B:289:LEU:O	18:B:1218:CLA:CBC	2.01	1.07
2:B:74:PHE:CE2	2:B:130:ARG:HA	1.89	1.07
1:A:81:ALA:HB1	1:A:82:HIS:HB2	1.07	1.07
2:B:195:VAL:HG23	2:B:274:ALA:HB1	1.36	1.07
2:B:334:LEU:HD12	2:B:389:HIS:HD2	0.92	1.07
2:B:649:MET:HE2	2:B:723:ALA:HB2	1.26	1.07
20:L:6020:BCR:H331	20:L:6020:BCR:HC8	1.37	1.07
2:B:532:LEU:HD12	2:B:533:ILE:N	1.67	1.07
12:L:102:TYR:HE2	12:L:105:ALA:HB3	1.16	1.07
18:L:1503:CLA:HAA2	18:L:1503:CLA:HBD	1.37	1.07
20:A:6011:BCR:HC8	20:A:6011:BCR:C32	1.82	1.07
2:B:344:ILE:HD13	18:B:1225:CLA:HBC1	1.37	1.07
2:B:348:VAL:HG21	18:B:1225:CLA:HMD3	1.32	1.07
13:N:63:ASP:HB2	13:N:64:ASP:CA	1.85	1.07
2:B:456:GLU:HG3	2:B:514:PRO:HB3	1.29	1.07
2:B:689:ASN:HD21	4:D:38:ARG:NH1	1.53	1.07
10:J:2:ARG:HB3	10:J:3:ASP:HB2	1.11	1.07
12:L:14:LEU:HD23	12:L:20:ILE:O	1.55	1.07
1:A:223:VAL:HG23	1:A:224:HIS:HD2	1.19	1.06
1:A:581:CYS:HB2	1:A:590:CYS:HA	1.08	1.06
17:4:59:LEU:HA	17:4:62:GLU:HB2	1.36	1.06
2:B:174:ARG:HB2	2:B:174:ARG:NH1	1.69	1.06
2:B:646:TRP:HE3	2:B:723:ALA:HB1	1.16	1.06
12:L:52:ARG:O	12:L:55:GLU:HG2	1.55	1.06
14:1:183:ASP:H	14:1:184:PRO:HA	0.99	1.06
15:2:161:THR:HG23	15:2:165:LYS:HG3	1.34	1.06
6:F:124:PRO:HG2	6:F:125:LEU:HG	1.11	1.06
7:G:63:PRO:HB3	18:G:1248:CLA:C2C	1.85	1.06
12:L:66:GLY:HA2	18:L:1503:CLA:HMB3	1.36	1.06
14:1:38:ARG:HA	14:1:39:TYR:CB	1.85	1.06
15:2:23:LEU:HB2	15:2:26:ASP:N	1.70	1.06
4:D:47:VAL:HG23	4:D:103:VAL:HG11	1.38	1.06
1:A:139:GLY:O	6:F:38:PRO:HB2	1.54	1.06
13:N:44:GLU:N	13:N:45:ASN:HB2	1.70	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:191:ASN:HA	15:2:192:LEU:CB	1.82	1.06
17:4:190:TRP:O	17:4:191:HIS:CD2	2.08	1.06
1:A:543:HIS:HA	1:A:546:ALA:HB3	1.16	1.06
12:L:63:LEU:HD21	18:L:1502:CLA:HMB3	1.07	1.06
15:2:185:GLY:O	15:2:187:GLY:HA3	1.55	1.06
1:A:658:TRP:CD1	2:B:625:TRP:NE1	2.24	1.06
3:C:3:HIS:NE2	3:C:48:CYS:O	1.86	1.06
2:B:646:TRP:HE3	2:B:723:ALA:CB	1.68	1.06
14:1:16:GLY:HA3	14:1:18:ALA:HA	1.11	1.05
6:F:73:VAL:HG21	6:F:83:PHE:H	1.21	1.05
15:2:23:LEU:HD23	15:2:26:ASP:CA	1.84	1.05
16:3:129:ARG:HD2	16:3:139:MET:SD	1.94	1.05
14:1:103:LEU:HA	14:1:106:ALA:HB3	1.35	1.05
15:2:28:GLY:C	15:2:29:PHE:CD2	2.29	1.05
2:B:569:ASP:CB	2:B:706:ARG:HH12	1.69	1.05
6:F:61:LEU:HD13	6:F:69:PRO:HB3	1.33	1.05
2:B:126:THR:HB	18:B:1215:CLA:HED1	1.37	1.05
15:2:27:PHE:HD1	15:2:29:PHE:N	1.53	1.05
16:3:132:ASP:CB	16:3:139:MET:HG3	1.87	1.05
13:N:30:ALA:HA	13:N:33:TYR:HB2	1.34	1.05
2:B:287:GLY:H	18:B:1218:CLA:CMC	1.58	1.05
2:B:464:GLN:OE1	18:B:1234:CLA:HMD1	1.55	1.05
4:D:144:ILE:H	4:D:144:ILE:HD12	1.15	1.05
12:L:58:LEU:HD13	12:L:153:TRP:CZ3	1.92	1.05
2:B:478:LEU:CD1	2:B:485:ALA:HB3	1.87	1.05
12:L:113:SER:N	12:L:114:ILE:HB	1.70	1.05
1:A:571:ASP:O	1:A:574:ASN:ND2	1.89	1.05
3:C:18:VAL:HG12	21:C:3103:SF4:S2	1.96	1.05
1:A:119:SER:HA	1:A:145:ILE:HG23	1.38	1.04
1:A:744:ALA:HB2	20:A:6011:BCR:H322	1.31	1.04
6:F:12:LYS:HD2	6:F:13:GLN:N	1.71	1.04
12:L:74:LEU:HB3	12:L:77:THR:HG21	1.39	1.04
15:2:28:GLY:C	15:2:29:PHE:CG	2.29	1.04
2:B:653:GLY:HA3	2:B:720:THR:HG23	1.38	1.04
4:D:102:ARG:HA	4:D:103:VAL:CB	1.83	1.04
13:N:51:ASP:N	13:N:52:LEU:HB2	1.72	1.04
14:1:189:ILE:N	14:1:190:GLY:HA2	1.72	1.04
1:A:450:CYS:CB	1:A:551:VAL:HG12	1.88	1.04
15:2:153:PRO:HB2	15:2:154:GLN:C	1.78	1.04
1:A:35:ALA:HA	1:A:36:LYS:HB2	1.04	1.04
6:F:5:LEU:HB3	6:F:62:LEU:HD23	1.07	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:79:SER:N	13:N:80:ASN:HA	1.72	1.04
2:B:658:ALA:O	2:B:661:PHE:HB2	1.56	1.04
2:B:83:HIS:N	2:B:84:VAL:HG23	1.73	1.04
2:B:621:ARG:HG3	2:B:622:ASP:N	1.68	1.04
4:D:102:ARG:CA	4:D:103:VAL:HB	1.86	1.04
10:J:2:ARG:HB2	10:J:7:TYR:CE1	1.93	1.04
2:B:58:PHE:CE2	18:B:1241:CLA:HBB	1.91	1.04
4:D:135:ARG:HG2	4:D:139:LYS:HD3	1.34	1.03
15:2:21:GLY:H	15:2:22:SER:HB3	1.23	1.03
15:2:23:LEU:HD12	15:2:26:ASP:O	1.56	1.03
15:2:20:ASP:CB	15:2:23:LEU:HD21	1.88	1.03
1:A:51:THR:HG23	1:A:722:PRO:HA	1.06	1.03
2:B:344:ILE:HD11	18:B:1225:CLA:CAC	1.89	1.03
18:F:1302:CLA:HMA1	18:F:1302:CLA:C9	1.87	1.03
15:2:32:LEU:CD2	15:2:32:LEU:O	2.06	1.03
1:A:629:ASN:HD21	1:A:633:VAL:HG23	0.88	1.03
2:B:646:TRP:CE3	2:B:723:ALA:HB1	1.93	1.03
5:E:36:VAL:CG2	5:E:52:VAL:HG13	1.87	1.03
8:H:24:TYR:HB2	8:H:25:GLY:HA2	1.39	1.03
12:L:163:LEU:N	12:L:164:PRO:HD2	1.73	1.03
15:2:22:SER:H	15:2:23:LEU:CA	1.71	1.03
1:A:268:PRO:HD2	1:A:277:TYR:HE1	1.22	1.03
1:A:81:ALA:CB	1:A:83:PHE:H	1.70	1.03
1:A:649:ILE:O	1:A:652:TRP:CD1	2.12	1.03
18:A:9011:CLA:HBB2	18:B:9010:CLA:ND	1.74	1.03
6:F:126:ALA:N	6:F:130:LEU:HD11	1.74	1.03
15:2:20:ASP:HB3	15:2:23:LEU:CD2	1.88	1.03
1:A:443:ILE:HD13	1:A:562:PHE:HE1	1.20	1.03
2:B:621:ARG:HG3	2:B:622:ASP:H	1.20	1.03
4:D:118:VAL:HB	4:D:127:ARG:HH21	1.20	1.03
20:L:6020:BCR:H331	20:L:6020:BCR:C8	1.84	1.03
14:1:57:ILE:O	14:1:60:PRO:HD2	1.58	1.02
15:2:19:LEU:HD12	15:2:22:SER:OG	1.59	1.02
2:B:661:PHE:HB3	18:B:9023:CLA:HMC3	1.41	1.02
7:G:88:THR:N	7:G:89:ALA:HA	1.70	1.02
20:I:6018:BCR:H383	20:L:6020:BCR:C34	1.88	1.02
1:A:483:GLN:CA	1:A:484:LEU:HB2	1.89	1.02
1:A:620:MET:HA	1:A:624:VAL:CG1	1.89	1.02
1:A:679:PHE:HA	1:A:682:ALA:HB3	1.03	1.02
10:J:5:LYS:HB3	10:J:6:THR:OG1	1.56	1.02
14:1:159:VAL:HA	14:1:162:CYS:SG	1.99	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ILE:H	1:A:493:GLN:CB	1.71	1.02
7:G:35:VAL:H	7:G:36:PRO:HD3	0.89	1.02
15:2:22:SER:H	15:2:25:GLY:H	1.05	1.02
1:A:489:ALA:HB1	1:A:490:GLN:O	1.56	1.02
18:B:1202:CLA:HBB2	18:B:1203:CLA:HBA1	1.33	1.02
15:2:22:SER:H	15:2:23:LEU:HA	1.24	1.02
17:4:180:ASP:H	17:4:185:HIS:CE1	1.78	1.02
14:1:179:THR:HG21	17:4:88:SER:HB3	1.41	1.02
1:A:354:TRP:HB3	18:A:1103:CLA:HHD	1.42	1.02
2:B:287:GLY:CA	18:B:1218:CLA:CMC	2.36	1.02
2:B:627:ASN:HA	2:B:732:LYS:HE3	1.42	1.02
18:L:1502:CLA:C4	18:L:1504:CLA:HMA1	1.88	1.02
12:L:22:GLY:O	12:L:23:LEU:HB2	1.58	1.02
7:G:35:VAL:HG13	7:G:36:PRO:CA	1.90	1.02
15:2:36:SER:HA	15:2:37:ASP:HB2	1.42	1.02
2:B:290:MET:HA	18:B:1218:CLA:HBC3	1.40	1.02
3:C:11:CYS:O	3:C:12:ILE:O	1.78	1.02
7:G:88:THR:H	7:G:89:ALA:HA	0.87	1.02
13:N:36:GLU:HB3	13:N:37:PHE:CA	1.90	1.02
13:N:48:GLY:CA	13:N:50:GLN:H	1.71	1.02
16:3:72:GLY:O	16:3:76:PRO:HD2	1.60	1.01
17:4:59:LEU:O	17:4:62:GLU:HB3	1.57	1.01
2:B:101:VAL:HG23	2:B:102:GLU:H	1.22	1.01
1:A:126:ILE:HD11	10:J:27:ILE:HG23	1.03	1.01
1:A:654:ARG:HH11	1:A:655:ASP:HB3	1.24	1.01
1:A:663:GLN:HG3	1:A:753:ARG:HA	1.38	1.01
2:B:191:ALA:HB1	2:B:277:HIS:O	1.59	1.01
12:L:66:GLY:HA2	18:L:1503:CLA:CMB	1.90	1.01
14:1:188:ASN:HA	14:1:189:ILE:HG12	1.05	1.01
1:A:213:LEU:O	1:A:217:SER:HB3	1.61	1.01
1:A:347:TYR:CD2	1:A:348:GLU:N	2.28	1.01
2:B:485:ALA:HA	18:B:1232:CLA:CMA	1.90	1.01
2:B:478:LEU:HD12	2:B:485:ALA:CB	1.89	1.01
2:B:344:ILE:HD11	18:B:1225:CLA:HBC2	1.43	1.01
2:B:463:ILE:HG21	18:B:1234:CLA:O2D	1.58	1.01
13:N:77:CYS:HB2	13:N:78:GLY:CA	1.90	1.01
1:A:452:PHE:HE2	18:A:1136:CLA:CBB	1.74	1.01
1:A:64:PHE:HE1	18:A:1103:CLA:HMC1	0.87	1.01
2:B:348:VAL:CG2	18:B:1225:CLA:HMD3	1.89	1.01
2:B:530:THR:HG21	2:B:583:MET:HB2	1.42	1.01
2:B:78:VAL:HG23	2:B:130:ARG:HD3	1.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:33:LYS:HB3	7:G:34:GLN:HB2	1.40	1.01
10:J:3:ASP:O	10:J:7:TYR:CE1	2.12	1.01
15:2:23:LEU:HD23	15:2:26:ASP:C	1.81	1.01
2:B:174:ARG:CB	2:B:174:ARG:HH11	1.73	1.01
6:F:5:LEU:HB3	6:F:62:LEU:CD2	1.91	1.01
17:4:77:ALA:CB	17:4:78:ALA:HA	1.90	1.01
1:A:109:TRP:HE1	1:A:113:PRO:HA	1.21	1.01
12:L:36:TYR:O	12:L:38:SER:N	1.94	1.01
15:2:22:SER:C	15:2:23:LEU:CG	2.30	1.01
2:B:454:LEU:HD12	2:B:614:THR:HG21	1.42	1.01
12:L:164:PRO:CG	18:L:1503:CLA:C2	2.39	1.01
15:2:21:GLY:HA2	15:2:25:GLY:O	1.61	1.00
2:B:334:LEU:CD1	2:B:389:HIS:HD2	1.74	1.00
7:G:35:VAL:CG1	7:G:36:PRO:HB3	1.91	1.00
10:J:11:ALA:HB3	10:J:12:PRO:HD3	1.37	1.00
13:N:32:ALA:HA	13:N:35:VAL:HG23	1.41	1.00
15:2:22:SER:C	15:2:23:LEU:HD13	1.81	1.00
1:A:147:SER:H	1:A:391:THR:HG21	1.25	1.00
15:2:22:SER:C	15:2:23:LEU:CD1	2.29	1.00
15:2:21:GLY:CA	15:2:25:GLY:C	2.30	1.00
2:B:305:LEU:O	2:B:307:ALA:N	1.93	1.00
2:B:341:LEU:HD12	2:B:341:LEU:O	1.59	1.00
18:B:1235:CLA:H8	18:F:1302:CLA:H52	1.43	1.00
7:G:83:TYR:HA	7:G:85:ILE:N	1.76	1.00
9:I:26:LEU:HG	9:I:29:GLU:O	1.59	1.00
2:B:422:LEU:HD21	2:B:531:THR:OG1	1.60	1.00
1:A:588:GLY:HA3	2:B:668:ARG:HD2	1.42	1.00
2:B:700:LEU:HD22	2:B:704:GLN:NE2	1.76	1.00
3:C:27:GLU:H	3:C:43:PRO:HG3	1.26	1.00
15:2:189:ILE:HA	15:2:191:ASN:N	1.75	1.00
15:2:33:GLY:N	15:2:35:SER:N	2.08	1.00
1:A:557:LEU:HA	1:A:560:VAL:CG2	1.90	1.00
1:A:637:ILE:HD12	1:A:637:ILE:N	1.74	1.00
15:2:23:LEU:HB2	15:2:25:GLY:CA	1.92	1.00
1:A:452:PHE:CD1	1:A:456:HIS:HE1	1.79	1.00
1:A:592:VAL:O	1:A:597:HIS:CE1	2.15	1.00
2:B:682:HIS:HB3	18:B:1237:CLA:HMA3	1.00	1.00
13:N:65:LEU:HD12	13:N:68:GLU:OE1	1.62	1.00
15:2:24:PRO:HG2	15:2:27:PHE:CE2	1.95	1.00
6:F:5:LEU:CB	6:F:62:LEU:HD23	1.92	1.00
15:2:22:SER:C	15:2:23:LEU:HG	1.81	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:HA	2:B:272:ASP:OD1	1.62	1.00
4:D:153:PRO:O	4:D:154:TYR:HD2	1.45	1.00
14:1:10:ARG:H	17:4:110:LYS:HD2	1.26	1.00
2:B:378:ILE:CG1	18:B:1225:CLA:HBB2	1.91	1.00
15:2:21:GLY:C	15:2:25:GLY:CA	2.30	0.99
14:1:10:ARG:N	17:4:110:LYS:HD2	1.75	0.99
15:2:17:GLU:CD	15:2:18:TRP:HB2	1.81	0.99
16:3:197:GLY:O	16:3:200:ILE:HG22	1.61	0.99
1:A:347:TYR:HD2	1:A:348:GLU:N	1.58	0.99
8:H:33:ASN:ND2	18:H:1501:CLA:HMD3	1.73	0.99
9:I:4:LEU:HD22	9:I:5:PRO:HA	1.44	0.99
15:2:191:ASN:HA	15:2:192:LEU:HB2	1.00	0.99
1:A:35:ALA:HA	1:A:36:LYS:CB	1.92	0.99
2:B:286:ILE:HD12	18:B:1218:CLA:HMC2	1.04	0.99
2:B:527:LEU:HD23	2:B:527:LEU:H	1.26	0.99
8:H:63:SER:O	8:H:67:TYR:HB2	1.61	0.99
10:J:2:ARG:CB	10:J:3:ASP:HB2	1.92	0.99
1:A:50:THR:HG21	1:A:723:ARG:HH12	1.25	0.99
2:B:428:PHE:CD2	2:B:432:HIS:CD2	2.50	0.99
12:L:66:GLY:HA2	18:L:1503:CLA:C2B	1.89	0.99
14:1:188:ASN:CA	14:1:189:ILE:HG12	1.92	0.99
15:2:44:ASN:HD21	15:2:113:ILE:CB	1.76	0.99
1:A:620:MET:HA	1:A:624:VAL:HG12	1.40	0.99
2:B:667:TRP:CZ3	21:B:3101:SF4:S3	2.55	0.99
18:B:9023:CLA:H3A	18:B:9023:CLA:CGA	1.93	0.99
6:F:39:ALA:O	6:F:41:ALA:N	1.94	0.99
12:L:33:ILE:HG23	12:L:35:TRP:HB3	1.43	0.99
17:4:66:SER:O	17:4:67:ILE:HG23	1.63	0.99
1:A:543:HIS:CA	1:A:546:ALA:HB3	1.93	0.99
2:B:317:ARG:HG2	2:B:317:ARG:HH21	1.23	0.99
3:C:51:CYS:O	3:C:53:ARG:N	1.95	0.99
4:D:155:ASP:HB3	4:D:156:LEU:CA	1.91	0.99
6:F:80:TRP:HE1	18:F:1302:CLA:HBC2	1.24	0.99
18:L:1503:CLA:CED	18:L:1503:CLA:C1	2.41	0.99
2:B:574:ASP:HA	2:B:577:TYR:HB3	1.44	0.99
2:B:73:ASN:HD22	2:B:108:GLY:HA3	1.28	0.99
12:L:66:GLY:HA3	18:L:1503:CLA:C2B	1.88	0.99
16:3:212:ASN:HB2	16:3:214:LEU:N	1.76	0.98
3:C:5:VAL:HG13	3:C:6:LYS:H	1.26	0.98
15:2:17:GLU:CB	15:2:18:TRP:C	2.30	0.98
15:2:19:LEU:CA	15:2:20:ASP:CG	2.30	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25:PHE:H	9:I:26:LEU:CB	1.70	0.98
15:2:194:ALA:CB	15:2:195:HIS:HA	1.92	0.98
1:A:38:GLY:HA2	1:A:44:ILE:HB	1.45	0.98
2:B:330:ILE:HG21	18:B:1202:CLA:CAC	1.92	0.98
9:I:12:VAL:HG11	18:I:1204:CLA:O1A	1.64	0.98
18:A:1132:CLA:C2B	12:L:72:GLY:CA	2.40	0.98
2:B:174:ARG:HH11	2:B:174:ARG:HB2	0.84	0.98
2:B:682:HIS:HB3	18:B:1237:CLA:CMA	1.94	0.98
2:B:720:THR:OG1	18:B:9010:CLA:O1D	1.78	0.98
13:N:46:PHE:O	13:N:47:THR:HG22	1.61	0.98
15:2:18:TRP:HA	15:2:20:ASP:O	1.63	0.98
2:B:331:HIS:CE1	2:B:392:ILE:HG21	1.98	0.98
2:B:492:ILE:H	2:B:492:ILE:HD13	1.25	0.98
4:D:43:GLU:O	4:D:43:GLU:HG2	1.63	0.98
18:B:1138:CLA:C3B	18:F:1139:CLA:HMD2	1.93	0.98
15:2:17:GLU:CB	15:2:18:TRP:CA	2.36	0.98
1:A:665:ILE:HD11	18:A:9011:CLA:HBC1	1.45	0.98
3:C:33:GLY:O	5:E:61:THR:HB	1.64	0.98
7:G:13:GLY:HA2	7:G:16:LEU:HB2	1.44	0.98
13:N:45:ASN:HD22	13:N:46:PHE:H	1.06	0.98
1:A:32:GLU:HB2	1:A:33:GLN:HA	1.42	0.98
1:A:482:ILE:O	1:A:484:LEU:HD12	1.64	0.98
4:D:133:ASN:ND2	4:D:135:ARG:H	1.60	0.98
15:2:27:PHE:CD1	15:2:29:PHE:N	2.30	0.98
1:A:43:THR:HG22	1:A:46:LYS:HG2	1.44	0.98
2:B:549:ASP:HA	2:B:551:LYS:HG2	1.43	0.98
6:F:105:LEU:HD11	6:F:118:GLU:OE2	1.62	0.98
2:B:478:LEU:HD12	2:B:485:ALA:HB3	0.99	0.98
18:A:1124:CLA:HHC	18:A:1137:CLA:CGA	1.94	0.97
1:A:123:VAL:H	1:A:133:ASN:HD22	1.01	0.97
1:A:446:LEU:HD22	1:A:449:VAL:CG1	1.94	0.97
2:B:101:VAL:HA	2:B:105:THR:OG1	1.64	0.97
18:A:1132:CLA:C2B	12:L:72:GLY:N	2.26	0.97
1:A:77:LYS:NZ	18:A:1109:CLA:C2B	2.27	0.97
1:A:97:TYR:CE2	1:A:153:TRP:CE3	2.52	0.97
1:A:380:PRO:HB3	1:A:385:LEU:HD12	1.46	0.97
2:B:547:MET:HB3	3:C:66:ARG:NH2	1.77	0.97
14:1:89:VAL:CG1	14:1:90:PRO:HD3	1.94	0.97
13:N:58:VAL:CG1	16:3:86:PRO:CA	2.43	0.97
1:A:654:ARG:NH1	1:A:655:ASP:HB3	1.78	0.97
13:N:57:LYS:CB	16:3:87:ALA:HB2	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:CYS:SG	1:A:582:ASP:N	2.37	0.97
18:B:1217:CLA:CMA	7:G:21:PHE:HD2	1.76	0.97
7:G:23:PHE:HB2	7:G:24:PHE:HD1	1.28	0.97
12:L:119:THR:H	12:L:120:LEU:HA	0.83	0.97
1:A:479:ASP:O	1:A:483:GLN:HB2	1.64	0.97
1:A:545:HIS:ND1	1:A:612:VAL:HG22	1.78	0.97
18:B:1227:CLA:HMB2	18:B:1228:CLA:C3D	1.94	0.97
18:B:1207:CLA:H61	8:H:65:LEU:HD22	1.44	0.97
15:2:20:ASP:OD2	15:2:22:SER:HB3	1.64	0.97
16:3:132:ASP:O	16:3:137:GLY:HA2	1.64	0.97
17:4:51:ALA:HB1	17:4:161:MET:HE1	1.45	0.97
2:B:109:ALA:O	2:B:110:LEU:HB2	1.64	0.97
18:B:9010:CLA:HED3	18:B:9010:CLA:H2A	1.45	0.97
15:2:84:GLU:OE2	17:4:186:ILE:HG13	1.65	0.97
15:2:63:PHE:HD2	15:2:63:PHE:H	0.98	0.97
1:A:744:ALA:HB2	20:A:6011:BCR:C32	1.95	0.97
1:A:618:TRP:CH2	1:A:646:SER:HB3	1.99	0.97
2:B:195:VAL:CG2	2:B:274:ALA:HB1	1.93	0.97
2:B:700:LEU:CD2	2:B:704:GLN:NE2	2.27	0.97
2:B:99:PRO:O	2:B:103:ALA:N	1.96	0.97
4:D:141:VAL:O	4:D:143:PRO:HD3	1.65	0.97
2:B:127:ILE:HD12	2:B:190:TRP:HZ3	1.30	0.97
2:B:628:SER:O	2:B:630:GLN:N	1.97	0.97
6:F:86:PRO:HG3	10:J:39:PHE:HB2	1.46	0.97
18:L:1503:CLA:CGA	18:L:1503:CLA:CGD	2.43	0.97
12:L:44:ARG:HD2	12:L:46:ALA:HA	1.46	0.97
20:L:6020:BCR:C33	20:L:6020:BCR:HC8	1.91	0.97
15:2:26:ASP:HB3	15:2:27:PHE:CG	1.99	0.96
15:2:32:LEU:HA	15:2:33:GLY:O	1.65	0.96
15:2:93:THR:N	15:2:94:LEU:HB2	1.79	0.96
1:A:475:ASP:OD2	12:L:75:ARG:HD3	1.64	0.96
1:A:581:CYS:CB	1:A:590:CYS:HA	1.94	0.96
12:L:92:VAL:CG1	12:L:93:VAL:H	1.77	0.96
14:1:152:ARG:CD	14:1:153:LEU:HD13	1.94	0.96
18:A:1103:CLA:HBA1	18:A:1123:CLA:H43	1.45	0.96
1:A:450:CYS:HB3	1:A:551:VAL:CG1	1.95	0.96
6:F:127:SER:HA	6:F:131:PHE:HB2	1.43	0.96
15:2:33:GLY:H	15:2:35:SER:CA	1.78	0.96
1:A:423:ASP:HB3	1:A:424:PRO:HD2	1.42	0.96
2:B:569:ASP:HB2	2:B:706:ARG:NH1	1.78	0.96
4:D:118:VAL:HB	4:D:127:ARG:NH2	1.80	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:19:LEU:HG	15:2:20:ASP:CG	1.84	0.96
2:B:291:TYR:HA	2:B:299:HIS:N	1.80	0.96
4:D:94:TYR:HB2	4:D:95:LYS:HZ2	1.29	0.96
6:F:49:THR:CA	6:F:56:TYR:OH	2.13	0.96
15:2:22:SER:H	15:2:25:GLY:N	1.64	0.96
16:3:120:ALA:O	16:3:124:PHE:HB2	1.66	0.96
1:A:141:ARG:CB	1:A:141:ARG:NH1	2.23	0.96
1:A:618:TRP:CZ3	1:A:646:SER:HB3	2.00	0.96
18:B:1202:CLA:HBB2	18:B:1203:CLA:CBA	1.95	0.96
2:B:78:VAL:HA	2:B:130:ARG:CZ	1.96	0.96
4:D:155:ASP:HB3	4:D:156:LEU:HA	1.44	0.96
1:A:126:ILE:HG22	1:A:129:GLN:CG	1.96	0.96
2:B:302:LYS:HA	2:B:302:LYS:HE2	1.47	0.96
10:J:11:ALA:HB1	10:J:12:PRO:HD3	1.46	0.96
1:A:126:ILE:CD1	10:J:27:ILE:HG23	1.93	0.96
15:2:28:GLY:HA3	15:2:29:PHE:HD2	1.22	0.96
1:A:277:TYR:CD2	18:A:1113:CLA:HBC1	2.01	0.96
1:A:231:GLN:HA	1:A:234:ASN:ND2	1.81	0.96
20:A:6011:BCR:HC8	20:A:6011:BCR:H321	0.96	0.96
1:A:725:LEU:HB3	19:A:5001:PQN:O4	1.66	0.96
2:B:125:TYR:CD1	2:B:359:ALA:HB2	2.00	0.96
2:B:517:PHE:HA	2:B:520:HIS:HB2	1.45	0.96
1:A:199:VAL:HG23	1:A:199:VAL:O	1.63	0.96
1:A:483:GLN:HA	1:A:484:LEU:HB2	0.98	0.96
2:B:17:THR:O	2:B:19:ARG:N	1.97	0.96
2:B:225:LEU:CA	2:B:230:TRP:HE1	1.78	0.96
6:F:116:GLN:C	6:F:118:GLU:H	1.67	0.96
12:L:58:LEU:HD13	12:L:153:TRP:HZ3	1.31	0.96
15:2:18:TRP:CD1	15:2:21:GLY:CA	2.29	0.95
1:A:543:HIS:HA	1:A:546:ALA:CB	1.94	0.95
1:A:84:GLY:O	1:A:88:ILE:N	1.97	0.95
15:2:23:LEU:HA	15:2:25:GLY:N	1.80	0.95
1:A:679:PHE:HA	1:A:682:ALA:CB	1.94	0.95
12:L:63:LEU:CD2	18:L:1502:CLA:HMB3	1.95	0.95
2:B:287:GLY:CA	18:B:1218:CLA:HMC3	1.93	0.95
2:B:361:ILE:HD12	2:B:367:THR:OG1	1.66	0.95
2:B:722:ALA:HB1	18:B:1224:CLA:H42	1.48	0.95
19:A:5001:PQN:H202	19:A:5001:PQN:H243	1.46	0.95
2:B:682:HIS:CE1	18:B:1238:CLA:HAC1	2.01	0.95
2:B:379:ALA:O	2:B:383:MET:HB2	1.65	0.95
15:2:23:LEU:CA	15:2:25:GLY:N	2.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:24:PRO:HB3	15:2:32:LEU:CG	1.97	0.95
1:A:521:VAL:CG1	1:A:522:ALA:N	2.28	0.95
1:A:611:VAL:HG13	1:A:612:VAL:HG23	1.48	0.95
2:B:694:ARG:HE	9:I:29:GLU:CD	1.68	0.95
1:A:492:ILE:H	1:A:493:GLN:HB3	1.31	0.95
7:G:83:TYR:HB2	7:G:85:ILE:HG12	1.48	0.95
15:2:23:LEU:CD2	15:2:26:ASP:N	2.30	0.95
6:F:136:TRP:CD2	6:F:137:PRO:HD3	2.00	0.95
1:A:700:TRP:CZ2	19:A:5001:PQN:H2M3	2.00	0.95
1:A:567:ARG:HG2	1:A:567:ARG:O	1.66	0.95
2:B:19:ARG:HH12	3:C:72:GLU:HB3	1.32	0.95
18:H:1501:CLA:HBB2	18:L:1502:CLA:HAA1	1.48	0.95
2:B:20:ARG:HH22	9:I:28:VAL:CG1	1.79	0.95
2:B:519:VAL:HG21	2:B:593:TYR:HD2	1.26	0.95
5:E:39:LEU:HD22	5:E:88:GLU:OE2	1.66	0.95
6:F:96:TRP:HD1	6:F:97:ILE:H	1.01	0.95
2:B:20:ARG:NH2	9:I:28:VAL:HG13	1.81	0.95
14:1:82:ALA:N	14:1:83:THR:HA	1.82	0.94
14:1:91:TRP:H	14:1:92:GLY:HA2	1.28	0.94
18:A:1123:CLA:HHD	18:A:1123:CLA:HBC2	1.48	0.94
2:B:400:PRO:HG3	4:D:141:VAL:HG21	1.46	0.94
2:B:518:LEU:CD2	2:B:614:THR:HG22	1.95	0.94
12:L:66:GLY:C	18:L:1503:CLA:CAB	2.34	0.94
13:N:63:ASP:HB2	13:N:64:ASP:CB	1.97	0.94
18:B:1209:CLA:O1A	18:B:1209:CLA:H51	1.66	0.94
2:B:365:PHE:CD1	2:B:602:TRP:CD1	2.55	0.94
4:D:55:GLU:HA	4:D:68:MET:O	1.67	0.94
6:F:96:TRP:CD1	6:F:97:ILE:N	2.35	0.94
7:G:33:LYS:HB3	7:G:34:GLN:CB	1.95	0.94
12:L:102:TYR:CE2	12:L:105:ALA:HB3	2.02	0.94
12:L:165:TYR:CE1	18:L:1503:CLA:OBD	2.20	0.94
13:N:51:ASP:HB3	13:N:52:LEU:CG	1.97	0.94
14:1:16:GLY:CA	14:1:18:ALA:HA	1.98	0.94
1:A:453:LEU:HB2	18:A:1136:CLA:HBB2	1.47	0.94
1:A:347:TYR:HD2	1:A:348:GLU:H	1.01	0.94
2:B:415:LYS:HZ1	2:B:540:ASP:HA	1.32	0.94
20:I:6018:BCR:C38	20:L:6020:BCR:H341	1.95	0.94
15:2:157:LYS:HA	15:2:160:ARG:CG	1.97	0.94
1:A:33:GLN:HE22	18:A:1109:CLA:C2C	1.81	0.94
18:A:9011:CLA:HBB1	2:B:624:LEU:CD1	1.97	0.94
13:N:81:VAL:HG23	13:N:82:PHE:HB3	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:LEU:HA	2:B:339:ALA:CB	1.97	0.94
10:J:39:PHE:CE2	10:J:41:PHE:HB3	2.02	0.94
1:A:744:ALA:CB	20:A:6011:BCR:H322	1.97	0.94
2:B:37:ILE:HA	2:B:41:ARG:HD2	1.49	0.94
15:2:23:LEU:CB	15:2:26:ASP:N	2.30	0.94
2:B:649:MET:O	2:B:652:PHE:HB3	1.67	0.94
15:2:23:LEU:CB	15:2:26:ASP:H	1.79	0.94
17:4:41:VAL:HG23	17:4:42:GLN:N	1.79	0.94
1:A:620:MET:O	1:A:621:GLN:HB2	1.68	0.94
2:B:102:GLU:OE2	2:B:639:VAL:CG1	2.16	0.94
18:B:1217:CLA:HMA2	7:G:21:PHE:CD2	2.01	0.94
2:B:64:ASN:HA	2:B:67:HIS:HB2	1.49	0.94
7:G:88:THR:H	7:G:89:ALA:CA	1.78	0.94
10:J:3:ASP:O	10:J:7:TYR:CZ	2.20	0.94
15:2:23:LEU:N	15:2:23:LEU:HD13	1.83	0.94
1:A:77:LYS:HZ1	18:A:1109:CLA:C2B	1.79	0.94
2:B:100:ALA:HA	2:B:103:ALA:HB3	1.46	0.94
2:B:639:VAL:CG1	2:B:640:CYS:H	1.80	0.94
7:G:67:ASN:O	7:G:71:VAL:HG22	1.68	0.94
15:2:175:MET:O	15:2:179:PHE:HB3	1.66	0.94
15:2:22:SER:N	15:2:23:LEU:CG	2.30	0.94
1:A:358:LEU:HG	18:A:1103:CLA:HMD3	1.47	0.94
18:B:1227:CLA:CHB	18:B:1228:CLA:OBD	2.15	0.94
2:B:284:PHE:HE1	18:B:1216:CLA:HHC	1.28	0.94
13:N:58:VAL:HG12	16:3:86:PRO:CA	1.98	0.94
18:A:1106:CLA:H2A	18:A:1106:CLA:O2D	1.68	0.94
1:A:414:ALA:O	1:A:417:PHE:HD2	1.49	0.94
18:B:1207:CLA:HMA2	18:B:1207:CLA:H2	1.46	0.94
2:B:351:HIS:O	2:B:352:MET:HB2	1.68	0.94
14:1:9:PRO:N	17:4:110:LYS:HZ3	1.63	0.93
2:B:215:VAL:HB	2:B:217:PRO:HD3	1.50	0.93
2:B:291:TYR:HA	2:B:299:HIS:H	1.30	0.93
2:B:591:THR:HG22	2:B:721:TYR:HE2	1.30	0.93
13:N:73:ASP:O	13:N:74:LYS:HG2	1.67	0.93
1:A:126:ILE:HG22	1:A:129:GLN:HG2	1.48	0.93
7:G:95:PRO:O	7:G:97:PHE:N	2.00	0.93
2:B:299:HIS:CE1	18:B:1218:CLA:HED3	2.04	0.93
2:B:573:TRP:CZ3	2:B:574:ASP:HB3	2.02	0.93
17:4:116:ASN:HA	17:4:117:GLN:HG3	1.50	0.93
18:B:1239:CLA:C1B	20:B:6017:BCR:H15C	1.99	0.93
4:D:141:VAL:HG22	4:D:142:SER:H	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:54:LEU:HD13	8:H:55:LYS:N	1.83	0.93
16:3:217:LEU:HA	16:3:218:ALA:HB3	1.48	0.93
18:A:1123:CLA:C10	18:A:1123:CLA:H12	1.99	0.93
1:A:141:ARG:HB2	1:A:141:ARG:HH11	0.78	0.93
1:A:675:TYR:HB3	1:A:748:ALA:O	1.68	0.93
6:F:100:VAL:HG12	6:F:125:LEU:HD22	1.46	0.93
14:1:183:ASP:N	14:1:184:PRO:HA	1.79	0.93
15:2:17:GLU:OE1	15:2:18:TRP:HE3	1.52	0.93
17:4:62:GLU:O	17:4:63:VAL:HG23	1.69	0.93
17:4:82:GLU:HG3	17:4:83:TYR:H	1.26	0.93
7:G:35:VAL:HG13	7:G:36:PRO:CB	1.99	0.93
5:E:60:LYS:O	5:E:61:THR:CG2	2.17	0.93
13:N:36:GLU:CB	13:N:37:PHE:HA	1.99	0.93
16:3:55:LEU:HD13	16:3:58:GLY:HA3	1.48	0.93
2:B:293:THR:HB	18:B:1209:CLA:HMA3	1.50	0.93
2:B:387:PHE:O	2:B:391:PRO:HD2	1.68	0.93
1:A:139:GLY:O	6:F:38:PRO:CB	2.15	0.93
6:F:1:ASP:N	6:F:62:LEU:HD13	1.82	0.93
7:G:30:ASN:ND2	7:G:34:GLN:O	2.01	0.93
14:1:16:GLY:HA3	14:1:18:ALA:CA	1.97	0.93
1:A:147:SER:OG	18:A:1126:CLA:CMA	2.17	0.93
1:A:150:PHE:HA	1:A:153:TRP:NE1	1.84	0.93
1:A:207:LEU:C	1:A:310:PHE:O	2.07	0.93
1:A:483:GLN:OE1	1:A:485:GLN:HA	1.69	0.93
1:A:547:PHE:HE1	1:A:551:VAL:HG13	1.33	0.93
2:B:593:TYR:HD1	2:B:594:TRP:N	1.66	0.93
1:A:119:SER:HA	1:A:145:ILE:CG2	1.97	0.93
3:C:42:ALA:C	3:C:44:ARG:H	1.71	0.93
6:F:28:SER:HB3	6:F:42:ILE:HG23	1.47	0.93
1:A:608:SER:HA	1:A:611:VAL:HG12	1.49	0.92
2:B:341:LEU:HD23	18:B:1202:CLA:HED2	1.51	0.92
2:B:415:LYS:NZ	2:B:540:ASP:HA	1.83	0.92
1:A:75:SER:HA	1:A:354:TRP:HZ2	1.31	0.92
2:B:225:LEU:HA	2:B:230:TRP:NE1	1.84	0.92
2:B:334:LEU:CD1	2:B:389:HIS:CD2	2.51	0.92
5:E:36:VAL:HG22	5:E:52:VAL:HG13	1.51	0.92
17:4:82:GLU:HB3	17:4:84:PHE:CE1	2.05	0.92
13:N:63:ASP:HB3	13:N:64:ASP:HA	1.50	0.92
15:2:154:GLN:HG2	15:2:155:LYS:N	1.85	0.92
1:A:442:ILE:HD11	1:A:561:LEU:HD21	1.52	0.92
2:B:485:ALA:CA	18:B:1232:CLA:HMA3	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:100:VAL:HG12	6:F:125:LEU:CD2	1.98	0.92
15:2:23:LEU:CB	15:2:25:GLY:N	2.29	0.92
1:A:454:GLY:O	1:A:456:HIS:N	2.03	0.92
1:A:476:MET:SD	1:A:476:MET:N	2.42	0.92
1:A:89:ILE:O	1:A:92:TRP:HB3	1.69	0.92
2:B:526:GLY:HA2	2:B:582:TRP:HZ3	1.34	0.92
14:1:89:VAL:CB	14:1:90:PRO:HD3	1.99	0.92
1:A:665:ILE:HD13	2:B:625:TRP:CD1	2.05	0.92
18:B:1217:CLA:CMA	7:G:21:PHE:CD2	2.53	0.92
2:B:589:TRP:HD1	2:B:592:PHE:HE2	1.14	0.92
3:C:4:SER:OG	3:C:68:TYR:O	1.86	0.92
4:D:102:ARG:HG2	4:D:110:GLN:HB2	1.52	0.92
6:F:115:THR:O	6:F:117:LYS:C	2.08	0.92
14:1:102:PHE:O	14:1:105:ILE:HG22	1.70	0.92
2:B:714:SER:O	2:B:718:ILE:N	2.01	0.92
12:L:66:GLY:CA	18:L:1503:CLA:CMB	2.48	0.92
1:A:569:ILE:O	1:A:569:ILE:HG22	1.69	0.92
1:A:97:TYR:HE2	1:A:153:TRP:CE3	1.88	0.92
2:B:355:LEU:HD21	18:B:1214:CLA:HED3	1.52	0.92
15:2:194:ALA:HB3	15:2:195:HIS:CG	2.05	0.92
17:4:120:ILE:O	17:4:120:ILE:HG13	1.70	0.92
1:A:147:SER:H	1:A:391:THR:CG2	1.83	0.92
2:B:287:GLY:HA2	18:B:1218:CLA:HMC3	1.51	0.92
2:B:523:ILE:HD12	2:B:590:VAL:HG21	1.48	0.92
16:3:134:TYR:CA	16:3:136:PRO:HD2	1.97	0.92
1:A:347:TYR:HD2	1:A:349:ILE:H	1.17	0.92
2:B:103:ALA:HB1	2:B:104:PHE:CD1	2.04	0.91
2:B:330:ILE:HG22	2:B:331:HIS:N	1.83	0.91
14:1:89:VAL:HG12	14:1:90:PRO:HD3	1.52	0.91
16:3:129:ARG:HD3	16:3:139:MET:SD	2.09	0.91
6:F:12:LYS:HD2	6:F:13:GLN:H	1.27	0.91
15:2:22:SER:CA	15:2:23:LEU:CG	2.48	0.91
2:B:519:VAL:HG21	2:B:593:TYR:CD2	2.05	0.91
12:L:165:TYR:HD1	18:L:1503:CLA:OBD	1.45	0.91
13:N:77:CYS:CB	13:N:78:GLY:CA	2.48	0.91
1:A:434:ARG:NH2	1:A:438:HIS:HB3	1.85	0.91
3:C:7:ILE:HD12	3:C:65:VAL:HA	1.50	0.91
4:D:26:SER:HB3	4:D:69:ARG:HB2	1.52	0.91
12:L:113:SER:H	12:L:114:ILE:CB	1.83	0.91
12:L:129:GLN:NE2	12:L:129:GLN:HA	1.83	0.91
12:L:14:LEU:HD22	12:L:23:LEU:H	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:63:ASP:HB2	13:N:64:ASP:HA	1.44	0.91
1:A:110:LEU:O	1:A:113:PRO:HD3	1.70	0.91
2:B:550:LYS:HA	2:B:553:PHE:HB2	1.52	0.91
2:B:631:LEU:HD13	2:B:632:ILE:H	1.36	0.91
2:B:71:GLN:NE2	2:B:89:HIS:O	2.03	0.91
4:D:107:GLY:O	4:D:108:GLU:HB3	1.70	0.91
4:D:26:SER:H	4:D:27:PRO:HB2	1.36	0.91
6:F:105:LEU:O	6:F:108:ILE:N	2.03	0.91
18:L:1503:CLA:H12	18:L:1503:CLA:CED	2.00	0.91
1:A:63:ASP:H	18:A:1128:CLA:HAA2	1.33	0.91
1:A:147:SER:CA	1:A:391:THR:HG21	1.99	0.91
2:B:174:ARG:HG3	18:B:1221:CLA:CMD	1.98	0.91
12:L:66:GLY:HA3	18:L:1503:CLA:C3B	2.01	0.91
14:I:40:LYS:HG2	14:I:41:GLU:N	1.84	0.91
16:3:132:ASP:CB	16:3:139:MET:CG	2.46	0.91
1:A:317:TYR:HA	1:A:325:HIS:H	1.35	0.91
1:A:50:THR:HG21	1:A:723:ARG:NH1	1.85	0.91
3:C:58:CYS:SG	21:C:3103:SF4:S3	2.69	0.91
4:D:86:LEU:HA	4:D:89:ARG:HB3	1.50	0.91
7:G:37:GLU:HG3	7:G:43:HIS:NE2	1.86	0.91
12:L:67:PRO:HD2	18:L:1503:CLA:CAB	1.98	0.91
13:N:48:GLY:HA2	13:N:50:GLN:N	1.83	0.91
13:N:60:PHE:HD2	13:N:60:PHE:N	1.69	0.91
2:B:83:HIS:H	2:B:84:VAL:HG23	1.33	0.91
4:D:102:ARG:HA	4:D:103:VAL:HB	0.93	0.91
8:H:58:ILE:O	8:H:58:ILE:HD12	1.69	0.91
1:A:521:VAL:HG13	1:A:522:ALA:N	1.83	0.91
3:C:81:TYR:HE1	4:D:37:LEU:O	1.53	0.91
15:2:194:ALA:HB1	15:2:195:HIS:HA	1.49	0.90
15:2:40:SER:CA	15:2:41:LEU:CB	2.45	0.90
4:D:54:LYS:HB2	4:D:56:GLN:HB2	1.53	0.90
4:D:94:TYR:HB2	4:D:95:LYS:NZ	1.85	0.90
6:F:126:ALA:H	6:F:130:LEU:HD13	1.35	0.90
18:B:1203:CLA:H2	18:B:1226:CLA:ND	1.86	0.90
2:B:133:GLU:HA	2:B:136:TYR:HE1	1.30	0.90
6:F:81:GLY:O	6:F:86:PRO:CD	2.19	0.90
8:H:27:ASP:O	8:H:29:PRO:HD3	1.72	0.90
10:J:19:PHE:O	10:J:23:ALA:HB3	1.71	0.90
12:L:87:ALA:O	12:L:90:GLY:N	2.03	0.90
1:A:620:MET:O	1:A:621:GLN:CB	2.18	0.90
3:C:55:GLU:HB3	3:C:65:VAL:HG21	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:PHE:CE2	18:A:1136:CLA:CBB	2.55	0.90
2:B:341:LEU:CD2	18:B:1202:CLA:HED2	2.01	0.90
18:B:9010:CLA:HMB3	18:B:9022:CLA:HMD1	1.51	0.90
16:3:132:ASP:HB3	16:3:139:MET:HG3	0.91	0.90
1:A:744:ALA:O	1:A:748:ALA:N	2.03	0.90
2:B:510:LEU:HD21	18:B:1234:CLA:HHD	1.51	0.90
6:F:28:SER:HB3	6:F:42:ILE:CG2	2.01	0.90
15:2:22:SER:CB	15:2:23:LEU:HG	2.01	0.90
2:B:657:TRP:HE1	2:B:717:TYR:HB2	1.35	0.90
7:G:82:ALA:HB3	7:G:83:TYR:HB3	1.53	0.90
1:A:557:LEU:CA	1:A:560:VAL:HG22	1.99	0.90
1:A:50:THR:CG2	1:A:723:ARG:HH12	1.84	0.90
1:A:81:ALA:CB	1:A:82:HIS:HB2	2.00	0.90
2:B:20:ARG:O	2:B:24:GLY:N	2.05	0.90
9:I:25:PHE:CD2	9:I:25:PHE:O	2.24	0.90
15:2:21:GLY:N	15:2:23:LEU:CD2	2.35	0.90
18:A:1113:CLA:HAA1	18:A:1113:CLA:HED2	1.52	0.90
1:A:396:PHE:HD2	1:A:396:PHE:O	1.55	0.90
1:A:467:MET:CA	1:A:471:GLY:HA3	2.01	0.90
2:B:177:HIS:CE1	18:B:1209:CLA:C4C	2.55	0.90
2:B:678:LEU:HD22	2:B:679:ALA:N	1.86	0.90
3:C:5:VAL:HG13	3:C:6:LYS:N	1.86	0.90
4:D:57:ILE:HG13	4:D:67:ILE:HA	1.54	0.90
12:L:69:VAL:HG21	12:L:83:ALA:HB1	1.52	0.90
15:2:178:TRP:C	15:2:180:GLN:H	1.76	0.90
2:B:519:VAL:CG2	2:B:593:TYR:HD2	1.85	0.90
3:C:12:ILE:CA	3:C:13:GLY:O	2.20	0.90
14:1:183:ASP:H	14:1:184:PRO:CA	1.85	0.89
2:B:287:GLY:CA	18:B:1218:CLA:HMC1	2.01	0.89
17:4:115:VAL:HG12	17:4:116:ASN:N	1.85	0.89
2:B:78:VAL:HA	2:B:130:ARG:NE	1.85	0.89
1:A:80:SER:N	1:A:81:ALA:HB2	1.87	0.89
15:2:154:GLN:HG2	15:2:155:LYS:H	1.36	0.89
15:2:63:PHE:HD2	15:2:63:PHE:N	1.70	0.89
1:A:569:ILE:HG13	1:A:586:ARG:NH1	1.86	0.89
2:B:627:ASN:HA	2:B:732:LYS:CE	2.03	0.89
3:C:9:ASP:OD2	3:C:10:THR:N	2.05	0.89
6:F:115:THR:HG23	6:F:116:GLN:N	1.87	0.89
15:2:106:GLU:HG2	18:2:2012:CLA:CHD	2.03	0.89
15:2:172:LEU:HB3	15:2:175:MET:SD	2.12	0.89
15:2:27:PHE:HD1	15:2:28:GLY:C	1.76	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:H	1:A:44:ILE:HD13	1.33	0.89
1:A:621:GLN:HA	1:A:637:ILE:CD1	2.02	0.89
2:B:479:SER:C	2:B:481:THR:H	1.75	0.89
2:B:707:LEU:O	2:B:710:LEU:N	2.04	0.89
4:D:96:ILE:CG1	4:D:97:LYS:H	1.86	0.89
15:2:19:LEU:HB2	15:2:22:SER:OG	1.72	0.89
1:A:650:ASN:HD22	2:B:651:LEU:HD11	1.36	0.89
1:A:51:THR:HG23	1:A:722:PRO:CA	1.98	0.89
1:A:86:LEU:HD11	1:A:90:PHE:CE1	2.07	0.89
18:B:1205:CLA:CAB	18:B:1205:CLA:H51	2.03	0.89
15:2:93:THR:HG22	15:2:94:LEU:HA	1.52	0.89
1:A:594:ALA:HA	1:A:597:HIS:HB2	1.55	0.89
6:F:144:LEU:HD11	20:F:6016:BCR:C33	2.03	0.89
2:B:310:PRO:HA	2:B:312:GLY:N	1.87	0.89
1:A:621:GLN:HA	1:A:637:ILE:HD13	1.55	0.88
2:B:671:TRP:O	2:B:675:ILE:HG23	1.73	0.88
2:B:573:TRP:HH2	2:B:706:ARG:HG3	1.34	0.88
2:B:653:GLY:HA3	2:B:720:THR:CG2	2.03	0.88
10:J:2:ARG:CB	10:J:7:TYR:HE1	1.86	0.88
17:4:115:VAL:CG1	17:4:116:ASN:H	1.86	0.88
1:A:223:VAL:HG23	1:A:224:HIS:CD2	2.08	0.88
18:B:1224:CLA:C3A	18:B:1224:CLA:CGA	2.51	0.88
13:N:58:VAL:HB	16:3:86:PRO:O	1.73	0.88
13:N:81:VAL:HB	13:N:82:PHE:HA	0.90	0.88
15:2:86:GLU:O	15:2:89:THR:HB	1.74	0.88
2:B:593:TYR:CD1	2:B:594:TRP:N	2.42	0.88
3:C:12:ILE:HG13	21:C:3103:SF4:S2	2.13	0.88
6:F:49:THR:HA	6:F:56:TYR:HH	1.33	0.88
8:H:55:LYS:HA	8:H:58:ILE:HG13	1.55	0.88
1:A:84:GLY:HA2	1:A:87:SER:HB3	1.56	0.88
2:B:344:ILE:CG1	18:B:1225:CLA:HBC1	2.02	0.88
2:B:700:LEU:HD23	2:B:704:GLN:HE22	1.38	0.88
6:F:81:GLY:O	6:F:86:PRO:HD2	1.72	0.88
2:B:176:ASN:HB2	2:B:291:TYR:CD1	2.08	0.88
1:A:658:TRP:HD1	2:B:625:TRP:NE1	1.68	0.88
17:4:147:LEU:O	17:4:148:GLU:HB2	1.71	0.88
1:A:349:ILE:HA	1:A:352:THR:OG1	1.74	0.88
2:B:284:PHE:CE1	18:B:1216:CLA:HHC	2.08	0.88
2:B:259:GLY:HA3	2:B:269:TRP:HZ2	1.36	0.88
4:D:90:LEU:O	4:D:91:ARG:HD3	1.72	0.88
2:B:98:GLN:HB2	8:H:78:PRO:HB3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:92:ARG:N	8:H:93:GLY:HA3	1.89	0.88
14:1:180:HIS:O	18:1:1003:CLA:C2A	2.21	0.88
16:3:134:TYR:C	16:3:136:PRO:CD	2.41	0.88
16:3:138:SER:H	16:3:139:MET:HB3	1.37	0.88
1:A:208:ALA:N	1:A:310:PHE:O	2.06	0.88
2:B:416:GLU:HA	2:B:419:ILE:HD12	1.56	0.88
4:D:27:PRO:O	4:D:28:ILE:CG1	2.18	0.88
6:F:48:LYS:O	6:F:52:ARG:HB2	1.73	0.88
1:A:342:GLY:O	1:A:431:LEU:CD2	2.22	0.88
6:F:105:LEU:HD21	18:F:1139:CLA:HED1	1.55	0.88
18:L:1502:CLA:H42	18:L:1504:CLA:HMA1	1.55	0.88
12:L:92:VAL:HG13	12:L:93:VAL:N	1.89	0.88
15:2:17:GLU:HB3	15:2:18:TRP:HB3	1.55	0.88
9:I:25:PHE:CA	9:I:26:LEU:HB2	2.03	0.88
13:N:47:THR:HA	13:N:49:CYS:SG	2.14	0.88
13:N:69:CYS:SG	13:N:72:LYS:HG3	2.14	0.88
17:4:172:ASN:O	17:4:173:VAL:HG23	1.72	0.88
18:B:1220:CLA:OBD	18:B:1221:CLA:CAB	2.21	0.88
2:B:5:ILE:CG2	2:B:6:PRO:HA	2.04	0.88
12:L:70:LYS:HG2	12:L:75:ARG:HG3	1.53	0.88
15:2:17:GLU:HG3	15:2:18:TRP:CB	1.96	0.87
17:4:51:ALA:HB1	17:4:161:MET:CE	2.03	0.87
1:A:409:GLY:HA3	18:A:1128:CLA:HAC1	1.54	0.87
2:B:86:PRO:HB2	2:B:116:ALA:O	1.74	0.87
6:F:126:ALA:N	6:F:130:LEU:CD1	2.32	0.87
6:F:76:ASP:O	6:F:77:GLN:O	1.91	0.87
7:G:8:ILE:CG1	7:G:9:SER:H	1.86	0.87
12:L:66:GLY:CA	18:L:1503:CLA:HMB3	2.03	0.87
13:N:58:VAL:HG23	13:N:59:PRO:HA	0.89	0.87
13:N:69:CYS:CB	13:N:72:LYS:HG3	2.04	0.87
17:4:58:MET:SD	17:4:58:MET:N	2.47	0.87
1:A:261:SER:HB2	1:A:277:TYR:CE2	2.09	0.87
2:B:103:ALA:HB1	2:B:104:PHE:HD1	1.38	0.87
2:B:378:ILE:HG22	2:B:382:ILE:CD1	2.04	0.87
2:B:553:PHE:CZ	3:C:66:ARG:HG3	2.08	0.87
6:F:134:PHE:CE2	18:F:4015:CLA:C3B	2.58	0.87
14:1:27:LEU:CB	14:1:28:GLY:HA2	2.04	0.87
1:A:455:PHE:HD1	1:A:456:HIS:HB3	1.40	0.87
2:B:275:HIS:ND1	18:B:1214:CLA:HMB1	1.88	0.87
2:B:84:VAL:CG1	2:B:85:ARG:H	1.87	0.87
2:B:549:ASP:OD2	3:C:63:LEU:HB3	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:86:PRO:CG	10:J:39:PHE:HB2	2.04	0.87
9:I:27:HIS:HA	9:I:30:LYS:HD3	1.52	0.87
17:4:82:GLU:HB3	17:4:84:PHE:CZ	2.09	0.87
2:B:530:THR:OG1	2:B:582:TRP:HB3	1.74	0.87
8:H:77:LEU:HD23	8:H:78:PRO:HD2	1.54	0.87
17:4:63:VAL:HG12	17:4:67:ILE:H	1.38	0.87
1:A:268:PRO:HB2	1:A:273:ASN:HB3	1.53	0.87
1:A:495:THR:C	1:A:497:ALA:H	1.74	0.87
3:C:41:SER:OG	4:D:132:LEU:HD21	1.75	0.87
4:D:135:ARG:HG2	4:D:139:LYS:CD	2.05	0.87
4:D:155:ASP:HB3	4:D:156:LEU:C	1.93	0.87
16:3:61:ILE:O	16:3:64:ARG:HB3	1.75	0.87
1:A:96:MET:HB3	1:A:149:PHE:HE2	1.40	0.87
1:A:493:GLN:HG3	1:A:515:TRP:CB	2.04	0.87
18:B:1138:CLA:H8	18:B:1138:CLA:CBB	2.03	0.87
2:B:302:LYS:CE	2:B:302:LYS:HA	2.05	0.87
4:D:122:LYS:O	4:D:127:ARG:NH2	2.08	0.87
4:D:137:ILE:HG13	4:D:140:ASN:ND2	1.89	0.87
6:F:115:THR:O	6:F:118:GLU:N	2.07	0.87
12:L:44:ARG:HH11	12:L:44:ARG:CB	1.86	0.87
12:L:69:VAL:CG2	12:L:83:ALA:HB1	2.05	0.87
17:4:190:TRP:HA	17:4:190:TRP:CE3	2.07	0.87
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.10	0.87
1:A:581:CYS:HB2	1:A:590:CYS:CA	2.02	0.87
1:A:658:TRP:CD1	2:B:625:TRP:CE2	2.63	0.87
2:B:704:GLN:C	2:B:706:ARG:H	1.78	0.87
1:A:211:LEU:O	1:A:214:GLY:N	2.06	0.87
6:F:42:ILE:HG12	6:F:43:LYS:H	1.39	0.87
18:A:1106:CLA:HMC3	18:A:1107:CLA:HMD2	1.55	0.86
1:A:109:TRP:O	1:A:112:ASP:N	2.08	0.86
1:A:318:ARG:HD3	1:A:319:THR:N	1.89	0.86
2:B:553:PHE:CE2	3:C:66:ARG:HG3	2.09	0.86
2:B:64:ASN:HA	2:B:67:HIS:CB	2.05	0.86
3:C:81:TYR:CE1	4:D:37:LEU:O	2.27	0.86
13:N:82:PHE:N	13:N:82:PHE:CD2	2.36	0.86
1:A:109:TRP:NE1	1:A:113:PRO:HA	1.90	0.86
1:A:374:GLN:O	1:A:378:SER:OG	1.92	0.86
1:A:645:SER:OG	2:B:637:PRO:HG2	1.75	0.86
3:C:60:THR:N	5:E:80:ASN:HD21	1.71	0.86
6:F:144:LEU:HD11	20:F:6016:BCR:H332	1.57	0.86
13:N:58:VAL:HG22	13:N:60:PHE:CG	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:TRP:CE3	18:A:9011:CLA:HMA2	2.09	0.86
18:B:1224:CLA:H3A	18:B:1224:CLA:O1A	1.73	0.86
2:B:286:ILE:HD12	18:B:1218:CLA:CMC	1.99	0.86
3:C:27:GLU:N	3:C:43:PRO:HG3	1.89	0.86
18:B:1207:CLA:HED1	12:L:73:PRO:HG3	1.56	0.86
13:N:57:LYS:HB2	16:3:87:ALA:CB	2.01	0.86
15:2:23:LEU:HB3	15:2:26:ASP:O	1.75	0.86
17:4:68:GLY:O	17:4:69:ILE:HG22	1.75	0.86
1:A:228:PRO:C	1:A:230:ASN:H	1.75	0.86
2:B:63:GLY:O	2:B:66:PHE:N	2.09	0.86
18:L:1503:CLA:CB	18:L:1503:CLA:CHD	2.37	0.86
2:B:393:PHE:HA	2:B:397:ASP:HB2	1.56	0.86
2:B:441:ASP:OD1	2:B:616:LEU:HD22	1.76	0.86
18:B:9010:CLA:H12	18:B:9012:CLA:CHD	2.05	0.86
18:L:1503:CLA:O1A	18:L:1503:CLA:HED3	1.75	0.86
12:L:97:MET:SD	12:L:98:CYS:N	2.48	0.86
15:2:23:LEU:HB2	15:2:26:ASP:H	1.31	0.86
1:A:101:ALA:HA	1:A:161:GLU:OE2	1.75	0.86
1:A:582:ASP:O	2:B:562:PRO:HD2	1.76	0.86
2:B:120:VAL:HG23	18:B:1225:CLA:HBA2	1.56	0.86
18:B:1218:CLA:C6	18:1:1012:CLA:C3A	2.54	0.86
3:C:63:LEU:HD22	3:C:64:SER:N	1.91	0.86
12:L:70:LYS:HA	12:L:75:ARG:HG3	1.58	0.86
16:3:134:TYR:C	16:3:136:PRO:HD3	1.95	0.86
18:A:9011:CLA:HBB1	2:B:624:LEU:HD11	1.57	0.86
2:B:199:ILE:HG12	2:B:271:THR:HG21	1.56	0.86
2:B:589:TRP:HD1	2:B:592:PHE:CE2	1.93	0.86
2:B:60:TRP:O	2:B:64:ASN:ND2	2.09	0.86
10:J:11:ALA:CB	10:J:12:PRO:CD	2.50	0.86
15:2:197:ALA:N	15:2:198:ASP:HA	1.89	0.86
17:4:156:ASN:HD22	17:4:156:ASN:N	1.73	0.86
1:A:553:VAL:HA	1:A:556:LEU:HD12	0.91	0.86
1:A:754:ILE:O	1:A:755:ILE:HG13	1.75	0.86
18:B:1218:CLA:H2A	18:B:1218:CLA:O1D	1.76	0.86
3:C:44:ARG:O	3:C:45:THR:OG1	1.94	0.86
18:B:1209:CLA:HAA2	7:G:38:GLN:HA	1.57	0.86
18:F:1302:CLA:H92	18:F:1302:CLA:HMA1	0.91	0.86
12:L:53:GLY:CA	12:L:139:PHE:CE1	2.58	0.86
15:2:86:GLU:OE1	17:4:187:SER:HB2	1.76	0.86
7:G:95:PRO:C	7:G:97:PHE:H	1.77	0.86
15:2:17:GLU:CD	15:2:18:TRP:N	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:O	1:A:199:VAL:HG22	1.76	0.85
2:B:450:GLU:HG3	2:B:451:LYS:H	1.38	0.85
2:B:411:MET:SD	18:B:1242:CLA:CMD	2.63	0.85
7:G:77:ILE:O	7:G:77:ILE:HG22	1.76	0.85
1:A:289:PRO:O	1:A:523:VAL:HG11	1.77	0.85
1:A:461:TYR:HB2	1:A:649:ILE:HG13	1.58	0.85
1:A:591:GLN:OE1	2:B:667:TRP:CB	2.25	0.85
1:A:707:ILE:HG22	1:A:711:HIS:HE1	1.40	0.85
3:C:60:THR:H	5:E:80:ASN:HD21	1.24	0.85
1:A:299:ILE:O	1:A:299:ILE:CG2	2.23	0.85
4:D:102:ARG:NH1	4:D:110:GLN:NE2	2.23	0.85
13:N:63:ASP:CB	13:N:64:ASP:CA	2.46	0.85
2:B:411:MET:SD	18:B:1242:CLA:HMD1	2.16	0.85
4:D:31:GLY:HA3	12:L:13:PRO:CB	2.02	0.85
8:H:49:LYS:HG3	12:L:140:THR:CG2	2.06	0.85
18:J:2107:CLA:H91	18:J:2107:CLA:H13	1.58	0.85
2:B:307:ALA:O	2:B:310:PRO:HD2	1.76	0.85
2:B:463:ILE:H	2:B:463:ILE:HD12	1.40	0.85
7:G:20:ARG:CZ	7:G:64:VAL:HB	2.07	0.85
12:L:44:ARG:NH1	12:L:44:ARG:HB2	1.91	0.85
15:2:28:GLY:O	15:2:29:PHE:CD1	2.30	0.85
1:A:35:ALA:CA	1:A:36:LYS:HB2	1.99	0.85
1:A:491:TRP:HA	1:A:492:ILE:CG1	2.06	0.85
6:F:148:GLU:O	6:F:149:LEU:HG	1.77	0.85
15:2:18:TRP:HD1	15:2:21:GLY:HA3	0.69	0.85
15:2:41:LEU:C	15:2:45:VAL:HG11	1.96	0.85
2:B:429:LEU:CD2	2:B:524:ALA:O	2.24	0.85
2:B:635:ILE:HG23	2:B:636:THR:H	1.40	0.85
2:B:663:PHE:H	2:B:663:PHE:HD2	0.89	0.85
2:B:92:TRP:HD1	9:I:9:VAL:HB	1.40	0.85
3:C:36:ALA:O	3:C:37:LYS:HB2	1.74	0.85
9:I:25:PHE:H	9:I:26:LEU:HB2	0.82	0.85
15:2:19:LEU:HD12	15:2:22:SER:HG	1.40	0.85
16:3:55:LEU:H	16:3:56:ALA:HA	1.41	0.85
18:B:1138:CLA:CAD	18:B:1138:CLA:HED2	2.07	0.85
15:2:22:SER:H	15:2:23:LEU:CB	1.89	0.85
16:3:83:GLY:HA2	16:3:86:PRO:HD2	0.87	0.85
1:A:535:GLY:O	1:A:538:ASP:HB2	1.75	0.85
12:L:50:LEU:HG	12:L:138:LYS:O	1.75	0.85
13:N:17:ASN:ND2	13:N:20:LYS:HD3	1.92	0.85
15:2:18:TRP:CD1	15:2:21:GLY:O	2.30	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1212:CLA:HHD	18:B:1212:CLA:HBC3	1.59	0.84
13:N:63:ASP:HB2	13:N:64:ASP:HB2	1.58	0.84
15:2:17:GLU:OE1	15:2:18:TRP:CE3	2.30	0.84
15:2:28:GLY:O	15:2:29:PHE:CE2	2.30	0.84
1:A:464:ASN:HD21	1:A:477:PHE:HB2	0.68	0.84
1:A:735:VAL:HG13	1:A:736:THR:N	1.91	0.84
18:A:9011:CLA:HBB2	18:B:9010:CLA:C4D	2.06	0.84
1:A:90:PHE:HD1	1:A:175:ALA:HA	1.42	0.84
2:B:299:HIS:NE2	18:B:1218:CLA:HED3	1.92	0.84
2:B:378:ILE:HG13	18:B:1225:CLA:CBB	2.06	0.84
13:N:57:LYS:HB3	13:N:58:VAL:HA	1.59	0.84
15:2:28:GLY:O	15:2:29:PHE:CE1	2.31	0.84
15:2:59:ALA:O	15:2:63:PHE:CE2	2.30	0.84
1:A:327:ILE:HG22	1:A:328:LYS:HD3	1.57	0.84
1:A:467:MET:HA	1:A:471:GLY:CA	2.06	0.84
2:B:333:GLN:O	2:B:334:LEU:HB2	1.76	0.84
6:F:92:TYR:CZ	6:F:96:TRP:HZ3	1.94	0.84
14:1:76:ALA:C	14:1:78:PRO:HD3	1.98	0.84
1:A:183:TRP:HZ3	1:A:188:LYS:HB2	1.41	0.84
1:A:408:VAL:HG11	1:A:605:MET:HB2	1.57	0.84
1:A:412:ALA:HB2	1:A:598:VAL:HG21	1.59	0.84
18:B:1203:CLA:HBA2	18:B:1203:CLA:CGD	2.08	0.84
7:G:61:ASN:O	7:G:64:VAL:HG22	1.77	0.84
13:N:51:ASP:CB	13:N:52:LEU:HG	2.07	0.84
15:2:21:GLY:CA	15:2:23:LEU:CD2	2.55	0.84
1:A:330:ILE:O	1:A:333:ALA:CB	2.26	0.84
1:A:718:PRO:CG	1:A:722:PRO:HD3	2.07	0.84
18:B:1205:CLA:C1A	18:B:1205:CLA:CGA	2.55	0.84
18:B:1220:CLA:C1B	18:B:1242:CLA:HBA1	2.07	0.84
2:B:224:PRO:HB2	2:B:229:GLN:O	1.76	0.84
2:B:663:PHE:HD2	2:B:663:PHE:N	1.74	0.84
2:B:655:LEU:HB2	18:B:9022:CLA:HAA1	1.58	0.84
1:A:496:HIS:HB3	1:A:515:TRP:CD1	2.12	0.84
4:D:44:GLU:OE1	4:D:102:ARG:HD3	1.76	0.84
5:E:62:ARG:HG3	5:E:63:TYR:HD1	1.40	0.84
16:3:54:TRP:CB	16:3:55:LEU:CA	2.38	0.84
16:3:82:ALA:HA	16:3:83:GLY:O	1.78	0.84
1:A:364:MET:HA	1:A:364:MET:CE	2.08	0.84
1:A:284:ARG:NH1	1:A:508:THR:OG1	2.10	0.84
1:A:520:LEU:HD22	1:A:521:VAL:N	1.93	0.84
2:B:104:PHE:O	2:B:106:ARG:N	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:SER:HB3	18:B:1222:CLA:O1D	1.78	0.84
6:F:124:PRO:CG	6:F:125:LEU:HG	2.05	0.84
7:G:85:ILE:HA	7:G:86:LEU:C	1.98	0.84
15:2:28:GLY:O	15:2:29:PHE:CZ	2.31	0.84
1:A:455:PHE:CD1	1:A:456:HIS:HB3	2.12	0.84
2:B:276:HIS:HE2	18:B:1215:CLA:HMB3	1.42	0.84
2:B:463:ILE:H	2:B:463:ILE:CD1	1.90	0.84
2:B:657:TRP:CZ3	2:B:661:PHE:HE1	1.96	0.84
2:B:688:ALA:O	2:B:691:ILE:HD11	1.78	0.84
3:C:58:CYS:HA	21:C:3103:SF4:S1	2.17	0.84
10:J:7:TYR:O	10:J:8:LEU:HB2	1.76	0.84
12:L:148:VAL:HA	12:L:151:VAL:CG2	2.07	0.84
14:1:7:GLY:HA2	14:1:9:PRO:N	1.93	0.84
1:A:261:SER:HB2	1:A:277:TYR:CD2	2.13	0.84
1:A:278:ALA:O	1:A:280:PHE:HD2	1.61	0.84
1:A:63:ASP:OD1	1:A:66:SER:OG	1.94	0.84
1:A:718:PRO:HG3	1:A:722:PRO:HD3	1.60	0.84
2:B:653:GLY:O	2:B:657:TRP:HB2	1.76	0.84
6:F:100:VAL:CG1	6:F:125:LEU:CD2	2.54	0.84
12:L:167:PHE:HB2	12:L:168:LYS:CB	2.07	0.84
15:2:28:GLY:O	15:2:29:PHE:CD2	2.30	0.84
2:B:537:GLY:HA3	2:B:575:ASP:HB3	1.59	0.84
4:D:144:ILE:N	4:D:144:ILE:HD12	1.93	0.84
2:B:458:ILE:HG12	6:F:74:SER:CB	2.07	0.84
14:1:89:VAL:HB	14:1:90:PRO:HD3	1.60	0.83
1:A:688:PHE:CD1	1:A:688:PHE:O	2.31	0.83
1:A:712:ASN:O	1:A:715:LYS:N	2.09	0.83
1:A:71:LEU:CD1	1:A:352:THR:HG22	2.07	0.83
18:B:1207:CLA:HBC3	20:I:6018:BCR:C21	2.03	0.83
2:B:564:ARG:O	2:B:564:ARG:HG2	1.76	0.83
2:B:663:PHE:CD2	2:B:663:PHE:N	2.45	0.83
3:C:12:ILE:HA	3:C:13:GLY:C	1.93	0.83
2:B:333:GLN:O	18:B:1202:CLA:HHD	1.78	0.83
9:I:26:LEU:HG	9:I:29:GLU:C	1.98	0.83
15:2:178:TRP:HA	15:2:179:PHE:CD1	2.13	0.83
15:2:96:ILE:O	15:2:100:VAL:HG13	1.78	0.83
1:A:423:ASP:HB3	1:A:424:PRO:CD	2.07	0.83
1:A:486:PRO:N	1:A:487:VAL:HB	1.92	0.83
2:B:358:TYR:O	2:B:360:PHE:N	2.12	0.83
2:B:645:VAL:O	2:B:648:TRP:N	2.10	0.83
3:C:60:THR:H	5:E:80:ASN:ND2	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:1503:CLA:HBC2	18:L:1503:CLA:HHD	0.87	0.83
15:2:36:SER:HA	15:2:37:ASP:CB	2.08	0.83
1:A:722:PRO:HB2	18:F:1139:CLA:HMC3	1.59	0.83
12:L:92:VAL:O	12:L:94:ILE:N	2.09	0.83
14:1:84:TYR:HB2	14:1:85:LEU:HG	1.60	0.83
1:A:658:TRP:HD1	2:B:625:TRP:CD1	1.96	0.83
4:D:108:GLU:HG2	4:D:109:VAL:HG22	1.57	0.83
15:2:197:ALA:H	15:2:198:ASP:CA	1.88	0.83
1:A:331:LEU:HD13	1:A:346:LEU:HB3	1.58	0.83
1:A:657:LEU:O	1:A:659:ALA:N	2.09	0.83
1:A:755:ILE:H	1:A:758:GLY:HA3	0.74	0.83
2:B:617:MET:O	2:B:621:ARG:N	2.09	0.83
18:A:9013:CLA:CHB	18:B:9012:CLA:HBB2	2.08	0.83
6:F:102:ARG:NH2	6:F:148:GLU:OE2	2.10	0.83
7:G:23:PHE:HB2	7:G:24:PHE:CD1	2.14	0.83
15:2:96:ILE:HG13	15:2:97:VAL:H	1.41	0.83
1:A:71:LEU:HA	1:A:74:ILE:CG2	2.09	0.83
2:B:395:ILE:O	2:B:395:ILE:HG22	1.78	0.83
2:B:464:GLN:O	2:B:469:LYS:CB	2.27	0.83
3:C:5:VAL:CG1	3:C:6:LYS:H	1.91	0.83
14:1:54:VAL:HA	14:1:57:ILE:CG2	2.08	0.83
1:A:311:LEU:HD21	18:A:1108:CLA:HMC3	1.58	0.83
1:A:398:HIS:HB2	18:A:1126:CLA:NB	1.93	0.83
1:A:85:GLN:HE21	1:A:85:GLN:HA	1.44	0.83
2:B:378:ILE:HG22	2:B:382:ILE:CG1	2.08	0.83
2:B:573:TRP:CE3	2:B:574:ASP:HB3	2.13	0.83
4:D:109:VAL:HB	4:D:110:GLN:HA	1.61	0.83
12:L:14:LEU:HD22	12:L:23:LEU:N	1.93	0.83
15:2:44:ASN:ND2	15:2:113:ILE:CB	2.41	0.83
1:A:255:LEU:H	1:A:255:LEU:HD12	1.43	0.83
1:A:305:ALA:HB2	18:A:1115:CLA:CMA	2.06	0.83
1:A:403:GLY:O	1:A:407:ILE:HG22	1.78	0.83
2:B:18:THR:HG21	18:B:1238:CLA:HBB2	1.60	0.83
17:4:72:VAL:H	17:4:73:PRO:HD2	1.44	0.83
1:A:472:ARG:O	1:A:474:GLN:N	2.11	0.83
18:B:1205:CLA:O2A	18:B:1205:CLA:NA	2.12	0.83
2:B:126:THR:CB	18:B:1215:CLA:HED1	2.07	0.83
2:B:200:PRO:O	2:B:205:GLU:N	2.10	0.83
2:B:646:TRP:CE3	2:B:723:ALA:CB	2.59	0.83
6:F:125:LEU:CA	6:F:130:LEU:HD11	2.09	0.83
17:4:102:GLU:O	17:4:105:ARG:HG3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:106:TRP:CZ2	17:4:110:LYS:NZ	2.46	0.82
1:A:125:PRO:HA	1:A:130:GLU:OE1	1.79	0.82
1:A:268:PRO:CB	1:A:273:ASN:HB2	2.06	0.82
19:A:5001:PQN:H212	18:B:1138:CLA:HBC1	1.61	0.82
2:B:5:ILE:O	2:B:13:ALA:O	1.96	0.82
2:B:646:TRP:CD1	2:B:646:TRP:N	2.47	0.82
1:A:331:LEU:HD13	1:A:346:LEU:CB	2.09	0.82
1:A:368:LEU:HA	1:A:371:VAL:CG2	2.09	0.82
1:A:430:ASP:OD2	1:A:432:LEU:N	2.11	0.82
1:A:488:PHE:CE2	18:A:1136:CLA:O2D	2.31	0.82
2:B:378:ILE:CD1	18:B:1225:CLA:HBB2	2.09	0.82
2:B:422:LEU:CB	18:B:1236:CLA:HBB2	2.07	0.82
2:B:265:THR:HA	2:B:360:PHE:HE2	1.42	0.82
2:B:709:GLY:O	2:B:713:PHE:HB2	1.78	0.82
9:I:29:GLU:OE1	12:L:104:ILE:HG21	1.77	0.82
18:A:1140:CLA:NC	18:A:1140:CLA:H42	1.94	0.82
20:A:6011:BCR:C8	20:A:6011:BCR:C32	2.49	0.82
2:B:294:ASN:ND2	18:B:1209:CLA:HMA2	1.93	0.82
3:C:27:GLU:HB2	4:D:127:ARG:HD2	1.60	0.82
15:2:19:LEU:HD23	15:2:20:ASP:OD1	1.79	0.82
2:B:120:VAL:CG2	18:B:1225:CLA:HBA2	2.09	0.82
20:B:6017:BCR:H351	20:B:6017:BCR:H16C	1.60	0.82
4:D:28:ILE:HB	4:D:67:ILE:CG2	2.10	0.82
4:D:90:LEU:O	4:D:91:ARG:NH1	2.12	0.82
1:A:584:PRO:HD3	2:B:561:GLY:HA3	1.62	0.82
2:B:564:ARG:HH12	3:C:66:ARG:HH22	1.24	0.82
7:G:16:LEU:HD23	7:G:68:ILE:HG12	1.61	0.82
18:A:1129:CLA:HMA1	18:L:1130:CLA:OBD	1.79	0.82
2:B:684:ARG:CZ	12:L:22:GLY:HA3	2.10	0.82
15:2:194:ALA:HB3	15:2:195:HIS:CD2	2.14	0.82
1:A:160:SER:O	1:A:163:GLN:HB3	1.80	0.82
1:A:402:ILE:HD12	1:A:402:ILE:H	1.41	0.82
2:B:593:TYR:CE1	18:B:1234:CLA:HAC2	2.13	0.82
2:B:262:HIS:CD2	2:B:264:GLN:HB3	2.13	0.82
2:B:668:ARG:HB2	2:B:702:ILE:HG22	1.60	0.82
3:C:63:LEU:O	3:C:63:LEU:HD13	1.79	0.82
7:G:35:VAL:HG13	7:G:36:PRO:HB3	1.56	0.82
17:4:62:GLU:O	17:4:63:VAL:CG2	2.27	0.82
1:A:458:PHE:CD1	18:B:9022:CLA:HMB3	2.14	0.82
2:B:294:ASN:CG	18:B:1209:CLA:HMA2	2.00	0.82
2:B:450:GLU:HA	6:F:68:LEU:HD11	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:79:TYR:N	12:L:80:ALA:HB2	1.94	0.82
13:N:57:LYS:HD2	16:3:87:ALA:HB1	0.82	0.82
6:F:130:LEU:N	6:F:130:LEU:HD12	1.95	0.82
7:G:25:ASN:HB3	7:G:31:MET:HG3	1.62	0.82
13:N:81:VAL:C	13:N:83:TRP:HD1	1.82	0.82
13:N:81:VAL:CB	13:N:83:TRP:HA	2.09	0.82
1:A:315:HIS:HB3	18:A:1108:CLA:O1D	1.80	0.82
1:A:725:LEU:HD22	19:A:5001:PQN:C6	2.09	0.82
1:A:665:ILE:CD1	18:A:9011:CLA:HBC1	2.09	0.82
2:B:424:TRP:HE1	18:B:1229:CLA:CED	1.91	0.82
2:B:58:PHE:CZ	18:B:1241:CLA:HHB	2.14	0.82
2:B:443:MET:SD	2:B:451:LYS:HE3	2.18	0.82
3:C:52:LYS:HZ3	3:C:66:ARG:HH11	1.28	0.82
1:A:735:VAL:HG13	1:A:736:THR:H	1.45	0.82
18:B:1216:CLA:CGA	18:B:1220:CLA:H11	2.09	0.82
2:B:536:LYS:O	2:B:538:ALA:N	2.12	0.82
2:B:648:TRP:HZ3	20:B:6017:BCR:HC21	1.44	0.82
2:B:6:PRO:HD3	2:B:20:ARG:HE	1.45	0.82
4:D:133:ASN:OD1	4:D:135:ARG:HB2	1.79	0.82
2:B:689:ASN:ND2	4:D:38:ARG:NH1	2.28	0.82
2:B:20:ARG:NH2	9:I:28:VAL:HA	1.95	0.82
13:N:67:LEU:O	13:N:67:LEU:HG	1.78	0.82
15:2:19:LEU:HG	15:2:20:ASP:OD1	1.79	0.81
1:A:147:SER:N	1:A:391:THR:CG2	2.39	0.81
2:B:378:ILE:HG22	2:B:382:ILE:HG13	1.60	0.81
4:D:50:TRP:O	4:D:73:ASN:OD1	1.98	0.81
18:L:1503:CLA:H12	18:L:1503:CLA:HED3	1.62	0.81
15:2:162:LYS:HG3	15:2:164:ILE:H	1.45	0.81
17:4:96:ILE:HG23	17:4:97:LEU:H	1.43	0.81
18:A:1107:CLA:HAA2	18:A:1107:CLA:HBD	1.61	0.81
1:A:159:THR:O	1:A:160:SER:HB3	1.78	0.81
1:A:399:HIS:NE2	18:A:1127:CLA:ND	2.27	0.81
1:A:542:HIS:HA	1:A:545:HIS:CD2	2.15	0.81
1:A:714:LEU:HD23	6:F:149:LEU:CD2	2.09	0.81
3:C:52:LYS:NZ	3:C:66:ARG:HH11	1.79	0.81
5:E:36:VAL:CG2	5:E:52:VAL:CG1	2.58	0.81
6:F:50:LYS:O	6:F:53:PHE:HB2	1.80	0.81
15:2:23:LEU:HD23	15:2:26:ASP:O	1.79	0.81
15:2:28:GLY:O	15:2:29:PHE:CG	2.33	0.81
15:2:94:LEU:HD21	15:2:98:GLU:OE1	1.80	0.81
18:B:1212:CLA:C2	18:B:1212:CLA:HAA1	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1216:CLA:HAA2	18:B:1221:CLA:HBB2	1.62	0.81
2:B:202:SER:HA	2:B:245:GLY:HA2	1.62	0.81
2:B:304:ILE:CG2	2:B:305:LEU:HD12	2.09	0.81
2:B:319:HIS:O	2:B:320:LYS:C	2.18	0.81
2:B:547:MET:CB	3:C:66:ARG:HH21	1.90	0.81
5:E:72:VAL:HG22	5:E:78:SER:HB3	1.62	0.81
8:H:44:ALA:HB3	8:H:45:ALA:HA	1.60	0.81
2:B:92:TRP:HD1	9:I:9:VAL:CB	1.93	0.81
15:2:178:TRP:HB2	15:2:183:TYR:OH	1.80	0.81
15:2:188:PRO:HA	15:2:192:LEU:HD12	1.62	0.81
2:B:663:PHE:O	2:B:664:LEU:HB2	1.78	0.81
7:G:35:VAL:CG1	7:G:36:PRO:CB	2.55	0.81
1:A:253:ASP:OD2	1:A:254:LEU:HG	1.80	0.81
1:A:288:ASP:HA	1:A:295:TRP:CZ3	2.15	0.81
1:A:446:LEU:CD2	1:A:449:VAL:HG11	2.10	0.81
1:A:453:LEU:CD1	1:A:547:PHE:HA	2.11	0.81
1:A:711:HIS:N	1:A:711:HIS:ND1	2.29	0.81
2:B:325:THR:O	2:B:329:SER:HB3	1.80	0.81
18:A:9013:CLA:C4A	18:B:9012:CLA:HBB2	2.09	0.81
2:B:92:TRP:CD1	9:I:9:VAL:HB	2.16	0.81
6:F:94:ALA:O	6:F:96:TRP:CD1	2.33	0.81
13:N:65:LEU:O	13:N:68:GLU:HG2	1.79	0.81
2:B:672:GLN:HE22	2:B:698:VAL:CA	1.93	0.81
10:J:2:ARG:HB3	10:J:3:ASP:CB	2.04	0.81
8:H:47:PHE:CZ	12:L:50:LEU:HD11	2.14	0.81
14:1:181:LEU:HA	14:1:182:ALA:O	1.80	0.81
14:1:38:ARG:CA	14:1:39:TYR:CB	2.59	0.81
15:2:24:PRO:CB	15:2:32:LEU:HG	2.09	0.81
1:A:368:LEU:HD22	1:A:371:VAL:HG21	1.62	0.81
1:A:520:LEU:HD21	1:A:530:LEU:HB3	1.62	0.81
12:L:58:LEU:CD1	12:L:153:TRP:CZ3	2.63	0.81
13:N:44:GLU:HG2	13:N:44:GLU:O	1.80	0.81
15:2:23:LEU:HB2	15:2:25:GLY:C	1.99	0.81
1:A:245:PRO:HA	1:A:248:PHE:HE1	1.46	0.81
2:B:253:ALA:O	2:B:254:ILE:HG22	1.80	0.81
2:B:37:ILE:O	4:D:148:PHE:HD1	1.59	0.81
2:B:458:ILE:H	18:B:1235:CLA:HMD1	1.45	0.81
12:L:70:LYS:HG2	12:L:75:ARG:CG	2.10	0.81
15:2:40:SER:CB	15:2:41:LEU:CB	2.58	0.81
14:1:10:ARG:O	17:4:110:LYS:HG3	1.80	0.81
1:A:238:ASP:CB	1:A:239:PRO:HD3	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LEU:CD1	1:A:346:LEU:HB3	2.09	0.81
18:B:1209:CLA:H3A	18:B:1209:CLA:CGA	2.10	0.81
2:B:527:LEU:CD2	2:B:586:THR:HG21	2.09	0.81
6:F:130:LEU:O	6:F:133:GLY:N	2.13	0.81
12:L:107:PHE:HA	12:L:133:ALA:CB	2.10	0.81
12:L:38:SER:O	12:L:44:ARG:NH1	2.13	0.81
12:L:51:LEU:O	12:L:51:LEU:HD13	1.80	0.81
2:B:174:ARG:O	2:B:175:LEU:HB2	1.78	0.81
2:B:571:SER:HB2	2:B:574:ASP:H	1.46	0.81
6:F:116:GLN:C	6:F:118:GLU:N	2.34	0.81
18:L:1503:CLA:H11	18:L:1503:CLA:CED	2.09	0.81
15:2:172:LEU:O	15:2:175:MET:SD	2.39	0.81
18:B:1218:CLA:HED2	18:B:1218:CLA:OBD	1.81	0.81
18:B:1232:CLA:HMB1	18:G:1233:CLA:C3B	2.11	0.81
7:G:61:ASN:HA	7:G:64:VAL:HG22	1.61	0.81
2:B:451:LYS:CD	10:J:35:ASP:OD1	2.29	0.81
10:J:39:PHE:CZ	10:J:41:PHE:HB3	2.16	0.81
8:H:47:PHE:CE2	12:L:138:LYS:HB2	2.16	0.81
2:B:684:ARG:CZ	12:L:22:GLY:CA	2.59	0.81
15:2:19:LEU:CD1	15:2:22:SER:OG	2.29	0.80
18:A:1108:CLA:HBC2	18:A:1110:CLA:C2C	2.11	0.80
1:A:147:SER:HA	1:A:391:THR:HG21	1.61	0.80
2:B:104:PHE:C	2:B:106:ARG:HD2	2.01	0.80
2:B:133:GLU:HA	2:B:136:TYR:CD1	2.15	0.80
4:D:28:ILE:HB	4:D:67:ILE:HG23	1.62	0.80
1:A:71:LEU:HD21	1:A:353:SER:HB2	1.63	0.80
2:B:420:SER:HA	18:B:1138:CLA:HED1	1.63	0.80
2:B:115:ASN:O	2:B:117:TYR:CD1	2.35	0.80
2:B:83:HIS:HB3	2:B:84:VAL:HA	1.62	0.80
2:B:674:LEU:HD11	18:B:9023:CLA:HED2	1.63	0.80
3:C:48:CYS:HA	3:C:49:VAL:HG12	1.63	0.80
4:D:75:LEU:HD13	4:D:76:LYS:H	1.47	0.80
9:I:4:LEU:CD2	9:I:5:PRO:HA	2.11	0.80
15:2:23:LEU:CD2	15:2:25:GLY:C	2.48	0.80
16:3:83:GLY:O	16:3:88:GLU:HA	1.81	0.80
1:A:358:LEU:HD13	1:A:413:HIS:CE1	2.16	0.80
1:A:434:ARG:HH21	1:A:438:HIS:HB3	1.46	0.80
1:A:442:ILE:HD11	1:A:561:LEU:CD2	2.11	0.80
4:D:133:ASN:HD22	4:D:134:MET:N	1.78	0.80
6:F:125:LEU:HA	6:F:130:LEU:HD11	1.64	0.80
14:1:34:ALA:HB3	14:1:37:GLU:HA	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:19:LEU:CD2	15:2:20:ASP:OD1	2.30	0.80
1:A:555:ILE:H	1:A:556:LEU:HB2	0.65	0.80
2:B:668:ARG:HH21	2:B:699:ALA:C	1.83	0.80
2:B:84:VAL:HG12	2:B:85:ARG:N	1.95	0.80
14:1:91:TRP:N	14:1:92:GLY:HA2	1.96	0.80
15:2:22:SER:O	15:2:23:LEU:HD13	1.81	0.80
6:F:127:SER:CA	6:F:131:PHE:HB2	2.12	0.80
14:1:181:LEU:O	18:1:1003:CLA:CHA	2.30	0.80
15:2:19:LEU:CG	15:2:20:ASP:OD1	2.30	0.80
15:2:19:LEU:CA	15:2:20:ASP:OD2	2.29	0.80
17:4:42:GLN:HG2	17:4:46:VAL:HG23	1.63	0.80
1:A:282:THR:HB	1:A:284:ARG:HH21	1.45	0.80
1:A:443:ILE:CD1	1:A:562:PHE:HE1	1.94	0.80
1:A:751:LEU:CD1	1:A:752:ALA:H	1.94	0.80
2:B:551:LYS:HE2	4:D:141:VAL:HA	1.63	0.80
8:H:42:THR:N	8:H:43:PHE:HB2	1.96	0.80
10:J:10:VAL:HG12	10:J:14:LEU:HD11	1.62	0.80
12:L:65:VAL:CG1	18:L:1503:CLA:HMA3	2.11	0.80
1:A:462:ILE:N	1:A:649:ILE:HD12	1.95	0.80
1:A:637:ILE:H	1:A:637:ILE:CD1	1.77	0.80
1:A:663:GLN:NE2	1:A:753:ARG:NH1	2.29	0.80
2:B:336:LEU:CA	2:B:339:ALA:HB3	2.09	0.80
4:D:45:PHE:O	4:D:78:ALA:HA	1.82	0.80
6:F:8:CYS:SG	6:F:63:CYS:HB3	2.22	0.80
17:4:41:VAL:CG2	17:4:42:GLN:H	1.85	0.80
2:B:174:ARG:NH2	18:B:1210:CLA:HHD	1.97	0.80
2:B:119:GLY:HA3	2:B:371:LEU:CD1	2.11	0.80
2:B:476:ILE:HB	2:B:477:PRO:CD	2.10	0.80
1:A:699:TYR:HE1	2:B:536:LYS:HE3	1.47	0.80
2:B:594:TRP:HA	2:B:598:HIS:CE1	2.16	0.80
20:I:6018:BCR:H371	20:L:6020:BCR:H342	1.63	0.80
15:2:32:LEU:HD12	15:2:33:GLY:O	1.81	0.80
2:B:117:TYR:CE2	2:B:366:THR:OG1	2.35	0.80
2:B:621:ARG:O	2:B:625:TRP:HB3	1.82	0.80
1:A:562:PHE:CZ	2:B:677:THR:HG21	2.17	0.80
5:E:37:LYS:HE2	5:E:39:LEU:HD12	1.62	0.80
6:F:137:PRO:O	6:F:139:ALA:N	2.13	0.80
14:1:187:ASN:O	14:1:188:ASN:HB2	1.81	0.80
15:2:20:ASP:OD2	15:2:22:SER:CB	2.30	0.80
1:A:284:ARG:HA	1:A:508:THR:OG1	1.82	0.80
1:A:443:ILE:HD13	1:A:562:PHE:CE1	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:ASN:HB3	2:B:614:THR:O	1.82	0.80
10:J:10:VAL:CG1	10:J:14:LEU:HD11	2.12	0.80
13:N:83:TRP:O	13:N:84:LYS:HB3	1.80	0.80
15:2:18:TRP:CA	15:2:20:ASP:O	2.30	0.79
16:3:133:TRP:O	16:3:137:GLY:HA3	1.81	0.79
16:3:134:TYR:H	16:3:136:PRO:HD2	1.44	0.79
1:A:527:VAL:HG13	1:A:528:ALA:H	1.45	0.79
18:B:1209:CLA:CHC	18:B:1217:CLA:HMD2	2.12	0.79
2:B:177:HIS:HE1	18:B:1209:CLA:C4C	1.93	0.79
4:D:96:ILE:HG13	4:D:97:LYS:H	1.47	0.79
14:1:98:LEU:HA	14:1:101:GLU:OE2	1.83	0.79
15:2:19:LEU:CB	15:2:22:SER:OG	2.30	0.79
15:2:22:SER:O	15:2:23:LEU:CD1	2.30	0.79
1:A:735:VAL:CG1	1:A:736:THR:H	1.95	0.79
2:B:508:LEU:HD13	2:B:509:PHE:CD1	2.17	0.79
1:A:295:TRP:HB2	1:A:298:ASP:HB2	1.64	0.79
2:B:86:PRO:O	2:B:116:ALA:N	2.15	0.79
7:G:83:TYR:CB	7:G:85:ILE:HG12	2.11	0.79
18:B:1207:CLA:CBC	20:I:6018:BCR:H21C	2.04	0.79
15:2:23:LEU:CD1	15:2:26:ASP:O	2.29	0.79
15:2:32:LEU:HA	15:2:33:GLY:C	2.02	0.79
17:4:180:ASP:OD2	17:4:185:HIS:CD2	2.35	0.79
18:B:1235:CLA:C1A	18:B:1235:CLA:CGA	2.59	0.79
2:B:393:PHE:HD2	2:B:398:TYR:HB2	1.45	0.79
3:C:8:TYR:CZ	4:D:137:ILE:HD13	2.16	0.79
4:D:108:GLU:HG2	4:D:109:VAL:N	1.97	0.79
6:F:2:ILE:HG13	6:F:2:ILE:O	1.81	0.79
14:1:185:TRP:CE3	14:1:185:TRP:HA	2.18	0.79
15:2:59:ALA:O	15:2:63:PHE:HE2	1.63	0.79
17:4:42:GLN:HA	17:4:45:LEU:HB3	1.65	0.79
1:A:486:PRO:CD	1:A:487:VAL:HB	2.12	0.79
18:F:1302:CLA:CMA	18:F:1302:CLA:C9	2.54	0.79
14:1:91:TRP:H	14:1:92:GLY:CA	1.95	0.79
3:C:25:VAL:HG21	3:C:48:CYS:CB	2.13	0.79
18:L:1503:CLA:CBD	18:L:1503:CLA:HAA2	2.00	0.79
14:1:85:LEU:C	14:1:87:ASN:HA	2.03	0.79
16:3:212:ASN:CB	16:3:213:LEU:HB2	2.13	0.79
1:A:185:HIS:CG	1:A:186:TYR:H	2.00	0.79
1:A:308:ILE:HD12	1:A:311:LEU:HD22	1.64	0.79
1:A:619:LYS:O	1:A:621:GLN:O	1.99	0.79
1:A:687:ALA:O	1:A:689:SER:N	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:652:PHE:CE1	2:B:656:VAL:HG21	2.17	0.79
4:D:119:TYR:O	4:D:121:GLU:N	2.15	0.79
4:D:123:VAL:H	4:D:127:ARG:NH1	1.80	0.79
8:H:64:LEU:HG	8:H:65:LEU:N	1.98	0.79
8:H:93:GLY:H	8:H:94:LYS:HA	1.46	0.79
1:A:289:PRO:O	1:A:523:VAL:CG1	2.30	0.79
1:A:495:THR:C	1:A:497:ALA:N	2.35	0.79
2:B:101:VAL:HG23	2:B:102:GLU:N	1.96	0.79
2:B:301:ILE:HG23	2:B:304:ILE:HG21	1.63	0.79
2:B:342:GLY:O	2:B:345:THR:OG1	2.00	0.79
2:B:331:HIS:ND1	2:B:392:ILE:CG2	2.43	0.79
3:C:42:ALA:CB	3:C:45:THR:HG23	2.13	0.79
7:G:8:ILE:HG13	7:G:9:SER:N	1.97	0.79
13:N:19:LYS:HD2	13:N:20:LYS:N	1.97	0.79
1:A:107:GLU:O	1:A:109:TRP:N	2.16	0.79
1:A:442:ILE:HD12	1:A:443:ILE:N	1.98	0.79
18:B:1239:CLA:HBD	19:B:5002:PQN:H262	1.64	0.79
2:B:646:TRP:HB3	2:B:723:ALA:HB1	1.63	0.79
6:F:130:LEU:H	6:F:130:LEU:HD12	1.48	0.79
13:N:58:VAL:HG23	13:N:59:PRO:N	1.97	0.79
14:1:52:LEU:HA	14:1:55:PRO:CD	2.12	0.79
1:A:362:LEU:O	1:A:366:GLY:N	2.14	0.79
2:B:57:ILE:CG2	18:B:1241:CLA:C3B	2.60	0.79
2:B:464:GLN:O	2:B:469:LYS:HB3	1.81	0.79
2:B:533:ILE:CD1	2:B:579:ALA:HA	2.13	0.79
2:B:651:LEU:HA	2:B:654:HIS:HB2	1.65	0.79
4:D:47:VAL:O	4:D:100:PHE:HB2	1.83	0.79
4:D:50:TRP:H	4:D:73:ASN:HB2	1.45	0.79
8:H:54:LEU:CD1	8:H:55:LYS:H	1.94	0.79
8:H:87:PRO:O	8:H:88:LYS:HB2	1.82	0.79
12:L:74:LEU:CB	12:L:77:THR:HG21	2.13	0.79
14:1:94:LEU:CB	14:1:95:PRO:CD	2.61	0.78
1:A:638:THR:OG1	1:A:641:ASN:ND2	2.15	0.78
18:B:1220:CLA:CHD	18:B:1220:CLA:HBC2	2.11	0.78
2:B:542:ARG:O	2:B:542:ARG:HD2	1.82	0.78
14:1:103:LEU:O	14:1:107:PHE:HD1	1.66	0.78
15:2:157:LYS:CA	15:2:160:ARG:HG2	2.10	0.78
15:2:56:MET:HB3	15:2:172:LEU:HD22	1.64	0.78
1:A:181:ALA:HA	1:A:184:PHE:HB3	1.64	0.78
1:A:368:LEU:HA	1:A:371:VAL:HG22	1.64	0.78
1:A:489:ALA:HB1	1:A:490:GLN:C	2.03	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ASN:HB2	2:B:291:TYR:HD1	1.45	0.78
2:B:391:PRO:HD3	2:B:538:ALA:CB	2.11	0.78
2:B:533:ILE:HD12	2:B:579:ALA:HA	1.65	0.78
2:B:700:LEU:O	2:B:701:SER:C	2.21	0.78
4:D:102:ARG:HH11	4:D:110:GLN:HE22	1.31	0.78
15:2:153:PRO:HB2	15:2:154:GLN:O	1.82	0.78
15:2:32:LEU:HD23	15:2:32:LEU:C	2.04	0.78
16:3:106:THR:OG1	16:3:109:ALA:HA	1.83	0.78
1:A:282:THR:HB	1:A:284:ARG:NH2	1.98	0.78
18:B:1138:CLA:HBB2	18:B:1138:CLA:C8	2.11	0.78
14:1:186:HIS:CB	14:1:188:ASN:O	2.32	0.78
16:3:84:LEU:HG	16:3:85:ILE:HA	1.63	0.78
15:2:21:GLY:N	15:2:22:SER:HB3	1.99	0.78
15:2:22:SER:N	15:2:25:GLY:N	2.32	0.78
16:3:73:ALA:HB1	18:3:3006:CLA:HBB	1.64	0.78
2:B:259:GLY:C	2:B:269:TRP:HE1	1.85	0.78
2:B:459:PHE:CZ	18:F:1302:CLA:O1D	2.37	0.78
2:B:591:THR:HG22	2:B:721:TYR:CE2	2.18	0.78
6:F:141:TYR:HD2	6:F:142:ARG:H	1.30	0.78
7:G:36:PRO:O	7:G:37:GLU:HB3	1.84	0.78
1:A:684:PHE:HE2	18:A:1140:CLA:HBB2	1.48	0.78
18:B:1202:CLA:H41	18:B:1221:CLA:O1A	1.84	0.78
2:B:311:PRO:O	18:B:1220:CLA:HMB3	1.83	0.78
2:B:218:TYR:CE2	2:B:253:ALA:O	2.36	0.78
2:B:176:ASN:ND2	2:B:292:ARG:H	1.82	0.78
2:B:720:THR:O	2:B:723:ALA:N	2.15	0.78
8:H:73:PRO:HB2	8:H:74:GLN:CA	2.14	0.78
15:2:177:ALA:O	18:2:2003:CLA:C2C	2.32	0.78
17:4:144:ALA:H	17:4:145:PRO:CD	1.96	0.78
1:A:330:ILE:O	1:A:333:ALA:HB2	1.84	0.78
1:A:609:ILE:O	1:A:611:VAL:O	2.02	0.78
2:B:119:GLY:HA3	2:B:371:LEU:HD12	1.65	0.78
2:B:393:PHE:CD2	2:B:398:TYR:HB2	2.18	0.78
8:H:42:THR:HG1	8:H:47:PHE:HE1	1.30	0.78
17:4:82:GLU:CG	17:4:83:TYR:H	1.96	0.78
1:A:103:PHE:HB2	1:A:140:PHE:HZ	1.48	0.78
1:A:326:GLY:HA3	1:A:330:ILE:HG13	1.63	0.78
2:B:330:ILE:CG2	18:B:1202:CLA:HAC1	2.13	0.78
2:B:290:MET:HA	18:B:1218:CLA:HBC2	0.81	0.78
6:F:52:ARG:HB3	6:F:56:TYR:CE1	2.18	0.78
1:A:493:GLN:HG3	1:A:515:TRP:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:OG1	1:A:52:THR:N	2.16	0.78
2:B:174:ARG:O	18:B:1221:CLA:HMD3	1.83	0.78
18:H:1501:CLA:HMA2	12:L:58:LEU:HB3	1.66	0.78
12:L:129:GLN:OE1	12:L:131:GLN:O	2.02	0.78
17:4:80:LYS:HD2	17:4:83:TYR:OH	1.84	0.78
2:B:73:ASN:ND2	2:B:108:GLY:HA3	1.99	0.78
4:D:79:ARG:HE	4:D:81:GLU:CD	1.87	0.78
5:E:35:LYS:CA	5:E:50:GLY:HA2	2.08	0.78
13:N:71:GLY:O	13:N:72:LYS:HB3	1.82	0.78
15:2:23:LEU:CD2	15:2:26:ASP:CA	2.62	0.77
17:4:72:VAL:H	17:4:73:PRO:CD	1.97	0.77
1:A:650:ASN:C	1:A:652:TRP:H	1.87	0.77
2:B:115:ASN:O	2:B:117:TYR:CE1	2.37	0.77
18:B:1212:CLA:H2	18:B:1212:CLA:HAA1	1.63	0.77
2:B:396:ARG:O	2:B:397:ASP:OD2	2.01	0.77
4:D:141:VAL:HG22	4:D:142:SER:N	1.98	0.77
5:E:65:VAL:HG23	5:E:83:ALA:CB	2.12	0.77
18:I:1204:CLA:HBB1	20:I:6018:BCR:HC32	1.65	0.77
13:N:57:LYS:CG	16:3:87:ALA:HB1	2.14	0.77
17:4:110:LYS:O	17:4:112:PRO:HD3	1.83	0.77
1:A:272:LEU:HD23	1:A:274:TRP:HE3	1.49	0.77
1:A:452:PHE:CD1	1:A:456:HIS:CE1	2.70	0.77
1:A:687:ALA:HB1	18:A:9013:CLA:HBB2	1.65	0.77
2:B:170:ASN:HD22	18:B:1209:CLA:HED2	1.48	0.77
4:D:19:GLU:N	4:D:20:LEU:HA	1.99	0.77
6:F:52:ARG:O	6:F:55:ASN:HB2	1.84	0.77
1:A:639:ALA:C	1:A:641:ASN:H	1.88	0.77
1:A:705:GLU:O	1:A:707:ILE:N	2.17	0.77
1:A:71:LEU:HD21	1:A:353:SER:CB	2.14	0.77
2:B:337:ALA:HB1	18:B:1202:CLA:OBD	1.85	0.77
2:B:170:ASN:ND2	18:B:1209:CLA:HED2	1.98	0.77
2:B:280:ILE:HA	18:B:1214:CLA:HMC3	1.65	0.77
1:A:353:SER:OG	1:A:354:TRP:CD1	2.37	0.77
1:A:679:PHE:CA	1:A:682:ALA:HB3	1.99	0.77
1:A:81:ALA:HB1	1:A:82:HIS:CA	2.13	0.77
18:B:1209:CLA:CGA	18:B:1209:CLA:C3A	2.63	0.77
2:B:74:PHE:HB3	2:B:132:ASN:HD21	1.46	0.77
4:D:79:ARG:HB3	4:D:81:GLU:HG3	1.67	0.77
12:L:119:THR:N	12:L:120:LEU:CA	2.30	0.77
1:A:735:VAL:O	1:A:739:LEU:CB	2.32	0.77
1:A:680:LEU:HB3	18:B:9012:CLA:C2	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:LEU:HD11	10:J:38:THR:HG21	1.67	0.77
14:1:184:PRO:O	14:1:185:TRP:HB2	1.83	0.77
1:A:485:GLN:HB3	1:A:486:PRO:HD3	1.67	0.77
1:A:554:LEU:O	1:A:554:LEU:HD22	1.85	0.77
2:B:631:LEU:HA	2:B:643:LEU:HD12	1.66	0.77
6:F:48:LYS:HE2	6:F:48:LYS:H	1.48	0.77
18:B:1207:CLA:HBB2	9:I:13:GLY:O	1.84	0.77
12:L:112:PRO:HB2	12:L:113:SER:HA	1.65	0.77
16:3:212:ASN:CB	16:3:214:LEU:H	1.96	0.77
1:A:450:CYS:SG	1:A:551:VAL:HG12	2.25	0.77
1:A:592:VAL:O	1:A:597:HIS:NE2	2.18	0.77
1:A:605:MET:O	1:A:609:ILE:N	2.18	0.77
2:B:431:PHE:O	2:B:435:GLY:N	2.18	0.77
2:B:463:ILE:HG22	2:B:464:GLN:N	2.00	0.77
5:E:74:TYR:N	5:E:74:TYR:HD2	1.83	0.77
6:F:47:GLU:HA	6:F:51:LYS:HG2	1.65	0.77
15:2:21:GLY:CA	15:2:25:GLY:O	2.29	0.77
16:3:200:ILE:O	16:3:204:VAL:HG22	1.85	0.77
18:A:1123:CLA:CHD	18:A:1123:CLA:HBC2	2.13	0.77
2:B:504:ASN:C	2:B:506:ASN:H	1.89	0.77
2:B:58:PHE:HE2	18:B:1241:CLA:HBB	1.50	0.77
14:1:85:LEU:O	14:1:87:ASN:HA	1.85	0.77
18:A:1137:CLA:CMC	18:L:1130:CLA:HMC3	2.15	0.77
1:A:81:ALA:HB3	1:A:82:HIS:C	2.05	0.77
18:A:9011:CLA:HBB2	18:B:9010:CLA:C1D	2.14	0.77
2:B:330:ILE:CG2	18:B:1202:CLA:CAC	2.63	0.77
2:B:387:PHE:O	2:B:391:PRO:CD	2.33	0.77
2:B:393:PHE:O	2:B:397:ASP:N	2.18	0.77
2:B:705:ALA:HB1	19:B:5002:PQN:C8	2.14	0.77
2:B:536:LYS:C	2:B:538:ALA:H	1.87	0.77
2:B:545:LYS:HA	2:B:548:PRO:HG3	1.67	0.77
2:B:657:TRP:HZ3	2:B:661:PHE:HE1	1.31	0.77
12:L:45:THR:HG23	12:L:126:GLN:NE2	1.99	0.77
12:L:85:SER:OG	12:L:151:VAL:HB	1.85	0.77
18:A:1140:CLA:HBC2	18:A:1140:CLA:HMC1	1.67	0.76
1:A:373:ALA:O	1:A:375:HIS:N	2.19	0.76
1:A:435:VAL:CG2	1:A:438:HIS:CE1	2.69	0.76
1:A:568:LEU:HD23	2:B:676:GLU:OE1	1.85	0.76
1:A:631:GLN:NE2	1:A:631:GLN:O	2.19	0.76
1:A:75:SER:CA	1:A:354:TRP:HZ2	1.98	0.76
18:B:1207:CLA:O2A	18:B:1207:CLA:H2A	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:TYR:HE2	18:B:9010:CLA:O1A	1.68	0.76
6:F:122:ASP:H	10:J:9:SER:HB2	1.50	0.76
6:F:1:ASP:H2	6:F:62:LEU:HD13	1.48	0.76
2:B:294:ASN:HA	7:G:37:GLU:OE1	1.85	0.76
15:2:22:SER:N	15:2:23:LEU:CB	2.48	0.76
15:2:26:ASP:CB	15:2:27:PHE:CD2	2.67	0.76
16:3:138:SER:H	16:3:139:MET:CB	1.97	0.76
1:A:101:ALA:HA	1:A:161:GLU:CD	2.05	0.76
1:A:543:HIS:NE2	18:A:1136:CLA:NA	2.33	0.76
2:B:378:ILE:HG22	2:B:382:ILE:HD12	1.67	0.76
2:B:382:ILE:O	2:B:384:THR:O	2.04	0.76
2:B:693:TRP:CD1	2:B:695:ASP:O	2.38	0.76
2:B:713:PHE:O	2:B:716:GLY:N	2.18	0.76
3:C:49:VAL:O	3:C:51:CYS:N	2.16	0.76
4:D:86:LEU:O	4:D:90:LEU:HG	1.85	0.76
13:N:60:PHE:CD2	13:N:60:PHE:N	2.43	0.76
13:N:82:PHE:N	13:N:82:PHE:HD2	1.82	0.76
17:4:114:SER:CB	17:4:120:ILE:HG12	2.14	0.76
1:A:197:GLN:HE22	1:A:352:THR:HG23	1.49	0.76
1:A:284:ARG:HD3	1:A:508:THR:HG1	1.50	0.76
18:B:1212:CLA:HBC3	18:B:1212:CLA:CHD	2.15	0.76
13:N:41:LYS:O	13:N:42:PHE:O	2.03	0.76
1:A:397:THR:HB	1:A:613:ILE:HG12	1.68	0.76
2:B:259:GLY:HA3	2:B:269:TRP:CZ2	2.19	0.76
2:B:657:TRP:NE1	2:B:717:TYR:HB2	2.00	0.76
3:C:20:ALA:O	3:C:22:PRO:HD2	1.85	0.76
3:C:12:ILE:HG12	3:C:28:MET:SD	2.26	0.76
3:C:27:GLU:H	3:C:43:PRO:CG	1.98	0.76
3:C:41:SER:OG	4:D:132:LEU:CD2	2.33	0.76
18:F:1303:CLA:C4B	20:F:6016:BCR:H403	2.15	0.76
14:1:112:ARG:CZ	14:1:113:SER:HA	2.15	0.76
15:2:37:ASP:HB3	15:2:38:PRO:HB2	1.68	0.76
16:3:209:PRO:HB2	16:3:211:GLN:H	1.46	0.76
17:4:59:LEU:CA	17:4:62:GLU:HB2	2.15	0.76
1:A:251:ASN:HD22	1:A:251:ASN:C	1.89	0.76
1:A:705:GLU:HA	1:A:708:VAL:HB	1.66	0.76
2:B:203:ARG:NH1	2:B:252:THR:HB	2.00	0.76
2:B:84:VAL:CG1	2:B:85:ARG:N	2.43	0.76
2:B:84:VAL:HG12	2:B:86:PRO:HD3	1.66	0.76
12:L:143:PHE:O	12:L:147:GLY:N	2.19	0.76
12:L:97:MET:C	12:L:97:MET:SD	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:THR:O	1:A:552:THR:OG1	2.04	0.76
1:A:547:PHE:HE1	1:A:551:VAL:CG1	1.98	0.76
1:A:751:LEU:HD13	1:A:752:ALA:H	1.51	0.76
18:B:1202:CLA:HBA1	18:B:1202:CLA:HBD	1.67	0.76
2:B:192:GLY:O	2:B:195:VAL:HB	1.85	0.76
7:G:20:ARG:CG	7:G:20:ARG:HH11	1.99	0.76
13:N:81:VAL:CB	13:N:82:PHE:CA	2.53	0.76
15:2:22:SER:N	15:2:23:LEU:HA	1.98	0.76
1:A:707:ILE:HG22	1:A:711:HIS:CE1	2.20	0.76
18:A:9011:CLA:HMC1	18:A:9011:CLA:HBC2	1.68	0.76
1:A:742:GLY:HA2	18:A:9011:CLA:O1D	1.85	0.76
2:B:205:GLU:O	2:B:207:VAL:N	2.18	0.76
2:B:479:SER:O	2:B:481:THR:N	2.18	0.76
2:B:553:PHE:CE1	3:C:63:LEU:HG	2.21	0.76
4:D:106:SER:O	4:D:107:GLY:O	2.04	0.76
6:F:144:LEU:CD1	20:F:6016:BCR:H332	2.16	0.76
7:G:27:GLN:O	7:G:28:ARG:HG2	1.86	0.76
18:L:1502:CLA:NC	20:L:6020:BCR:H271	2.01	0.76
13:N:2:VAL:HA	13:N:3:ILE:CG1	2.15	0.76
15:2:19:LEU:CG	15:2:20:ASP:OD2	2.30	0.76
15:2:21:GLY:N	15:2:23:LEU:HD22	1.99	0.76
18:A:1137:CLA:HBD	18:A:1137:CLA:CBA	2.14	0.76
2:B:68:VAL:CA	2:B:71:GLN:O	2.31	0.76
2:B:93:ASP:OD2	2:B:96:PHE:HE2	1.69	0.76
8:H:73:PRO:HB2	8:H:74:GLN:HA	1.68	0.76
1:A:435:VAL:HG12	1:A:436:LEU:HD23	1.65	0.76
1:A:71:LEU:HA	1:A:74:ILE:HG22	1.68	0.76
2:B:19:ARG:HA	2:B:22:TRP:CD1	2.21	0.76
2:B:536:LYS:C	2:B:538:ALA:N	2.36	0.76
4:D:111:TYR:HD1	4:D:111:TYR:N	1.82	0.76
15:2:26:ASP:HB3	15:2:27:PHE:CD2	2.21	0.76
1:A:195:TRP:CZ3	18:A:1118:CLA:C2C	2.69	0.76
6:F:65:SER:O	6:F:66:ASP:HB3	1.84	0.76
7:G:36:PRO:O	7:G:37:GLU:CB	2.34	0.76
15:2:159:LEU:O	15:2:162:LYS:HB3	1.84	0.75
15:2:194:ALA:CB	15:2:195:HIS:CA	2.64	0.75
15:2:26:ASP:CG	15:2:27:PHE:HB3	2.05	0.75
3:C:55:GLU:HB3	3:C:65:VAL:CG2	2.15	0.75
4:D:122:LYS:HA	4:D:123:VAL:HG12	1.67	0.75
6:F:136:TRP:N	6:F:136:TRP:CD1	2.53	0.75
6:F:17:ARG:NH2	6:F:66:ASP:OD1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:188:PRO:HB2	15:2:193:PHE:CD2	2.20	0.75
15:2:106:GLU:HG2	18:2:2012:CLA:C4C	2.16	0.75
18:A:1124:CLA:HHC	18:A:1137:CLA:O1A	1.85	0.75
18:B:1222:CLA:HBB2	18:B:1236:CLA:HHB	1.67	0.75
2:B:174:ARG:NE	18:B:1210:CLA:HHD	2.00	0.75
2:B:89:HIS:O	2:B:90:ALA:CB	2.34	0.75
4:D:150:GLY:HA2	4:D:151:LYS:C	2.06	0.75
14:1:186:HIS:HB3	14:1:188:ASN:O	1.85	0.75
1:A:268:PRO:O	1:A:269:PHE:HB3	1.85	0.75
1:A:283:PHE:CE2	18:A:1116:CLA:HHC	2.21	0.75
1:A:402:ILE:HD12	1:A:402:ILE:N	2.01	0.75
1:A:457:SER:HA	1:A:460:LEU:HD22	1.68	0.75
3:C:72:GLU:OE2	3:C:77:MET:HG3	1.86	0.75
7:G:77:ILE:CG2	7:G:77:ILE:O	2.34	0.75
12:L:162:ASP:C	12:L:164:PRO:HD2	2.05	0.75
15:2:17:GLU:HB3	15:2:19:LEU:N	2.00	0.75
15:2:21:GLY:N	15:2:23:LEU:HD21	2.00	0.75
18:A:1107:CLA:HMB3	10:J:27:ILE:HG12	1.69	0.75
1:A:133:ASN:HB2	1:A:142:GLY:HA2	1.67	0.75
1:A:64:PHE:CE1	18:A:1103:CLA:CMC	2.50	0.75
18:A:9013:CLA:C1	18:A:9013:CLA:HMA2	2.17	0.75
2:B:387:PHE:CE2	18:B:1242:CLA:HMC1	2.21	0.75
2:B:344:ILE:HG13	2:B:345:THR:N	2.01	0.75
2:B:549:ASP:HA	2:B:551:LYS:CG	2.15	0.75
4:D:45:PHE:C	4:D:45:PHE:CD1	2.56	0.75
6:F:100:VAL:HG11	6:F:125:LEU:HD22	1.66	0.75
12:L:37:LEU:HD22	12:L:37:LEU:H	1.51	0.75
15:2:86:GLU:OE2	17:4:187:SER:HB3	1.87	0.75
20:A:6011:BCR:H23C	20:A:6011:BCR:H403	1.68	0.75
2:B:100:ALA:HA	2:B:103:ALA:CB	2.16	0.75
18:B:1212:CLA:H3A	18:B:1212:CLA:CGA	2.16	0.75
2:B:458:ILE:H	18:B:1235:CLA:CMD	1.98	0.75
3:C:16:GLN:O	3:C:16:GLN:NE2	2.20	0.75
3:C:48:CYS:SG	3:C:49:VAL:O	2.45	0.75
6:F:45:THR:O	6:F:48:LYS:HG2	1.87	0.75
6:F:85:THR:HB	10:J:39:PHE:CD2	2.21	0.75
18:L:1503:CLA:O2D	18:L:1503:CLA:C1	2.34	0.75
6:F:124:PRO:HG2	6:F:125:LEU:CG	2.06	0.75
6:F:81:GLY:HA2	6:F:85:THR:H	1.50	0.75
9:I:9:VAL:HA	9:I:12:VAL:HG12	1.68	0.75
13:N:45:ASN:HD22	13:N:46:PHE:N	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:89:VAL:HB	14:1:90:PRO:CD	2.16	0.75
1:A:223:VAL:HA	1:A:227:LEU:HD12	1.68	0.75
1:A:629:ASN:OD1	1:A:633:VAL:O	2.05	0.75
1:A:478:SER:CB	1:A:647:ILE:HD13	2.16	0.75
2:B:439:HIS:CD2	18:B:1230:CLA:NC	2.54	0.75
2:B:392:ILE:HG22	2:B:393:PHE:N	2.02	0.75
2:B:547:MET:SD	2:B:550:LYS:HB3	2.27	0.75
6:F:45:THR:O	6:F:47:GLU:N	2.19	0.75
13:N:55:GLN:HG3	13:N:56:LYS:N	2.01	0.75
14:1:74:TRP:CZ3	14:1:81:GLN:HG3	2.22	0.75
18:A:1105:CLA:C2B	18:A:1107:CLA:HED2	2.17	0.75
1:A:396:PHE:O	1:A:396:PHE:CD2	2.38	0.75
1:A:754:ILE:O	1:A:755:ILE:CG1	2.35	0.75
5:E:89:GLU:HG2	5:E:90:VAL:O	1.85	0.75
6:F:115:THR:CG2	6:F:116:GLN:H	1.95	0.75
6:F:13:GLN:O	6:F:14:PHE:CB	2.35	0.75
6:F:25:LEU:O	6:F:28:SER:HB2	1.86	0.75
7:G:8:ILE:CG1	7:G:9:SER:N	2.49	0.75
8:H:44:ALA:N	8:H:45:ALA:HB2	2.02	0.75
14:1:90:PRO:HG2	14:1:92:GLY:HA2	1.69	0.75
2:B:345:THR:HB	2:B:379:ALA:HB2	1.68	0.75
4:D:111:TYR:O	4:D:115:LYS:HD3	1.87	0.75
2:B:451:LYS:HD2	10:J:35:ASP:OD1	1.87	0.75
12:L:165:TYR:HE1	18:L:1503:CLA:CBD	2.00	0.75
13:N:2:VAL:HA	13:N:3:ILE:CB	2.16	0.75
16:3:217:LEU:CA	16:3:218:ALA:HB3	2.15	0.74
17:4:137:ILE:HG23	17:4:141:LEU:HD23	1.69	0.74
1:A:289:PRO:HD3	1:A:295:TRP:CH2	2.20	0.74
1:A:458:PHE:CD2	1:A:458:PHE:C	2.60	0.74
1:A:489:ALA:HA	1:A:490:GLN:HB2	1.67	0.74
2:B:646:TRP:HA	2:B:649:MET:HB2	1.68	0.74
2:B:672:GLN:OE1	2:B:698:VAL:HB	1.86	0.74
3:C:17:CYS:SG	3:C:18:VAL:N	2.60	0.74
6:F:49:THR:O	6:F:53:PHE:N	2.20	0.74
7:G:21:PHE:HA	7:G:23:PHE:CG	2.21	0.74
1:A:112:ASP:O	1:A:113:PRO:O	2.04	0.74
1:A:446:LEU:O	1:A:449:VAL:CG1	2.31	0.74
2:B:33:SER:O	2:B:34:HIS:HD2	1.69	0.74
2:B:493:TRP:HB2	2:B:494:LEU:HD22	1.69	0.74
2:B:527:LEU:HD23	2:B:527:LEU:N	2.02	0.74
2:B:702:ILE:HD12	2:B:703:VAL:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:81:VAL:C	13:N:83:TRP:CD1	2.60	0.74
15:2:161:THR:CG2	15:2:165:LYS:HG3	2.14	0.74
16:3:132:ASP:CG	16:3:139:MET:HB2	2.08	0.74
18:A:1119:CLA:HBC2	18:A:1119:CLA:HHD	1.69	0.74
1:A:299:ILE:O	1:A:299:ILE:HG23	1.87	0.74
2:B:187:SER:O	2:B:190:TRP:N	2.20	0.74
5:E:39:LEU:O	5:E:86:GLU:HA	1.86	0.74
6:F:83:PHE:O	6:F:87:GLY:CA	2.36	0.74
7:G:22:VAL:C	7:G:23:PHE:HD2	1.90	0.74
14:1:70:LYS:HB3	14:1:73:GLU:HG3	1.69	0.74
1:A:558:LYS:O	1:A:562:PHE:HD1	1.70	0.74
1:A:625:TRP:HB2	1:A:637:ILE:CD1	2.14	0.74
1:A:687:ALA:CB	18:A:9013:CLA:CBB	2.59	0.74
2:B:454:LEU:CD1	2:B:614:THR:HG21	2.18	0.74
18:B:9022:CLA:NB	18:B:9023:CLA:HBB2	2.01	0.74
4:D:50:TRP:N	4:D:73:ASN:HB2	2.02	0.74
13:N:8:GLU:HG2	13:N:11:LYS:HB2	1.67	0.74
17:4:144:ALA:O	17:4:146:THR:N	2.20	0.74
2:B:344:ILE:CG1	18:B:1225:CLA:CAC	2.64	0.74
18:B:1227:CLA:H41	18:B:1228:CLA:H92	1.67	0.74
2:B:257:ILE:CD1	18:B:1214:CLA:HMB2	2.18	0.74
2:B:479:SER:C	2:B:481:THR:N	2.39	0.74
2:B:639:VAL:CG1	2:B:640:CYS:N	2.39	0.74
2:B:720:THR:OG1	18:B:9010:CLA:CGD	2.35	0.74
4:D:155:ASP:CB	4:D:156:LEU:HA	2.17	0.74
7:G:23:PHE:CD1	7:G:24:PHE:HB2	2.23	0.74
15:2:183:TYR:O	15:2:184:THR:HG22	1.87	0.74
1:A:158:ILE:O	1:A:163:GLN:NE2	2.19	0.74
1:A:198:ASP:CG	1:A:199:VAL:H	1.91	0.74
18:B:1239:CLA:CHA	19:B:5002:PQN:H251	2.18	0.74
4:D:44:GLU:OE1	4:D:110:GLN:NE2	2.20	0.74
6:F:18:GLU:C	6:F:20:GLN:H	1.90	0.74
13:N:8:GLU:CG	13:N:11:LYS:HB2	2.18	0.74
14:1:164:GLN:HA	14:1:167:ALA:HB3	1.70	0.74
14:1:70:LYS:CB	14:1:73:GLU:HG3	2.16	0.74
15:2:18:TRP:CD1	15:2:21:GLY:C	2.60	0.74
17:4:82:GLU:O	17:4:83:TYR:CD2	2.41	0.74
1:A:367:SER:O	1:A:371:VAL:HG22	1.87	0.74
2:B:101:VAL:CG2	2:B:102:GLU:H	1.99	0.74
18:B:1239:CLA:H11	19:B:5002:PQN:H271	1.70	0.74
2:B:391:PRO:HD3	2:B:538:ALA:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:ILE:CD1	2:B:590:VAL:HG21	2.17	0.74
1:A:588:GLY:CA	2:B:668:ARG:HD2	2.18	0.74
3:C:55:GLU:HG2	3:C:58:CYS:O	1.88	0.74
5:E:51:SER:OG	5:E:68:ARG:O	2.04	0.74
9:I:12:VAL:CG1	18:I:1204:CLA:O1A	2.35	0.74
18:A:1129:CLA:CMA	18:L:1130:CLA:OBD	2.36	0.74
18:A:1132:CLA:HHB	12:L:72:GLY:HA2	1.68	0.74
14:1:189:ILE:N	14:1:190:GLY:CA	2.51	0.74
15:2:23:LEU:HD22	15:2:26:ASP:N	1.99	0.74
18:A:1106:CLA:CBB	18:A:1126:CLA:H8	2.18	0.74
1:A:238:ASP:HB3	1:A:239:PRO:CD	2.12	0.74
1:A:364:MET:HG2	18:A:1123:CLA:HMA1	1.70	0.74
1:A:369:THR:HG23	1:A:402:ILE:O	1.88	0.74
1:A:492:ILE:N	1:A:493:GLN:HB3	2.02	0.74
12:L:123:ARG:O	12:L:125:LYS:N	2.20	0.74
12:L:53:GLY:HA3	12:L:139:PHE:CZ	2.23	0.74
12:L:62:PHE:N	12:L:150:GLY:O	2.21	0.74
15:2:21:GLY:HA2	15:2:23:LEU:CD2	2.06	0.74
13:N:58:VAL:CB	16:3:86:PRO:O	2.36	0.74
1:A:478:SER:HB2	1:A:647:ILE:HD13	1.68	0.74
1:A:700:TRP:HH2	18:A:9013:CLA:O1D	1.69	0.74
12:L:137:ALA:C	12:L:138:LYS:HZ2	1.91	0.74
15:2:22:SER:N	15:2:25:GLY:CA	2.51	0.74
17:4:120:ILE:HA	17:4:121:PHE:CD2	2.23	0.74
18:4:1304:CLA:CAA	18:4:1304:CLA:C2	2.64	0.74
1:A:171:ALA:HA	1:A:174:PHE:HB3	1.69	0.74
1:A:463:HIS:NE2	1:A:467:MET:SD	2.61	0.74
1:A:625:TRP:CB	1:A:637:ILE:HD11	2.13	0.74
2:B:428:PHE:CG	18:B:1229:CLA:OBD	2.41	0.74
4:D:111:TYR:H	4:D:111:TYR:HD1	1.33	0.74
15:2:187:GLY:C	15:2:189:ILE:H	1.91	0.73
17:4:63:VAL:HG12	17:4:67:ILE:N	2.02	0.73
1:A:126:ILE:CD1	10:J:27:ILE:CG2	2.60	0.73
1:A:583:GLY:N	1:A:589:THR:OG1	2.21	0.73
1:A:697:ARG:NH2	1:A:724:ALA:O	2.20	0.73
2:B:311:PRO:HD2	18:B:1220:CLA:CMA	2.11	0.73
3:C:12:ILE:HG22	3:C:13:GLY:HA2	1.70	0.73
4:D:60:MET:SD	4:D:66:ALA:HB2	2.27	0.73
17:4:113:GLY:O	17:4:114:SER:HB2	1.88	0.73
1:A:435:VAL:CG2	1:A:438:HIS:HE1	2.01	0.73
18:A:1126:CLA:C1C	20:A:6011:BCR:HC42	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ARG:CG	2:B:4:ARG:HH11	2.01	0.73
2:B:589:TRP:CD1	2:B:592:PHE:HE2	2.02	0.73
1:A:453:LEU:HD13	1:A:547:PHE:HA	1.69	0.73
1:A:527:VAL:HG13	1:A:528:ALA:N	2.03	0.73
1:A:735:VAL:CG1	1:A:736:THR:N	2.52	0.73
1:A:735:VAL:O	1:A:739:LEU:HB2	1.87	0.73
2:B:395:ILE:HG12	2:B:551:LYS:HA	1.69	0.73
2:B:698:VAL:HG12	3:C:79:LEU:CD2	2.12	0.73
4:D:123:VAL:H	4:D:127:ARG:HH12	1.35	0.73
7:G:8:ILE:CD1	7:G:9:SER:H	2.00	0.73
7:G:90:SER:H	7:G:93:TYR:N	1.86	0.73
13:N:58:VAL:CG2	13:N:59:PRO:CA	2.47	0.73
14:1:150:ASN:HD22	14:1:153:LEU:HD23	1.52	0.73
1:A:366:GLY:O	1:A:369:THR:N	2.20	0.73
1:A:404:GLY:O	1:A:405:PHE:C	2.27	0.73
1:A:527:VAL:CG1	1:A:528:ALA:N	2.52	0.73
18:B:1237:CLA:HAC1	18:B:1238:CLA:CHC	2.18	0.73
4:D:26:SER:CB	4:D:69:ARG:HB2	2.17	0.73
6:F:81:GLY:O	6:F:86:PRO:HD3	1.87	0.73
17:4:55:VAL:O	17:4:59:LEU:HB2	1.88	0.73
1:A:223:VAL:CG2	1:A:224:HIS:HD2	1.98	0.73
1:A:486:PRO:HD2	1:A:487:VAL:HB	1.70	0.73
1:A:64:PHE:CA	1:A:67:HIS:HB2	2.15	0.73
18:B:1216:CLA:HAA2	18:B:1221:CLA:CBB	2.17	0.73
2:B:335:GLY:O	2:B:339:ALA:HB2	1.89	0.73
2:B:265:THR:HA	2:B:360:PHE:CE2	2.24	0.73
3:C:27:GLU:OE1	3:C:43:PRO:HB3	1.88	0.73
1:A:715:LYS:NZ	6:F:153:ASN:HD21	1.87	0.73
6:F:89:LEU:O	6:F:93:ILE:N	2.20	0.73
18:L:1502:CLA:H2A	18:L:1502:CLA:O1D	1.87	0.73
7:G:8:ILE:HD13	14:1:95:PRO:HB3	1.71	0.73
16:3:116:VAL:O	16:3:117:LEU:HD12	1.89	0.73
1:A:520:LEU:HD22	1:A:521:VAL:H	1.51	0.73
2:B:317:ARG:HD3	2:B:407:VAL:CG1	2.19	0.73
4:D:112:LEU:CG	4:D:113:HIS:CE1	2.67	0.73
1:A:511:THR:HB	1:A:515:TRP:HZ2	1.54	0.73
18:B:1220:CLA:OBD	18:B:1221:CLA:CBB	2.37	0.73
2:B:346:SER:OG	18:B:1222:CLA:OBD	2.04	0.73
2:B:573:TRP:CZ3	2:B:703:VAL:HG22	2.23	0.73
8:H:65:LEU:O	8:H:69:SER:N	2.22	0.73
9:I:16:PHE:HB3	9:I:17:PRO:HD3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:107:PHE:HD2	12:L:133:ALA:HB2	1.53	0.73
20:I:6018:BCR:H371	20:L:6020:BCR:C34	2.18	0.73
1:A:493:GLN:HG3	1:A:515:TRP:HB3	1.69	0.73
1:A:679:PHE:CB	1:A:745:THR:HA	2.18	0.73
2:B:598:HIS:HB3	2:B:602:TRP:CH2	2.24	0.73
5:E:44:TYR:HE1	5:E:74:TYR:HE2	1.37	0.73
6:F:4:GLY:CA	6:F:5:LEU:HB2	2.19	0.73
13:N:75:TYR:CE2	13:N:76:LYS:HD3	2.23	0.73
14:1:188:ASN:HB3	14:1:190:GLY:N	2.04	0.73
15:2:22:SER:N	15:2:25:GLY:HA2	2.02	0.73
17:4:102:GLU:O	17:4:105:ARG:HD2	1.88	0.73
1:A:160:SER:O	1:A:163:GLN:CB	2.36	0.73
1:A:493:GLN:C	1:A:496:HIS:HB2	2.09	0.73
1:A:497:ALA:HB2	1:A:516:GLY:HA2	1.70	0.73
1:A:578:ARG:HA	1:A:595:TRP:CB	2.19	0.73
12:L:86:LEU:C	12:L:88:ALA:H	1.92	0.73
15:2:179:PHE:C	15:2:179:PHE:CD1	2.62	0.72
1:A:594:ALA:O	1:A:598:VAL:N	2.19	0.72
1:A:611:VAL:O	1:A:612:VAL:HB	1.85	0.72
1:A:462:ILE:H	1:A:649:ILE:HD12	1.52	0.72
2:B:273:VAL:HG11	18:B:1215:CLA:HMA3	1.69	0.72
3:C:42:ALA:C	3:C:44:ARG:N	2.39	0.72
3:C:63:LEU:HD22	3:C:64:SER:H	1.51	0.72
5:E:37:LYS:HE3	5:E:47:LYS:HD3	1.69	0.72
5:E:74:TYR:N	5:E:74:TYR:CD2	2.57	0.72
6:F:68:LEU:HD12	6:F:69:PRO:HD2	1.71	0.72
16:3:133:TRP:O	16:3:137:GLY:N	2.22	0.72
16:3:67:MET:HB2	18:3:3005:CLA:C2C	2.19	0.72
1:A:568:LEU:HA	4:D:79:ARG:NH1	2.03	0.72
1:A:679:PHE:HB3	1:A:745:THR:HA	1.71	0.72
2:B:355:LEU:HD21	18:B:1214:CLA:CED	2.19	0.72
5:E:35:LYS:HA	5:E:50:GLY:CA	2.08	0.72
20:I:6018:BCR:C23	20:L:6020:BCR:H342	2.19	0.72
14:1:103:LEU:HA	14:1:106:ALA:CB	2.18	0.72
1:A:526:LYS:HA	1:A:627:THR:CA	2.19	0.72
1:A:700:TRP:CH2	19:A:5001:PQN:H2M3	2.23	0.72
2:B:287:GLY:HA2	18:B:1218:CLA:CMC	2.14	0.72
3:C:60:THR:HA	5:E:80:ASN:ND2	2.03	0.72
6:F:133:GLY:O	6:F:136:TRP:CD1	2.43	0.72
2:B:98:GLN:OE1	8:H:79:ILE:N	2.21	0.72
2:B:159:PRO:HA	2:B:162:LYS:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ARG:O	2:B:23:PHE:C	2.27	0.72
2:B:378:ILE:CG2	2:B:382:ILE:HG13	2.18	0.72
1:A:309:LEU:O	1:A:310:PHE:HB2	1.89	0.72
1:A:340:GLY:C	1:A:342:GLY:H	1.92	0.72
1:A:684:PHE:C	1:A:684:PHE:HD2	1.93	0.72
2:B:284:PHE:O	2:B:288:GLY:N	2.23	0.72
2:B:348:VAL:HG21	18:B:1225:CLA:CMD	2.14	0.72
7:G:83:TYR:HA	7:G:85:ILE:H	1.51	0.72
17:4:136:GLY:HA3	17:4:139:ASN:O	1.89	0.72
17:4:42:GLN:O	17:4:46:VAL:N	2.22	0.72
1:A:204:ASN:OD1	1:A:315:HIS:HA	1.88	0.72
1:A:606:TYR:O	1:A:610:SER:CB	2.33	0.72
1:A:681:GLY:O	20:A:6011:BCR:H351	1.88	0.72
18:B:1202:CLA:H2	18:B:1210:CLA:C4D	2.18	0.72
2:B:276:HIS:HA	18:B:1214:CLA:C3B	2.19	0.72
2:B:304:ILE:HG22	2:B:305:LEU:H	1.55	0.72
2:B:626:LEU:O	2:B:627:ASN:HB2	1.88	0.72
7:G:34:GLN:HE21	7:G:36:PRO:HG3	1.54	0.72
1:A:105:ASN:HB3	1:A:150:PHE:CE2	2.23	0.72
1:A:461:TYR:CB	1:A:649:ILE:HG13	2.20	0.72
1:A:569:ILE:O	1:A:569:ILE:CG2	2.37	0.72
1:A:572:LYS:O	1:A:574:ASN:N	2.22	0.72
1:A:656:PHE:O	1:A:657:LEU:HD23	1.90	0.72
1:A:687:ALA:C	1:A:689:SER:H	1.92	0.72
2:B:331:HIS:O	2:B:332:PHE:HB2	1.87	0.72
2:B:410:ARG:HA	2:B:413:GLU:OE2	1.88	0.72
3:C:35:LYS:HG3	3:C:35:LYS:O	1.89	0.72
4:D:52:SER:HB3	4:D:73:ASN:HD21	1.54	0.72
6:F:136:TRP:CG	6:F:137:PRO:CD	2.66	0.72
6:F:18:GLU:O	6:F:20:GLN:N	2.22	0.72
6:F:22:LEU:HD22	6:F:49:THR:HG21	1.72	0.72
6:F:22:LEU:O	6:F:23:LYS:HB2	1.89	0.72
1:A:185:HIS:CG	1:A:186:TYR:N	2.58	0.72
1:A:389:TYR:CE2	1:A:625:TRP:CD1	2.78	0.72
1:A:81:ALA:CB	1:A:82:HIS:CA	2.66	0.72
18:B:1222:CLA:HAA1	18:B:1236:CLA:HED1	1.72	0.72
2:B:22:TRP:CH2	18:B:1238:CLA:HMB1	2.25	0.72
3:C:27:GLU:HG2	3:C:28:MET:N	2.05	0.72
6:F:80:TRP:NE1	18:F:1302:CLA:HBC2	2.02	0.72
15:2:179:PHE:CE1	15:2:180:GLN:HG2	2.25	0.72
1:A:250:LEU:HD23	1:A:251:ASN:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:682:HIS:HE1	18:B:1238:CLA:HAC1	1.54	0.72
2:B:303:TYR:HD2	2:B:307:ALA:HB2	1.53	0.72
2:B:635:ILE:H	2:B:636:THR:HG22	1.54	0.72
2:B:74:PHE:HD1	2:B:121:TYR:CZ	2.07	0.72
4:D:111:TYR:CD1	4:D:111:TYR:N	2.53	0.72
7:G:35:VAL:HG13	7:G:36:PRO:HA	1.70	0.72
10:J:26:LEU:O	10:J:29:ILE:HG22	1.90	0.72
15:2:161:THR:HG23	15:2:165:LYS:CG	2.17	0.72
1:A:347:TYR:HD2	1:A:349:ILE:N	1.88	0.72
2:B:176:ASN:CB	2:B:291:TYR:HD1	2.03	0.72
1:A:437:ARG:O	4:D:32:SER:OG	2.08	0.72
7:G:67:ASN:O	7:G:71:VAL:CG2	2.38	0.72
7:G:83:TYR:H	7:G:85:ILE:H	1.36	0.72
12:L:63:LEU:HD21	18:L:1502:CLA:CMB	2.03	0.72
18:A:1106:CLA:HBB2	18:A:1126:CLA:H8	1.72	0.71
1:A:120:ALA:H	1:A:145:ILE:HG21	1.53	0.71
1:A:390:ALA:O	1:A:391:THR:HG23	1.90	0.71
2:B:104:PHE:HB2	2:B:112:PRO:C	2.11	0.71
2:B:280:ILE:HA	18:B:1214:CLA:CMC	2.19	0.71
2:B:378:ILE:CG2	2:B:382:ILE:CD1	2.67	0.71
2:B:697:PRO:HB3	18:B:1238:CLA:C2C	2.19	0.71
7:G:37:GLU:CB	7:G:43:HIS:HE1	2.03	0.71
14:1:39:TYR:O	14:1:40:LYS:HB3	1.89	0.71
15:2:46:GLN:HA	15:2:49:LEU:HB3	1.73	0.71
2:B:170:ASN:ND2	18:B:1209:CLA:CED	2.53	0.71
2:B:332:PHE:H	2:B:335:GLY:N	1.87	0.71
2:B:694:ARG:NE	9:I:29:GLU:OE1	2.23	0.71
2:B:714:SER:HA	2:B:717:TYR:HB3	1.70	0.71
7:G:10:LEU:O	7:G:13:GLY:N	2.23	0.71
2:B:451:LYS:HD3	10:J:35:ASP:OD1	1.90	0.71
12:L:49:PRO:O	12:L:52:ARG:N	2.22	0.71
13:N:22:LEU:HG	13:N:24:THR:OG1	1.90	0.71
15:2:103:GLY:HA2	18:2:2012:CLA:C3C	2.19	0.71
17:4:142:ASN:O	17:4:143:PHE:HB2	1.88	0.71
1:A:575:LEU:HB3	1:A:579:PHE:HB2	1.70	0.71
2:B:177:HIS:HE1	18:B:1209:CLA:C3C	2.03	0.71
2:B:317:ARG:CG	2:B:317:ARG:HH21	2.00	0.71
4:D:149:THR:HB	4:D:152:GLN:C	2.10	0.71
4:D:43:GLU:O	4:D:44:GLU:HB2	1.88	0.71
10:J:11:ALA:HB1	10:J:12:PRO:CD	2.18	0.71
1:A:64:PHE:O	1:A:420:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:N	1:A:44:ILE:HD13	2.05	0.71
1:A:493:GLN:CG	1:A:515:TRP:HB2	2.21	0.71
2:B:174:ARG:CZ	18:B:1210:CLA:HHD	2.20	0.71
2:B:343:VAL:HG12	2:B:347:LEU:HD13	1.73	0.71
2:B:400:PRO:O	2:B:404:ALA:HB2	1.90	0.71
16:3:214:LEU:HG	16:3:215:ASP:HB3	1.72	0.71
17:4:156:ASN:H	17:4:156:ASN:ND2	1.88	0.71
18:A:1137:CLA:HBD	18:A:1137:CLA:HBA1	1.72	0.71
1:A:688:PHE:CZ	18:A:1140:CLA:C2C	2.73	0.71
1:A:158:ILE:C	1:A:163:GLN:HE22	1.94	0.71
1:A:387:THR:HA	1:A:527:VAL:O	1.91	0.71
1:A:49:ASP:O	1:A:721:GLN:HB2	1.89	0.71
1:A:728:VAL:HA	1:A:731:ARG:HG3	1.71	0.71
12:L:165:TYR:HE1	18:L:1503:CLA:HBD	1.54	0.71
18:4:1304:CLA:H2	18:4:1304:CLA:HAA2	1.69	0.71
1:A:553:VAL:CG1	1:A:556:LEU:HD12	2.21	0.71
1:A:71:LEU:HD11	1:A:352:THR:CG2	2.18	0.71
18:B:1227:CLA:CMB	18:B:1228:CLA:C4D	2.65	0.71
2:B:117:TYR:HE2	2:B:366:THR:HG1	1.31	0.71
1:A:709:TRP:CZ3	2:B:417:ALA:HA	2.25	0.71
1:A:552:THR:O	1:A:556:LEU:HG	1.90	0.71
2:B:200:PRO:HB2	2:B:207:VAL:HG11	1.73	0.71
2:B:338:LEU:H	2:B:338:LEU:HD12	1.55	0.71
2:B:57:ILE:O	2:B:60:TRP:HB3	1.91	0.71
2:B:591:THR:CG2	2:B:721:TYR:HE2	2.04	0.71
1:A:604:TRP:HE1	18:B:9023:CLA:CHD	2.03	0.71
5:E:40:ARG:NH2	5:E:62:ARG:NH2	2.39	0.71
14:1:89:VAL:CB	14:1:90:PRO:CD	2.69	0.71
15:2:178:TRP:HA	15:2:179:PHE:HD1	1.53	0.71
15:2:178:TRP:CB	15:2:183:TYR:CE2	2.74	0.71
1:A:55:TRP:CZ3	18:A:1140:CLA:HMD2	2.26	0.71
1:A:149:PHE:HA	1:A:152:ILE:HB	1.72	0.71
1:A:299:ILE:HG23	1:A:303:HIS:CD2	2.25	0.71
1:A:398:HIS:HB2	18:A:1126:CLA:C1B	2.21	0.71
1:A:684:PHE:C	1:A:684:PHE:CD2	2.64	0.71
2:B:117:TYR:CD2	2:B:366:THR:OG1	2.44	0.71
6:F:144:LEU:HB3	6:F:145:LEU:HG	1.72	0.71
12:L:91:LEU:HD13	20:L:6020:BCR:H333	1.72	0.71
14:1:9:PRO:O	14:1:10:ARG:CB	2.38	0.71
17:4:180:ASP:N	17:4:185:HIS:CE1	2.55	0.71
1:A:377:TYR:CD2	1:A:396:PHE:CE1	2.79	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:ILE:HG21	18:B:1202:CLA:HAC1	1.72	0.71
2:B:67:HIS:NE2	2:B:89:HIS:CB	2.54	0.71
3:C:10:THR:HG21	5:E:63:TYR:CE2	2.26	0.71
8:H:73:PRO:HG3	9:I:3:ASN:OD1	1.91	0.71
15:2:17:GLU:OE1	15:2:18:TRP:HB2	1.90	0.71
15:2:185:GLY:C	15:2:187:GLY:HA3	2.11	0.71
1:A:402:ILE:H	1:A:402:ILE:CD1	2.04	0.71
1:A:356:ALA:N	1:A:421:ASP:OD1	2.24	0.71
1:A:54:ILE:HG22	1:A:54:ILE:O	1.91	0.71
1:A:615:HIS:C	1:A:615:HIS:CD2	2.63	0.71
1:A:40:PHE:CZ	1:A:61:ALA:HA	2.26	0.71
2:B:428:PHE:CD2	2:B:432:HIS:NE2	2.59	0.71
2:B:439:HIS:HA	2:B:442:VAL:HB	1.71	0.71
2:B:56:ILE:O	2:B:60:TRP:N	2.24	0.71
5:E:39:LEU:CD2	5:E:88:GLU:OE2	2.38	0.71
6:F:93:ILE:O	6:F:96:TRP:NE1	2.24	0.71
1:A:33:GLN:OE1	18:A:1109:CLA:CHC	2.38	0.70
1:A:590:CYS:O	1:A:591:GLN:C	2.28	0.70
1:A:684:PHE:CE2	18:A:1140:CLA:HBB2	2.26	0.70
2:B:372:TYR:HD2	2:B:373:THR:N	1.88	0.70
13:N:57:LYS:CB	13:N:58:VAL:HA	2.21	0.70
15:2:17:GLU:C	15:2:17:GLU:OE2	2.30	0.70
1:A:218:TRP:O	1:A:222:GLN:N	2.22	0.70
2:B:411:MET:HE3	2:B:411:MET:HA	1.73	0.70
2:B:428:PHE:HB2	18:B:1229:CLA:O1D	1.91	0.70
2:B:678:LEU:O	2:B:682:HIS:CD2	2.43	0.70
12:L:127:PRO:O	12:L:128:ASP:HB2	1.89	0.70
1:A:141:ARG:HB3	1:A:141:ARG:HH11	1.51	0.70
1:A:152:ILE:HA	1:A:382:TYR:CD2	2.26	0.70
1:A:522:ALA:HA	1:A:528:ALA:HB3	1.71	0.70
1:A:64:PHE:O	1:A:66:SER:N	2.24	0.70
2:B:428:PHE:CD2	18:B:1229:CLA:OBD	2.44	0.70
2:B:585:ASN:HB2	18:B:9012:CLA:HBC2	1.72	0.70
3:C:34:CYS:SG	3:C:38:GLN:HG2	2.31	0.70
4:D:26:SER:N	4:D:27:PRO:O	2.24	0.70
4:D:72:PRO:HD2	4:D:73:ASN:ND2	2.05	0.70
12:L:148:VAL:HA	12:L:151:VAL:HG23	1.71	0.70
18:B:1202:CLA:H2	18:B:1210:CLA:CHA	2.21	0.70
18:B:1236:CLA:H2A	18:B:1236:CLA:HED3	1.72	0.70
2:B:174:ARG:HH21	18:B:1210:CLA:HHD	1.53	0.70
2:B:388:ALA:O	2:B:390:GLY:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:HIS:HD2	18:B:1230:CLA:NC	1.89	0.70
2:B:415:LYS:HE3	2:B:540:ASP:HB2	1.73	0.70
8:H:92:ARG:H	8:H:93:GLY:HA3	1.55	0.70
12:L:57:GLY:HA3	12:L:143:PHE:HA	1.72	0.70
13:N:2:VAL:HA	13:N:3:ILE:HB	1.73	0.70
16:3:54:TRP:HB2	16:3:55:LEU:HA	0.79	0.70
1:A:385:LEU:O	1:A:388:ASP:N	2.24	0.70
2:B:276:HIS:HA	18:B:1214:CLA:C2B	2.21	0.70
2:B:3:LEU:O	2:B:14:GLN:HA	1.92	0.70
2:B:304:ILE:CG2	2:B:305:LEU:N	2.54	0.70
4:D:135:ARG:CG	4:D:139:LYS:HD3	2.17	0.70
9:I:26:LEU:O	9:I:28:VAL:HG23	1.91	0.70
14:1:83:THR:O	14:1:84:TYR:HB2	1.92	0.70
15:2:70:LYS:HE2	15:2:193:PHE:CE1	2.25	0.70
1:A:245:PRO:HA	1:A:248:PHE:CE1	2.27	0.70
1:A:407:ILE:HG13	18:A:1124:CLA:C2D	2.21	0.70
1:A:462:ILE:HD12	1:A:649:ILE:HD13	1.72	0.70
2:B:679:ALA:O	2:B:680:TRP:HB2	1.91	0.70
6:F:102:ARG:HH11	6:F:103:SER:HB2	1.56	0.70
2:B:98:GLN:HB2	8:H:78:PRO:CB	2.20	0.70
9:I:25:PHE:HB3	9:I:26:LEU:HD13	1.71	0.70
1:A:305:ALA:CB	18:A:1115:CLA:HMA1	2.10	0.70
18:A:1133:CLA:HHC	18:A:1134:CLA:C2B	2.21	0.70
1:A:126:ILE:HG22	1:A:129:GLN:HG3	1.72	0.70
2:B:549:ASP:CA	2:B:551:LYS:HG2	2.21	0.70
2:B:530:THR:HG21	2:B:583:MET:CB	2.19	0.70
2:B:652:PHE:CE1	2:B:656:VAL:CG2	2.74	0.70
18:B:9010:CLA:O2A	18:B:9012:CLA:HMD3	1.92	0.70
2:B:546:LEU:HD21	5:E:74:TYR:HE1	1.55	0.70
8:H:22:ASP:C	8:H:24:TYR:H	1.95	0.70
4:D:32:SER:HA	12:L:23:LEU:HD21	1.73	0.70
12:L:65:VAL:HG13	18:L:1503:CLA:HMA3	1.73	0.70
16:3:128:ARG:O	16:3:132:ASP:HB2	1.92	0.70
17:4:56:ALA:HA	17:4:59:LEU:HB3	1.74	0.70
1:A:367:SER:HA	1:A:370:ILE:HG23	1.72	0.70
1:A:654:ARG:HH11	1:A:655:ASP:CB	2.01	0.70
2:B:428:PHE:HA	2:B:432:HIS:CD2	2.27	0.70
2:B:51:PHE:O	2:B:53:GLN:N	2.24	0.70
4:D:42:VAL:O	4:D:44:GLU:N	2.24	0.70
4:D:50:TRP:CD1	4:D:51:GLU:C	2.65	0.70
8:H:49:LYS:HD3	8:H:50:ARG:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1132:CLA:CHB	12:L:72:GLY:HA2	2.21	0.70
15:2:17:GLU:C	15:2:18:TRP:O	2.29	0.70
18:A:1103:CLA:H2A	18:A:1103:CLA:O2D	1.90	0.70
18:B:1208:CLA:HED3	18:B:1208:CLA:H2A	1.72	0.70
2:B:559:CYS:SG	2:B:702:ILE:HG12	2.31	0.70
4:D:108:GLU:CG	4:D:109:VAL:HG22	2.22	0.70
7:G:8:ILE:HD12	7:G:9:SER:H	1.56	0.70
12:L:103:GLY:O	12:L:104:ILE:HG13	1.90	0.70
15:2:23:LEU:CB	15:2:26:ASP:O	2.40	0.70
1:A:62:HIS:O	1:A:63:ASP:O	2.10	0.70
2:B:40:GLY:O	2:B:42:LEU:N	2.25	0.70
12:L:47:VAL:HG22	12:L:48:ASN:HB3	1.72	0.70
14:1:82:ALA:N	14:1:83:THR:CA	2.55	0.69
16:3:126:GLU:O	16:3:130:LEU:HG	1.91	0.69
1:A:123:VAL:N	1:A:133:ASN:HD22	1.83	0.69
1:A:393:LEU:HG	1:A:394:SER:H	1.56	0.69
2:B:543:GLY:O	2:B:544:SER:HB3	1.91	0.69
2:B:718:ILE:O	2:B:722:ALA:HB2	1.92	0.69
2:B:729:THR:HA	2:B:732:LYS:O	1.91	0.69
1:A:604:TRP:HE1	18:B:9023:CLA:C1D	2.04	0.69
5:E:51:SER:HB2	5:E:69:PHE:HD2	1.56	0.69
8:H:56:PHE:O	8:H:57:LEU:HD23	1.92	0.69
10:J:6:THR:O	10:J:7:TYR:HB2	1.92	0.69
15:2:19:LEU:CG	15:2:22:SER:OG	2.40	0.69
15:2:27:PHE:HE1	15:2:30:ASP:H	1.39	0.69
17:4:156:ASN:N	17:4:156:ASN:ND2	2.39	0.69
1:A:62:HIS:ND1	18:A:1128:CLA:O1A	2.25	0.69
1:A:246:HIS:HA	18:A:1147:CLA:C1D	2.22	0.69
1:A:315:HIS:ND1	18:A:1108:CLA:HMA3	2.06	0.69
1:A:335:LYS:O	1:A:342:GLY:HA2	1.92	0.69
1:A:534:LEU:H	1:A:534:LEU:HD13	1.57	0.69
2:B:531:THR:O	2:B:533:ILE:N	2.25	0.69
2:B:544:SER:OG	2:B:545:LYS:N	2.22	0.69
2:B:596:TRP:HE1	2:B:608:GLN:NE2	1.90	0.69
8:H:49:LYS:O	8:H:50:ARG:NH1	2.25	0.69
12:L:54:VAL:O	12:L:58:LEU:HB2	1.91	0.69
15:2:18:TRP:O	15:2:19:LEU:C	2.29	0.69
2:B:345:THR:HG23	18:B:1225:CLA:HMC1	1.73	0.69
2:B:291:TYR:CD2	2:B:299:HIS:HB2	2.27	0.69
2:B:77:TRP:NE1	2:B:81:PRO:HA	2.08	0.69
4:D:96:ILE:CG1	4:D:97:LYS:N	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:9:SER:OG	10:J:10:VAL:N	2.23	0.69
12:L:163:LEU:N	12:L:164:PRO:CD	2.54	0.69
13:N:2:VAL:HB	13:N:4:GLU:HB2	1.72	0.69
13:N:54:LYS:HD2	13:N:54:LYS:N	2.06	0.69
17:4:96:ILE:HG23	17:4:97:LEU:N	2.07	0.69
1:A:112:ASP:CG	1:A:112:ASP:O	2.31	0.69
1:A:250:LEU:HA	18:A:1113:CLA:O2D	1.91	0.69
1:A:87:SER:O	1:A:91:LEU:HB2	1.92	0.69
2:B:415:LYS:HB2	2:B:539:LEU:HD21	1.75	0.69
2:B:440:ASN:ND2	2:B:614:THR:O	2.23	0.69
2:B:463:ILE:N	2:B:463:ILE:HD12	2.06	0.69
2:B:59:LEU:CD2	2:B:59:LEU:O	2.40	0.69
3:C:12:ILE:HG21	3:C:28:MET:SD	2.31	0.69
3:C:63:LEU:HD22	3:C:65:VAL:H	1.57	0.69
4:D:50:TRP:HD1	4:D:51:GLU:C	1.93	0.69
6:F:115:THR:CG2	6:F:116:GLN:N	2.55	0.69
12:L:107:PHE:HA	12:L:133:ALA:HB2	1.75	0.69
15:2:26:ASP:CB	15:2:27:PHE:HD2	2.05	0.69
16:3:85:ILE:N	16:3:86:PRO:HD3	2.06	0.69
1:A:696:GLY:HA2	2:B:569:ASP:OD2	1.91	0.69
1:A:679:PHE:HB2	1:A:745:THR:HG22	1.74	0.69
1:A:86:LEU:HD21	1:A:90:PHE:CE2	2.27	0.69
1:A:97:TYR:CE2	1:A:153:TRP:HE3	2.09	0.69
18:B:1216:CLA:O2A	18:B:1220:CLA:C1	2.36	0.69
2:B:64:ASN:CA	2:B:67:HIS:HB2	2.22	0.69
12:L:160:VAL:O	12:L:161:LEU:O	2.11	0.69
15:2:180:GLN:O	15:2:182:ILE:HD13	1.92	0.69
15:2:189:ILE:CA	15:2:191:ASN:H	1.95	0.69
16:3:134:TYR:C	16:3:136:PRO:HD2	2.11	0.69
1:A:690:LEU:HD13	1:A:690:LEU:H	1.58	0.69
1:A:685:VAL:O	1:A:741:GLY:HA2	1.92	0.69
4:D:86:LEU:HA	4:D:89:ARG:CB	2.22	0.69
8:H:39:PHE:N	8:H:41:GLU:O	2.24	0.69
18:L:1503:CLA:H11	18:L:1503:CLA:HED1	1.74	0.69
12:L:87:ALA:O	12:L:90:GLY:CA	2.40	0.69
1:A:373:ALA:C	1:A:375:HIS:H	1.92	0.69
1:A:395:LEU:O	1:A:397:THR:N	2.25	0.69
2:B:104:PHE:HA	2:B:106:ARG:CD	2.23	0.69
18:B:1227:CLA:HMB2	18:B:1228:CLA:CHA	2.22	0.69
2:B:530:THR:O	2:B:530:THR:HG22	1.91	0.69
7:G:43:HIS:CD2	7:G:43:HIS:N	2.60	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:58:VAL:HG22	13:N:60:PHE:CD2	2.27	0.69
16:3:75:ALA:HB3	16:3:76:PRO:HD3	1.75	0.69
14:1:11:PRO:N	17:4:107:GLN:HG3	2.07	0.69
1:A:491:TRP:N	1:A:492:ILE:HG23	2.08	0.69
1:A:693:LEU:HD23	2:B:665:ILE:HG12	1.75	0.69
2:B:174:ARG:HE	18:B:1210:CLA:HHD	1.56	0.69
2:B:344:ILE:CD1	18:B:1225:CLA:CAC	2.58	0.69
2:B:367:THR:O	2:B:368:GLN:NE2	2.25	0.69
2:B:395:ILE:HG23	2:B:551:LYS:O	1.91	0.69
2:B:70:TRP:HB3	2:B:71:GLN:HB3	1.73	0.69
2:B:84:VAL:HG13	2:B:85:ARG:H	1.57	0.69
2:B:84:VAL:HG12	2:B:86:PRO:CD	2.23	0.69
6:F:12:LYS:CD	6:F:13:GLN:H	2.04	0.69
18:A:1136:CLA:H91	18:L:1504:CLA:HMC2	1.75	0.69
1:A:318:ARG:HD3	1:A:319:THR:H	1.55	0.69
1:A:347:TYR:CE2	1:A:349:ILE:HG22	2.28	0.69
1:A:458:PHE:O	1:A:460:LEU:N	2.26	0.69
1:A:685:VAL:O	1:A:685:VAL:CG1	2.40	0.69
2:B:478:LEU:C	2:B:480:SER:H	1.94	0.69
3:C:62:PHE:HE2	5:E:43:SER:O	1.75	0.69
6:F:55:ASN:O	6:F:56:TYR:C	2.31	0.69
2:B:458:ILE:HG12	6:F:74:SER:HB3	1.75	0.69
7:G:20:ARG:O	7:G:23:PHE:HB2	1.92	0.69
12:L:149:SER:O	12:L:153:TRP:HB3	1.93	0.69
12:L:90:GLY:O	12:L:93:VAL:HG22	1.93	0.69
18:A:1107:CLA:HAC1	2:B:446:PHE:CZ	2.27	0.69
1:A:401:TRP:CH2	1:A:610:SER:HB2	2.27	0.69
1:A:484:LEU:HD22	1:A:539:PHE:HE2	1.57	0.69
18:A:9011:CLA:CBB	2:B:624:LEU:CD1	2.71	0.69
2:B:456:GLU:HG3	2:B:514:PRO:CB	2.14	0.69
2:B:57:ILE:O	2:B:60:TRP:CB	2.41	0.69
4:D:100:PHE:CE1	4:D:113:HIS:NE2	2.61	0.69
4:D:149:THR:HB	4:D:152:GLN:O	1.93	0.69
3:C:60:THR:CA	5:E:80:ASN:HD21	2.06	0.69
8:H:55:LYS:HA	8:H:58:ILE:CG1	2.21	0.69
12:L:45:THR:HG23	12:L:126:GLN:HE21	1.57	0.69
1:A:335:LYS:O	1:A:342:GLY:CA	2.41	0.69
1:A:347:TYR:CD2	1:A:349:ILE:N	2.56	0.69
19:A:5001:PQN:H202	19:A:5001:PQN:C24	2.23	0.69
18:B:1209:CLA:O1A	18:B:1209:CLA:C5	2.39	0.69
18:B:1215:CLA:HMC1	18:B:1215:CLA:HBC3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:LEU:HD23	2:B:617:MET:N	2.08	0.69
2:B:700:LEU:HD23	2:B:704:GLN:NE2	2.01	0.69
11:K:14:UNK:HA	18:K:1141:CLA:HHD	1.74	0.69
4:D:30:ALA:HA	12:L:13:PRO:HD3	1.73	0.69
15:2:85:GLN:O	15:2:86:GLU:HG3	1.93	0.68
16:3:86:PRO:HB2	16:3:87:ALA:HB3	1.76	0.68
17:4:124:TYR:CA	17:4:125:SER:HB3	2.22	0.68
15:2:84:GLU:OE2	17:4:186:ILE:CG1	2.41	0.68
17:4:190:TRP:HE3	17:4:190:TRP:HA	1.57	0.68
1:A:84:GLY:O	1:A:87:SER:N	2.26	0.68
2:B:524:ALA:HB2	18:B:1235:CLA:HMA1	1.74	0.68
2:B:569:ASP:CG	2:B:706:ARG:HH22	1.95	0.68
5:E:66:VAL:CA	5:E:81:ASN:ND2	2.37	0.68
6:F:86:PRO:CD	10:J:39:PHE:HB2	2.23	0.68
18:A:1132:CLA:C1B	12:L:72:GLY:HA2	2.22	0.68
12:L:87:ALA:O	12:L:91:LEU:N	2.25	0.68
17:4:185:HIS:O	17:4:186:ILE:HG12	1.93	0.68
1:A:414:ALA:O	1:A:417:PHE:CD2	2.40	0.68
18:B:1242:CLA:HBC3	18:B:1242:CLA:HHD	1.74	0.68
2:B:93:ASP:OD2	2:B:96:PHE:CE2	2.46	0.68
3:C:27:GLU:OE2	3:C:29:ILE:HG23	1.93	0.68
15:2:31:PRO:O	15:2:33:GLY:HA3	1.94	0.68
18:B:1208:CLA:H62	18:B:1209:CLA:C4	2.23	0.68
18:B:1227:CLA:CBC	18:B:1242:CLA:HMD3	2.23	0.68
2:B:388:ALA:O	2:B:391:PRO:HD2	1.94	0.68
2:B:542:ARG:C	2:B:542:ARG:HD2	2.13	0.68
6:F:4:GLY:HA3	6:F:5:LEU:HB2	1.76	0.68
7:G:83:TYR:CA	7:G:85:ILE:H	2.05	0.68
7:G:88:THR:N	7:G:90:SER:HA	2.08	0.68
8:H:49:LYS:HG3	12:L:140:THR:HG23	1.75	0.68
17:4:137:ILE:HG13	17:4:140:PRO:HD2	1.74	0.68
1:A:391:THR:HG22	1:A:394:SER:HB3	1.75	0.68
2:B:302:LYS:CA	2:B:302:LYS:HE2	2.21	0.68
2:B:355:LEU:HD22	2:B:355:LEU:O	1.94	0.68
2:B:448:THR:HG21	2:B:451:LYS:HE2	1.76	0.68
2:B:567:THR:O	2:B:568:CYS:HB2	1.92	0.68
2:B:584:LEU:O	2:B:588:GLY:N	2.25	0.68
2:B:440:ASN:O	2:B:615:TYR:HA	1.93	0.68
2:B:631:LEU:HA	2:B:643:LEU:CD1	2.23	0.68
6:F:141:TYR:CD2	6:F:142:ARG:N	2.60	0.68
4:D:31:GLY:HA2	12:L:13:PRO:HB3	1.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:1503:CLA:O2D	18:L:1503:CLA:H11	1.93	0.68
12:L:27:VAL:HG13	18:L:1130:CLA:H12	1.74	0.68
15:2:178:TRP:HE3	15:2:178:TRP:N	1.90	0.68
1:A:552:THR:HG22	1:A:604:TRP:HB3	1.74	0.68
2:B:167:TRP:CZ2	18:B:1208:CLA:HMA1	2.28	0.68
2:B:399:ASN:ND2	2:B:402:GLN:HB2	2.07	0.68
3:C:27:GLU:CG	3:C:28:MET:N	2.55	0.68
6:F:1:ASP:HA	6:F:62:LEU:HD11	1.75	0.68
7:G:43:HIS:O	7:G:48:ASP:OD1	2.09	0.68
12:L:66:GLY:CA	18:L:1503:CLA:C1B	2.71	0.68
13:N:58:VAL:N	13:N:60:PHE:CE2	2.61	0.68
13:N:58:VAL:CG2	13:N:60:PHE:CG	2.76	0.68
16:3:193:LEU:HA	16:3:196:LEU:HG	1.75	0.68
1:A:105:ASN:O	1:A:109:TRP:HB3	1.92	0.68
1:A:131:ILE:HD11	2:B:446:PHE:HA	1.75	0.68
1:A:76:ARG:HD2	1:A:191:PRO:O	1.94	0.68
1:A:290:LEU:O	1:A:291:THR:CG2	2.32	0.68
1:A:620:MET:HA	1:A:624:VAL:HG11	1.72	0.68
1:A:654:ARG:CD	1:A:655:ASP:OD2	2.42	0.68
1:A:664:VAL:CG2	1:A:675:TYR:O	2.41	0.68
18:A:9011:CLA:CBB	2:B:624:LEU:HD12	2.23	0.68
2:B:85:ARG:NH1	2:B:115:ASN:OD1	2.26	0.68
18:B:1222:CLA:O1A	18:B:1222:CLA:H2	1.94	0.68
2:B:415:LYS:HE3	2:B:540:ASP:CB	2.23	0.68
2:B:37:ILE:CA	2:B:41:ARG:HD2	2.23	0.68
2:B:703:VAL:O	2:B:704:GLN:HB2	1.93	0.68
1:A:568:LEU:HA	4:D:79:ARG:HH12	1.58	0.68
6:F:122:ASP:N	10:J:9:SER:HB2	2.08	0.68
6:F:73:VAL:HG21	6:F:83:PHE:N	2.02	0.68
6:F:96:TRP:C	6:F:96:TRP:CD1	2.65	0.68
15:2:17:GLU:CB	15:2:18:TRP:HB3	2.15	0.68
15:2:70:LYS:HD2	15:2:70:LYS:H	1.58	0.68
1:A:246:HIS:CE1	18:A:1147:CLA:C4A	2.76	0.68
1:A:96:MET:CB	1:A:149:PHE:HE2	2.06	0.68
1:A:43:THR:HG22	1:A:46:LYS:CG	2.23	0.68
1:A:620:MET:HB3	1:A:625:TRP:CZ2	2.29	0.68
1:A:733:VAL:C	1:A:735:VAL:H	1.95	0.68
2:B:341:LEU:HA	2:B:344:ILE:HG23	1.76	0.68
2:B:351:HIS:O	2:B:352:MET:CB	2.41	0.68
2:B:377:TYR:CE1	2:B:587:ILE:HD13	2.28	0.68
2:B:42:LEU:HG	2:B:43:TYR:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:672:GLN:NE2	2:B:698:VAL:HA	1.97	0.68
7:G:35:VAL:N	7:G:36:PRO:CD	2.30	0.68
8:H:54:LEU:HD23	12:L:100:THR:OG1	1.93	0.68
15:2:175:MET:HG2	15:2:176:GLY:N	2.09	0.68
17:4:187:SER:O	17:4:188:ASP:HB2	1.91	0.68
18:A:1132:CLA:C2B	12:L:72:GLY:H	2.02	0.68
18:A:1140:CLA:C4C	18:A:1140:CLA:C4	2.72	0.68
1:A:278:ALA:O	1:A:280:PHE:CD2	2.47	0.68
1:A:579:PHE:O	1:A:593:SER:OG	2.11	0.68
1:A:641:ASN:OD1	1:A:642:PHE:HB2	1.93	0.68
1:A:685:VAL:O	1:A:741:GLY:CA	2.41	0.68
1:A:95:GLY:CA	1:A:96:MET:SD	2.82	0.68
2:B:284:PHE:CZ	18:B:1216:CLA:HBB2	2.29	0.68
2:B:683:GLU:O	2:B:684:ARG:HD2	1.94	0.68
4:D:83:CYS:O	4:D:84:LEU:C	2.31	0.68
1:A:675:TYR:CE2	18:A:1106:CLA:HBC1	2.28	0.68
1:A:701:GLN:OE1	1:A:723:ARG:HG3	1.93	0.68
18:B:1203:CLA:HBA2	18:B:1203:CLA:O1D	1.94	0.68
2:B:120:VAL:CG2	18:B:1225:CLA:CBA	2.72	0.68
18:B:1215:CLA:C6	18:B:1215:CLA:HBB2	2.23	0.68
2:B:276:HIS:ND1	2:B:277:HIS:N	2.41	0.68
2:B:519:VAL:CG2	2:B:593:TYR:CD2	2.70	0.68
2:B:652:PHE:CD1	2:B:656:VAL:CG2	2.77	0.68
7:G:83:TYR:N	7:G:85:ILE:H	1.92	0.68
13:N:64:ASP:OD2	13:N:65:LEU:N	2.27	0.68
16:3:192:MET:O	16:3:196:LEU:HG	1.93	0.68
17:4:141:LEU:O	17:4:142:ASN:HB2	1.92	0.68
18:B:1239:CLA:HBC1	20:B:6017:BCR:H392	1.75	0.68
2:B:262:HIS:NE2	2:B:264:GLN:HB3	2.07	0.68
2:B:377:TYR:CD1	2:B:587:ILE:HD13	2.29	0.68
2:B:498:LEU:HA	2:B:501:ILE:HG23	1.76	0.68
3:C:5:VAL:CG1	3:C:6:LYS:N	2.54	0.68
6:F:94:ALA:O	6:F:97:ILE:HG13	1.93	0.68
8:H:47:PHE:CE2	12:L:50:LEU:HD11	2.28	0.68
15:2:192:LEU:HA	15:2:195:HIS:NE2	2.02	0.67
17:4:137:ILE:CG1	17:4:140:PRO:HD2	2.23	0.67
1:A:599:PHE:HZ	1:A:693:LEU:HD21	1.59	0.67
2:B:317:ARG:NH1	18:B:1227:CLA:CAD	2.57	0.67
2:B:283:LEU:O	2:B:284:PHE:CD1	2.48	0.67
2:B:717:TYR:CE2	18:B:9010:CLA:O1A	2.47	0.67
18:B:9012:CLA:H41	18:B:9012:CLA:C7	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:PRO:HD2	4:D:73:ASN:CG	2.14	0.67
8:H:58:ILE:HD12	8:H:58:ILE:C	2.14	0.67
10:J:4:PHE:HB2	10:J:5:LYS:O	1.94	0.67
2:B:687:LEU:HD11	12:L:40:LEU:HD12	1.75	0.67
13:N:43:PRO:HD2	13:N:44:GLU:O	1.94	0.67
13:N:77:CYS:SG	13:N:81:VAL:HA	2.33	0.67
15:2:178:TRP:C	15:2:180:GLN:N	2.47	0.67
1:A:268:PRO:HD2	1:A:277:TYR:CD1	2.29	0.67
2:B:235:GLN:C	2:B:236:ASN:HD22	1.98	0.67
6:F:61:LEU:CD1	6:F:69:PRO:HB3	2.16	0.67
8:H:41:GLU:HA	8:H:41:GLU:OE1	1.94	0.67
15:2:176:GLY:O	15:2:178:TRP:CE3	2.48	0.67
17:4:99:HIS:CE1	17:4:103:ILE:HG12	2.28	0.67
17:4:118:ASP:N	17:4:119:PRO:HD3	2.08	0.67
1:A:373:ALA:C	1:A:375:HIS:N	2.47	0.67
1:A:398:HIS:HB2	18:A:1126:CLA:C4B	2.23	0.67
2:B:127:ILE:HD12	2:B:190:TRP:CZ3	2.22	0.67
2:B:209:TRP:CG	2:B:210:ASN:N	2.62	0.67
2:B:373:THR:O	2:B:376:GLN:N	2.27	0.67
2:B:708:VAL:HG11	18:B:1239:CLA:OBD	1.94	0.67
2:B:92:TRP:O	2:B:94:PRO:HD3	1.94	0.67
9:I:27:HIS:O	9:I:28:VAL:O	2.12	0.67
10:J:2:ARG:HE	10:J:5:LYS:HD3	1.58	0.67
12:L:40:LEU:O	12:L:42:ALA:N	2.28	0.67
20:I:6018:BCR:C38	20:L:6020:BCR:C34	2.64	0.67
1:A:604:TRP:O	1:A:608:SER:N	2.28	0.67
1:A:72:GLU:HG3	1:A:76:ARG:NH1	2.08	0.67
2:B:104:PHE:HA	2:B:106:ARG:HD2	1.74	0.67
2:B:19:ARG:HA	2:B:22:TRP:HD1	1.58	0.67
2:B:561:GLY:N	21:B:3101:SF4:S4	2.68	0.67
2:B:334:LEU:HD21	18:B:1226:CLA:C2B	2.25	0.67
3:C:11:CYS:C	3:C:12:ILE:O	2.32	0.67
5:E:40:ARG:NH2	5:E:62:ARG:HH22	1.92	0.67
8:H:73:PRO:HB2	8:H:74:GLN:HB3	1.76	0.67
18:L:1503:CLA:HED1	18:L:1503:CLA:C1	2.24	0.67
14:1:84:TYR:CB	14:1:85:LEU:CA	2.42	0.67
15:2:178:TRP:HB2	15:2:183:TYR:CE2	2.30	0.67
15:2:187:GLY:H	15:2:189:ILE:H	1.43	0.67
16:3:209:PRO:HB2	16:3:211:GLN:N	2.08	0.67
1:A:343:HIS:ND1	1:A:343:HIS:N	2.43	0.67
1:A:569:ILE:HG13	1:A:586:ARG:HH12	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TRP:O	1:A:94:SER:N	2.27	0.67
2:B:338:LEU:O	2:B:342:GLY:N	2.27	0.67
2:B:351:HIS:H	2:B:351:HIS:CD2	2.11	0.67
5:E:53:VAL:HG23	5:E:66:VAL:O	1.94	0.67
8:H:24:TYR:CB	8:H:25:GLY:HA2	2.19	0.67
9:I:8:PHE:O	9:I:11:LEU:HB2	1.93	0.67
14:1:40:LYS:O	14:1:42:SER:N	2.28	0.67
15:2:21:GLY:H	15:2:23:LEU:HD21	1.59	0.67
17:4:106:TRP:CE2	17:4:110:LYS:NZ	2.61	0.67
1:A:277:TYR:CG	18:A:1113:CLA:HBC1	2.29	0.67
1:A:186:TYR:HA	1:A:191:PRO:HD3	1.76	0.67
1:A:205:HIS:O	1:A:209:GLY:N	2.27	0.67
1:A:364:MET:HG2	18:A:1123:CLA:CMA	2.25	0.67
1:A:604:TRP:O	1:A:607:ASN:N	2.27	0.67
2:B:276:HIS:HE2	18:B:1215:CLA:CMB	2.07	0.67
2:B:464:GLN:O	2:B:469:LYS:HB2	1.94	0.67
2:B:63:GLY:O	2:B:65:LEU:C	2.32	0.67
2:B:644:SER:O	2:B:647:ALA:HB3	1.94	0.67
2:B:721:TYR:N	18:B:9010:CLA:O1D	2.28	0.67
12:L:33:ILE:CG2	12:L:35:TRP:HB3	2.21	0.67
14:1:75:ALA:O	14:1:78:PRO:CD	2.43	0.67
15:2:170:ALA:O	15:2:173:ALA:HB3	1.95	0.67
15:2:178:TRP:HB2	15:2:183:TYR:CZ	2.29	0.67
15:2:19:LEU:CG	15:2:20:ASP:CG	2.60	0.67
15:2:63:PHE:CD2	15:2:63:PHE:N	2.42	0.67
1:A:31:PHE:CD2	1:A:31:PHE:C	2.67	0.67
1:A:342:GLY:C	1:A:431:LEU:HD23	2.15	0.67
1:A:452:PHE:CD2	1:A:453:LEU:N	2.63	0.67
1:A:472:ARG:O	1:A:472:ARG:HG2	1.95	0.67
1:A:750:PHE:CZ	18:A:1126:CLA:HMB1	2.29	0.67
2:B:17:THR:HG22	2:B:696:LYS:HG3	1.77	0.67
2:B:463:ILE:CG2	2:B:467:HIS:CE1	2.60	0.67
2:B:627:ASN:OD1	2:B:732:LYS:HE3	1.95	0.67
2:B:658:ALA:O	2:B:661:PHE:CB	2.40	0.67
1:A:590:CYS:H	2:B:669:GLY:H	1.43	0.67
5:E:90:VAL:HG13	5:E:91:ALA:N	2.10	0.67
7:G:42:SER:H	7:G:43:HIS:HD2	1.40	0.67
2:B:684:ARG:NH2	12:L:22:GLY:HA3	2.09	0.67
12:L:59:ALA:HA	12:L:62:PHE:CE2	2.29	0.67
1:A:690:LEU:N	1:A:690:LEU:HD13	2.10	0.67
1:A:86:LEU:HD11	1:A:90:PHE:CD1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1214:CLA:CHD	18:B:1214:CLA:H43	2.24	0.67
18:B:1205:CLA:O1A	18:B:1224:CLA:HAA1	1.94	0.67
2:B:305:LEU:O	2:B:308:HIS:N	2.27	0.67
2:B:422:LEU:HD22	2:B:532:LEU:HB3	1.77	0.67
2:B:557:PHE:HZ	2:B:570:ILE:HG13	1.60	0.67
5:E:44:TYR:HE1	5:E:74:TYR:CE2	2.12	0.67
18:F:1139:CLA:C3D	18:F:1139:CLA:HED2	2.24	0.67
18:A:1115:CLA:HBB2	18:K:1141:CLA:C3B	2.25	0.67
15:2:153:PRO:HB2	15:2:154:GLN:CA	2.24	0.67
15:2:19:LEU:HA	15:2:21:GLY:N	2.10	0.67
2:B:174:ARG:HG3	18:B:1221:CLA:HMD3	1.73	0.67
18:B:1227:CLA:HBC3	18:B:1242:CLA:HMD3	1.77	0.67
2:B:266:GLN:NE2	2:B:505:SER:OG	2.28	0.67
2:B:344:ILE:CG1	2:B:345:THR:N	2.56	0.67
2:B:372:TYR:O	2:B:375:HIS:N	2.27	0.67
18:B:9023:CLA:HMA2	20:B:6017:BCR:H403	1.77	0.67
18:I:1204:CLA:HBC3	18:I:1204:CLA:HMC1	1.77	0.67
18:L:1130:CLA:H43	18:L:1504:CLA:HMA2	1.77	0.67
13:N:81:VAL:H	13:N:82:PHE:HD2	1.41	0.67
18:A:1129:CLA:HMA2	12:L:25:THR:HG21	1.76	0.67
1:A:149:PHE:HB3	1:A:153:TRP:CH2	2.30	0.67
1:A:535:GLY:O	1:A:538:ASP:CB	2.42	0.67
1:A:679:PHE:CD1	1:A:679:PHE:C	2.68	0.67
1:A:750:PHE:O	1:A:751:LEU:HB2	1.95	0.67
2:B:276:HIS:ND1	2:B:276:HIS:C	2.48	0.67
2:B:596:TRP:HZ3	2:B:613:SER:HB2	1.60	0.67
5:E:40:ARG:CZ	5:E:42:GLU:HG2	2.24	0.67
8:H:50:ARG:HH11	8:H:50:ARG:HG3	1.59	0.67
12:L:138:LYS:HB3	12:L:138:LYS:HZ2	1.58	0.67
13:N:32:ALA:HA	13:N:35:VAL:CG2	2.23	0.67
13:N:48:GLY:CA	13:N:50:GLN:N	2.50	0.67
13:N:81:VAL:C	13:N:82:PHE:HD2	1.97	0.67
15:2:194:ALA:HB3	15:2:195:HIS:HA	1.78	0.66
1:A:48:PRO:HB3	1:A:53:TRP:CZ3	2.30	0.66
1:A:547:PHE:CE1	1:A:551:VAL:HG13	2.23	0.66
2:B:104:PHE:HB2	2:B:112:PRO:CA	2.25	0.66
18:B:1202:CLA:HED3	18:B:1203:CLA:CMB	2.25	0.66
2:B:188:LEU:O	2:B:192:GLY:N	2.26	0.66
2:B:609:PHE:CD1	2:B:610:ASN:N	2.63	0.66
2:B:704:GLN:O	2:B:706:ARG:N	2.28	0.66
2:B:569:ASP:HB3	2:B:706:ARG:HH12	1.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:THR:HA	5:E:80:ASN:HD21	1.57	0.66
7:G:71:VAL:O	7:G:75:GLY:N	2.27	0.66
9:I:26:LEU:HA	9:I:29:GLU:N	2.10	0.66
10:J:11:ALA:HB3	10:J:12:PRO:CD	2.19	0.66
1:A:555:ILE:CA	1:A:556:LEU:HB2	2.24	0.66
2:B:350:GLN:HA	2:B:353:TYR:HD1	1.59	0.66
2:B:371:LEU:HD11	18:B:1225:CLA:HED2	1.78	0.66
2:B:571:SER:HB3	2:B:573:TRP:HB3	1.77	0.66
3:C:63:LEU:HD23	3:C:66:ARG:HG2	1.77	0.66
1:A:715:LYS:HZ3	6:F:153:ASN:HD21	1.42	0.66
6:F:1:ASP:HA	6:F:62:LEU:CD1	2.25	0.66
8:H:26:SER:HA	8:H:28:ALA:N	2.11	0.66
8:H:33:ASN:HD21	18:H:1501:CLA:CMD	1.93	0.66
16:3:132:ASP:HB3	16:3:139:MET:CB	2.26	0.66
18:A:1136:CLA:HAA1	18:A:1136:CLA:O1D	1.95	0.66
1:A:308:ILE:HD12	1:A:311:LEU:CB	2.25	0.66
2:B:330:ILE:O	2:B:333:GLN:N	2.26	0.66
3:C:62:PHE:CE2	5:E:43:SER:O	2.48	0.66
5:E:51:SER:O	5:E:53:VAL:N	2.28	0.66
6:F:115:THR:O	6:F:117:LYS:N	2.28	0.66
6:F:92:TYR:CE2	6:F:96:TRP:HZ3	2.11	0.66
7:G:8:ILE:O	7:G:10:LEU:N	2.28	0.66
15:2:27:PHE:CD1	15:2:28:GLY:C	2.63	0.66
1:A:114:THR:HB	1:A:115:HIS:CD2	2.30	0.66
1:A:284:ARG:HD3	1:A:508:THR:OG1	1.95	0.66
1:A:364:MET:HA	1:A:364:MET:HE3	1.76	0.66
1:A:545:HIS:HD1	1:A:612:VAL:HG22	1.55	0.66
1:A:65:ASP:C	1:A:67:HIS:H	1.99	0.66
1:A:75:SER:HA	1:A:354:TRP:CH2	2.30	0.66
2:B:187:SER:O	2:B:189:ALA:N	2.29	0.66
2:B:395:ILE:CG2	2:B:395:ILE:O	2.43	0.66
1:A:658:TRP:CD1	2:B:625:TRP:CD1	2.81	0.66
2:B:708:VAL:CG1	18:B:1239:CLA:O1D	2.43	0.66
6:F:127:SER:N	6:F:130:LEU:HD13	2.11	0.66
6:F:55:ASN:O	6:F:58:LYS:HB2	1.95	0.66
12:L:111:GLU:OE1	12:L:134:ASP:O	2.14	0.66
8:H:49:LYS:HG3	12:L:140:THR:HG21	1.77	0.66
13:N:38:GLY:N	13:N:39:SER:HA	2.08	0.66
15:2:19:LEU:HA	15:2:22:SER:HB3	1.77	0.66
16:3:85:ILE:N	16:3:86:PRO:CD	2.58	0.66
1:A:370:ILE:HD13	18:A:1124:CLA:C3A	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1131:CLA:HBC2	18:A:1131:CLA:HMC1	1.77	0.66
1:A:684:PHE:HA	1:A:687:ALA:HB3	1.77	0.66
1:A:81:ALA:HB3	1:A:83:PHE:H	0.85	0.66
18:B:1138:CLA:C4C	18:F:1139:CLA:HBC2	2.26	0.66
2:B:463:ILE:HG23	2:B:467:HIS:ND1	2.10	0.66
5:E:62:ARG:HG3	5:E:63:TYR:CD1	2.28	0.66
7:G:37:GLU:CB	7:G:43:HIS:CE1	2.79	0.66
9:I:24:LEU:HA	9:I:27:HIS:H	1.61	0.66
18:H:1501:CLA:HBB2	18:L:1502:CLA:CAA	2.22	0.66
14:1:185:TRP:HA	14:1:185:TRP:HE3	1.56	0.66
14:1:84:TYR:OH	14:1:92:GLY:N	2.28	0.66
17:4:93:ILE:HG13	17:4:94:GLU:H	1.60	0.66
18:A:1129:CLA:CBB	18:L:1130:CLA:HBC3	2.25	0.66
18:A:1137:CLA:HMC1	18:L:1130:CLA:HMC3	1.78	0.66
1:A:588:GLY:O	2:B:668:ARG:HD3	1.95	0.66
1:A:677:LEU:HD21	2:B:441:ASP:O	1.95	0.66
1:A:726:SER:OG	1:A:729:GLN:NE2	2.28	0.66
18:B:1208:CLA:C1	18:B:1209:CLA:H2	2.26	0.66
18:B:1202:CLA:H2	18:B:1210:CLA:C3D	2.25	0.66
2:B:346:SER:O	2:B:350:GLN:OE1	2.13	0.66
2:B:58:PHE:CD1	2:B:145:LEU:HB3	2.30	0.66
2:B:365:PHE:CE1	2:B:602:TRP:CD1	2.83	0.66
2:B:617:MET:O	2:B:621:ARG:HG2	1.95	0.66
2:B:655:LEU:CB	18:B:9022:CLA:HAA1	2.24	0.66
3:C:27:GLU:HB3	3:C:43:PRO:CB	2.24	0.66
3:C:50:GLY:C	3:C:52:LYS:H	1.98	0.66
3:C:11:CYS:SG	3:C:59:PRO:HD2	2.36	0.66
7:G:20:ARG:O	7:G:23:PHE:CB	2.43	0.66
7:G:33:LYS:C	7:G:33:LYS:HD3	2.16	0.66
8:H:50:ARG:NH1	8:H:50:ARG:HG3	2.10	0.66
8:H:63:SER:O	8:H:67:TYR:CB	2.42	0.66
12:L:27:VAL:HG13	18:L:1130:CLA:C1	2.26	0.66
13:N:73:ASP:O	13:N:74:LYS:CG	2.42	0.66
15:2:162:LYS:HZ2	15:2:163:GLU:H	1.42	0.66
15:2:23:LEU:CG	15:2:26:ASP:O	2.44	0.66
1:A:579:PHE:O	1:A:580:PRO:O	2.12	0.66
1:A:696:GLY:CA	2:B:569:ASP:OD2	2.44	0.66
1:A:81:ALA:CB	1:A:82:HIS:C	2.63	0.66
2:B:193:HIS:CD2	2:B:197:VAL:O	2.48	0.66
2:B:703:VAL:O	2:B:704:GLN:CB	2.44	0.66
2:B:67:HIS:NE2	2:B:89:HIS:HB2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:LEU:HD21	18:B:9010:CLA:HBC2	1.75	0.66
6:F:105:LEU:O	6:F:107:ALA:N	2.27	0.66
1:A:751:LEU:HD13	1:A:752:ALA:N	2.11	0.66
1:A:80:SER:N	1:A:81:ALA:CB	2.57	0.66
2:B:200:PRO:HB2	2:B:207:VAL:CG1	2.26	0.66
2:B:652:PHE:O	2:B:655:LEU:N	2.28	0.66
3:C:55:GLU:CB	3:C:65:VAL:CG2	2.73	0.66
3:C:5:VAL:C	3:C:6:LYS:HG2	2.15	0.66
12:L:15:ASN:N	12:L:24:GLU:OE1	2.29	0.66
1:A:458:PHE:CD2	1:A:459:GLY:N	2.64	0.66
1:A:727:ILE:HG22	1:A:728:VAL:N	2.09	0.66
2:B:246:THR:HG22	2:B:247:THR:H	1.61	0.66
2:B:407:VAL:HB	18:B:1220:CLA:HMC3	1.78	0.66
2:B:415:LYS:O	2:B:417:ALA:N	2.27	0.66
2:B:596:TRP:O	2:B:597:LYS:HB2	1.96	0.66
2:B:678:LEU:O	2:B:682:HIS:HD2	1.78	0.66
4:D:112:LEU:HG	4:D:113:HIS:NE2	2.09	0.66
4:D:47:VAL:HG23	4:D:103:VAL:CG1	2.21	0.66
6:F:115:THR:O	6:F:118:GLU:HB2	1.95	0.66
18:F:1302:CLA:HMC2	14:I:191:ASP:HB2	1.78	0.66
6:F:141:TYR:HE2	6:F:142:ARG:HD3	1.60	0.66
7:G:20:ARG:HH21	7:G:68:ILE:CG2	2.09	0.66
15:2:33:GLY:HA2	15:2:34:LEU:C	2.15	0.66
17:4:96:ILE:CG2	17:4:97:LEU:H	2.08	0.66
1:A:196:PHE:CD2	1:A:196:PHE:C	2.69	0.66
1:A:613:ILE:O	1:A:616:PHE:HB3	1.96	0.66
2:B:375:HIS:CE1	18:B:1225:CLA:NA	2.64	0.66
2:B:261:PHE:O	2:B:262:HIS:ND1	2.29	0.66
2:B:722:ALA:CB	18:B:1224:CLA:H42	2.23	0.66
3:C:25:VAL:O	3:C:25:VAL:HG12	1.96	0.66
4:D:45:PHE:C	4:D:45:PHE:HD1	1.98	0.66
18:B:1207:CLA:C6	8:H:65:LEU:HD22	2.25	0.66
10:J:2:ARG:HD3	10:J:7:TYR:HD1	1.60	0.66
1:A:160:SER:OG	1:A:163:GLN:HB2	1.95	0.65
1:A:183:TRP:HE3	1:A:183:TRP:O	1.79	0.65
1:A:397:THR:O	1:A:398:HIS:C	2.34	0.65
2:B:259:GLY:C	2:B:269:TRP:NE1	2.49	0.65
2:B:319:HIS:O	2:B:321:GLY:N	2.30	0.65
2:B:383:MET:O	2:B:386:ALA:HB3	1.96	0.65
1:A:582:ASP:HA	2:B:562:PRO:HG2	1.78	0.65
2:B:569:ASP:CB	2:B:706:ARG:NH1	2.48	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:GLU:HB3	3:C:43:PRO:HB3	1.76	0.65
13:N:77:CYS:CB	13:N:78:GLY:HA2	2.25	0.65
15:2:19:LEU:CD1	15:2:22:SER:HG	2.07	0.65
17:4:124:TYR:HA	17:4:125:SER:HB3	1.77	0.65
17:4:62:GLU:C	17:4:63:VAL:CG2	2.65	0.65
1:A:246:HIS:H	1:A:246:HIS:CD2	2.14	0.65
1:A:526:LYS:HA	1:A:627:THR:N	2.11	0.65
1:A:80:SER:H	1:A:81:ALA:HA	1.59	0.65
2:B:53:GLN:HE22	18:B:1202:CLA:H3A	1.61	0.65
18:B:1202:CLA:HED3	18:B:1203:CLA:HMB2	1.78	0.65
2:B:126:THR:CG2	18:B:1215:CLA:HED1	2.26	0.65
2:B:330:ILE:CG2	18:B:1202:CLA:HBC1	2.26	0.65
2:B:532:LEU:HA	2:B:535:VAL:HG23	1.78	0.65
13:N:40:CYS:O	13:N:41:LYS:O	2.13	0.65
15:2:17:GLU:N	15:2:18:TRP:O	2.28	0.65
15:2:103:GLY:HA2	18:2:2012:CLA:C2C	2.27	0.65
16:3:106:THR:HG23	16:3:109:ALA:HB2	1.77	0.65
16:3:196:LEU:HB3	18:3:3005:CLA:C3B	2.26	0.65
13:N:57:LYS:CB	16:3:87:ALA:CB	2.66	0.65
1:A:105:ASN:HB3	1:A:150:PHE:HE2	1.60	0.65
1:A:115:HIS:O	1:A:116:ILE:HB	1.95	0.65
1:A:435:VAL:HG22	1:A:438:HIS:CE1	2.31	0.65
1:A:585:GLY:C	1:A:587:GLY:N	2.49	0.65
1:A:89:ILE:O	1:A:92:TRP:CB	2.43	0.65
2:B:589:TRP:O	2:B:591:THR:N	2.27	0.65
2:B:78:VAL:HG23	2:B:130:ARG:CD	2.23	0.65
12:L:66:GLY:HA2	18:L:1503:CLA:C1B	2.26	0.65
17:4:105:ARG:O	17:4:108:ASP:HB3	1.95	0.65
17:4:190:TRP:CA	17:4:190:TRP:CE3	2.79	0.65
1:A:435:VAL:HG23	1:A:438:HIS:CE1	2.31	0.65
1:A:663:GLN:O	1:A:667:SER:CB	2.40	0.65
2:B:100:ALA:CA	2:B:103:ALA:HB3	2.24	0.65
18:B:1221:CLA:HMC1	18:B:1221:CLA:HBC2	1.77	0.65
2:B:636:THR:HG23	2:B:636:THR:O	1.95	0.65
2:B:458:ILE:HG22	6:F:72:ILE:HG21	1.78	0.65
12:L:113:SER:CA	12:L:114:ILE:HB	2.26	0.65
12:L:63:LEU:HD11	18:L:1502:CLA:CHB	2.27	0.65
13:N:36:GLU:O	13:N:40:CYS:HB3	1.95	0.65
14:1:181:LEU:HA	14:1:182:ALA:C	2.17	0.65
18:B:1138:CLA:H51	18:B:1138:CLA:CBB	2.27	0.65
2:B:39:GLU:HA	2:B:39:GLU:OE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:ILE:H	2:B:492:ILE:CD1	1.95	0.65
2:B:521:HIS:O	2:B:524:ALA:N	2.29	0.65
2:B:646:TRP:O	2:B:650:PHE:CB	2.45	0.65
5:E:38:ILE:HB	5:E:46:PHE:O	1.97	0.65
5:E:40:ARG:HB3	5:E:42:GLU:HG3	1.79	0.65
6:F:149:LEU:HA	6:F:151:ASP:CG	2.16	0.65
16:3:57:TYR:HE2	16:3:185:VAL:CB	2.10	0.65
18:A:1131:CLA:CBC	18:A:1136:CLA:HAC1	2.26	0.65
1:A:488:PHE:H	1:A:535:GLY:HA2	1.62	0.65
2:B:197:VAL:HG21	18:B:1211:CLA:C2D	2.26	0.65
2:B:330:ILE:CG2	2:B:331:HIS:N	2.57	0.65
2:B:341:LEU:HA	2:B:344:ILE:CG2	2.26	0.65
2:B:117:TYR:HB3	2:B:370:ALA:HB2	1.79	0.65
3:C:49:VAL:O	3:C:49:VAL:CG1	2.44	0.65
9:I:16:PHE:CD1	9:I:17:PRO:N	2.65	0.65
18:L:1503:CLA:O1A	18:L:1503:CLA:CGD	2.45	0.65
1:A:58:HIS:HE1	18:A:1101:CLA:NC	1.94	0.65
2:B:348:VAL:HG23	18:B:1215:CLA:H42	1.77	0.65
1:A:665:ILE:CD1	2:B:625:TRP:CD1	2.79	0.65
2:B:646:TRP:CZ3	18:B:1205:CLA:HBC1	2.31	0.65
12:L:64:LEU:O	12:L:66:GLY:N	2.30	0.65
14:1:75:ALA:O	14:1:78:PRO:HD2	1.96	0.65
16:3:107:TYR:H	16:3:108:TRP:C	1.98	0.65
16:3:126:GLU:CD	16:3:127:HIS:H	1.98	0.65
17:4:81:GLU:O	17:4:84:PHE:HE1	1.80	0.65
1:A:283:PHE:HB3	1:A:507:ALA:HA	1.79	0.65
1:A:546:ALA:O	1:A:550:HIS:CE1	2.50	0.65
1:A:735:VAL:O	1:A:739:LEU:HB3	1.95	0.65
18:B:1215:CLA:HMC1	18:B:1215:CLA:CBC	2.27	0.65
2:B:120:VAL:HG23	18:B:1225:CLA:CBA	2.27	0.65
2:B:424:TRP:HE1	18:B:1229:CLA:HED1	1.62	0.65
2:B:568:CYS:SG	2:B:569:ASP:N	2.69	0.65
2:B:365:PHE:HB3	2:B:602:TRP:CD2	2.32	0.65
2:B:518:LEU:HD22	2:B:614:THR:HG22	1.79	0.65
2:B:89:HIS:O	2:B:90:ALA:HB3	1.97	0.65
3:C:51:CYS:C	21:C:3102:SF4:S1	2.75	0.65
3:C:52:LYS:HE2	3:C:66:ARG:CA	2.16	0.65
4:D:141:VAL:CG2	4:D:142:SER:H	2.05	0.65
6:F:153:ASN:CG	6:F:154:PHE:N	2.48	0.65
1:A:126:ILE:HG13	10:J:27:ILE:HG21	1.77	0.65
13:N:81:VAL:N	13:N:82:PHE:CD2	2.63	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:102:PHE:O	14:1:105:ILE:CG2	2.44	0.65
15:2:22:SER:HB3	15:2:23:LEU:HG	1.74	0.65
15:2:96:ILE:HG13	15:2:97:VAL:N	2.11	0.65
16:3:67:MET:HE2	16:3:71:ALA:N	2.11	0.65
1:A:161:GLU:O	1:A:165:TYR:HB3	1.96	0.65
1:A:653:LEU:HD21	18:B:9010:CLA:CBC	2.26	0.65
1:A:686:TRP:CE3	18:A:9011:CLA:CMA	2.77	0.65
1:A:700:TRP:CH2	18:A:9013:CLA:O1D	2.50	0.65
2:B:193:HIS:HB2	18:B:1211:CLA:C1C	2.25	0.65
2:B:414:HIS:CD2	18:B:1227:CLA:C4A	2.80	0.65
2:B:265:THR:O	2:B:360:PHE:HD2	1.80	0.65
2:B:432:HIS:CE1	18:B:1229:CLA:C4D	2.79	0.65
7:G:8:ILE:HG13	7:G:9:SER:H	1.58	0.65
15:2:54:TRP:CE3	15:2:54:TRP:HA	2.32	0.65
16:3:80:GLY:O	16:3:81:LYS:HB2	1.96	0.65
17:4:53:LEU:HA	17:4:56:ALA:HB3	1.77	0.65
1:A:197:GLN:O	1:A:198:ASP:HB3	1.95	0.65
1:A:621:GLN:CA	1:A:637:ILE:HD13	2.25	0.65
18:A:9011:CLA:HBB1	2:B:624:LEU:HD12	1.75	0.65
2:B:96:PHE:HZ	18:B:1206:CLA:C1D	2.10	0.65
18:B:1228:CLA:HMC3	18:B:1236:CLA:HMC1	1.78	0.65
2:B:478:LEU:O	2:B:480:SER:N	2.30	0.65
2:B:91:ILE:HD11	2:B:114:ASN:ND2	2.12	0.65
3:C:8:TYR:CE1	4:D:137:ILE:HD13	2.32	0.65
4:D:58:PHE:O	4:D:65:ALA:HA	1.97	0.65
5:E:34:SER:O	5:E:36:VAL:N	2.30	0.65
16:3:185:VAL:O	16:3:189:ARG:CB	2.45	0.64
17:4:144:ALA:H	17:4:145:PRO:HD3	1.60	0.64
1:A:661:ALA:O	1:A:664:VAL:N	2.29	0.64
2:B:189:ALA:HB1	18:B:1211:CLA:C2C	2.28	0.64
2:B:432:HIS:C	2:B:434:LEU:N	2.51	0.64
2:B:631:LEU:HD13	2:B:632:ILE:N	2.11	0.64
2:B:37:ILE:O	4:D:148:PHE:CG	2.50	0.64
6:F:82:GLU:O	10:J:38:THR:CG2	2.45	0.64
12:L:102:TYR:HE2	12:L:105:ALA:CB	2.02	0.64
13:N:59:PRO:HA	13:N:60:PHE:CB	2.26	0.64
13:N:81:VAL:O	13:N:83:TRP:CD1	2.50	0.64
17:4:81:GLU:N	17:4:82:GLU:HA	2.12	0.64
1:A:246:HIS:CE1	18:A:1147:CLA:NA	2.65	0.64
1:A:349:ILE:HD12	1:A:352:THR:HB	1.78	0.64
1:A:588:GLY:O	2:B:668:ARG:CD	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ALA:O	2:B:193:HIS:N	2.31	0.64
2:B:242:HIS:HB2	2:B:249:GLY:HA3	1.79	0.64
2:B:345:THR:CG2	18:B:1225:CLA:CMC	2.74	0.64
2:B:689:ASN:HD21	4:D:38:ARG:HH11	1.38	0.64
4:D:83:CYS:O	4:D:86:LEU:N	2.30	0.64
11:K:76:UNK:C	11:K:78:UNK:N	2.56	0.64
12:L:155:CYS:SG	12:L:156:PHE:N	2.71	0.64
12:L:86:LEU:C	12:L:88:ALA:N	2.51	0.64
15:2:114:LEU:CB	15:2:115:ASN:HA	2.27	0.64
15:2:196:LEU:HD12	15:2:196:LEU:H	1.62	0.64
1:A:453:LEU:HD11	1:A:547:PHE:HA	1.80	0.64
1:A:454:GLY:C	1:A:456:HIS:H	1.97	0.64
1:A:594:ALA:HA	1:A:597:HIS:CB	2.27	0.64
2:B:290:MET:CB	18:B:1218:CLA:HBC2	2.18	0.64
18:B:1222:CLA:CAD	18:B:1234:CLA:HBB2	2.28	0.64
2:B:284:PHE:CE1	18:B:1216:CLA:CHC	2.80	0.64
2:B:325:THR:O	2:B:329:SER:CB	2.46	0.64
18:G:1233:CLA:C4C	18:G:1233:CLA:H52	2.27	0.64
15:2:188:PRO:HB2	15:2:193:PHE:HD2	1.62	0.64
16:3:55:LEU:N	16:3:56:ALA:HA	2.08	0.64
1:A:65:ASP:C	1:A:67:HIS:N	2.50	0.64
1:A:753:ARG:NH1	1:A:757:VAL:HB	2.13	0.64
2:B:293:THR:O	2:B:295:PHE:CD1	2.51	0.64
2:B:304:ILE:HD11	18:B:1216:CLA:O1D	1.97	0.64
2:B:392:ILE:O	2:B:393:PHE:C	2.35	0.64
3:C:27:GLU:HB3	3:C:43:PRO:HG3	1.80	0.64
13:N:47:THR:OG1	13:N:50:GLN:HB2	1.98	0.64
16:3:140:GLY:H	16:3:141:LYS:HB3	1.63	0.64
17:4:98:SER:O	17:4:101:VAL:HG22	1.96	0.64
1:A:736:THR:O	1:A:740:LEU:N	2.31	0.64
2:B:275:HIS:HE1	18:B:1214:CLA:CBB	2.10	0.64
18:B:1222:CLA:CBD	18:B:1234:CLA:HBB2	2.28	0.64
2:B:124:TRP:HZ3	2:B:135:LEU:HG	1.63	0.64
2:B:361:ILE:HG13	2:B:368:GLN:HE22	1.63	0.64
1:A:139:GLY:C	6:F:38:PRO:HB2	2.18	0.64
9:I:4:LEU:HD22	9:I:5:PRO:CA	2.24	0.64
14:1:188:ASN:C	14:1:190:GLY:HA2	2.17	0.64
15:2:17:GLU:OE2	15:2:18:TRP:N	2.30	0.64
17:4:156:ASN:HD22	17:4:156:ASN:H	1.40	0.64
1:A:354:TRP:CB	18:A:1103:CLA:HHD	2.25	0.64
18:A:1107:CLA:CBD	18:A:1107:CLA:HAA2	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:CB	18:A:1136:CLA:HBB2	2.25	0.64
1:A:491:TRP:CA	1:A:492:ILE:HG12	2.21	0.64
1:A:620:MET:CA	1:A:624:VAL:HG12	2.23	0.64
1:A:76:ARG:HH21	1:A:190:ALA:HB1	1.62	0.64
2:B:216:LEU:HD11	2:B:221:GLY:HA2	1.80	0.64
2:B:247:THR:OG1	2:B:248:GLN:NE2	2.30	0.64
2:B:283:LEU:HG	18:B:1216:CLA:HMC1	1.78	0.64
2:B:306:GLU:O	2:B:306:GLU:HG2	1.96	0.64
2:B:439:HIS:CE1	2:B:453:ILE:HB	2.33	0.64
2:B:585:ASN:ND2	18:B:9012:CLA:HMC3	2.12	0.64
3:C:51:CYS:O	3:C:51:CYS:SG	2.55	0.64
7:G:61:ASN:HA	7:G:64:VAL:CG2	2.28	0.64
14:1:91:TRP:HB2	14:1:92:GLY:O	1.97	0.64
15:2:17:GLU:CA	15:2:18:TRP:C	2.61	0.64
17:4:190:TRP:C	17:4:191:HIS:CD2	2.71	0.64
18:A:1131:CLA:HBC1	18:A:1136:CLA:HAC1	1.80	0.64
1:A:446:LEU:HD13	1:A:450:CYS:SG	2.37	0.64
2:B:330:ILE:O	2:B:331:HIS:C	2.33	0.64
2:B:64:ASN:N	2:B:64:ASN:OD1	2.30	0.64
2:B:93:ASP:OD2	18:B:1206:CLA:C1A	2.46	0.64
4:D:64:GLY:O	4:D:65:ALA:CB	2.45	0.64
4:D:48:ILE:O	4:D:73:ASN:O	2.16	0.64
5:E:58:ASP:N	5:E:59:PRO:HD3	2.13	0.64
6:F:13:GLN:O	6:F:14:PHE:HB3	1.97	0.64
12:L:78:GLU:O	12:L:80:ALA:HA	1.97	0.64
14:1:167:ALA:O	14:1:169:PRO:HD3	1.97	0.64
17:4:106:TRP:CE2	17:4:110:LYS:HE3	2.33	0.64
1:A:203:LEU:HD21	18:A:1119:CLA:O2D	1.97	0.64
1:A:143:ILE:HD13	1:A:144:GLN:O	1.98	0.64
2:B:464:GLN:OE1	18:B:1234:CLA:CMD	2.41	0.64
2:B:46:ILE:O	2:B:49:SER:OG	2.07	0.64
2:B:547:MET:O	2:B:549:ASP:N	2.29	0.64
2:B:651:LEU:O	2:B:655:LEU:N	2.31	0.64
2:B:684:ARG:CZ	12:L:22:GLY:HA2	2.27	0.64
4:D:64:GLY:O	4:D:65:ALA:HB3	1.98	0.64
6:F:43:LYS:HG3	6:F:44:ALA:H	1.61	0.64
9:I:19:VAL:HA	9:I:22:ALA:HB3	1.80	0.64
12:L:64:LEU:C	12:L:66:GLY:H	2.01	0.64
14:1:70:LYS:HB2	14:1:73:GLU:CG	2.28	0.64
15:2:94:LEU:HD13	15:2:95:PHE:N	2.13	0.64
16:3:82:ALA:HB1	16:3:84:LEU:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:SER:HB2	1:A:161:GLU:CD	2.18	0.64
1:A:188:LYS:NZ	16:3:54:TRP:CH2	2.65	0.64
1:A:434:ARG:HD3	18:A:1129:CLA:OBD	1.97	0.64
1:A:562:PHE:HB3	1:A:566:SER:HA	1.80	0.64
1:A:71:LEU:CD2	1:A:353:SER:HB2	2.27	0.64
1:A:606:TYR:HE1	1:A:742:GLY:O	1.81	0.64
18:B:1239:CLA:C2B	20:B:6017:BCR:H15C	2.27	0.64
18:B:1242:CLA:HBA2	18:B:1242:CLA:O1D	1.97	0.64
4:D:75:LEU:HD13	4:D:76:LYS:N	2.12	0.64
6:F:136:TRP:HD1	6:F:136:TRP:H	1.46	0.64
6:F:98:GLY:O	6:F:102:ARG:N	2.24	0.64
12:L:94:ILE:O	12:L:98:CYS:N	2.30	0.64
16:3:212:ASN:HB2	16:3:213:LEU:CB	2.28	0.64
17:4:49:ARG:HH21	18:4:4001:CLA:C1C	2.11	0.64
1:A:58:HIS:HE1	18:A:1101:CLA:C1C	2.10	0.64
1:A:441:ALA:O	1:A:445:HIS:HE1	1.81	0.64
2:B:341:LEU:HD21	18:B:1202:CLA:HED2	1.80	0.64
18:B:1208:CLA:O2A	18:B:1209:CLA:H2	1.96	0.64
2:B:289:LEU:O	18:B:1218:CLA:HBC3	1.95	0.64
2:B:194:LEU:O	2:B:195:VAL:HG23	1.97	0.64
2:B:508:LEU:HD13	2:B:509:PHE:HD1	1.63	0.64
2:B:583:MET:SD	2:B:584:LEU:N	2.71	0.64
2:B:5:ILE:CG2	2:B:6:PRO:CA	2.76	0.64
2:B:705:ALA:HB1	19:B:5002:PQN:C7	2.28	0.64
2:B:92:TRP:HD1	9:I:9:VAL:CG1	2.11	0.64
12:L:18:PRO:HG2	12:L:19:PHE:CE1	2.33	0.64
15:2:19:LEU:CA	15:2:20:ASP:C	2.66	0.63
15:2:23:LEU:CD2	15:2:26:ASP:O	2.46	0.63
16:3:132:ASP:O	16:3:133:TRP:HD1	1.80	0.63
1:A:246:HIS:HA	18:A:1147:CLA:C2D	2.28	0.63
1:A:120:ALA:N	1:A:145:ILE:HG21	2.13	0.63
1:A:397:THR:OG1	18:A:1126:CLA:CMB	2.46	0.63
1:A:699:TYR:O	1:A:700:TRP:CD1	2.51	0.63
1:A:725:LEU:HD23	1:A:725:LEU:O	1.97	0.63
18:B:1235:CLA:HBB2	18:B:1236:CLA:HAC2	1.78	0.63
2:B:432:HIS:HE1	18:B:1229:CLA:CHA	2.11	0.63
3:C:69:LEU:HB3	3:C:72:GLU:HG2	1.79	0.63
13:N:49:CYS:SG	13:N:50:GLN:HG3	2.37	0.63
14:1:54:VAL:HA	14:1:57:ILE:HG22	1.79	0.63
1:A:504:ALA:HA	18:A:1134:CLA:NA	2.13	0.63
1:A:649:ILE:O	1:A:652:TRP:HD1	1.73	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1216:CLA:H42	18:B:1242:CLA:HMA1	1.80	0.63
2:B:705:ALA:CB	19:B:5002:PQN:C7	2.76	0.63
2:B:659:THR:HB	18:B:9023:CLA:C3B	2.28	0.63
2:B:703:VAL:HA	2:B:706:ARG:HG2	1.80	0.63
3:C:52:LYS:HZ3	3:C:66:ARG:NH1	1.96	0.63
4:D:109:VAL:CG2	4:D:110:GLN:HG3	2.28	0.63
15:2:178:TRP:N	15:2:178:TRP:CE3	2.66	0.63
15:2:56:MET:HB3	15:2:172:LEU:CD2	2.28	0.63
18:A:1119:CLA:CHD	18:A:1119:CLA:HBC2	2.28	0.63
1:A:216:LEU:HB3	1:A:304:LEU:HG	1.79	0.63
1:A:318:ARG:CD	1:A:319:THR:H	2.12	0.63
1:A:441:ALA:HA	1:A:444:SER:HG	1.61	0.63
1:A:449:VAL:HG13	1:A:450:CYS:H	1.63	0.63
1:A:546:ALA:O	1:A:550:HIS:ND1	2.32	0.63
1:A:96:MET:HB3	1:A:149:PHE:CE2	2.28	0.63
2:B:330:ILE:HG21	18:B:1202:CLA:CBC	2.27	0.63
18:B:1237:CLA:HBC3	18:B:1237:CLA:HMC1	1.80	0.63
2:B:19:ARG:O	2:B:23:PHE:N	2.32	0.63
7:G:83:TYR:CA	7:G:85:ILE:N	2.56	0.63
12:L:66:GLY:C	18:L:1503:CLA:CMB	2.66	0.63
12:L:37:LEU:C	12:L:42:ALA:CB	2.67	0.63
12:L:53:GLY:O	12:L:56:VAL:HG22	1.99	0.63
14:1:52:LEU:HD23	14:1:55:PRO:HG3	1.79	0.63
15:2:188:PRO:C	15:2:192:LEU:HG	2.18	0.63
15:2:23:LEU:HD23	15:2:26:ASP:N	2.00	0.63
1:A:431:LEU:CD1	18:A:1122:CLA:HMC3	2.12	0.63
1:A:126:ILE:HD13	1:A:127:VAL:HG13	1.79	0.63
1:A:360:ILE:O	1:A:364:MET:HB2	1.97	0.63
1:A:371:VAL:HG23	1:A:372:VAL:H	1.63	0.63
1:A:491:TRP:HA	1:A:492:ILE:CB	2.27	0.63
2:B:280:ILE:HG13	2:B:281:ALA:H	1.63	0.63
2:B:393:PHE:HB2	2:B:397:ASP:HB2	1.79	0.63
2:B:508:LEU:CD1	2:B:509:PHE:HD1	2.10	0.63
2:B:704:GLN:C	2:B:706:ARG:N	2.48	0.63
2:B:573:TRP:CH2	2:B:706:ARG:HG3	2.25	0.63
4:D:137:ILE:HD11	4:D:140:ASN:OD1	1.99	0.63
4:D:150:GLY:HA2	4:D:151:LYS:O	1.97	0.63
13:N:66:ASP:O	13:N:67:LEU:HB3	1.98	0.63
15:2:19:LEU:HA	15:2:21:GLY:H	1.63	0.63
16:3:134:TYR:O	16:3:135:ASN:HB2	1.98	0.63
17:4:63:VAL:CG1	17:4:67:ILE:H	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1129:CLA:HMB2	18:L:1130:CLA:C1D	2.28	0.63
18:A:1137:CLA:HBD	18:A:1137:CLA:HBA2	1.81	0.63
1:A:397:THR:OG1	18:A:1126:CLA:HMB1	1.99	0.63
1:A:545:HIS:CE1	1:A:612:VAL:HG22	2.34	0.63
1:A:658:TRP:O	1:A:658:TRP:CG	2.51	0.63
2:B:344:ILE:CG1	18:B:1225:CLA:CBC	2.69	0.63
2:B:693:TRP:HA	18:B:1238:CLA:OBD	1.99	0.63
2:B:77:TRP:CZ3	2:B:130:ARG:NE	2.66	0.63
2:B:596:TRP:CZ3	2:B:613:SER:HB2	2.33	0.63
2:B:648:TRP:HE1	18:B:9022:CLA:H42	0.65	0.63
3:C:29:ILE:HG22	4:D:127:ARG:O	1.99	0.63
6:F:48:LYS:HE2	6:F:48:LYS:N	2.13	0.63
15:2:54:TRP:HE3	15:2:54:TRP:HA	1.63	0.63
17:4:181:ASN:C	17:4:183:LEU:H	2.02	0.63
17:4:40:PHE:O	17:4:41:VAL:C	2.37	0.63
17:4:59:LEU:O	17:4:62:GLU:CB	2.39	0.63
1:A:164:LEU:CD2	1:A:164:LEU:H	2.11	0.63
1:A:658:TRP:CD2	1:A:658:TRP:O	2.51	0.63
1:A:687:ALA:HB1	18:A:9013:CLA:HBB1	1.73	0.63
1:A:95:GLY:HA3	1:A:96:MET:CE	2.28	0.63
2:B:143:LEU:C	2:B:145:LEU:N	2.51	0.63
2:B:372:TYR:CD2	2:B:373:THR:N	2.67	0.63
2:B:478:LEU:CD2	2:B:486:LEU:HB2	2.29	0.63
1:A:591:GLN:OE1	2:B:667:TRP:N	2.31	0.63
18:F:1139:CLA:HMC1	18:F:1139:CLA:HBC3	1.81	0.63
6:F:92:TYR:CZ	6:F:96:TRP:CZ3	2.84	0.63
8:H:64:LEU:HG	8:H:65:LEU:H	1.62	0.63
1:A:284:ARG:HA	1:A:508:THR:HG1	1.63	0.63
1:A:536:THR:O	1:A:537:ALA:CB	2.46	0.63
1:A:582:ASP:HA	2:B:562:PRO:CG	2.29	0.63
1:A:612:VAL:O	1:A:613:ILE:C	2.34	0.63
1:A:663:GLN:NE2	1:A:753:ARG:HH12	1.96	0.63
1:A:666:GLN:O	1:A:668:TYR:N	2.32	0.63
2:B:243:LEU:HA	2:B:264:GLN:HE22	1.63	0.63
2:B:432:HIS:C	2:B:434:LEU:H	2.01	0.63
4:D:82:GLN:O	4:D:85:ALA:HB3	1.99	0.63
8:H:65:LEU:O	8:H:66:THR:O	2.16	0.63
8:H:77:LEU:HD23	8:H:78:PRO:CD	2.28	0.63
13:N:65:LEU:HD12	13:N:68:GLU:CD	2.18	0.63
14:1:94:LEU:CB	14:1:95:PRO:HD3	2.29	0.63
1:A:195:TRP:CZ3	18:A:1118:CLA:C1C	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:O	1:A:310:PHE:CB	2.47	0.63
1:A:407:ILE:HG21	18:A:1124:CLA:C3D	2.28	0.63
1:A:78:VAL:O	1:A:82:HIS:CD2	2.51	0.63
2:B:177:HIS:CE1	18:B:1209:CLA:C3C	2.81	0.63
18:B:1216:CLA:H2A	18:B:1216:CLA:O2D	1.98	0.63
2:B:458:ILE:N	18:B:1235:CLA:HMD1	2.14	0.63
2:B:533:ILE:HG21	2:B:579:ALA:N	2.14	0.63
2:B:657:TRP:HZ3	2:B:661:PHE:CE1	2.14	0.63
2:B:720:THR:OG1	18:B:9010:CLA:HED2	1.99	0.63
4:D:23:ASN:HB2	12:L:17:ASP:OD2	1.99	0.63
18:B:1217:CLA:HMB3	7:G:18:LEU:HD22	1.78	0.63
8:H:47:PHE:HZ	12:L:50:LEU:HD11	1.61	0.63
14:1:70:LYS:CB	14:1:73:GLU:CG	2.77	0.63
17:4:180:ASP:N	17:4:185:HIS:NE2	2.40	0.63
1:A:439:ARG:HG3	1:A:440:ASP:OD2	1.99	0.63
1:A:754:ILE:HA	1:A:758:GLY:HA2	1.81	0.63
2:B:195:VAL:O	2:B:254:ILE:HD11	1.99	0.63
2:B:49:SER:HG	2:B:50:HIS:H	1.46	0.63
2:B:618:GLY:HA2	2:B:621:ARG:HH11	1.63	0.63
2:B:622:ASP:OD1	2:B:626:LEU:HB3	1.99	0.63
2:B:69:ALA:HB2	2:B:132:ASN:HB3	1.80	0.63
4:D:77:LEU:HD12	4:D:77:LEU:O	1.98	0.63
5:E:61:THR:HG23	5:E:62:ARG:H	1.63	0.63
6:F:52:ARG:C	6:F:55:ASN:HB2	2.19	0.63
6:F:92:TYR:CE2	6:F:96:TRP:CZ3	2.87	0.63
18:L:1503:CLA:CED	18:L:1503:CLA:O1A	2.44	0.63
15:2:86:GLU:OE1	17:4:187:SER:CB	2.47	0.62
1:A:118:PRO:HA	1:A:150:PHE:CE2	2.34	0.62
1:A:371:VAL:O	1:A:375:HIS:HB2	1.99	0.62
1:A:690:LEU:HG	1:A:694:PHE:CZ	2.34	0.62
18:B:1214:CLA:HBA1	18:B:1223:CLA:C2B	2.28	0.62
18:B:1239:CLA:CHB	20:B:6017:BCR:H15C	2.29	0.62
2:B:314:ARG:HB3	18:B:1301:CLA:C2A	2.28	0.62
2:B:415:LYS:HD3	2:B:539:LEU:HG	1.80	0.62
6:F:97:ILE:HG23	18:F:1240:CLA:CHD	2.29	0.62
14:1:89:VAL:HG12	14:1:90:PRO:CD	2.27	0.62
15:2:187:GLY:C	15:2:189:ILE:N	2.53	0.62
15:2:23:LEU:HB3	15:2:26:ASP:H	1.62	0.62
17:4:56:ALA:CA	17:4:59:LEU:HB3	2.29	0.62
1:A:90:PHE:CD1	1:A:175:ALA:HA	2.30	0.62
1:A:235:ALA:O	1:A:236:GLY:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PHE:CD1	1:A:237:VAL:HG21	2.34	0.62
1:A:253:ASP:O	1:A:257:GLN:N	2.31	0.62
1:A:425:THR:HG21	1:A:428:TYR:HE2	1.64	0.62
1:A:441:ALA:C	1:A:445:HIS:CE1	2.73	0.62
1:A:542:HIS:HA	1:A:545:HIS:HD2	1.61	0.62
1:A:572:LYS:HD2	1:A:579:PHE:CE2	2.34	0.62
1:A:590:CYS:O	1:A:592:VAL:HG23	2.00	0.62
1:A:603:PHE:O	1:A:606:TYR:HB3	1.99	0.62
1:A:654:ARG:HD3	1:A:655:ASP:OD2	1.99	0.62
1:A:663:GLN:CG	1:A:753:ARG:HA	2.23	0.62
2:B:104:PHE:CA	2:B:106:ARG:HD2	2.29	0.62
18:B:1205:CLA:HMD2	18:B:1224:CLA:O1A	1.98	0.62
18:B:1212:CLA:CAA	18:B:1212:CLA:H2	2.29	0.62
2:B:149:SER:O	2:B:152:ALA:HB3	1.99	0.62
2:B:304:ILE:HG22	2:B:305:LEU:HD12	1.79	0.62
2:B:414:HIS:O	2:B:414:HIS:CG	2.52	0.62
2:B:678:LEU:HD22	2:B:678:LEU:C	2.18	0.62
2:B:712:HIS:O	2:B:713:PHE:O	2.18	0.62
7:G:35:VAL:HG12	7:G:36:PRO:HB3	1.79	0.62
12:L:148:VAL:HA	12:L:151:VAL:HG22	1.80	0.62
12:L:147:GLY:O	12:L:151:VAL:N	2.28	0.62
12:L:83:ALA:HA	12:L:86:LEU:CD2	2.29	0.62
13:N:57:LYS:CG	16:3:87:ALA:CB	2.73	0.62
14:1:186:HIS:HB2	14:1:188:ASN:O	1.99	0.62
15:2:19:LEU:H	15:2:22:SER:HB2	1.63	0.62
16:3:200:ILE:C	16:3:204:VAL:HG22	2.19	0.62
1:A:126:ILE:HG23	1:A:127:VAL:HG22	1.80	0.62
1:A:340:GLY:C	1:A:342:GLY:N	2.53	0.62
1:A:688:PHE:HZ	18:A:1140:CLA:C2C	2.12	0.62
2:B:102:GLU:OE1	2:B:641:ASN:HB3	1.99	0.62
3:C:49:VAL:HG13	3:C:49:VAL:O	1.99	0.62
4:D:83:CYS:O	4:D:85:ALA:N	2.33	0.62
4:D:88:THR:O	4:D:91:ARG:HB2	1.99	0.62
6:F:125:LEU:HB3	6:F:130:LEU:HD21	1.79	0.62
6:F:83:PHE:O	6:F:87:GLY:HA3	1.99	0.62
1:A:150:PHE:HA	1:A:153:TRP:HE1	1.62	0.62
1:A:57:LEU:C	1:A:57:LEU:HD23	2.20	0.62
1:A:674:ALA:O	1:A:678:PHE:N	2.32	0.62
2:B:697:PRO:HG2	18:B:1238:CLA:HBC2	1.81	0.62
2:B:77:TRP:O	2:B:130:ARG:NH2	2.33	0.62
2:B:416:GLU:HA	2:B:419:ILE:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:PHE:O	2:B:521:HIS:N	2.33	0.62
2:B:52:GLY:O	2:B:55:ALA:CB	2.47	0.62
2:B:614:THR:O	2:B:615:TYR:HB3	1.99	0.62
4:D:133:ASN:CG	4:D:135:ARG:HB2	2.20	0.62
6:F:80:TRP:HE1	18:F:1302:CLA:CBC	2.06	0.62
15:2:19:LEU:N	15:2:20:ASP:C	2.53	0.62
16:3:186:LYS:HA	18:3:3004:CLA:C2C	2.29	0.62
16:3:207:VAL:O	16:3:208:GLY:C	2.37	0.62
13:N:57:LYS:CD	16:3:87:ALA:CB	2.39	0.62
1:A:364:MET:HG2	18:A:1123:CLA:H3A	1.81	0.62
1:A:434:ARG:O	1:A:438:HIS:CD2	2.51	0.62
2:B:510:LEU:HD13	18:B:1234:CLA:HMD3	1.82	0.62
2:B:557:PHE:CZ	2:B:570:ILE:HG13	2.34	0.62
2:B:65:LEU:HG	2:B:124:TRP:CH2	2.34	0.62
2:B:8:PHE:N	2:B:8:PHE:CD1	2.67	0.62
2:B:91:ILE:CD1	2:B:114:ASN:HD22	2.13	0.62
6:F:127:SER:O	6:F:129:LEU:N	2.33	0.62
8:H:47:PHE:HE2	12:L:138:LYS:HB2	1.61	0.62
12:L:132:SER:HB2	12:L:135:GLY:HA3	1.80	0.62
14:1:52:LEU:HA	14:1:55:PRO:CG	2.29	0.62
15:2:70:LYS:H	15:2:70:LYS:CD	2.12	0.62
13:N:58:VAL:CB	16:3:86:PRO:HA	2.27	0.62
1:A:460:LEU:HD13	18:A:1132:CLA:C3C	2.30	0.62
2:B:330:ILE:HG22	2:B:331:HIS:H	1.62	0.62
2:B:407:VAL:O	2:B:411:MET:N	2.25	0.62
2:B:504:ASN:C	2:B:506:ASN:N	2.52	0.62
2:B:659:THR:C	2:B:661:PHE:H	2.02	0.62
3:C:35:LYS:O	3:C:35:LYS:CG	2.48	0.62
5:E:44:TYR:CE1	5:E:74:TYR:HE2	2.18	0.62
7:G:34:GLN:NE2	7:G:36:PRO:CG	2.50	0.62
7:G:83:TYR:HB2	7:G:85:ILE:CG1	2.27	0.62
13:N:47:THR:CA	13:N:49:CYS:SG	2.87	0.62
14:1:160:GLY:O	14:1:163:VAL:HG12	1.99	0.62
15:2:32:LEU:O	15:2:32:LEU:HD22	1.96	0.62
15:2:86:GLU:HG2	17:4:184:GLN:CD	2.20	0.62
1:A:203:LEU:HD13	18:A:1123:CLA:CHD	2.29	0.62
1:A:346:LEU:HD22	1:A:347:TYR:H	1.64	0.62
1:A:387:THR:O	1:A:389:TYR:CZ	2.53	0.62
1:A:499:ALA:O	1:A:503:THR:O	2.16	0.62
1:A:64:PHE:C	1:A:67:HIS:H	2.03	0.62
1:A:681:GLY:CA	20:A:6011:BCR:H17C	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LEU:O	1:A:743:ILE:HD13	2.00	0.62
2:B:374:HIS:O	2:B:376:GLN:N	2.33	0.62
2:B:58:PHE:CE1	2:B:145:LEU:HB3	2.34	0.62
2:B:59:LEU:O	2:B:59:LEU:HD22	1.98	0.62
2:B:609:PHE:O	2:B:611:GLU:N	2.32	0.62
3:C:22:PRO:O	4:D:84:LEU:HD11	2.00	0.62
3:C:41:SER:HG	4:D:132:LEU:HD21	1.64	0.62
1:A:714:LEU:HD23	6:F:149:LEU:HD22	1.80	0.62
18:A:1129:CLA:H3A	18:L:1130:CLA:OBD	2.00	0.62
18:L:1503:CLA:CBD	18:L:1503:CLA:CAA	2.77	0.62
12:L:73:PRO:HB2	12:L:74:LEU:HG	1.82	0.62
13:N:47:THR:N	13:N:49:CYS:SG	2.73	0.62
14:1:44:LEU:H	14:1:44:LEU:HD22	1.64	0.62
1:A:404:GLY:HA3	1:A:609:ILE:HG13	1.81	0.62
1:A:494:ASN:O	1:A:495:THR:HB	1.99	0.62
1:A:548:THR:C	1:A:550:HIS:H	2.01	0.62
1:A:558:LYS:O	1:A:562:PHE:CD1	2.53	0.62
2:B:126:THR:HB	18:B:1215:CLA:CED	2.22	0.62
6:F:136:TRP:N	6:F:136:TRP:HD1	1.97	0.62
6:F:82:GLU:O	10:J:38:THR:HG21	1.99	0.62
14:1:153:LEU:HD22	14:1:153:LEU:H	1.64	0.62
16:3:132:ASP:OD1	16:3:139:MET:CB	2.38	0.62
1:A:214:GLY:O	1:A:217:SER:N	2.30	0.62
1:A:326:GLY:CA	1:A:330:ILE:HG13	2.28	0.62
1:A:328:LYS:O	1:A:332:GLU:OE2	2.18	0.62
18:B:1208:CLA:H62	18:B:1209:CLA:H43	1.82	0.62
2:B:215:VAL:CB	2:B:217:PRO:HD3	2.28	0.62
2:B:31:PHE:HD2	2:B:34:HIS:HD1	1.46	0.62
2:B:593:TYR:CZ	18:B:1234:CLA:HAC2	2.34	0.62
18:B:1237:CLA:HMD2	20:B:6017:BCR:H281	1.81	0.62
3:C:62:PHE:CE2	5:E:43:SER:N	2.62	0.62
5:E:51:SER:HB2	5:E:69:PHE:CD2	2.34	0.62
6:F:86:PRO:HD3	10:J:39:PHE:HB2	1.82	0.62
8:H:41:GLU:CD	12:L:50:LEU:HD13	2.20	0.62
15:2:26:ASP:HB2	15:2:27:PHE:CD2	2.35	0.62
1:A:441:ALA:C	1:A:445:HIS:HE1	2.03	0.62
1:A:449:VAL:HG13	1:A:450:CYS:N	2.15	0.62
1:A:486:PRO:HD2	1:A:487:VAL:CB	2.30	0.62
1:A:88:ILE:O	1:A:92:TRP:N	2.30	0.62
2:B:207:VAL:HA	2:B:211:ASN:HD21	1.63	0.62
2:B:280:ILE:CA	18:B:1214:CLA:HMC3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:SER:O	2:B:34:HIS:CD2	2.52	0.62
2:B:715:VAL:HA	2:B:718:ILE:HD12	1.81	0.62
2:B:724:PHE:O	2:B:726:ILE:N	2.33	0.62
18:B:9023:CLA:HMA2	20:B:6017:BCR:C40	2.30	0.62
2:B:19:ARG:NH1	3:C:72:GLU:HB3	2.10	0.62
5:E:37:LYS:HB2	5:E:89:GLU:HB2	1.80	0.62
15:2:24:PRO:HB3	15:2:32:LEU:CB	2.30	0.61
17:4:158:ARG:HH11	17:4:158:ARG:HG2	1.65	0.61
1:A:282:THR:O	1:A:284:ARG:HG2	2.00	0.61
1:A:308:ILE:CD1	1:A:311:LEU:HD22	2.30	0.61
18:B:1215:CLA:CBB	18:B:1215:CLA:H62	2.29	0.61
2:B:290:MET:HG3	18:B:1218:CLA:C2C	2.29	0.61
2:B:420:SER:CA	18:B:1138:CLA:HED1	2.30	0.61
2:B:425:ALA:HB1	2:B:528:HIS:CD2	2.35	0.61
2:B:52:GLY:O	2:B:55:ALA:HB3	2.00	0.61
7:G:33:LYS:HB3	7:G:34:GLN:HB3	1.80	0.61
13:N:78:GLY:HA3	13:N:80:ASN:OD1	2.00	0.61
17:4:81:GLU:H	17:4:82:GLU:HA	1.66	0.61
1:A:466:THR:O	1:A:470:LEU:HB3	1.99	0.61
1:A:685:VAL:O	1:A:685:VAL:HG13	2.01	0.61
2:B:622:ASP:OD1	2:B:626:LEU:HD22	1.99	0.61
2:B:680:TRP:C	2:B:680:TRP:HE3	2.03	0.61
4:D:58:PHE:HE2	4:D:90:LEU:CD2	2.13	0.61
18:G:1233:CLA:HBC2	18:G:1233:CLA:HHD	1.80	0.61
1:A:383:PRO:C	1:A:384:TYR:HD1	2.03	0.61
1:A:435:VAL:HG22	1:A:438:HIS:HE1	1.64	0.61
1:A:463:HIS:O	1:A:467:MET:N	2.33	0.61
2:B:403:ASN:O	2:B:406:ASN:ND2	2.34	0.61
2:B:69:ALA:CB	2:B:132:ASN:HB3	2.31	0.61
1:A:567:ARG:HH22	4:D:37:LEU:CG	2.13	0.61
4:D:88:THR:O	4:D:91:ARG:N	2.33	0.61
5:E:37:LYS:CE	5:E:39:LEU:HD12	2.30	0.61
5:E:45:TRP:O	5:E:45:TRP:CG	2.51	0.61
10:J:13:VAL:O	10:J:17:LEU:HB2	2.00	0.61
12:L:94:ILE:C	12:L:96:SER:H	2.04	0.61
15:2:24:PRO:HD2	15:2:27:PHE:CD2	2.32	0.61
15:2:94:LEU:HD11	15:2:98:GLU:OE2	2.00	0.61
16:3:74:ILE:HD13	16:3:199:PHE:CD2	2.36	0.61
17:4:126:LEU:C	17:4:153:GLU:OE2	2.39	0.61
17:4:185:HIS:C	17:4:186:ILE:HG12	2.20	0.61
1:A:369:THR:HB	18:A:1127:CLA:C3C	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:HD11	18:A:1108:CLA:HAC1	1.82	0.61
1:A:317:TYR:C	1:A:324:GLY:HA3	2.21	0.61
1:A:330:ILE:O	1:A:333:ALA:HB3	2.00	0.61
1:A:663:GLN:HE21	1:A:753:ARG:HH11	1.47	0.61
1:A:95:GLY:N	1:A:96:MET:SD	2.73	0.61
18:B:1218:CLA:C2A	18:B:1218:CLA:O1D	2.46	0.61
4:D:45:PHE:O	4:D:45:PHE:HD1	1.83	0.61
8:H:26:SER:HA	8:H:27:ASP:C	2.20	0.61
8:H:41:GLU:OE1	12:L:50:LEU:HD22	2.00	0.61
8:H:73:PRO:HB2	8:H:74:GLN:CB	2.29	0.61
13:N:77:CYS:SG	13:N:81:VAL:O	2.57	0.61
13:N:9:LYS:O	13:N:13:ASN:N	2.32	0.61
14:1:102:PHE:O	14:1:106:ALA:N	2.33	0.61
17:4:149:ALA:HB1	17:4:150:LYS:HG2	1.81	0.61
18:A:1126:CLA:C4A	18:A:1126:CLA:HBA2	2.31	0.61
1:A:585:GLY:C	1:A:587:GLY:H	2.03	0.61
2:B:257:ILE:HG12	18:B:1214:CLA:HMB2	1.81	0.61
2:B:432:HIS:HE1	18:B:1229:CLA:C4D	2.12	0.61
2:B:649:MET:O	2:B:652:PHE:CB	2.46	0.61
18:B:9023:CLA:CGA	18:B:9023:CLA:C3A	2.74	0.61
6:F:137:PRO:HA	6:F:141:TYR:HB3	0.73	0.61
6:F:5:LEU:O	6:F:62:LEU:HG	2.01	0.61
6:F:66:ASP:OD2	6:F:68:LEU:HB2	2.00	0.61
8:H:76:VAL:O	8:H:77:LEU:O	2.18	0.61
18:J:2107:CLA:H52	18:2:2005:CLA:C2A	2.30	0.61
11:K:7:UNK:O	11:K:11:UNK:N	2.34	0.61
12:L:66:GLY:C	18:L:1503:CLA:HMB3	2.19	0.61
13:N:59:PRO:HA	13:N:60:PHE:HB3	1.80	0.61
15:2:194:ALA:HB3	15:2:195:HIS:CA	2.29	0.61
18:A:1133:CLA:CHC	18:A:1134:CLA:C2B	2.79	0.61
1:A:133:ASN:CB	1:A:142:GLY:HA2	2.30	0.61
1:A:347:TYR:CD2	1:A:349:ILE:HG22	2.36	0.61
1:A:700:TRP:CE2	19:A:5001:PQN:H2M3	2.35	0.61
2:B:312:GLY:H	18:B:1301:CLA:C2D	2.13	0.61
2:B:344:ILE:HG13	18:B:1225:CLA:CAC	2.30	0.61
2:B:508:LEU:CD1	2:B:509:PHE:CD1	2.83	0.61
2:B:518:LEU:HD23	2:B:614:THR:HA	1.82	0.61
2:B:636:THR:O	2:B:638:LEU:N	2.32	0.61
2:B:646:TRP:CE3	2:B:723:ALA:CA	2.83	0.61
2:B:35:ASP:HB3	4:D:154:TYR:HE1	1.66	0.61
5:E:79:THR:O	5:E:80:ASN:O	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:61:ASN:CA	7:G:64:VAL:HG22	2.29	0.61
8:H:42:THR:OG1	8:H:47:PHE:HE1	1.82	0.61
12:L:107:PHE:HA	12:L:133:ALA:HB3	1.82	0.61
12:L:53:GLY:N	12:L:139:PHE:HE1	1.98	0.61
16:3:143:TYR:O	16:3:144:PHE:HB2	2.00	0.61
1:A:222:GLN:NE2	1:A:222:GLN:O	2.33	0.61
1:A:242:ILE:O	1:A:244:LEU:N	2.33	0.61
1:A:427:ARG:O	1:A:430:ASP:HB2	2.01	0.61
18:A:1140:CLA:H51	19:A:5001:PQN:C19	2.29	0.61
19:A:5001:PQN:H212	18:B:1138:CLA:CBC	2.30	0.61
1:A:718:PRO:HG2	1:A:722:PRO:HD3	1.80	0.61
18:B:1238:CLA:O1A	9:I:21:MET:SD	2.58	0.61
2:B:708:VAL:HG12	18:B:1239:CLA:O1D	2.00	0.61
2:B:196:HIS:HE1	18:B:1211:CLA:C3C	2.12	0.61
2:B:463:ILE:C	2:B:465:SER:H	2.03	0.61
2:B:593:TYR:O	2:B:594:TRP:HB2	2.01	0.61
2:B:365:PHE:CD1	2:B:602:TRP:CG	2.89	0.61
2:B:73:ASN:O	2:B:77:TRP:N	2.31	0.61
2:B:84:VAL:HG12	2:B:85:ARG:H	1.59	0.61
4:D:96:ILE:HG12	4:D:97:LYS:H	1.63	0.61
5:E:75:ALA:O	5:E:76:ASN:HB2	2.00	0.61
18:A:1105:CLA:C2B	18:A:1107:CLA:CED	2.78	0.61
1:A:369:THR:HG21	18:A:1127:CLA:C2C	2.30	0.61
1:A:442:ILE:HD12	1:A:443:ILE:H	1.65	0.61
1:A:461:TYR:HB2	1:A:649:ILE:CG1	2.29	0.61
1:A:688:PHE:CG	1:A:688:PHE:O	2.53	0.61
2:B:341:LEU:HD21	18:B:1202:CLA:CED	2.30	0.61
18:B:1209:CLA:HBA2	7:G:38:GLN:HG2	1.82	0.61
2:B:273:VAL:HG22	18:B:1214:CLA:CMA	2.30	0.61
2:B:19:ARG:HH11	2:B:19:ARG:HG3	1.65	0.61
2:B:350:GLN:O	2:B:354:SER:N	2.28	0.61
2:B:4:ARG:HG3	2:B:4:ARG:HH11	1.66	0.61
3:C:31:TRP:CH2	3:C:33:GLY:HA3	2.35	0.61
4:D:102:ARG:CG	4:D:110:GLN:HB2	2.28	0.61
5:E:40:ARG:HB2	5:E:86:GLU:HG3	1.82	0.61
8:H:86:PRO:O	8:H:87:PRO:O	2.19	0.61
13:N:69:CYS:HB3	13:N:72:LYS:HG3	1.80	0.61
13:N:72:LYS:CA	13:N:75:TYR:O	2.49	0.61
14:1:164:GLN:OE1	14:1:181:LEU:HD11	2.00	0.61
1:A:346:LEU:HG	18:A:1122:CLA:HMD3	1.81	0.61
1:A:392:GLN:OE1	1:A:392:GLN:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:HH21	1:A:438:HIS:CB	2.14	0.61
1:A:473:PRO:O	1:A:474:GLN:C	2.37	0.61
1:A:496:HIS:ND1	1:A:515:TRP:CD2	2.61	0.61
1:A:81:ALA:HB3	1:A:83:PHE:CA	2.24	0.61
2:B:371:LEU:HD22	18:B:1225:CLA:O1D	2.01	0.61
2:B:478:LEU:HG	2:B:486:LEU:HB2	1.82	0.61
2:B:53:GLN:C	2:B:55:ALA:N	2.51	0.61
4:D:24:THR:OG1	4:D:24:THR:O	2.19	0.61
12:L:70:LYS:HA	12:L:75:ARG:HA	1.82	0.61
13:N:73:ASP:N	13:N:75:TYR:O	2.33	0.61
15:2:33:GLY:CA	15:2:35:SER:HB3	2.31	0.61
17:4:136:GLY:HA3	17:4:139:ASN:HA	1.83	0.61
1:A:654:ARG:HD2	1:A:655:ASP:OD2	2.01	0.61
1:A:679:PHE:C	1:A:679:PHE:HD1	2.03	0.61
1:A:79:PHE:C	1:A:81:ALA:HB2	2.20	0.61
2:B:175:LEU:HA	18:B:1221:CLA:HED1	1.83	0.61
2:B:577:TYR:O	2:B:578:LEU:HB2	2.00	0.61
3:C:52:LYS:NZ	3:C:66:ARG:NH1	2.49	0.61
5:E:56:ASP:OD1	5:E:56:ASP:N	2.33	0.61
6:F:100:VAL:HG12	6:F:125:LEU:HD21	1.82	0.61
6:F:42:ILE:HG12	6:F:43:LYS:N	2.14	0.61
6:F:84:ILE:HA	6:F:87:GLY:HA3	1.83	0.61
18:B:1209:CLA:HBA2	7:G:38:GLN:CG	2.31	0.61
11:K:55:UNK:O	11:K:57:UNK:N	2.34	0.61
14:1:185:TRP:O	14:1:186:HIS:HB2	2.00	0.60
14:1:86:GLY:N	14:1:87:ASN:HA	2.15	0.60
15:2:36:SER:CA	15:2:37:ASP:HB2	2.26	0.60
17:4:194:ILE:O	17:4:196:GLN:HG2	1.99	0.60
17:4:37:LEU:O	17:4:39:TRP:N	2.28	0.60
1:A:364:MET:HG2	18:A:1123:CLA:C3A	2.31	0.60
1:A:32:GLU:HB2	1:A:33:GLN:CA	2.24	0.60
1:A:377:TYR:CD2	1:A:396:PHE:HE1	2.18	0.60
1:A:369:THR:O	1:A:403:GLY:HA3	2.01	0.60
1:A:439:ARG:C	1:A:441:ALA:H	2.04	0.60
1:A:387:THR:OG1	1:A:526:LYS:HG3	2.01	0.60
1:A:50:THR:CG2	1:A:723:ARG:NH1	2.53	0.60
18:B:1237:CLA:HAC1	18:B:1238:CLA:C4B	2.31	0.60
2:B:195:VAL:HG13	2:B:254:ILE:HD11	1.83	0.60
2:B:271:THR:HA	2:B:274:ALA:HB2	1.83	0.60
3:C:27:GLU:CB	3:C:43:PRO:HG3	2.30	0.60
6:F:49:THR:O	6:F:52:ARG:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:73:PRO:HA	8:H:75:ASP:OD2	2.01	0.60
13:N:16:LEU:HG	13:N:19:LYS:NZ	2.16	0.60
13:N:58:VAL:HG22	13:N:60:PHE:CD1	2.36	0.60
15:2:159:LEU:O	15:2:162:LYS:CG	2.49	0.60
15:2:44:ASN:OD1	15:2:46:GLN:HB2	2.01	0.60
1:A:199:VAL:CG2	1:A:199:VAL:O	2.36	0.60
1:A:41:SER:O	1:A:43:THR:N	2.33	0.60
1:A:505:PRO:HD3	18:A:1134:CLA:C4D	2.32	0.60
1:A:556:LEU:C	1:A:560:VAL:HG13	2.21	0.60
2:B:122:GLN:O	2:B:126:THR:OG1	2.19	0.60
2:B:171:ALA:HB1	2:B:172:GLU:OE2	2.02	0.60
2:B:284:PHE:C	2:B:286:ILE:H	2.05	0.60
2:B:393:PHE:HE2	2:B:398:TYR:CD1	2.19	0.60
2:B:525:LEU:HG	2:B:526:GLY:N	2.16	0.60
2:B:526:GLY:HA2	2:B:582:TRP:CZ3	2.25	0.60
3:C:7:ILE:CD1	3:C:65:VAL:HA	2.26	0.60
6:F:108:ILE:O	6:F:114:PRO:HB3	2.01	0.60
15:2:33:GLY:CA	15:2:34:LEU:C	2.69	0.60
1:A:323:ILE:HG12	18:A:1108:CLA:HMA2	1.84	0.60
1:A:751:LEU:O	1:A:754:ILE:N	2.34	0.60
2:B:101:VAL:CA	2:B:105:THR:OG1	2.46	0.60
18:B:1138:CLA:CAD	18:B:1138:CLA:CED	2.78	0.60
2:B:178:HIS:CE1	18:B:1210:CLA:NC	2.69	0.60
2:B:398:TYR:O	4:D:142:SER:CB	2.50	0.60
4:D:153:PRO:O	4:D:154:TYR:CD2	2.38	0.60
12:L:33:ILE:O	12:L:33:ILE:HG22	2.01	0.60
14:1:118:PRO:N	14:1:119:GLU:HA	2.16	0.60
15:2:97:VAL:HG23	15:2:98:GLU:N	2.17	0.60
16:3:82:ALA:HB1	16:3:83:GLY:C	2.22	0.60
1:A:224:HIS:HB3	1:A:248:PHE:CD2	2.36	0.60
1:A:42:ARG:HG2	1:A:43:THR:H	1.66	0.60
1:A:55:TRP:O	1:A:59:ALA:HB3	2.01	0.60
1:A:578:ARG:O	1:A:593:SER:OG	2.14	0.60
1:A:639:ALA:C	1:A:641:ASN:N	2.55	0.60
1:A:697:ARG:CD	1:A:727:ILE:H	2.14	0.60
2:B:63:GLY:O	2:B:65:LEU:N	2.35	0.60
2:B:595:HIS:CE1	2:B:725:LEU:HD22	2.36	0.60
3:C:22:PRO:CD	3:C:51:CYS:SG	2.89	0.60
4:D:136:SER:N	4:D:139:LYS:HZ2	1.99	0.60
6:F:26:GLN:C	6:F:28:SER:H	2.05	0.60
9:I:6:SER:O	9:I:7:LEU:C	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:109:GLU:HA	12:L:134:ASP:HB2	1.83	0.60
12:L:138:LYS:HB3	12:L:138:LYS:NZ	2.16	0.60
12:L:145:PHE:O	12:L:148:VAL:O	2.19	0.60
12:L:83:ALA:HA	12:L:86:LEU:HD21	1.84	0.60
16:3:134:TYR:CA	16:3:136:PRO:CD	2.75	0.60
1:A:688:PHE:CZ	18:A:1140:CLA:C1C	2.84	0.60
1:A:605:MET:HE3	1:A:606:TYR:N	2.16	0.60
1:A:613:ILE:HG22	1:A:614:PHE:N	2.16	0.60
1:A:603:PHE:CE2	1:A:735:VAL:HA	2.35	0.60
1:A:750:PHE:CD1	1:A:750:PHE:C	2.74	0.60
2:B:239:SER:OG	2:B:249:GLY:O	2.17	0.60
2:B:382:ILE:O	2:B:386:ALA:HB2	2.01	0.60
2:B:448:THR:CG2	2:B:451:LYS:HE2	2.30	0.60
5:E:40:ARG:HG3	5:E:85:ASP:O	2.02	0.60
6:F:141:TYR:C	6:F:143:GLU:H	2.04	0.60
18:A:1136:CLA:C9	18:L:1504:CLA:HMC2	2.30	0.60
15:2:162:LYS:NZ	15:2:163:GLU:HB2	2.16	0.60
15:2:180:GLN:O	15:2:182:ILE:N	2.32	0.60
15:2:178:TRP:HB3	15:2:183:TYR:CE2	2.37	0.60
16:3:133:TRP:HB3	16:3:135:ASN:H	1.65	0.60
16:3:196:LEU:HD22	18:3:3005:CLA:C3B	2.31	0.60
17:4:118:ASP:H	17:4:119:PRO:HD3	1.66	0.60
1:A:109:TRP:CZ3	1:A:150:PHE:HB3	2.37	0.60
1:A:200:GLU:HG2	1:A:318:ARG:HG3	1.82	0.60
1:A:688:PHE:CE1	1:A:737:HIS:HD2	2.20	0.60
2:B:593:TYR:OH	18:B:1234:CLA:CAC	2.50	0.60
18:B:9023:CLA:HMB3	18:B:1239:CLA:HMC3	1.83	0.60
2:B:317:ARG:HG2	2:B:317:ARG:NH2	2.04	0.60
2:B:606:VAL:HG22	2:B:610:ASN:ND2	2.17	0.60
13:N:23:ALA:HB1	13:N:27:ALA:HB3	1.83	0.60
15:2:103:GLY:O	15:2:106:GLU:HG3	2.02	0.60
17:4:102:GLU:O	17:4:105:ARG:CG	2.49	0.60
1:A:113:PRO:HG3	1:A:154:ARG:HH12	1.66	0.60
1:A:308:ILE:HA	1:A:311:LEU:HB3	1.84	0.60
1:A:462:ILE:HG22	1:A:463:HIS:N	2.15	0.60
1:A:657:LEU:C	1:A:659:ALA:H	2.05	0.60
2:B:351:HIS:NE2	18:B:1223:CLA:ND	2.49	0.60
2:B:19:ARG:O	2:B:20:ARG:C	2.39	0.60
2:B:428:PHE:HD2	2:B:432:HIS:NE2	1.95	0.60
3:C:44:ARG:HH22	4:D:115:LYS:HE3	1.67	0.60
3:C:55:GLU:CB	3:C:65:VAL:HG21	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:133:TRP:NE1	16:3:139:MET:O	2.33	0.60
2:B:133:GLU:CA	2:B:136:TYR:HE1	2.11	0.60
2:B:50:HIS:ND1	2:B:50:HIS:O	2.33	0.60
2:B:558:PRO:HA	2:B:703:VAL:HG23	1.84	0.60
3:C:4:SER:CB	3:C:5:VAL:HA	2.31	0.60
9:I:15:LEU:O	9:I:18:ALA:HB3	2.02	0.60
13:N:58:VAL:HG12	16:3:86:PRO:CB	2.31	0.60
15:2:32:LEU:CA	15:2:33:GLY:C	2.67	0.60
15:2:45:VAL:N	15:2:46:GLN:OE1	2.35	0.60
17:4:114:SER:HB2	17:4:120:ILE:HG12	1.84	0.60
1:A:99:HIS:ND1	1:A:103:PHE:HZ	2.00	0.60
18:A:1137:CLA:CB	18:A:1137:CLA:HBA1	2.32	0.60
1:A:198:ASP:CG	1:A:199:VAL:N	2.54	0.60
1:A:218:TRP:HZ3	18:A:1148:CLA:C4D	2.14	0.60
1:A:250:LEU:HD23	1:A:251:ASN:H	1.66	0.60
1:A:346:LEU:O	1:A:347:TYR:O	2.19	0.60
1:A:743:ILE:O	1:A:746:THR:N	2.33	0.60
1:A:751:LEU:O	1:A:753:ARG:N	2.35	0.60
2:B:520:HIS:NE2	18:B:1234:CLA:NC	2.50	0.60
2:B:187:SER:O	2:B:188:LEU:C	2.40	0.60
2:B:537:GLY:CA	2:B:575:ASP:HB3	2.30	0.60
2:B:546:LEU:HD21	5:E:74:TYR:CE1	2.35	0.60
3:C:63:LEU:CD2	3:C:66:ARG:HG2	2.32	0.60
3:C:63:LEU:C	3:C:63:LEU:HD13	2.21	0.60
7:G:16:LEU:CD2	7:G:68:ILE:HG12	2.32	0.60
12:L:37:LEU:C	12:L:42:ALA:HB3	2.21	0.60
13:N:36:GLU:HA	13:N:39:SER:HB3	1.83	0.60
15:2:93:THR:N	15:2:94:LEU:CB	2.61	0.60
1:A:109:TRP:O	1:A:111:ASN:OD1	2.20	0.60
1:A:347:TYR:HB3	1:A:350:LEU:HG	1.84	0.60
1:A:383:PRO:C	1:A:384:TYR:CD1	2.75	0.60
1:A:541:VAL:O	1:A:544:ILE:N	2.35	0.60
1:A:704:ILE:HG13	1:A:724:ALA:HB2	1.84	0.60
1:A:87:SER:OG	1:A:179:LEU:HB2	2.02	0.60
2:B:260:GLY:N	2:B:269:TRP:CE2	2.70	0.60
2:B:436:LEU:HD23	2:B:453:ILE:HG13	1.84	0.60
2:B:720:THR:CB	18:B:9010:CLA:O1D	2.50	0.60
13:N:45:ASN:O	13:N:49:CYS:SG	2.60	0.60
13:N:77:CYS:HB2	13:N:78:GLY:HA2	1.80	0.60
16:3:55:LEU:CD1	16:3:58:GLY:HA3	2.27	0.59
1:A:135:ASP:H	1:A:136:VAL:HG22	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLN:OE1	1:A:351:THR:HB	2.02	0.59
1:A:479:ASP:C	1:A:481:ALA:H	2.05	0.59
1:A:582:ASP:CG	1:A:583:GLY:H	2.06	0.59
1:A:649:ILE:HG22	1:A:650:ASN:N	2.17	0.59
2:B:311:PRO:HD3	18:B:1219:CLA:CBB	2.31	0.59
2:B:216:LEU:N	2:B:217:PRO:HD3	2.17	0.59
2:B:680:TRP:C	2:B:680:TRP:CE3	2.75	0.59
4:D:55:GLU:O	4:D:57:ILE:HD12	2.02	0.59
6:F:73:VAL:HB	6:F:83:PHE:CE2	2.37	0.59
7:G:5:SER:HA	18:G:1233:CLA:HBA1	1.82	0.59
11:K:13:UNK:O	11:K:17:UNK:CB	2.50	0.59
12:L:40:LEU:HD13	18:L:1502:CLA:HBD	1.83	0.59
17:4:60:LEU:C	17:4:62:GLU:N	2.53	0.59
18:A:1129:CLA:HAA2	18:A:1129:CLA:HBD	1.84	0.59
1:A:232:PHE:CZ	1:A:243:PRO:HG2	2.37	0.59
1:A:483:GLN:OE1	1:A:485:GLN:CA	2.48	0.59
1:A:572:LYS:O	1:A:574:ASN:HB2	2.02	0.59
2:B:101:VAL:O	2:B:106:ARG:NH1	2.34	0.59
2:B:346:SER:CB	18:B:1222:CLA:O1D	2.48	0.59
2:B:344:ILE:CD1	18:B:1225:CLA:CBC	1.81	0.59
18:B:1235:CLA:O1A	18:B:1235:CLA:CHA	2.49	0.59
2:B:20:ARG:HH21	9:I:28:VAL:HA	1.66	0.59
2:B:395:ILE:O	2:B:396:ARG:HB2	2.03	0.59
1:A:668:TYR:CG	2:B:445:ALA:HA	2.37	0.59
2:B:537:GLY:O	2:B:572:ALA:HB1	2.02	0.59
18:B:1239:CLA:H41	9:I:21:MET:HG3	1.83	0.59
9:I:18:ALA:O	9:I:22:ALA:HB2	2.02	0.59
12:L:126:GLN:O	12:L:127:PRO:C	2.40	0.59
12:L:71:ALA:O	12:L:73:PRO:HD2	2.01	0.59
13:N:25:THR:HB	15:2:201:HIS:CB	2.32	0.59
14:1:88:PRO:C	14:1:89:VAL:HG23	2.23	0.59
15:2:54:TRP:CE3	15:2:57:LEU:HB2	2.38	0.59
16:3:87:ALA:O	16:3:89:THR:N	2.34	0.59
17:4:106:TRP:CE2	17:4:110:LYS:CE	2.85	0.59
17:4:113:GLY:O	17:4:120:ILE:HD11	2.02	0.59
1:A:239:PRO:HB2	1:A:240:LYS:HG3	1.84	0.59
1:A:308:ILE:HD12	1:A:311:LEU:CD2	2.33	0.59
1:A:646:SER:O	1:A:652:TRP:HZ2	1.83	0.59
1:A:709:TRP:CZ2	18:B:1228:CLA:HED1	2.37	0.59
2:B:439:HIS:HD2	18:B:1230:CLA:C1C	2.15	0.59
18:B:1222:CLA:HBD	18:B:1234:CLA:HBB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:LEU:HD22	2:B:129:LEU:H	1.67	0.59
2:B:132:ASN:O	2:B:136:TYR:CD1	2.55	0.59
2:B:330:ILE:HG21	18:B:1202:CLA:HAC2	1.78	0.59
1:A:665:ILE:HD13	2:B:625:TRP:CG	2.36	0.59
2:B:675:ILE:O	2:B:679:ALA:CB	2.50	0.59
19:A:5001:PQN:H171	18:F:1139:CLA:HBB2	1.84	0.59
6:F:56:TYR:O	6:F:58:LYS:CB	2.50	0.59
8:H:24:TYR:HB2	8:H:25:GLY:CA	2.25	0.59
8:H:73:PRO:CB	8:H:74:GLN:HA	2.31	0.59
12:L:92:VAL:CG1	12:L:93:VAL:N	2.53	0.59
15:2:27:PHE:HD1	15:2:28:GLY:CA	2.16	0.59
15:2:76:THR:OG1	15:2:77:PRO:HD3	2.02	0.59
1:A:397:THR:HA	1:A:613:ILE:HD11	1.84	0.59
1:A:602:LEU:O	1:A:604:TRP:N	2.35	0.59
2:B:224:PRO:CB	2:B:229:GLN:O	2.49	0.59
2:B:464:GLN:HE22	2:B:512:ILE:HG13	1.67	0.59
2:B:4:ARG:HD3	2:B:5:ILE:H	1.67	0.59
2:B:91:ILE:CD1	2:B:114:ASN:ND2	2.65	0.59
7:G:91:ASN:H	7:G:93:TYR:H	1.48	0.59
13:N:36:GLU:HA	13:N:39:SER:CB	2.32	0.59
14:1:152:ARG:HD3	14:1:153:LEU:N	2.16	0.59
15:2:166:ASN:OD1	18:2:2004:CLA:C4C	2.51	0.59
15:2:24:PRO:HG3	15:2:27:PHE:CE2	2.34	0.59
17:4:51:ALA:CB	17:4:161:MET:CE	2.79	0.59
1:A:120:ALA:CB	18:A:1106:CLA:HED3	2.32	0.59
1:A:150:PHE:HD1	1:A:153:TRP:CZ2	2.21	0.59
1:A:83:PHE:HE1	1:A:182:GLY:HA2	1.68	0.59
1:A:456:HIS:CD2	1:A:456:HIS:C	2.76	0.59
1:A:566:SER:O	1:A:568:LEU:N	2.34	0.59
1:A:58:HIS:CE1	18:A:1101:CLA:NC	2.70	0.59
1:A:95:GLY:C	1:A:96:MET:SD	2.80	0.59
2:B:49:SER:OG	2:B:50:HIS:N	2.35	0.59
3:C:31:TRP:O	3:C:37:LYS:HG2	2.02	0.59
3:C:23:THR:OG1	3:C:48:CYS:HA	2.02	0.59
6:F:153:ASN:CG	6:F:154:PHE:H	2.04	0.59
9:I:26:LEU:HD12	9:I:29:GLU:HG3	1.82	0.59
12:L:56:VAL:O	12:L:60:HIS:N	2.31	0.59
16:3:138:SER:N	16:3:139:MET:HB3	2.13	0.59
1:A:287:LEU:HA	1:A:294:LEU:HA	1.85	0.59
1:A:39:HIS:H	1:A:44:ILE:CD1	2.12	0.59
1:A:443:ILE:HG22	1:A:444:SER:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:SER:HB2	1:A:596:ASP:H	1.67	0.59
1:A:652:TRP:HA	1:A:656:PHE:HB2	1.85	0.59
1:A:688:PHE:CE1	1:A:737:HIS:CD2	2.91	0.59
2:B:439:HIS:HD2	18:B:1230:CLA:C4C	2.16	0.59
18:B:1239:CLA:CBD	19:B:5002:PQN:H251	2.32	0.59
2:B:497:TRP:O	2:B:501:ILE:HG23	2.02	0.59
2:B:674:LEU:O	2:B:678:LEU:HD13	2.01	0.59
2:B:680:TRP:CZ3	2:B:684:ARG:HG2	2.38	0.59
4:D:113:HIS:HA	4:D:117:GLY:HA2	1.85	0.59
4:D:137:ILE:CD1	4:D:140:ASN:OD1	2.50	0.59
4:D:43:GLU:CG	4:D:43:GLU:O	2.46	0.59
2:B:546:LEU:CD2	5:E:74:TYR:CE1	2.85	0.59
6:F:120:ILE:HG23	10:J:9:SER:HB3	1.85	0.59
6:F:73:VAL:HB	6:F:83:PHE:CD2	2.37	0.59
12:L:111:GLU:CD	12:L:138:LYS:HE3	2.22	0.59
13:N:12:THR:C	13:N:14:LYS:H	2.06	0.59
14:1:190:GLY:O	14:1:191:ASP:HB2	2.03	0.59
17:4:61:PRO:HA	17:4:68:GLY:HA2	1.82	0.59
1:A:149:PHE:H	1:A:152:ILE:HD12	1.67	0.59
1:A:218:TRP:HZ3	18:A:1148:CLA:ND	2.01	0.59
1:A:230:ASN:O	1:A:234:ASN:OD1	2.20	0.59
1:A:317:TYR:OH	18:A:1119:CLA:CAD	2.50	0.59
1:A:664:VAL:HG23	1:A:675:TYR:O	2.02	0.59
18:B:1222:CLA:CHB	18:B:1236:CLA:HAA2	2.33	0.59
18:B:1239:CLA:C1	19:B:5002:PQN:H271	2.33	0.59
2:B:174:ARG:CZ	18:B:1210:CLA:C3C	2.81	0.59
2:B:277:HIS:O	2:B:278:LEU:HB2	2.03	0.59
2:B:310:PRO:HA	2:B:311:PRO:C	2.19	0.59
2:B:350:GLN:HA	2:B:353:TYR:CD1	2.37	0.59
2:B:548:PRO:HB2	3:C:62:PHE:CD1	2.38	0.59
2:B:627:ASN:OD1	2:B:732:LYS:CE	2.51	0.59
4:D:56:GLN:O	4:D:68:MET:SD	2.60	0.59
5:E:43:SER:OG	5:E:82:TYR:HE1	1.86	0.59
18:B:1229:CLA:ND	6:F:90:PHE:CZ	2.70	0.59
14:1:188:ASN:HA	14:1:189:ILE:CB	2.26	0.59
14:1:86:GLY:N	14:1:87:ASN:CA	2.66	0.59
10:J:5:LYS:NZ	15:2:120:ASN:O	2.22	0.59
15:2:188:PRO:HA	15:2:192:LEU:CD1	2.32	0.59
15:2:21:GLY:H	15:2:23:LEU:CD2	2.08	0.59
1:A:383:PRO:O	1:A:384:TYR:HD1	1.86	0.59
1:A:425:THR:HG21	1:A:428:TYR:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:PHE:HB2	18:B:9023:CLA:CGA	2.33	0.59
1:A:454:GLY:HA3	1:A:547:PHE:CD2	2.38	0.59
1:A:599:PHE:CZ	1:A:693:LEU:HD11	2.37	0.59
2:B:143:LEU:C	2:B:145:LEU:H	2.05	0.59
2:B:153:GLY:O	2:B:154:TRP:C	2.41	0.59
2:B:41:ARG:HA	2:B:44:GLN:OE1	2.02	0.59
18:B:1239:CLA:HMB2	20:B:6017:BCR:C14	2.33	0.59
2:B:646:TRP:HB3	2:B:723:ALA:CB	2.33	0.59
18:A:1129:CLA:C3A	18:L:1130:CLA:OBD	2.50	0.59
12:L:27:VAL:HG12	12:L:27:VAL:O	2.02	0.59
14:1:84:TYR:HB3	14:1:85:LEU:HA	0.74	0.59
15:2:159:LEU:O	15:2:162:LYS:HG2	2.03	0.59
15:2:23:LEU:HD22	15:2:25:GLY:O	2.02	0.59
15:2:32:LEU:HD12	15:2:33:GLY:C	2.23	0.59
16:3:119:MET:HG3	18:3:3010:CLA:C3D	2.32	0.59
1:A:401:TRP:CD1	18:A:1126:CLA:HHC	2.38	0.59
1:A:133:ASN:O	1:A:134:GLY:O	2.21	0.59
1:A:251:ASN:ND2	1:A:251:ASN:C	2.56	0.59
1:A:301:HIS:C	1:A:301:HIS:CD2	2.76	0.59
1:A:435:VAL:HG23	1:A:438:HIS:HE1	1.66	0.59
1:A:462:ILE:CD1	1:A:649:ILE:HD13	2.33	0.59
1:A:663:GLN:HE21	1:A:753:ARG:NH1	1.96	0.59
1:A:684:PHE:CE1	18:A:9013:CLA:CMB	2.86	0.59
2:B:104:PHE:CD1	2:B:104:PHE:N	2.71	0.59
2:B:270:LEU:HD23	2:B:271:THR:H	1.68	0.59
3:C:22:PRO:HG3	3:C:53:ARG:HH21	1.67	0.59
4:D:28:ILE:HD12	4:D:67:ILE:HD13	1.84	0.59
4:D:79:ARG:HB3	4:D:81:GLU:CG	2.32	0.59
5:E:87:VAL:HG12	5:E:89:GLU:OE1	2.03	0.59
7:G:63:PRO:HB3	18:G:1248:CLA:C3C	2.32	0.59
18:L:1130:CLA:HMC2	18:L:1504:CLA:C3B	2.33	0.59
13:N:46:PHE:O	13:N:47:THR:CG2	2.46	0.59
14:1:27:LEU:CB	14:1:28:GLY:CA	2.79	0.59
15:2:114:LEU:H	15:2:115:ASN:CB	2.16	0.59
15:2:117:GLY:O	15:2:120:ASN:N	2.36	0.59
17:4:116:ASN:HA	17:4:117:GLN:CG	2.30	0.59
1:A:149:PHE:CD2	1:A:153:TRP:CZ3	2.91	0.59
1:A:200:GLU:OE2	1:A:327:ILE:HD13	2.03	0.59
1:A:654:ARG:HG2	2:B:633:ASN:OD1	2.03	0.59
1:A:86:LEU:HB2	18:A:1103:CLA:C2	2.33	0.59
2:B:103:ALA:CB	2:B:104:PHE:HD1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:ILE:HG21	18:B:1234:CLA:CED	2.32	0.59
2:B:711:VAL:HG11	18:B:1239:CLA:HED3	1.83	0.59
2:B:441:ASP:OD1	2:B:616:LEU:N	2.28	0.59
2:B:53:GLN:O	2:B:55:ALA:N	2.36	0.59
2:B:714:SER:O	2:B:718:ILE:HG13	2.03	0.59
3:C:4:SER:OG	3:C:68:TYR:C	2.41	0.59
6:F:127:SER:HA	6:F:131:PHE:CB	2.26	0.59
8:H:34:SER:O	8:H:36:GLN:N	2.36	0.59
12:L:126:GLN:O	12:L:128:ASP:N	2.36	0.59
13:N:30:ALA:CA	13:N:33:TYR:HB2	2.22	0.59
15:2:23:LEU:HD23	15:2:26:ASP:HA	1.83	0.58
1:A:77:LYS:HZ2	18:A:1109:CLA:C2B	2.15	0.58
1:A:299:ILE:O	1:A:299:ILE:HG22	2.03	0.58
2:B:374:HIS:C	2:B:376:GLN:N	2.57	0.58
2:B:446:PHE:O	2:B:447:GLY:C	2.40	0.58
2:B:594:TRP:HA	2:B:598:HIS:ND1	2.17	0.58
2:B:368:GLN:HG2	2:B:594:TRP:HH2	1.68	0.58
2:B:676:GLU:O	2:B:678:LEU:N	2.35	0.58
2:B:697:PRO:HG3	18:B:1238:CLA:C4C	2.32	0.58
2:B:672:GLN:CD	2:B:698:VAL:HB	2.23	0.58
4:D:146:VAL:O	4:D:149:THR:HG23	2.03	0.58
4:D:150:GLY:CA	4:D:151:LYS:C	2.70	0.58
5:E:36:VAL:HG21	5:E:52:VAL:CG1	2.33	0.58
14:1:90:PRO:HG2	14:1:92:GLY:CA	2.33	0.58
18:A:1119:CLA:H2	18:A:1123:CLA:HMB1	1.84	0.58
1:A:214:GLY:O	1:A:215:SER:C	2.42	0.58
1:A:228:PRO:C	1:A:230:ASN:N	2.50	0.58
1:A:397:THR:HB	1:A:613:ILE:CG1	2.31	0.58
1:A:536:THR:O	1:A:537:ALA:HB3	2.03	0.58
1:A:461:TYR:HB3	1:A:649:ILE:N	2.17	0.58
2:B:174:ARG:NH2	18:B:1210:CLA:CHD	2.66	0.58
2:B:135:LEU:C	2:B:137:THR:H	2.06	0.58
2:B:553:PHE:CZ	3:C:63:LEU:HG	2.38	0.58
2:B:593:TYR:OH	18:B:1234:CLA:HAC2	2.03	0.58
2:B:678:LEU:HD22	2:B:679:ALA:H	1.67	0.58
1:A:653:LEU:CD2	18:B:9010:CLA:HBC2	2.32	0.58
8:H:29:PRO:HB2	12:L:35:TRP:CD1	2.38	0.58
8:H:55:LYS:CA	8:H:58:ILE:HG13	2.29	0.58
12:L:85:SER:HA	12:L:88:ALA:HB3	1.84	0.58
15:2:63:PHE:O	15:2:67:PHE:N	2.25	0.58
16:3:126:GLU:OE1	16:3:127:HIS:N	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:SER:CA	1:A:611:VAL:HG12	2.28	0.58
1:A:40:PHE:CE1	1:A:61:ALA:HA	2.37	0.58
1:A:478:SER:HB3	1:A:647:ILE:HD13	1.85	0.58
2:B:330:ILE:HG21	18:B:1202:CLA:HBC1	1.85	0.58
2:B:510:LEU:HD21	18:B:1234:CLA:CHD	2.30	0.58
2:B:596:TRP:NE1	2:B:608:GLN:NE2	2.52	0.58
2:B:441:ASP:CG	2:B:616:LEU:HD22	2.23	0.58
4:D:144:ILE:N	4:D:144:ILE:CD1	2.61	0.58
18:B:1228:CLA:C2B	20:F:6016:BCR:C34	2.81	0.58
18:B:1217:CLA:CMB	7:G:18:LEU:HD22	2.32	0.58
18:H:1501:CLA:HMA1	12:L:59:ALA:HB2	1.83	0.58
12:L:89:ALA:O	12:L:92:VAL:HG12	2.03	0.58
15:2:17:GLU:CA	15:2:18:TRP:O	2.51	0.58
1:A:750:PHE:HZ	18:A:1126:CLA:HMB1	1.66	0.58
1:A:452:PHE:CE2	18:A:1136:CLA:HBB2	2.37	0.58
1:A:620:MET:HE3	1:A:624:VAL:HG11	1.85	0.58
2:B:104:PHE:HB2	2:B:112:PRO:HA	1.85	0.58
2:B:284:PHE:HE1	18:B:1216:CLA:CHC	2.09	0.58
2:B:533:ILE:HG22	2:B:575:ASP:O	2.03	0.58
2:B:582:TRP:O	2:B:585:ASN:HB3	2.03	0.58
2:B:652:PHE:CD1	2:B:656:VAL:HG21	2.37	0.58
2:B:67:HIS:NE2	2:B:89:HIS:HB3	2.18	0.58
2:B:700:LEU:HD22	2:B:704:GLN:HE22	1.36	0.58
5:E:63:TYR:HA	5:E:82:TYR:O	2.03	0.58
7:G:83:TYR:CD2	7:G:83:TYR:O	2.56	0.58
8:H:26:SER:HB2	8:H:29:PRO:CA	2.34	0.58
12:L:69:VAL:O	12:L:75:ARG:HA	2.04	0.58
13:N:43:PRO:C	13:N:45:ASN:HB2	2.22	0.58
13:N:69:CYS:HB2	13:N:72:LYS:N	2.19	0.58
14:1:14:LEU:O	14:1:15:ASP:CB	2.52	0.58
15:2:26:ASP:CB	15:2:27:PHE:CB	2.29	0.58
17:4:62:GLU:C	17:4:63:VAL:HG22	2.23	0.58
1:A:110:LEU:HG	1:A:111:ASN:N	2.18	0.58
1:A:294:LEU:HG	1:A:380:PRO:O	2.02	0.58
1:A:679:PHE:HB3	1:A:748:ALA:HB3	1.85	0.58
2:B:104:PHE:HB2	2:B:112:PRO:O	2.03	0.58
2:B:53:GLN:NE2	18:B:1202:CLA:H3A	2.18	0.58
2:B:459:PHE:C	2:B:461:GLN:HB2	2.24	0.58
2:B:646:TRP:HE3	2:B:723:ALA:CA	2.17	0.58
2:B:73:ASN:HB2	2:B:76:ALA:HB3	1.84	0.58
3:C:27:GLU:HB3	3:C:43:PRO:CG	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:166:TYR:N	12:L:167:PHE:C	2.56	0.58
16:3:126:GLU:OE2	16:3:127:HIS:CG	2.56	0.58
16:3:209:PRO:CD	16:3:210:TYR:HA	2.34	0.58
1:A:355:HIS:NE2	1:A:416:ILE:HD12	2.19	0.58
2:B:293:THR:CB	18:B:1209:CLA:HMA3	2.31	0.58
10:J:2:ARG:HD3	10:J:7:TYR:CD1	2.39	0.58
13:N:81:VAL:CG2	13:N:82:PHE:HA	2.32	0.58
15:2:26:ASP:HB2	15:2:27:PHE:HD2	1.67	0.58
16:3:212:ASN:CB	16:3:213:LEU:CB	2.82	0.58
1:A:448:TRP:HE1	18:A:1131:CLA:HED3	1.69	0.58
1:A:611:VAL:HG22	1:A:612:VAL:H	1.67	0.58
2:B:119:GLY:HA3	2:B:371:LEU:HD11	1.84	0.58
2:B:341:LEU:CD2	18:B:1202:CLA:CED	2.80	0.58
1:A:645:SER:OG	2:B:637:PRO:CG	2.50	0.58
2:B:729:THR:HG23	2:B:733:PHE:HA	1.86	0.58
18:B:9010:CLA:CMB	18:B:9022:CLA:HMD1	2.28	0.58
3:C:69:LEU:O	3:C:71:HIS:N	2.37	0.58
4:D:144:ILE:H	4:D:144:ILE:CD1	1.98	0.58
5:E:40:ARG:CZ	5:E:62:ARG:NH2	2.66	0.58
11:K:6:UNK:C	11:K:8:UNK:N	2.64	0.58
12:L:64:LEU:C	12:L:66:GLY:N	2.56	0.58
12:L:93:VAL:HA	12:L:96:SER:HB2	1.86	0.58
14:1:105:ILE:O	14:1:108:VAL:HG22	2.03	0.58
14:1:63:LEU:HD23	14:1:66:GLY:HA2	1.85	0.58
17:4:56:ALA:C	17:4:59:LEU:HB3	2.24	0.58
1:A:377:TYR:C	1:A:377:TYR:CD1	2.74	0.58
1:A:434:ARG:HH21	1:A:438:HIS:CD2	2.22	0.58
1:A:521:VAL:HG12	1:A:522:ALA:N	2.17	0.58
2:B:183:PHE:O	2:B:186:SER:HB2	2.03	0.58
2:B:478:LEU:C	2:B:480:SER:N	2.57	0.58
2:B:621:ARG:HD3	2:B:622:ASP:HB2	1.85	0.58
4:D:119:TYR:HB3	4:D:121:GLU:O	2.03	0.58
4:D:69:ARG:HD2	4:D:70:GLU:H	1.67	0.58
15:2:109:ARG:CB	18:2:2011:CLA:C2C	2.81	0.58
16:3:82:ALA:CA	16:3:83:GLY:C	2.72	0.58
1:A:504:ALA:HB2	18:A:1134:CLA:CHB	2.33	0.58
1:A:311:LEU:HD21	18:A:1108:CLA:CMC	2.32	0.58
1:A:478:SER:O	1:A:481:ALA:HB3	2.03	0.58
1:A:493:GLN:CG	1:A:515:TRP:CB	2.78	0.58
1:A:567:ARG:HH22	4:D:37:LEU:HG	1.68	0.58
2:B:135:LEU:HD22	2:B:136:TYR:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:VAL:O	2:B:216:LEU:HB3	2.03	0.58
2:B:254:ILE:HG13	2:B:255:LEU:H	1.68	0.58
2:B:283:LEU:O	18:B:1216:CLA:HMC3	2.03	0.58
2:B:476:ILE:HB	2:B:477:PRO:HD2	1.86	0.58
2:B:456:GLU:CG	2:B:514:PRO:HB3	2.19	0.58
2:B:54:LEU:HA	2:B:57:ILE:HD12	1.86	0.58
2:B:675:ILE:O	2:B:679:ALA:HB3	2.04	0.58
3:C:56:SER:O	3:C:57:ALA:HB3	2.04	0.58
4:D:75:LEU:HD11	12:L:19:PHE:CG	2.39	0.58
8:H:32:TYR:CD1	8:H:32:TYR:C	2.77	0.58
13:N:2:VAL:CB	13:N:4:GLU:HB2	2.34	0.58
15:2:192:LEU:HD13	15:2:195:HIS:CE1	2.39	0.58
16:3:134:TYR:O	16:3:136:PRO:HD3	2.03	0.58
1:A:484:LEU:CD2	1:A:539:PHE:CE2	2.87	0.58
1:A:569:ILE:HG13	1:A:586:ARG:CZ	2.33	0.58
1:A:646:SER:O	1:A:652:TRP:CZ2	2.57	0.58
1:A:83:PHE:CE1	1:A:182:GLY:HA2	2.39	0.58
18:B:1207:CLA:C2A	18:B:1207:CLA:O2A	2.51	0.58
2:B:120:VAL:HA	2:B:123:TRP:HB3	1.86	0.58
2:B:596:TRP:CD2	2:B:623:TYR:HB2	2.38	0.58
1:A:566:SER:OG	2:B:673:GLU:OE2	2.14	0.58
9:I:10:PRO:O	9:I:14:LEU:HB3	2.04	0.58
12:L:10:VAL:HB	12:L:11:ILE:HD12	1.86	0.58
12:L:66:GLY:C	12:L:68:PHE:H	2.08	0.58
13:N:71:GLY:HA3	13:N:75:TYR:CZ	2.39	0.58
16:3:126:GLU:CD	16:3:127:HIS:N	2.57	0.57
18:4:1304:CLA:H11	18:4:1304:CLA:HBD	1.86	0.57
17:4:77:ALA:CB	17:4:78:ALA:CA	2.72	0.57
18:A:1123:CLA:HBD	18:A:1123:CLA:HBA1	1.84	0.57
1:A:223:VAL:HA	1:A:227:LEU:CD1	2.33	0.57
1:A:398:HIS:C	1:A:400:MET:H	2.07	0.57
1:A:697:ARG:HD3	1:A:727:ILE:H	1.69	0.57
1:A:71:LEU:HA	1:A:74:ILE:HG23	1.85	0.57
2:B:254:ILE:HG21	18:B:1212:CLA:HBC1	1.85	0.57
2:B:493:TRP:HH2	18:B:1213:CLA:C3D	2.17	0.57
18:B:1220:CLA:NB	18:B:1242:CLA:HBA1	2.19	0.57
2:B:144:PHE:CD2	2:B:145:LEU:HD22	2.39	0.57
2:B:259:GLY:CA	2:B:269:TRP:HZ2	2.10	0.57
2:B:466:ALA:C	2:B:468:GLY:H	2.07	0.57
2:B:525:LEU:HD11	2:B:582:TRP:CH2	2.38	0.57
3:C:42:ALA:O	3:C:44:ARG:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:TYR:CB	4:D:37:LEU:HD12	2.34	0.57
4:D:27:PRO:C	4:D:28:ILE:HG13	2.13	0.57
6:F:25:LEU:CD1	6:F:41:ALA:O	2.52	0.57
7:G:43:HIS:CD2	7:G:43:HIS:H	2.22	0.57
7:G:86:LEU:O	7:G:87:ALA:HB2	2.03	0.57
9:I:6:SER:O	9:I:10:PRO:CD	2.52	0.57
10:J:28:GLU:CD	10:J:31:ARG:HH11	2.07	0.57
12:L:77:THR:O	12:L:80:ALA:HB1	2.03	0.57
15:2:177:ALA:C	15:2:178:TRP:HE3	2.08	0.57
14:1:10:ARG:O	17:4:110:LYS:CG	2.51	0.57
1:A:51:THR:O	1:A:53:TRP:N	2.31	0.57
1:A:590:CYS:H	2:B:669:GLY:N	2.01	0.57
1:A:552:THR:CG2	1:A:604:TRP:HB3	2.33	0.57
2:B:103:ALA:HB1	2:B:104:PHE:CE1	2.38	0.57
6:F:125:LEU:C	6:F:130:LEU:HD11	2.23	0.57
12:L:24:GLU:HA	12:L:28:THR:HG21	1.86	0.57
15:2:54:TRP:HE3	15:2:57:LEU:HB2	1.68	0.57
17:4:99:HIS:CE1	17:4:103:ILE:CG1	2.87	0.57
17:4:124:TYR:CD2	17:4:125:SER:HB3	2.40	0.57
17:4:63:VAL:HB	17:4:65:THR:O	2.05	0.57
1:A:286:GLY:O	1:A:287:LEU:HB3	2.04	0.57
1:A:283:PHE:O	1:A:507:ALA:HA	2.04	0.57
1:A:605:MET:HA	1:A:608:SER:OG	2.04	0.57
1:A:638:THR:HG1	1:A:641:ASN:HD21	1.49	0.57
1:A:652:TRP:CD1	1:A:652:TRP:N	2.71	0.57
2:B:340:SER:OG	18:B:1242:CLA:HBB1	2.03	0.57
2:B:325:THR:O	2:B:329:SER:N	2.35	0.57
2:B:365:PHE:HD1	2:B:602:TRP:NE1	2.02	0.57
2:B:393:PHE:CA	2:B:397:ASP:HB2	2.33	0.57
5:E:62:ARG:O	5:E:83:ALA:HB3	2.04	0.57
7:G:20:ARG:HG2	7:G:20:ARG:HH11	1.68	0.57
7:G:21:PHE:C	7:G:23:PHE:HB3	2.24	0.57
13:N:69:CYS:HG	13:N:72:LYS:C	2.08	0.57
13:N:71:GLY:HA2	13:N:76:LYS:CB	2.34	0.57
14:1:40:LYS:CG	14:1:41:GLU:H	1.93	0.57
14:1:74:TRP:HB3	14:1:77:LEU:HG	1.86	0.57
1:A:479:ASP:O	1:A:483:GLN:CB	2.47	0.57
1:A:568:LEU:O	1:A:569:ILE:CD1	2.39	0.57
1:A:605:MET:O	1:A:608:SER:N	2.37	0.57
2:B:257:ILE:CG1	18:B:1214:CLA:HMB2	2.34	0.57
2:B:171:ALA:HB2	18:B:1221:CLA:HBC1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:SER:O	2:B:168:PHE:N	2.37	0.57
2:B:4:ARG:HG2	2:B:5:ILE:N	2.19	0.57
2:B:700:LEU:O	2:B:701:SER:O	2.21	0.57
4:D:149:THR:HG22	4:D:152:GLN:HB3	1.85	0.57
5:E:44:TYR:CD2	5:E:45:TRP:HB3	2.39	0.57
5:E:61:THR:HG23	5:E:62:ARG:N	2.20	0.57
12:L:163:LEU:HD12	12:L:166:TYR:CZ	2.39	0.57
13:N:41:LYS:O	13:N:42:PHE:C	2.43	0.57
14:1:186:HIS:O	14:1:187:ASN:HB2	2.04	0.57
15:2:19:LEU:CB	15:2:20:ASP:OD2	2.52	0.57
15:2:41:LEU:O	15:2:45:VAL:HG11	2.05	0.57
17:4:113:GLY:O	17:4:114:SER:CB	2.52	0.57
1:A:377:TYR:CG	1:A:378:SER:N	2.71	0.57
1:A:465:ASP:C	1:A:467:MET:N	2.57	0.57
1:A:472:ARG:HG2	1:A:474:GLN:HB3	1.85	0.57
1:A:495:THR:O	1:A:497:ALA:N	2.37	0.57
1:A:52:THR:HA	1:A:55:TRP:HE1	1.69	0.57
18:B:1207:CLA:HMC1	18:B:1207:CLA:HBC2	1.85	0.57
18:B:1220:CLA:CHB	18:B:1242:CLA:HBA1	2.35	0.57
2:B:156:HIS:HE1	2:B:162:LYS:O	1.86	0.57
2:B:338:LEU:CB	2:B:382:ILE:HG23	2.34	0.57
2:B:393:PHE:O	2:B:398:TYR:N	2.30	0.57
2:B:595:HIS:O	2:B:597:LYS:O	2.21	0.57
2:B:648:TRP:HZ3	20:B:6017:BCR:C2	2.15	0.57
3:C:46:GLU:HA	3:C:46:GLU:OE2	2.02	0.57
7:G:20:ARG:NH1	7:G:20:ARG:HG2	2.17	0.57
8:H:77:LEU:CD2	8:H:78:PRO:HD2	2.29	0.57
8:H:85:GLN:O	8:H:86:PRO:C	2.42	0.57
11:K:57:UNK:O	11:K:61:UNK:N	2.37	0.57
1:A:251:ASN:ND2	1:A:251:ASN:O	2.38	0.57
1:A:334:HIS:N	1:A:334:HIS:ND1	2.53	0.57
1:A:621:GLN:HA	1:A:637:ILE:HD11	1.85	0.57
1:A:90:PHE:O	1:A:92:TRP:N	2.36	0.57
2:B:121:TYR:C	2:B:122:GLN:HE21	2.07	0.57
2:B:301:ILE:HG22	2:B:302:LYS:H	1.70	0.57
2:B:377:TYR:CE1	2:B:587:ILE:HG21	2.39	0.57
2:B:464:GLN:HG3	2:B:509:PHE:HB3	1.86	0.57
2:B:650:PHE:O	2:B:720:THR:HG22	2.04	0.57
2:B:65:LEU:O	2:B:67:HIS:N	2.37	0.57
2:B:693:TRP:HB3	18:B:1238:CLA:HMD3	1.86	0.57
2:B:646:TRP:CE3	2:B:723:ALA:HA	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PHE:HB2	1:A:140:PHE:CZ	2.35	0.57
1:A:525:ASN:O	1:A:628:ILE:HB	2.03	0.57
1:A:534:LEU:N	1:A:534:LEU:HD13	2.20	0.57
1:A:743:ILE:N	1:A:743:ILE:HD12	2.20	0.57
2:B:421:HIS:NE2	18:B:1228:CLA:NB	2.53	0.57
2:B:309:ILE:N	2:B:310:PRO:HD2	2.20	0.57
2:B:412:LEU:HD13	2:B:415:LYS:HG2	1.86	0.57
2:B:713:PHE:O	2:B:715:VAL:N	2.38	0.57
2:B:717:TYR:CD1	2:B:717:TYR:O	2.58	0.57
4:D:122:LYS:HA	4:D:123:VAL:CG1	2.32	0.57
13:N:69:CYS:CB	13:N:72:LYS:CG	2.80	0.57
15:2:159:LEU:O	15:2:162:LYS:CB	2.51	0.57
15:2:86:GLU:HG2	17:4:184:GLN:NE2	2.20	0.57
17:4:69:ILE:HG23	17:4:70:ILE:O	2.05	0.57
17:4:91:PHE:O	17:4:95:PHE:HD2	1.87	0.57
18:A:1105:CLA:C2B	18:A:1107:CLA:H11	2.34	0.57
1:A:308:ILE:HD12	1:A:311:LEU:HB3	1.86	0.57
1:A:678:PHE:CD1	1:A:747:TRP:HZ3	2.22	0.57
1:A:714:LEU:HD23	6:F:149:LEU:HD21	1.86	0.57
1:A:80:SER:N	1:A:81:ALA:CA	2.67	0.57
2:B:330:ILE:CG2	18:B:1202:CLA:CBC	2.82	0.57
2:B:686:PRO:HA	2:B:689:ASN:HB2	1.87	0.57
3:C:48:CYS:HA	3:C:49:VAL:CG1	2.34	0.57
4:D:111:TYR:CE2	4:D:115:LYS:HA	2.39	0.57
4:D:72:PRO:HB2	4:D:73:ASN:HA	0.72	0.57
6:F:47:GLU:HA	6:F:51:LYS:CG	2.35	0.57
9:I:20:ALA:O	9:I:24:LEU:HD12	2.05	0.57
17:4:118:ASP:N	17:4:119:PRO:CD	2.67	0.57
1:A:126:ILE:CG1	10:J:27:ILE:CG2	2.82	0.57
2:B:273:VAL:HG22	18:B:1214:CLA:HMA1	1.87	0.57
2:B:340:SER:C	2:B:342:GLY:N	2.57	0.57
2:B:398:TYR:OH	2:B:409:ALA:HB2	2.05	0.57
3:C:10:THR:O	3:C:11:CYS:O	2.23	0.57
3:C:29:ILE:HD11	3:C:39:ILE:HG23	1.86	0.57
4:D:58:PHE:CE2	4:D:90:LEU:CD2	2.87	0.57
12:L:53:GLY:N	12:L:139:PHE:CE1	2.73	0.57
14:1:173:PRO:C	14:1:175:GLU:N	2.56	0.57
1:A:569:ILE:HA	1:A:586:ARG:HH12	1.69	0.57
2:B:531:THR:HG22	18:B:1222:CLA:HMC2	1.86	0.57
2:B:42:LEU:HA	2:B:45:ASN:HB2	1.86	0.57
2:B:62:SER:HA	2:B:139:ALA:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:646:TRP:O	2:B:650:PHE:HB3	2.05	0.57
1:A:694:PHE:HE1	2:B:665:ILE:CD1	2.18	0.57
18:B:9012:CLA:H72	18:B:9012:CLA:H41	1.85	0.57
6:F:134:PHE:CZ	18:F:4015:CLA:C3B	2.88	0.57
6:F:149:LEU:HA	6:F:151:ASP:OD1	2.03	0.57
9:I:6:SER:O	9:I:10:PRO:HD3	2.04	0.57
18:A:1115:CLA:HBB2	18:K:1141:CLA:C2B	2.34	0.57
13:N:2:VAL:CG1	13:N:4:GLU:HB2	2.35	0.57
13:N:74:LYS:O	13:N:74:LYS:HG3	2.05	0.57
13:N:81:VAL:N	13:N:82:PHE:HD2	1.99	0.57
14:1:72:GLN:HE22	18:1:1013:CLA:C2D	2.16	0.56
15:2:56:MET:SD	15:2:175:MET:SD	3.03	0.56
17:4:102:GLU:O	17:4:105:ARG:CD	2.53	0.56
1:A:195:TRP:CZ3	18:A:1118:CLA:C3C	2.88	0.56
1:A:289:PRO:HD3	1:A:295:TRP:HH2	1.66	0.56
1:A:396:PHE:HD2	1:A:396:PHE:C	2.07	0.56
1:A:415:ALA:O	1:A:416:ILE:HG12	2.05	0.56
1:A:476:MET:O	1:A:481:ALA:HB1	2.04	0.56
1:A:564:ARG:HG3	1:A:565:SER:N	2.21	0.56
1:A:686:TRP:CD2	18:A:9011:CLA:HMA2	2.40	0.56
2:B:333:GLN:O	18:B:1202:CLA:CHD	2.52	0.56
2:B:365:PHE:HB3	2:B:602:TRP:CE3	2.41	0.56
2:B:422:LEU:O	2:B:532:LEU:HD23	2.05	0.56
4:D:57:ILE:HG13	4:D:67:ILE:CA	2.32	0.56
2:B:450:GLU:CA	6:F:68:LEU:HD11	2.33	0.56
7:G:88:THR:H	7:G:90:SER:HA	1.69	0.56
9:I:25:PHE:CD1	9:I:26:LEU:HD13	2.40	0.56
12:L:53:GLY:CA	12:L:139:PHE:HE1	2.14	0.56
1:A:181:ALA:HA	1:A:184:PHE:CB	2.33	0.56
1:A:283:PHE:HE2	18:A:1116:CLA:CHC	2.18	0.56
1:A:415:ALA:C	1:A:416:ILE:HG12	2.24	0.56
1:A:464:ASN:CG	1:A:477:PHE:HB2	2.21	0.56
1:A:484:LEU:CD2	1:A:539:PHE:HE2	2.18	0.56
1:A:566:SER:C	1:A:568:LEU:H	2.09	0.56
1:A:699:TYR:HE1	2:B:536:LYS:CE	2.17	0.56
18:B:1219:CLA:HBC2	18:B:1219:CLA:HMC1	1.88	0.56
3:C:9:ASP:CG	3:C:10:THR:N	2.58	0.56
4:D:96:ILE:HG12	4:D:97:LYS:N	2.18	0.56
16:3:119:MET:O	16:3:123:GLY:N	2.38	0.56
16:3:132:ASP:HB3	16:3:139:MET:HG2	1.75	0.56
18:A:1140:CLA:C4C	18:A:1140:CLA:H42	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:143:ILE:HB	2.05	0.56
1:A:435:VAL:O	1:A:438:HIS:N	2.37	0.56
1:A:545:HIS:H	1:A:545:HIS:CD2	2.21	0.56
1:A:54:ILE:O	1:A:54:ILE:CG2	2.53	0.56
1:A:673:SER:OG	2:B:446:PHE:CE1	2.58	0.56
1:A:742:GLY:C	1:A:743:ILE:HD12	2.26	0.56
1:A:744:ALA:O	1:A:747:TRP:N	2.32	0.56
2:B:257:ILE:HD13	18:B:1214:CLA:HMB2	1.86	0.56
2:B:463:ILE:O	2:B:465:SER:N	2.38	0.56
3:C:27:GLU:N	3:C:43:PRO:CG	2.63	0.56
3:C:36:ALA:O	3:C:37:LYS:CB	2.49	0.56
3:C:17:CYS:HA	3:C:57:ALA:HA	1.88	0.56
6:F:5:LEU:C	6:F:62:LEU:HG	2.26	0.56
12:L:124:LYS:O	12:L:124:LYS:HD3	2.05	0.56
12:L:33:ILE:O	12:L:34:ALA:C	2.43	0.56
14:1:108:VAL:O	14:1:109:GLU:OE2	2.24	0.56
15:2:19:LEU:C	15:2:20:ASP:CG	2.64	0.56
1:A:370:ILE:HD13	18:A:1124:CLA:C2A	2.35	0.56
1:A:579:PHE:HE1	1:A:581:CYS:O	1.89	0.56
1:A:693:LEU:HD12	1:A:730:GLY:O	2.04	0.56
2:B:345:THR:CG2	18:B:1225:CLA:HMC1	2.34	0.56
2:B:17:THR:C	2:B:19:ARG:H	2.09	0.56
2:B:290:MET:CA	18:B:1218:CLA:HBC3	2.10	0.56
2:B:374:HIS:C	2:B:376:GLN:H	2.08	0.56
2:B:428:PHE:HD2	2:B:432:HIS:HD2	1.42	0.56
2:B:439:HIS:HA	2:B:442:VAL:CB	2.35	0.56
2:B:50:HIS:HE1	18:B:1210:CLA:C3D	2.18	0.56
2:B:707:LEU:O	2:B:710:LEU:CA	2.53	0.56
2:B:71:GLN:CD	2:B:89:HIS:O	2.42	0.56
6:F:144:LEU:HA	6:F:149:LEU:HD13	1.87	0.56
14:1:15:ASP:O	14:1:18:ALA:HB1	2.06	0.56
16:3:126:GLU:O	16:3:130:LEU:N	2.37	0.56
17:4:74:LYS:O	17:4:75:TRP:O	2.23	0.56
1:A:198:ASP:OD2	1:A:199:VAL:N	2.38	0.56
1:A:197:GLN:NE2	1:A:352:THR:HG23	2.20	0.56
1:A:555:ILE:HD11	18:B:9023:CLA:HMD1	1.86	0.56
1:A:80:SER:O	18:A:1109:CLA:C2A	2.53	0.56
2:B:191:ALA:HB1	2:B:277:HIS:C	2.25	0.56
2:B:192:GLY:HA2	2:B:195:VAL:HB	1.86	0.56
2:B:293:THR:HG22	18:B:1209:CLA:O1D	2.05	0.56
1:A:694:PHE:HE1	2:B:665:ILE:HD11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:PHE:HB3	2:B:132:ASN:ND2	2.19	0.56
9:I:5:PRO:O	9:I:7:LEU:N	2.39	0.56
12:L:34:ALA:O	12:L:36:TYR:N	2.38	0.56
13:N:51:ASP:N	13:N:52:LEU:CB	2.58	0.56
14:1:40:LYS:NZ	14:1:41:GLU:HG3	2.19	0.56
1:A:113:PRO:HB3	1:A:384:TYR:CD2	2.40	0.56
1:A:113:PRO:CB	1:A:384:TYR:CE2	2.88	0.56
1:A:441:ALA:HA	1:A:444:SER:OG	2.05	0.56
1:A:621:GLN:H	1:A:624:VAL:HG12	1.69	0.56
1:A:709:TRP:HZ2	18:B:1228:CLA:HED1	1.69	0.56
18:B:1237:CLA:C1A	18:B:1237:CLA:CGA	2.84	0.56
2:B:195:VAL:HG22	2:B:274:ALA:HB1	1.84	0.56
2:B:308:HIS:O	2:B:310:PRO:O	2.23	0.56
2:B:323:TYR:CD1	2:B:323:TYR:C	2.79	0.56
2:B:53:GLN:O	2:B:56:ILE:N	2.38	0.56
3:C:48:CYS:CB	21:C:3102:SF4:S2	2.50	0.56
2:B:672:GLN:NE2	3:C:79:LEU:HD22	2.20	0.56
4:D:133:ASN:CG	4:D:135:ARG:H	2.08	0.56
4:D:52:SER:CB	4:D:73:ASN:HD21	2.18	0.56
5:E:45:TRP:HZ3	5:E:82:TYR:HH	1.53	0.56
6:F:122:ASP:O	6:F:123:VAL:C	2.43	0.56
6:F:130:LEU:O	6:F:132:ARG:N	2.38	0.56
6:F:81:GLY:CA	6:F:85:THR:H	2.18	0.56
7:G:82:ALA:CB	7:G:83:TYR:HB3	2.30	0.56
12:L:7:THR:OG1	12:L:8:TYR:N	2.36	0.56
16:3:200:ILE:O	16:3:204:VAL:N	2.35	0.56
17:4:99:HIS:HE1	17:4:103:ILE:CG1	2.19	0.56
17:4:142:ASN:ND2	17:4:145:PRO:HD3	2.19	0.56
17:4:81:GLU:O	17:4:84:PHE:CE1	2.59	0.56
1:A:152:ILE:O	1:A:155:ALA:HB3	2.06	0.56
1:A:551:VAL:O	1:A:551:VAL:HG23	2.06	0.56
1:A:690:LEU:N	1:A:690:LEU:CD1	2.68	0.56
1:A:71:LEU:HB2	1:A:193:LEU:HD22	1.88	0.56
2:B:337:ALA:CB	18:B:1202:CLA:OBD	2.52	0.56
2:B:304:ILE:CD1	18:B:1220:CLA:HED2	2.36	0.56
2:B:12:ILE:HA	2:B:15:ASP:HB3	1.87	0.56
2:B:260:GLY:O	2:B:261:PHE:HB2	2.05	0.56
2:B:292:ARG:HD2	2:B:299:HIS:O	2.06	0.56
2:B:338:LEU:HD21	2:B:385:GLY:O	2.05	0.56
2:B:443:MET:O	2:B:445:ALA:N	2.39	0.56
2:B:652:PHE:CZ	2:B:656:VAL:HG21	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:GLY:HA2	21:C:3102:SF4:S3	2.46	0.56
6:F:39:ALA:C	6:F:41:ALA:H	2.09	0.56
7:G:20:ARG:HH21	7:G:68:ILE:HG21	1.71	0.56
12:L:66:GLY:HA3	18:L:1503:CLA:C1B	2.32	0.56
14:1:21:ASP:N	14:1:22:PHE:C	2.59	0.56
1:A:106:TYR:HE2	1:A:164:LEU:HD11	1.70	0.56
1:A:374:GLN:O	1:A:378:SER:CB	2.53	0.56
1:A:401:TRP:HB3	18:A:1126:CLA:HMC3	1.86	0.56
1:A:603:PHE:CZ	1:A:735:VAL:HA	2.41	0.56
2:B:286:ILE:C	18:B:1218:CLA:CMC	2.71	0.56
4:D:50:TRP:CE2	4:D:73:ASN:ND2	2.74	0.56
4:D:84:LEU:HD13	4:D:85:ALA:H	1.70	0.56
7:G:91:ASN:N	7:G:93:TYR:H	2.04	0.56
15:2:180:GLN:C	15:2:182:ILE:N	2.59	0.56
15:2:59:ALA:C	15:2:61:GLY:H	2.07	0.56
1:A:51:THR:CG2	1:A:722:PRO:CA	2.63	0.56
1:A:627:THR:OG1	1:A:635:THR:O	2.18	0.56
18:B:1227:CLA:H12	18:B:1228:CLA:HMD1	1.88	0.56
2:B:291:TYR:CD2	2:B:299:HIS:CB	2.89	0.56
2:B:301:ILE:O	2:B:304:ILE:HB	2.06	0.56
2:B:348:VAL:O	2:B:351:HIS:O	2.24	0.56
2:B:365:PHE:CD1	2:B:602:TRP:NE1	2.74	0.56
2:B:587:ILE:O	2:B:588:GLY:C	2.42	0.56
2:B:83:HIS:CA	2:B:84:VAL:HG23	2.36	0.56
4:D:123:VAL:N	4:D:127:ARG:HH12	2.03	0.56
4:D:135:ARG:HD3	4:D:139:LYS:O	2.06	0.56
5:E:63:TYR:N	5:E:64:PRO:HD3	2.21	0.56
7:G:69:VAL:HA	7:G:72:LEU:HD23	1.88	0.56
9:I:6:SER:O	9:I:8:PHE:N	2.39	0.56
10:J:10:VAL:HG13	10:J:14:LEU:HD11	1.88	0.56
12:L:66:GLY:O	12:L:68:PHE:N	2.39	0.56
14:1:75:ALA:O	14:1:78:PRO:HD3	2.06	0.56
15:2:19:LEU:CA	15:2:22:SER:CB	2.84	0.56
15:2:76:THR:OG1	15:2:77:PRO:CD	2.54	0.56
16:3:56:ALA:O	16:3:58:GLY:N	2.38	0.56
16:3:82:ALA:CA	16:3:83:GLY:O	2.53	0.56
1:A:210:LEU:HD22	18:A:1111:CLA:HHC	1.88	0.56
1:A:161:GLU:O	1:A:163:GLN:N	2.35	0.56
1:A:396:PHE:C	1:A:396:PHE:CD2	2.77	0.56
1:A:692:PHE:CD2	19:A:5001:PQN:C1	2.89	0.56
1:A:559:GLY:HA3	1:A:597:HIS:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:THR:OG1	1:A:635:THR:HB	2.06	0.56
1:A:78:VAL:O	1:A:82:HIS:HB2	2.06	0.56
18:B:1205:CLA:CAD	18:B:1224:CLA:HAA2	2.36	0.56
2:B:216:LEU:N	2:B:217:PRO:CD	2.69	0.56
2:B:463:ILE:CG2	2:B:464:GLN:N	2.66	0.56
2:B:468:GLY:HA2	2:B:498:LEU:HD21	1.88	0.56
2:B:655:LEU:HB2	18:B:9022:CLA:CAA	2.32	0.56
2:B:693:TRP:HB3	18:B:1238:CLA:CMD	2.36	0.56
3:C:2:SER:O	3:C:3:HIS:ND1	2.39	0.56
5:E:33:GLY:HA2	5:E:52:VAL:HG23	1.88	0.56
6:F:102:ARG:HH11	6:F:103:SER:CB	2.19	0.56
6:F:140:ALA:O	6:F:143:GLU:N	2.39	0.56
12:L:49:PRO:HG2	12:L:138:LYS:HD3	1.87	0.56
12:L:70:LYS:CA	12:L:75:ARG:HG3	2.32	0.56
13:N:59:PRO:HA	13:N:60:PHE:CG	2.40	0.56
15:2:182:ILE:HG22	15:2:188:PRO:HG2	1.87	0.56
17:4:81:GLU:N	17:4:82:GLU:CA	2.69	0.56
1:A:106:TYR:O	1:A:110:LEU:HB3	2.06	0.56
1:A:283:PHE:CE2	18:A:1116:CLA:CHC	2.88	0.56
1:A:472:ARG:O	1:A:473:PRO:C	2.44	0.56
1:A:543:HIS:C	1:A:546:ALA:HB3	2.27	0.56
2:B:533:ILE:HD13	2:B:579:ALA:HA	1.87	0.56
2:B:618:GLY:HA2	2:B:621:ARG:HG2	1.88	0.56
2:B:672:GLN:OE1	2:B:699:ALA:N	2.36	0.56
6:F:92:TYR:HA	6:F:136:TRP:CZ2	2.41	0.56
7:G:35:VAL:HG13	7:G:36:PRO:N	2.21	0.56
14:1:44:LEU:CD2	14:1:44:LEU:H	2.18	0.55
14:1:74:TRP:CB	14:1:77:LEU:HG	2.36	0.55
15:2:19:LEU:HB2	15:2:22:SER:CB	2.36	0.55
1:A:103:PHE:CB	1:A:140:PHE:HZ	2.19	0.55
2:B:37:ILE:HG23	2:B:41:ARG:HB3	1.89	0.55
2:B:49:SER:HG	2:B:50:HIS:N	2.03	0.55
2:B:564:ARG:O	2:B:565:GLY:C	2.44	0.55
2:B:620:LEU:O	2:B:625:TRP:N	2.31	0.55
1:A:658:TRP:HD1	2:B:625:TRP:CE2	2.13	0.55
2:B:661:PHE:HB3	18:B:9023:CLA:CMC	2.27	0.55
3:C:22:PRO:O	4:D:84:LEU:HD21	2.06	0.55
5:E:58:ASP:N	5:E:59:PRO:CD	2.69	0.55
6:F:2:ILE:O	6:F:3:ALA:HB3	2.06	0.55
9:I:16:PHE:C	9:I:16:PHE:CD1	2.79	0.55
13:N:16:LEU:HG	13:N:19:LYS:HZ1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PRO:HB3	1:A:384:TYR:CE2	2.41	0.55
1:A:532:ILE:HG23	1:A:624:VAL:HG23	1.87	0.55
1:A:86:LEU:HD13	1:A:87:SER:N	2.21	0.55
2:B:332:PHE:C	2:B:335:GLY:H	2.10	0.55
2:B:487:ASN:OD1	2:B:490:ARG:HG3	2.07	0.55
2:B:713:PHE:O	2:B:714:SER:C	2.44	0.55
2:B:90:ALA:C	2:B:91:ILE:HD12	2.27	0.55
2:B:98:GLN:O	2:B:98:GLN:NE2	2.39	0.55
3:C:25:VAL:HA	3:C:44:ARG:HB2	1.87	0.55
3:C:5:VAL:HG22	3:C:6:LYS:HG2	1.88	0.55
18:H:1501:CLA:CMA	12:L:58:LEU:HB3	2.35	0.55
13:N:81:VAL:HG23	13:N:82:PHE:CB	2.28	0.55
18:4:1304:CLA:HBD	18:4:1304:CLA:CGA	2.37	0.55
1:A:391:THR:HB	1:A:395:LEU:HD12	1.87	0.55
1:A:472:ARG:C	1:A:474:GLN:N	2.56	0.55
1:A:629:ASN:ND2	1:A:630:ASP:N	2.55	0.55
1:A:692:PHE:CE2	1:A:725:LEU:HD13	2.41	0.55
1:A:693:LEU:HB2	1:A:734:GLY:HA3	1.87	0.55
1:A:86:LEU:HD22	1:A:86:LEU:O	2.07	0.55
18:B:1215:CLA:HBB2	18:B:1215:CLA:H62	1.87	0.55
2:B:363:GLN:HA	2:B:365:PHE:CE1	2.41	0.55
2:B:616:LEU:O	2:B:619:TRP:HB2	2.05	0.55
2:B:655:LEU:O	2:B:658:ALA:HB3	2.06	0.55
3:C:23:THR:O	3:C:25:VAL:HG23	2.06	0.55
6:F:108:ILE:HG22	6:F:108:ILE:O	2.06	0.55
18:I:1204:CLA:CHA	18:I:1204:CLA:CBA	2.81	0.55
12:L:36:TYR:C	12:L:38:SER:H	2.02	0.55
15:2:18:TRP:C	15:2:20:ASP:O	2.44	0.55
16:3:209:PRO:HD2	16:3:210:TYR:HA	1.89	0.55
17:4:66:SER:O	17:4:67:ILE:CG2	2.47	0.55
1:A:195:TRP:CE3	18:A:1118:CLA:C3C	2.90	0.55
1:A:470:LEU:HD11	2:B:95:HIS:HB3	1.88	0.55
1:A:547:PHE:O	1:A:549:ILE:N	2.40	0.55
18:B:1227:CLA:O1D	18:B:1227:CLA:OBD	2.23	0.55
2:B:284:PHE:O	2:B:288:GLY:HA3	2.07	0.55
2:B:680:TRP:HE1	4:D:37:LEU:HD21	1.71	0.55
2:B:64:ASN:O	2:B:68:VAL:HG12	2.05	0.55
1:A:567:ARG:HH12	4:D:37:LEU:HD21	1.70	0.55
5:E:62:ARG:HD3	5:E:63:TYR:CE1	2.41	0.55
18:B:1232:CLA:CMB	18:G:1233:CLA:C3B	2.83	0.55
12:L:137:ALA:O	12:L:138:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:53:GLY:C	12:L:55:GLU:N	2.59	0.55
12:L:92:VAL:C	12:L:94:ILE:H	2.06	0.55
1:A:675:TYR:CZ	18:A:1106:CLA:HBC1	2.42	0.55
18:A:1106:CLA:C2A	18:A:1106:CLA:O2D	2.48	0.55
1:A:186:TYR:H	1:A:191:PRO:HG3	1.71	0.55
1:A:393:LEU:HG	1:A:394:SER:N	2.22	0.55
1:A:488:PHE:HE2	18:A:1136:CLA:O2D	1.85	0.55
1:A:578:ARG:HA	1:A:595:TRP:CG	2.41	0.55
2:B:260:GLY:N	2:B:269:TRP:NE1	2.53	0.55
2:B:353:TYR:CG	2:B:354:SER:N	2.74	0.55
2:B:361:ILE:HD12	2:B:367:THR:HG1	1.70	0.55
2:B:37:ILE:HG22	4:D:148:PHE:CE1	2.42	0.55
18:H:1501:CLA:HAA1	18:H:1505:CLA:C3C	2.36	0.55
8:H:41:GLU:CA	8:H:41:GLU:OE1	2.55	0.55
8:H:86:PRO:O	8:H:87:PRO:C	2.44	0.55
14:1:86:GLY:N	14:1:87:ASN:CB	2.69	0.55
1:A:208:ALA:O	1:A:209:GLY:C	2.45	0.55
1:A:578:ARG:HE	1:A:728:VAL:HG11	1.71	0.55
2:B:593:TYR:HE1	18:B:1234:CLA:HAC2	1.67	0.55
2:B:247:THR:O	2:B:248:GLN:O	2.25	0.55
2:B:399:ASN:C	2:B:401:GLU:H	2.09	0.55
2:B:532:LEU:CD1	2:B:533:ILE:N	2.55	0.55
12:L:47:VAL:HG12	12:L:52:ARG:NH1	2.21	0.55
14:1:188:ASN:C	14:1:190:GLY:CA	2.75	0.55
15:2:85:GLN:C	15:2:86:GLU:HG3	2.27	0.55
16:3:109:ALA:O	16:3:111:ASN:N	2.40	0.55
16:3:82:ALA:HA	16:3:83:GLY:C	2.26	0.55
1:A:205:HIS:O	1:A:209:GLY:CA	2.55	0.55
1:A:477:PHE:HA	1:A:482:ILE:CB	2.18	0.55
1:A:579:PHE:CE1	1:A:581:CYS:O	2.60	0.55
1:A:642:PHE:O	1:A:643:ALA:C	2.45	0.55
1:A:713:LYS:O	1:A:714:LEU:HB2	2.07	0.55
2:B:459:PHE:HB3	18:B:1234:CLA:H11	1.88	0.55
2:B:166:SER:O	2:B:169:LYS:N	2.40	0.55
2:B:279:ALA:HB3	18:B:1214:CLA:HHC	1.89	0.55
2:B:344:ILE:CG1	18:B:1225:CLA:HAC1	2.36	0.55
2:B:432:HIS:CE1	18:B:1229:CLA:CHA	2.90	0.55
2:B:438:VAL:O	2:B:442:VAL:N	2.39	0.55
2:B:46:ILE:O	2:B:50:HIS:N	2.32	0.55
2:B:621:ARG:CG	2:B:622:ASP:N	2.50	0.55
2:B:632:ILE:HD11	2:B:651:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:PHE:CD1	2:B:720:THR:HB	2.42	0.55
3:C:65:VAL:O	3:C:66:ARG:HG2	2.07	0.55
4:D:102:ARG:O	4:D:108:GLU:C	2.45	0.55
4:D:34:GLY:C	4:D:62:THR:HB	2.26	0.55
4:D:49:THR:N	4:D:99:GLN:O	2.39	0.55
5:E:58:ASP:H	5:E:59:PRO:HD3	1.72	0.55
5:E:66:VAL:HA	5:E:81:ASN:HD21	0.70	0.55
6:F:19:LYS:HE2	6:F:19:LYS:O	2.06	0.55
12:L:49:PRO:O	12:L:50:LEU:C	2.45	0.55
15:2:185:GLY:O	15:2:186:THR:HB	2.06	0.55
17:4:105:ARG:HA	17:4:108:ASP:HB3	1.89	0.55
17:4:61:PRO:HG3	17:4:71:ASN:OD1	2.06	0.55
1:A:380:PRO:CB	1:A:385:LEU:HD12	2.28	0.55
1:A:486:PRO:CA	1:A:487:VAL:HB	2.36	0.55
1:A:725:LEU:HG	1:A:729:GLN:CD	2.27	0.55
1:A:733:VAL:C	1:A:735:VAL:N	2.61	0.55
18:B:1208:CLA:H2	7:G:39:ASN:OD1	2.06	0.55
2:B:117:TYR:HB3	2:B:370:ALA:CB	2.36	0.55
2:B:478:LEU:HG	2:B:486:LEU:H	1.71	0.55
2:B:524:ALA:CB	18:B:1235:CLA:HMA1	2.36	0.55
2:B:530:THR:O	2:B:530:THR:CG2	2.55	0.55
2:B:548:PRO:HG2	3:C:62:PHE:CG	2.42	0.55
2:B:672:GLN:HA	2:B:675:ILE:HG12	1.89	0.55
2:B:687:LEU:N	2:B:687:LEU:CD2	2.70	0.55
2:B:458:ILE:HG12	6:F:74:SER:HB2	1.85	0.55
7:G:83:TYR:CG	7:G:83:TYR:O	2.60	0.55
8:H:49:LYS:CD	8:H:50:ARG:H	2.19	0.55
12:L:107:PHE:CD2	12:L:133:ALA:HB2	2.40	0.55
15:2:19:LEU:HA	15:2:20:ASP:CB	2.26	0.55
1:A:126:ILE:CD1	1:A:127:VAL:HG13	2.37	0.55
1:A:418:MET:HB3	1:A:564:ARG:HH11	1.71	0.55
1:A:439:ARG:O	1:A:441:ALA:N	2.28	0.55
1:A:612:VAL:O	1:A:613:ILE:O	2.25	0.55
2:B:150:LEU:O	2:B:154:TRP:N	2.40	0.55
2:B:291:TYR:C	2:B:292:ARG:HG3	2.27	0.55
2:B:387:PHE:O	2:B:390:GLY:CA	2.55	0.55
2:B:433:THR:O	2:B:433:THR:HG22	2.07	0.55
2:B:442:VAL:O	2:B:445:ALA:HB3	2.07	0.55
2:B:600:THR:HG22	2:B:608:GLN:HB3	1.88	0.55
2:B:609:PHE:CE1	2:B:613:SER:HB3	2.42	0.55
3:C:8:TYR:HA	4:D:132:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:ALA:O	5:E:84:LEU:HB2	2.07	0.55
7:G:22:VAL:C	7:G:23:PHE:CD2	2.76	0.55
13:N:19:LYS:HD2	13:N:20:LYS:CA	2.36	0.55
13:N:19:LYS:HD2	13:N:20:LYS:HA	1.89	0.55
13:N:48:GLY:HA2	13:N:49:CYS:CB	2.36	0.55
15:2:182:ILE:HA	15:2:188:PRO:HG3	1.87	0.55
16:3:143:TYR:O	16:3:144:PHE:CB	2.54	0.55
16:3:193:LEU:HA	16:3:196:LEU:CG	2.37	0.55
1:A:725:LEU:HD12	18:A:1140:CLA:HMD3	1.89	0.55
1:A:119:SER:HA	1:A:145:ILE:HG21	1.87	0.55
1:A:183:TRP:CZ3	1:A:188:LYS:HB2	2.32	0.55
1:A:202:MET:HG3	1:A:203:LEU:N	2.21	0.55
1:A:230:ASN:O	1:A:234:ASN:CG	2.45	0.55
1:A:380:PRO:HD2	1:A:529:LEU:HD11	1.89	0.55
1:A:688:PHE:HE1	1:A:737:HIS:CD2	2.25	0.55
1:A:88:ILE:HG22	1:A:89:ILE:N	2.21	0.55
2:B:242:HIS:HB2	2:B:249:GLY:C	2.28	0.55
2:B:378:ILE:O	2:B:382:ILE:N	2.37	0.55
2:B:410:ARG:HA	2:B:413:GLU:CD	2.27	0.55
7:G:81:VAL:CG1	7:G:83:TYR:CE1	2.89	0.55
9:I:25:PHE:N	9:I:26:LEU:CA	2.68	0.55
4:D:30:ALA:CA	12:L:13:PRO:HD3	2.36	0.55
12:L:59:ALA:HB3	18:L:1502:CLA:HED2	1.89	0.55
12:L:97:MET:SD	12:L:101:MET:HB2	2.47	0.55
14:1:150:ASN:ND2	14:1:153:LEU:HD23	2.21	0.54
15:2:61:GLY:O	15:2:65:PRO:HG2	2.07	0.54
16:3:133:TRP:CD1	16:3:137:GLY:CA	2.90	0.54
18:4:1304:CLA:CAA	18:4:1304:CLA:H2	2.31	0.54
17:4:137:ILE:CG2	17:4:141:LEU:HD23	2.35	0.54
1:A:407:ILE:HD12	18:A:1124:CLA:C3D	2.37	0.54
1:A:453:LEU:HD23	18:A:1136:CLA:CAB	2.37	0.54
1:A:496:HIS:ND1	1:A:515:TRP:CE2	2.75	0.54
1:A:663:GLN:NE2	1:A:753:ARG:O	2.39	0.54
1:A:682:ALA:HB1	1:A:745:THR:HG23	1.90	0.54
18:B:1218:CLA:HAA2	18:B:1218:CLA:HBD	1.88	0.54
2:B:165:VAL:O	2:B:168:PHE:HB2	2.06	0.54
2:B:211:ASN:HD22	2:B:215:VAL:HG22	1.72	0.54
2:B:646:TRP:O	2:B:650:PHE:N	2.37	0.54
2:B:663:PHE:HA	19:B:5002:PQN:H9	1.89	0.54
3:C:55:GLU:CB	3:C:65:VAL:HG22	2.36	0.54
5:E:62:ARG:HD3	5:E:63:TYR:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:150:VAL:HA	6:F:151:ASP:CB	2.36	0.54
7:G:62:ASP:HB2	7:G:63:PRO:HD3	1.89	0.54
1:A:187:HIS:CE1	18:A:1109:CLA:C3C	2.90	0.54
1:A:130:GLU:N	1:A:130:GLU:CD	2.60	0.54
1:A:318:ARG:CD	1:A:319:THR:N	2.67	0.54
1:A:417:PHE:N	1:A:420:ARG:HB2	2.23	0.54
1:A:449:VAL:CG1	1:A:450:CYS:H	2.19	0.54
1:A:618:TRP:HB2	1:A:656:PHE:HE1	1.71	0.54
1:A:86:LEU:HD21	1:A:90:PHE:CD2	2.41	0.54
2:B:146:SER:O	2:B:150:LEU:HD12	2.07	0.54
2:B:676:GLU:C	2:B:678:LEU:H	2.10	0.54
9:I:11:LEU:O	9:I:13:GLY:N	2.40	0.54
9:I:26:LEU:C	9:I:28:VAL:N	2.61	0.54
12:L:27:VAL:HG13	18:L:1130:CLA:O2A	2.06	0.54
12:L:69:VAL:HG12	12:L:75:ARG:O	2.08	0.54
17:4:142:ASN:HD21	17:4:145:PRO:HG3	1.70	0.54
1:A:327:ILE:CG2	1:A:328:LYS:HD3	2.32	0.54
1:A:349:ILE:HA	1:A:352:THR:CB	2.38	0.54
1:A:417:PHE:HD1	1:A:421:ASP:OD2	1.91	0.54
1:A:629:ASN:ND2	1:A:633:VAL:CG2	2.49	0.54
1:A:686:TRP:HA	1:A:741:GLY:HA3	1.88	0.54
18:B:1209:CLA:C5	18:B:1209:CLA:CGA	2.85	0.54
18:B:1214:CLA:HBA1	18:B:1214:CLA:HBD	1.88	0.54
18:B:1203:CLA:H2	18:B:1226:CLA:C4D	2.37	0.54
2:B:304:ILE:O	2:B:308:HIS:HB2	2.02	0.54
2:B:98:GLN:C	2:B:100:ALA:H	2.10	0.54
3:C:12:ILE:C	3:C:38:GLN:HG3	2.28	0.54
4:D:109:VAL:HB	4:D:110:GLN:CA	2.35	0.54
4:D:102:ARG:O	4:D:109:VAL:N	2.41	0.54
8:H:26:SER:HB2	8:H:29:PRO:HA	1.89	0.54
12:L:40:LEU:HB3	12:L:55:GLU:OE2	2.07	0.54
13:N:71:GLY:CA	13:N:76:LYS:HB3	2.38	0.54
14:1:70:LYS:HB2	14:1:73:GLU:HG2	1.90	0.54
15:2:148:TRP:HB2	15:2:151:ALA:HA	1.89	0.54
16:3:135:ASN:N	16:3:136:PRO:CD	2.69	0.54
17:4:94:GLU:HB2	17:4:95:PHE:CE2	2.43	0.54
1:A:96:MET:CB	1:A:149:PHE:CE2	2.90	0.54
1:A:288:ASP:OD1	1:A:295:TRP:HE3	1.91	0.54
1:A:450:CYS:CB	1:A:551:VAL:CG1	2.69	0.54
1:A:742:GLY:CA	18:A:9011:CLA:O1D	2.53	0.54
2:B:246:THR:HG22	2:B:247:THR:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:HIS:CD2	18:B:1230:CLA:C1C	2.89	0.54
1:A:668:TYR:CD1	2:B:445:ALA:HA	2.43	0.54
2:B:597:LYS:O	2:B:599:ILE:N	2.40	0.54
2:B:594:TRP:CE2	2:B:598:HIS:NE2	2.75	0.54
2:B:68:VAL:HG23	2:B:72:GLY:H	1.73	0.54
2:B:68:VAL:O	2:B:69:ALA:HB3	2.07	0.54
3:C:81:TYR:HB3	4:D:37:LEU:HD12	1.89	0.54
3:C:33:GLY:C	5:E:61:THR:HB	2.28	0.54
7:G:16:LEU:HB3	7:G:17:PHE:CE1	2.41	0.54
13:N:19:LYS:CD	13:N:20:LYS:N	2.69	0.54
13:N:50:GLN:C	13:N:52:LEU:HB2	2.26	0.54
13:N:72:LYS:HD2	13:N:72:LYS:O	2.07	0.54
13:N:71:GLY:HA2	13:N:76:LYS:HB2	1.90	0.54
13:N:76:LYS:O	13:N:77:CYS:SG	2.66	0.54
14:1:52:LEU:C	14:1:55:PRO:HD2	2.28	0.54
1:A:149:PHE:O	1:A:153:TRP:CD2	2.60	0.54
1:A:258:LEU:O	1:A:259:TYR:C	2.46	0.54
1:A:599:PHE:CZ	1:A:693:LEU:HD21	2.40	0.54
1:A:92:TRP:O	1:A:94:SER:C	2.46	0.54
2:B:310:PRO:C	18:B:1219:CLA:HBB1	2.27	0.54
2:B:557:PHE:HA	3:C:68:TYR:OH	2.06	0.54
2:B:601:LEU:O	2:B:604:GLY:N	2.36	0.54
2:B:660:GLY:O	2:B:664:LEU:HD12	2.08	0.54
8:H:54:LEU:HD22	8:H:58:ILE:HG12	1.89	0.54
8:H:82:GLY:O	8:H:84:GLN:HG3	2.08	0.54
16:3:56:ALA:C	16:3:58:GLY:H	2.11	0.54
1:A:371:VAL:HG23	1:A:372:VAL:N	2.23	0.54
1:A:451:ILE:O	1:A:455:PHE:HB3	2.07	0.54
1:A:542:HIS:C	1:A:544:ILE:H	2.11	0.54
1:A:401:TRP:HH2	1:A:610:SER:HB2	1.72	0.54
1:A:722:PRO:HB2	18:F:1139:CLA:CMC	2.34	0.54
1:A:78:VAL:HG21	1:A:354:TRP:CE2	2.43	0.54
2:B:242:HIS:HB2	2:B:249:GLY:CA	2.36	0.54
2:B:410:ARG:O	2:B:413:GLU:N	2.40	0.54
2:B:531:THR:CG2	18:B:1222:CLA:HMC2	2.38	0.54
4:D:46:TYR:CD2	4:D:80:LYS:HB3	2.43	0.54
7:G:68:ILE:C	7:G:68:ILE:HD12	2.27	0.54
8:H:44:ALA:H	8:H:45:ALA:HB2	1.72	0.54
18:A:1137:CLA:HMC1	18:L:1130:CLA:CMC	2.38	0.54
15:2:44:ASN:HA	15:2:46:GLN:OE1	2.08	0.54
16:3:107:TYR:HB2	16:3:108:TRP:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:201:GLN:HA	16:3:204:VAL:HG22	1.90	0.54
1:A:118:PRO:O	1:A:119:SER:HB2	2.08	0.54
1:A:135:ASP:HA	1:A:141:ARG:HA	1.88	0.54
1:A:673:SER:OG	2:B:446:PHE:CD1	2.60	0.54
2:B:125:TYR:CE1	2:B:359:ALA:HB2	2.41	0.54
2:B:18:THR:HG23	2:B:22:TRP:HE1	1.72	0.54
2:B:39:GLU:OE2	2:B:39:GLU:CA	2.56	0.54
2:B:521:HIS:O	2:B:523:ILE:N	2.40	0.54
4:D:136:SER:H	4:D:139:LYS:NZ	2.06	0.54
10:J:26:LEU:O	10:J:29:ILE:CG2	2.56	0.54
10:J:4:PHE:CB	10:J:5:LYS:O	2.56	0.54
13:N:69:CYS:HB3	13:N:72:LYS:CG	2.38	0.54
14:1:110:HIS:NE2	18:1:1012:CLA:NB	2.56	0.54
17:4:144:ALA:C	17:4:146:THR:H	2.10	0.54
17:4:158:ARG:NH2	17:4:161:MET:SD	2.79	0.54
18:A:1103:CLA:NB	18:A:1128:CLA:CMB	2.71	0.54
1:A:427:ARG:O	1:A:430:ASP:N	2.37	0.54
2:B:241:ASN:O	2:B:242:HIS:C	2.46	0.54
2:B:311:PRO:HG2	18:B:1220:CLA:HHB	1.89	0.54
2:B:388:ALA:O	2:B:391:PRO:CD	2.56	0.54
2:B:527:LEU:C	2:B:529:THR:H	2.11	0.54
2:B:630:GLN:OE1	2:B:630:GLN:HA	2.07	0.54
6:F:105:LEU:C	6:F:107:ALA:H	2.11	0.54
6:F:42:ILE:CG1	6:F:43:LYS:H	2.13	0.54
15:2:191:ASN:N	15:2:192:LEU:HB2	2.19	0.54
16:3:212:ASN:HB2	16:3:213:LEU:CA	2.37	0.54
17:4:120:ILE:HA	17:4:121:PHE:CG	2.43	0.54
18:A:1137:CLA:HMC1	18:A:1137:CLA:HBC3	1.90	0.54
1:A:123:VAL:HG13	1:A:133:ASN:ND2	2.23	0.54
1:A:490:GLN:N	1:A:491:TRP:O	2.40	0.54
2:B:584:LEU:HD23	2:B:587:ILE:HD12	1.90	0.54
2:B:518:LEU:HD21	2:B:614:THR:HG22	1.85	0.54
4:D:133:ASN:C	4:D:135:ARG:N	2.60	0.54
20:I:6018:BCR:H383	20:L:6020:BCR:H342	1.85	0.54
13:N:73:ASP:CG	13:N:76:LYS:HA	2.28	0.54
14:1:70:LYS:HB2	14:1:73:GLU:HG3	1.88	0.54
17:4:49:ARG:HH21	18:4:4001:CLA:CHC	2.21	0.54
1:A:737:HIS:CE1	18:A:1140:CLA:NA	2.76	0.54
1:A:133:ASN:HA	1:A:143:ILE:N	2.23	0.54
1:A:425:THR:HG22	1:A:426:THR:N	2.23	0.54
1:A:520:LEU:HD21	1:A:530:LEU:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ALA:HB1	1:A:528:ALA:HB1	1.90	0.54
2:B:93:ASP:OD2	18:B:1206:CLA:NA	2.41	0.54
2:B:457:PRO:HB3	18:B:1235:CLA:OBD	2.08	0.54
2:B:391:PRO:HG2	2:B:555:TYR:CE1	2.43	0.54
2:B:693:TRP:HD1	2:B:695:ASP:O	1.87	0.54
1:A:458:PHE:CD1	18:B:9022:CLA:CMB	2.89	0.54
2:B:91:ILE:HG12	2:B:114:ASN:ND2	2.23	0.54
6:F:78:ARG:HA	6:F:80:TRP:CZ3	2.43	0.54
6:F:96:TRP:O	6:F:100:VAL:HG23	2.08	0.54
9:I:25:PHE:CD2	9:I:25:PHE:C	2.80	0.54
1:A:126:ILE:CG1	10:J:27:ILE:HG21	2.38	0.54
14:1:140:LEU:O	14:1:142:GLU:N	2.40	0.53
15:2:180:GLN:C	15:2:182:ILE:H	2.11	0.53
1:A:109:TRP:HE1	1:A:113:PRO:CA	2.08	0.53
1:A:369:THR:CB	18:A:1127:CLA:C3C	2.86	0.53
1:A:223:VAL:HG23	1:A:224:HIS:N	2.23	0.53
1:A:408:VAL:HG12	1:A:408:VAL:O	2.08	0.53
1:A:492:ILE:H	1:A:493:GLN:HB2	1.66	0.53
2:B:304:ILE:CD1	18:B:1216:CLA:O1D	2.56	0.53
2:B:448:THR:CB	2:B:451:LYS:HE2	2.37	0.53
2:B:641:ASN:O	2:B:643:LEU:N	2.41	0.53
4:D:112:LEU:C	4:D:113:HIS:CG	2.80	0.53
4:D:50:TRP:O	4:D:73:ASN:N	2.40	0.53
5:E:45:TRP:HA	5:E:46:PHE:HB3	1.90	0.53
6:F:38:PRO:O	6:F:39:ALA:HB2	2.08	0.53
12:L:14:LEU:CD2	12:L:22:GLY:H	2.19	0.53
12:L:164:PRO:CB	18:L:1503:CLA:C2	2.86	0.53
14:1:156:LEU:HD13	14:1:159:VAL:HB	1.91	0.53
15:2:188:PRO:HB2	15:2:193:PHE:CE2	2.42	0.53
17:4:143:PHE:O	17:4:144:ALA:CB	2.55	0.53
1:A:155:ALA:HB2	1:A:382:TYR:HB3	1.90	0.53
1:A:211:LEU:O	1:A:214:GLY:CA	2.55	0.53
1:A:302:HIS:ND1	18:A:1116:CLA:C1C	2.72	0.53
1:A:302:HIS:CE1	1:A:306:ILE:HD12	2.44	0.53
1:A:341:GLN:NE2	1:A:344:LYS:HD2	2.23	0.53
1:A:398:HIS:C	1:A:398:HIS:CD2	2.81	0.53
1:A:397:THR:O	1:A:399:HIS:N	2.41	0.53
1:A:425:THR:O	1:A:426:THR:HG23	2.08	0.53
1:A:58:HIS:CE1	18:A:1101:CLA:C1C	2.90	0.53
1:A:661:ALA:O	1:A:665:ILE:N	2.31	0.53
2:B:476:ILE:HB	2:B:477:PRO:HD3	1.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:583:MET:SD	2:B:583:MET:C	2.86	0.53
2:B:674:LEU:O	2:B:678:LEU:CD1	2.56	0.53
2:B:650:PHE:CE1	2:B:720:THR:HB	2.43	0.53
4:D:58:PHE:CE2	4:D:90:LEU:HD23	2.44	0.53
5:E:32:ARG:HE	5:E:54:ALA:HA	1.72	0.53
18:B:1228:CLA:C2B	20:F:6016:BCR:H341	2.38	0.53
9:I:5:PRO:O	9:I:6:SER:C	2.47	0.53
16:3:193:LEU:HA	16:3:196:LEU:CD1	2.39	0.53
17:4:142:ASN:ND2	17:4:145:PRO:CD	2.71	0.53
1:A:283:PHE:CG	1:A:301:HIS:HE1	2.26	0.53
1:A:500:PRO:HG3	1:A:510:SER:HA	1.89	0.53
2:B:284:PHE:O	2:B:288:GLY:CA	2.56	0.53
2:B:334:LEU:HD23	18:B:1202:CLA:CHD	2.37	0.53
2:B:428:PHE:HA	2:B:432:HIS:HD2	1.71	0.53
2:B:518:LEU:CD2	2:B:614:THR:CG2	2.81	0.53
2:B:640:CYS:O	2:B:644:SER:HB2	2.07	0.53
4:D:154:TYR:N	4:D:155:ASP:HA	2.22	0.53
4:D:85:ALA:O	4:D:89:ARG:N	2.36	0.53
7:G:16:LEU:HB3	7:G:17:PHE:CD1	2.43	0.53
7:G:88:THR:N	7:G:89:ALA:CA	2.52	0.53
8:H:43:PHE:CD1	8:H:43:PHE:N	2.72	0.53
8:H:45:ALA:O	8:H:47:PHE:HB2	2.08	0.53
12:L:7:THR:O	12:L:8:TYR:HB3	2.07	0.53
13:N:74:LYS:HG3	13:N:85:TRP:HZ2	1.74	0.53
14:1:15:ASP:O	14:1:18:ALA:HA	2.07	0.53
14:1:188:ASN:HB3	14:1:190:GLY:C	2.29	0.53
1:A:31:PHE:HD2	1:A:31:PHE:C	2.12	0.53
1:A:344:LYS:HD3	1:A:344:LYS:C	2.29	0.53
1:A:434:ARG:HH21	1:A:438:HIS:CG	2.26	0.53
1:A:448:TRP:CZ2	18:A:1131:CLA:HMD1	2.43	0.53
1:A:608:SER:O	1:A:611:VAL:O	2.27	0.53
18:B:1235:CLA:CHA	18:B:1235:CLA:CGA	2.86	0.53
2:B:218:TYR:HE1	2:B:232:LEU:HD22	1.72	0.53
2:B:262:HIS:CG	2:B:262:HIS:O	2.62	0.53
2:B:510:LEU:HD13	2:B:510:LEU:N	2.22	0.53
2:B:558:PRO:HG3	2:B:703:VAL:HB	1.90	0.53
18:B:9012:CLA:OBD	18:B:9012:CLA:O2D	2.24	0.53
4:D:44:GLU:OE2	4:D:45:PHE:N	2.30	0.53
7:G:50:ARG:NH1	7:G:51:ALA:CB	2.72	0.53
8:H:47:PHE:O	8:H:48:THR:OG1	2.22	0.53
9:I:16:PHE:HD1	9:I:17:PRO:N	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:VAL:O	12:L:27:VAL:CG1	2.55	0.53
14:1:152:ARG:O	14:1:154:ALA:N	2.42	0.53
14:1:15:ASP:O	14:1:18:ALA:CB	2.57	0.53
15:2:26:ASP:HB3	15:2:27:PHE:HB3	0.59	0.53
17:4:93:ILE:HG13	17:4:94:GLU:N	2.23	0.53
1:A:367:SER:C	1:A:369:THR:N	2.62	0.53
1:A:63:ASP:OD2	1:A:420:ARG:NH2	2.41	0.53
1:A:504:ALA:O	1:A:505:PRO:C	2.46	0.53
1:A:545:HIS:HD1	1:A:612:VAL:CG2	2.21	0.53
1:A:549:ILE:O	1:A:549:ILE:HG22	2.09	0.53
1:A:62:HIS:HB2	18:A:1128:CLA:HAA2	1.90	0.53
18:B:1202:CLA:HBB2	18:B:1203:CLA:CGA	2.37	0.53
2:B:273:VAL:HG12	2:B:273:VAL:O	2.08	0.53
2:B:448:THR:HG21	2:B:451:LYS:CE	2.38	0.53
2:B:558:PRO:HB3	2:B:702:ILE:HG13	1.90	0.53
2:B:594:TRP:O	2:B:595:HIS:C	2.45	0.53
2:B:440:ASN:CB	2:B:614:THR:O	2.56	0.53
10:J:16:THR:O	10:J:19:PHE:N	2.42	0.53
10:J:28:GLU:HA	10:J:31:ARG:HD2	1.90	0.53
12:L:65:VAL:HG11	18:L:1503:CLA:HMA3	1.89	0.53
13:N:47:THR:CB	13:N:50:GLN:HB2	2.38	0.53
13:N:78:GLY:C	13:N:80:ASN:HA	2.28	0.53
14:1:180:HIS:CE1	18:1:1008:CLA:NA	2.77	0.53
15:2:97:VAL:HG23	15:2:98:GLU:H	1.72	0.53
13:N:58:VAL:HG12	16:3:86:PRO:C	2.29	0.53
17:4:89:THR:C	17:4:91:PHE:N	2.62	0.53
1:A:120:ALA:HB3	18:A:1106:CLA:HED3	1.91	0.53
18:A:1137:CLA:CB	18:A:1137:CLA:CBA	2.86	0.53
1:A:737:HIS:HE1	18:A:1140:CLA:NA	2.07	0.53
1:A:115:HIS:O	1:A:116:ILE:CB	2.57	0.53
1:A:431:LEU:O	1:A:432:LEU:C	2.45	0.53
1:A:593:SER:O	1:A:597:HIS:N	2.39	0.53
1:A:605:MET:HE3	1:A:606:TYR:H	1.74	0.53
1:A:668:TYR:HB3	2:B:445:ALA:HA	1.91	0.53
2:B:652:PHE:HE1	18:B:1239:CLA:HMB1	1.74	0.53
2:B:31:PHE:O	2:B:34:HIS:HB2	2.09	0.53
2:B:387:PHE:O	2:B:390:GLY:HA3	2.09	0.53
2:B:440:ASN:OD1	2:B:453:ILE:HG22	2.09	0.53
2:B:670:TYR:CD2	2:B:670:TYR:O	2.62	0.53
4:D:116:ASP:CG	4:D:118:VAL:HG13	2.28	0.53
18:H:1501:CLA:C1D	18:H:1501:CLA:H62	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1237:CLA:H42	20:L:6020:BCR:H361	1.90	0.53
15:2:185:GLY:O	15:2:187:GLY:CA	2.44	0.53
1:A:75:SER:CA	1:A:354:TRP:CZ2	2.73	0.53
1:A:405:PHE:N	1:A:605:MET:SD	2.82	0.53
1:A:50:THR:O	1:A:51:THR:O	2.27	0.53
1:A:714:LEU:CD2	6:F:149:LEU:HD22	2.39	0.53
1:A:74:ILE:O	1:A:78:VAL:HG23	2.08	0.53
1:A:80:SER:HA	1:A:83:PHE:CD1	2.43	0.53
2:B:284:PHE:CE1	18:B:1216:CLA:CAB	2.91	0.53
2:B:186:SER:HB3	18:B:1215:CLA:HBC1	1.91	0.53
2:B:364:ASP:O	2:B:365:PHE:C	2.44	0.53
2:B:689:ASN:ND2	4:D:38:ARG:HH12	2.06	0.53
3:C:52:LYS:HG2	3:C:65:VAL:HB	1.91	0.53
3:C:61:ASP:OD1	5:E:80:ASN:HB3	2.08	0.53
18:B:1138:CLA:C4B	18:F:1139:CLA:HMD2	2.38	0.53
6:F:130:LEU:CD1	6:F:130:LEU:H	2.20	0.53
6:F:60:GLY:C	6:F:62:LEU:N	2.62	0.53
7:G:10:LEU:O	7:G:12:THR:N	2.42	0.53
8:H:45:ALA:O	8:H:47:PHE:CB	2.57	0.53
13:N:35:VAL:HG12	13:N:35:VAL:O	2.08	0.53
13:N:64:ASP:CG	13:N:65:LEU:N	2.62	0.53
14:1:57:ILE:HG13	14:1:57:ILE:O	2.09	0.53
14:1:63:LEU:CD1	14:1:68:TRP:HE1	2.22	0.53
15:2:194:ALA:HB3	15:2:195:HIS:CB	2.39	0.53
1:A:106:TYR:CZ	1:A:153:TRP:CD1	2.96	0.53
2:B:26:ALA:O	2:B:28:ALA:N	2.41	0.53
3:C:60:THR:N	5:E:80:ASN:ND2	2.43	0.53
4:D:67:ILE:HG12	4:D:68:MET:O	2.09	0.53
4:D:27:PRO:HG2	4:D:75:LEU:HB2	1.88	0.53
5:E:51:SER:CB	5:E:69:PHE:HD2	2.22	0.53
10:J:33:PHE:O	10:J:35:ASP:O	2.26	0.53
4:D:28:ILE:HA	12:L:19:PHE:CZ	2.43	0.53
14:1:181:LEU:N	14:1:182:ALA:HB3	2.24	0.53
15:2:162:LYS:HZ1	15:2:163:GLU:HB2	1.74	0.53
16:3:118:GLU:O	16:3:122:MET:HB2	2.09	0.53
16:3:54:TRP:HA	16:3:54:TRP:HE3	1.74	0.53
17:4:99:HIS:HE1	17:4:103:ILE:HG13	1.74	0.53
1:A:347:TYR:HA	1:A:348:GLU:OE2	2.08	0.53
1:A:621:GLN:C	1:A:623:ASP:N	2.58	0.53
2:B:399:ASN:O	2:B:401:GLU:N	2.37	0.53
2:B:523:ILE:O	2:B:527:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:TRP:CD2	2:B:598:HIS:NE2	2.77	0.53
6:F:102:ARG:HH21	6:F:148:GLU:CD	2.12	0.53
6:F:2:ILE:O	6:F:2:ILE:CG1	2.55	0.53
8:H:50:ARG:NH1	12:L:134:ASP:OD2	2.42	0.53
12:L:69:VAL:HG22	12:L:83:ALA:HB1	1.86	0.53
16:3:132:ASP:O	16:3:139:MET:HB3	2.09	0.53
18:A:1137:CLA:HMC1	18:A:1137:CLA:CB	2.39	0.53
1:A:228:PRO:HA	1:A:231:GLN:HB3	1.91	0.53
1:A:302:HIS:C	1:A:303:HIS:ND1	2.62	0.53
1:A:407:ILE:CD1	18:A:1124:CLA:C2D	2.86	0.53
1:A:486:PRO:HB2	1:A:487:VAL:HG23	1.91	0.53
1:A:749:PHE:CG	1:A:750:PHE:N	2.77	0.53
18:B:1227:CLA:C1	18:B:1228:CLA:HMD1	2.39	0.53
2:B:423:SER:HG	2:B:424:TRP:H	1.56	0.53
2:B:557:PHE:HD2	2:B:557:PHE:H	1.57	0.53
2:B:627:ASN:OD1	2:B:732:LYS:HD2	2.09	0.53
3:C:6:LYS:C	3:C:8:TYR:CZ	2.82	0.53
4:D:58:PHE:C	4:D:58:PHE:CD1	2.83	0.53
5:E:46:PHE:CG	5:E:47:LYS:N	2.76	0.53
7:G:68:ILE:HG13	7:G:69:VAL:HG22	1.90	0.53
9:I:15:LEU:HA	9:I:18:ALA:HB3	1.90	0.53
12:L:36:TYR:OH	18:L:1504:CLA:H71	2.09	0.53
12:L:44:ARG:HH11	12:L:44:ARG:CG	2.22	0.53
13:N:74:LYS:O	13:N:74:LYS:CG	2.57	0.53
15:2:178:TRP:HB2	15:2:183:TYR:HH	1.74	0.52
15:2:192:LEU:HB3	15:2:193:PHE:HA	1.90	0.52
1:A:246:HIS:H	1:A:246:HIS:HD2	1.55	0.52
1:A:398:HIS:CD2	1:A:399:HIS:N	2.77	0.52
1:A:452:PHE:HZ	18:A:1136:CLA:HMC3	1.74	0.52
1:A:512:SER:O	1:A:512:SER:OG	2.26	0.52
1:A:602:LEU:HD21	18:A:1128:CLA:HBC1	1.91	0.52
1:A:63:ASP:CG	1:A:64:PHE:N	2.62	0.52
1:A:664:VAL:HG21	1:A:675:TYR:O	2.09	0.52
18:B:1208:CLA:HAA1	18:B:1208:CLA:H12	1.91	0.52
2:B:260:GLY:N	2:B:269:TRP:CZ2	2.77	0.52
2:B:458:ILE:HA	2:B:461:GLN:OE1	2.09	0.52
3:C:22:PRO:HG3	3:C:53:ARG:HE	1.74	0.52
4:D:102:ARG:NH2	4:D:104:PHE:CD2	2.76	0.52
6:F:56:TYR:O	6:F:58:LYS:HB2	2.08	0.52
7:G:4:PRO:HG2	18:G:1233:CLA:HED1	1.89	0.52
12:L:107:PHE:CD2	12:L:133:ALA:CB	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:29:PHE:CG	16:3:107:TYR:HE2	2.27	0.52
13:N:7:LEU:O	13:N:12:THR:OG1	2.27	0.52
14:1:84:TYR:CE2	14:1:90:PRO:HD2	2.43	0.52
15:2:38:PRO:O	15:2:39:GLU:HB2	2.09	0.52
1:A:125:PRO:HA	1:A:130:GLU:CD	2.29	0.52
1:A:362:LEU:O	1:A:366:GLY:CA	2.56	0.52
1:A:437:ARG:HH12	4:D:31:GLY:N	2.08	0.52
1:A:500:PRO:HD2	1:A:501:GLY:H	1.74	0.52
1:A:497:ALA:CB	1:A:516:GLY:HA2	2.38	0.52
1:A:588:GLY:O	2:B:668:ARG:HD2	2.10	0.52
1:A:737:HIS:HE1	18:A:1140:CLA:C1A	2.22	0.52
2:B:115:ASN:ND2	2:B:117:TYR:CZ	2.78	0.52
18:B:1214:CLA:HBA1	18:B:1223:CLA:C3B	2.39	0.52
18:B:1221:CLA:O1D	18:B:1221:CLA:HBA1	2.09	0.52
18:B:1242:CLA:HBC3	18:B:1242:CLA:CHD	2.39	0.52
2:B:201:GLY:O	2:B:204:GLY:HA2	2.09	0.52
2:B:42:LEU:O	2:B:46:ILE:HG13	2.09	0.52
2:B:53:GLN:HE21	2:B:57:ILE:HD11	1.74	0.52
2:B:555:TYR:CD1	2:B:572:ALA:HB3	2.45	0.52
2:B:724:PHE:O	2:B:727:ALA:N	2.41	0.52
5:E:72:VAL:HG22	5:E:78:SER:CB	2.37	0.52
6:F:92:TYR:HE1	6:F:136:TRP:HE1	1.57	0.52
7:G:61:ASN:C	7:G:64:VAL:HG22	2.29	0.52
14:1:164:GLN:NE2	14:1:168:TYR:O	2.37	0.52
15:2:188:PRO:CB	15:2:193:PHE:HD2	2.22	0.52
1:A:274:TRP:HE1	18:A:1115:CLA:CED	2.22	0.52
18:A:1119:CLA:CGA	18:A:1123:CLA:HBB2	2.40	0.52
18:A:1136:CLA:C7	18:A:1137:CLA:HAC2	2.19	0.52
1:A:217:SER:O	18:A:1148:CLA:C2A	2.57	0.52
1:A:363:ALA:O	1:A:366:GLY:HA3	2.10	0.52
1:A:472:ARG:C	1:A:474:GLN:H	2.11	0.52
1:A:599:PHE:CD2	1:A:731:ARG:O	2.63	0.52
2:B:104:PHE:HA	2:B:106:ARG:HD3	1.91	0.52
2:B:663:PHE:HZ	18:B:1239:CLA:CHD	2.23	0.52
2:B:186:SER:CB	18:B:1215:CLA:HBC1	2.38	0.52
2:B:334:LEU:O	2:B:389:HIS:HB2	2.09	0.52
2:B:478:LEU:HG	2:B:486:LEU:N	2.25	0.52
6:F:126:ALA:N	6:F:130:LEU:HD13	2.15	0.52
15:2:106:GLU:CG	18:2:2012:CLA:CHD	2.82	0.52
16:3:209:PRO:HB2	16:3:210:TYR:CA	2.40	0.52
16:3:217:LEU:CA	16:3:218:ALA:CB	2.84	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:179:PHE:N	17:4:179:PHE:CD1	2.78	0.52
1:A:283:PHE:CZ	18:A:1116:CLA:HHC	2.45	0.52
1:A:452:PHE:CD1	18:A:1131:CLA:C2D	2.93	0.52
1:A:123:VAL:H	1:A:133:ASN:ND2	1.86	0.52
1:A:173:VAL:O	1:A:176:GLY:CA	2.54	0.52
1:A:243:PRO:O	1:A:244:LEU:C	2.48	0.52
2:B:194:LEU:CD1	18:B:1215:CLA:HED3	2.39	0.52
4:D:146:VAL:O	4:D:148:PHE:N	2.43	0.52
5:E:45:TRP:O	5:E:45:TRP:CD2	2.62	0.52
5:E:44:TYR:CZ	5:E:73:ASN:HA	2.45	0.52
6:F:93:ILE:HD11	18:F:1240:CLA:C3A	2.39	0.52
9:I:5:PRO:HG2	18:I:1204:CLA:OBD	2.08	0.52
12:L:113:SER:H	12:L:114:ILE:CG2	2.22	0.52
12:L:118:LEU:HB3	12:L:119:THR:OG1	2.10	0.52
12:L:38:SER:O	12:L:44:ARG:NH2	2.41	0.52
12:L:97:MET:O	12:L:99:LEU:N	2.42	0.52
13:N:81:VAL:O	13:N:83:TRP:NE1	2.43	0.52
16:3:140:GLY:H	16:3:141:LYS:CB	2.22	0.52
17:4:59:LEU:C	17:4:62:GLU:CB	2.78	0.52
1:A:106:TYR:O	1:A:110:LEU:CB	2.57	0.52
1:A:332:GLU:CB	1:A:344:LYS:HG2	2.39	0.52
1:A:562:PHE:HB3	1:A:566:SER:OG	2.09	0.52
1:A:599:PHE:HZ	1:A:693:LEU:HD11	1.74	0.52
2:B:189:ALA:O	18:B:1211:CLA:C2C	2.57	0.52
2:B:317:ARG:HH11	18:B:1227:CLA:CAD	2.23	0.52
18:B:1227:CLA:CMB	18:B:1228:CLA:CHA	2.87	0.52
2:B:619:TRP:O	2:B:624:LEU:N	2.39	0.52
3:C:8:TYR:CE1	4:D:137:ILE:CD1	2.92	0.52
4:D:58:PHE:C	4:D:58:PHE:HD1	2.12	0.52
7:G:21:PHE:N	7:G:23:PHE:HB3	2.21	0.52
12:L:111:GLU:OE2	12:L:138:LYS:HE3	2.09	0.52
12:L:33:ILE:HG23	12:L:35:TRP:CB	2.28	0.52
13:N:75:TYR:CD2	13:N:76:LYS:HG2	2.44	0.52
14:1:84:TYR:OH	14:1:92:GLY:CA	2.57	0.52
16:3:197:GLY:O	16:3:200:ILE:N	2.42	0.52
16:3:209:PRO:CB	16:3:210:TYR:HA	2.39	0.52
17:4:106:TRP:NE1	17:4:110:LYS:CE	2.72	0.52
17:4:194:ILE:HD12	17:4:195:VAL:HG23	1.92	0.52
17:4:40:PHE:O	17:4:42:GLN:N	2.43	0.52
17:4:63:VAL:HG12	17:4:66:SER:HA	1.91	0.52
1:A:326:GLY:O	1:A:328:LYS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:TYR:CB	1:A:754:ILE:HD11	2.40	0.52
1:A:416:ILE:O	1:A:419:VAL:N	2.42	0.52
1:A:452:PHE:O	1:A:454:GLY:O	2.27	0.52
1:A:578:ARG:HA	1:A:595:TRP:HB3	1.90	0.52
1:A:654:ARG:HD3	1:A:655:ASP:N	2.24	0.52
1:A:725:LEU:C	1:A:725:LEU:HD23	2.29	0.52
18:B:1209:CLA:C1C	18:B:1217:CLA:HMD2	2.40	0.52
2:B:215:VAL:O	2:B:216:LEU:CB	2.57	0.52
2:B:391:PRO:HB3	2:B:538:ALA:HA	1.90	0.52
2:B:61:THR:O	2:B:65:LEU:HB2	2.10	0.52
2:B:678:LEU:C	2:B:678:LEU:CD2	2.77	0.52
3:C:64:SER:C	3:C:65:VAL:HG22	2.29	0.52
3:C:49:VAL:HA	3:C:76:SER:HB3	1.90	0.52
4:D:122:LYS:HA	4:D:123:VAL:CB	2.39	0.52
4:D:133:ASN:ND2	4:D:135:ARG:N	2.43	0.52
6:F:110:ASP:C	6:F:112:LYS:H	2.12	0.52
7:G:20:ARG:C	7:G:23:PHE:HB3	2.29	0.52
9:I:3:ASN:O	9:I:4:LEU:HB3	2.10	0.52
10:J:38:THR:O	10:J:40:PRO:HD3	2.10	0.52
12:L:117:ALA:H	12:L:121:THR:HG1	1.58	0.52
12:L:118:LEU:N	12:L:119:THR:OG1	2.43	0.52
14:1:54:VAL:O	14:1:57:ILE:HG23	2.09	0.52
15:2:20:ASP:CG	15:2:23:LEU:HD21	2.30	0.52
13:N:58:VAL:CA	16:3:86:PRO:O	2.58	0.52
1:A:195:TRP:HZ3	18:A:1118:CLA:C1C	2.21	0.52
1:A:373:ALA:HB2	1:A:399:HIS:O	2.10	0.52
1:A:443:ILE:CD1	1:A:562:PHE:CE1	2.82	0.52
1:A:691:MET:O	1:A:695:SER:HB2	2.09	0.52
18:B:1209:CLA:O2A	18:B:1209:CLA:C4A	2.58	0.52
2:B:211:ASN:O	2:B:211:ASN:ND2	2.41	0.52
2:B:285:LEU:O	2:B:286:ILE:HG22	2.10	0.52
2:B:338:LEU:HD12	2:B:338:LEU:N	2.25	0.52
2:B:35:ASP:HB3	4:D:154:TYR:CE1	2.44	0.52
2:B:392:ILE:CG2	2:B:393:PHE:N	2.72	0.52
2:B:487:ASN:C	2:B:489:GLY:H	2.13	0.52
2:B:551:LYS:HB2	4:D:141:VAL:C	2.29	0.52
2:B:629:SER:HA	2:B:632:ILE:HG22	1.91	0.52
2:B:711:VAL:HG22	2:B:711:VAL:O	2.09	0.52
1:A:586:ARG:HA	3:C:76:SER:O	2.09	0.52
2:B:551:LYS:CB	4:D:141:VAL:O	2.44	0.52
6:F:130:LEU:CD1	6:F:130:LEU:N	2.69	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:62:ASP:N	7:G:63:PRO:HD2	2.25	0.52
18:A:1137:CLA:CMC	18:L:1130:CLA:CMC	2.86	0.52
14:1:63:LEU:HD11	14:1:68:TRP:NE1	2.24	0.52
1:A:110:LEU:O	1:A:113:PRO:CD	2.52	0.52
1:A:141:ARG:HB3	1:A:141:ARG:NH1	2.13	0.52
1:A:493:GLN:O	1:A:496:HIS:N	2.32	0.52
1:A:668:TYR:CB	2:B:445:ALA:HA	2.40	0.52
1:A:680:LEU:HB3	18:B:9012:CLA:H2	1.89	0.52
18:B:1221:CLA:OBD	18:B:1221:CLA:HED3	2.10	0.52
2:B:176:ASN:ND2	2:B:292:ARG:N	2.55	0.52
2:B:609:PHE:HD1	2:B:610:ASN:N	2.04	0.52
2:B:689:ASN:HD21	4:D:38:ARG:HH12	1.52	0.52
4:D:27:PRO:HD2	4:D:72:PRO:HG2	1.92	0.52
5:E:32:ARG:NE	5:E:54:ALA:HA	2.25	0.52
8:H:22:ASP:C	8:H:24:TYR:N	2.63	0.52
9:I:26:LEU:O	9:I:28:VAL:N	2.43	0.52
2:B:92:TRP:CD1	9:I:9:VAL:CG1	2.90	0.52
12:L:136:TRP:CD1	12:L:137:ALA:N	2.77	0.52
13:N:65:LEU:O	13:N:68:GLU:CG	2.55	0.52
15:2:147:GLY:O	15:2:148:TRP:HB2	2.10	0.52
17:4:42:GLN:OE1	17:4:120:ILE:CG2	2.58	0.52
1:A:202:MET:CE	18:A:1123:CLA:HMD2	2.39	0.52
18:A:1129:CLA:HMB2	18:L:1130:CLA:ND	2.25	0.52
18:A:1137:CLA:CHA	18:A:1137:CLA:HBA1	2.40	0.52
1:A:229:ILE:HA	1:A:232:PHE:CZ	2.45	0.52
1:A:733:VAL:HG23	18:A:1140:CLA:O1D	2.10	0.52
1:A:76:ARG:NH2	1:A:190:ALA:C	2.63	0.52
2:B:19:ARG:O	2:B:22:TRP:N	2.43	0.52
2:B:330:ILE:HG23	18:B:1202:CLA:HAC1	1.88	0.52
2:B:534:LEU:HD22	2:B:579:ALA:HB1	1.92	0.52
2:B:588:GLY:HA2	2:B:717:TYR:OH	2.10	0.52
18:A:9013:CLA:HMC2	18:B:9012:CLA:CAC	2.40	0.52
7:G:78:GLY:O	7:G:79:HIS:O	2.28	0.52
12:L:148:VAL:O	12:L:149:SER:CB	2.57	0.52
13:N:2:VAL:HA	13:N:3:ILE:HD12	1.92	0.52
13:N:70:GLU:OE1	13:N:76:LYS:HB2	2.10	0.52
14:1:146:LYS:HA	14:1:149:LYS:HG2	1.90	0.52
1:A:458:PHE:HD2	1:A:459:GLY:N	2.07	0.52
1:A:462:ILE:H	1:A:649:ILE:CD1	2.22	0.52
19:A:5001:PQN:C20	19:A:5001:PQN:H243	2.32	0.52
1:A:556:LEU:O	1:A:560:VAL:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ILE:N	1:A:637:ILE:CD1	2.50	0.52
2:B:323:TYR:O	2:B:325:THR:N	2.43	0.52
2:B:506:ASN:C	2:B:508:LEU:H	2.12	0.52
2:B:415:LYS:HZ2	2:B:540:ASP:HA	1.74	0.52
2:B:649:MET:SD	18:B:1205:CLA:HBC3	2.49	0.52
4:D:102:ARG:NE	4:D:104:PHE:HB3	2.25	0.52
6:F:89:LEU:O	6:F:92:TYR:HB3	2.10	0.52
18:G:1233:CLA:HBC2	18:G:1233:CLA:CHD	2.41	0.52
7:G:53:GLU:H	7:G:53:GLU:CD	2.13	0.52
7:G:68:ILE:HG13	7:G:69:VAL:HG13	1.91	0.52
12:L:165:TYR:CE1	18:L:1503:CLA:CB	2.89	0.52
12:L:13:PRO:CG	12:L:18:PRO:HA	2.40	0.52
12:L:25:THR:OG1	12:L:26:PRO:O	2.24	0.52
12:L:33:ILE:C	12:L:35:TRP:N	2.60	0.52
12:L:97:MET:O	12:L:100:THR:HG23	2.10	0.52
14:1:70:LYS:NZ	18:1:1013:CLA:CHD	2.73	0.51
17:4:117:GLN:O	17:4:122:LYS:N	2.43	0.51
17:4:185:HIS:O	17:4:186:ILE:CG1	2.58	0.51
1:A:304:LEU:HA	1:A:307:ALA:CB	2.39	0.51
1:A:318:ARG:HG2	1:A:327:ILE:HD11	1.92	0.51
1:A:553:VAL:HA	1:A:556:LEU:CG	2.38	0.51
1:A:716:VAL:O	1:A:717:ALA:O	2.28	0.51
18:B:1209:CLA:H51	18:B:1209:CLA:CGA	2.36	0.51
2:B:302:LYS:CA	2:B:302:LYS:CE	2.85	0.51
2:B:301:ILE:HG22	2:B:302:LYS:N	2.25	0.51
2:B:517:PHE:C	2:B:517:PHE:HD1	2.13	0.51
3:C:12:ILE:CD1	21:C:3103:SF4:S4	2.98	0.51
3:C:3:HIS:CE1	3:C:48:CYS:O	2.58	0.51
4:D:72:PRO:CB	4:D:73:ASN:CA	2.51	0.51
6:F:118:GLU:OE2	18:F:1139:CLA:CED	2.59	0.51
6:F:147:GLY:O	6:F:152:ASN:O	2.27	0.51
6:F:29:LEU:O	6:F:31:LEU:O	2.27	0.51
13:N:29:PHE:O	13:N:33:TYR:N	2.43	0.51
14:1:40:LYS:HZ2	14:1:41:GLU:HG3	1.74	0.51
15:2:19:LEU:CB	15:2:22:SER:CB	2.88	0.51
15:2:44:ASN:ND2	15:2:47:ALA:HB2	2.25	0.51
1:A:195:TRP:HZ3	18:A:1118:CLA:C2C	2.22	0.51
18:A:1126:CLA:H41	18:A:1126:CLA:H93	1.92	0.51
1:A:130:GLU:H	1:A:130:GLU:CD	2.12	0.51
1:A:224:HIS:HB3	1:A:248:PHE:CE2	2.45	0.51
1:A:382:TYR:N	1:A:382:TYR:CD1	2.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:CG2	1:A:402:ILE:O	2.58	0.51
1:A:689:SER:HB2	1:A:738:TYR:N	2.26	0.51
1:A:80:SER:H	1:A:81:ALA:CA	2.21	0.51
2:B:330:ILE:HG22	18:B:1202:CLA:HBC1	1.91	0.51
18:B:1205:CLA:H51	18:B:1205:CLA:CBB	2.40	0.51
2:B:194:LEU:O	2:B:274:ALA:CB	2.58	0.51
2:B:442:VAL:O	2:B:443:MET:C	2.49	0.51
6:F:45:THR:C	6:F:47:GLU:N	2.62	0.51
6:F:144:LEU:HD11	20:F:6016:BCR:H333	1.87	0.51
6:F:65:SER:O	6:F:66:ASP:CB	2.56	0.51
7:G:18:LEU:O	7:G:20:ARG:N	2.44	0.51
6:F:121:ILE:H	10:J:9:SER:CB	2.22	0.51
14:1:90:PRO:CG	14:1:92:GLY:HA2	2.39	0.51
1:A:354:TRP:CB	18:A:1103:CLA:HAC1	2.41	0.51
1:A:692:PHE:CD1	1:A:733:VAL:HG11	2.46	0.51
1:A:93:LEU:O	1:A:96:MET:SD	2.68	0.51
18:B:1208:CLA:HAA1	18:B:1208:CLA:HBD	1.93	0.51
2:B:174:ARG:HH21	18:B:1210:CLA:CHD	2.23	0.51
2:B:199:ILE:HD11	2:B:271:THR:OG1	2.09	0.51
2:B:317:ARG:CG	2:B:317:ARG:NH2	2.66	0.51
2:B:368:GLN:O	2:B:369:ALA:CB	2.58	0.51
2:B:414:HIS:CD2	18:B:1227:CLA:NA	2.75	0.51
2:B:478:LEU:HA	2:B:483:GLY:HA3	1.90	0.51
2:B:562:PRO:O	2:B:563:GLY:C	2.48	0.51
5:E:40:ARG:C	5:E:42:GLU:H	2.13	0.51
8:H:24:TYR:CB	8:H:25:GLY:CA	2.88	0.51
13:N:42:PHE:O	13:N:45:ASN:N	2.43	0.51
14:1:51:MET:SD	14:1:150:ASN:HB3	2.50	0.51
16:3:134:TYR:O	16:3:135:ASN:CB	2.59	0.51
16:3:67:MET:CE	16:3:70:ALA:HB3	2.40	0.51
18:A:1110:CLA:C2D	18:A:1146:CLA:C3C	2.88	0.51
1:A:401:TRP:CZ2	1:A:610:SER:HB2	2.45	0.51
18:B:1216:CLA:CAA	18:B:1221:CLA:HBB2	2.37	0.51
2:B:133:GLU:CA	2:B:136:TYR:CE1	2.78	0.51
2:B:156:HIS:CE1	2:B:161:TRP:O	2.63	0.51
2:B:177:HIS:CD2	2:B:177:HIS:C	2.84	0.51
2:B:340:SER:C	2:B:342:GLY:H	2.14	0.51
2:B:651:LEU:O	18:B:9022:CLA:HBA1	2.10	0.51
3:C:73:THR:C	3:C:75:ARG:H	2.13	0.51
18:L:1502:CLA:H42	18:L:1504:CLA:CMA	2.35	0.51
14:1:180:HIS:O	14:1:181:LEU:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:15:ASP:O	14:1:18:ALA:CA	2.59	0.51
16:3:138:SER:N	16:3:139:MET:CB	2.70	0.51
17:4:116:ASN:N	17:4:117:GLN:HA	2.25	0.51
1:A:504:ALA:HB2	18:A:1134:CLA:C1B	2.41	0.51
1:A:185:HIS:CD2	1:A:191:PRO:HG3	2.46	0.51
1:A:288:ASP:OD1	1:A:295:TRP:CE3	2.63	0.51
1:A:397:THR:HG22	1:A:613:ILE:HG13	1.93	0.51
1:A:562:PHE:CZ	2:B:677:THR:CG2	2.92	0.51
1:A:558:LYS:NZ	1:A:597:HIS:CE1	2.78	0.51
1:A:750:PHE:CD1	1:A:750:PHE:O	2.63	0.51
18:B:1220:CLA:CHC	18:B:1242:CLA:HBD	2.40	0.51
2:B:270:LEU:HD22	2:B:271:THR:HG23	1.92	0.51
2:B:332:PHE:HA	2:B:335:GLY:HA3	1.92	0.51
2:B:398:TYR:O	4:D:142:SER:HB2	2.11	0.51
2:B:517:PHE:CD1	2:B:517:PHE:C	2.83	0.51
2:B:687:LEU:HD22	2:B:687:LEU:N	2.26	0.51
4:D:102:ARG:HB3	4:D:110:GLN:HB2	1.92	0.51
18:F:1139:CLA:OBD	18:F:1139:CLA:O2D	2.27	0.51
12:L:136:TRP:HD1	12:L:137:ALA:N	2.09	0.51
18:L:1503:CLA:O2D	18:L:1503:CLA:CGA	2.58	0.51
12:L:78:GLU:C	12:L:80:ALA:HA	2.31	0.51
12:L:99:LEU:HA	12:L:102:TYR:HB2	1.93	0.51
13:N:72:LYS:N	13:N:75:TYR:O	2.43	0.51
15:2:191:ASN:CA	15:2:192:LEU:CB	2.60	0.51
15:2:19:LEU:HA	15:2:20:ASP:C	2.30	0.51
1:A:149:PHE:CD2	1:A:153:TRP:CH2	2.98	0.51
1:A:317:TYR:CA	1:A:325:HIS:H	2.15	0.51
2:B:510:LEU:HD11	18:B:1234:CLA:HHD	1.92	0.51
2:B:452:GLN:HG3	2:B:453:ILE:N	2.24	0.51
1:A:680:LEU:HD23	18:B:9012:CLA:H2	1.92	0.51
2:B:680:TRP:CD1	4:D:37:LEU:HD11	2.46	0.51
7:G:14:LEU:O	7:G:18:LEU:HG	2.10	0.51
10:J:19:PHE:CD1	10:J:20:GLY:N	2.78	0.51
15:2:34:LEU:HD23	15:2:34:LEU:N	2.24	0.51
1:A:150:PHE:CD1	1:A:153:TRP:HZ2	2.28	0.51
1:A:393:LEU:HA	1:A:616:PHE:CZ	2.45	0.51
2:B:284:PHE:CZ	18:B:1216:CLA:CBB	2.93	0.51
6:F:116:GLN:HG3	6:F:119:ILE:HB	1.93	0.51
7:G:35:VAL:HG12	7:G:36:PRO:CD	2.40	0.51
9:I:16:PHE:HD1	9:I:17:PRO:CD	2.22	0.51
9:I:23:SER:O	9:I:26:LEU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:22:LEU:C	13:N:24:THR:H	2.14	0.51
13:N:58:VAL:HG12	16:3:86:PRO:HB3	1.92	0.51
14:1:171:THR:HG23	14:1:171:THR:O	2.10	0.51
15:2:141:LEU:N	15:2:141:LEU:HD23	2.25	0.51
15:2:178:TRP:CB	15:2:183:TYR:CZ	2.92	0.51
1:A:187:HIS:NE2	18:A:1109:CLA:C2C	2.74	0.51
1:A:151:GLN:OE1	1:A:384:TYR:HB2	2.10	0.51
1:A:491:TRP:CD1	18:A:1135:CLA:O1A	2.64	0.51
1:A:695:SER:HB3	19:A:5001:PQN:H9	1.93	0.51
1:A:55:TRP:N	1:A:55:TRP:CD1	2.78	0.51
1:A:90:PHE:O	1:A:92:TRP:C	2.49	0.51
2:B:98:GLN:O	2:B:100:ALA:N	2.44	0.51
2:B:22:TRP:HH2	18:B:1238:CLA:HMB1	1.75	0.51
2:B:393:PHE:CE2	2:B:398:TYR:CD1	2.98	0.51
2:B:53:GLN:C	2:B:55:ALA:H	2.14	0.51
2:B:571:SER:CB	2:B:574:ASP:H	2.20	0.51
2:B:65:LEU:O	2:B:66:PHE:C	2.48	0.51
4:D:116:ASP:OD1	4:D:118:VAL:HG22	2.11	0.51
4:D:121:GLU:O	4:D:122:LYS:HB2	2.10	0.51
18:F:1302:CLA:C2	18:F:1302:CLA:H71	2.41	0.51
7:G:20:ARG:HH21	7:G:68:ILE:HG22	1.76	0.51
10:J:24:GLY:O	10:J:27:ILE:N	2.43	0.51
15:2:27:PHE:CD1	15:2:28:GLY:HA2	2.46	0.51
16:3:54:TRP:CE3	16:3:54:TRP:HA	2.45	0.51
17:4:114:SER:O	17:4:115:VAL:O	2.28	0.51
17:4:106:TRP:CZ3	18:4:1304:CLA:HMA2	2.46	0.51
1:A:210:LEU:HD13	18:A:1111:CLA:C3B	2.41	0.51
1:A:112:ASP:OD2	1:A:112:ASP:O	2.29	0.51
1:A:555:ILE:N	1:A:556:LEU:CB	2.30	0.51
1:A:78:VAL:O	1:A:82:HIS:CG	2.64	0.51
2:B:45:ASN:O	2:B:46:ILE:C	2.48	0.51
2:B:589:TRP:HA	2:B:592:PHE:CD2	2.45	0.51
3:C:62:PHE:CE1	5:E:41:ARG:O	2.64	0.51
4:D:29:PHE:CZ	4:D:62:THR:HG23	2.46	0.51
8:H:41:GLU:HA	8:H:42:THR:HB	1.92	0.51
10:J:3:ASP:HB3	10:J:5:LYS:HG3	1.93	0.51
18:4:1304:CLA:HAA2	18:4:1304:CLA:C1	2.39	0.51
18:4:4013:CLA:C2C	18:4:4010:CLA:C4C	2.89	0.51
1:A:63:ASP:HA	18:A:1128:CLA:HMA2	1.93	0.51
1:A:280:PHE:H	1:A:280:PHE:HD2	1.57	0.51
1:A:452:PHE:HD2	1:A:453:LEU:N	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:PHE:CD1	1:A:737:HIS:HD2	2.28	0.51
1:A:754:ILE:C	1:A:755:ILE:HG13	2.26	0.51
1:A:93:LEU:O	1:A:95:GLY:N	2.43	0.51
2:B:284:PHE:O	2:B:286:ILE:N	2.44	0.51
2:B:378:ILE:CG2	2:B:382:ILE:HD12	2.37	0.51
2:B:393:PHE:CB	2:B:397:ASP:HB2	2.40	0.51
2:B:411:MET:HE1	2:B:414:HIS:HE1	1.76	0.51
2:B:594:TRP:CE3	2:B:598:HIS:CD2	2.99	0.51
2:B:703:VAL:O	2:B:704:GLN:HG3	2.10	0.51
5:E:51:SER:OG	5:E:51:SER:O	2.25	0.51
5:E:82:TYR:O	5:E:83:ALA:CB	2.59	0.51
18:B:1138:CLA:HMC3	18:F:1139:CLA:CHD	2.41	0.51
6:F:136:TRP:CB	6:F:137:PRO:HD3	2.37	0.51
10:J:9:SER:HG	10:J:10:VAL:N	2.08	0.51
17:4:143:PHE:O	17:4:144:ALA:HB2	2.10	0.50
17:4:171:HIS:HA	17:4:175:GLY:HA2	1.92	0.50
17:4:170:GLN:HB3	17:4:174:THR:HG23	1.93	0.50
1:A:364:MET:C	1:A:366:GLY:N	2.62	0.50
1:A:434:ARG:CD	18:A:1129:CLA:OBD	2.59	0.50
1:A:558:LYS:HZ1	1:A:597:HIS:CE1	2.29	0.50
1:A:581:CYS:SG	1:A:590:CYS:SG	3.09	0.50
1:A:599:PHE:CG	1:A:599:PHE:O	2.64	0.50
1:A:397:THR:HG21	1:A:750:PHE:CZ	2.46	0.50
1:A:99:HIS:HD1	1:A:103:PHE:HZ	1.57	0.50
18:B:1203:CLA:HBD	18:B:1203:CLA:HBA2	1.93	0.50
18:B:1225:CLA:HAA2	18:B:1225:CLA:HBD	1.92	0.50
2:B:703:VAL:HA	2:B:706:ARG:CG	2.41	0.50
4:D:55:GLU:HB3	4:D:67:ILE:HG13	1.93	0.50
4:D:93:LYS:O	4:D:94:TYR:CD1	2.64	0.50
5:E:63:TYR:N	5:E:64:PRO:CD	2.74	0.50
5:E:44:TYR:CE1	5:E:74:TYR:CE2	2.95	0.50
9:I:12:VAL:CB	18:I:1204:CLA:O1A	2.59	0.50
12:L:109:GLU:N	12:L:133:ALA:O	2.31	0.50
12:L:36:TYR:C	12:L:38:SER:N	2.61	0.50
12:L:65:VAL:HG23	12:L:84:GLY:HA2	0.80	0.50
15:2:190:ASP:C	15:2:192:LEU:HD23	2.32	0.50
16:3:133:TRP:CD1	16:3:133:TRP:O	2.64	0.50
1:A:186:TYR:N	1:A:189:ALA:O	2.44	0.50
1:A:253:ASP:HA	1:A:256:ALA:HB3	1.94	0.50
1:A:368:LEU:HA	1:A:371:VAL:HG21	1.90	0.50
1:A:462:ILE:HD12	1:A:649:ILE:CD1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:PHE:CG	1:A:548:THR:N	2.79	0.50
2:B:351:HIS:CD2	2:B:351:HIS:N	2.77	0.50
2:B:564:ARG:O	2:B:564:ARG:CG	2.55	0.50
2:B:722:ALA:O	2:B:726:ILE:HG13	2.11	0.50
2:B:650:PHE:HZ	18:B:9010:CLA:C2D	2.24	0.50
4:D:46:TYR:HD2	4:D:78:ALA:O	1.94	0.50
4:D:52:SER:HB2	4:D:68:MET:HB2	1.94	0.50
6:F:115:THR:C	6:F:117:LYS:N	2.65	0.50
18:G:1233:CLA:NC	18:G:1233:CLA:H52	2.26	0.50
7:G:87:ALA:HA	7:G:90:SER:HA	1.93	0.50
13:N:17:ASN:HA	13:N:20:LYS:HB2	1.92	0.50
15:2:33:GLY:N	15:2:35:SER:H	2.02	0.50
15:2:54:TRP:O	15:2:55:ALA:C	2.49	0.50
16:3:133:TRP:CD1	16:3:137:GLY:HA2	2.46	0.50
16:3:207:VAL:O	16:3:209:PRO:N	2.44	0.50
16:3:85:ILE:H	16:3:86:PRO:HD3	1.75	0.50
1:A:556:LEU:O	1:A:560:VAL:HG13	2.11	0.50
2:B:135:LEU:HD22	2:B:136:TYR:H	1.76	0.50
2:B:192:GLY:O	2:B:196:HIS:N	2.40	0.50
2:B:303:TYR:O	2:B:305:LEU:O	2.28	0.50
2:B:428:PHE:O	2:B:429:LEU:HB2	2.11	0.50
2:B:439:HIS:CD2	18:B:1230:CLA:C4C	2.93	0.50
2:B:540:ASP:C	2:B:542:ARG:H	2.14	0.50
1:A:470:LEU:CD2	2:B:96:PHE:CD2	2.94	0.50
3:C:24:ASP:O	3:C:25:VAL:HB	2.10	0.50
5:E:44:TYR:HD2	5:E:45:TRP:HB3	1.76	0.50
5:E:52:VAL:HA	5:E:67:VAL:HG12	1.93	0.50
8:H:93:GLY:N	8:H:94:LYS:HA	2.15	0.50
13:N:21:ARG:O	13:N:23:ALA:N	2.41	0.50
13:N:44:GLU:H	13:N:45:ASN:HB2	1.66	0.50
15:2:19:LEU:CA	15:2:21:GLY:N	2.75	0.50
16:3:125:ALA:O	16:3:129:ARG:HB3	2.11	0.50
17:4:126:LEU:O	17:4:153:GLU:OE2	2.29	0.50
17:4:91:PHE:O	17:4:95:PHE:CD2	2.64	0.50
1:A:328:LYS:O	1:A:331:LEU:N	2.44	0.50
1:A:455:PHE:C	1:A:455:PHE:CD1	2.84	0.50
1:A:463:HIS:CD2	1:A:467:MET:SD	3.04	0.50
1:A:491:TRP:CA	1:A:492:ILE:HG23	2.42	0.50
1:A:542:HIS:O	1:A:546:ALA:N	2.23	0.50
1:A:627:THR:OG1	1:A:634:VAL:O	2.30	0.50
18:B:1220:CLA:CHD	18:B:1220:CLA:CBC	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:SER:HA	2:B:190:TRP:HB3	1.92	0.50
2:B:331:HIS:O	2:B:332:PHE:CB	2.57	0.50
2:B:361:ILE:HG13	2:B:368:GLN:NE2	2.26	0.50
2:B:492:ILE:HB	2:B:493:TRP:CE2	2.45	0.50
2:B:659:THR:C	2:B:661:PHE:N	2.64	0.50
2:B:670:TYR:CD2	2:B:670:TYR:C	2.84	0.50
4:D:103:VAL:H	4:D:108:GLU:H	1.60	0.50
4:D:29:PHE:O	4:D:30:ALA:HB3	2.12	0.50
5:E:61:THR:HG23	5:E:63:TYR:H	1.75	0.50
5:E:87:VAL:CG1	5:E:89:GLU:OE1	2.59	0.50
18:B:1138:CLA:HMC3	18:F:1139:CLA:C1D	2.42	0.50
7:G:20:ARG:NH1	7:G:20:ARG:CG	2.63	0.50
7:G:83:TYR:CA	7:G:85:ILE:HG12	2.41	0.50
8:H:64:LEU:CG	8:H:65:LEU:N	2.72	0.50
10:J:1:MET:C	10:J:2:ARG:HG3	2.30	0.50
10:J:23:ALA:O	10:J:24:GLY:C	2.47	0.50
13:N:2:VAL:HA	13:N:3:ILE:HG13	1.93	0.50
15:2:157:LYS:HA	15:2:160:ARG:CB	2.41	0.50
1:A:204:ASN:CG	1:A:315:HIS:HA	2.31	0.50
1:A:591:GLN:OE1	2:B:667:TRP:CA	2.59	0.50
1:A:611:VAL:O	1:A:612:VAL:CB	2.55	0.50
1:A:629:ASN:HD22	1:A:630:ASP:H	1.57	0.50
1:A:663:GLN:OE1	1:A:663:GLN:HA	2.12	0.50
1:A:726:SER:O	1:A:729:GLN:N	2.36	0.50
18:B:1207:CLA:HMA2	18:B:1207:CLA:C2	2.31	0.50
18:B:1215:CLA:H61	18:B:1215:CLA:HBB2	1.94	0.50
2:B:137:THR:O	2:B:141:PHE:N	2.43	0.50
2:B:144:PHE:HD2	2:B:145:LEU:CD2	2.24	0.50
2:B:342:GLY:O	2:B:343:VAL:C	2.49	0.50
2:B:506:ASN:O	2:B:508:LEU:N	2.29	0.50
2:B:517:PHE:HD1	2:B:518:LEU:N	2.10	0.50
2:B:540:ASP:C	2:B:542:ARG:N	2.65	0.50
2:B:618:GLY:CA	2:B:621:ARG:HG2	2.42	0.50
2:B:560:ASP:O	3:C:52:LYS:HE3	2.10	0.50
3:C:69:LEU:O	3:C:72:GLU:N	2.43	0.50
6:F:110:ASP:OD2	6:F:111:GLU:N	2.38	0.50
7:G:43:HIS:HD2	7:G:43:HIS:H	1.58	0.50
8:H:89:LEU:O	8:H:89:LEU:HD13	2.11	0.50
12:L:17:ASP:O	12:L:19:PHE:N	2.36	0.50
15:2:183:TYR:O	15:2:184:THR:CG2	2.59	0.50
15:2:27:PHE:CE1	15:2:29:PHE:N	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:33:GLY:H	15:2:35:SER:HA	1.71	0.50
15:2:63:PHE:O	15:2:66:GLU:HB3	2.12	0.50
16:3:212:ASN:HA	16:3:213:LEU:CB	2.18	0.50
16:3:83:GLY:C	16:3:88:GLU:HA	2.31	0.50
17:4:94:GLU:O	17:4:95:PHE:CD1	2.64	0.50
1:A:484:LEU:HD21	1:A:539:PHE:CE2	2.47	0.50
1:A:687:ALA:C	1:A:689:SER:N	2.60	0.50
18:B:1221:CLA:CHC	18:B:1221:CLA:CBB	2.83	0.50
2:B:375:HIS:NE2	18:B:1225:CLA:C4D	2.73	0.50
2:B:368:GLN:O	2:B:369:ALA:HB3	2.12	0.50
2:B:388:ALA:C	2:B:390:GLY:H	2.14	0.50
2:B:422:LEU:HD21	2:B:531:THR:HG1	1.68	0.50
2:B:463:ILE:HD11	18:B:1231:CLA:HMC3	1.94	0.50
4:D:102:ARG:HB3	4:D:110:GLN:CB	2.42	0.50
4:D:103:VAL:O	4:D:104:PHE:HB3	2.11	0.50
3:C:29:ILE:HG21	4:D:128:GLN:O	2.12	0.50
4:D:137:ILE:O	4:D:139:LYS:N	2.45	0.50
4:D:45:PHE:CE1	4:D:46:TYR:O	2.64	0.50
5:E:44:TYR:CD1	5:E:73:ASN:HB3	2.46	0.50
7:G:81:VAL:HG12	7:G:83:TYR:CD1	2.46	0.50
8:H:66:THR:O	8:H:69:SER:N	2.43	0.50
2:B:92:TRP:CD1	9:I:9:VAL:HG11	2.47	0.50
18:J:2107:CLA:H91	18:J:2107:CLA:C13	2.35	0.50
12:L:97:MET:SD	12:L:98:CYS:CA	2.99	0.50
13:N:19:LYS:CG	13:N:20:LYS:N	2.74	0.50
13:N:43:PRO:HB2	13:N:44:GLU:HB3	1.94	0.50
14:1:173:PRO:O	14:1:174:LEU:C	2.49	0.50
15:2:56:MET:SD	15:2:175:MET:CE	3.00	0.50
1:A:33:GLN:OE1	18:A:1109:CLA:HHC	2.10	0.50
1:A:146:THR:HB	1:A:390:ALA:O	2.11	0.50
1:A:511:THR:HB	1:A:515:TRP:CZ2	2.41	0.50
1:A:684:PHE:O	1:A:685:VAL:HB	2.11	0.50
1:A:723:ARG:HG3	1:A:724:ALA:H	1.77	0.50
2:B:132:ASN:O	2:B:136:TYR:CE1	2.64	0.50
2:B:183:PHE:O	2:B:186:SER:CB	2.60	0.50
2:B:448:THR:HB	2:B:451:LYS:HE2	1.94	0.50
2:B:547:MET:HE1	2:B:557:PHE:CE1	2.46	0.50
2:B:549:ASP:C	2:B:551:LYS:N	2.65	0.50
2:B:588:GLY:O	2:B:592:PHE:CE2	2.65	0.50
2:B:656:VAL:HG22	18:B:1239:CLA:HBB2	1.94	0.50
2:B:681:ALA:O	2:B:685:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ALA:HA	2:B:132:ASN:HD22	1.76	0.50
3:C:12:ILE:CA	3:C:13:GLY:C	2.74	0.50
3:C:63:LEU:CD2	3:C:65:VAL:H	2.23	0.50
1:A:721:GLN:HE22	5:E:72:VAL:H	1.58	0.50
6:F:148:GLU:C	6:F:149:LEU:HG	2.32	0.50
7:G:20:ARG:HG3	7:G:20:ARG:HH11	1.76	0.50
7:G:35:VAL:CG1	7:G:36:PRO:CD	2.89	0.50
7:G:83:TYR:C	7:G:83:TYR:CD2	2.84	0.50
12:L:108:LYS:HB2	12:L:132:SER:HB3	1.93	0.50
14:1:185:TRP:O	14:1:186:HIS:CB	2.60	0.50
17:4:106:TRP:O	17:4:110:LYS:HG2	2.11	0.50
1:A:369:THR:HG21	18:A:1127:CLA:C3C	2.42	0.50
1:A:246:HIS:ND1	18:A:1147:CLA:C1A	2.75	0.50
1:A:281:LEU:HA	1:A:297:THR:O	2.12	0.50
1:A:435:VAL:HA	1:A:438:HIS:ND1	2.25	0.50
1:A:618:TRP:CD2	1:A:642:PHE:HD1	2.29	0.50
1:A:676:GLY:O	1:A:680:LEU:HD22	2.12	0.50
18:B:1209:CLA:CGA	18:B:1209:CLA:C4A	2.89	0.50
2:B:120:VAL:HG13	2:B:124:TRP:CD1	2.47	0.50
2:B:190:TRP:CZ2	18:B:1215:CLA:C3D	2.94	0.50
18:B:1215:CLA:CAB	18:B:1215:CLA:H62	2.41	0.50
18:B:1239:CLA:CBC	20:B:6017:BCR:H392	2.40	0.50
2:B:388:ALA:C	2:B:390:GLY:N	2.64	0.50
2:B:398:TYR:O	4:D:142:SER:HB3	2.12	0.50
2:B:682:HIS:CD2	2:B:682:HIS:H	2.29	0.50
3:C:17:CYS:HB2	3:C:58:CYS:N	2.26	0.50
4:D:56:GLN:OE1	4:D:95:LYS:HE2	2.12	0.50
4:D:86:LEU:CA	4:D:89:ARG:HB3	2.33	0.50
6:F:51:LYS:N	6:F:51:LYS:HD3	2.27	0.50
8:H:42:THR:HG23	8:H:42:THR:O	2.11	0.50
12:L:94:ILE:C	12:L:96:SER:N	2.63	0.50
13:N:1:GLY:O	13:N:3:ILE:HG13	2.12	0.50
13:N:51:ASP:OD1	13:N:52:LEU:HG	2.11	0.50
14:1:180:HIS:C	14:1:182:ALA:HB3	2.33	0.50
15:2:177:ALA:HA	15:2:178:TRP:CE3	2.47	0.50
15:2:96:ILE:O	15:2:100:VAL:CG1	2.56	0.50
16:3:86:PRO:HB2	16:3:87:ALA:CB	2.40	0.50
17:4:136:GLY:HA3	17:4:139:ASN:C	2.33	0.50
1:A:316:MET:O	1:A:325:HIS:N	2.44	0.50
1:A:348:GLU:O	1:A:352:THR:OG1	2.29	0.50
1:A:417:PHE:CE2	1:A:418:MET:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:VAL:HG23	1:A:561:LEU:HD12	1.94	0.50
1:A:671:SER:C	1:A:673:SER:H	2.15	0.50
1:A:86:LEU:O	1:A:90:PHE:N	2.32	0.50
18:B:1225:CLA:HAA2	18:B:1225:CLA:CBD	2.42	0.50
2:B:31:PHE:HA	2:B:34:HIS:HB2	1.94	0.50
2:B:532:LEU:C	2:B:532:LEU:HD12	2.31	0.50
3:C:49:VAL:N	3:C:76:SER:HB3	2.27	0.50
18:H:1501:CLA:HBD	18:H:1505:CLA:C3C	2.42	0.50
11:K:62:UNK:O	11:K:66:UNK:N	2.45	0.50
1:A:448:TRP:CE3	18:L:1130:CLA:HBB2	2.47	0.50
12:L:79:TYR:H	12:L:80:ALA:HB2	1.75	0.50
13:N:19:LYS:HG3	13:N:20:LYS:H	1.76	0.50
15:2:186:THR:HB	15:2:187:GLY:CA	2.42	0.49
15:2:50:VAL:HA	15:2:53:ARG:NE	2.27	0.49
17:4:170:GLN:O	17:4:172:ASN:N	2.45	0.49
1:A:475:ASP:C	1:A:476:MET:SD	2.90	0.49
1:A:564:ARG:HB2	1:A:564:ARG:CZ	2.42	0.49
1:A:541:VAL:HG21	1:A:615:HIS:ND1	2.26	0.49
1:A:662:SER:N	1:A:665:ILE:HD12	2.26	0.49
2:B:275:HIS:CE1	18:B:1214:CLA:CBB	2.92	0.49
2:B:175:LEU:O	2:B:179:LEU:N	2.45	0.49
2:B:411:MET:CE	2:B:411:MET:HA	2.40	0.49
2:B:593:TYR:CD1	2:B:593:TYR:C	2.86	0.49
4:D:113:HIS:CD2	4:D:113:HIS:N	2.78	0.49
13:N:69:CYS:HB2	13:N:72:LYS:CA	2.42	0.49
1:A:130:GLU:O	1:A:133:ASN:N	2.45	0.49
1:A:204:ASN:ND2	1:A:317:TYR:CD1	2.79	0.49
1:A:541:VAL:HG13	1:A:542:HIS:H	1.76	0.49
1:A:604:TRP:O	1:A:607:ASN:CA	2.60	0.49
2:B:284:PHE:CD1	18:B:1216:CLA:HMC3	2.47	0.49
2:B:498:LEU:HA	2:B:501:ILE:CG2	2.42	0.49
20:B:6017:BCR:H351	20:B:6017:BCR:C16	2.31	0.49
2:B:626:LEU:HG	2:B:627:ASN:H	1.77	0.49
2:B:91:ILE:HD11	2:B:114:ASN:HD22	1.74	0.49
6:F:115:THR:O	6:F:118:GLU:CB	2.58	0.49
6:F:28:SER:HB3	6:F:42:ILE:HG22	1.90	0.49
7:G:35:VAL:HG12	7:G:36:PRO:HD3	1.94	0.49
7:G:35:VAL:CG1	7:G:36:PRO:CA	2.78	0.49
18:L:1503:CLA:HBD	18:L:1503:CLA:CAA	2.26	0.49
13:N:36:GLU:HB2	13:N:37:PHE:CD2	2.47	0.49
13:N:38:GLY:N	13:N:39:SER:CA	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:53:ARG:O	15:2:57:LEU:HG	2.12	0.49
16:3:214:LEU:CG	16:3:215:ASP:HB3	2.40	0.49
17:4:114:SER:CB	17:4:120:ILE:CG1	2.90	0.49
17:4:142:ASN:HD22	17:4:145:PRO:HD3	1.76	0.49
1:A:661:ALA:HB3	1:A:665:ILE:HD11	1.93	0.49
2:B:18:THR:OG1	2:B:22:TRP:CZ2	2.63	0.49
2:B:218:TYR:CE1	2:B:232:LEU:HD22	2.48	0.49
2:B:262:HIS:HB3	2:B:269:TRP:CZ3	2.48	0.49
2:B:448:THR:N	2:B:449:PRO:CD	2.74	0.49
2:B:700:LEU:CD1	19:B:5002:PQN:H12	2.42	0.49
2:B:652:PHE:O	2:B:653:GLY:C	2.51	0.49
2:B:7:ARG:HB3	2:B:8:PHE:CD1	2.47	0.49
2:B:98:GLN:NE2	8:H:80:THR:CG2	2.75	0.49
6:F:46:MET:O	6:F:50:LYS:N	2.45	0.49
6:F:49:THR:O	6:F:52:ARG:CA	2.61	0.49
6:F:52:ARG:HA	6:F:55:ASN:OD1	2.12	0.49
2:B:98:GLN:OE1	8:H:78:PRO:C	2.50	0.49
12:L:47:VAL:HG12	12:L:52:ARG:HH12	1.77	0.49
14:1:152:ARG:HH11	14:1:153:LEU:HA	1.77	0.49
14:1:164:GLN:HA	14:1:167:ALA:CB	2.38	0.49
15:2:177:ALA:CA	15:2:178:TRP:HE3	2.25	0.49
15:2:27:PHE:CD1	15:2:28:GLY:CA	2.96	0.49
18:4:1304:CLA:HBA1	18:4:1304:CLA:O1D	2.13	0.49
1:A:681:GLY:HA2	20:A:6011:BCR:H17C	1.94	0.49
1:A:79:PHE:HA	1:A:82:HIS:HB2	1.93	0.49
18:B:1214:CLA:HBD	18:B:1223:CLA:C2B	2.43	0.49
2:B:141:PHE:C	2:B:143:LEU:H	2.14	0.49
2:B:300:SER:O	2:B:301:ILE:HB	2.13	0.49
2:B:355:LEU:O	2:B:356:PRO:O	2.31	0.49
2:B:489:GLY:O	2:B:492:ILE:HG12	2.12	0.49
6:F:26:GLN:C	6:F:28:SER:N	2.65	0.49
7:G:20:ARG:NE	7:G:64:VAL:HB	2.27	0.49
12:L:111:GLU:HG3	12:L:134:ASP:O	2.13	0.49
14:1:155:LEU:HD13	14:1:158:PHE:CE1	2.48	0.49
14:1:91:TRP:N	14:1:92:GLY:CA	2.62	0.49
15:2:36:SER:CA	15:2:37:ASP:CB	2.87	0.49
15:2:44:ASN:C	15:2:46:GLN:H	2.16	0.49
17:4:60:LEU:O	17:4:61:PRO:C	2.50	0.49
1:A:519:ASP:OD2	1:A:519:ASP:O	2.29	0.49
1:A:581:CYS:CB	1:A:590:CYS:SG	3.01	0.49
18:B:1138:CLA:H2A	18:B:1138:CLA:O1D	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:THR:CG2	2:B:521:HIS:HB3	2.42	0.49
2:B:564:ARG:HH12	3:C:66:ARG:NH2	2.02	0.49
2:B:574:ASP:CA	2:B:577:TYR:HB3	2.29	0.49
2:B:57:ILE:O	2:B:60:TRP:HB2	2.13	0.49
3:C:64:SER:O	3:C:65:VAL:HG22	2.13	0.49
4:D:26:SER:N	4:D:27:PRO:HB2	2.17	0.49
6:F:127:SER:C	6:F:131:PHE:HB2	2.33	0.49
6:F:99:TRP:CZ2	6:F:143:GLU:HG2	2.47	0.49
7:G:35:VAL:HG12	7:G:36:PRO:CB	2.36	0.49
13:N:51:ASP:CA	13:N:52:LEU:HB2	2.41	0.49
15:2:197:ALA:N	15:2:198:ASP:CA	2.58	0.49
16:3:111:ASN:O	16:3:112:TYR:HD1	1.95	0.49
1:A:111:ASN:OD1	1:A:112:ASP:N	2.46	0.49
1:A:213:LEU:O	1:A:213:LEU:HD13	2.13	0.49
1:A:354:TRP:O	1:A:357:GLN:HB3	2.12	0.49
1:A:462:ILE:CG2	1:A:463:HIS:N	2.75	0.49
1:A:378:SER:O	1:A:514:THR:HG21	2.13	0.49
1:A:567:ARG:HH22	4:D:37:LEU:HD21	1.77	0.49
1:A:615:HIS:HD2	1:A:615:HIS:C	2.13	0.49
1:A:622:SER:N	1:A:637:ILE:HD13	2.28	0.49
1:A:704:ILE:CG1	1:A:724:ALA:HB2	2.42	0.49
2:B:120:VAL:O	2:B:122:GLN:N	2.46	0.49
2:B:304:ILE:HG12	18:B:1220:CLA:HED2	1.94	0.49
2:B:304:ILE:HG23	2:B:305:LEU:HD12	1.94	0.49
2:B:374:HIS:C	2:B:374:HIS:ND1	2.66	0.49
2:B:332:PHE:CE1	2:B:393:PHE:CD1	3.00	0.49
2:B:71:GLN:OE1	2:B:89:HIS:HA	2.13	0.49
3:C:42:ALA:HB1	3:C:44:ARG:C	2.33	0.49
4:D:102:ARG:HG2	4:D:109:VAL:HG23	1.94	0.49
6:F:127:SER:H	6:F:130:LEU:HD13	1.77	0.49
6:F:127:SER:O	6:F:130:LEU:N	2.39	0.49
7:G:86:LEU:O	7:G:87:ALA:CB	2.60	0.49
8:H:64:LEU:O	8:H:65:LEU:C	2.50	0.49
10:J:5:LYS:HE3	10:J:6:THR:OG1	2.11	0.49
12:L:108:LYS:O	12:L:109:GLU:HB2	2.10	0.49
12:L:70:LYS:HG2	12:L:75:ARG:HG2	1.92	0.49
15:2:28:GLY:CA	15:2:29:PHE:CE2	2.91	0.49
15:2:37:ASP:HB3	15:2:38:PRO:CB	2.42	0.49
1:A:106:TYR:CE2	1:A:164:LEU:HD11	2.48	0.49
1:A:584:PRO:HG3	2:B:560:ASP:O	2.13	0.49
18:B:1208:CLA:C6	18:B:1209:CLA:H43	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1218:CLA:HAA2	18:B:1218:CLA:CBD	2.42	0.49
2:B:408:LEU:HD22	18:B:1220:CLA:HAC2	1.95	0.49
18:B:1229:CLA:C4D	6:F:90:PHE:CZ	2.96	0.49
2:B:510:LEU:CD2	18:B:1234:CLA:HHD	2.34	0.49
2:B:141:PHE:HA	2:B:144:PHE:HB3	1.94	0.49
2:B:304:ILE:HG23	2:B:305:LEU:N	2.25	0.49
2:B:70:TRP:N	2:B:71:GLN:O	2.44	0.49
6:F:1:ASP:H1	6:F:62:LEU:HD13	1.70	0.49
7:G:8:ILE:O	7:G:11:SER:N	2.45	0.49
12:L:57:GLY:CA	12:L:143:PHE:HA	2.40	0.49
17:4:59:LEU:C	17:4:62:GLU:HB3	2.28	0.49
1:A:567:ARG:HH12	2:B:680:TRP:HE1	1.60	0.49
1:A:657:LEU:HD13	18:B:9010:CLA:HMC3	1.94	0.49
1:A:678:PHE:CD1	1:A:747:TRP:CZ3	3.00	0.49
18:B:1229:CLA:C1D	6:F:90:PHE:CE2	2.96	0.49
2:B:635:ILE:HG23	2:B:636:THR:N	2.20	0.49
2:B:96:PHE:CZ	18:B:1206:CLA:C1D	2.94	0.49
3:C:7:ILE:C	3:C:8:TYR:CG	2.86	0.49
6:F:121:ILE:N	10:J:9:SER:CB	2.76	0.49
6:F:125:LEU:HB3	6:F:130:LEU:CD2	2.43	0.49
6:F:25:LEU:HD12	6:F:25:LEU:C	2.33	0.49
6:F:46:MET:HB2	6:F:51:LYS:NZ	2.28	0.49
8:H:30:SER:HB2	12:L:35:TRP:HE1	1.78	0.49
14:1:40:LYS:C	14:1:42:SER:H	2.13	0.49
15:2:179:PHE:CD1	15:2:180:GLN:HG2	2.46	0.49
16:3:138:SER:O	16:3:141:LYS:HB3	2.13	0.49
17:4:53:LEU:HA	17:4:56:ALA:CB	2.40	0.49
18:A:1123:CLA:CBD	18:A:1123:CLA:HBA1	2.42	0.49
1:A:434:ARG:NE	18:A:1129:CLA:OBD	2.45	0.49
1:A:130:GLU:O	1:A:132:LEU:N	2.46	0.49
1:A:149:PHE:CG	1:A:153:TRP:CZ3	3.01	0.49
1:A:710:ALA:O	1:A:714:LEU:HB2	2.13	0.49
18:B:1138:CLA:C3C	18:F:1139:CLA:HBC2	2.43	0.49
2:B:171:ALA:CB	18:B:1221:CLA:HBC1	2.42	0.49
18:B:1239:CLA:HBD	19:B:5002:PQN:C26	2.40	0.49
2:B:284:PHE:C	2:B:286:ILE:N	2.67	0.49
2:B:402:GLN:C	2:B:403:ASN:HD22	2.16	0.49
2:B:42:LEU:CD2	2:B:43:TYR:HD2	2.26	0.49
2:B:47:PHE:CE2	2:B:51:PHE:CZ	3.00	0.49
2:B:525:LEU:C	2:B:525:LEU:HD12	2.33	0.49
2:B:553:PHE:CE2	3:C:66:ARG:CG	2.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:PHE:O	2:B:654:HIS:N	2.42	0.49
6:F:49:THR:O	6:F:52:ARG:C	2.51	0.49
9:I:8:PHE:O	9:I:11:LEU:CB	2.59	0.49
13:N:2:VAL:HA	13:N:3:ILE:CD1	2.42	0.49
15:2:40:SER:HA	15:2:41:LEU:CB	2.38	0.49
17:4:68:GLY:O	17:4:69:ILE:CG2	2.55	0.49
18:A:1126:CLA:NC	20:A:6011:BCR:HC42	2.28	0.49
1:A:238:ASP:CB	1:A:239:PRO:CD	2.81	0.49
1:A:387:THR:O	1:A:389:TYR:CE2	2.66	0.49
1:A:490:GLN:HG3	1:A:494:ASN:CB	2.43	0.49
1:A:52:THR:CB	1:A:55:TRP:HE1	2.25	0.49
1:A:450:CYS:SG	1:A:550:HIS:HB3	2.53	0.49
1:A:623:ASP:OD2	1:A:623:ASP:O	2.31	0.49
2:B:338:LEU:HB2	2:B:382:ILE:HG23	1.95	0.49
2:B:440:ASN:HD22	2:B:614:THR:HB	1.77	0.49
2:B:440:ASN:HA	2:B:452:GLN:NE2	2.28	0.49
2:B:478:LEU:CG	2:B:486:LEU:HB2	2.42	0.49
3:C:63:LEU:HD23	3:C:66:ARG:CG	2.42	0.49
4:D:136:SER:N	4:D:139:LYS:NZ	2.60	0.49
6:F:27:ALA:C	6:F:29:LEU:H	2.16	0.49
7:G:81:VAL:HG11	7:G:83:TYR:CE1	2.48	0.49
8:H:58:ILE:CD1	8:H:58:ILE:O	2.51	0.49
15:2:176:GLY:O	15:2:178:TRP:CZ3	2.65	0.48
15:2:17:GLU:CD	15:2:18:TRP:CB	2.66	0.48
18:A:1123:CLA:CBC	18:A:1123:CLA:CHD	2.86	0.48
1:A:347:TYR:HB3	1:A:350:LEU:CG	2.43	0.48
1:A:358:LEU:HD21	18:A:1128:CLA:HBB1	1.94	0.48
1:A:442:ILE:O	1:A:443:ILE:C	2.52	0.48
1:A:490:GLN:HA	1:A:491:TRP:O	2.12	0.48
1:A:692:PHE:HD2	19:A:5001:PQN:C10	2.26	0.48
1:A:581:CYS:HB3	1:A:590:CYS:SG	2.53	0.48
1:A:461:TYR:HB2	1:A:649:ILE:CD1	2.43	0.48
1:A:665:ILE:CG1	18:A:9011:CLA:HBC1	2.43	0.48
2:B:402:GLN:HB3	2:B:403:ASN:HD22	1.77	0.48
2:B:427:LEU:CD1	18:B:1138:CLA:HMD2	2.42	0.48
2:B:42:LEU:HD21	2:B:43:TYR:CD2	2.48	0.48
2:B:4:ARG:HG3	2:B:4:ARG:NH1	2.28	0.48
2:B:510:LEU:N	2:B:510:LEU:CD1	2.76	0.48
4:D:133:ASN:HD22	4:D:134:MET:H	1.57	0.48
1:A:437:ARG:C	4:D:32:SER:OG	2.50	0.48
1:A:567:ARG:HH22	4:D:37:LEU:CD2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:64:GLY:O	6:F:67:GLY:N	2.43	0.48
8:H:39:PHE:HA	8:H:43:PHE:HD2	1.78	0.48
2:B:66:PHE:CE1	18:I:1204:CLA:HAC1	2.47	0.48
18:L:1502:CLA:C4	18:L:1504:CLA:CMA	2.78	0.48
12:L:62:PHE:O	12:L:65:VAL:HG12	2.13	0.48
12:L:70:LYS:O	12:L:75:ARG:HD2	2.13	0.48
13:N:59:PRO:HA	13:N:60:PHE:CD2	2.48	0.48
13:N:79:SER:H	13:N:82:PHE:HE2	1.59	0.48
13:N:8:GLU:HG2	13:N:11:LYS:CB	2.38	0.48
17:4:51:ALA:CB	17:4:161:MET:HE2	2.43	0.48
1:A:452:PHE:CZ	18:A:1136:CLA:HMC3	2.49	0.48
1:A:354:TRP:CG	18:A:1103:CLA:HAC1	2.49	0.48
1:A:389:TYR:HB3	1:A:754:ILE:HD11	1.95	0.48
1:A:415:ALA:O	1:A:416:ILE:CG1	2.61	0.48
1:A:386:ALA:CB	1:A:528:ALA:HB1	2.43	0.48
2:B:193:HIS:C	2:B:195:VAL:H	2.17	0.48
2:B:534:LEU:O	2:B:538:ALA:N	2.46	0.48
2:B:595:HIS:O	2:B:599:ILE:HG22	2.13	0.48
2:B:720:THR:HG1	18:B:9010:CLA:HED2	1.78	0.48
7:G:60:SER:C	7:G:64:VAL:HG13	2.21	0.48
17:4:194:ILE:O	17:4:195:VAL:C	2.51	0.48
18:A:1124:CLA:C4A	18:A:1135:CLA:HBB2	2.29	0.48
1:A:207:LEU:HD13	1:A:310:PHE:CD1	2.48	0.48
1:A:331:LEU:HD13	1:A:346:LEU:HB2	1.91	0.48
1:A:416:ILE:C	1:A:420:ARG:HB2	2.33	0.48
1:A:491:TRP:HA	1:A:492:ILE:CG2	2.43	0.48
1:A:525:ASN:C	1:A:627:THR:O	2.51	0.48
1:A:520:LEU:HD23	1:A:531:PRO:HD3	1.95	0.48
1:A:570:PRO:O	1:A:571:ASP:HB3	2.13	0.48
1:A:559:GLY:CA	1:A:597:HIS:CD2	2.97	0.48
1:A:681:GLY:O	20:A:6011:BCR:C15	2.62	0.48
2:B:412:LEU:HA	2:B:415:LYS:HB3	1.94	0.48
2:B:422:LEU:HA	2:B:425:ALA:HB3	1.95	0.48
2:B:433:THR:O	2:B:437:TYR:HD2	1.95	0.48
2:B:657:TRP:HE1	2:B:717:TYR:CB	2.16	0.48
4:D:102:ARG:CA	4:D:103:VAL:CB	2.66	0.48
2:B:680:TRP:HE1	4:D:37:LEU:CD2	2.26	0.48
5:E:51:SER:C	5:E:53:VAL:H	2.16	0.48
6:F:105:LEU:C	6:F:107:ALA:N	2.67	0.48
6:F:115:THR:O	6:F:117:LYS:CA	2.61	0.48
6:F:49:THR:C	6:F:56:TYR:OH	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:THR:O	10:J:7:TYR:CB	2.59	0.48
12:L:37:LEU:HD21	18:L:1130:CLA:C5	2.43	0.48
12:L:79:TYR:N	12:L:80:ALA:CB	2.73	0.48
18:B:1207:CLA:H62	12:L:91:LEU:CD2	2.44	0.48
15:2:20:ASP:OD2	15:2:22:SER:OG	2.30	0.48
16:3:125:ALA:O	16:3:129:ARG:CB	2.60	0.48
16:3:209:PRO:HB2	16:3:210:TYR:HA	1.95	0.48
1:A:99:HIS:HA	1:A:103:PHE:CE1	2.48	0.48
1:A:162:LEU:HA	1:A:165:TYR:CD2	2.48	0.48
1:A:171:ALA:CA	1:A:174:PHE:HB3	2.42	0.48
1:A:185:HIS:HA	1:A:189:ALA:HB3	1.95	0.48
1:A:214:GLY:O	1:A:216:LEU:N	2.47	0.48
1:A:615:HIS:CD2	1:A:615:HIS:O	2.66	0.48
1:A:619:LYS:HD2	1:A:619:LYS:HA	1.49	0.48
1:A:709:TRP:HZ2	18:B:1228:CLA:CED	2.25	0.48
2:B:649:MET:HG3	20:B:6017:BCR:HC41	1.94	0.48
6:F:111:GLU:O	6:F:111:GLU:CD	2.52	0.48
7:G:42:SER:H	7:G:43:HIS:CD2	2.27	0.48
2:B:20:ARG:HH22	9:I:28:VAL:HA	1.76	0.48
18:A:1129:CLA:O1A	18:L:1130:CLA:HMD1	2.13	0.48
12:L:32:LEU:O	12:L:33:ILE:HB	2.12	0.48
13:N:25:THR:HB	15:2:201:HIS:HB3	1.94	0.48
14:1:44:LEU:CD2	14:1:44:LEU:N	2.77	0.48
14:1:86:GLY:N	14:1:87:ASN:HB3	2.28	0.48
15:2:63:PHE:HA	15:2:66:GLU:HB3	1.96	0.48
16:3:78:ILE:H	16:3:79:LEU:HA	1.79	0.48
1:A:109:TRP:CH2	1:A:150:PHE:HB3	2.48	0.48
1:A:158:ILE:HG13	1:A:164:LEU:HD13	1.95	0.48
1:A:216:LEU:O	1:A:219:ALA:HB3	2.12	0.48
1:A:393:LEU:CG	1:A:394:SER:N	2.77	0.48
2:B:111:GLY:O	2:B:113:VAL:N	2.36	0.48
18:B:1237:CLA:HMC3	18:B:1238:CLA:ND	2.29	0.48
2:B:176:ASN:CB	2:B:291:TYR:CD1	2.85	0.48
1:A:709:TRP:CE3	2:B:416:GLU:O	2.66	0.48
4:D:58:PHE:O	4:D:58:PHE:HD1	1.96	0.48
6:F:100:VAL:HG22	6:F:130:LEU:HA	1.96	0.48
6:F:50:LYS:HG2	6:F:53:PHE:CD1	2.49	0.48
7:G:37:GLU:HB2	7:G:43:HIS:HE1	1.76	0.48
7:G:50:ARG:NH1	7:G:51:ALA:HB1	2.27	0.48
10:J:25:LEU:O	10:J:26:LEU:C	2.52	0.48
14:1:77:LEU:N	14:1:78:PRO:HD3	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:8:GLU:C	17:4:110:LYS:HZ3	2.16	0.48
17:4:124:TYR:CB	17:4:125:SER:HB3	2.44	0.48
17:4:193:THR:HG23	17:4:194:ILE:N	2.29	0.48
1:A:196:PHE:HD2	1:A:196:PHE:C	2.17	0.48
1:A:500:PRO:O	1:A:505:PRO:O	2.31	0.48
1:A:510:SER:O	1:A:512:SER:N	2.39	0.48
1:A:544:ILE:HA	1:A:547:PHE:HB3	1.96	0.48
1:A:555:ILE:N	1:A:556:LEU:CA	2.76	0.48
1:A:754:ILE:HA	1:A:758:GLY:CA	2.43	0.48
2:B:6:PRO:HD2	2:B:13:ALA:HA	1.95	0.48
2:B:364:ASP:C	2:B:365:PHE:CG	2.86	0.48
2:B:468:GLY:O	2:B:479:SER:OG	2.25	0.48
1:A:590:CYS:H	2:B:669:GLY:CA	2.27	0.48
2:B:697:PRO:HG3	18:B:1238:CLA:C3C	2.44	0.48
2:B:672:GLN:CD	2:B:699:ALA:H	2.16	0.48
2:B:67:HIS:CD2	2:B:71:GLN:OE1	2.66	0.48
2:B:720:THR:OG1	18:B:9010:CLA:CED	2.61	0.48
3:C:51:CYS:N	21:C:3102:SF4:S3	2.86	0.48
4:D:48:ILE:CG2	4:D:77:LEU:HD21	2.44	0.48
6:F:115:THR:C	6:F:118:GLU:HB2	2.33	0.48
6:F:136:TRP:CD1	6:F:137:PRO:HD3	2.38	0.48
13:N:42:PHE:CG	13:N:43:PRO:HA	2.48	0.48
13:N:51:ASP:HB3	13:N:52:LEU:CB	2.41	0.48
14:1:34:ALA:HB3	14:1:37:GLU:CA	2.40	0.48
18:2:2007:CLA:C4B	18:2:2002:CLA:HHC	2.43	0.48
1:A:126:ILE:CG2	1:A:129:GLN:HG2	2.32	0.48
1:A:173:VAL:O	1:A:175:ALA:N	2.47	0.48
1:A:367:SER:O	1:A:370:ILE:N	2.47	0.48
1:A:419:VAL:HG11	1:A:572:LYS:HE3	1.96	0.48
1:A:473:PRO:O	1:A:475:ASP:N	2.46	0.48
1:A:657:LEU:C	1:A:659:ALA:N	2.66	0.48
18:B:1209:CLA:O1A	18:B:1209:CLA:H3A	2.12	0.48
2:B:255:LEU:CD2	18:B:1212:CLA:HAC2	2.43	0.48
2:B:177:HIS:CE1	18:B:1209:CLA:CHD	2.96	0.48
2:B:407:VAL:O	2:B:411:MET:HB2	2.14	0.48
2:B:533:ILE:O	2:B:537:GLY:N	2.43	0.48
2:B:61:THR:C	2:B:63:GLY:N	2.66	0.48
2:B:595:HIS:CE1	2:B:725:LEU:HA	2.48	0.48
4:D:108:GLU:HG2	4:D:109:VAL:H	1.74	0.48
18:F:1302:CLA:O1D	18:F:1302:CLA:H2A	2.13	0.48
6:F:137:PRO:HA	6:F:141:TYR:CA	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:137:PRO:CB	6:F:141:TYR:HB3	2.36	0.48
12:L:97:MET:O	12:L:100:THR:N	2.30	0.48
17:4:63:VAL:O	17:4:64:PHE:O	2.32	0.48
1:A:206:HIS:HD2	18:A:1123:CLA:OBD	1.96	0.48
1:A:747:TRP:HB2	18:A:1126:CLA:HBB2	1.95	0.48
1:A:542:HIS:C	1:A:544:ILE:N	2.67	0.48
2:B:32:GLU:O	2:B:32:GLU:HG2	2.13	0.48
19:B:5002:PQN:H192	19:B:5002:PQN:H161	1.58	0.48
2:B:633:ASN:HA	2:B:636:THR:HB	1.96	0.48
2:B:84:VAL:HG12	2:B:86:PRO:N	2.27	0.48
4:D:107:GLY:O	4:D:108:GLU:CB	2.49	0.48
4:D:135:ARG:HA	4:D:139:LYS:HZ3	1.78	0.48
5:E:40:ARG:NH1	5:E:42:GLU:HG2	2.29	0.48
5:E:37:LYS:HB3	5:E:89:GLU:HB3	1.95	0.48
12:L:136:TRP:CD1	12:L:136:TRP:C	2.86	0.48
12:L:46:ALA:HB1	12:L:52:ARG:CZ	2.44	0.48
15:2:189:ILE:CB	15:2:190:ASP:HA	2.44	0.48
16:3:84:LEU:H	16:3:88:GLU:CD	2.17	0.48
17:4:97:LEU:O	17:4:101:VAL:HG13	2.14	0.48
1:A:364:MET:CG	18:A:1123:CLA:HMA1	2.42	0.48
1:A:347:TYR:CB	1:A:350:LEU:HG	2.44	0.48
1:A:637:ILE:HG22	1:A:757:VAL:HG12	1.96	0.48
1:A:71:LEU:CD1	1:A:352:THR:CG2	2.85	0.48
1:A:79:PHE:O	1:A:79:PHE:CG	2.67	0.48
18:B:1220:CLA:C1B	18:B:1242:CLA:CBA	2.87	0.48
2:B:415:LYS:NZ	2:B:540:ASP:CA	2.67	0.48
2:B:444:LEU:HB3	2:B:615:TYR:CD1	2.49	0.48
2:B:465:SER:O	2:B:468:GLY:N	2.45	0.48
2:B:558:PRO:O	2:B:559:CYS:O	2.32	0.48
2:B:702:ILE:HD12	2:B:702:ILE:C	2.32	0.48
3:C:70:TRP:O	3:C:71:HIS:C	2.51	0.48
4:D:134:MET:O	4:D:134:MET:HG2	2.14	0.48
4:D:48:ILE:HD13	4:D:86:LEU:HD22	1.95	0.48
6:F:59:TYR:N	6:F:59:TYR:CD1	2.81	0.48
8:H:33:ASN:ND2	8:H:34:SER:H	2.12	0.48
10:J:10:VAL:HG13	10:J:11:ALA:H	1.79	0.48
12:L:164:PRO:HB3	18:L:1503:CLA:C2	2.44	0.48
14:1:82:ALA:H	14:1:83:THR:HA	1.75	0.48
15:2:28:GLY:C	15:2:29:PHE:CD1	2.80	0.48
15:2:81:THR:HG23	15:2:82:ALA:H	1.78	0.48
1:A:228:PRO:HD2	1:A:229:ILE:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HB2	1:A:294:LEU:HB3	1.96	0.48
1:A:398:HIS:HD2	1:A:399:HIS:N	2.11	0.48
1:A:687:ALA:CB	18:A:9013:CLA:HBB2	2.39	0.48
18:B:1138:CLA:C3B	18:F:1139:CLA:CMD	2.82	0.48
2:B:50:HIS:CE1	18:B:1210:CLA:C3D	2.97	0.48
2:B:174:ARG:CG	18:B:1221:CLA:CMD	2.83	0.48
2:B:443:MET:O	2:B:446:PHE:N	2.47	0.48
2:B:631:LEU:CA	2:B:643:LEU:HD12	2.39	0.48
4:D:26:SER:H	4:D:27:PRO:CB	2.18	0.48
4:D:76:LYS:C	4:D:77:LEU:HG	2.35	0.48
6:F:92:TYR:HA	6:F:136:TRP:HZ2	1.77	0.48
18:B:1205:CLA:HMB3	18:I:1204:CLA:CMA	2.44	0.48
15:2:153:PRO:HD2	15:2:154:GLN:HA	1.96	0.47
15:2:186:THR:CB	15:2:187:GLY:CA	2.91	0.47
18:A:1106:CLA:HBB2	18:A:1126:CLA:C8	2.42	0.47
1:A:575:LEU:HB3	1:A:579:PHE:CB	2.40	0.47
1:A:594:ALA:HA	1:A:597:HIS:CG	2.49	0.47
1:A:645:SER:CB	2:B:637:PRO:HG2	2.44	0.47
1:A:606:TYR:CE1	1:A:742:GLY:O	2.66	0.47
18:A:9013:CLA:HBB1	18:A:9013:CLA:HHC	1.95	0.47
18:B:1218:CLA:OBD	18:B:1218:CLA:CED	2.56	0.47
2:B:22:TRP:HZ2	18:B:1238:CLA:CBB	2.27	0.47
2:B:31:PHE:HD2	2:B:34:HIS:ND1	2.11	0.47
2:B:495:PRO:HD2	2:B:496:GLY:H	1.79	0.47
2:B:496:GLY:O	2:B:499:ASN:N	2.47	0.47
2:B:576:PHE:CZ	2:B:580:VAL:HG21	2.49	0.47
2:B:58:PHE:CE2	18:B:1241:CLA:CHB	2.82	0.47
2:B:591:THR:CG2	2:B:721:TYR:CE2	2.88	0.47
2:B:593:TYR:HD1	2:B:593:TYR:C	2.17	0.47
3:C:12:ILE:CG1	21:C:3103:SF4:S2	2.96	0.47
3:C:26:LEU:HD23	4:D:120:PRO:CB	2.43	0.47
4:D:61:PRO:O	4:D:63:GLY:N	2.47	0.47
4:D:50:TRP:O	4:D:73:ASN:CG	2.52	0.47
18:B:1235:CLA:HBC1	6:F:83:PHE:CZ	2.49	0.47
7:G:74:TRP:HA	7:G:78:GLY:HA3	1.95	0.47
8:H:84:GLN:O	8:H:85:GLN:HB3	2.14	0.47
15:2:27:PHE:HE1	15:2:30:ASP:N	2.10	0.47
16:3:200:ILE:HG23	16:3:201:GLN:N	2.29	0.47
17:4:47:ASN:HD21	18:4:4005:CLA:C1A	2.27	0.47
1:A:407:ILE:CG1	18:A:1124:CLA:C2D	2.90	0.47
1:A:160:SER:O	1:A:163:GLN:HB2	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:O	1:A:175:ALA:C	2.51	0.47
1:A:248:PHE:HB2	1:A:255:LEU:HD21	1.96	0.47
1:A:457:SER:HA	1:A:460:LEU:CD2	2.42	0.47
18:B:1219:CLA:C4B	18:B:1219:CLA:H42	2.45	0.47
2:B:144:PHE:CD2	2:B:145:LEU:CD2	2.97	0.47
2:B:350:GLN:O	2:B:353:TYR:N	2.38	0.47
2:B:668:ARG:NH2	2:B:672:GLN:OE1	2.48	0.47
2:B:703:VAL:O	2:B:704:GLN:CG	2.62	0.47
3:C:49:VAL:C	3:C:51:CYS:N	2.66	0.47
18:F:1303:CLA:C3B	20:F:6016:BCR:H403	2.44	0.47
6:F:73:VAL:CG2	6:F:83:PHE:H	2.08	0.47
7:G:33:LYS:CB	7:G:34:GLN:HB2	2.28	0.47
7:G:70:ASP:O	7:G:73:ALA:N	2.37	0.47
14:I:19:PRO:N	14:I:20:GLY:HA3	2.29	0.47
15:2:70:LYS:HB3	15:2:191:ASN:ND2	2.29	0.47
15:2:73:ILE:O	15:2:73:ILE:HG13	2.13	0.47
16:3:217:LEU:HA	16:3:218:ALA:CB	2.21	0.47
17:4:75:TRP:O	17:4:76:TYR:CD2	2.68	0.47
17:4:95:PHE:O	17:4:98:SER:OG	2.32	0.47
1:A:205:HIS:NE2	18:A:1108:CLA:HMD1	2.29	0.47
1:A:282:THR:CB	1:A:284:ARG:HH21	2.23	0.47
1:A:331:LEU:CD1	1:A:346:LEU:CB	2.81	0.47
1:A:397:THR:O	1:A:399:HIS:C	2.51	0.47
1:A:64:PHE:C	1:A:420:ARG:NH2	2.67	0.47
1:A:435:VAL:HG12	1:A:436:LEU:N	2.29	0.47
1:A:449:VAL:CG1	1:A:450:CYS:N	2.77	0.47
1:A:540:LEU:O	1:A:541:VAL:C	2.50	0.47
1:A:570:PRO:O	1:A:571:ASP:CB	2.62	0.47
1:A:396:PHE:CD1	1:A:616:PHE:CZ	3.02	0.47
2:B:101:VAL:CG2	2:B:102:GLU:N	2.66	0.47
2:B:190:TRP:HZ2	18:B:1215:CLA:O1D	1.97	0.47
18:B:1227:CLA:H41	18:B:1228:CLA:C9	2.41	0.47
2:B:308:HIS:HE1	18:B:1219:CLA:NB	2.03	0.47
2:B:450:GLU:HG3	2:B:451:LYS:N	2.18	0.47
2:B:531:THR:O	2:B:533:ILE:HG13	2.14	0.47
2:B:580:VAL:HG12	2:B:580:VAL:O	2.13	0.47
1:A:590:CYS:H	2:B:669:GLY:HA3	1.78	0.47
4:D:44:GLU:OE2	4:D:46:TYR:CD2	2.67	0.47
6:F:32:TYR:CD2	6:F:32:TYR:N	2.81	0.47
9:I:16:PHE:HD1	9:I:17:PRO:CG	2.27	0.47
13:N:64:ASP:O	13:N:65:LEU:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:82:ALA:CB	16:3:83:GLY:C	2.82	0.47
17:4:85:ALA:HA	17:4:86:SER:HA	1.61	0.47
1:A:409:GLY:CA	18:A:1128:CLA:HAC1	2.35	0.47
1:A:688:PHE:HZ	18:A:1140:CLA:C3C	2.27	0.47
1:A:232:PHE:C	1:A:232:PHE:CD1	2.87	0.47
1:A:327:ILE:O	1:A:330:ILE:HD11	2.15	0.47
1:A:443:ILE:HD13	1:A:558:LYS:HA	1.97	0.47
18:B:1205:CLA:HBA1	18:B:1224:CLA:HBD	1.96	0.47
2:B:235:GLN:O	2:B:236:ASN:ND2	2.48	0.47
2:B:280:ILE:HG13	2:B:281:ALA:N	2.28	0.47
2:B:48:ALA:O	2:B:49:SER:C	2.53	0.47
2:B:53:GLN:HG2	2:B:57:ILE:HD11	1.95	0.47
2:B:548:PRO:HG2	3:C:62:PHE:CD2	2.50	0.47
18:B:1239:CLA:C2B	20:B:6017:BCR:C15	2.91	0.47
2:B:645:VAL:O	2:B:648:TRP:CA	2.62	0.47
3:C:72:GLU:CD	3:C:77:MET:HG3	2.33	0.47
6:F:19:LYS:HG2	6:F:53:PHE:CZ	2.49	0.47
7:G:50:ARG:HH11	7:G:51:ALA:CB	2.28	0.47
12:L:103:GLY:C	12:L:104:ILE:HG13	2.34	0.47
12:L:45:THR:CG2	12:L:126:GLN:HE21	2.27	0.47
13:N:59:PRO:CA	13:N:60:PHE:HB3	2.45	0.47
13:N:6:TYR:CD2	13:N:9:LYS:HE2	2.50	0.47
14:1:63:LEU:HD21	14:1:68:TRP:CD1	2.49	0.47
14:1:81:GLN:HA	14:1:82:ALA:HA	1.74	0.47
18:A:1124:CLA:HHB	18:A:1135:CLA:CBB	2.44	0.47
1:A:170:GLY:O	1:A:174:PHE:HB2	2.15	0.47
1:A:565:SER:O	1:A:566:SER:C	2.53	0.47
2:B:233:TYR:O	2:B:253:ALA:HB1	2.14	0.47
2:B:263:PRO:O	2:B:266:GLN:HG2	2.13	0.47
2:B:433:THR:HG21	2:B:521:HIS:HB3	1.97	0.47
2:B:527:LEU:O	2:B:531:THR:N	2.41	0.47
2:B:619:TRP:O	2:B:623:TYR:HB3	2.15	0.47
2:B:663:PHE:CZ	18:B:1239:CLA:CHD	2.97	0.47
2:B:668:ARG:CB	2:B:702:ILE:HG22	2.39	0.47
2:B:717:TYR:C	2:B:717:TYR:CD1	2.87	0.47
2:B:68:VAL:C	2:B:71:GLN:O	2.52	0.47
6:F:2:ILE:O	6:F:3:ALA:CB	2.61	0.47
7:G:21:PHE:N	7:G:21:PHE:CD1	2.82	0.47
14:1:189:ILE:O	14:1:189:ILE:HG13	2.13	0.47
15:2:180:GLN:HB3	15:2:182:ILE:O	2.14	0.47
15:2:187:GLY:N	15:2:189:ILE:H	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:18:TRP:CG	15:2:21:GLY:O	2.68	0.47
15:2:20:ASP:OD2	15:2:23:LEU:HD21	2.15	0.47
1:A:315:HIS:CD2	18:A:1108:CLA:NA	2.82	0.47
18:A:1140:CLA:H51	19:A:5001:PQN:H191	1.95	0.47
1:A:316:MET:O	1:A:324:GLY:HA2	2.15	0.47
1:A:358:LEU:HG	18:A:1103:CLA:CMD	2.32	0.47
1:A:407:ILE:C	1:A:407:ILE:HD13	2.34	0.47
1:A:416:ILE:HG22	1:A:420:ARG:HD2	1.96	0.47
1:A:715:LYS:HZ3	6:F:109:ARG:HH12	1.62	0.47
1:A:82:HIS:CE1	18:A:1103:CLA:CHA	2.97	0.47
2:B:145:LEU:HD13	2:B:148:ILE:HG21	1.96	0.47
2:B:179:LEU:HD12	2:B:288:GLY:HA2	1.97	0.47
2:B:302:LYS:HE3	2:B:323:TYR:CD2	2.49	0.47
2:B:338:LEU:HB3	2:B:382:ILE:HG23	1.95	0.47
2:B:433:THR:HG21	2:B:522:ALA:N	2.30	0.47
2:B:606:VAL:O	2:B:610:ASN:ND2	2.47	0.47
1:A:586:ARG:NH2	3:C:53:ARG:HH22	2.13	0.47
7:G:54:TYR:CD1	7:G:54:TYR:O	2.67	0.47
13:N:21:ARG:C	13:N:23:ALA:H	2.18	0.47
13:N:48:GLY:CA	13:N:49:CYS:HB3	2.45	0.47
13:N:61:LEU:HA	13:N:62:SER:HA	1.54	0.47
13:N:77:CYS:HB3	13:N:78:GLY:HA2	1.95	0.47
18:B:1218:CLA:C6	18:1:1012:CLA:C2A	2.93	0.47
15:2:167:GLY:O	15:2:170:ALA:HB3	2.14	0.47
15:2:59:ALA:O	15:2:61:GLY:N	2.46	0.47
16:3:81:LYS:HA	16:3:82:ALA:C	2.34	0.47
17:4:192:ASN:ND2	17:4:196:GLN:HE22	2.12	0.47
1:A:139:GLY:O	6:F:38:PRO:CG	2.63	0.47
1:A:71:LEU:HD12	1:A:193:LEU:HD13	1.96	0.47
1:A:436:LEU:O	1:A:439:ARG:HD2	2.14	0.47
1:A:463:HIS:ND1	1:A:477:PHE:CE1	2.81	0.47
1:A:680:LEU:C	1:A:682:ALA:H	2.18	0.47
1:A:697:ARG:HH22	1:A:701:GLN:HB2	1.79	0.47
18:B:1216:CLA:HAA2	18:B:1221:CLA:CAB	2.45	0.47
2:B:711:VAL:CG1	18:B:1239:CLA:HED3	2.43	0.47
2:B:16:PRO:HG3	3:C:74:THR:HG22	1.96	0.47
2:B:323:TYR:HD1	2:B:323:TYR:C	2.18	0.47
2:B:527:LEU:O	2:B:529:THR:N	2.44	0.47
2:B:705:ALA:HB2	19:B:5002:PQN:C7	2.44	0.47
5:E:37:LYS:HB2	5:E:89:GLU:CB	2.43	0.47
5:E:42:GLU:O	5:E:43:SER:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:56:TYR:O	6:F:58:LYS:HB3	2.12	0.47
7:G:20:ARG:NH2	7:G:68:ILE:HG21	2.29	0.47
7:G:35:VAL:CG1	7:G:36:PRO:N	2.77	0.47
12:L:14:LEU:HD22	12:L:22:GLY:CA	2.45	0.47
12:L:91:LEU:CD1	20:L:6020:BCR:H333	2.42	0.47
12:L:93:VAL:N	12:L:96:SER:OG	2.48	0.47
13:N:75:TYR:CE2	13:N:76:LYS:CD	2.97	0.47
17:4:124:TYR:HD2	17:4:125:SER:HB3	1.79	0.47
17:4:56:ALA:O	17:4:59:LEU:HB3	2.14	0.47
17:4:59:LEU:HG	17:4:62:GLU:OE1	2.14	0.47
1:A:543:HIS:NE2	18:A:1136:CLA:C4A	2.78	0.47
1:A:133:ASN:HB2	1:A:142:GLY:CA	2.42	0.47
1:A:542:HIS:CA	1:A:545:HIS:HD2	2.27	0.47
2:B:280:ILE:N	18:B:1214:CLA:HMC3	2.30	0.47
2:B:301:ILE:CG2	2:B:304:ILE:HG21	2.40	0.47
2:B:258:LEU:HD11	2:B:495:PRO:CD	2.44	0.47
2:B:536:LYS:O	2:B:537:GLY:C	2.53	0.47
2:B:567:THR:O	2:B:568:CYS:CB	2.61	0.47
2:B:96:PHE:HZ	18:B:1206:CLA:C2D	2.27	0.47
2:B:696:LYS:NZ	3:C:79:LEU:O	2.39	0.47
4:D:135:ARG:HA	4:D:139:LYS:NZ	2.29	0.47
6:F:133:GLY:O	6:F:136:TRP:NE1	2.47	0.47
6:F:73:VAL:O	6:F:83:PHE:CE2	2.68	0.47
12:L:15:ASN:ND2	12:L:16:GLY:N	2.63	0.47
13:N:76:LYS:O	13:N:77:CYS:CB	2.62	0.47
15:2:66:GLU:C	15:2:68:LEU:H	2.18	0.47
16:3:138:SER:C	16:3:141:LYS:HB3	2.35	0.47
1:A:31:PHE:HB2	1:A:32:GLU:HA	1.97	0.47
1:A:354:TRP:HB3	18:A:1103:CLA:CHD	2.29	0.47
1:A:463:HIS:O	1:A:467:MET:HB2	2.15	0.47
1:A:552:THR:HG22	1:A:604:TRP:CB	2.40	0.47
1:A:69:SER:O	1:A:71:LEU:N	2.48	0.47
1:A:728:VAL:HA	1:A:731:ARG:CG	2.41	0.47
1:A:755:ILE:N	1:A:758:GLY:CA	2.43	0.47
1:A:95:GLY:HA3	1:A:96:MET:SD	2.55	0.47
18:B:1227:CLA:HBD	18:B:1227:CLA:HAA1	1.96	0.47
2:B:341:LEU:CD1	18:B:1225:CLA:HMC1	2.45	0.47
2:B:545:LYS:CA	2:B:548:PRO:HG3	2.41	0.47
2:B:649:MET:HE3	2:B:719:PHE:CD1	2.50	0.47
2:B:69:ALA:N	2:B:71:GLN:O	2.48	0.47
3:C:23:THR:OG1	3:C:49:VAL:CG1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:73:VAL:O	6:F:83:PHE:HE2	1.97	0.47
12:L:85:SER:OG	12:L:85:SER:O	2.30	0.47
13:N:42:PHE:O	13:N:45:ASN:HA	2.14	0.47
14:1:44:LEU:O	14:1:47:CYS:SG	2.73	0.47
15:2:21:GLY:N	15:2:22:SER:CB	2.76	0.47
15:2:93:THR:H	15:2:94:LEU:HB2	1.68	0.47
17:4:55:VAL:O	17:4:59:LEU:CB	2.59	0.47
1:A:134:GLY:H	1:A:142:GLY:C	2.18	0.47
1:A:200:GLU:OE1	1:A:318:ARG:NH1	2.47	0.47
1:A:206:HIS:O	1:A:211:LEU:HG	2.15	0.47
1:A:354:TRP:O	1:A:358:LEU:N	2.46	0.47
1:A:425:THR:CG2	1:A:426:THR:N	2.77	0.47
1:A:620:MET:O	1:A:621:GLN:HB3	2.06	0.47
18:A:9013:CLA:HHC	18:A:9013:CLA:CBB	2.44	0.47
18:B:1202:CLA:HED3	18:B:1203:CLA:HMB1	1.96	0.47
2:B:343:VAL:O	2:B:344:ILE:C	2.53	0.47
2:B:344:ILE:HG13	18:B:1225:CLA:HAC2	1.95	0.47
2:B:436:LEU:HB3	2:B:453:ILE:HG21	1.95	0.47
2:B:533:ILE:CG2	2:B:575:ASP:O	2.63	0.47
2:B:587:ILE:C	2:B:589:TRP:N	2.66	0.47
2:B:4:ARG:CG	2:B:5:ILE:N	2.77	0.47
2:B:680:TRP:CD1	4:D:37:LEU:CD1	2.98	0.47
6:F:89:LEU:HD11	6:F:93:ILE:HD13	1.96	0.47
10:J:37:LEU:O	10:J:38:THR:HG23	2.15	0.47
10:J:3:ASP:CB	10:J:5:LYS:HG3	2.45	0.47
13:N:14:LYS:O	13:N:14:LYS:HG3	2.14	0.47
17:4:105:ARG:O	17:4:109:ILE:N	2.39	0.47
17:4:169:ILE:HG13	17:4:170:GLN:N	2.30	0.47
1:A:188:LYS:NZ	16:3:54:TRP:HH2	2.11	0.47
1:A:326:GLY:HA2	1:A:329:ASP:HB2	1.97	0.47
1:A:486:PRO:HD2	1:A:487:VAL:CG2	2.45	0.47
1:A:82:HIS:CE1	18:A:1103:CLA:C1A	2.98	0.47
2:B:521:HIS:O	2:B:522:ALA:C	2.53	0.47
2:B:557:PHE:CA	3:C:68:TYR:OH	2.63	0.47
2:B:694:ARG:HG3	12:L:104:ILE:HG21	1.97	0.47
3:C:28:MET:H	4:D:127:ARG:HH11	1.62	0.47
4:D:57:ILE:CG1	4:D:67:ILE:HA	2.36	0.47
9:I:10:PRO:O	9:I:14:LEU:CB	2.63	0.47
10:J:27:ILE:O	10:J:27:ILE:HG22	2.14	0.47
13:N:15:GLU:C	13:N:17:ASN:H	2.19	0.47
13:N:59:PRO:HD2	16:3:86:PRO:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:70:GLU:OE2	13:N:76:LYS:HD2	2.14	0.47
17:4:114:SER:HB3	17:4:120:ILE:HG12	1.96	0.46
1:A:282:THR:O	1:A:284:ARG:NE	2.48	0.46
1:A:475:ASP:OD2	12:L:75:ARG:CD	2.52	0.46
1:A:491:TRP:HA	1:A:492:ILE:HG23	1.96	0.46
20:A:6011:BCR:H392	20:A:6011:BCR:C23	2.45	0.46
1:A:618:TRP:HB2	1:A:656:PHE:CE1	2.49	0.46
18:B:1203:CLA:HBA2	18:B:1203:CLA:CBD	2.44	0.46
18:B:1205:CLA:CHA	18:B:1205:CLA:CGA	2.92	0.46
18:B:1228:CLA:HMB2	20:F:6016:BCR:H342	1.97	0.46
2:B:708:VAL:HG11	18:B:1239:CLA:O1D	2.14	0.46
2:B:164:SER:OG	2:B:165:VAL:N	2.45	0.46
2:B:329:SER:HA	2:B:397:ASP:OD1	2.15	0.46
2:B:423:SER:OG	2:B:424:TRP:N	2.47	0.46
2:B:520:HIS:NE2	18:B:1234:CLA:C1C	2.78	0.46
2:B:53:GLN:O	2:B:54:LEU:C	2.53	0.46
2:B:680:TRP:CE3	2:B:680:TRP:O	2.68	0.46
2:B:73:ASN:ND2	2:B:108:GLY:CA	2.74	0.46
2:B:91:ILE:HG22	2:B:91:ILE:O	2.14	0.46
4:D:50:TRP:HH2	4:D:58:PHE:HZ	1.63	0.46
1:A:51:THR:HB	18:F:1139:CLA:C3B	2.45	0.46
6:F:90:PHE:HA	6:F:93:ILE:HG22	1.97	0.46
7:G:72:LEU:O	7:G:77:ILE:N	2.48	0.46
8:H:65:LEU:O	8:H:66:THR:C	2.53	0.46
2:B:98:GLN:NE2	8:H:80:THR:HG22	2.30	0.46
14:1:153:LEU:O	14:1:157:ALA:HB2	2.15	0.46
18:A:1107:CLA:H111	18:A:1107:CLA:H91	1.66	0.46
1:A:291:THR:HA	1:A:523:VAL:HG21	1.97	0.46
1:A:326:GLY:CA	1:A:329:ASP:HB2	2.45	0.46
1:A:441:ALA:HB3	4:D:33:THR:HG21	1.97	0.46
1:A:446:LEU:HD23	18:A:1137:CLA:C3B	2.46	0.46
1:A:464:ASN:ND2	1:A:477:PHE:CB	2.31	0.46
1:A:493:GLN:CA	1:A:496:HIS:HB2	2.45	0.46
1:A:697:ARG:HD2	1:A:727:ILE:H	1.81	0.46
1:A:80:SER:CA	1:A:81:ALA:HB2	2.44	0.46
18:B:1220:CLA:HMC2	18:B:1242:CLA:CAD	2.45	0.46
2:B:459:PHE:HB2	18:B:1235:CLA:CAD	2.45	0.46
1:A:587:GLY:O	2:B:668:ARG:NH1	2.49	0.46
2:B:74:PHE:CE1	2:B:77:TRP:CZ3	3.03	0.46
6:F:109:ARG:HH12	6:F:153:ASN:HD21	1.63	0.46
6:F:36:SER:O	6:F:37:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:49:THR:O	6:F:56:TYR:OH	2.31	0.46
6:F:57:GLY:HA3	6:F:58:LYS:HB2	1.96	0.46
6:F:88:ILE:O	6:F:89:LEU:C	2.53	0.46
7:G:43:HIS:HD2	7:G:43:HIS:N	2.10	0.46
7:G:64:VAL:O	7:G:68:ILE:HG22	2.15	0.46
7:G:6:LEU:HD13	7:G:8:ILE:HG21	1.97	0.46
8:H:36:GLN:NE2	18:H:1501:CLA:OBD	2.46	0.46
9:I:25:PHE:CB	9:I:26:LEU:HD13	2.44	0.46
12:L:165:TYR:CE1	18:L:1503:CLA:HBD	2.42	0.46
12:L:59:ALA:HA	12:L:62:PHE:HE2	1.75	0.46
15:2:62:ILE:HA	18:2:2006:CLA:C2B	2.46	0.46
16:3:185:VAL:CB	18:3:3004:CLA:HHD	2.45	0.46
1:A:33:GLN:HB2	1:A:33:GLN:HE21	1.59	0.46
1:A:367:SER:HB3	1:A:371:VAL:HG13	1.97	0.46
1:A:405:PHE:HD2	1:A:605:MET:SD	2.39	0.46
1:A:71:LEU:HD21	1:A:353:SER:HB3	1.94	0.46
1:A:740:LEU:C	1:A:743:ILE:HD13	2.36	0.46
1:A:679:PHE:HB2	1:A:745:THR:HA	1.94	0.46
1:A:84:GLY:O	1:A:85:GLN:C	2.52	0.46
18:B:1208:CLA:HAC2	18:B:1208:CLA:HMC1	1.80	0.46
2:B:279:ALA:CB	18:B:1214:CLA:HHC	2.45	0.46
2:B:51:PHE:CE2	2:B:152:ALA:HB1	2.50	0.46
2:B:214:ASP:C	2:B:214:ASP:OD2	2.54	0.46
2:B:283:LEU:HD12	2:B:283:LEU:HA	1.74	0.46
2:B:308:HIS:HE1	18:B:1219:CLA:C4B	2.28	0.46
2:B:340:SER:N	2:B:342:GLY:H	2.12	0.46
2:B:38:THR:H	2:B:41:ARG:CD	2.28	0.46
2:B:41:ARG:O	2:B:45:ASN:ND2	2.48	0.46
2:B:596:TRP:CD1	2:B:608:GLN:NE2	2.83	0.46
19:A:5001:PQN:H171	18:F:1139:CLA:CBB	2.45	0.46
10:J:7:TYR:O	10:J:8:LEU:CB	2.56	0.46
12:L:147:GLY:O	12:L:150:GLY:CA	2.63	0.46
13:N:59:PRO:CA	13:N:60:PHE:CB	2.93	0.46
14:1:81:GLN:C	14:1:83:THR:HA	2.33	0.46
1:A:245:PRO:O	1:A:248:PHE:CE1	2.68	0.46
1:A:258:LEU:HG	1:A:259:TYR:H	1.81	0.46
1:A:437:ARG:HB3	4:D:32:SER:HB3	1.98	0.46
1:A:608:SER:O	1:A:611:VAL:HG12	2.15	0.46
1:A:737:HIS:O	1:A:738:TYR:C	2.53	0.46
1:A:84:GLY:HA2	1:A:87:SER:CB	2.38	0.46
2:B:333:GLN:C	18:B:1202:CLA:HMD3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1237:CLA:HAC1	18:B:1238:CLA:C1C	2.45	0.46
2:B:216:LEU:H	2:B:217:PRO:HD3	1.80	0.46
2:B:25:ILE:O	2:B:26:ALA:O	2.32	0.46
2:B:290:MET:HB3	2:B:291:TYR:CE1	2.51	0.46
2:B:373:THR:O	2:B:376:GLN:CB	2.63	0.46
2:B:596:TRP:CE2	2:B:608:GLN:O	2.69	0.46
2:B:649:MET:SD	18:B:1205:CLA:CBC	3.03	0.46
2:B:686:PRO:O	2:B:688:ALA:N	2.47	0.46
4:D:43:GLU:O	4:D:44:GLU:CB	2.62	0.46
4:D:26:SER:OG	4:D:67:ILE:O	2.23	0.46
5:E:45:TRP:HA	5:E:46:PHE:CB	2.45	0.46
12:L:72:GLY:HA3	12:L:73:PRO:HD3	1.41	0.46
12:L:80:ALA:C	12:L:82:ALA:H	2.19	0.46
13:N:42:PHE:CD2	13:N:43:PRO:HA	2.50	0.46
14:1:13:TYR:CB	17:4:107:GLN:HE21	2.28	0.46
14:1:188:ASN:O	14:1:191:ASP:N	2.48	0.46
1:A:105:ASN:HB3	1:A:150:PHE:CZ	2.50	0.46
1:A:301:HIS:HD2	1:A:301:HIS:C	2.19	0.46
1:A:338:PHE:O	1:A:339:THR:OG1	2.23	0.46
1:A:368:LEU:CA	1:A:371:VAL:HG22	2.42	0.46
1:A:439:ARG:HD3	4:D:34:GLY:HA3	1.97	0.46
1:A:453:LEU:HB2	18:A:1136:CLA:CBB	2.33	0.46
1:A:495:THR:O	1:A:499:ALA:HB2	2.16	0.46
18:A:1140:CLA:H41	19:A:5001:PQN:H192	1.97	0.46
1:A:684:PHE:CD1	18:A:9013:CLA:HMB1	2.51	0.46
1:A:706:SER:OG	1:A:707:ILE:N	2.48	0.46
1:A:86:LEU:HD22	1:A:86:LEU:C	2.36	0.46
18:A:9013:CLA:C1	18:A:9013:CLA:CMA	2.91	0.46
18:B:1207:CLA:H61	8:H:65:LEU:CD2	2.31	0.46
18:B:1216:CLA:HBD	18:B:1216:CLA:HAA1	1.97	0.46
18:B:1228:CLA:HAA1	18:B:1228:CLA:H12	1.98	0.46
2:B:174:ARG:HG3	18:B:1221:CLA:HMD2	1.89	0.46
2:B:265:THR:O	2:B:360:PHE:CD2	2.66	0.46
2:B:423:SER:HG	2:B:424:TRP:N	2.14	0.46
2:B:426:SER:O	2:B:430:GLY:N	2.48	0.46
2:B:519:VAL:O	2:B:523:ILE:HG22	2.15	0.46
2:B:717:TYR:HA	18:B:9010:CLA:HED1	1.97	0.46
6:F:141:TYR:C	6:F:143:GLU:N	2.69	0.46
6:F:16:LYS:O	6:F:17:ARG:C	2.50	0.46
8:H:48:THR:OG1	8:H:49:LYS:N	2.44	0.46
9:I:19:VAL:O	9:I:19:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:62:UNK:C	11:K:64:UNK:N	2.79	0.46
15:2:66:GLU:O	15:2:68:LEU:N	2.48	0.46
18:A:1136:CLA:H91	18:L:1504:CLA:CMC	2.44	0.46
1:A:104:SER:O	1:A:140:PHE:CE1	2.69	0.46
1:A:371:VAL:O	1:A:375:HIS:ND1	2.48	0.46
1:A:113:PRO:CG	1:A:384:TYR:CE2	2.98	0.46
1:A:524:GLY:O	1:A:526:LYS:N	2.48	0.46
1:A:393:LEU:HD13	1:A:617:SER:OG	2.16	0.46
18:B:1222:CLA:HBC2	18:B:1222:CLA:HHD	1.97	0.46
2:B:192:GLY:C	2:B:195:VAL:HB	2.36	0.46
2:B:273:VAL:HG11	18:B:1215:CLA:CMA	2.42	0.46
1:A:132:LEU:HD11	2:B:446:PHE:HZ	1.80	0.46
2:B:460:ALA:HA	18:B:1234:CLA:CBA	2.46	0.46
2:B:658:ALA:O	2:B:661:PHE:CD1	2.69	0.46
2:B:704:GLN:O	2:B:707:LEU:N	2.48	0.46
3:C:26:LEU:HD23	4:D:120:PRO:HB2	1.98	0.46
3:C:55:GLU:HB2	3:C:65:VAL:HG22	1.96	0.46
3:C:7:ILE:N	3:C:8:TYR:CE2	2.84	0.46
4:D:123:VAL:N	4:D:127:ARG:NH1	2.57	0.46
1:A:570:PRO:HD3	4:D:79:ARG:NH2	2.31	0.46
6:F:1:ASP:CA	6:F:62:LEU:CD1	2.92	0.46
6:F:77:GLN:O	6:F:80:TRP:CD2	2.69	0.46
18:H:1501:CLA:HBB1	12:L:36:TYR:HE1	1.80	0.46
9:I:16:PHE:CB	9:I:17:PRO:HD3	2.43	0.46
11:K:75:UNK:C	11:K:77:UNK:N	2.78	0.46
8:H:49:LYS:CG	12:L:140:THR:HG21	2.44	0.46
12:L:37:LEU:H	12:L:37:LEU:CD2	2.24	0.46
12:L:97:MET:CE	12:L:98:CYS:HA	2.45	0.46
13:N:64:ASP:O	13:N:65:LEU:HB2	2.16	0.46
14:1:60:PRO:HD3	18:1:1006:CLA:C4D	2.46	0.46
15:2:192:LEU:CB	15:2:193:PHE:HA	2.46	0.46
15:2:85:GLN:HA	15:2:89:THR:HG21	1.97	0.46
16:3:132:ASP:O	16:3:133:TRP:O	2.34	0.46
18:A:1140:CLA:CMC	18:A:1140:CLA:HBC2	2.43	0.46
1:A:146:THR:O	1:A:147:SER:CB	2.63	0.46
1:A:364:MET:HG2	18:A:1123:CLA:HHB	1.96	0.46
1:A:490:GLN:CA	1:A:491:TRP:O	2.64	0.46
1:A:545:HIS:ND1	1:A:612:VAL:CG2	2.66	0.46
1:A:548:THR:O	1:A:552:THR:N	2.49	0.46
1:A:750:PHE:CZ	18:A:1126:CLA:CMB	2.96	0.46
18:B:1209:CLA:HBA1	7:G:39:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:VAL:C	2:B:122:GLN:N	2.69	0.46
2:B:255:LEU:HD23	18:B:1212:CLA:HAC2	1.97	0.46
2:B:323:TYR:HA	2:B:326:ILE:HG23	1.96	0.46
2:B:460:ALA:HB1	18:B:1234:CLA:HAA2	1.96	0.46
2:B:459:PHE:N	2:B:461:GLN:HG3	2.31	0.46
2:B:527:LEU:CD2	2:B:586:THR:CG2	2.90	0.46
4:D:93:LYS:O	4:D:95:LYS:NZ	2.49	0.46
4:D:48:ILE:HG13	4:D:99:GLN:O	2.16	0.46
5:E:36:VAL:HG21	5:E:52:VAL:HG11	1.98	0.46
6:F:79:HIS:O	6:F:82:GLU:N	2.45	0.46
11:K:77:UNK:C	11:K:6:UNK:N	2.77	0.46
12:L:123:ARG:C	12:L:125:LYS:H	2.16	0.46
14:1:63:LEU:HD13	14:1:68:TRP:HE1	1.80	0.46
15:2:189:ILE:CG1	15:2:190:ASP:HA	2.46	0.46
15:2:33:GLY:CA	15:2:35:SER:N	2.78	0.46
17:4:114:SER:HB3	17:4:120:ILE:CG1	2.46	0.46
17:4:40:PHE:O	17:4:43:ALA:N	2.48	0.46
17:4:48:GLY:O	17:4:51:ALA:HB3	2.16	0.46
1:A:231:GLN:HA	1:A:234:ASN:HD22	1.74	0.46
1:A:483:GLN:HG3	1:A:484:LEU:O	2.07	0.46
1:A:682:ALA:CB	1:A:745:THR:HG23	2.46	0.46
1:A:90:PHE:O	1:A:91:LEU:C	2.54	0.46
2:B:109:ALA:HB1	2:B:111:GLY:H	1.80	0.46
18:B:1220:CLA:OBD	18:B:1221:CLA:HBB2	2.11	0.46
2:B:334:LEU:HD21	18:B:1226:CLA:C3B	2.46	0.46
18:B:1237:CLA:HBB1	18:B:1238:CLA:CAD	2.45	0.46
2:B:257:ILE:HA	2:B:272:ASP:CG	2.35	0.46
2:B:334:LEU:HD23	18:B:1202:CLA:C1D	2.45	0.46
18:B:1239:CLA:HBA2	19:B:5002:PQN:H252	1.96	0.46
2:B:509:PHE:O	2:B:510:LEU:O	2.33	0.46
2:B:530:THR:CG2	2:B:583:MET:HB2	2.30	0.46
6:F:130:LEU:C	6:F:132:ARG:H	2.19	0.46
20:F:6016:BCR:C8	20:F:6016:BCR:C33	2.91	0.46
7:G:78:GLY:C	7:G:79:HIS:O	2.53	0.46
8:H:30:SER:CB	12:L:35:TRP:HZ2	2.29	0.46
10:J:26:LEU:HA	10:J:29:ILE:HG22	1.97	0.46
13:N:81:VAL:CG2	13:N:82:PHE:HB3	2.33	0.46
16:3:132:ASP:CB	16:3:139:MET:CB	2.91	0.46
17:4:141:LEU:O	17:4:142:ASN:CB	2.60	0.46
17:4:152:LYS:HB3	17:4:153:GLU:H	1.48	0.46
17:4:82:GLU:HG2	17:4:84:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HG21	18:A:1127:CLA:HHD	1.98	0.46
1:A:449:VAL:O	1:A:453:LEU:N	2.49	0.46
2:B:98:GLN:C	2:B:100:ALA:N	2.69	0.46
2:B:135:LEU:C	2:B:137:THR:N	2.68	0.46
2:B:166:SER:C	2:B:168:PHE:N	2.69	0.46
2:B:209:TRP:CD1	2:B:210:ASN:N	2.83	0.46
2:B:343:VAL:CG1	2:B:347:LEU:HD13	2.43	0.46
2:B:439:HIS:HE1	2:B:453:ILE:HG12	1.81	0.46
2:B:496:GLY:C	2:B:498:LEU:N	2.69	0.46
2:B:16:PRO:O	2:B:696:LYS:CG	2.64	0.46
7:G:54:TYR:CG	7:G:54:TYR:O	2.69	0.46
6:F:85:THR:HB	10:J:39:PHE:CE2	2.49	0.46
12:L:137:ALA:C	12:L:138:LYS:NZ	2.65	0.46
12:L:58:LEU:O	12:L:62:PHE:HE2	1.99	0.46
15:2:65:PRO:O	15:2:68:LEU:HB3	2.15	0.46
17:4:40:PHE:HB3	17:4:43:ALA:HB3	1.97	0.46
1:A:130:GLU:C	1:A:132:LEU:N	2.67	0.46
1:A:287:LEU:CB	1:A:294:LEU:HB3	2.46	0.46
1:A:331:LEU:C	1:A:333:ALA:H	2.18	0.46
1:A:379:MET:HA	1:A:380:PRO:HD2	1.60	0.46
1:A:416:ILE:HG23	1:A:577:PHE:CG	2.51	0.46
1:A:569:ILE:HA	1:A:586:ARG:NH1	2.31	0.46
2:B:104:PHE:HD1	2:B:104:PHE:N	2.13	0.46
2:B:311:PRO:CD	18:B:1219:CLA:CBB	2.94	0.46
18:B:1220:CLA:H101	18:B:1220:CLA:H62	1.63	0.46
2:B:414:HIS:HD2	18:B:1227:CLA:HMA3	1.81	0.46
2:B:254:ILE:O	2:B:255:LEU:C	2.54	0.46
2:B:257:ILE:HD13	18:B:1214:CLA:CMB	2.45	0.46
2:B:436:LEU:HB3	2:B:453:ILE:CG2	2.45	0.46
2:B:460:ALA:HA	18:B:1234:CLA:CGA	2.46	0.46
2:B:469:LYS:HG3	2:B:501:ILE:O	2.17	0.46
4:D:87:GLY:HA2	4:D:90:LEU:HD12	1.98	0.46
6:F:150:VAL:HA	6:F:151:ASP:HB2	1.98	0.46
6:F:7:PRO:CA	6:F:62:LEU:HD12	2.46	0.46
18:L:1503:CLA:O2D	18:L:1503:CLA:O2A	2.34	0.46
13:N:79:SER:OG	13:N:79:SER:O	2.29	0.46
14:1:45:ILE:C	14:1:47:CYS:H	2.19	0.45
16:3:61:ILE:O	16:3:64:ARG:CB	2.57	0.45
16:3:67:MET:HE2	16:3:71:ALA:H	1.79	0.45
1:A:181:ALA:CA	1:A:184:PHE:HB3	2.41	0.45
1:A:252:ARG:HD3	1:A:263:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HA	1:A:315:HIS:CE1	2.50	0.45
1:A:492:ILE:N	1:A:493:GLN:CB	2.56	0.45
1:A:530:LEU:HB2	1:A:531:PRO:HD2	1.98	0.45
1:A:553:VAL:HG12	1:A:556:LEU:HD12	1.96	0.45
1:A:553:VAL:CB	1:A:556:LEU:HD12	2.43	0.45
1:A:671:SER:C	1:A:673:SER:N	2.70	0.45
1:A:718:PRO:O	1:A:719:ALA:HB2	2.15	0.45
18:B:1209:CLA:HBB2	18:B:1217:CLA:C1D	2.46	0.45
18:B:1218:CLA:CGD	18:B:1218:CLA:C2A	2.94	0.45
2:B:340:SER:OG	18:B:1242:CLA:CBB	2.64	0.45
2:B:158:GLN:OE1	2:B:159:PRO:O	2.33	0.45
2:B:399:ASN:OD1	2:B:402:GLN:N	2.48	0.45
2:B:459:PHE:O	2:B:460:ALA:C	2.55	0.45
2:B:534:LEU:O	2:B:538:ALA:CB	2.64	0.45
2:B:628:SER:C	2:B:630:GLN:H	2.09	0.45
2:B:645:VAL:O	2:B:648:TRP:HB3	2.16	0.45
1:A:470:LEU:HD23	2:B:96:PHE:CE2	2.51	0.45
4:D:104:PHE:CD1	4:D:108:GLU:OE2	2.68	0.45
4:D:77:LEU:HD13	4:D:83:CYS:SG	2.57	0.45
16:3:111:ASN:O	16:3:112:TYR:CD1	2.68	0.45
1:A:99:HIS:ND1	1:A:103:PHE:CZ	2.82	0.45
1:A:185:HIS:O	1:A:187:HIS:N	2.45	0.45
1:A:302:HIS:CG	1:A:303:HIS:CE1	2.98	0.45
1:A:568:LEU:HD22	4:D:79:ARG:NH1	2.30	0.45
1:A:578:ARG:O	1:A:579:PHE:O	2.33	0.45
1:A:725:LEU:CD1	18:A:1140:CLA:HMD3	2.46	0.45
1:A:393:LEU:HD23	1:A:754:ILE:HD13	1.99	0.45
2:B:106:ARG:O	2:B:107:GLY:C	2.55	0.45
2:B:177:HIS:ND1	18:B:1217:CLA:HMD3	2.31	0.45
2:B:259:GLY:CA	2:B:269:TRP:CZ2	2.93	0.45
2:B:303:TYR:CD2	2:B:307:ALA:HB2	2.43	0.45
2:B:368:GLN:HE21	2:B:368:GLN:HB2	1.48	0.45
2:B:440:ASN:ND2	2:B:614:THR:HB	2.31	0.45
4:D:104:PHE:CD2	4:D:105:PRO:HD2	2.51	0.45
2:B:39:GLU:HA	4:D:148:PHE:CE2	2.51	0.45
4:D:50:TRP:NE1	4:D:73:ASN:ND2	2.64	0.45
5:E:33:GLY:HA2	5:E:52:VAL:C	2.37	0.45
6:F:45:THR:O	6:F:46:MET:C	2.52	0.45
6:F:73:VAL:CG2	6:F:82:GLU:N	2.79	0.45
7:G:20:ARG:HA	7:G:20:ARG:HD3	1.53	0.45
8:H:24:TYR:N	8:H:24:TYR:CD1	2.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:155:LEU:HD13	14:1:158:PHE:HE1	1.80	0.45
15:2:32:LEU:HD12	15:2:34:LEU:N	2.30	0.45
17:4:180:ASP:O	17:4:185:HIS:CG	2.69	0.45
17:4:60:LEU:O	17:4:62:GLU:N	2.49	0.45
17:4:96:ILE:CG2	17:4:97:LEU:N	2.72	0.45
1:A:304:LEU:C	1:A:307:ALA:HB3	2.36	0.45
1:A:315:HIS:HB3	18:A:1108:CLA:CGD	2.45	0.45
1:A:427:ARG:HA	1:A:430:ASP:HB2	1.99	0.45
1:A:725:LEU:CD2	19:A:5001:PQN:C6	2.88	0.45
1:A:553:VAL:CG1	1:A:556:LEU:CD1	2.92	0.45
1:A:60:ASP:O	1:A:62:HIS:N	2.49	0.45
1:A:621:GLN:N	1:A:624:VAL:HG12	2.31	0.45
2:B:175:LEU:H	2:B:178:HIS:HB3	1.81	0.45
2:B:218:TYR:CD2	2:B:253:ALA:O	2.69	0.45
2:B:360:PHE:HB3	2:B:363:GLN:HE22	1.82	0.45
2:B:374:HIS:HB2	18:B:1224:CLA:C1B	2.46	0.45
2:B:446:PHE:O	2:B:447:GLY:O	2.34	0.45
2:B:504:ASN:HB3	2:B:601:LEU:HD21	1.98	0.45
2:B:391:PRO:CB	2:B:538:ALA:HA	2.47	0.45
2:B:546:LEU:HD23	2:B:546:LEU:HA	1.82	0.45
2:B:693:TRP:CD1	2:B:693:TRP:O	2.70	0.45
3:C:56:SER:O	3:C:57:ALA:CB	2.65	0.45
7:G:15:SER:O	7:G:18:LEU:HB2	2.17	0.45
8:H:30:SER:CB	12:L:35:TRP:CZ2	2.99	0.45
8:H:49:LYS:O	8:H:50:ARG:CZ	2.65	0.45
12:L:14:LEU:HD23	12:L:22:GLY:H	1.82	0.45
13:N:65:LEU:HB3	13:N:68:GLU:OE2	2.16	0.45
10:J:2:ARG:CZ	15:2:119:VAL:CB	2.95	0.45
15:2:193:PHE:O	15:2:194:ALA:HB2	2.16	0.45
15:2:19:LEU:CB	15:2:20:ASP:CG	2.85	0.45
15:2:22:SER:HB3	15:2:23:LEU:CG	2.46	0.45
15:2:94:LEU:HD11	15:2:98:GLU:CD	2.37	0.45
17:4:45:LEU:O	17:4:46:VAL:C	2.55	0.45
1:A:126:ILE:O	1:A:129:GLN:N	2.50	0.45
1:A:132:LEU:HD21	1:A:673:SER:O	2.16	0.45
1:A:477:PHE:CD2	1:A:482:ILE:HG21	2.51	0.45
1:A:50:THR:O	1:A:51:THR:C	2.52	0.45
1:A:514:THR:HG22	1:A:529:LEU:HD22	1.98	0.45
1:A:549:ILE:HA	1:A:552:THR:OG1	2.17	0.45
18:B:1138:CLA:H51	18:B:1138:CLA:H8	1.75	0.45
18:B:1202:CLA:CBB	18:B:1203:CLA:HBA1	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:ILE:HG22	2:B:149:SER:N	2.31	0.45
2:B:436:LEU:O	2:B:438:VAL:N	2.49	0.45
2:B:467:HIS:NE2	18:B:1231:CLA:NC	2.65	0.45
2:B:547:MET:CE	2:B:557:PHE:CE1	3.00	0.45
2:B:64:ASN:HA	2:B:67:HIS:HB3	1.91	0.45
2:B:7:ARG:HB3	2:B:8:PHE:H	1.50	0.45
2:B:98:GLN:OE1	8:H:78:PRO:HB2	2.17	0.45
3:C:48:CYS:SG	3:C:49:VAL:C	2.95	0.45
4:D:23:ASN:ND2	4:D:25:PRO:HD3	2.31	0.45
5:E:61:THR:CG2	5:E:62:ARG:H	2.26	0.45
18:F:1302:CLA:HMC2	14:1:190:GLY:O	2.17	0.45
6:F:31:LEU:C	6:F:32:TYR:CD2	2.89	0.45
6:F:42:ILE:HD13	6:F:42:ILE:H	1.80	0.45
6:F:1:ASP:CA	6:F:62:LEU:HD13	2.43	0.45
7:G:34:GLN:OE1	7:G:35:VAL:HG12	2.16	0.45
13:N:69:CYS:SG	13:N:72:LYS:C	2.94	0.45
14:1:103:LEU:H	14:1:103:LEU:HD22	1.81	0.45
14:1:159:VAL:O	14:1:161:PHE:N	2.50	0.45
15:2:152:SER:HA	15:2:153:PRO:HA	1.73	0.45
17:4:120:ILE:O	17:4:120:ILE:CG1	2.52	0.45
17:4:147:LEU:O	17:4:148:GLU:CB	2.53	0.45
17:4:54:GLY:O	17:4:57:GLY:N	2.39	0.45
1:A:132:LEU:HG	2:B:446:PHE:CZ	2.52	0.45
1:A:104:SER:O	1:A:140:PHE:CD1	2.70	0.45
1:A:460:LEU:HA	1:A:460:LEU:HD12	1.81	0.45
1:A:467:MET:HG3	1:A:471:GLY:HA3	1.98	0.45
1:A:602:LEU:O	1:A:605:MET:N	2.48	0.45
1:A:65:ASP:N	1:A:67:HIS:H	2.15	0.45
1:A:721:GLN:OE1	5:E:71:LYS:HG2	2.16	0.45
1:A:599:PHE:CE2	1:A:735:VAL:HB	2.51	0.45
18:B:1219:CLA:HBA2	18:B:1219:CLA:H3A	1.30	0.45
18:B:1239:CLA:C4B	20:B:6017:BCR:H17C	2.46	0.45
2:B:4:ARG:HH11	2:B:4:ARG:HG2	1.79	0.45
20:B:6017:BCR:H311	20:B:6017:BCR:HC8	1.99	0.45
2:B:613:SER:O	2:B:614:THR:HG23	2.16	0.45
2:B:696:LYS:HB2	2:B:696:LYS:HE3	1.41	0.45
2:B:558:PRO:HA	2:B:702:ILE:HD11	1.97	0.45
2:B:77:TRP:CG	2:B:77:TRP:O	2.70	0.45
3:C:23:THR:OG1	3:C:49:VAL:HG12	2.16	0.45
3:C:8:TYR:CE1	4:D:137:ILE:HG12	2.52	0.45
4:D:109:VAL:HG21	4:D:110:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:34:SER:OG	5:E:35:LYS:N	2.48	0.45
6:F:6:THR:O	6:F:8:CYS:N	2.49	0.45
6:F:99:TRP:HZ2	6:F:143:GLU:HG2	1.81	0.45
12:L:38:SER:O	12:L:44:ARG:CZ	2.65	0.45
13:N:66:ASP:OD2	13:N:70:GLU:O	2.34	0.45
14:1:11:PRO:N	17:4:107:GLN:CG	2.77	0.45
15:2:86:GLU:N	15:2:86:GLU:OE2	2.50	0.45
16:3:57:TYR:CE2	16:3:185:VAL:CB	2.97	0.45
1:A:218:TRP:CZ3	18:A:1148:CLA:C4D	2.97	0.45
1:A:200:GLU:HG2	1:A:327:ILE:HG12	1.97	0.45
1:A:202:MET:SD	18:A:1123:CLA:CMD	3.05	0.45
1:A:207:LEU:HD13	1:A:310:PHE:HA	1.99	0.45
1:A:287:LEU:HB2	1:A:294:LEU:CA	2.46	0.45
1:A:465:ASP:C	1:A:467:MET:H	2.19	0.45
1:A:465:ASP:OD2	1:A:648:THR:HG23	2.17	0.45
1:A:611:VAL:HG22	1:A:612:VAL:N	2.32	0.45
1:A:527:VAL:HG21	1:A:634:VAL:HG11	1.99	0.45
1:A:678:PHE:O	1:A:682:ALA:N	2.50	0.45
1:A:81:ALA:CA	1:A:83:PHE:H	2.28	0.45
2:B:190:TRP:CH2	18:B:1215:CLA:CAD	2.99	0.45
18:B:1227:CLA:HHD	18:B:1242:CLA:OBD	2.16	0.45
2:B:282:PHE:HA	2:B:285:LEU:HB2	1.99	0.45
2:B:176:ASN:CG	2:B:291:TYR:HD1	2.20	0.45
2:B:342:GLY:CA	2:B:383:MET:HG3	2.47	0.45
2:B:606:VAL:HG22	2:B:606:VAL:O	2.16	0.45
2:B:634:GLY:O	2:B:644:SER:HA	2.16	0.45
3:C:12:ILE:HD12	21:C:3103:SF4:S4	2.57	0.45
2:B:16:PRO:HG2	3:C:74:THR:HB	1.98	0.45
4:D:133:ASN:ND2	4:D:134:MET:N	2.57	0.45
5:E:45:TRP:N	5:E:46:PHE:HB2	2.32	0.45
6:F:125:LEU:HB3	6:F:130:LEU:CG	2.46	0.45
6:F:141:TYR:CE2	6:F:142:ARG:HD3	2.46	0.45
6:F:25:LEU:HG	6:F:26:GLN:N	2.31	0.45
6:F:53:PHE:C	6:F:55:ASN:N	2.70	0.45
6:F:94:ALA:HA	6:F:97:ILE:CD1	2.47	0.45
12:L:127:PRO:O	12:L:128:ASP:CB	2.62	0.45
12:L:78:GLU:HG3	12:L:79:TYR:N	2.31	0.45
13:N:8:GLU:OE2	13:N:11:LYS:HB3	2.16	0.45
15:2:63:PHE:HZ	15:2:172:LEU:HG	1.81	0.45
15:2:177:ALA:HA	15:2:178:TRP:HE3	1.82	0.45
16:3:57:TYR:O	16:3:60:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:158:ARG:NH1	17:4:158:ARG:HG2	2.30	0.45
18:A:1119:CLA:H2	18:A:1123:CLA:CMB	2.46	0.45
1:A:368:LEU:O	1:A:369:THR:HB	2.16	0.45
1:A:618:TRP:CG	1:A:642:PHE:HD1	2.34	0.45
18:B:1205:CLA:NB	18:B:1205:CLA:C2	2.80	0.45
18:B:1228:CLA:CMB	20:F:6016:BCR:H342	2.47	0.45
2:B:242:HIS:CD2	2:B:250:ALA:HA	2.52	0.45
2:B:291:TYR:HD2	2:B:299:HIS:CB	2.30	0.45
2:B:373:THR:O	2:B:376:GLN:CA	2.65	0.45
2:B:536:LYS:NZ	2:B:536:LYS:HB3	2.32	0.45
2:B:620:LEU:HA	2:B:624:LEU:HB2	1.98	0.45
2:B:675:ILE:O	2:B:679:ALA:HB2	2.17	0.45
18:B:9010:CLA:C1	18:B:9012:CLA:CHD	2.87	0.45
3:C:49:VAL:HG13	3:C:51:CYS:CB	2.46	0.45
18:B:1228:CLA:HMB2	20:F:6016:BCR:C34	2.46	0.45
8:H:43:PHE:HA	8:H:44:ALA:HA	1.80	0.45
18:A:1129:CLA:HBB2	18:L:1130:CLA:HBC3	1.98	0.45
4:D:36:LEU:HD23	12:L:19:PHE:O	2.17	0.45
2:B:684:ARG:NH1	12:L:22:GLY:CA	2.80	0.45
13:N:58:VAL:CG2	13:N:60:PHE:CD2	2.99	0.45
13:N:77:CYS:CB	13:N:78:GLY:HA3	2.12	0.45
15:2:19:LEU:N	15:2:21:GLY:N	2.65	0.45
17:4:56:ALA:HA	17:4:59:LEU:CB	2.44	0.45
1:A:323:ILE:CG2	18:A:1108:CLA:HAA2	2.47	0.45
1:A:398:HIS:C	1:A:400:MET:N	2.70	0.45
1:A:407:ILE:C	1:A:409:GLY:H	2.20	0.45
1:A:49:ASP:CG	1:A:50:THR:HG23	2.37	0.45
1:A:547:PHE:CE1	1:A:551:VAL:CG1	2.90	0.45
20:A:6011:BCR:H392	20:A:6011:BCR:H23C	1.99	0.45
18:A:9011:CLA:CMC	18:A:9011:CLA:HBC2	2.44	0.45
2:B:88:ALA:CA	2:B:116:ALA:HB2	2.47	0.45
18:B:1215:CLA:C7	18:B:1215:CLA:C2	2.95	0.45
2:B:697:PRO:HB3	18:B:1238:CLA:C1C	2.46	0.45
2:B:248:GLN:O	2:B:250:ALA:N	2.49	0.45
2:B:282:PHE:O	2:B:286:ILE:HG23	2.16	0.45
2:B:593:TYR:O	2:B:594:TRP:CB	2.61	0.45
4:D:151:LYS:O	4:D:152:GLN:O	2.35	0.45
4:D:61:PRO:C	4:D:63:GLY:N	2.69	0.45
5:E:39:LEU:HD13	5:E:88:GLU:OE2	2.17	0.45
7:G:73:ALA:HA	7:G:77:ILE:O	2.17	0.45
8:H:23:VAL:C	8:H:24:TYR:CG	2.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:45:ALA:C	8:H:47:PHE:HB2	2.37	0.45
8:H:66:THR:HG22	9:I:10:PRO:CB	2.47	0.45
12:L:56:VAL:O	12:L:60:HIS:HB2	2.16	0.45
12:L:93:VAL:HA	12:L:96:SER:CB	2.47	0.45
13:N:54:LYS:HD2	13:N:54:LYS:H	1.77	0.45
14:1:146:LYS:O	14:1:148:ILE:N	2.50	0.45
14:1:146:LYS:O	14:1:149:LYS:N	2.50	0.45
15:2:159:LEU:HB3	15:2:160:ARG:HH21	1.82	0.45
15:2:33:GLY:N	15:2:35:SER:HB3	2.32	0.45
16:3:196:LEU:CD2	18:3:3005:CLA:C3B	2.95	0.45
1:A:302:HIS:O	1:A:303:HIS:ND1	2.45	0.45
1:A:339:THR:O	1:A:342:GLY:HA2	2.17	0.45
1:A:389:TYR:CD2	1:A:625:TRP:CE2	3.05	0.45
1:A:478:SER:C	1:A:481:ALA:HB3	2.37	0.45
1:A:494:ASN:O	1:A:495:THR:CB	2.63	0.45
1:A:550:HIS:C	1:A:552:THR:H	2.21	0.45
1:A:621:GLN:HB2	1:A:621:GLN:HE21	1.42	0.45
1:A:76:ARG:H	1:A:76:ARG:HG2	1.60	0.45
1:A:707:ILE:HD13	18:B:1138:CLA:HMD3	1.99	0.45
18:B:1218:CLA:HMA3	18:B:1219:CLA:CAD	2.47	0.45
2:B:192:GLY:O	2:B:195:VAL:CB	2.61	0.45
2:B:597:LYS:HB3	2:B:598:HIS:ND1	2.32	0.45
2:B:672:GLN:NE2	2:B:698:VAL:HB	2.32	0.45
3:C:12:ILE:HG21	3:C:28:MET:CE	2.46	0.45
3:C:31:TRP:O	3:C:31:TRP:CE3	2.70	0.45
4:D:112:LEU:HG	4:D:113:HIS:ND1	2.26	0.45
9:I:25:PHE:CA	9:I:26:LEU:CB	2.81	0.45
10:J:2:ARG:HE	10:J:5:LYS:CD	2.30	0.45
12:L:112:PRO:CB	12:L:113:SER:HA	2.39	0.45
12:L:151:VAL:HG23	12:L:152:THR:H	1.82	0.45
18:L:1502:CLA:H52	20:L:6020:BCR:H402	1.99	0.45
16:3:132:ASP:CG	16:3:139:MET:CB	2.82	0.45
16:3:138:SER:O	16:3:141:LYS:CB	2.65	0.45
16:3:74:ILE:HD11	16:3:199:PHE:HA	1.99	0.45
18:A:1140:CLA:H51	19:A:5001:PQN:H192	1.97	0.45
1:A:331:LEU:O	1:A:334:HIS:CE1	2.70	0.45
1:A:462:ILE:HD11	18:B:9022:CLA:O1A	2.17	0.45
1:A:482:ILE:HA	1:A:482:ILE:HD13	1.86	0.45
1:A:497:ALA:HB2	1:A:516:GLY:CA	2.43	0.45
1:A:525:ASN:ND2	1:A:526:LYS:H	2.14	0.45
1:A:389:TYR:CE2	1:A:625:TRP:CG	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:SER:OG	1:A:672:LEU:CB	2.64	0.45
1:A:667:SER:OG	1:A:672:LEU:HB3	2.17	0.45
1:A:76:ARG:HH21	1:A:190:ALA:CB	2.29	0.45
1:A:85:GLN:NE2	1:A:85:GLN:HA	2.23	0.45
2:B:345:THR:HG23	18:B:1225:CLA:HAC1	1.99	0.45
18:B:1138:CLA:HAA2	18:B:1228:CLA:HMB1	1.99	0.45
2:B:245:GLY:C	2:B:246:THR:HG1	2.19	0.45
2:B:378:ILE:C	2:B:380:GLY:N	2.71	0.45
2:B:438:VAL:O	2:B:442:VAL:HG23	2.16	0.45
2:B:636:THR:HA	2:B:637:PRO:HD2	1.70	0.45
2:B:7:ARG:O	2:B:8:PHE:C	2.54	0.45
4:D:109:VAL:HG23	4:D:110:GLN:HB2	1.99	0.45
4:D:124:ASN:HB2	4:D:125:PRO:HD3	1.98	0.45
2:B:689:ASN:ND2	4:D:38:ARG:HH11	2.06	0.45
4:D:79:ARG:CB	4:D:81:GLU:HG3	2.42	0.45
6:F:75:GLY:O	18:F:1302:CLA:C4C	2.65	0.45
6:F:144:LEU:CG	20:F:6016:BCR:H332	2.47	0.45
8:H:26:SER:OG	8:H:29:PRO:HB3	2.17	0.45
9:I:17:PRO:O	9:I:20:ALA:N	2.50	0.45
12:L:18:PRO:HG2	12:L:19:PHE:HE1	1.82	0.45
12:L:33:ILE:O	12:L:35:TRP:N	2.50	0.45
15:2:147:GLY:O	15:2:148:TRP:CB	2.66	0.44
16:3:64:ARG:HH21	18:3:3002:CLA:CHA	2.29	0.44
17:4:108:ASP:O	17:4:109:ILE:O	2.35	0.44
1:A:121:GLN:NE2	18:A:1107:CLA:HED3	2.32	0.44
18:A:1136:CLA:O1D	18:A:1136:CLA:CAA	2.64	0.44
1:A:244:LEU:O	1:A:246:HIS:HB2	2.16	0.44
1:A:296:LEU:C	1:A:298:ASP:H	2.20	0.44
1:A:441:ALA:O	1:A:445:HIS:CE1	2.67	0.44
1:A:446:LEU:C	1:A:449:VAL:HG12	2.32	0.44
1:A:58:HIS:O	18:A:1128:CLA:C2	2.65	0.44
1:A:618:TRP:CE3	1:A:656:PHE:HD1	2.35	0.44
18:B:1216:CLA:O1A	18:B:1220:CLA:H11	2.17	0.44
18:B:1228:CLA:HBC2	20:F:6016:BCR:C17	2.47	0.44
2:B:141:PHE:C	2:B:143:LEU:N	2.71	0.44
2:B:144:PHE:HD2	2:B:145:LEU:HD22	1.80	0.44
2:B:156:HIS:CE1	2:B:162:LYS:O	2.69	0.44
2:B:206:TYR:O	2:B:208:ARG:HG3	2.17	0.44
2:B:311:PRO:N	18:B:1219:CLA:HBB1	2.32	0.44
2:B:375:HIS:NE2	18:B:1225:CLA:C1A	2.80	0.44
2:B:439:HIS:C	2:B:441:ASP:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLY:O	2:B:446:PHE:CD2	2.69	0.44
2:B:77:TRP:HE1	2:B:81:PRO:HA	1.80	0.44
18:A:9011:CLA:CBB	18:B:9010:CLA:ND	2.63	0.44
2:B:721:TYR:HD1	18:B:9010:CLA:OBD	1.99	0.44
5:E:37:LYS:C	5:E:38:ILE:HD12	2.37	0.44
5:E:44:TYR:CG	5:E:73:ASN:HB3	2.52	0.44
5:E:72:VAL:CG1	5:E:73:ASN:O	2.65	0.44
5:E:72:VAL:HG13	5:E:73:ASN:O	2.17	0.44
6:F:124:PRO:O	6:F:125:LEU:HD23	2.17	0.44
6:F:75:GLY:O	18:F:1302:CLA:CHD	2.64	0.44
6:F:73:VAL:HG13	6:F:80:TRP:HA	1.99	0.44
7:G:85:ILE:CA	7:G:86:LEU:C	2.77	0.44
13:N:73:ASP:OD1	13:N:76:LYS:HA	2.17	0.44
13:N:7:LEU:O	13:N:7:LEU:HG	2.16	0.44
15:2:16:PRO:N	15:2:19:LEU:O	2.49	0.44
16:3:67:MET:SD	16:3:71:ALA:HB2	2.58	0.44
17:4:137:ILE:N	17:4:141:LEU:HD23	2.32	0.44
17:4:89:THR:OG1	17:4:91:PHE:HB2	2.17	0.44
1:A:595:TRP:CD1	18:A:1128:CLA:HMD1	2.51	0.44
1:A:260:PRO:O	1:A:261:SER:HB3	2.17	0.44
18:A:9011:CLA:HMB2	18:B:9010:CLA:C4A	2.47	0.44
2:B:311:PRO:N	18:B:1219:CLA:CBB	2.80	0.44
2:B:156:HIS:ND1	2:B:161:TRP:O	2.50	0.44
2:B:167:TRP:HH2	2:B:174:ARG:HH22	1.60	0.44
2:B:291:TYR:O	2:B:292:ARG:HG3	2.18	0.44
2:B:388:ALA:CA	2:B:391:PRO:HD2	2.47	0.44
18:B:1239:CLA:C4D	19:B:5002:PQN:H251	2.46	0.44
1:A:444:SER:HB3	2:B:677:THR:O	2.17	0.44
2:B:725:LEU:H	2:B:725:LEU:HD23	1.82	0.44
6:F:7:PRO:O	6:F:8:CYS:HB2	2.18	0.44
12:L:33:ILE:CG2	12:L:33:ILE:O	2.65	0.44
13:N:22:LEU:C	13:N:24:THR:N	2.70	0.44
13:N:59:PRO:C	13:N:60:PHE:HD2	2.20	0.44
13:N:8:GLU:HG2	13:N:8:GLU:O	2.16	0.44
15:2:142:TRP:O	15:2:143:PHE:CD2	2.70	0.44
15:2:163:GLU:HA	15:2:166:ASN:HB3	1.99	0.44
15:2:17:GLU:CB	15:2:19:LEU:N	2.72	0.44
16:3:75:ALA:CB	16:3:76:PRO:HD3	2.46	0.44
1:A:123:VAL:O	1:A:133:ASN:ND2	2.51	0.44
1:A:159:THR:HG21	1:A:242:ILE:HG12	2.00	0.44
1:A:52:THR:CA	1:A:55:TRP:HE1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:C	1:A:92:TRP:N	2.70	0.44
2:B:179:LEU:CD1	2:B:287:GLY:O	2.65	0.44
2:B:195:VAL:HG13	2:B:254:ILE:CG1	2.47	0.44
2:B:334:LEU:HD23	18:B:1202:CLA:C4C	2.47	0.44
2:B:319:HIS:HA	2:B:406:ASN:HB3	1.98	0.44
1:A:668:TYR:CD1	2:B:445:ALA:CB	3.01	0.44
2:B:463:ILE:HG22	2:B:464:GLN:H	1.79	0.44
18:A:9013:CLA:C1D	2:B:582:TRP:HD1	2.30	0.44
2:B:85:ARG:HH11	2:B:85:ARG:HB3	1.82	0.44
2:B:91:ILE:HD13	2:B:113:VAL:HA	1.98	0.44
3:C:25:VAL:O	3:C:25:VAL:CG1	2.65	0.44
4:D:46:TYR:HE1	4:D:110:GLN:HB3	1.83	0.44
6:F:121:ILE:HB	6:F:124:PRO:HD3	1.99	0.44
6:F:141:TYR:HD2	6:F:142:ARG:HH11	1.65	0.44
7:G:89:ALA:HA	7:G:90:SER:HA	1.73	0.44
8:H:47:PHE:O	8:H:49:LYS:N	2.51	0.44
18:J:2107:CLA:H62	18:J:2107:CLA:H93	1.62	0.44
12:L:66:GLY:O	18:L:1503:CLA:HMB3	2.17	0.44
12:L:14:LEU:CD2	12:L:23:LEU:H	2.16	0.44
14:1:159:VAL:O	14:1:160:GLY:C	2.56	0.44
15:2:175:MET:O	15:2:176:GLY:C	2.54	0.44
15:2:92:THR:C	15:2:94:LEU:HB2	2.33	0.44
16:3:119:MET:O	16:3:120:ALA:C	2.55	0.44
1:A:127:VAL:CG1	10:J:30:ASN:ND2	2.80	0.44
1:A:367:SER:O	1:A:369:THR:N	2.51	0.44
19:A:5001:PQN:H221	19:A:5001:PQN:H261	1.66	0.44
1:A:578:ARG:NH2	1:A:728:VAL:HB	2.32	0.44
1:A:744:ALA:HB2	20:A:6011:BCR:H323	1.90	0.44
1:A:92:TRP:O	1:A:93:LEU:C	2.56	0.44
18:B:1138:CLA:H91	18:B:1229:CLA:H2	1.98	0.44
18:B:1208:CLA:CAA	18:B:1208:CLA:H12	2.48	0.44
2:B:387:PHE:O	2:B:390:GLY:N	2.50	0.44
2:B:415:LYS:O	2:B:418:ILE:HG23	2.17	0.44
2:B:448:THR:N	2:B:449:PRO:HD2	2.32	0.44
18:A:9013:CLA:C1D	2:B:582:TRP:CD1	3.01	0.44
18:B:9022:CLA:HAC2	18:B:9023:CLA:HBC3	1.99	0.44
3:C:14:CYS:C	3:C:16:GLN:H	2.20	0.44
3:C:30:PRO:O	3:C:31:TRP:O	2.35	0.44
2:B:37:ILE:CG2	4:D:148:PHE:CE1	3.00	0.44
5:E:45:TRP:CA	5:E:46:PHE:CB	2.96	0.44
6:F:53:PHE:C	6:F:55:ASN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:6:SER:O	9:I:10:PRO:HD2	2.18	0.44
10:J:39:PHE:HA	10:J:40:PRO:HD2	1.90	0.44
12:L:165:TYR:CE1	18:L:1503:CLA:CAD	2.99	0.44
12:L:167:PHE:N	12:L:167:PHE:CD1	2.74	0.44
13:N:58:VAL:HG11	16:3:86:PRO:CA	2.22	0.44
14:1:84:TYR:CD2	14:1:88:PRO:O	2.71	0.44
17:4:99:HIS:ND1	17:4:99:HIS:C	2.71	0.44
18:A:1131:CLA:HBC3	18:A:1136:CLA:HAC1	1.95	0.44
1:A:164:LEU:HD23	1:A:164:LEU:H	1.81	0.44
1:A:239:PRO:HG2	1:A:240:LYS:HE3	2.00	0.44
1:A:151:GLN:CD	1:A:384:TYR:HB2	2.38	0.44
1:A:430:ASP:OD2	1:A:431:LEU:N	2.50	0.44
1:A:432:LEU:HD23	1:A:433:ASP:N	2.33	0.44
1:A:725:LEU:O	19:A:5001:PQN:H6	2.18	0.44
1:A:493:GLN:HG2	1:A:515:TRP:HB2	2.00	0.44
1:A:711:HIS:HB3	1:A:716:VAL:HB	2.00	0.44
2:B:427:LEU:HD12	18:B:1138:CLA:HMD2	1.99	0.44
18:B:1235:CLA:H92	18:B:1235:CLA:HBB1	2.00	0.44
2:B:332:PHE:N	2:B:335:GLY:N	2.62	0.44
2:B:392:ILE:HG22	2:B:393:PHE:H	1.82	0.44
2:B:38:THR:H	2:B:41:ARG:HD2	1.83	0.44
2:B:594:TRP:CD2	2:B:598:HIS:CD2	3.06	0.44
3:C:51:CYS:O	21:C:3102:SF4:S1	2.76	0.44
3:C:76:SER:C	3:C:78:GLY:N	2.71	0.44
5:E:40:ARG:C	5:E:42:GLU:N	2.70	0.44
12:L:77:THR:OG1	12:L:78:GLU:N	2.50	0.44
13:N:71:GLY:HA2	13:N:76:LYS:HB3	1.97	0.44
15:2:90:ASP:HB3	15:2:91:THR:OG1	2.18	0.44
18:A:1107:CLA:H43	18:A:1107:CLA:O1A	2.17	0.44
1:A:747:TRP:CZ2	18:A:1126:CLA:O2A	2.71	0.44
1:A:126:ILE:O	1:A:128:GLY:N	2.50	0.44
18:B:1218:CLA:CAA	18:B:1218:CLA:CBD	2.96	0.44
18:B:1219:CLA:O2D	18:B:1219:CLA:H2A	2.17	0.44
18:B:1224:CLA:O1D	18:B:1225:CLA:HMA1	2.18	0.44
18:B:1231:CLA:H3A	18:B:1231:CLA:HBA2	1.57	0.44
2:B:12:ILE:HG13	2:B:12:ILE:H	1.55	0.44
2:B:225:LEU:O	2:B:226:LEU:O	2.35	0.44
2:B:290:MET:HA	18:B:1218:CLA:CAC	2.27	0.44
2:B:37:ILE:O	4:D:148:PHE:HB3	2.18	0.44
2:B:406:ASN:O	2:B:408:LEU:N	2.50	0.44
2:B:543:GLY:HA2	2:B:551:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASN:HB2	2:B:651:LEU:HD13	2.00	0.44
2:B:657:TRP:CH2	2:B:713:PHE:CZ	3.05	0.44
3:C:3:HIS:NE2	3:C:48:CYS:C	2.65	0.44
4:D:102:ARG:CB	4:D:110:GLN:HB2	2.48	0.44
4:D:57:ILE:CG2	4:D:65:ALA:HB1	2.47	0.44
4:D:99:GLN:HB3	4:D:114:PRO:HD3	2.00	0.44
7:G:35:VAL:HG12	7:G:36:PRO:CG	2.47	0.44
8:H:43:PHE:HD1	8:H:43:PHE:N	2.15	0.44
10:J:16:THR:O	10:J:18:TRP:N	2.50	0.44
10:J:3:ASP:O	10:J:5:LYS:N	2.50	0.44
18:L:1502:CLA:HBC2	18:L:1502:CLA:HHD	2.00	0.44
14:1:10:ARG:CB	14:1:11:PRO:CB	2.95	0.44
16:3:64:ARG:O	16:3:68:LEU:HB2	2.17	0.44
17:4:60:LEU:C	17:4:62:GLU:H	2.20	0.44
14:1:183:ASP:HA	17:4:87:SER:HA	2.00	0.44
18:A:1107:CLA:OBD	18:A:1107:CLA:HED3	2.18	0.44
1:A:147:SER:H	1:A:391:THR:HG23	1.76	0.44
1:A:362:LEU:HD11	18:A:1128:CLA:HBB2	2.00	0.44
1:A:629:ASN:HD22	1:A:630:ASP:N	2.15	0.44
2:B:196:HIS:CE1	18:B:1211:CLA:C3C	2.99	0.44
18:B:1235:CLA:OBD	18:B:1235:CLA:O2D	2.35	0.44
2:B:243:LEU:HA	2:B:264:GLN:NE2	2.32	0.44
2:B:273:VAL:HG13	2:B:276:HIS:HB3	1.98	0.44
2:B:317:ARG:HD3	2:B:407:VAL:HG13	1.99	0.44
2:B:331:HIS:CD2	18:B:1202:CLA:HBC1	2.53	0.44
4:D:84:LEU:CD1	4:D:85:ALA:H	2.31	0.44
4:D:93:LYS:O	4:D:94:TYR:CG	2.71	0.44
6:F:124:PRO:C	6:F:125:LEU:HD23	2.38	0.44
18:F:1302:CLA:H2	18:F:1302:CLA:H71	1.98	0.44
6:F:96:TRP:N	6:F:96:TRP:CD1	2.83	0.44
7:G:20:ARG:O	7:G:23:PHE:HB3	2.15	0.44
9:I:16:PHE:CE1	20:I:6018:BCR:H341	2.52	0.44
12:L:56:VAL:HG23	12:L:57:GLY:N	2.33	0.44
12:L:97:MET:SD	12:L:98:CYS:HA	2.58	0.44
14:1:109:GLU:O	14:1:112:ARG:HG3	2.18	0.44
16:3:188:GLY:O	16:3:191:ALA:HB3	2.18	0.44
17:4:63:VAL:O	17:4:64:PHE:C	2.55	0.44
18:A:1107:CLA:HAC1	2:B:446:PHE:HZ	1.76	0.44
1:A:331:LEU:O	1:A:334:HIS:ND1	2.50	0.44
1:A:364:MET:HA	1:A:364:MET:HE2	1.95	0.44
1:A:692:PHE:CE2	19:A:5001:PQN:C2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:9011:CLA:H41	18:A:9011:CLA:H62	1.76	0.44
2:B:103:ALA:O	2:B:106:ARG:NH1	2.51	0.44
18:B:1212:CLA:CBA	18:B:1212:CLA:H2	2.48	0.44
2:B:209:TRP:CD1	2:B:209:TRP:C	2.91	0.44
2:B:230:TRP:O	2:B:232:LEU:N	2.51	0.44
2:B:257:ILE:CA	2:B:272:ASP:OD1	2.50	0.44
2:B:648:TRP:CZ3	20:B:6017:BCR:H332	2.52	0.44
3:C:49:VAL:CA	3:C:76:SER:HB3	2.47	0.44
3:C:55:GLU:CD	3:C:55:GLU:C	2.76	0.44
18:F:1139:CLA:HAA1	18:F:1139:CLA:HBD	2.00	0.44
6:F:44:ALA:O	6:F:46:MET:N	2.51	0.44
12:L:159:TYR:HD1	12:L:159:TYR:HA	1.55	0.44
12:L:69:VAL:HG22	12:L:83:ALA:CB	2.47	0.44
15:2:19:LEU:C	15:2:20:ASP:OD1	2.57	0.44
16:3:140:GLY:N	16:3:141:LYS:HB3	2.31	0.44
17:4:103:ILE:HG13	18:4:1304:CLA:HMA3	2.00	0.44
17:4:118:ASP:HB2	17:4:119:PRO:HD3	2.00	0.44
18:A:1115:CLA:H12	18:K:1141:CLA:C3B	2.48	0.44
1:A:277:TYR:CD2	18:A:1113:CLA:CBC	2.88	0.44
1:A:393:LEU:HD11	1:A:750:PHE:CE1	2.53	0.44
1:A:450:CYS:SG	1:A:551:VAL:CG1	3.04	0.44
1:A:488:PHE:HB3	1:A:535:GLY:HA2	1.99	0.44
1:A:618:TRP:CE2	1:A:642:PHE:HD1	2.36	0.44
1:A:683:HIS:HB3	18:B:9012:CLA:HBD	1.99	0.44
1:A:82:HIS:CE1	18:A:1103:CLA:C4D	3.01	0.44
2:B:337:ALA:O	18:B:1202:CLA:O1D	2.36	0.44
2:B:345:THR:CG2	18:B:1225:CLA:HMC3	2.47	0.44
2:B:141:PHE:O	2:B:144:PHE:HB3	2.18	0.44
2:B:262:HIS:CE1	2:B:265:THR:OG1	2.71	0.44
2:B:392:ILE:O	2:B:394:PHE:N	2.51	0.44
2:B:496:GLY:C	2:B:498:LEU:H	2.22	0.44
3:C:69:LEU:CB	3:C:72:GLU:HG2	2.46	0.44
4:D:31:GLY:CA	12:L:13:PRO:CB	2.63	0.44
6:F:128:SER:O	6:F:132:ARG:HB2	2.17	0.44
6:F:53:PHE:HB3	6:F:54:ASP:H	1.30	0.44
8:H:26:SER:CA	8:H:27:ASP:C	2.85	0.44
8:H:85:GLN:O	8:H:87:PRO:O	2.36	0.44
18:J:2107:CLA:H3A	18:J:2107:CLA:HBA1	1.68	0.44
13:N:25:THR:O	13:N:26:GLY:C	2.55	0.44
13:N:47:THR:HA	13:N:48:GLY:HA2	1.67	0.44
13:N:72:LYS:HA	13:N:75:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:8:GLU:HA	17:4:110:LYS:NZ	2.33	0.43
15:2:74:LEU:O	15:2:75:ASN:HB2	2.18	0.43
16:3:114:LEU:O	16:3:115:PHE:HD1	2.01	0.43
16:3:206:GLY:O	16:3:207:VAL:C	2.56	0.43
17:4:166:GLY:O	17:4:169:ILE:HG12	2.18	0.43
17:4:186:ILE:O	17:4:187:SER:OG	2.36	0.43
18:A:1113:CLA:HAA1	18:A:1113:CLA:CED	2.36	0.43
1:A:453:LEU:HD23	18:A:1136:CLA:CBB	2.47	0.43
1:A:200:GLU:OE2	1:A:327:ILE:CD1	2.65	0.43
1:A:203:LEU:HD13	18:A:1123:CLA:C1D	2.47	0.43
1:A:293:GLY:O	1:A:294:LEU:HB3	2.17	0.43
1:A:520:LEU:CD2	1:A:530:LEU:CB	2.95	0.43
1:A:733:VAL:O	1:A:737:HIS:N	2.33	0.43
2:B:693:TRP:HE3	18:B:1238:CLA:HMD3	1.83	0.43
2:B:141:PHE:CE2	2:B:145:LEU:HD23	2.53	0.43
2:B:169:LYS:O	2:B:327:ASN:ND2	2.50	0.43
2:B:375:HIS:NE2	18:B:1225:CLA:CHA	2.81	0.43
2:B:436:LEU:HD23	2:B:453:ILE:CG1	2.46	0.43
2:B:439:HIS:HE1	2:B:453:ILE:CG1	2.31	0.43
2:B:601:LEU:O	2:B:603:ARG:N	2.51	0.43
3:C:6:LYS:O	3:C:8:TYR:CZ	2.71	0.43
6:F:88:ILE:HG13	6:F:89:LEU:H	1.83	0.43
7:G:74:TRP:CA	7:G:78:GLY:HA3	2.48	0.43
10:J:26:LEU:O	10:J:29:ILE:N	2.50	0.43
10:J:28:GLU:OE1	18:J:2107:CLA:C4A	2.66	0.43
10:J:31:ARG:HH22	18:J:2107:CLA:C1C	2.31	0.43
12:L:58:LEU:O	12:L:62:PHE:CE2	2.71	0.43
14:1:70:LYS:HZ1	18:1:1013:CLA:C4C	2.31	0.43
14:1:5:MET:O	14:1:9:PRO:O	2.36	0.43
15:2:170:ALA:HA	18:2:2004:CLA:C3B	2.48	0.43
16:3:78:ILE:HB	16:3:79:LEU:CA	2.48	0.43
17:4:48:GLY:HA2	17:4:51:ALA:CB	2.48	0.43
1:A:204:ASN:ND2	1:A:317:TYR:HD1	2.16	0.43
1:A:272:LEU:HD23	1:A:274:TRP:CE3	2.40	0.43
1:A:154:ARG:CZ	1:A:384:TYR:CE1	3.01	0.43
18:B:1207:CLA:CMA	18:B:1207:CLA:H2	2.33	0.43
2:B:276:HIS:HB2	18:B:1214:CLA:C1B	2.47	0.43
2:B:287:GLY:H	18:B:1218:CLA:HMC1	0.61	0.43
2:B:303:TYR:HB3	18:B:1219:CLA:HED3	2.00	0.43
18:B:1238:CLA:HHD	18:B:1238:CLA:HBC3	1.99	0.43
2:B:205:GLU:O	2:B:207:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:HIS:O	2:B:243:LEU:C	2.57	0.43
2:B:586:THR:HG22	2:B:586:THR:O	2.17	0.43
2:B:444:LEU:HG	2:B:615:TYR:CZ	2.53	0.43
2:B:680:TRP:NE1	4:D:37:LEU:CD2	2.81	0.43
2:B:88:ALA:HB3	2:B:114:ASN:CB	2.48	0.43
3:C:70:TRP:HA	3:C:70:TRP:CE3	2.52	0.43
2:B:399:ASN:CB	4:D:144:ILE:HD13	2.49	0.43
4:D:90:LEU:HG	4:D:90:LEU:H	1.69	0.43
7:G:53:GLU:O	7:G:54:TYR:HB3	2.18	0.43
7:G:71:VAL:O	7:G:74:TRP:N	2.48	0.43
9:I:26:LEU:HA	9:I:29:GLU:C	2.39	0.43
12:L:37:LEU:HA	12:L:42:ALA:CB	2.48	0.43
12:L:93:VAL:HG12	12:L:144:PHE:HE1	1.81	0.43
12:L:97:MET:O	12:L:98:CYS:C	2.56	0.43
13:N:70:GLU:OE1	13:N:70:GLU:HA	2.17	0.43
14:1:37:GLU:O	14:1:38:ARG:CB	2.66	0.43
15:2:193:PHE:O	15:2:194:ALA:CB	2.66	0.43
18:2:2007:CLA:C3B	18:2:2002:CLA:HHC	2.48	0.43
18:A:1108:CLA:HMD2	18:A:1110:CLA:C3B	2.48	0.43
1:A:130:GLU:N	1:A:130:GLU:OE1	2.51	0.43
1:A:158:ILE:CA	1:A:163:GLN:HE22	2.31	0.43
19:A:5001:PQN:H23	19:A:5001:PQN:H191	2.00	0.43
1:A:613:ILE:CG2	1:A:614:PHE:N	2.81	0.43
1:A:63:ASP:O	1:A:67:HIS:ND1	2.51	0.43
1:A:715:LYS:NZ	6:F:153:ASN:ND2	2.62	0.43
1:A:83:PHE:HB3	1:A:84:GLY:H	1.46	0.43
2:B:420:SER:CB	18:B:1138:CLA:CED	2.96	0.43
18:B:1208:CLA:CB	18:B:1208:CLA:HAA1	2.46	0.43
2:B:120:VAL:O	2:B:124:TRP:HD1	2.01	0.43
2:B:120:VAL:C	2:B:122:GLN:H	2.22	0.43
2:B:77:TRP:HH2	2:B:125:TYR:CD2	2.36	0.43
2:B:81:PRO:HB3	2:B:130:ARG:NH2	2.33	0.43
2:B:174:ARG:HD2	18:B:1221:CLA:HMD1	2.00	0.43
2:B:19:ARG:CG	2:B:19:ARG:HH11	2.31	0.43
2:B:353:TYR:CE2	2:B:354:SER:HA	2.53	0.43
2:B:583:MET:SD	2:B:584:LEU:HD23	2.58	0.43
2:B:599:ILE:CG2	2:B:600:THR:N	2.82	0.43
3:C:27:GLU:CD	3:C:29:ILE:HG23	2.38	0.43
3:C:31:TRP:CD2	3:C:31:TRP:C	2.90	0.43
4:D:115:LYS:NZ	4:D:116:ASP:OD1	2.39	0.43
4:D:23:ASN:ND2	12:L:17:ASP:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:166:ASN:HD21	18:2:2004:CLA:C1C	2.31	0.43
15:2:190:ASP:O	15:2:191:ASN:C	2.57	0.43
15:2:56:MET:O	15:2:60:ALA:N	2.49	0.43
17:4:136:GLY:HA2	17:4:141:LEU:HD21	2.00	0.43
1:A:120:ALA:HB1	18:A:1106:CLA:HED3	1.98	0.43
1:A:222:GLN:HA	1:A:226:SER:HB2	2.00	0.43
1:A:609:ILE:C	1:A:611:VAL:O	2.57	0.43
2:B:193:HIS:C	2:B:195:VAL:N	2.71	0.43
2:B:279:ALA:O	2:B:280:ILE:C	2.56	0.43
2:B:287:GLY:HA2	2:B:290:MET:HE2	2.01	0.43
2:B:468:GLY:CA	2:B:498:LEU:CD2	2.96	0.43
2:B:56:ILE:H	2:B:56:ILE:HG13	1.68	0.43
2:B:672:GLN:O	2:B:676:GLU:N	2.50	0.43
2:B:680:TRP:HZ2	4:D:33:THR:HA	1.83	0.43
6:F:94:ALA:O	6:F:96:TRP:HD1	1.98	0.43
6:F:96:TRP:CD1	6:F:97:ILE:HG13	2.53	0.43
8:H:65:LEU:HD23	8:H:69:SER:HB2	1.99	0.43
10:J:6:THR:OG1	10:J:7:TYR:N	2.52	0.43
12:L:23:LEU:CB	18:L:1130:CLA:HED1	2.49	0.43
15:2:151:ALA:O	15:2:153:PRO:O	2.36	0.43
15:2:36:SER:OG	15:2:38:PRO:C	2.57	0.43
15:2:56:MET:HA	15:2:59:ALA:H	1.83	0.43
17:4:142:ASN:HD22	17:4:145:PRO:CD	2.30	0.43
17:4:82:GLU:C	17:4:83:TYR:CG	2.91	0.43
1:A:365:LEU:HD22	18:A:1123:CLA:O1A	2.18	0.43
1:A:127:VAL:HG12	10:J:30:ASN:HD21	1.83	0.43
1:A:185:HIS:CD2	1:A:186:TYR:H	2.34	0.43
1:A:260:PRO:O	1:A:261:SER:CB	2.66	0.43
1:A:377:TYR:O	1:A:380:PRO:HD3	2.19	0.43
1:A:415:ALA:O	1:A:417:PHE:HB3	2.19	0.43
1:A:448:TRP:HZ2	18:A:1131:CLA:HMD1	1.84	0.43
1:A:613:ILE:O	1:A:614:PHE:C	2.57	0.43
1:A:86:LEU:HD13	1:A:86:LEU:C	2.39	0.43
18:B:1202:CLA:O2A	18:B:1210:CLA:CHA	2.66	0.43
2:B:326:ILE:HG12	18:B:1221:CLA:C2C	2.48	0.43
2:B:652:PHE:CE1	18:B:1239:CLA:HMB1	2.53	0.43
2:B:467:HIS:CD2	2:B:467:HIS:N	2.86	0.43
2:B:57:ILE:HA	2:B:60:TRP:HB2	2.01	0.43
2:B:74:PHE:HE2	2:B:130:ARG:CA	2.05	0.43
3:C:27:GLU:CA	3:C:43:PRO:HG3	2.48	0.43
6:F:52:ARG:CA	6:F:55:ASN:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:63:PRO:HG3	18:G:1248:CLA:C3C	2.47	0.43
7:G:50:ARG:HD3	7:G:51:ALA:HB2	2.01	0.43
6:F:121:ILE:N	10:J:9:SER:HB2	2.33	0.43
18:A:1115:CLA:CBB	18:K:1141:CLA:C2B	2.96	0.43
13:N:9:LYS:C	13:N:11:LYS:H	2.22	0.43
15:2:22:SER:O	15:2:22:SER:OG	2.30	0.43
16:3:198:TYR:HA	16:3:198:TYR:HD1	1.62	0.43
17:4:156:ASN:HA	17:4:159:LEU:HB2	2.00	0.43
17:4:193:THR:OG1	17:4:194:ILE:N	2.51	0.43
1:A:150:PHE:HD1	1:A:153:TRP:HZ2	1.58	0.43
1:A:227:LEU:HD21	1:A:297:THR:HA	2.00	0.43
1:A:253:ASP:C	1:A:256:ALA:HB3	2.38	0.43
1:A:436:LEU:O	4:D:62:THR:O	2.37	0.43
1:A:493:GLN:O	1:A:494:ASN:C	2.56	0.43
1:A:443:ILE:HD11	1:A:561:LEU:HD13	2.01	0.43
1:A:585:GLY:HA3	3:C:50:GLY:O	2.18	0.43
1:A:632:GLY:N	1:A:633:VAL:HG22	2.33	0.43
1:A:622:SER:H	1:A:637:ILE:HD13	1.83	0.43
1:A:679:PHE:O	1:A:679:PHE:HD1	2.01	0.43
1:A:92:TRP:HB3	1:A:93:LEU:H	1.54	0.43
18:B:1239:CLA:HMB2	20:B:6017:BCR:C15	2.49	0.43
2:B:135:LEU:CD2	2:B:136:TYR:N	2.81	0.43
2:B:160:LYS:C	2:B:162:LYS:H	2.22	0.43
2:B:199:ILE:HD13	2:B:199:ILE:HA	1.63	0.43
2:B:266:GLN:NE2	2:B:505:SER:HG	2.17	0.43
2:B:276:HIS:HB2	18:B:1214:CLA:CHB	2.49	0.43
2:B:332:PHE:H	2:B:335:GLY:CA	2.31	0.43
2:B:341:LEU:O	2:B:341:LEU:CD1	2.47	0.43
2:B:657:TRP:CZ3	2:B:661:PHE:CE1	2.87	0.43
2:B:5:ILE:HG22	2:B:6:PRO:N	2.34	0.43
4:D:114:PRO:HA	4:D:117:GLY:H	1.84	0.43
4:D:135:ARG:CD	4:D:139:LYS:O	2.67	0.43
6:F:88:ILE:HG13	6:F:89:LEU:N	2.34	0.43
7:G:48:ASP:OD2	7:G:48:ASP:N	2.51	0.43
8:H:42:THR:H	8:H:43:PHE:HB2	1.79	0.43
10:J:3:ASP:OD1	15:2:117:GLY:HA2	2.18	0.43
12:L:55:GLU:C	18:L:1502:CLA:HED1	2.39	0.43
13:N:25:THR:HB	15:2:201:HIS:HB2	1.98	0.43
14:1:53:ALA:C	14:1:55:PRO:HD2	2.39	0.43
1:A:110:LEU:HG	1:A:111:ASN:H	1.81	0.43
1:A:222:GLN:O	1:A:227:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLY:O	1:A:367:SER:C	2.56	0.43
1:A:393:LEU:HA	1:A:616:PHE:HZ	1.82	0.43
1:A:356:ALA:HA	1:A:417:PHE:CD1	2.54	0.43
1:A:550:HIS:O	1:A:552:THR:N	2.52	0.43
1:A:695:SER:OG	1:A:696:GLY:N	2.51	0.43
1:A:753:ARG:HH12	1:A:757:VAL:HB	1.81	0.43
2:B:280:ILE:HG22	18:B:1214:CLA:C3C	2.49	0.43
18:B:1242:CLA:CGD	18:B:1242:CLA:HBA2	2.48	0.43
2:B:222:LEU:HA	2:B:222:LEU:HD12	1.80	0.43
2:B:23:PHE:CD2	2:B:23:PHE:N	2.87	0.43
2:B:393:PHE:CZ	2:B:394:PHE:HE1	2.37	0.43
2:B:520:HIS:O	2:B:521:HIS:O	2.35	0.43
2:B:536:LYS:O	2:B:541:ALA:CB	2.66	0.43
2:B:64:ASN:N	2:B:67:HIS:HB2	2.33	0.43
2:B:720:THR:O	2:B:721:TYR:C	2.57	0.43
2:B:724:PHE:C	2:B:726:ILE:H	2.21	0.43
18:A:9011:CLA:HMB2	18:B:9010:CLA:CHB	2.49	0.43
1:A:455:PHE:HA	18:B:9023:CLA:O1A	2.18	0.43
3:C:17:CYS:HB2	3:C:58:CYS:H	1.83	0.43
3:C:32:GLY:HA2	3:C:37:LYS:HG2	2.01	0.43
5:E:90:VAL:CG1	5:E:91:ALA:N	2.79	0.43
6:F:113:LYS:HA	6:F:114:PRO:HD3	1.81	0.43
6:F:14:PHE:O	6:F:18:GLU:CB	2.67	0.43
6:F:47:GLU:HA	6:F:51:LYS:HB2	2.00	0.43
6:F:86:PRO:HD3	10:J:39:PHE:CB	2.48	0.43
18:B:1209:CLA:HBA2	7:G:38:GLN:HG3	2.00	0.43
7:G:86:LEU:HD13	7:G:86:LEU:H	1.84	0.43
7:G:8:ILE:O	7:G:9:SER:C	2.57	0.43
7:G:92:GLY:C	7:G:93:TYR:O	2.56	0.43
9:I:26:LEU:HB3	9:I:30:LYS:HA	2.00	0.43
12:L:120:LEU:HD23	12:L:121:THR:H	1.84	0.43
14:1:162:CYS:CA	14:1:165:GLN:HB2	2.21	0.43
13:N:29:PHE:HE1	15:2:201:HIS:CD2	2.37	0.43
15:2:94:LEU:C	15:2:96:ILE:N	2.71	0.43
16:3:131:GLN:HB3	16:3:134:TYR:CE1	2.54	0.43
1:A:184:PHE:CD1	1:A:184:PHE:C	2.92	0.43
1:A:548:THR:C	1:A:550:HIS:N	2.70	0.43
1:A:572:LYS:HD2	1:A:579:PHE:HE2	1.83	0.43
1:A:80:SER:O	1:A:83:PHE:HD1	2.02	0.43
2:B:12:ILE:O	2:B:20:ARG:HG3	2.19	0.43
2:B:238:SER:HA	2:B:251:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:MET:HB3	2:B:291:TYR:CD1	2.54	0.43
18:A:9011:CLA:CBB	2:B:624:LEU:HD11	2.36	0.43
2:B:650:PHE:CE2	2:B:654:HIS:CE1	3.07	0.43
2:B:675:ILE:HD11	2:B:698:VAL:C	2.39	0.43
2:B:68:VAL:HG23	2:B:69:ALA:H	1.84	0.43
2:B:653:GLY:CA	2:B:720:THR:CG2	2.88	0.43
18:B:9012:CLA:HAA2	18:B:9012:CLA:O1D	2.19	0.43
3:C:8:TYR:H	4:D:132:LEU:HD22	1.82	0.43
4:D:80:LYS:HE3	4:D:100:PHE:CE2	2.53	0.43
3:C:60:THR:CA	5:E:80:ASN:ND2	2.73	0.43
5:E:62:ARG:NH2	5:E:83:ALA:O	2.50	0.43
6:F:45:THR:C	6:F:47:GLU:H	2.21	0.43
6:F:52:ARG:HA	6:F:55:ASN:HB2	1.99	0.43
9:I:16:PHE:HD1	9:I:17:PRO:HG3	1.83	0.43
13:N:36:GLU:HA	13:N:39:SER:HB2	2.00	0.43
13:N:36:GLU:C	13:N:40:CYS:HA	2.38	0.43
13:N:56:LYS:HB3	13:N:57:LYS:H	1.66	0.43
13:N:58:VAL:CG2	13:N:59:PRO:N	2.65	0.43
14:1:43:GLU:HB3	14:1:44:LEU:H	1.45	0.43
15:2:19:LEU:CG	15:2:22:SER:HG	2.26	0.43
16:3:133:TRP:CD1	16:3:133:TRP:N	2.86	0.43
18:A:1123:CLA:HHD	18:A:1123:CLA:CBC	2.31	0.43
18:A:1103:CLA:HMC3	18:A:1128:CLA:HMA1	2.01	0.43
1:A:158:ILE:C	1:A:163:GLN:NE2	2.66	0.43
1:A:176:GLY:O	1:A:180:PHE:N	2.51	0.43
1:A:208:ALA:HA	1:A:311:LEU:HA	2.00	0.43
1:A:385:LEU:O	1:A:388:ASP:CB	2.67	0.43
2:B:126:THR:O	2:B:127:ILE:C	2.55	0.43
2:B:155:LEU:O	2:B:158:GLN:N	2.51	0.43
2:B:534:LEU:O	2:B:538:ALA:HB3	2.19	0.43
2:B:56:ILE:O	2:B:57:ILE:C	2.58	0.43
2:B:533:ILE:HG21	2:B:579:ALA:CA	2.49	0.43
3:C:12:ILE:O	3:C:38:GLN:HG3	2.19	0.43
3:C:24:ASP:HB2	3:C:25:VAL:H	1.68	0.43
3:C:29:ILE:HB	3:C:30:PRO:CD	2.49	0.43
3:C:8:TYR:CD1	4:D:137:ILE:HB	2.53	0.43
4:D:88:THR:O	4:D:89:ARG:C	2.55	0.43
7:G:90:SER:H	7:G:93:TYR:H	1.61	0.43
8:H:49:LYS:HE3	12:L:100:THR:HG21	2.01	0.43
8:H:66:THR:HB	8:H:67:TYR:H	1.74	0.43
10:J:10:VAL:HG13	10:J:11:ALA:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:128:ASP:HB3	12:L:129:GLN:H	1.67	0.43
18:B:1207:CLA:H41	12:L:91:LEU:HD21	2.01	0.43
13:N:8:GLU:HG3	13:N:11:LYS:HB2	1.97	0.43
13:N:74:LYS:HG3	13:N:85:TRP:CZ2	2.52	0.43
14:1:160:GLY:HA2	18:1:1003:CLA:C2C	2.49	0.43
16:3:61:ILE:C	16:3:64:ARG:HB3	2.36	0.43
16:3:78:ILE:HB	16:3:79:LEU:O	2.19	0.43
18:A:1124:CLA:CHC	18:A:1137:CLA:CGA	2.81	0.43
1:A:253:ASP:CA	1:A:256:ALA:HB3	2.49	0.43
1:A:646:SER:HB2	1:A:652:TRP:CZ2	2.54	0.43
1:A:733:VAL:O	1:A:735:VAL:N	2.51	0.43
18:B:1217:CLA:C4A	18:B:1217:CLA:O1A	2.67	0.43
18:B:1224:CLA:CBC	18:B:1225:CLA:HBB1	2.49	0.43
2:B:190:TRP:CZ2	2:B:194:LEU:HD13	2.53	0.43
2:B:243:LEU:O	2:B:246:THR:HB	2.19	0.43
2:B:338:LEU:HB2	2:B:382:ILE:CG2	2.49	0.43
2:B:466:ALA:C	2:B:468:GLY:N	2.70	0.43
2:B:705:ALA:CB	19:B:5002:PQN:C8	2.93	0.43
2:B:503:GLU:H	2:B:506:ASN:HD22	1.67	0.43
2:B:515:GLY:O	2:B:518:LEU:HB2	2.19	0.43
2:B:645:VAL:HG12	2:B:646:TRP:N	2.34	0.43
3:C:24:ASP:CG	4:D:112:LEU:HD21	2.39	0.43
4:D:46:TYR:CG	4:D:80:LYS:HB3	2.54	0.43
5:E:38:ILE:N	5:E:38:ILE:HD12	2.34	0.43
6:F:33:ALA:HA	6:F:42:ILE:HD11	2.01	0.43
11:K:55:UNK:C	11:K:57:UNK:N	2.81	0.43
14:1:82:ALA:C	14:1:84:TYR:H	2.22	0.42
15:2:179:PHE:C	15:2:179:PHE:HD1	2.19	0.42
15:2:86:GLU:OE1	17:4:184:GLN:HB3	2.19	0.42
18:3:3002:CLA:C3B	18:3:3007:CLA:C3C	2.97	0.42
17:4:144:ALA:N	17:4:145:PRO:CD	2.71	0.42
17:4:41:VAL:CG2	17:4:42:GLN:N	2.53	0.42
17:4:82:GLU:CG	17:4:83:TYR:N	2.49	0.42
1:A:80:SER:C	18:A:1109:CLA:C2A	2.87	0.42
1:A:63:ASP:N	18:A:1128:CLA:HAA2	2.16	0.42
18:A:1140:CLA:H3A	18:A:1140:CLA:HBA2	1.54	0.42
1:A:149:PHE:O	1:A:153:TRP:CG	2.72	0.42
1:A:367:SER:C	1:A:369:THR:H	2.22	0.42
1:A:479:ASP:C	1:A:481:ALA:N	2.71	0.42
1:A:78:VAL:HG21	1:A:354:TRP:CD2	2.53	0.42
18:B:1217:CLA:CHA	18:B:1217:CLA:HBA1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1236:CLA:O1D	18:B:1236:CLA:OBD	2.35	0.42
2:B:151:LEU:HB3	2:B:155:LEU:HD12	2.01	0.42
2:B:192:GLY:CA	2:B:195:VAL:HB	2.47	0.42
2:B:42:LEU:O	2:B:45:ASN:HB2	2.19	0.42
2:B:558:PRO:CA	2:B:702:ILE:HD11	2.49	0.42
2:B:646:TRP:C	2:B:648:TRP:N	2.72	0.42
2:B:65:LEU:HG	2:B:124:TRP:CZ3	2.54	0.42
2:B:710:LEU:HD12	2:B:710:LEU:HA	1.84	0.42
2:B:90:ALA:H	2:B:91:ILE:HD12	1.84	0.42
4:D:53:PRO:CB	4:D:95:LYS:HD2	2.49	0.42
6:F:73:VAL:HG21	6:F:82:GLU:N	2.33	0.42
9:I:14:LEU:HA	9:I:14:LEU:HD22	1.85	0.42
12:L:138:LYS:N	12:L:138:LYS:HD2	2.34	0.42
18:L:1502:CLA:OBD	18:L:1502:CLA:O2D	2.37	0.42
13:N:58:VAL:HB	13:N:59:PRO:HD2	2.01	0.42
13:N:60:PHE:HD2	13:N:60:PHE:H	1.60	0.42
14:1:173:PRO:O	14:1:175:GLU:N	2.52	0.42
16:3:64:ARG:HG2	16:3:65:PHE:N	2.34	0.42
17:4:137:ILE:HG12	17:4:140:PRO:O	2.19	0.42
15:2:86:GLU:HG2	17:4:184:GLN:OE1	2.18	0.42
1:A:90:PHE:HB3	1:A:175:ALA:HB2	2.00	0.42
1:A:228:PRO:O	1:A:230:ASN:N	2.49	0.42
1:A:692:PHE:HA	19:A:5001:PQN:H9	2.01	0.42
1:A:71:LEU:HD23	1:A:74:ILE:HG23	2.01	0.42
2:B:88:ALA:N	2:B:116:ALA:HB2	2.35	0.42
2:B:254:ILE:CG2	18:B:1212:CLA:HBC1	2.50	0.42
2:B:550:LYS:NZ	2:B:570:ILE:O	2.52	0.42
2:B:549:ASP:C	2:B:551:LYS:HG2	2.38	0.42
2:B:724:PHE:C	2:B:726:ILE:N	2.73	0.42
2:B:81:PRO:HB3	2:B:130:ARG:HH22	1.84	0.42
1:A:567:ARG:O	4:D:79:ARG:NH1	2.51	0.42
6:F:13:GLN:C	6:F:67:GLY:HA3	2.39	0.42
6:F:5:LEU:O	6:F:63:CYS:O	2.37	0.42
2:B:456:GLU:HB2	6:F:70:HIS:HB3	2.01	0.42
18:B:1217:CLA:HMA1	7:G:21:PHE:CD2	2.48	0.42
7:G:21:PHE:C	7:G:23:PHE:CG	2.92	0.42
12:L:118:LEU:HB3	12:L:119:THR:HA	2.00	0.42
15:2:174:VAL:HG12	15:2:175:MET:N	2.34	0.42
15:2:20:ASP:OD2	15:2:23:LEU:HD11	2.19	0.42
17:4:114:SER:O	17:4:115:VAL:C	2.57	0.42
17:4:81:GLU:C	17:4:84:PHE:CE1	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLN:HB3	1:A:144:GLN:HE21	1.63	0.42
1:A:159:THR:O	1:A:160:SER:CB	2.57	0.42
1:A:163:GLN:O	1:A:166:CYS:HB3	2.19	0.42
1:A:442:ILE:HD11	1:A:561:LEU:HD22	1.98	0.42
1:A:624:VAL:HG13	1:A:625:TRP:CD1	2.54	0.42
1:A:650:ASN:ND2	2:B:632:ILE:HD11	2.35	0.42
1:A:668:TYR:CE1	2:B:445:ALA:HB2	2.54	0.42
1:A:744:ALA:O	1:A:745:THR:C	2.57	0.42
2:B:119:GLY:O	2:B:121:TYR:N	2.52	0.42
18:B:1237:CLA:H52	18:B:1237:CLA:H11	1.70	0.42
2:B:226:LEU:O	2:B:227:THR:C	2.57	0.42
2:B:344:ILE:O	2:B:348:VAL:N	2.53	0.42
2:B:388:ALA:C	2:B:391:PRO:HD2	2.39	0.42
2:B:510:LEU:HD22	18:B:1234:CLA:HMD2	2.01	0.42
2:B:556:SER:O	3:C:68:TYR:OH	2.37	0.42
2:B:557:PHE:HA	2:B:558:PRO:HD2	1.78	0.42
2:B:589:TRP:CD1	2:B:592:PHE:CE2	2.85	0.42
2:B:592:PHE:HD1	2:B:623:TYR:HE2	1.66	0.42
3:C:72:GLU:OE2	3:C:77:MET:CG	2.64	0.42
4:D:102:ARG:HH11	4:D:110:GLN:HE21	1.52	0.42
4:D:52:SER:CB	4:D:68:MET:HB2	2.48	0.42
6:F:115:THR:O	6:F:116:GLN:C	2.56	0.42
6:F:93:ILE:HA	6:F:96:TRP:HZ2	1.64	0.42
7:G:50:ARG:CG	7:G:51:ALA:HB2	2.49	0.42
8:H:88:LYS:C	8:H:90:GLY:N	2.73	0.42
8:H:90:GLY:HA3	8:H:91:PRO:HA	1.79	0.42
12:L:56:VAL:CG2	12:L:57:GLY:N	2.82	0.42
12:L:6:PRO:O	12:L:7:THR:C	2.57	0.42
13:N:81:VAL:CG1	13:N:83:TRP:HA	2.48	0.42
14:1:152:ARG:CD	14:1:153:LEU:N	2.82	0.42
15:2:74:LEU:O	15:2:75:ASN:CB	2.67	0.42
17:4:60:LEU:HD11	17:4:76:TYR:OH	2.19	0.42
18:A:1132:CLA:HHB	12:L:72:GLY:O	2.18	0.42
1:A:219:ALA:O	1:A:223:VAL:HG22	2.19	0.42
1:A:367:SER:HA	1:A:370:ILE:CG2	2.45	0.42
1:A:395:LEU:C	1:A:397:THR:N	2.73	0.42
1:A:46:LYS:HB3	5:E:76:ASN:HD21	1.84	0.42
1:A:503:THR:O	1:A:504:ALA:HB3	2.19	0.42
1:A:62:HIS:CG	18:A:1128:CLA:O1A	2.73	0.42
1:A:680:LEU:C	1:A:682:ALA:N	2.72	0.42
1:A:751:LEU:HD12	1:A:752:ALA:H	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1138:CLA:CHC	18:F:1139:CLA:HMD2	2.49	0.42
2:B:174:ARG:CD	18:B:1221:CLA:HMD1	2.49	0.42
18:B:1239:CLA:H11	19:B:5002:PQN:C27	2.47	0.42
2:B:124:TRP:CZ3	2:B:135:LEU:HG	2.49	0.42
2:B:310:PRO:HA	2:B:312:GLY:H	1.74	0.42
2:B:345:THR:HG23	18:B:1225:CLA:CMC	2.42	0.42
2:B:372:TYR:C	2:B:372:TYR:CD2	2.93	0.42
2:B:383:MET:O	2:B:386:ALA:CB	2.67	0.42
2:B:456:GLU:HA	2:B:457:PRO:HD2	1.76	0.42
2:B:663:PHE:O	2:B:664:LEU:CB	2.59	0.42
1:A:447:ASN:OD1	2:B:674:LEU:HD21	2.19	0.42
2:B:714:SER:O	2:B:717:TYR:N	2.53	0.42
2:B:91:ILE:CG1	2:B:114:ASN:ND2	2.81	0.42
4:D:102:ARG:NH1	4:D:110:GLN:HE22	2.06	0.42
4:D:112:LEU:HA	4:D:115:LYS:CE	2.49	0.42
4:D:58:PHE:CE1	4:D:66:ALA:HB3	2.54	0.42
6:F:18:GLU:C	6:F:20:GLN:N	2.58	0.42
7:G:22:VAL:CA	7:G:23:PHE:CD2	3.02	0.42
7:G:62:ASP:N	7:G:63:PRO:CD	2.82	0.42
7:G:81:VAL:CG1	7:G:83:TYR:CD1	3.02	0.42
9:I:29:GLU:H	9:I:29:GLU:HG2	1.33	0.42
10:J:3:ASP:O	10:J:7:TYR:OH	2.36	0.42
10:J:5:LYS:HB2	10:J:7:TYR:CD1	2.55	0.42
15:2:110:TRP:C	15:2:112:ASP:N	2.73	0.42
16:3:126:GLU:OE2	16:3:127:HIS:CD2	2.72	0.42
16:3:196:LEU:HB2	16:3:197:GLY:H	1.75	0.42
16:3:209:PRO:CB	16:3:211:GLN:H	2.23	0.42
1:A:106:TYR:CE1	1:A:153:TRP:CD1	3.08	0.42
1:A:299:ILE:HG23	1:A:303:HIS:HD2	1.82	0.42
1:A:389:TYR:HB2	1:A:754:ILE:HD11	2.01	0.42
1:A:452:PHE:HA	1:A:456:HIS:ND1	2.35	0.42
1:A:465:ASP:O	1:A:467:MET:N	2.52	0.42
1:A:692:PHE:CD2	19:A:5001:PQN:C10	3.02	0.42
18:A:9013:CLA:H3A	18:A:9013:CLA:CGA	2.50	0.42
2:B:297:ILE:HD11	18:B:1218:CLA:HMD1	2.01	0.42
2:B:429:LEU:HD21	18:B:1235:CLA:CMB	2.50	0.42
1:A:654:ARG:CG	2:B:633:ASN:OD1	2.67	0.42
2:B:687:LEU:HD11	12:L:40:LEU:CD1	2.47	0.42
2:B:585:ASN:CG	18:B:9012:CLA:HMC3	2.40	0.42
2:B:92:TRP:HD1	9:I:9:VAL:HG11	1.80	0.42
3:C:30:PRO:HD2	3:C:31:TRP:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:VAL:HG13	3:C:51:CYS:HB2	2.02	0.42
8:H:58:ILE:HA	8:H:61:GLY:HA3	2.01	0.42
12:L:14:LEU:N	12:L:24:GLU:HB2	2.33	0.42
13:N:48:GLY:HA3	13:N:50:GLN:H	1.73	0.42
14:1:188:ASN:HB3	14:1:190:GLY:CA	2.49	0.42
15:2:196:LEU:HD12	15:2:196:LEU:N	2.30	0.42
13:N:58:VAL:HA	16:3:86:PRO:O	2.19	0.42
17:4:194:ILE:HB	17:4:195:VAL:H	1.60	0.42
17:4:48:GLY:CA	17:4:158:ARG:HH22	2.32	0.42
1:A:146:THR:H	18:A:1106:CLA:HMD1	1.82	0.42
1:A:216:LEU:C	1:A:218:TRP:H	2.22	0.42
1:A:239:PRO:HB2	1:A:240:LYS:H	1.43	0.42
1:A:262:PHE:HA	1:A:262:PHE:HD2	1.71	0.42
1:A:293:GLY:O	1:A:380:PRO:HB2	2.20	0.42
1:A:427:ARG:O	1:A:430:ASP:CB	2.68	0.42
1:A:452:PHE:HA	18:A:1131:CLA:O1D	2.20	0.42
1:A:462:ILE:CD1	1:A:649:ILE:CD1	2.98	0.42
1:A:485:GLN:CB	1:A:486:PRO:HD3	2.42	0.42
1:A:500:PRO:O	1:A:506:GLY:HA2	2.20	0.42
1:A:57:LEU:C	1:A:59:ALA:H	2.22	0.42
1:A:401:TRP:CE3	1:A:609:ILE:HG21	2.54	0.42
1:A:664:VAL:HG23	1:A:675:TYR:C	2.40	0.42
2:B:375:HIS:HE1	18:B:1225:CLA:C4A	2.32	0.42
2:B:232:LEU:HA	2:B:235:GLN:NE2	2.34	0.42
2:B:446:PHE:O	2:B:448:THR:OG1	2.36	0.42
2:B:466:ALA:O	2:B:478:LEU:HD22	2.19	0.42
2:B:648:TRP:CZ3	20:B:6017:BCR:HC21	2.36	0.42
2:B:616:LEU:HD23	2:B:616:LEU:C	2.39	0.42
2:B:643:LEU:HD21	2:B:727:ALA:HA	2.01	0.42
2:B:627:ASN:OD1	2:B:732:LYS:CD	2.67	0.42
3:C:69:LEU:O	3:C:70:TRP:C	2.57	0.42
6:F:43:LYS:HG3	6:F:44:ALA:N	2.31	0.42
6:F:50:LYS:C	6:F:52:ARG:H	2.23	0.42
7:G:22:VAL:N	7:G:23:PHE:HB3	2.34	0.42
10:J:28:GLU:OE2	10:J:31:ARG:HD3	2.20	0.42
12:L:138:LYS:HZ2	12:L:138:LYS:CB	2.29	0.42
12:L:30:SER:H	12:L:34:ALA:HB2	1.85	0.42
13:N:74:LYS:O	13:N:85:TRP:NE1	2.43	0.42
14:1:67:ASN:HB3	14:1:68:TRP:H	1.49	0.42
15:2:22:SER:O	15:2:23:LEU:HD11	2.17	0.42
16:3:133:TRP:CD1	16:3:139:MET:HE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:131:GLN:C	16:3:133:TRP:N	2.73	0.42
18:A:1140:CLA:HAC1	19:A:5001:PQN:H152	2.02	0.42
1:A:162:LEU:HD23	1:A:165:TYR:CE2	2.54	0.42
1:A:242:ILE:HA	1:A:243:PRO:HD3	1.81	0.42
1:A:246:HIS:CE1	18:A:1147:CLA:C1A	3.02	0.42
1:A:526:LYS:HA	1:A:627:THR:HA	1.99	0.42
1:A:673:SER:OG	2:B:446:PHE:HE1	2.03	0.42
1:A:697:ARG:HH11	1:A:697:ARG:CG	2.33	0.42
18:B:1220:CLA:CBB	18:B:1227:CLA:HMD2	2.49	0.42
2:B:290:MET:HA	18:B:1218:CLA:C3C	2.48	0.42
2:B:322:LEU:O	2:B:324:ASP:N	2.52	0.42
2:B:571:SER:O	2:B:574:ASP:OD2	2.37	0.42
2:B:580:VAL:CG1	2:B:580:VAL:O	2.67	0.42
2:B:596:TRP:CH2	2:B:612:SER:HB2	2.54	0.42
2:B:615:TYR:O	2:B:615:TYR:CG	2.72	0.42
2:B:80:ASP:HA	2:B:81:PRO:HD3	1.70	0.42
18:B:9012:CLA:HBA1	18:B:9012:CLA:H3A	1.68	0.42
6:F:79:HIS:C	6:F:81:GLY:N	2.61	0.42
9:I:26:LEU:CG	9:I:29:GLU:O	2.47	0.42
12:L:36:TYR:OH	18:L:1504:CLA:H12	2.19	0.42
15:2:180:GLN:O	15:2:182:ILE:CD1	2.66	0.42
16:3:78:ILE:N	16:3:79:LEU:HA	2.35	0.42
17:4:141:LEU:H	17:4:141:LEU:HG	1.62	0.42
17:4:197:THR:OG1	17:4:198:LEU:N	2.53	0.42
17:4:49:ARG:HG2	17:4:49:ARG:HH11	1.85	0.42
17:4:60:LEU:HB3	17:4:61:PRO:CD	2.49	0.42
18:A:1122:CLA:HBA1	18:A:1122:CLA:H3A	1.91	0.42
1:A:249:ILE:HB	1:A:250:LEU:H	1.42	0.42
1:A:308:ILE:C	1:A:311:LEU:H	2.22	0.42
1:A:312:ILE:O	1:A:315:HIS:N	2.38	0.42
1:A:341:GLN:HB3	1:A:344:LYS:CB	2.50	0.42
1:A:547:PHE:CD1	1:A:548:THR:N	2.88	0.42
1:A:55:TRP:CH2	18:F:1139:CLA:HBB2	2.55	0.42
1:A:648:THR:HG22	1:A:651:GLY:H	1.84	0.42
1:A:725:LEU:HD22	19:A:5001:PQN:H6	1.98	0.42
18:B:1212:CLA:CBC	18:B:1212:CLA:CHD	2.86	0.42
2:B:414:HIS:CD2	18:B:1227:CLA:HMA3	2.54	0.42
2:B:251:GLY:O	2:B:252:THR:O	2.38	0.42
2:B:46:ILE:O	2:B:47:PHE:C	2.58	0.42
2:B:700:LEU:HD12	19:B:5002:PQN:C4	2.49	0.42
2:B:520:HIS:O	2:B:521:HIS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:672:GLN:HE22	2:B:698:VAL:CB	2.33	0.42
2:B:655:LEU:HB2	18:B:9022:CLA:CGA	2.50	0.42
1:A:470:LEU:HD23	2:B:96:PHE:CD2	2.55	0.42
3:C:55:GLU:CG	3:C:58:CYS:O	2.63	0.42
18:F:1139:CLA:HED2	18:F:1139:CLA:C4D	2.50	0.42
6:F:65:SER:C	6:F:67:GLY:H	2.23	0.42
8:H:26:SER:CB	8:H:29:PRO:HB3	2.50	0.42
12:L:118:LEU:C	12:L:120:LEU:HA	2.30	0.42
13:N:37:PHE:N	13:N:40:CYS:HA	2.35	0.42
13:N:82:PHE:HA	13:N:83:TRP:HA	1.54	0.42
14:1:60:PRO:HD3	18:1:1006:CLA:C3D	2.49	0.42
14:1:172:GLY:C	14:1:174:LEU:H	2.22	0.42
15:2:180:GLN:HB3	15:2:182:ILE:HG12	2.00	0.42
14:1:9:PRO:HA	17:4:110:LYS:CD	2.50	0.42
17:4:166:GLY:O	17:4:170:GLN:NE2	2.53	0.42
17:4:91:PHE:HB3	17:4:92:VAL:H	1.64	0.42
1:A:164:LEU:H	1:A:164:LEU:HD22	1.83	0.42
1:A:302:HIS:HB3	1:A:303:HIS:CE1	2.54	0.42
1:A:360:ILE:HG12	18:A:1123:CLA:C2B	2.50	0.42
1:A:367:SER:OG	1:A:370:ILE:HG12	2.20	0.42
1:A:385:LEU:HB2	1:A:386:ALA:H	1.71	0.42
1:A:400:MET:HE1	18:A:1135:CLA:HMC3	2.01	0.42
1:A:48:PRO:HB3	1:A:53:TRP:HZ3	1.81	0.42
1:A:53:TRP:C	1:A:55:TRP:H	2.23	0.42
1:A:599:PHE:O	1:A:599:PHE:CD1	2.73	0.42
1:A:675:TYR:CE1	1:A:751:LEU:HD11	2.54	0.42
1:A:751:LEU:HA	1:A:751:LEU:HD22	1.86	0.42
18:B:1209:CLA:H61	18:B:1209:CLA:H41	1.70	0.42
18:B:1212:CLA:C4D	18:B:1212:CLA:HED3	2.50	0.42
2:B:176:ASN:OD1	2:B:291:TYR:HD1	2.02	0.42
2:B:476:ILE:CB	2:B:477:PRO:CD	2.91	0.42
2:B:487:ASN:O	2:B:488:ALA:HB3	2.20	0.42
2:B:537:GLY:CA	2:B:575:ASP:CB	2.98	0.42
2:B:692:ARG:O	2:B:693:TRP:CG	2.73	0.42
2:B:79:GLN:CD	2:B:80:ASP:OD1	2.58	0.42
2:B:724:PHE:CD1	18:B:9010:CLA:HMD1	2.55	0.42
3:C:32:GLY:O	5:E:60:LYS:HD3	2.19	0.42
6:F:111:GLU:OE1	6:F:111:GLU:O	2.38	0.42
6:F:38:PRO:O	6:F:39:ALA:CB	2.68	0.42
6:F:5:LEU:HB3	6:F:62:LEU:CG	2.48	0.42
6:F:92:TYR:CE1	6:F:96:TRP:CZ3	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:38:SER:C	12:L:44:ARG:HH12	2.16	0.42
14:1:150:ASN:O	14:1:152:ARG:N	2.53	0.42
15:2:97:VAL:O	15:2:101:PHE:CD1	2.73	0.42
15:2:23:LEU:CB	15:2:25:GLY:CA	2.80	0.42
14:1:13:TYR:CB	17:4:107:GLN:NE2	2.82	0.42
1:A:195:TRP:CE3	18:A:1118:CLA:C2C	3.03	0.42
1:A:383:PRO:HB2	1:A:384:TYR:CD1	2.55	0.42
1:A:451:ILE:O	1:A:452:PHE:C	2.57	0.42
1:A:548:THR:O	1:A:550:HIS:N	2.52	0.42
1:A:585:GLY:O	1:A:587:GLY:N	2.52	0.42
2:B:355:LEU:CD2	18:B:1214:CLA:CED	2.96	0.42
2:B:218:TYR:HE2	2:B:253:ALA:HA	1.85	0.42
2:B:287:GLY:CA	2:B:290:MET:HE2	2.50	0.42
2:B:421:HIS:O	2:B:425:ALA:HB2	2.20	0.42
2:B:427:LEU:CD2	2:B:431:PHE:CZ	3.02	0.42
2:B:468:GLY:HA2	2:B:498:LEU:CD2	2.49	0.42
2:B:577:TYR:CD2	2:B:578:LEU:HD22	2.55	0.42
2:B:585:ASN:O	2:B:588:GLY:CA	2.68	0.42
3:C:18:VAL:HB	3:C:58:CYS:HB2	2.02	0.42
3:C:21:CYS:HB3	3:C:24:ASP:O	2.20	0.42
4:D:125:PRO:HB2	4:D:126:GLY:H	1.56	0.42
4:D:41:GLN:HG3	4:D:41:GLN:H	1.64	0.42
5:E:40:ARG:O	5:E:42:GLU:N	2.53	0.42
7:G:61:ASN:O	7:G:64:VAL:N	2.53	0.42
2:B:70:TRP:CH2	18:I:1204:CLA:HMD3	2.55	0.42
12:L:27:VAL:CG1	18:L:1130:CLA:H12	2.45	0.42
12:L:36:TYR:OH	18:L:1504:CLA:H52	2.20	0.42
12:L:16:GLY:O	12:L:17:ASP:C	2.58	0.42
15:2:94:LEU:O	15:2:96:ILE:HG13	2.20	0.41
17:4:181:ASN:O	17:4:183:LEU:N	2.45	0.41
18:A:1136:CLA:HMB2	18:A:1137:CLA:C3D	2.50	0.41
1:A:196:PHE:O	1:A:196:PHE:CD2	2.73	0.41
1:A:461:TYR:O	1:A:464:ASN:N	2.53	0.41
2:B:334:LEU:O	2:B:389:HIS:CB	2.68	0.41
2:B:332:PHE:CA	2:B:335:GLY:HA3	2.49	0.41
2:B:444:LEU:O	2:B:445:ALA:HB2	2.20	0.41
2:B:478:LEU:CA	2:B:483:GLY:HA3	2.50	0.41
2:B:483:GLY:O	2:B:487:ASN:N	2.52	0.41
2:B:46:ILE:C	2:B:49:SER:HG	2.11	0.41
2:B:559:CYS:HA	2:B:570:ILE:HG22	2.02	0.41
2:B:722:ALA:HB2	18:B:1224:CLA:HBB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:102:ARG:HD3	6:F:103:SER:HB2	2.02	0.41
6:F:116:GLN:HA	6:F:119:ILE:HB	2.02	0.41
6:F:13:GLN:O	6:F:14:PHE:HB2	2.15	0.41
7:G:18:LEU:C	7:G:20:ARG:H	2.23	0.41
7:G:22:VAL:CA	7:G:23:PHE:HD2	2.32	0.41
12:L:25:THR:O	12:L:28:THR:OG1	2.28	0.41
13:N:35:VAL:CG1	13:N:35:VAL:O	2.68	0.41
13:N:51:ASP:H	13:N:52:LEU:C	2.23	0.41
16:3:217:LEU:N	16:3:218:ALA:HB3	2.34	0.41
17:4:74:LYS:O	17:4:75:TRP:C	2.59	0.41
1:A:207:LEU:CD1	1:A:310:PHE:HA	2.50	0.41
1:A:631:GLN:H	1:A:633:VAL:HG22	1.85	0.41
1:A:664:VAL:O	1:A:667:SER:HB3	2.19	0.41
1:A:697:ARG:NH1	1:A:697:ARG:HG3	2.34	0.41
2:B:104:PHE:C	2:B:106:ARG:N	2.72	0.41
18:B:1235:CLA:H72	18:B:1235:CLA:HBB2	2.02	0.41
2:B:22:TRP:HB2	2:B:23:PHE:HD2	1.85	0.41
2:B:309:ILE:HB	2:B:319:HIS:HB2	2.02	0.41
2:B:515:GLY:CA	2:B:518:LEU:HB2	2.49	0.41
2:B:548:PRO:HB2	3:C:62:PHE:CE1	2.55	0.41
2:B:595:HIS:HB3	2:B:623:TYR:CE1	2.55	0.41
2:B:596:TRP:CH2	2:B:618:GLY:C	2.93	0.41
2:B:656:VAL:HA	18:B:1239:CLA:CBB	2.49	0.41
4:D:102:ARG:NE	4:D:108:GLU:OE2	2.53	0.41
3:C:28:MET:O	4:D:123:VAL:HA	2.19	0.41
6:F:46:MET:HB2	6:F:51:LYS:HZ2	1.84	0.41
7:G:76:SER:HB2	7:G:77:ILE:H	1.72	0.41
8:H:66:THR:O	8:H:67:TYR:C	2.58	0.41
9:I:23:SER:O	9:I:26:LEU:HD23	2.21	0.41
9:I:25:PHE:CD1	9:I:26:LEU:CD1	3.03	0.41
13:N:54:LYS:HA	13:N:55:GLN:HA	1.50	0.41
1:A:325:HIS:CE1	18:A:1120:CLA:CHA	3.03	0.41
1:A:200:GLU:CG	1:A:327:ILE:HG12	2.51	0.41
1:A:349:ILE:HD12	1:A:352:THR:CB	2.48	0.41
1:A:473:PRO:O	1:A:476:MET:SD	2.78	0.41
1:A:57:LEU:HD23	1:A:57:LEU:O	2.20	0.41
1:A:627:THR:O	1:A:628:ILE:HB	2.19	0.41
1:A:751:LEU:O	1:A:754:ILE:HG22	2.19	0.41
1:A:707:ILE:HG12	18:B:1138:CLA:HED3	2.02	0.41
18:B:1224:CLA:H11	18:B:1224:CLA:H51	1.76	0.41
2:B:122:GLN:N	2:B:122:GLN:HE21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:PHE:HD2	2:B:132:ASN:OD1	2.02	0.41
2:B:195:VAL:HG13	2:B:254:ILE:CD1	2.48	0.41
2:B:322:LEU:HA	2:B:322:LEU:HD12	1.74	0.41
2:B:330:ILE:HD13	18:B:1202:CLA:HAC2	2.01	0.41
2:B:357:ALA:C	2:B:358:TYR:CG	2.93	0.41
2:B:443:MET:SD	2:B:451:LYS:CE	3.00	0.41
2:B:585:ASN:O	2:B:588:GLY:N	2.53	0.41
2:B:595:HIS:O	2:B:599:ILE:HB	2.21	0.41
2:B:16:PRO:O	2:B:696:LYS:HG3	2.20	0.41
18:B:9023:CLA:HMB3	18:B:1239:CLA:CMC	2.49	0.41
4:D:105:PRO:HA	4:D:106:SER:HA	1.78	0.41
4:D:108:GLU:CG	4:D:109:VAL:N	2.74	0.41
4:D:52:SER:OG	4:D:72:PRO:CD	2.69	0.41
6:F:77:GLN:HA	6:F:80:TRP:CZ2	2.56	0.41
7:G:37:GLU:CD	7:G:43:HIS:CE1	2.93	0.41
9:I:23:SER:O	9:I:26:LEU:CD2	2.68	0.41
10:J:2:ARG:NH1	10:J:2:ARG:HG2	2.35	0.41
18:A:1129:CLA:HBB1	18:L:1130:CLA:HBC3	2.00	0.41
13:N:51:ASP:H	13:N:52:LEU:HB2	1.73	0.41
14:1:84:TYR:CZ	14:1:90:PRO:HD2	2.55	0.41
14:1:9:PRO:HA	17:4:110:LYS:HD2	2.02	0.41
16:3:138:SER:N	16:3:139:MET:CA	2.83	0.41
18:4:1304:CLA:CED	18:4:4012:CLA:HBB	2.50	0.41
17:4:186:ILE:C	17:4:187:SER:OG	2.59	0.41
18:A:1107:CLA:HED3	18:A:1107:CLA:CAD	2.51	0.41
18:A:1140:CLA:O1D	18:A:1140:CLA:OBD	2.33	0.41
1:A:439:ARG:HH11	4:D:62:THR:C	2.23	0.41
1:A:443:ILE:CD1	1:A:558:LYS:HA	2.50	0.41
1:A:499:ALA:N	1:A:500:PRO:CD	2.84	0.41
1:A:586:ARG:HG3	3:C:49:VAL:CG2	2.50	0.41
1:A:697:ARG:HH11	1:A:697:ARG:HG3	1.85	0.41
1:A:743:ILE:O	1:A:744:ALA:C	2.57	0.41
1:A:750:PHE:HZ	18:A:1126:CLA:CMB	2.32	0.41
1:A:97:TYR:CE2	1:A:153:TRP:CZ3	3.05	0.41
2:B:103:ALA:CB	2:B:104:PHE:CD1	2.90	0.41
2:B:311:PRO:HA	18:B:1301:CLA:HHD	2.03	0.41
2:B:193:HIS:NE2	2:B:197:VAL:O	2.53	0.41
2:B:391:PRO:HD3	2:B:538:ALA:HB1	1.97	0.41
2:B:534:LEU:HA	2:B:534:LEU:HD13	1.64	0.41
2:B:582:TRP:HZ2	18:B:9012:CLA:CBB	2.33	0.41
2:B:59:LEU:HD23	2:B:59:LEU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:HIS:N	3:C:71:HIS:ND1	2.48	0.41
9:I:4:LEU:HB2	9:I:5:PRO:HA	2.02	0.41
12:L:136:TRP:O	12:L:138:LYS:HD2	2.21	0.41
12:L:146:GLY:O	12:L:150:GLY:N	2.52	0.41
18:L:1503:CLA:O1A	18:L:1503:CLA:O1D	2.37	0.41
12:L:70:LYS:CG	12:L:75:ARG:HG3	2.38	0.41
14:1:150:ASN:HA	14:1:153:LEU:HD23	2.03	0.41
14:1:47:CYS:O	14:1:151:GLY:HA2	2.21	0.41
15:2:44:ASN:HD22	15:2:47:ALA:HB2	1.84	0.41
15:2:97:VAL:CG2	15:2:98:GLU:N	2.83	0.41
16:3:133:TRP:CD1	16:3:137:GLY:HA3	2.55	0.41
17:4:126:LEU:HD12	17:4:126:LEU:N	2.36	0.41
17:4:60:LEU:CD1	17:4:76:TYR:OH	2.69	0.41
1:A:127:VAL:HG12	10:J:30:ASN:ND2	2.36	0.41
1:A:242:ILE:HG23	1:A:242:ILE:O	2.21	0.41
1:A:292:GLY:O	1:A:294:LEU:N	2.54	0.41
1:A:367:SER:O	1:A:371:VAL:N	2.48	0.41
1:A:413:HIS:HA	1:A:416:ILE:HD11	2.01	0.41
1:A:452:PHE:C	1:A:452:PHE:CD2	2.94	0.41
1:A:50:THR:HA	1:A:721:GLN:N	2.35	0.41
1:A:660:GLN:HG2	1:A:753:ARG:NE	2.36	0.41
19:A:5001:PQN:C21	18:B:1138:CLA:HBC1	2.42	0.41
2:B:429:LEU:HB3	2:B:525:LEU:HB2	2.02	0.41
2:B:595:HIS:O	2:B:599:ILE:CG2	2.69	0.41
2:B:84:VAL:O	2:B:85:ARG:CZ	2.68	0.41
3:C:12:ILE:HG22	3:C:13:GLY:CA	2.44	0.41
4:D:41:GLN:OE1	4:D:42:VAL:N	2.54	0.41
1:A:428:TYR:CZ	4:D:57:ILE:HG21	2.56	0.41
4:D:88:THR:O	4:D:91:ARG:CB	2.68	0.41
8:H:22:ASP:O	8:H:24:TYR:N	2.52	0.41
10:J:11:ALA:O	10:J:14:LEU:HD13	2.20	0.41
10:J:14:LEU:N	10:J:14:LEU:HD12	2.36	0.41
2:B:691:ILE:HG22	12:L:102:TYR:HE1	1.84	0.41
12:L:53:GLY:HA2	12:L:56:VAL:HG13	2.01	0.41
20:L:6020:BCR:H24C	20:L:6020:BCR:H371	1.78	0.41
13:N:36:GLU:CB	13:N:37:PHE:CA	2.74	0.41
13:N:51:ASP:CG	13:N:52:LEU:HG	2.40	0.41
14:1:84:TYR:OH	14:1:91:TRP:C	2.58	0.41
15:2:162:LYS:HG3	15:2:163:GLU:N	2.35	0.41
15:2:177:ALA:O	15:2:178:TRP:HB2	2.21	0.41
15:2:186:THR:HB	15:2:187:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:92:THR:C	15:2:94:LEU:CB	2.88	0.41
1:A:236:GLY:O	1:A:237:VAL:C	2.58	0.41
1:A:308:ILE:HA	1:A:311:LEU:CB	2.49	0.41
1:A:35:ALA:HB1	1:A:36:LYS:O	2.20	0.41
1:A:641:ASN:OD1	1:A:642:PHE:CB	2.66	0.41
1:A:668:TYR:O	1:A:670:SER:OG	2.33	0.41
1:A:718:PRO:O	1:A:719:ALA:CB	2.68	0.41
1:A:675:TYR:CZ	1:A:751:LEU:HD11	2.54	0.41
2:B:341:LEU:HD11	18:B:1225:CLA:HMC1	2.01	0.41
2:B:193:HIS:HE1	18:B:1211:CLA:C4D	2.33	0.41
2:B:267:SER:HA	2:B:356:PRO:HG2	2.02	0.41
2:B:289:LEU:HD23	18:B:1217:CLA:HMA3	2.02	0.41
2:B:301:ILE:C	2:B:304:ILE:HB	2.41	0.41
2:B:373:THR:O	2:B:374:HIS:C	2.59	0.41
2:B:410:ARG:O	2:B:411:MET:C	2.59	0.41
2:B:479:SER:O	2:B:480:SER:C	2.59	0.41
2:B:551:LYS:HG3	4:D:141:VAL:N	2.36	0.41
2:B:557:PHE:CB	3:C:68:TYR:CE2	3.03	0.41
2:B:55:ALA:O	2:B:58:PHE:HB2	2.20	0.41
2:B:594:TRP:N	2:B:596:TRP:O	2.54	0.41
2:B:518:LEU:HD23	2:B:614:THR:HG22	1.97	0.41
2:B:83:HIS:HB3	2:B:84:VAL:CA	2.42	0.41
2:B:84:VAL:CG1	2:B:86:PRO:HD3	2.43	0.41
3:C:63:LEU:CD2	3:C:66:ARG:CG	2.98	0.41
4:D:50:TRP:O	4:D:73:ASN:CB	2.69	0.41
6:F:116:GLN:O	6:F:118:GLU:N	2.36	0.41
7:G:12:THR:HG22	7:G:16:LEU:CD1	2.50	0.41
10:J:16:THR:OG1	10:J:17:LEU:N	2.53	0.41
12:L:125:LYS:O	12:L:125:LYS:HG2	2.19	0.41
12:L:17:ASP:HA	12:L:18:PRO:HD2	1.57	0.41
15:2:178:TRP:CB	15:2:183:TYR:HH	2.32	0.41
15:2:94:LEU:O	15:2:96:ILE:N	2.54	0.41
17:4:109:ILE:HA	17:4:120:ILE:HD13	2.02	0.41
17:4:136:GLY:HA3	17:4:139:ASN:CA	2.49	0.41
17:4:56:ALA:HA	17:4:59:LEU:HD13	2.01	0.41
1:A:108:ALA:HB1	1:A:138:GLY:O	2.20	0.41
1:A:602:LEU:O	1:A:603:PHE:C	2.59	0.41
1:A:663:GLN:CA	1:A:663:GLN:OE1	2.69	0.41
1:A:694:PHE:HZ	2:B:661:PHE:CE2	2.39	0.41
1:A:697:ARG:NH2	1:A:701:GLN:HB2	2.35	0.41
2:B:20:ARG:HH22	9:I:28:VAL:CB	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:PRO:CG	2:B:538:ALA:HA	2.50	0.41
2:B:455:ILE:HG13	2:B:455:ILE:O	2.20	0.41
2:B:517:PHE:O	2:B:521:HIS:HB2	2.20	0.41
2:B:51:PHE:HB2	2:B:52:GLY:H	1.60	0.41
2:B:697:PRO:HB3	18:B:1238:CLA:CMC	2.51	0.41
2:B:577:TYR:CE1	2:B:706:ARG:HB2	2.56	0.41
2:B:729:THR:O	2:B:730:SER:HB2	2.21	0.41
2:B:91:ILE:HG12	2:B:114:ASN:HD21	1.85	0.41
3:C:55:GLU:HG3	3:C:64:SER:HB2	2.02	0.41
6:F:47:GLU:HA	6:F:51:LYS:CB	2.51	0.41
18:B:1228:CLA:C1B	20:F:6016:BCR:H341	2.50	0.41
6:F:78:ARG:HE	6:F:78:ARG:HB2	1.58	0.41
17:4:105:ARG:HG3	17:4:105:ARG:H	1.72	0.41
18:A:1135:CLA:HBA1	18:A:1135:CLA:H3A	1.63	0.41
1:A:186:TYR:HA	1:A:189:ALA:O	2.20	0.41
1:A:192:LYS:CB	1:A:195:TRP:HE1	2.34	0.41
1:A:200:GLU:HB2	1:A:318:ARG:HD2	2.02	0.41
1:A:204:ASN:ND2	1:A:317:TYR:CE1	2.89	0.41
1:A:451:ILE:C	1:A:455:PHE:HB3	2.41	0.41
1:A:690:LEU:H	1:A:690:LEU:CD1	2.30	0.41
1:A:721:GLN:O	1:A:723:ARG:N	2.53	0.41
1:A:86:LEU:C	1:A:88:ILE:N	2.74	0.41
2:B:144:PHE:C	2:B:145:LEU:HD22	2.41	0.41
2:B:349:ALA:O	2:B:372:TYR:CE1	2.74	0.41
2:B:393:PHE:CE2	2:B:394:PHE:CD1	3.08	0.41
2:B:415:LYS:HB2	2:B:539:LEU:CD2	2.49	0.41
2:B:463:ILE:CG2	2:B:464:GLN:H	2.34	0.41
2:B:666:SER:O	19:B:5002:PQN:C9	2.68	0.41
1:A:568:LEU:HD22	4:D:79:ARG:CZ	2.51	0.41
6:F:90:PHE:O	6:F:91:LEU:C	2.59	0.41
7:G:34:GLN:HB3	7:G:36:PRO:CD	2.51	0.41
13:N:32:ALA:O	13:N:35:VAL:HB	2.21	0.41
14:1:54:VAL:N	14:1:55:PRO:HD2	2.35	0.41
14:1:97:ILE:HG23	14:1:98:LEU:N	2.36	0.41
15:2:33:GLY:H	15:2:35:SER:CB	2.31	0.41
16:3:84:LEU:HG	16:3:85:ILE:CA	2.43	0.41
1:A:121:GLN:HE21	18:A:1107:CLA:CED	2.34	0.41
1:A:212:GLY:C	1:A:214:GLY:N	2.68	0.41
1:A:502:THR:OG1	1:A:503:THR:N	2.54	0.41
1:A:733:VAL:HG22	1:A:737:HIS:CE1	2.56	0.41
1:A:749:PHE:CD2	1:A:750:PHE:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:1235:CLA:HBC3	18:B:1235:CLA:HHD	2.03	0.41
2:B:142:LEU:HA	2:B:142:LEU:HD13	1.50	0.41
2:B:216:LEU:H	2:B:217:PRO:CD	2.34	0.41
2:B:373:THR:O	2:B:377:TYR:N	2.52	0.41
2:B:453:ILE:O	2:B:455:ILE:N	2.54	0.41
2:B:47:PHE:O	2:B:48:ALA:C	2.58	0.41
2:B:591:THR:O	2:B:721:TYR:OH	2.36	0.41
18:A:9011:CLA:HMB3	18:B:9012:CLA:HMD1	2.03	0.41
4:D:47:VAL:HG12	4:D:48:ILE:N	2.36	0.41
5:E:32:ARG:NH2	5:E:54:ALA:HB2	2.36	0.41
6:F:31:LEU:C	6:F:32:TYR:HD2	2.24	0.41
7:G:6:LEU:HA	7:G:6:LEU:HD23	1.76	0.41
7:G:91:ASN:HD22	7:G:91:ASN:HA	1.55	0.41
8:H:85:GLN:CD	8:H:86:PRO:HD2	2.41	0.41
9:I:25:PHE:HD2	9:I:25:PHE:O	1.95	0.41
9:I:28:VAL:HB	9:I:29:GLU:H	1.47	0.41
18:J:2107:CLA:HBA2	18:J:2107:CLA:H91	2.03	0.41
10:J:24:GLY:O	10:J:26:LEU:N	2.54	0.41
12:L:10:VAL:O	12:L:11:ILE:O	2.37	0.41
18:L:1504:CLA:H52	18:L:1504:CLA:H12	1.94	0.41
14:1:173:PRO:C	14:1:175:GLU:H	2.23	0.41
14:1:52:LEU:HA	14:1:55:PRO:HG3	2.01	0.41
14:1:94:LEU:CB	14:1:95:PRO:HD2	2.46	0.41
15:2:192:LEU:N	15:2:195:HIS:CE1	2.86	0.41
15:2:62:ILE:HG13	18:2:2006:CLA:C2B	2.50	0.41
16:3:121:LEU:O	16:3:125:ALA:HB2	2.21	0.41
17:4:190:TRP:HB3	17:4:191:HIS:H	1.59	0.41
18:A:1129:CLA:CBD	18:A:1129:CLA:HAA2	2.45	0.41
18:A:1131:CLA:OBD	18:A:1131:CLA:HED3	2.21	0.41
1:A:158:ILE:O	1:A:159:THR:HG23	2.21	0.41
1:A:204:ASN:HD21	1:A:316:MET:H	1.69	0.41
1:A:205:HIS:O	1:A:208:ALA:C	2.60	0.41
1:A:241:GLU:HG3	1:A:241:GLU:H	1.73	0.41
1:A:492:ILE:H	1:A:493:GLN:CA	2.32	0.41
1:A:725:LEU:HD22	19:A:5001:PQN:C5	2.48	0.41
2:B:57:ILE:HG23	18:B:1203:CLA:HMC2	2.03	0.41
2:B:78:VAL:HB	2:B:130:ARG:HG2	2.02	0.41
2:B:421:HIS:N	2:B:423:SER:OG	2.54	0.41
2:B:42:LEU:HA	2:B:45:ASN:HD22	1.86	0.41
2:B:462:TRP:C	2:B:463:ILE:O	2.59	0.41
2:B:632:ILE:HD12	2:B:647:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LEU:O	2:B:68:VAL:N	2.54	0.41
2:B:89:HIS:O	2:B:90:ALA:HB2	2.18	0.41
3:C:42:ALA:HB1	3:C:45:THR:HG23	1.98	0.41
1:A:715:LYS:O	6:F:106:ILE:HD11	2.20	0.41
8:H:58:ILE:CD1	8:H:58:ILE:C	2.82	0.41
9:I:5:PRO:C	9:I:7:LEU:N	2.74	0.41
10:J:26:LEU:CA	10:J:29:ILE:HG22	2.51	0.41
13:N:16:LEU:O	13:N:20:LYS:HB2	2.21	0.41
13:N:36:GLU:CB	13:N:37:PHE:CD2	3.04	0.41
14:1:155:LEU:O	14:1:158:PHE:N	2.50	0.41
15:2:17:GLU:CD	15:2:18:TRP:H	2.18	0.41
15:2:189:ILE:HG13	15:2:190:ASP:N	2.34	0.41
15:2:18:TRP:C	15:2:20:ASP:C	2.79	0.41
15:2:27:PHE:HD1	15:2:28:GLY:HA2	1.80	0.41
15:2:27:PHE:HB2	15:2:28:GLY:CA	2.45	0.41
16:3:62:ASN:N	16:3:62:ASN:OD1	2.42	0.41
13:N:58:VAL:HB	16:3:86:PRO:HA	2.01	0.41
17:4:90:LEU:HD23	17:4:94:GLU:OE1	2.21	0.41
1:A:157:GLY:O	1:A:159:THR:N	2.54	0.41
1:A:186:TYR:CA	1:A:189:ALA:O	2.69	0.41
1:A:213:LEU:C	1:A:213:LEU:HD13	2.41	0.41
1:A:287:LEU:HB2	1:A:294:LEU:HA	2.03	0.41
1:A:326:GLY:O	1:A:329:ASP:N	2.54	0.41
1:A:675:TYR:CE2	18:A:1106:CLA:CBC	3.01	0.41
18:B:1214:CLA:HBA1	18:B:1214:CLA:CBD	2.51	0.41
18:B:1228:CLA:H12	18:B:1228:CLA:HBD	2.02	0.41
2:B:460:ALA:CB	18:B:1234:CLA:HAA2	2.51	0.41
2:B:656:VAL:O	2:B:712:HIS:O	2.39	0.41
2:B:657:TRP:O	2:B:659:THR:N	2.54	0.41
2:B:548:PRO:HD2	3:C:63:LEU:H	1.86	0.41
4:D:146:VAL:O	4:D:147:LYS:C	2.59	0.41
4:D:87:GLY:O	4:D:90:LEU:HB2	2.20	0.41
6:F:105:LEU:HA	6:F:105:LEU:HD12	1.65	0.41
6:F:29:LEU:C	6:F:31:LEU:N	2.75	0.41
6:F:83:PHE:O	6:F:87:GLY:N	2.54	0.41
8:H:91:PRO:HA	8:H:92:ARG:HA	1.90	0.41
12:L:108:LYS:C	12:L:109:GLU:OE2	2.60	0.41
12:L:44:ARG:O	12:L:45:THR:CB	2.69	0.41
12:L:48:ASN:OD1	12:L:48:ASN:C	2.58	0.41
13:N:81:VAL:HB	13:N:83:TRP:CA	2.19	0.41
14:1:54:VAL:N	14:1:55:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:17:GLU:OE2	15:2:17:GLU:CA	2.69	0.40
15:2:59:ALA:C	15:2:61:GLY:N	2.71	0.40
18:A:1107:CLA:H43	18:A:1107:CLA:CGA	2.51	0.40
18:A:1129:CLA:H51	18:A:1129:CLA:H12	1.82	0.40
1:A:223:VAL:HG23	1:A:224:HIS:H	1.86	0.40
1:A:568:LEU:HA	4:D:79:ARG:CZ	2.51	0.40
1:A:582:ASP:CG	1:A:583:GLY:N	2.72	0.40
1:A:621:GLN:NE2	1:A:625:TRP:CZ3	2.89	0.40
2:B:115:ASN:HB3	2:B:117:TYR:CE1	2.55	0.40
2:B:561:GLY:HA2	21:B:3101:SF4:S2	2.60	0.40
2:B:317:ARG:HA	2:B:410:ARG:CZ	2.51	0.40
2:B:399:ASN:CG	2:B:402:GLN:HB2	2.42	0.40
2:B:409:ALA:O	2:B:412:LEU:HB2	2.22	0.40
2:B:465:SER:O	2:B:479:SER:HB2	2.21	0.40
2:B:523:ILE:HB	2:B:590:VAL:CG2	2.52	0.40
2:B:616:LEU:C	2:B:618:GLY:N	2.74	0.40
2:B:99:PRO:HB3	2:B:102:GLU:HB3	2.03	0.40
3:C:50:GLY:C	3:C:52:LYS:N	2.68	0.40
1:A:570:PRO:HD3	4:D:79:ARG:HH22	1.85	0.40
12:L:155:CYS:O	12:L:156:PHE:C	2.59	0.40
14:1:188:ASN:CB	14:1:190:GLY:N	2.81	0.40
14:1:57:ILE:O	14:1:58:LEU:C	2.60	0.40
15:2:163:GLU:HG2	15:2:166:ASN:HB3	2.02	0.40
17:4:158:ARG:HA	17:4:158:ARG:NE	2.36	0.40
1:A:208:ALA:O	1:A:212:GLY:N	2.52	0.40
1:A:557:LEU:HG	1:A:561:LEU:CD1	2.50	0.40
1:A:57:LEU:C	1:A:59:ALA:N	2.75	0.40
1:A:649:ILE:CG2	1:A:650:ASN:N	2.83	0.40
1:A:701:GLN:O	1:A:703:LEU:N	2.54	0.40
1:A:83:PHE:HD2	1:A:83:PHE:HA	1.77	0.40
18:B:1214:CLA:H43	18:B:1214:CLA:HHD	2.02	0.40
18:B:1235:CLA:O1A	18:B:1235:CLA:HBD	2.21	0.40
2:B:429:LEU:HD21	18:B:1235:CLA:HMB3	2.02	0.40
2:B:525:LEU:CG	2:B:526:GLY:N	2.83	0.40
2:B:539:LEU:HD12	2:B:539:LEU:C	2.40	0.40
2:B:78:VAL:HA	2:B:130:ARG:NH2	2.33	0.40
3:C:27:GLU:HB2	4:D:127:ARG:CD	2.41	0.40
3:C:41:SER:OG	4:D:132:LEU:HD23	2.15	0.40
2:B:672:GLN:HE21	3:C:79:LEU:HD22	1.86	0.40
4:D:61:PRO:O	4:D:62:THR:C	2.59	0.40
4:D:54:LYS:O	4:D:68:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:PRO:HD2	4:D:73:ASN:OD1	2.21	0.40
6:F:2:ILE:N	6:F:62:LEU:HD22	2.35	0.40
6:F:59:TYR:HD1	6:F:59:TYR:N	2.19	0.40
7:G:63:PRO:CG	18:G:1248:CLA:C3C	2.99	0.40
9:I:20:ALA:C	9:I:22:ALA:H	2.24	0.40
12:L:158:MET:O	12:L:159:TYR:CG	2.74	0.40
12:L:67:PRO:HA	12:L:71:ALA:HB3	2.03	0.40
15:2:178:TRP:CB	15:2:183:TYR:HE2	2.29	0.40
16:3:209:PRO:HD2	16:3:210:TYR:CD1	2.56	0.40
14:1:9:PRO:C	17:4:110:LYS:HD2	2.39	0.40
18:A:1136:CLA:H71	18:A:1137:CLA:CAC	2.20	0.40
1:A:247:GLU:O	1:A:248:PHE:CG	2.74	0.40
1:A:505:PRO:HD3	18:A:1134:CLA:CHA	2.51	0.40
1:A:562:PHE:CB	1:A:566:SER:OG	2.70	0.40
1:A:600:LEU:O	1:A:601:GLY:C	2.60	0.40
1:A:697:ARG:NE	1:A:725:LEU:O	2.53	0.40
18:B:1218:CLA:H52	18:B:1218:CLA:H11	1.90	0.40
18:B:1214:CLA:CBA	18:B:1223:CLA:C3B	2.99	0.40
2:B:422:LEU:N	18:B:1236:CLA:HBB2	2.37	0.40
2:B:20:ARG:NH2	9:I:28:VAL:CA	2.78	0.40
2:B:392:ILE:HA	2:B:392:ILE:HD13	1.55	0.40
2:B:453:ILE:HA	2:B:453:ILE:HD12	1.96	0.40
2:B:561:GLY:O	2:B:563:GLY:N	2.54	0.40
2:B:592:PHE:C	2:B:593:TYR:O	2.59	0.40
2:B:596:TRP:HH2	2:B:612:SER:HB2	1.87	0.40
2:B:596:TRP:CE2	2:B:623:TYR:HB2	2.56	0.40
2:B:654:HIS:O	18:B:9022:CLA:HAA2	2.22	0.40
2:B:85:ARG:HA	2:B:85:ARG:NH1	2.37	0.40
2:B:98:GLN:HE22	8:H:80:THR:CG2	2.35	0.40
5:E:32:ARG:NE	5:E:53:VAL:O	2.39	0.40
6:F:4:GLY:N	6:F:5:LEU:HB2	2.36	0.40
6:F:79:HIS:O	6:F:81:GLY:CA	2.65	0.40
7:G:85:ILE:HA	7:G:86:LEU:O	2.20	0.40
18:I:1204:CLA:O1D	18:I:1204:CLA:H2A	2.22	0.40
8:H:30:SER:HB2	12:L:35:TRP:CZ2	2.57	0.40
12:L:55:GLU:HG3	12:L:56:VAL:N	2.36	0.40
13:N:8:GLU:CG	13:N:11:LYS:CB	2.94	0.40
14:1:52:LEU:HA	14:1:55:PRO:HD3	1.98	0.40
16:3:64:ARG:HD3	16:3:65:PHE:CE2	2.56	0.40
17:4:40:PHE:HD1	17:4:40:PHE:HA	1.66	0.40
18:A:1108:CLA:CBC	18:A:1110:CLA:C2C	2.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASP:HB2	18:A:1128:CLA:HAA1	2.04	0.40
1:A:341:GLN:NE2	1:A:344:LYS:CD	2.84	0.40
1:A:376:MET:HB2	1:A:376:MET:HE2	1.94	0.40
1:A:502:THR:O	1:A:505:PRO:O	2.39	0.40
1:A:52:THR:HA	1:A:55:TRP:NE1	2.36	0.40
1:A:596:ASP:HA	1:A:599:PHE:HB3	2.04	0.40
1:A:712:ASN:O	1:A:715:LYS:CA	2.69	0.40
1:A:80:SER:O	1:A:83:PHE:CD1	2.75	0.40
2:B:74:PHE:CD1	2:B:121:TYR:CZ	2.98	0.40
2:B:36:ASP:O	2:B:41:ARG:CD	2.69	0.40
2:B:474:PHE:CD2	2:B:476:ILE:HG12	2.57	0.40
2:B:493:TRP:HE1	18:B:1232:CLA:HBB2	1.87	0.40
19:B:5002:PQN:H141	19:B:5002:PQN:H161	1.87	0.40
3:C:48:CYS:HA	3:C:49:VAL:CB	2.52	0.40
6:F:109:ARG:HH12	6:F:153:ASN:ND2	2.20	0.40
6:F:6:THR:C	6:F:8:CYS:H	2.25	0.40
7:G:43:HIS:O	7:G:48:ASP:CG	2.60	0.40
7:G:57:LEU:HD23	7:G:57:LEU:H	1.87	0.40
13:N:71:GLY:HA3	13:N:76:LYS:HB3	2.03	0.40
14:1:111:GLN:CD	14:1:111:GLN:C	2.80	0.40
15:2:157:LYS:C	15:2:160:ARG:H	2.24	0.40
15:2:47:ALA:HA	15:2:50:VAL:HG12	2.02	0.40
1:A:177:LEU:HA	1:A:180:PHE:HB3	2.03	0.40
1:A:204:ASN:HA	1:A:204:ASN:HD22	1.57	0.40
1:A:258:LEU:CG	1:A:259:TYR:H	2.35	0.40
1:A:42:ARG:HG2	1:A:43:THR:N	2.35	0.40
1:A:526:LYS:N	1:A:627:THR:O	2.55	0.40
2:B:421:HIS:NE2	18:B:1228:CLA:C1B	2.85	0.40
2:B:69:ALA:HB1	2:B:132:ASN:HB3	2.04	0.40
2:B:199:ILE:HG13	2:B:254:ILE:HD12	2.04	0.40
2:B:309:ILE:N	2:B:310:PRO:CD	2.85	0.40
2:B:372:TYR:HD2	2:B:373:THR:CA	2.35	0.40
2:B:576:PHE:C	2:B:576:PHE:CD2	2.94	0.40
3:C:70:TRP:O	3:C:72:GLU:HB2	2.21	0.40
4:D:50:TRP:CZ3	4:D:86:LEU:HD21	2.56	0.40
5:E:45:TRP:CE3	5:E:45:TRP:C	2.95	0.40
6:F:14:PHE:CG	6:F:15:ALA:N	2.89	0.40
6:F:16:LYS:C	6:F:18:GLU:N	2.74	0.40
6:F:60:GLY:C	6:F:62:LEU:H	2.23	0.40
9:I:11:LEU:HB3	9:I:12:VAL:H	1.46	0.40
12:L:108:LYS:H	12:L:133:ALA:HB3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:12:THR:C	13:N:14:LYS:N	2.74	0.40
13:N:36:GLU:HB3	13:N:37:PHE:CB	2.50	0.40
13:N:70:GLU:CD	13:N:76:LYS:HD2	2.42	0.40

All (2) 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)
12:L:161:LEU:O	17:4:141:LEU:O[1_655]	1.55	0.65
14:1:71:ALA:CB	15:2:30:ASP:OD1[1_556]	1.96	0.24

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	726/754 (96%)	290 (40%)	201 (28%)	235 (32%)	0	0
2	B	730/732 (100%)	290 (40%)	209 (29%)	231 (32%)	0	0
3	C	78/80 (98%)	20 (26%)	23 (30%)	35 (45%)	0	0
4	D	136/138 (99%)	50 (37%)	28 (21%)	58 (43%)	0	0
5	E	60/62 (97%)	28 (47%)	13 (22%)	19 (32%)	0	0
6	F	152/154 (99%)	59 (39%)	40 (26%)	53 (35%)	0	0
7	G	93/95 (98%)	40 (43%)	22 (24%)	31 (33%)	0	0
8	H	73/75 (97%)	21 (29%)	18 (25%)	34 (47%)	0	0
9	I	28/30 (93%)	9 (32%)	11 (39%)	8 (29%)	0	0
10	J	40/42 (95%)	16 (40%)	14 (35%)	10 (25%)	0	0
12	L	162/164 (99%)	64 (40%)	40 (25%)	58 (36%)	0	0
13	N	83/85 (98%)	26 (31%)	26 (31%)	31 (37%)	0	0
14	1	171/187 (91%)	74 (43%)	43 (25%)	54 (32%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2	162/186 (87%)	72 (44%)	46 (28%)	44 (27%)	0	0
16	3	109/165 (66%)	49 (45%)	36 (33%)	24 (22%)	0	0
17	4	163/165 (99%)	69 (42%)	48 (29%)	46 (28%)	0	0
All	All	2966/3114 (95%)	1177 (40%)	818 (28%)	971 (33%)	0	0

All (971) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	48	PRO
1	A	51	THR
1	A	52	THR
1	A	61	ALA
1	A	63	ASP
1	A	65	ASP
1	A	70	ASP
1	A	81	ALA
1	A	92	TRP
1	A	93	LEU
1	A	108	ALA
1	A	113	PRO
1	A	118	PRO
1	A	130	GLU
1	A	134	GLY
1	A	136	VAL
1	A	147	SER
1	A	148	GLY
1	A	158	ILE
1	A	159	THR
1	A	160	SER
1	A	162	LEU
1	A	174	PHE
1	A	186	TYR
1	A	189	ALA
1	A	192	LYS
1	A	198	ASP
1	A	207	LEU
1	A	208	ALA
1	A	215	SER
1	A	229	ILE
1	A	236	GLY

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Mol	Chain	Res	Type
1	A	237	VAL
1	A	238	ASP
1	A	239	PRO
1	A	246	HIS
1	A	249	ILE
1	A	253	ASP
1	A	261	SER
1	A	262	PHE
1	A	278	ALA
1	A	283	PHE
1	A	286	GLY
1	A	294	LEU
1	A	329	ASP
1	A	347	TYR
1	A	374	GLN
1	A	384	TYR
1	A	394	SER
1	A	396	PHE
1	A	398	HIS
1	A	399	HIS
1	A	417	PHE
1	A	423	ASP
1	A	424	PRO
1	A	432	LEU
1	A	439	ARG
1	A	455	PHE
1	A	462	ILE
1	A	491	TRP
1	A	492	ILE
1	A	494	ASN
1	A	495	THR
1	A	505	PRO
1	A	511	THR
1	A	519	ASP
1	A	522	ALA
1	A	523	VAL
1	A	524	GLY
1	A	525	ASN
1	A	542	HIS
1	A	548	THR
1	A	551	VAL
1	A	563	ALA

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Mol	Chain	Res	Type
1	A	567	ARG
1	A	571	ASP
1	A	573	ALA
1	A	579	PHE
1	A	580	PRO
1	A	618	TRP
1	A	621	GLN
1	A	622	SER
1	A	628	ILE
1	A	641	ASN
1	A	642	PHE
1	A	651	GLY
1	A	658	TRP
1	A	667	SER
1	A	680	LEU
1	A	688	PHE
1	A	700	TRP
1	A	702	GLU
1	A	706	SER
1	A	714	LEU
1	A	715	LYS
1	A	717	ALA
1	A	725	LEU
1	A	727	ILE
1	A	751	LEU
1	A	752	ALA
1	A	756	ALA
2	B	6	PRO
2	B	18	THR
2	B	20	ARG
2	B	26	ALA
2	B	27	THR
2	B	36	ASP
2	B	41	ARG
2	B	52	GLY
2	B	64	ASN
2	B	90	ALA
2	B	99	PRO
2	B	101	VAL
2	B	105	THR
2	B	109	ALA
2	B	120	VAL

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Mol	Chain	Res	Type
2	B	121	TYR
2	B	125	TYR
2	B	148	ILE
2	B	160	LYS
2	B	167	TRP
2	B	175	LEU
2	B	187	SER
2	B	188	LEU
2	B	195	VAL
2	B	206	TYR
2	B	210	ASN
2	B	226	LEU
2	B	248	GLN
2	B	252	THR
2	B	254	ILE
2	B	255	LEU
2	B	257	ILE
2	B	261	PHE
2	B	262	HIS
2	B	278	LEU
2	B	281	ALA
2	B	285	LEU
2	B	295	PHE
2	B	302	LYS
2	B	306	GLU
2	B	323	TYR
2	B	332	PHE
2	B	334	LEU
2	B	343	VAL
2	B	356	PRO
2	B	359	ALA
2	B	370	ALA
2	B	371	LEU
2	B	374	HIS
2	B	381	PHE
2	B	392	ILE
2	B	396	ARG
2	B	407	VAL
2	B	416	GLU
2	B	423	SER
2	B	428	PHE
2	B	441	ASP

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Mol	Chain	Res	Type
2	B	445	ALA
2	B	454	LEU
2	B	461	GLN
2	B	463	ILE
2	B	490	ARG
2	B	507	SER
2	B	510	LEU
2	B	512	ILE
2	B	522	ALA
2	B	527	LEU
2	B	528	HIS
2	B	532	LEU
2	B	559	CYS
2	B	562	PRO
2	B	565	GLY
2	B	569	ASP
2	B	590	VAL
2	B	598	HIS
2	B	612	SER
2	B	614	THR
2	B	615	TYR
2	B	628	SER
2	B	629	SER
2	B	635	ILE
2	B	637	PRO
2	B	656	VAL
2	B	657	TRP
2	B	658	ALA
2	B	664	LEU
2	B	667	TRP
2	B	677	THR
2	B	680	TRP
2	B	684	ARG
2	B	704	GLN
2	B	705	ALA
2	B	711	VAL
2	B	713	PHE
2	B	714	SER
2	B	725	LEU
2	B	728	SER
2	B	730	SER
3	C	10	THR

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Mol	Chain	Res	Type
3	C	11	CYS
3	C	12	ILE
3	C	18	VAL
3	C	22	PRO
3	C	31	TRP
3	C	37	LYS
3	C	43	PRO
3	C	45	THR
3	C	52	LYS
3	C	58	CYS
3	C	65	VAL
3	C	67	VAL
3	C	68	TYR
3	C	70	TRP
3	C	80	ALA
4	D	22	PRO
4	D	23	ASN
4	D	26	SER
4	D	27	PRO
4	D	33	THR
4	D	38	ARG
4	D	42	VAL
4	D	43	GLU
4	D	56	GLN
4	D	64	GLY
4	D	72	PRO
4	D	83	CYS
4	D	103	VAL
4	D	104	PHE
4	D	107	GLY
4	D	108	GLU
4	D	120	PRO
4	D	124	ASN
4	D	125	PRO
4	D	138	GLY
4	D	141	VAL
4	D	147	LYS
4	D	152	GLN
5	E	35	LYS
5	E	43	SER
5	E	46	PHE
5	E	53	VAL

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Mol	Chain	Res	Type
5	E	76	ASN
5	E	80	ASN
5	E	83	ALA
5	E	84	LEU
5	E	87	VAL
6	F	5	LEU
6	F	14	PHE
6	F	19	LYS
6	F	23	LYS
6	F	34	ASP
6	F	40	LEU
6	F	53	PHE
6	F	58	LYS
6	F	77	GLN
6	F	80	TRP
6	F	106	ILE
6	F	112	LYS
6	F	115	THR
6	F	116	GLN
6	F	117	LYS
6	F	126	ALA
6	F	128	SER
6	F	131	PHE
6	F	136	TRP
6	F	138	VAL
7	G	9	SER
7	G	10	LEU
7	G	23	PHE
7	G	24	PHE
7	G	37	GLU
7	G	38	GLN
7	G	48	ASP
7	G	79	HIS
7	G	81	VAL
7	G	84	TYR
7	G	93	TYR
7	G	96	SER
8	H	23	VAL
8	H	27	ASP
8	H	28	ALA
8	H	35	LEU
8	H	50	ARG

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Mol	Chain	Res	Type
8	H	53	LEU
8	H	58	ILE
8	H	64	LEU
8	H	66	THR
8	H	67	TYR
8	H	77	LEU
8	H	83	PRO
8	H	87	PRO
8	H	88	LYS
9	I	3	ASN
9	I	4	LEU
9	I	12	VAL
9	I	27	HIS
9	I	28	VAL
10	J	4	PHE
10	J	8	LEU
10	J	11	ALA
10	J	17	LEU
10	J	25	LEU
10	J	26	LEU
12	L	11	ILE
12	L	23	LEU
12	L	33	ILE
12	L	35	TRP
12	L	36	TYR
12	L	37	LEU
12	L	41	PRO
12	L	42	ALA
12	L	49	PRO
12	L	50	LEU
12	L	65	VAL
12	L	69	VAL
12	L	73	PRO
12	L	80	ALA
12	L	93	VAL
12	L	98	CYS
12	L	103	GLY
12	L	114	ILE
12	L	117	ALA
12	L	124	LYS
12	L	127	PRO
12	L	128	ASP

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Mol	Chain	Res	Type
12	L	138	LYS
12	L	161	LEU
13	N	4	GLU
13	N	5	GLU
13	N	20	LYS
13	N	41	LYS
13	N	42	PHE
13	N	45	ASN
13	N	53	ALA
13	N	58	VAL
13	N	59	PRO
13	N	61	LEU
13	N	65	LEU
13	N	67	LEU
13	N	72	LYS
13	N	74	LYS
13	N	77	CYS
13	N	83	TRP
14	1	6	PRO
14	1	8	GLU
14	1	9	PRO
14	1	10	ARG
14	1	11	PRO
14	1	15	ASP
14	1	18	ALA
14	1	26	PRO
14	1	38	ARG
14	1	39	TYR
14	1	40	LYS
14	1	41	GLU
14	1	43	GLU
14	1	63	LEU
14	1	70	LYS
14	1	73	GLU
14	1	74	TRP
14	1	77	LEU
14	1	84	TYR
14	1	89	VAL
14	1	90	PRO
14	1	94	LEU
14	1	102	PHE
14	1	118	PRO

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Mol	Chain	Res	Type
14	1	123	TYR
14	1	124	PRO
14	1	146	LYS
14	1	147	GLU
14	1	178	ALA
14	1	186	HIS
15	2	18	TRP
15	2	19	LEU
15	2	22	SER
15	2	29	PHE
15	2	30	ASP
15	2	31	PRO
15	2	37	ASP
15	2	38	PRO
15	2	39	GLU
15	2	41	LEU
15	2	43	TRP
15	2	76	THR
15	2	90	ASP
15	2	116	PRO
15	2	142	TRP
15	2	148	TRP
15	2	153	PRO
15	2	179	PHE
15	2	181	HIS
15	2	186	THR
15	2	191	ASN
15	2	194	ALA
16	3	83	GLY
16	3	87	ALA
16	3	88	GLU
16	3	110	ASP
16	3	133	TRP
16	3	135	ASN
16	3	144	PHE
16	3	213	LEU
16	3	215	ASP
17	4	36	ASN
17	4	38	ARG
17	4	41	VAL
17	4	64	PHE
17	4	67	ILE

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Mol	Chain	Res	Type
17	4	69	ILE
17	4	75	TRP
17	4	82	GLU
17	4	91	PHE
17	4	109	ILE
17	4	110	LYS
17	4	114	SER
17	4	115	VAL
17	4	125	SER
17	4	127	PRO
17	4	129	GLY
17	4	142	ASN
17	4	143	PHE
17	4	144	ALA
17	4	148	GLU
17	4	152	LYS
17	4	154	ILE
17	4	173	VAL
17	4	188	ASP
17	4	189	PRO
17	4	195	VAL
1	A	49	ASP
1	A	74	ILE
1	A	84	GLY
1	A	91	LEU
1	A	94	SER
1	A	109	TRP
1	A	111	ASN
1	A	114	THR
1	A	116	ILE
1	A	127	VAL
1	A	155	ALA
1	A	209	GLY
1	A	243	PRO
1	A	269	PHE
1	A	291	THR
1	A	292	GLY
1	A	293	GLY
1	A	307	ALA
1	A	354	TRP
1	A	366	GLY
1	A	368	LEU

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Mol	Chain	Res	Type
1	A	373	ALA
1	A	380	PRO
1	A	388	ASP
1	A	395	LEU
1	A	408	VAL
1	A	426	THR
1	A	443	ILE
1	A	450	CYS
1	A	460	LEU
1	A	469	ALA
1	A	472	ARG
1	A	473	PRO
1	A	483	GLN
1	A	487	VAL
1	A	496	HIS
1	A	503	THR
1	A	513	LEU
1	A	526	LYS
1	A	541	VAL
1	A	543	HIS
1	A	547	PHE
1	A	549	ILE
1	A	569	ILE
1	A	578	ARG
1	A	582	ASP
1	A	620	MET
1	A	631	GLN
1	A	643	ALA
1	A	647	ILE
1	A	654	ARG
1	A	670	SER
1	A	685	VAL
1	A	705	GLU
1	A	711	HIS
1	A	712	ASN
1	A	718	PRO
1	A	719	ALA
1	A	755	ILE
2	B	8	PHE
2	B	11	GLY
2	B	19	ARG
2	B	54	LEU

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Mol	Chain	Res	Type
2	B	65	LEU
2	B	66	PHE
2	B	71	GLN
2	B	83	HIS
2	B	84	VAL
2	B	103	ALA
2	B	107	GLY
2	B	110	LEU
2	B	136	TYR
2	B	139	ALA
2	B	140	ILE
2	B	146	SER
2	B	154	TRP
2	B	172	GLU
2	B	184	GLY
2	B	198	ALA
2	B	215	VAL
2	B	223	GLY
2	B	227	THR
2	B	231	ASN
2	B	242	HIS
2	B	249	GLY
2	B	253	ALA
2	B	268	LEU
2	B	294	ASN
2	B	301	ILE
2	B	315	LEU
2	B	318	GLY
2	B	320	LYS
2	B	321	GLY
2	B	342	GLY
2	B	352	MET
2	B	357	ALA
2	B	369	ALA
2	B	389	HIS
2	B	433	THR
2	B	437	TYR
2	B	442	VAL
2	B	447	GLY
2	B	450	GLU
2	B	479	SER
2	B	480	SER

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Mol	Chain	Res	Type
2	B	495	PRO
2	B	501	ILE
2	B	504	ASN
2	B	516	ASP
2	B	521	HIS
2	B	526	GLY
2	B	533	ILE
2	B	537	GLY
2	B	539	LEU
2	B	543	GLY
2	B	544	SER
2	B	563	GLY
2	B	578	LEU
2	B	593	TYR
2	B	639	VAL
2	B	687	LEU
2	B	701	SER
3	C	13	GLY
3	C	30	PRO
3	C	36	ALA
3	C	46	GLU
3	C	49	VAL
3	C	50	GLY
3	C	61	ASP
4	D	29	PHE
4	D	30	ALA
4	D	40	ALA
4	D	54	LYS
4	D	77	LEU
4	D	94	TYR
4	D	109	VAL
4	D	132	LEU
5	E	41	ARG
5	E	52	VAL
5	E	61	THR
5	E	62	ARG
6	F	8	CYS
6	F	27	ALA
6	F	28	SER
6	F	39	ALA
6	F	42	ILE
6	F	43	LYS

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Mol	Chain	Res	Type
6	F	45	THR
6	F	46	MET
6	F	71	LEU
6	F	78	ARG
6	F	86	PRO
6	F	95	GLY
6	F	144	LEU
7	G	11	SER
7	G	16	LEU
7	G	19	GLY
7	G	35	VAL
7	G	36	PRO
7	G	87	ALA
8	H	31	PRO
8	H	51	GLY
8	H	52	LEU
8	H	61	GLY
8	H	71	ASN
8	H	76	VAL
8	H	79	ILE
9	I	6	SER
9	I	7	LEU
10	J	7	TYR
12	L	7	THR
12	L	12	GLN
12	L	14	LEU
12	L	18	PRO
12	L	32	LEU
12	L	45	THR
12	L	51	LEU
12	L	75	ARG
12	L	86	LEU
12	L	104	ILE
12	L	109	GLU
12	L	119	THR
12	L	159	TYR
13	N	3	ILE
13	N	7	LEU
13	N	8	GLU
13	N	26	GLY
13	N	35	VAL
13	N	51	ASP

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Mol	Chain	Res	Type
13	N	54	LYS
13	N	56	LYS
14	1	33	PRO
14	1	49	TRP
14	1	68	TRP
14	1	93	THR
14	1	117	ASP
14	1	121	LYS
14	1	141	GLU
14	1	145	VAL
14	1	151	GLY
14	1	152	ARG
14	1	160	GLY
14	1	182	ALA
15	2	60	ALA
15	2	67	PHE
15	2	87	TYR
15	2	143	PHE
15	2	151	ALA
15	2	162	LYS
16	3	114	LEU
16	3	141	LYS
16	3	207	VAL
16	3	208	GLY
17	4	88	SER
17	4	90	LEU
17	4	119	PRO
1	A	83	PHE
1	A	119	SER
1	A	135	ASP
1	A	185	HIS
1	A	191	PRO
1	A	228	PRO
1	A	235	ALA
1	A	245	PRO
1	A	250	LEU
1	A	274	TRP
1	A	279	ASP
1	A	310	PHE
1	A	318	ARG
1	A	337	PRO
1	A	341	GLN

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Mol	Chain	Res	Type
1	A	370	ILE
1	A	381	PRO
1	A	474	GLN
1	A	480	THR
1	A	498	LEU
1	A	507	ALA
1	A	509	ALA
1	A	566	SER
1	A	574	ASN
1	A	586	ARG
1	A	602	LEU
1	A	648	THR
1	A	708	VAL
1	A	733	VAL
2	B	16	PRO
2	B	81	PRO
2	B	86	PRO
2	B	173	SER
2	B	216	LEU
2	B	233	TYR
2	B	330	ILE
2	B	390	GLY
2	B	397	ASP
2	B	400	PRO
2	B	421	HIS
2	B	440	ASN
2	B	491	ASN
2	B	497	TRP
2	B	529	THR
2	B	545	LYS
2	B	549	ASP
2	B	558	PRO
2	B	566	GLY
2	B	568	CYS
2	B	594	TRP
2	B	600	THR
2	B	610	ASN
2	B	613	SER
2	B	642	SER
2	B	686	PRO
2	B	693	TRP
2	B	707	LEU

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Mol	Chain	Res	Type
2	B	720	THR
2	B	727	ALA
3	C	8	TYR
3	C	16	GLN
3	C	60	THR
3	C	74	THR
3	C	79	LEU
4	D	25	PRO
4	D	45	PHE
4	D	61	PRO
4	D	84	LEU
4	D	90	LEU
4	D	97	LYS
4	D	143	PRO
5	E	51	SER
5	E	59	PRO
6	F	3	ALA
6	F	12	LYS
6	F	18	GLU
6	F	65	SER
6	F	66	ASP
6	F	108	ILE
6	F	134	PHE
6	F	152	ASN
7	G	7	VAL
7	G	8	ILE
7	G	44	PHE
7	G	54	TYR
7	G	59	LYS
7	G	86	LEU
8	H	24	TYR
8	H	33	ASN
8	H	34	SER
8	H	39	PHE
8	H	47	PHE
8	H	55	LYS
8	H	73	PRO
8	H	86	PRO
12	L	29	SER
12	L	48	ASN
12	L	63	LEU
12	L	87	ALA

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Mol	Chain	Res	Type
12	L	108	LYS
12	L	123	ARG
12	L	164	PRO
13	N	10	SER
13	N	22	LEU
14	1	46	HIS
14	1	100	ILE
14	1	170	GLY
14	1	183	ASP
14	1	185	TRP
15	2	75	ASN
15	2	79	TRP
15	2	95	PHE
16	3	75	ALA
17	4	72	VAL
17	4	139	ASN
17	4	153	GLU
17	4	182	LEU
17	4	187	SER
1	A	60	ASP
1	A	299	ILE
1	A	327	ILE
1	A	382	TYR
1	A	416	ILE
1	A	444	SER
1	A	452	PHE
1	A	537	ALA
1	A	561	LEU
1	A	591	GLN
1	A	603	PHE
1	A	613	ILE
1	A	629	ASN
1	A	630	ASP
2	B	32	GLU
2	B	47	PHE
2	B	51	PHE
2	B	135	LEU
2	B	153	GLY
2	B	165	VAL
2	B	305	LEU
2	B	311	PRO
2	B	325	THR

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Mol	Chain	Res	Type
2	B	375	HIS
2	B	394	PHE
2	B	448	THR
2	B	472	TYR
2	B	478	LEU
2	B	482	ASN
2	B	508	LEU
2	B	511	THR
2	B	553	PHE
2	B	627	ASN
2	B	636	THR
2	B	641	ASN
2	B	691	ILE
3	C	25	VAL
3	C	44	ARG
3	C	56	SER
3	C	72	GLU
4	D	21	ASP
4	D	44	GLU
4	D	65	ALA
4	D	85	ALA
4	D	123	VAL
4	D	139	LYS
5	E	58	ASP
6	F	44	ALA
6	F	54	ASP
6	F	61	LEU
6	F	74	SER
6	F	114	PRO
6	F	137	PRO
6	F	142	ARG
7	G	25	ASN
7	G	32	ALA
9	I	26	LEU
10	J	3	ASP
10	J	40	PRO
12	L	17	ASP
12	L	34	ALA
12	L	67	PRO
12	L	92	VAL
12	L	115	ALA
14	1	153	LEU

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Mol	Chain	Res	Type
14	1	172	GLY
14	1	188	ASN
15	2	36	SER
15	2	74	LEU
15	2	117	GLY
16	3	66	ALA
16	3	111	ASN
17	4	97	LEU
17	4	123	GLN
17	4	134	PRO
17	4	171	HIS
17	4	194	ILE
1	A	34	TRP
1	A	110	LEU
1	A	234	ASN
1	A	281	LEU
1	A	376	MET
1	A	402	ILE
1	A	420	ARG
1	A	466	THR
1	A	500	PRO
1	A	553	VAL
1	A	593	SER
1	A	624	VAL
1	A	666	GLN
1	A	716	VAL
2	B	3	LEU
2	B	144	PHE
2	B	194	LEU
2	B	211	ASN
2	B	228	GLY
2	B	339	ALA
3	C	38	GLN
4	D	46	TYR
4	D	53	PRO
4	D	122	LYS
5	E	78	SER
6	F	21	ALA
7	G	34	GLN
7	G	49	THR
7	G	66	PHE
8	H	30	SER

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Mol	Chain	Res	Type
8	H	41	GLU
8	H	80	THR
8	H	85	GLN
12	L	9	GLN
12	L	13	PRO
12	L	21	GLY
12	L	106	SER
12	L	151	VAL
12	L	158	MET
13	N	14	LYS
13	N	44	GLU
14	1	181	LEU
15	2	27	PHE
15	2	35	SER
15	2	45	VAL
15	2	53	ARG
15	2	77	PRO
15	2	188	PRO
15	2	199	PRO
16	3	64	ARG
16	3	81	LYS
16	3	113	THR
16	3	120	ALA
16	3	136	PRO
1	A	95	GLY
1	A	176	GLY
1	A	405	PHE
1	A	486	PRO
1	A	635	THR
1	A	674	ALA
1	A	681	GLY
1	A	726	SER
2	B	128	GLY
2	B	345	THR
2	B	391	PRO
2	B	535	VAL
2	B	552	ASP
3	C	59	PRO
4	D	28	ILE
4	D	62	THR
4	D	71	GLY
4	D	116	ASP

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Mol	Chain	Res	Type
4	D	129	GLY
4	D	136	SER
5	E	45	TRP
6	F	123	VAL
7	G	29	GLU
10	J	24	GLY
12	L	44	ARG
12	L	112	PRO
12	L	163	LEU
13	N	13	ASN
13	N	60	PHE
16	3	80	GLY
16	3	217	LEU
17	4	63	VAL
17	4	73	PRO
17	4	145	PRO
1	A	669	GLY
1	A	704	ILE
2	B	25	ILE
2	B	477	PRO
2	B	645	VAL
3	C	33	GLY
4	D	137	ILE
4	D	153	PRO
8	H	72	ALA
15	2	96	ILE
1	A	137	GLY
1	A	199	VAL
1	A	322	GLY
1	A	409	GLY
1	A	612	VAL
2	B	112	PRO
4	D	130	VAL
4	D	146	VAL
6	F	7	PRO
14	1	69	VAL
15	2	149	GLY
16	3	206	GLY
17	4	46	VAL
1	A	54	ILE
1	A	531	PRO
2	B	127	ILE

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Mol	Chain	Res	Type
2	B	548	PRO
2	B	697	PRO
5	E	63	TYR
7	G	77	ILE
14	1	189	ILE
17	4	61	PRO
17	4	96	ILE
4	D	105	PRO
6	F	69	PRO
14	1	32	VAL
15	2	21	GLY
13	N	81	VAL
17	4	137	ILE
6	F	38	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	588/613 (96%)	350 (60%)	238 (40%)	0	0
2	B	598/598 (100%)	397 (66%)	201 (34%)	0	1
3	C	69/69 (100%)	40 (58%)	29 (42%)	0	0
4	D	118/118 (100%)	77 (65%)	41 (35%)	0	1
5	E	55/55 (100%)	36 (66%)	19 (34%)	0	1
6	F	127/127 (100%)	80 (63%)	47 (37%)	0	0
7	G	80/80 (100%)	37 (46%)	43 (54%)	0	0
8	H	62/62 (100%)	40 (64%)	22 (36%)	0	1
9	I	26/26 (100%)	18 (69%)	8 (31%)	0	1
10	J	37/37 (100%)	27 (73%)	10 (27%)	0	1
12	L	127/127 (100%)	78 (61%)	49 (39%)	0	0
13	N	74/74 (100%)	48 (65%)	26 (35%)	0	1
14	1	92/147 (63%)	63 (68%)	29 (32%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	2	122/151 (81%)	80 (66%)	42 (34%)	0	1
16	3	74/123 (60%)	45 (61%)	29 (39%)	0	0
17	4	130/139 (94%)	84 (65%)	46 (35%)	0	1
All	All	2379/2546 (93%)	1500 (63%)	879 (37%)	0	0

All (879) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PHE
1	A	33	GLN
1	A	39	HIS
1	A	40	PHE
1	A	41	SER
1	A	42	ARG
1	A	43	THR
1	A	44	ILE
1	A	53	TRP
1	A	55	TRP
1	A	56	ASN
1	A	63	ASP
1	A	68	THR
1	A	75	SER
1	A	76	ARG
1	A	77	LYS
1	A	79	PHE
1	A	83	PHE
1	A	85	GLN
1	A	86	LEU
1	A	91	LEU
1	A	93	LEU
1	A	96	MET
1	A	98	PHE
1	A	103	PHE
1	A	110	LEU
1	A	112	ASP
1	A	114	THR
1	A	115	HIS
1	A	122	VAL
1	A	123	VAL
1	A	126	ILE
1	A	130	GLU

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Mol	Chain	Res	Type
1	A	135	ASP
1	A	136	VAL
1	A	140	PHE
1	A	141	ARG
1	A	143	ILE
1	A	144	GLN
1	A	145	ILE
1	A	149	PHE
1	A	154	ARG
1	A	158	ILE
1	A	159	THR
1	A	160	SER
1	A	164	LEU
1	A	165	TYR
1	A	167	THR
1	A	169	ILE
1	A	173	VAL
1	A	178	MET
1	A	179	LEU
1	A	183	TRP
1	A	184	PHE
1	A	192	LYS
1	A	193	LEU
1	A	195	TRP
1	A	202	MET
1	A	204	ASN
1	A	207	LEU
1	A	213	LEU
1	A	216	LEU
1	A	222	GLN
1	A	227	LEU
1	A	232	PHE
1	A	233	LEU
1	A	240	LYS
1	A	241	GLU
1	A	244	LEU
1	A	249	ILE
1	A	250	LEU
1	A	251	ASN
1	A	252	ARG
1	A	254	LEU
1	A	255	LEU

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Mol	Chain	Res	Type
1	A	262	PHE
1	A	267	THR
1	A	269	PHE
1	A	272	LEU
1	A	274	TRP
1	A	275	SER
1	A	277	TYR
1	A	279	ASP
1	A	280	PHE
1	A	281	LEU
1	A	282	THR
1	A	283	PHE
1	A	284	ARG
1	A	288	ASP
1	A	290	LEU
1	A	294	LEU
1	A	295	TRP
1	A	297	THR
1	A	299	ILE
1	A	301	HIS
1	A	304	LEU
1	A	308	ILE
1	A	311	LEU
1	A	318	ARG
1	A	328	LYS
1	A	330	ILE
1	A	331	LEU
1	A	334	HIS
1	A	339	THR
1	A	343	HIS
1	A	346	LEU
1	A	349	ILE
1	A	350	LEU
1	A	351	THR
1	A	352	THR
1	A	354	TRP
1	A	355	HIS
1	A	358	LEU
1	A	364	MET
1	A	367	SER
1	A	368	LEU
1	A	370	ILE

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Mol	Chain	Res	Type
1	A	371	VAL
1	A	372	VAL
1	A	374	GLN
1	A	375	HIS
1	A	376	MET
1	A	377	TYR
1	A	382	TYR
1	A	389	TYR
1	A	392	GLN
1	A	393	LEU
1	A	396	PHE
1	A	397	THR
1	A	399	HIS
1	A	405	PHE
1	A	407	ILE
1	A	416	ILE
1	A	419	VAL
1	A	426	THR
1	A	427	ARG
1	A	431	LEU
1	A	434	ARG
1	A	438	HIS
1	A	440	ASP
1	A	445	HIS
1	A	446	LEU
1	A	447	ASN
1	A	453	LEU
1	A	455	PHE
1	A	456	HIS
1	A	458	PHE
1	A	462	ILE
1	A	465	ASP
1	A	467	MET
1	A	472	ARG
1	A	476	MET
1	A	478	SER
1	A	479	ASP
1	A	480	THR
1	A	482	ILE
1	A	483	GLN
1	A	484	LEU
1	A	485	GLN

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Mol	Chain	Res	Type
1	A	490	GLN
1	A	495	THR
1	A	503	THR
1	A	508	THR
1	A	511	THR
1	A	514	THR
1	A	519	ASP
1	A	523	VAL
1	A	527	VAL
1	A	532	ILE
1	A	534	LEU
1	A	536	THR
1	A	540	LEU
1	A	542	HIS
1	A	545	HIS
1	A	551	VAL
1	A	553	VAL
1	A	554	LEU
1	A	555	ILE
1	A	556	LEU
1	A	558	LYS
1	A	562	PHE
1	A	564	ARG
1	A	566	SER
1	A	568	LEU
1	A	569	ILE
1	A	571	ASP
1	A	578	ARG
1	A	579	PHE
1	A	590	CYS
1	A	605	MET
1	A	608	SER
1	A	615	HIS
1	A	619	LYS
1	A	620	MET
1	A	624	VAL
1	A	627	THR
1	A	628	ILE
1	A	631	GLN
1	A	633	VAL
1	A	637	ILE
1	A	638	THR

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Mol	Chain	Res	Type
1	A	644	GLN
1	A	648	THR
1	A	649	ILE
1	A	654	ARG
1	A	657	LEU
1	A	662	SER
1	A	671	SER
1	A	678	PHE
1	A	679	PHE
1	A	680	LEU
1	A	684	PHE
1	A	685	VAL
1	A	690	LEU
1	A	692	PHE
1	A	697	ARG
1	A	702	GLU
1	A	703	LEU
1	A	704	ILE
1	A	706	SER
1	A	709	TRP
1	A	711	HIS
1	A	713	LYS
1	A	714	LEU
1	A	720	THR
1	A	723	ARG
1	A	731	ARG
1	A	733	VAL
1	A	736	THR
1	A	737	HIS
1	A	740	LEU
1	A	743	ILE
1	A	745	THR
1	A	747	TRP
1	A	750	PHE
1	A	753	ARG
1	A	754	ILE
1	A	757	VAL
2	B	3	LEU
2	B	4	ARG
2	B	7	ARG
2	B	8	PHE
2	B	12	ILE

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Mol	Chain	Res	Type
2	B	15	ASP
2	B	23	PHE
2	B	42	LEU
2	B	47	PHE
2	B	50	HIS
2	B	53	GLN
2	B	54	LEU
2	B	56	ILE
2	B	64	ASN
2	B	65	LEU
2	B	68	VAL
2	B	77	TRP
2	B	79	GLN
2	B	85	ARG
2	B	102	GLU
2	B	104	PHE
2	B	105	THR
2	B	106	ARG
2	B	110	LEU
2	B	115	ASN
2	B	120	VAL
2	B	122	GLN
2	B	123	TRP
2	B	124	TRP
2	B	126	THR
2	B	129	LEU
2	B	133	GLU
2	B	135	LEU
2	B	140	ILE
2	B	142	LEU
2	B	143	LEU
2	B	148	ILE
2	B	150	LEU
2	B	157	LEU
2	B	158	GLN
2	B	161	TRP
2	B	162	LYS
2	B	172	GLU
2	B	174	ARG
2	B	182	LEU
2	B	187	SER
2	B	199	ILE

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Mol	Chain	Res	Type
2	B	203	ARG
2	B	209	TRP
2	B	211	ASN
2	B	213	LEU
2	B	214	ASP
2	B	215	VAL
2	B	227	THR
2	B	232	LEU
2	B	235	GLN
2	B	236	ASN
2	B	239	SER
2	B	243	LEU
2	B	248	GLN
2	B	258	LEU
2	B	266	GLN
2	B	268	LEU
2	B	269	TRP
2	B	270	LEU
2	B	276	HIS
2	B	283	LEU
2	B	286	ILE
2	B	302	LYS
2	B	308	HIS
2	B	309	ILE
2	B	315	LEU
2	B	317	ARG
2	B	320	LYS
2	B	323	TYR
2	B	326	ILE
2	B	330	ILE
2	B	334	LEU
2	B	336	LEU
2	B	338	LEU
2	B	341	LEU
2	B	344	ILE
2	B	345	THR
2	B	346	SER
2	B	348	VAL
2	B	350	GLN
2	B	351	HIS
2	B	352	MET
2	B	353	TYR

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Mol	Chain	Res	Type
2	B	355	LEU
2	B	358	TYR
2	B	361	ILE
2	B	364	ASP
2	B	365	PHE
2	B	368	GLN
2	B	374	HIS
2	B	375	HIS
2	B	376	GLN
2	B	383	MET
2	B	392	ILE
2	B	393	PHE
2	B	399	ASN
2	B	402	GLN
2	B	406	ASN
2	B	408	LEU
2	B	414	HIS
2	B	415	LYS
2	B	418	ILE
2	B	420	SER
2	B	427	LEU
2	B	432	HIS
2	B	434	LEU
2	B	437	TYR
2	B	438	VAL
2	B	439	HIS
2	B	441	ASP
2	B	444	LEU
2	B	448	THR
2	B	454	LEU
2	B	455	ILE
2	B	458	ILE
2	B	462	TRP
2	B	463	ILE
2	B	470	THR
2	B	472	TYR
2	B	475	ASP
2	B	480	SER
2	B	481	THR
2	B	487	ASN
2	B	492	ILE
2	B	493	TRP

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Mol	Chain	Res	Type
2	B	494	LEU
2	B	497	TRP
2	B	499	ASN
2	B	503	GLU
2	B	508	LEU
2	B	510	LEU
2	B	511	THR
2	B	516	ASP
2	B	517	PHE
2	B	518	LEU
2	B	523	ILE
2	B	525	LEU
2	B	527	LEU
2	B	529	THR
2	B	532	LEU
2	B	534	LEU
2	B	539	LEU
2	B	540	ASP
2	B	545	LYS
2	B	546	LEU
2	B	549	ASP
2	B	550	LYS
2	B	551	LYS
2	B	552	ASP
2	B	557	PHE
2	B	560	ASP
2	B	564	ARG
2	B	569	ASP
2	B	575	ASP
2	B	576	PHE
2	B	578	LEU
2	B	582	TRP
2	B	583	MET
2	B	593	TYR
2	B	594	TRP
2	B	595	HIS
2	B	596	TRP
2	B	607	SER
2	B	609	PHE
2	B	611	GLU
2	B	612	SER
2	B	614	THR

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Mol	Chain	Res	Type
2	B	615	TYR
2	B	616	LEU
2	B	620	LEU
2	B	622	ASP
2	B	628	SER
2	B	630	GLN
2	B	631	LEU
2	B	643	LEU
2	B	646	TRP
2	B	657	TRP
2	B	659	THR
2	B	661	PHE
2	B	663	PHE
2	B	668	ARG
2	B	678	LEU
2	B	680	TRP
2	B	682	HIS
2	B	684	ARG
2	B	685	THR
2	B	687	LEU
2	B	690	LEU
2	B	692	ARG
2	B	694	ARG
2	B	696	LYS
2	B	704	GLN
2	B	707	LEU
2	B	710	LEU
2	B	725	LEU
3	C	4	SER
3	C	6	LYS
3	C	8	TYR
3	C	11	CYS
3	C	12	ILE
3	C	16	GLN
3	C	17	CYS
3	C	18	VAL
3	C	19	ARG
3	C	24	ASP
3	C	27	GLU
3	C	29	ILE
3	C	35	LYS
3	C	38	GLN

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Mol	Chain	Res	Type
3	C	46	GLU
3	C	48	CYS
3	C	49	VAL
3	C	51	CYS
3	C	52	LYS
3	C	53	ARG
3	C	54	CYS
3	C	56	SER
3	C	63	LEU
3	C	65	VAL
3	C	68	TYR
3	C	69	LEU
3	C	71	HIS
3	C	72	GLU
3	C	75	ARG
4	D	20	LEU
4	D	21	ASP
4	D	23	ASN
4	D	29	PHE
4	D	37	LEU
4	D	38	ARG
4	D	41	GLN
4	D	43	GLU
4	D	45	PHE
4	D	51	GLU
4	D	58	PHE
4	D	62	THR
4	D	67	ILE
4	D	69	ARG
4	D	70	GLU
4	D	74	LEU
4	D	75	LEU
4	D	76	LYS
4	D	77	LEU
4	D	84	LEU
4	D	86	LEU
4	D	89	ARG
4	D	90	LEU
4	D	91	ARG
4	D	102	ARG
4	D	104	PHE
4	D	108	GLU

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Mol	Chain	Res	Type
4	D	109	VAL
4	D	111	TYR
4	D	112	LEU
4	D	113	HIS
4	D	115	LYS
4	D	123	VAL
4	D	128	GLN
4	D	130	VAL
4	D	133	ASN
4	D	134	MET
4	D	139	LYS
4	D	144	ILE
4	D	146	VAL
4	D	156	LEU
5	E	32	ARG
5	E	34	SER
5	E	39	LEU
5	E	45	TRP
5	E	53	VAL
5	E	56	ASP
5	E	62	ARG
5	E	65	VAL
5	E	66	VAL
5	E	71	LYS
5	E	73	ASN
5	E	74	TYR
5	E	76	ASN
5	E	77	ILE
5	E	84	LEU
5	E	85	ASP
5	E	87	VAL
5	E	89	GLU
5	E	90	VAL
6	F	1	ASP
6	F	2	ILE
6	F	10	GLU
6	F	12	LYS
6	F	18	GLU
6	F	19	LYS
6	F	22	LEU
6	F	24	LYS
6	F	25	LEU

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Mol	Chain	Res	Type
6	F	28	SER
6	F	32	TYR
6	F	35	ASP
6	F	42	ILE
6	F	43	LYS
6	F	45	THR
6	F	46	MET
6	F	48	LYS
6	F	49	THR
6	F	52	ARG
6	F	53	PHE
6	F	59	TYR
6	F	61	LEU
6	F	63	CYS
6	F	72	ILE
6	F	78	ARG
6	F	80	TRP
6	F	88	ILE
6	F	90	PHE
6	F	93	ILE
6	F	96	TRP
6	F	99	TRP
6	F	100	VAL
6	F	102	ARG
6	F	105	LEU
6	F	115	THR
6	F	117	LYS
6	F	118	GLU
6	F	120	ILE
6	F	121	ILE
6	F	122	ASP
6	F	130	LEU
6	F	136	TRP
6	F	141	TYR
6	F	143	GLU
6	F	144	LEU
6	F	151	ASP
6	F	152	ASN
7	G	5	SER
7	G	7	VAL
7	G	8	ILE
7	G	10	LEU

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Mol	Chain	Res	Type
7	G	15	SER
7	G	16	LEU
7	G	20	ARG
7	G	21	PHE
7	G	22	VAL
7	G	23	PHE
7	G	26	PHE
7	G	27	GLN
7	G	28	ARG
7	G	29	GLU
7	G	30	ASN
7	G	31	MET
7	G	34	GLN
7	G	39	ASN
7	G	41	MET
7	G	43	HIS
7	G	45	GLU
7	G	49	THR
7	G	50	ARG
7	G	53	GLU
7	G	56	SER
7	G	57	LEU
7	G	60	SER
7	G	62	ASP
7	G	66	PHE
7	G	68	ILE
7	G	69	VAL
7	G	70	ASP
7	G	71	VAL
7	G	72	LEU
7	G	76	SER
7	G	77	ILE
7	G	79	HIS
7	G	80	ILE
7	G	83	TYR
7	G	86	LEU
7	G	91	ASN
7	G	94	ASP
7	G	97	PHE
8	H	24	TYR
8	H	32	TYR
8	H	33	ASN

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Mol	Chain	Res	Type
8	H	41	GLU
8	H	43	PHE
8	H	47	PHE
8	H	50	ARG
8	H	52	LEU
8	H	53	LEU
8	H	54	LEU
8	H	57	LEU
8	H	59	LEU
8	H	63	SER
8	H	65	LEU
8	H	66	THR
8	H	67	TYR
8	H	77	LEU
8	H	84	GLN
8	H	85	GLN
8	H	88	LYS
8	H	92	ARG
8	H	95	ILE
9	I	1	MET
9	I	4	LEU
9	I	7	LEU
9	I	11	LEU
9	I	14	LEU
9	I	21	MET
9	I	24	LEU
9	I	29	GLU
10	J	8	LEU
10	J	10	VAL
10	J	13	VAL
10	J	19	PHE
10	J	22	LEU
10	J	26	LEU
10	J	31	ARG
10	J	32	PHE
10	J	38	THR
10	J	42	PHE
12	L	7	THR
12	L	9	GLN
12	L	10	VAL
12	L	11	ILE
12	L	15	ASN

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Mol	Chain	Res	Type
12	L	17	ASP
12	L	23	LEU
12	L	36	TYR
12	L	37	LEU
12	L	40	LEU
12	L	44	ARG
12	L	48	ASN
12	L	50	LEU
12	L	52	ARG
12	L	55	GLU
12	L	58	LEU
12	L	60	HIS
12	L	64	LEU
12	L	70	LYS
12	L	75	ARG
12	L	76	ASN
12	L	79	TYR
12	L	94	ILE
12	L	96	SER
12	L	100	THR
12	L	101	MET
12	L	102	TYR
12	L	107	PHE
12	L	108	LYS
12	L	114	ILE
12	L	118	LEU
12	L	120	LEU
12	L	121	THR
12	L	124	LYS
12	L	126	GLN
12	L	128	ASP
12	L	129	GLN
12	L	132	SER
12	L	136	TRP
12	L	138	LYS
12	L	145	PHE
12	L	151	VAL
12	L	152	THR
12	L	153	TRP
12	L	155	CYS
12	L	157	LEU
12	L	161	LEU

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Mol	Chain	Res	Type
12	L	167	PHE
12	L	168	LYS
13	N	8	GLU
13	N	11	LYS
13	N	18	ASP
13	N	21	ARG
13	N	22	LEU
13	N	24	THR
13	N	33	TYR
13	N	35	VAL
13	N	39	SER
13	N	45	ASN
13	N	49	CYS
13	N	51	ASP
13	N	54	LYS
13	N	56	LYS
13	N	57	LYS
13	N	60	PHE
13	N	61	LEU
13	N	65	LEU
13	N	69	CYS
13	N	70	GLU
13	N	72	LYS
13	N	81	VAL
13	N	82	PHE
13	N	83	TRP
13	N	84	LYS
13	N	85	TRP
14	1	40	LYS
14	1	41	GLU
14	1	43	GLU
14	1	44	LEU
14	1	45	ILE
14	1	48	ARG
14	1	49	TRP
14	1	57	ILE
14	1	61	GLU
14	1	67	ASN
14	1	69	VAL
14	1	73	GLU
14	1	87	ASN
14	1	96	THR

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Mol	Chain	Res	Type
14	1	100	ILE
14	1	101	GLU
14	1	111	GLN
14	1	112	ARG
14	1	147	GLU
14	1	149	LYS
14	1	150	ASN
14	1	153	LEU
14	1	155	LEU
14	1	156	LEU
14	1	158	PHE
14	1	164	GLN
14	1	174	LEU
14	1	185	TRP
14	1	189	ILE
15	2	17	GLU
15	2	18	TRP
15	2	23	LEU
15	2	26	ASP
15	2	27	PHE
15	2	29	PHE
15	2	30	ASP
15	2	31	PRO
15	2	36	SER
15	2	38	PRO
15	2	49	LEU
15	2	53	ARG
15	2	54	TRP
15	2	63	PHE
15	2	67	PHE
15	2	70	LYS
15	2	74	LEU
15	2	81	THR
15	2	86	GLU
15	2	91	THR
15	2	93	THR
15	2	94	LEU
15	2	99	LEU
15	2	108	ARG
15	2	141	LEU
15	2	142	TRP
15	2	143	PHE

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Mol	Chain	Res	Type
15	2	144	ASP
15	2	154	GLN
15	2	156	LEU
15	2	157	LYS
15	2	159	LEU
15	2	162	LYS
15	2	164	ILE
15	2	169	LEU
15	2	174	VAL
15	2	175	MET
15	2	178	TRP
15	2	179	PHE
15	2	181	HIS
15	2	182	ILE
15	2	189	ILE
16	3	54	TRP
16	3	57	TYR
16	3	60	ILE
16	3	64	ARG
16	3	67	MET
16	3	68	LEU
16	3	77	GLU
16	3	78	ILE
16	3	84	LEU
16	3	89	THR
16	3	108	TRP
16	3	111	ASN
16	3	115	PHE
16	3	116	VAL
16	3	118	GLU
16	3	119	MET
16	3	121	LEU
16	3	124	PHE
16	3	126	GLU
16	3	129	ARG
16	3	132	ASP
16	3	138	SER
16	3	139	MET
16	3	141	LYS
16	3	142	GLN
16	3	144	PHE
16	3	200	ILE

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Mol	Chain	Res	Type
16	3	203	LEU
16	3	205	THR
17	4	39	TRP
17	4	40	PHE
17	4	44	GLU
17	4	55	VAL
17	4	58	MET
17	4	63	VAL
17	4	69	ILE
17	4	70	ILE
17	4	72	VAL
17	4	75	TRP
17	4	82	GLU
17	4	86	SER
17	4	88	SER
17	4	89	THR
17	4	91	PHE
17	4	101	VAL
17	4	103	ILE
17	4	105	ARG
17	4	116	ASN
17	4	123	GLN
17	4	124	TYR
17	4	126	LEU
17	4	141	LEU
17	4	143	PHE
17	4	150	LYS
17	4	151	GLU
17	4	152	LYS
17	4	154	ILE
17	4	156	ASN
17	4	159	LEU
17	4	161	MET
17	4	164	PHE
17	4	165	LEU
17	4	168	ILE
17	4	170	GLN
17	4	171	HIS
17	4	174	THR
17	4	179	PHE
17	4	180	ASP
17	4	182	LEU

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Mol	Chain	Res	Type
17	4	183	LEU
17	4	187	SER
17	4	190	TRP
17	4	194	ILE
17	4	196	GLN
17	4	198	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	58	HIS
1	A	115	HIS
1	A	121	GLN
1	A	133	ASN
1	A	144	GLN
1	A	204	ASN
1	A	205	HIS
1	A	206	HIS
1	A	224	HIS
1	A	231	GLN
1	A	246	HIS
1	A	251	ASN
1	A	301	HIS
1	A	302	HIS
1	A	303	HIS
1	A	320	ASN
1	A	341	GLN
1	A	438	HIS
1	A	445	HIS
1	A	456	HIS
1	A	464	ASN
1	A	525	ASN
1	A	597	HIS
1	A	621	GLN
1	A	629	ASN
1	A	631	GLN
1	A	663	GLN
1	A	729	GLN
1	A	737	HIS
2	B	14	GLN
2	B	45	ASN

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Mol	Chain	Res	Type
2	B	53	GLN
2	B	73	ASN
2	B	114	ASN
2	B	122	GLN
2	B	132	ASN
2	B	170	ASN
2	B	177	HIS
2	B	196	HIS
2	B	210	ASN
2	B	211	ASN
2	B	235	GLN
2	B	236	ASN
2	B	248	GLN
2	B	262	HIS
2	B	266	GLN
2	B	333	GLN
2	B	363	GLN
2	B	368	GLN
2	B	376	GLN
2	B	389	HIS
2	B	403	ASN
2	B	406	ASN
2	B	439	HIS
2	B	502	ASN
2	B	506	ASN
2	B	521	HIS
2	B	595	HIS
2	B	608	GLN
2	B	682	HIS
2	B	689	ASN
2	B	704	GLN
3	C	16	GLN
4	D	23	ASN
4	D	73	ASN
4	D	110	GLN
4	D	133	ASN
5	E	80	ASN
6	F	20	GLN
6	F	153	ASN
7	G	27	GLN
7	G	30	ASN
7	G	38	GLN

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Mol	Chain	Res	Type
7	G	39	ASN
7	G	43	HIS
7	G	61	ASN
7	G	91	ASN
8	H	33	ASN
8	H	36	GLN
8	H	84	GLN
12	L	9	GLN
12	L	15	ASN
12	L	39	ASN
12	L	126	GLN
12	L	129	GLN
13	N	17	ASN
13	N	45	ASN
14	1	72	GLN
14	1	150	ASN
14	1	180	HIS
14	1	186	HIS
15	2	44	ASN
15	2	181	HIS
15	2	191	ASN
15	2	195	HIS
16	3	127	HIS
17	4	47	ASN
17	4	99	HIS
17	4	142	ASN
17	4	156	ASN
17	4	170	GLN
17	4	172	ASN
17	4	191	HIS
17	4	192	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

178 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	CLA	H	1501	-	49,63,73	2.22	12 (24%)	55,101,113	3.61	23 (41%)
21	SF4	C	3102	3	0,12,12	0.00	-	-		
18	CLA	4	1009	-	22,32,73	1.90	5 (22%)	26,54,113	2.79	13 (50%)
18	CLA	1	1002	-	22,32,73	1.89	6 (27%)	26,54,113	2.97	15 (57%)
18	CLA	J	1308	-	22,32,73	1.87	5 (22%)	26,54,113	3.17	16 (61%)
18	CLA	3	3006	16	22,32,73	1.84	5 (22%)	26,54,113	2.92	14 (53%)
18	CLA	A	1133	-	22,32,73	1.88	5 (22%)	26,54,113	3.03	15 (57%)
18	CLA	A	1140	-	49,63,73	2.27	13 (26%)	55,101,113	3.68	21 (38%)
18	CLA	A	1122	-	49,63,73	2.28	13 (26%)	55,101,113	3.20	20 (36%)
18	CLA	A	1152	-	22,32,73	1.91	6 (27%)	26,54,113	2.97	17 (65%)
18	CLA	1	1001	-	22,32,73	1.95	6 (27%)	26,54,113	3.04	16 (61%)
18	CLA	3	3012	-	22,32,73	1.84	7 (31%)	26,54,113	2.90	15 (57%)
20	BCR	F	6016	-	41,41,41	1.56	2 (4%)	56,56,56	4.86	33 (58%)
18	CLA	H	1505	8	22,32,73	1.92	7 (31%)	26,54,113	3.04	15 (57%)
18	CLA	4	4005	-	22,32,73	1.90	5 (22%)	26,54,113	3.28	14 (53%)
18	CLA	A	1101	-	22,32,73	1.91	5 (22%)	26,54,113	3.12	14 (53%)
18	CLA	3	3002	-	22,32,73	1.88	6 (27%)	26,54,113	2.98	16 (61%)
18	CLA	B	1211	2	22,32,73	1.82	7 (31%)	26,54,113	3.03	14 (53%)
18	CLA	A	1106	-	35,49,73	2.51	12 (34%)	38,84,113	3.73	19 (50%)
18	CLA	B	1216	-	50,64,73	2.27	11 (22%)	56,102,113	3.43	20 (35%)
18	CLA	3	3015	-	22,32,73	1.82	5 (22%)	26,54,113	2.98	18 (69%)
18	CLA	1	1006	-	22,32,73	1.93	7 (31%)	26,54,113	3.08	17 (65%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1309	-	22,32,73	1.88	6 (27%)	26,54,113	2.95	15 (57%)
18	CLA	B	9010	2	41,55,73	2.44	15 (36%)	45,91,113	3.59	23 (51%)
18	CLA	G	1248	-	22,32,73	1.91	7 (31%)	26,54,113	3.14	14 (53%)
18	CLA	A	1107	1	51,65,73	2.34	13 (25%)	57,103,113	3.42	22 (38%)
18	CLA	A	1108	-	44,58,73	2.29	12 (27%)	49,95,113	3.85	18 (36%)
18	CLA	B	1238	-	48,62,73	2.32	12 (25%)	53,99,113	3.56	26 (49%)
18	CLA	B	1215	2	46,60,73	2.33	12 (26%)	51,97,113	3.06	25 (49%)
18	CLA	4	4010	-	22,32,73	1.90	5 (22%)	26,54,113	3.02	16 (61%)
18	CLA	3	3013	-	22,32,73	1.94	7 (31%)	26,54,113	3.06	17 (65%)
18	CLA	1	1005	-	22,32,73	1.90	5 (22%)	26,54,113	3.03	17 (65%)
18	CLA	A	1127	1	22,32,73	1.94	8 (36%)	26,54,113	2.87	13 (50%)
18	CLA	3	3010	-	22,32,73	1.84	5 (22%)	26,54,113	2.89	14 (53%)
18	CLA	2	2004	-	22,32,73	1.91	6 (27%)	26,54,113	3.07	15 (57%)
18	CLA	3	3001	-	22,32,73	1.91	5 (22%)	26,54,113	3.13	16 (61%)
18	CLA	B	1202	-	44,58,73	2.41	13 (29%)	49,95,113	4.00	23 (46%)
18	CLA	B	1224	-	45,59,73	2.21	13 (28%)	50,96,113	2.75	22 (44%)
18	CLA	1	1010	-	22,32,73	1.92	5 (22%)	26,54,113	3.03	17 (65%)
18	CLA	K	1141	-	22,32,73	1.84	5 (22%)	26,54,113	2.89	16 (61%)
18	CLA	B	1212	-	54,68,73	2.11	13 (24%)	61,107,113	3.28	19 (31%)
18	CLA	A	1111	-	22,32,73	1.95	5 (22%)	26,54,113	3.00	15 (57%)
18	CLA	B	1213	2	22,32,73	1.84	5 (22%)	26,54,113	2.96	16 (61%)
18	CLA	2	2006	-	22,32,73	1.82	5 (22%)	26,54,113	2.91	14 (53%)
18	CLA	4	4008	-	22,32,73	1.87	5 (22%)	26,54,113	2.94	15 (57%)
18	CLA	B	1208	-	49,63,73	2.24	12 (24%)	55,101,113	3.45	28 (50%)
18	CLA	A	1104	1	22,32,73	1.88	6 (27%)	26,54,113	3.00	15 (57%)
18	CLA	A	1142	-	22,32,73	1.91	5 (22%)	26,54,113	2.89	15 (57%)
18	CLA	F	1139	-	38,52,73	2.39	9 (23%)	40,87,113	3.37	18 (45%)
18	CLA	3	3008	-	22,32,73	1.96	6 (27%)	26,54,113	3.08	14 (53%)
18	CLA	A	1110	-	22,32,73	1.88	6 (27%)	26,54,113	3.26	15 (57%)
18	CLA	4	4006	-	22,32,73	1.97	5 (22%)	26,54,113	3.10	16 (61%)
18	CLA	L	1502	12	45,59,73	2.31	12 (26%)	50,96,113	3.24	22 (44%)
18	CLA	B	1220	-	54,68,73	2.06	11 (20%)	61,107,113	3.76	20 (32%)
18	CLA	A	1134	-	22,32,73	1.85	6 (27%)	26,54,113	3.25	18 (69%)
18	CLA	L	1125	-	22,32,73	1.88	5 (22%)	26,54,113	2.84	14 (53%)
18	CLA	B	1206	2	22,32,73	1.91	6 (27%)	26,54,113	3.13	16 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	1232	-	49,63,73	2.18	11 (22%)	55,101,113	3.61	20 (36%)
18	CLA	4	4012	-	22,32,73	2.02	7 (31%)	26,54,113	3.14	12 (46%)
21	SF4	C	3103	3	0,12,12	0.00	-	-		
18	CLA	B	9023	-	41,55,73	2.37	12 (29%)	45,91,113	3.60	19 (42%)
18	CLA	1	1003	-	22,32,73	1.86	5 (22%)	26,54,113	3.04	16 (61%)
18	CLA	2	2002	-	22,32,73	1.92	7 (31%)	26,54,113	2.99	15 (57%)
18	CLA	B	9012	-	49,63,73	2.33	12 (24%)	55,101,113	3.25	24 (43%)
18	CLA	2	2003	-	22,32,73	1.89	7 (31%)	26,54,113	3.24	14 (53%)
18	CLA	B	1218	-	45,59,73	2.62	14 (31%)	50,96,113	3.57	22 (44%)
18	CLA	F	1306	-	22,32,73	1.99	6 (27%)	26,54,113	3.04	15 (57%)
18	CLA	A	1109	-	23,30,73	2.57	10 (43%)	16,49,113	2.93	8 (50%)
18	CLA	2	2015	-	22,32,73	1.86	5 (22%)	26,54,113	2.99	17 (65%)
18	CLA	F	1303	-	22,32,73	1.87	5 (22%)	26,54,113	3.02	15 (57%)
18	CLA	4	4011	-	22,32,73	1.88	6 (27%)	26,54,113	2.96	17 (65%)
18	CLA	3	2009	-	22,32,73	1.91	7 (31%)	26,54,113	3.02	15 (57%)
18	CLA	2	2010	-	22,32,73	1.89	5 (22%)	26,54,113	3.09	15 (57%)
18	CLA	L	1503	-	40,54,73	2.80	14 (35%)	48,90,113	5.25	24 (50%)
18	CLA	1	1012	-	22,32,73	1.81	5 (22%)	26,54,113	3.14	15 (57%)
18	CLA	4	4013	-	22,32,73	1.92	7 (31%)	26,54,113	3.02	14 (53%)
18	CLA	A	1117	-	22,32,73	1.78	5 (22%)	26,54,113	2.92	16 (61%)
18	CLA	B	1219	2	45,59,73	2.30	9 (20%)	50,96,113	3.09	21 (42%)
18	CLA	A	1118	-	22,32,73	1.91	7 (31%)	26,54,113	3.05	15 (57%)
18	CLA	A	1144	-	22,32,73	1.84	5 (22%)	26,54,113	3.07	15 (57%)
18	CLA	B	9022	-	48,62,73	2.27	13 (27%)	53,99,113	4.31	23 (43%)
18	CLA	F	4015	-	22,32,73	1.87	5 (22%)	26,54,113	3.15	16 (61%)
18	CLA	B	1301	-	22,32,73	1.92	5 (22%)	26,54,113	2.95	15 (57%)
18	CLA	A	1147	-	22,32,73	1.92	7 (31%)	26,54,113	2.95	15 (57%)
18	CLA	F	1302	-	49,63,73	2.14	12 (24%)	55,101,113	3.43	21 (38%)
18	CLA	A	1128	-	49,63,73	2.13	14 (28%)	55,101,113	3.04	20 (36%)
18	CLA	4	1304	-	49,63,73	2.16	11 (22%)	55,101,113	3.49	19 (34%)
18	CLA	3	3009	-	22,32,73	1.90	6 (27%)	26,54,113	3.03	14 (53%)
18	CLA	B	1205	-	49,63,73	2.17	12 (24%)	55,101,113	3.86	23 (41%)
18	CLA	1	1007	-	22,32,73	1.97	7 (31%)	26,54,113	2.91	15 (57%)
18	CLA	4	4002	-	22,32,73	1.85	6 (27%)	26,54,113	3.04	14 (53%)
18	CLA	A	1123	-	49,63,73	2.30	13 (26%)	55,101,113	3.47	20 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PQN	A	5001	-	34,34,34	1.75	2 (5%)	42,45,45	1.35	4 (9%)
18	CLA	I	1204	-	49,63,73	2.24	12 (24%)	55,101,113	3.21	18 (32%)
18	CLA	A	1135	-	36,53,73	2.48	13 (36%)	39,89,113	3.85	15 (38%)
18	CLA	B	1229	-	43,57,73	2.54	12 (27%)	52,94,113	4.77	21 (40%)
21	SF4	B	3101	1,2	0,12,12	0.00	-	-		
18	CLA	B	1225	-	36,53,73	2.53	12 (33%)	39,89,113	4.48	21 (53%)
18	CLA	B	1241	-	22,32,73	2.07	8 (36%)	26,54,113	2.94	17 (65%)
18	CLA	A	1136	-	49,63,73	2.20	12 (24%)	55,101,113	3.58	23 (41%)
18	CLA	2	2012	-	22,32,73	1.96	8 (36%)	26,54,113	3.01	16 (61%)
18	CLA	4	4007	-	22,32,73	1.96	7 (31%)	26,54,113	3.10	16 (61%)
18	CLA	1	1008	-	22,32,73	1.88	5 (22%)	26,54,113	3.01	16 (61%)
18	CLA	A	1151	-	22,32,73	1.87	6 (27%)	26,54,113	2.94	14 (53%)
20	BCR	I	6018	-	41,41,41	1.84	4 (9%)	56,56,56	4.81	33 (58%)
18	CLA	F	1305	-	22,32,73	1.84	5 (22%)	26,54,113	3.01	16 (61%)
18	CLA	A	1102	-	22,32,73	1.87	5 (22%)	26,54,113	2.91	14 (53%)
18	CLA	B	1231	-	40,54,73	2.43	13 (32%)	44,90,113	4.12	16 (36%)
18	CLA	B	1237	-	45,59,73	2.27	12 (26%)	50,96,113	3.94	20 (40%)
18	CLA	3	3005	-	22,32,73	1.88	7 (31%)	26,54,113	3.25	16 (61%)
18	CLA	A	1132	-	22,32,73	2.09	8 (36%)	26,54,113	3.08	18 (69%)
20	BCR	A	6011	-	41,41,41	1.54	3 (7%)	56,56,56	4.49	15 (26%)
18	CLA	F	1240	-	22,32,73	1.91	6 (27%)	26,54,113	3.37	15 (57%)
18	CLA	A	9011	-	49,63,73	2.15	11 (22%)	55,101,113	3.70	22 (40%)
18	CLA	2	2011	-	22,32,73	1.86	6 (27%)	26,54,113	3.06	16 (61%)
18	CLA	1	1004	-	22,32,73	1.92	7 (31%)	26,54,113	2.89	16 (61%)
18	CLA	A	1131	-	35,52,73	2.57	10 (28%)	42,88,113	4.02	21 (50%)
18	CLA	1	1013	-	22,32,73	1.90	5 (22%)	26,54,113	2.99	16 (61%)
18	CLA	A	1143	-	22,32,73	1.91	5 (22%)	26,54,113	2.98	15 (57%)
18	CLA	B	1242	-	41,55,73	2.46	13 (31%)	45,91,113	4.04	17 (37%)
18	CLA	2	2013	-	22,32,73	1.97	6 (27%)	26,54,113	2.90	14 (53%)
18	CLA	B	1236	-	40,54,73	2.40	11 (27%)	44,90,113	4.41	17 (38%)
18	CLA	A	1120	-	22,32,73	1.95	6 (27%)	26,54,113	3.20	17 (65%)
18	CLA	B	1221	-	42,56,73	2.31	11 (26%)	46,92,113	3.17	20 (43%)
18	CLA	G	1233	-	45,59,73	2.37	13 (28%)	50,96,113	3.70	17 (34%)
18	CLA	K	1153	-	22,32,73	1.90	7 (31%)	26,54,113	2.82	15 (57%)
18	CLA	2	2001	-	22,32,73	1.87	5 (22%)	26,54,113	2.96	15 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1124	-	22,32,73	1.91	5 (22%)	26,54,113	3.17	15 (57%)
18	CLA	J	1307	-	22,32,73	1.87	5 (22%)	26,54,113	3.03	18 (69%)
18	CLA	B	1223	-	22,32,73	1.97	8 (36%)	26,54,113	2.91	14 (53%)
18	CLA	A	1115	-	41,55,73	2.38	13 (31%)	45,91,113	3.69	21 (46%)
18	CLA	B	1207	-	49,63,73	2.09	12 (24%)	55,101,113	4.16	25 (45%)
18	CLA	4	4009	-	22,32,73	1.84	5 (22%)	26,54,113	3.08	16 (61%)
18	CLA	L	1504	-	49,63,73	2.11	11 (22%)	55,101,113	3.41	16 (29%)
18	CLA	A	9013	-	40,54,73	2.34	10 (25%)	44,90,113	3.27	18 (40%)
20	BCR	L	6020	-	41,41,41	1.88	3 (7%)	56,56,56	4.82	25 (44%)
18	CLA	4	4001	-	22,32,73	1.88	5 (22%)	26,54,113	3.07	16 (61%)
18	CLA	B	1201	-	22,32,73	1.98	6 (27%)	26,54,113	3.17	14 (53%)
18	CLA	2	2005	-	22,32,73	1.94	5 (22%)	26,54,113	3.02	17 (65%)
18	CLA	4	4003	-	22,32,73	1.87	5 (22%)	26,54,113	2.87	16 (61%)
18	CLA	2	2007	-	22,32,73	1.91	6 (27%)	26,54,113	3.16	15 (57%)
18	CLA	B	1214	-	43,57,73	2.38	12 (27%)	46,93,113	3.18	21 (45%)
18	CLA	J	2107	-	55,69,73	2.04	11 (20%)	62,108,113	3.44	21 (33%)
18	CLA	3	3004	-	22,32,73	1.91	7 (31%)	26,54,113	3.07	16 (61%)
18	CLA	B	1203	18	40,56,73	2.48	12 (30%)	46,92,113	3.55	19 (41%)
18	CLA	A	1148	-	22,32,73	1.90	6 (27%)	26,54,113	3.17	16 (61%)
18	CLA	K	1150	-	22,32,73	1.86	5 (22%)	26,54,113	3.07	14 (53%)
18	CLA	3	3011	-	22,32,73	1.85	5 (22%)	26,54,113	2.91	17 (65%)
18	CLA	B	1138	-	50,64,73	2.16	14 (28%)	56,102,113	3.22	26 (46%)
18	CLA	A	1137	-	49,63,73	2.24	11 (22%)	55,101,113	3.12	23 (41%)
18	CLA	B	1227	2	44,58,73	2.22	14 (31%)	49,95,113	4.01	19 (38%)
18	CLA	B	1226	18	22,32,73	1.97	7 (31%)	26,54,113	2.91	15 (57%)
18	CLA	B	1230	-	22,32,73	1.86	6 (27%)	26,54,113	2.86	15 (57%)
18	CLA	B	1217	-	44,58,73	2.29	13 (29%)	49,95,113	4.00	21 (42%)
18	CLA	A	1119	-	49,63,73	2.26	12 (24%)	55,101,113	3.40	18 (32%)
18	CLA	A	1113	-	44,58,73	2.35	12 (27%)	49,95,113	4.17	22 (44%)
18	CLA	1	1011	14	22,32,73	1.92	5 (22%)	26,54,113	3.05	16 (61%)
18	CLA	A	1146	-	22,32,73	1.95	7 (31%)	26,54,113	2.93	16 (61%)
18	CLA	1	1014	-	22,32,73	1.91	5 (22%)	26,54,113	2.95	14 (53%)
18	CLA	B	1239	-	49,63,73	2.22	12 (24%)	55,101,113	3.14	19 (34%)
19	PQN	B	5002	-	34,34,34	1.78	2 (5%)	42,45,45	1.65	8 (19%)
18	CLA	A	1129	-	49,63,73	2.17	12 (24%)	55,101,113	3.69	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1126	1	49,63,73	2.19	13 (26%)	55,101,113	4.40	26 (47%)
18	CLA	A	1105	1	22,32,73	1.88	7 (31%)	26,54,113	3.10	16 (61%)
18	CLA	A	1116	-	22,32,73	1.92	7 (31%)	26,54,113	3.18	17 (65%)
18	CLA	B	1210	-	22,32,73	1.99	6 (27%)	26,54,113	2.97	17 (65%)
20	BCR	B	6017	-	41,41,41	1.54	3 (7%)	56,56,56	4.28	24 (42%)
18	CLA	B	1209	-	49,63,73	2.15	11 (22%)	55,101,113	3.86	23 (41%)
18	CLA	B	1228	-	49,63,73	2.18	12 (24%)	55,101,113	3.94	24 (43%)
18	CLA	3	3003	-	22,32,73	1.93	6 (27%)	26,54,113	2.90	17 (65%)
18	CLA	A	1103	1	41,55,73	2.39	12 (29%)	45,91,113	3.89	21 (46%)
18	CLA	4	4004	-	22,32,73	1.93	7 (31%)	26,54,113	2.95	15 (57%)
18	CLA	B	1234	-	44,58,73	2.29	12 (27%)	49,95,113	3.43	18 (36%)
18	CLA	3	3007	-	22,32,73	1.85	7 (31%)	26,54,113	3.14	16 (61%)
18	CLA	B	1235	-	49,63,73	2.20	13 (26%)	55,101,113	3.53	19 (34%)
18	CLA	L	1130	-	44,58,73	2.25	12 (27%)	49,95,113	3.42	20 (40%)
18	CLA	2	2008	-	22,32,73	1.91	6 (27%)	26,54,113	3.02	15 (57%)
18	CLA	B	1222	-	59,73,73	1.97	11 (18%)	67,113,113	2.74	21 (31%)

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
18	CLA	H	1501	-	4/4/18/25	9/25/123/135	-
21	SF4	C	3102	3	-	-	0/6/5/5
18	CLA	4	1009	-	3/3/7/25	-	-
18	CLA	1	1002	-	3/3/7/25	-	-
18	CLA	J	1308	-	3/3/7/25	-	-
18	CLA	3	3006	16	3/3/7/25	-	-
18	CLA	A	1133	-	3/3/7/25	-	-
18	CLA	A	1140	-	4/4/18/25	12/25/123/135	-
18	CLA	A	1122	-	4/4/18/25	7/25/123/135	-
18	CLA	A	1152	-	3/3/7/25	-	-
18	CLA	1	1001	-	3/3/7/25	-	-
18	CLA	3	3012	-	3/3/7/25	-	-
20	BCR	F	6016	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	H	1505	8	3/3/7/25	-	-
18	CLA	4	4005	-	3/3/7/25	-	-
18	CLA	A	1101	-	3/3/7/25	-	-
18	CLA	3	3002	-	3/3/7/25	-	-
18	CLA	B	1211	2	3/3/7/25	-	-
18	CLA	A	1106	-	3/3/15/25	2/8/106/135	-
18	CLA	B	1216	-	4/4/18/25	10/27/125/135	-
18	CLA	3	3015	-	3/3/7/25	-	-
18	CLA	1	1006	-	3/3/7/25	-	-
18	CLA	A	1309	-	3/3/7/25	-	-
18	CLA	B	9010	2	3/3/16/25	9/16/114/135	-
18	CLA	G	1248	-	3/3/7/25	-	-
18	CLA	A	1107	1	4/4/18/25	17/28/126/135	-
18	CLA	A	1108	-	3/3/17/25	5/19/117/135	-
18	CLA	B	1238	-	3/3/17/25	9/24/122/135	-
18	CLA	B	1215	2	3/3/17/25	12/22/120/135	-
18	CLA	4	4010	-	3/3/7/25	-	-
18	CLA	3	3013	-	3/3/7/25	-	-
18	CLA	1	1005	-	3/3/7/25	-	-
18	CLA	A	1127	1	3/3/7/25	-	-
18	CLA	3	3010	-	3/3/7/25	-	-
18	CLA	2	2004	-	3/3/7/25	-	-
18	CLA	3	3001	-	3/3/7/25	-	-
18	CLA	B	1202	-	3/3/17/25	8/19/117/135	-
18	CLA	B	1224	-	3/3/17/25	4/21/119/135	-
18	CLA	1	1010	-	3/3/7/25	-	-
18	CLA	K	1141	-	3/3/7/25	-	-
18	CLA	B	1212	-	4/4/19/25	19/31/129/135	-
18	CLA	A	1111	-	3/3/7/25	-	-
18	CLA	B	1213	2	3/3/7/25	-	-
18	CLA	2	2006	-	3/3/7/25	-	-
18	CLA	4	4008	-	3/3/7/25	-	-
18	CLA	B	1208	-	4/4/18/25	15/25/123/135	-
18	CLA	A	1104	1	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1142	-	3/3/7/25	-	-
18	CLA	F	1139	-	3/3/15/25	9/11/110/135	-
18	CLA	3	3008	-	3/3/7/25	-	-
18	CLA	A	1110	-	3/3/7/25	-	-
18	CLA	4	4006	-	3/3/7/25	-	-
18	CLA	L	1502	12	3/3/17/25	10/21/119/135	-
18	CLA	B	1220	-	4/4/19/25	18/31/129/135	-
18	CLA	A	1134	-	3/3/7/25	-	-
18	CLA	L	1125	-	3/3/7/25	-	-
18	CLA	B	1206	2	3/3/7/25	-	-
18	CLA	B	1232	-	4/4/18/25	9/25/123/135	-
18	CLA	4	4012	-	3/3/7/25	-	-
21	SF4	C	3103	3	-	-	0/6/5/5
18	CLA	B	9023	-	3/3/16/25	5/16/114/135	-
18	CLA	1	1003	-	3/3/7/25	-	-
18	CLA	2	2002	-	3/3/7/25	-	-
18	CLA	B	9012	-	4/4/18/25	15/25/123/135	-
18	CLA	2	2003	-	3/3/7/25	-	-
18	CLA	B	1218	-	3/3/17/25	12/21/119/135	-
18	CLA	F	1306	-	3/3/7/25	-	-
18	CLA	A	1109	-	3/3/6/25	-	-
18	CLA	2	2015	-	3/3/7/25	-	-
18	CLA	F	1303	-	3/3/7/25	-	-
18	CLA	4	4011	-	3/3/7/25	-	-
18	CLA	3	2009	-	3/3/7/25	-	-
18	CLA	2	2010	-	3/3/7/25	-	-
18	CLA	L	1503	-	3/3/16/25	6/16/112/135	-
18	CLA	1	1012	-	3/3/7/25	-	-
18	CLA	4	4013	-	3/3/7/25	-	-
18	CLA	A	1117	-	3/3/7/25	-	-
18	CLA	B	1219	2	3/3/17/25	11/21/119/135	-
18	CLA	A	1118	-	3/3/7/25	-	-
18	CLA	A	1144	-	3/3/7/25	-	-
18	CLA	B	9022	-	3/3/17/25	12/24/122/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	4015	-	3/3/7/25	-	-
18	CLA	B	1301	-	3/3/7/25	-	-
18	CLA	A	1147	-	3/3/7/25	-	-
18	CLA	F	1302	-	4/4/18/25	6/25/123/135	-
18	CLA	A	1128	-	4/4/18/25	9/25/123/135	-
18	CLA	4	1304	-	4/4/18/25	11/25/123/135	-
18	CLA	3	3009	-	3/3/7/25	-	-
18	CLA	B	1205	-	4/4/18/25	12/25/123/135	-
18	CLA	1	1007	-	3/3/7/25	-	-
18	CLA	4	4002	-	3/3/7/25	-	-
18	CLA	A	1123	-	4/4/18/25	14/25/123/135	-
19	PQN	A	5001	-	1/1/8/9	11/23/43/43	0/2/2/2
18	CLA	I	1204	-	4/4/18/25	14/25/123/135	-
18	CLA	A	1135	-	3/3/16/25	5/11/111/135	-
18	CLA	B	1229	-	3/3/17/25	8/19/115/135	-
21	SF4	B	3101	1,2	-	-	0/6/5/5
18	CLA	B	1225	-	3/3/16/25	3/11/111/135	-
18	CLA	B	1241	-	3/3/7/25	-	-
18	CLA	A	1136	-	4/4/18/25	12/25/123/135	-
18	CLA	2	2012	-	3/3/7/25	-	-
18	CLA	4	4007	-	3/3/7/25	-	-
18	CLA	1	1008	-	3/3/7/25	-	-
18	CLA	A	1151	-	3/3/7/25	-	-
20	BCR	I	6018	-	-	12/29/63/63	0/2/2/2
18	CLA	F	1305	-	3/3/7/25	-	-
18	CLA	A	1102	-	3/3/7/25	-	-
18	CLA	B	1231	-	3/3/16/25	10/15/113/135	-
18	CLA	B	1237	-	3/3/17/25	11/21/119/135	-
18	CLA	3	3005	-	3/3/7/25	-	-
18	CLA	A	1132	-	3/3/7/25	-	-
20	BCR	A	6011	-	-	15/29/63/63	0/2/2/2
18	CLA	F	1240	-	3/3/7/25	-	-
18	CLA	A	9011	-	4/4/18/25	11/25/123/135	-
18	CLA	2	2011	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	1004	-	3/3/7/25	-	-
18	CLA	A	1131	-	3/3/16/25	6/11/109/135	-
18	CLA	1	1013	-	3/3/7/25	-	-
18	CLA	A	1143	-	3/3/7/25	-	-
18	CLA	B	1242	-	3/3/16/25	13/16/114/135	-
18	CLA	2	2013	-	3/3/7/25	-	-
18	CLA	B	1236	-	3/3/16/25	6/15/113/135	-
18	CLA	A	1120	-	3/3/7/25	-	-
18	CLA	B	1221	-	3/3/16/25	14/17/115/135	-
18	CLA	G	1233	-	3/3/17/25	12/21/119/135	-
18	CLA	K	1153	-	3/3/7/25	-	-
18	CLA	2	2001	-	3/3/7/25	-	-
18	CLA	A	1124	-	3/3/7/25	-	-
18	CLA	J	1307	-	3/3/7/25	-	-
18	CLA	B	1223	-	3/3/7/25	-	-
18	CLA	A	1115	-	3/3/16/25	7/16/114/135	-
18	CLA	B	1207	-	4/4/18/25	11/25/123/135	-
18	CLA	4	4009	-	3/3/7/25	-	-
18	CLA	L	1504	-	4/4/18/25	9/25/123/135	-
18	CLA	A	9013	-	3/3/16/25	4/15/113/135	-
20	BCR	L	6020	-	-	16/29/63/63	0/2/2/2
18	CLA	4	4001	-	3/3/7/25	-	-
18	CLA	B	1201	-	3/3/7/25	-	-
18	CLA	2	2005	-	3/3/7/25	-	-
18	CLA	4	4003	-	3/3/7/25	-	-
18	CLA	2	2007	-	3/3/7/25	-	-
18	CLA	B	1214	-	3/3/16/25	7/18/116/135	-
18	CLA	J	2107	-	4/4/19/25	13/33/131/135	-
18	CLA	3	3004	-	3/3/7/25	-	-
18	CLA	B	1203	18	3/3/17/25	9/17/115/135	-
18	CLA	A	1148	-	3/3/7/25	-	-
18	CLA	K	1150	-	3/3/7/25	-	-
18	CLA	3	3011	-	3/3/7/25	-	-
18	CLA	B	1138	-	4/4/18/25	12/27/125/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1137	-	4/4/18/25	13/25/123/135	-
18	CLA	B	1227	2	3/3/17/25	10/19/117/135	-
18	CLA	B	1226	18	3/3/7/25	-	-
18	CLA	B	1230	-	3/3/7/25	-	-
18	CLA	B	1217	-	3/3/17/25	6/19/117/135	-
18	CLA	A	1119	-	4/4/18/25	14/25/123/135	-
18	CLA	A	1113	-	3/3/17/25	5/19/117/135	-
18	CLA	1	1011	14	3/3/7/25	-	-
18	CLA	A	1146	-	3/3/7/25	-	-
18	CLA	1	1014	-	3/3/7/25	-	-
18	CLA	B	1239	-	4/4/18/25	6/25/123/135	-
19	PQN	B	5002	-	1/1/8/9	8/23/43/43	0/2/2/2
18	CLA	A	1129	-	4/4/18/25	9/25/123/135	-
18	CLA	A	1126	1	4/4/18/25	12/25/123/135	-
18	CLA	A	1105	1	3/3/7/25	-	-
18	CLA	A	1116	-	3/3/7/25	-	-
18	CLA	B	1210	-	3/3/7/25	-	-
20	BCR	B	6017	-	-	19/29/63/63	0/2/2/2
18	CLA	B	1209	-	4/4/18/25	13/25/123/135	-
18	CLA	B	1228	-	4/4/18/25	9/25/123/135	-
18	CLA	3	3003	-	3/3/7/25	-	-
18	CLA	A	1103	1	3/3/16/25	8/16/114/135	-
18	CLA	4	4004	-	3/3/7/25	-	-
18	CLA	B	1234	-	3/3/17/25	9/19/117/135	-
18	CLA	3	3007	-	3/3/7/25	-	-
18	CLA	B	1235	-	4/4/18/25	11/25/123/135	-
18	CLA	L	1130	-	3/3/17/25	3/19/117/135	-
18	CLA	2	2008	-	3/3/7/25	-	-
18	CLA	B	1222	-	4/4/20/25	20/37/135/135	-

All (1418) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	5002	PQN	C3-C2	8.48	1.50	1.35
19	A	5001	PQN	C3-C2	8.17	1.50	1.35
18	B	1229	CLA	CAB-C3B	-8.17	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1131	CLA	CAB-C3B	-8.10	1.34	1.51
20	L	6020	BCR	C11-C10	-7.70	1.19	1.43
20	I	6018	BCR	C10-C9	-7.54	1.25	1.35
18	B	9012	CLA	C3B-CAB	-7.34	1.33	1.47
18	L	1503	CLA	CAB-C3B	-7.34	1.36	1.51
18	A	1106	CLA	C3B-CAB	-7.34	1.33	1.47
18	B	1217	CLA	C3B-CAB	-7.23	1.33	1.47
18	A	1107	CLA	C3B-CAB	-7.21	1.33	1.47
18	B	1242	CLA	C3B-CAB	-7.18	1.33	1.47
18	A	1137	CLA	C3B-CAB	-7.06	1.33	1.47
18	B	1238	CLA	C3B-CAB	-7.03	1.33	1.47
18	B	1239	CLA	C3B-CAB	-6.96	1.33	1.47
18	B	1215	CLA	C3B-CAB	-6.96	1.33	1.47
18	B	1202	CLA	C3B-CAB	-6.94	1.33	1.47
18	B	1220	CLA	C3B-CAB	-6.93	1.33	1.47
18	G	1233	CLA	CHC-C1C	6.90	1.52	1.35
18	B	1225	CLA	C3B-CAB	-6.88	1.33	1.47
20	L	6020	BCR	C10-C9	-6.85	1.26	1.35
18	B	1208	CLA	CHC-C1C	6.85	1.52	1.35
18	L	1502	CLA	C3B-CAB	-6.82	1.34	1.47
20	F	6016	BCR	C10-C9	-6.82	1.26	1.35
18	A	1126	CLA	C3B-CAB	-6.80	1.34	1.47
18	A	1123	CLA	C3B-CAB	-6.79	1.34	1.47
18	F	1139	CLA	C3B-CAB	-6.76	1.34	1.47
18	B	1237	CLA	C3B-CAB	-6.74	1.34	1.47
18	A	1122	CLA	C3B-CAB	-6.74	1.34	1.47
18	B	9022	CLA	C3B-CAB	-6.72	1.34	1.47
18	G	1233	CLA	C3B-CAB	-6.71	1.34	1.47
18	B	1232	CLA	C3B-CAB	-6.70	1.34	1.47
18	B	1218	CLA	C3B-CAB	-6.69	1.34	1.47
18	B	1231	CLA	C3B-CAB	-6.69	1.34	1.47
18	J	2107	CLA	C3B-CAB	-6.68	1.34	1.47
18	B	1235	CLA	C3B-CAB	-6.65	1.34	1.47
18	A	1119	CLA	CHC-C1C	6.64	1.52	1.35
18	B	1219	CLA	C3B-CAB	-6.63	1.34	1.47
18	A	1103	CLA	C3B-CAB	-6.60	1.34	1.47
18	A	9013	CLA	C3B-CAB	-6.55	1.34	1.47
18	A	1136	CLA	C3B-CAB	-6.55	1.34	1.47
18	B	1219	CLA	CHC-C1C	6.55	1.51	1.35
18	B	1229	CLA	CHC-C1C	6.55	1.51	1.35
18	B	1214	CLA	C3B-CAB	-6.54	1.34	1.47
18	B	1218	CLA	CHC-C1C	6.53	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1236	CLA	CHC-C1C	6.52	1.51	1.35
18	A	1135	CLA	C3B-CAB	-6.52	1.34	1.47
18	H	1501	CLA	C3B-CAB	-6.50	1.34	1.47
18	B	9010	CLA	C3B-CAB	-6.50	1.34	1.47
18	B	1215	CLA	O2D-CGD	6.49	1.49	1.33
18	B	1209	CLA	C3B-CAB	-6.48	1.34	1.47
18	B	1242	CLA	CHC-C1C	6.47	1.51	1.35
18	B	9023	CLA	C3B-CAB	-6.46	1.34	1.47
18	F	1139	CLA	O2D-CGD	6.45	1.48	1.33
18	A	1129	CLA	CHC-C1C	6.44	1.51	1.35
18	A	9011	CLA	O2D-CGD	6.43	1.48	1.33
18	L	1502	CLA	CHC-C1C	6.41	1.51	1.35
18	B	1216	CLA	CHC-C1C	6.41	1.51	1.35
18	B	1216	CLA	C3B-CAB	-6.40	1.34	1.47
18	L	1130	CLA	CHC-C1C	6.40	1.51	1.35
18	B	1214	CLA	CHC-C1C	6.38	1.51	1.35
18	B	9012	CLA	O2D-CGD	6.36	1.48	1.33
18	B	1222	CLA	C3B-CAB	-6.35	1.35	1.47
18	B	1224	CLA	CHC-C1C	6.34	1.51	1.35
18	B	1203	CLA	C3B-CAB	-6.33	1.35	1.47
18	B	1205	CLA	CHC-C1C	6.30	1.51	1.35
18	4	1304	CLA	CHC-C1C	6.30	1.51	1.35
18	B	1227	CLA	O2D-CGD	6.30	1.48	1.33
18	F	1302	CLA	C3B-CAB	-6.29	1.35	1.47
18	B	1218	CLA	O2D-CGD	6.28	1.48	1.33
18	B	9012	CLA	CHC-C1C	6.28	1.51	1.35
18	F	1302	CLA	CHC-C1C	6.26	1.51	1.35
18	A	1108	CLA	C3B-CAB	-6.26	1.35	1.47
18	I	1204	CLA	CHC-C1C	6.26	1.51	1.35
18	A	1115	CLA	C3B-CAB	-6.25	1.35	1.47
18	B	1234	CLA	C3B-CAB	-6.22	1.35	1.47
18	B	1222	CLA	CHC-C1C	6.22	1.50	1.35
18	B	1212	CLA	CHC-C1C	6.22	1.50	1.35
18	B	1232	CLA	CHC-C1C	6.22	1.50	1.35
18	B	9022	CLA	CHC-C1C	6.21	1.50	1.35
18	L	1504	CLA	C3B-CAB	-6.21	1.35	1.47
18	B	1236	CLA	C3B-CAB	-6.21	1.35	1.47
18	A	9011	CLA	C3B-CAB	-6.20	1.35	1.47
18	A	1129	CLA	C3B-CAB	-6.16	1.35	1.47
18	A	1140	CLA	C3B-CAB	-6.15	1.35	1.47
18	A	1126	CLA	CHC-C1C	6.15	1.50	1.35
18	B	1203	CLA	C3D-CAD	-6.15	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1113	CLA	O2D-CGD	6.14	1.48	1.33
20	F	6016	BCR	C11-C10	-6.12	1.24	1.43
18	A	1137	CLA	CHC-C1C	6.12	1.50	1.35
18	B	1221	CLA	C3B-CAB	-6.12	1.35	1.47
18	J	2107	CLA	CHC-C1C	6.10	1.50	1.35
20	I	6018	BCR	C11-C10	-6.10	1.24	1.43
18	I	1204	CLA	C3B-CAB	-6.07	1.35	1.47
18	H	1501	CLA	CHC-C1C	6.07	1.50	1.35
18	B	1238	CLA	CHC-C1C	6.05	1.50	1.35
18	B	9023	CLA	CHC-C1C	6.05	1.50	1.35
18	A	1128	CLA	CHC-C1C	6.04	1.50	1.35
18	B	1209	CLA	CHC-C1C	6.04	1.50	1.35
18	4	1304	CLA	C3B-CAB	-6.03	1.35	1.47
18	L	1504	CLA	CHC-C1C	6.03	1.50	1.35
18	A	1113	CLA	C3B-CAB	-6.02	1.35	1.47
18	A	1119	CLA	C3B-CAB	-5.99	1.35	1.47
18	A	1122	CLA	CHC-C1C	5.93	1.50	1.35
18	A	1108	CLA	CHC-C1C	5.93	1.50	1.35
18	B	1231	CLA	CHC-C1C	5.93	1.50	1.35
18	B	1202	CLA	CHC-C1C	5.92	1.50	1.35
18	B	1208	CLA	O2D-CGD	5.91	1.47	1.33
18	B	1138	CLA	CHC-C1C	5.91	1.50	1.35
18	B	1217	CLA	CHC-C1C	5.90	1.50	1.35
18	B	1234	CLA	CHC-C1C	5.88	1.50	1.35
18	A	1122	CLA	OBD-CAD	5.88	1.30	1.22
18	H	1501	CLA	O2D-CGD	5.88	1.47	1.33
18	B	1228	CLA	C3B-CAB	-5.88	1.36	1.47
18	A	1128	CLA	C3B-CAB	-5.87	1.36	1.47
18	A	1123	CLA	CHC-C1C	5.85	1.50	1.35
18	B	1225	CLA	CHC-C1C	5.85	1.50	1.35
18	F	1139	CLA	CHC-C1C	5.84	1.50	1.35
18	B	1228	CLA	CHC-C1C	5.84	1.49	1.35
18	B	1238	CLA	O2D-CGD	5.84	1.47	1.33
18	B	1237	CLA	CHC-C1C	5.83	1.49	1.35
18	L	1503	CLA	CHC-C1C	5.82	1.49	1.35
18	A	1115	CLA	CHC-C1C	5.82	1.49	1.35
18	F	1139	CLA	OBD-CAD	5.82	1.30	1.22
18	B	1220	CLA	CHC-C1C	5.81	1.49	1.35
18	A	1140	CLA	O2D-CGD	5.80	1.47	1.33
18	B	1216	CLA	O2D-CGD	5.80	1.47	1.33
18	B	1207	CLA	CHC-C1C	5.79	1.49	1.35
18	B	1207	CLA	C3B-CAB	-5.79	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	1503	CLA	O2D-CGD	5.79	1.47	1.33
18	I	1204	CLA	O2D-CGD	5.77	1.47	1.33
18	B	1203	CLA	CHC-C1C	5.76	1.49	1.35
18	A	1108	CLA	O2D-CGD	5.74	1.47	1.33
18	B	9023	CLA	O2D-CGD	5.74	1.47	1.33
18	A	1135	CLA	CHC-C1C	5.73	1.49	1.35
18	J	2107	CLA	O2D-CGD	5.73	1.47	1.33
18	A	1119	CLA	OBD-CAD	5.73	1.30	1.22
18	B	1203	CLA	O2D-CGD	5.72	1.47	1.33
18	A	1103	CLA	CHC-C1C	5.71	1.49	1.35
18	B	1227	CLA	C3B-CAB	-5.71	1.36	1.47
18	A	1136	CLA	CHC-C1C	5.70	1.49	1.35
18	B	1209	CLA	O2D-CGD	5.70	1.47	1.33
18	A	1123	CLA	OBD-CAD	5.69	1.30	1.22
18	A	1131	CLA	CHC-C1C	5.68	1.49	1.35
18	A	1107	CLA	CHC-C1C	5.67	1.49	1.35
20	B	6017	BCR	C11-C10	-5.66	1.25	1.43
18	G	1233	CLA	O2D-CGD	5.65	1.47	1.33
18	B	1221	CLA	O2D-CGD	5.65	1.47	1.33
18	B	1212	CLA	O2D-CGD	5.60	1.46	1.33
18	A	1137	CLA	OBD-CAD	5.59	1.30	1.22
18	A	1113	CLA	CHC-C1C	5.58	1.49	1.35
18	B	1216	CLA	OBD-CAD	5.58	1.30	1.22
18	A	1135	CLA	OBD-CAD	5.58	1.30	1.22
18	A	1106	CLA	CHC-C1C	5.57	1.49	1.35
18	B	1138	CLA	C3B-CAB	-5.57	1.36	1.47
18	B	1219	CLA	OBD-CAD	5.57	1.30	1.22
18	B	1231	CLA	OBD-CAD	5.56	1.30	1.22
18	A	1119	CLA	O2D-CGD	5.56	1.46	1.33
18	B	9010	CLA	O2D-CGD	5.54	1.46	1.33
18	B	1239	CLA	CHC-C1C	5.53	1.49	1.35
18	B	1224	CLA	C3B-CAB	-5.53	1.36	1.47
18	B	1208	CLA	O2A-CGA	5.52	1.49	1.33
18	B	1218	CLA	OBD-CAD	5.51	1.30	1.22
18	A	1123	CLA	O2D-CGD	5.51	1.46	1.33
18	L	1503	CLA	C4C-C3C	-5.51	1.35	1.45
18	L	1503	CLA	C1B-NB	-5.51	1.30	1.35
18	B	1205	CLA	C3B-CAB	-5.49	1.36	1.47
18	A	1140	CLA	OBD-CAD	5.48	1.30	1.22
18	B	1229	CLA	O2D-CGD	5.48	1.46	1.33
18	A	9011	CLA	CHC-C1C	5.47	1.49	1.35
18	B	1224	CLA	O2D-CGD	5.44	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1136	CLA	O2D-CGD	5.44	1.46	1.33
18	A	1140	CLA	CHC-C1C	5.44	1.48	1.35
18	B	1235	CLA	CHC-C1C	5.43	1.48	1.35
18	4	1304	CLA	O2D-CGD	5.43	1.46	1.33
18	B	1202	CLA	O2D-CGD	5.42	1.46	1.33
18	B	1232	CLA	O2D-CGD	5.42	1.46	1.33
18	A	1128	CLA	O2D-CGD	5.42	1.46	1.33
18	A	9013	CLA	O2D-CGD	5.42	1.46	1.33
18	B	1234	CLA	O2D-CGD	5.42	1.46	1.33
18	B	1242	CLA	O2D-CGD	5.41	1.46	1.33
18	B	1237	CLA	O2D-CGD	5.40	1.46	1.33
18	A	1131	CLA	OBD-CAD	5.40	1.29	1.22
18	B	1225	CLA	O2D-CGD	5.40	1.46	1.33
18	B	1228	CLA	O2A-CGA	5.38	1.49	1.33
18	A	1103	CLA	O2D-CGD	5.37	1.46	1.33
18	B	1138	CLA	O2D-CGD	5.37	1.46	1.33
18	L	1130	CLA	C3B-CAB	-5.37	1.37	1.47
18	A	1122	CLA	O2D-CGD	5.35	1.46	1.33
18	B	1222	CLA	O2D-CGD	5.34	1.46	1.33
18	B	1220	CLA	O2D-CGD	5.33	1.46	1.33
18	A	1109	CLA	C4D-C3D	-5.31	1.39	1.49
18	B	1208	CLA	C3B-CAB	-5.31	1.37	1.47
18	B	1222	CLA	OBD-CAD	5.30	1.29	1.22
18	B	1214	CLA	O2D-CGD	5.29	1.46	1.33
18	B	9010	CLA	CHC-C1C	5.28	1.48	1.35
18	A	1135	CLA	O2D-CGD	5.27	1.46	1.33
20	A	6011	BCR	C11-C10	-5.27	1.27	1.43
18	A	1107	CLA	OBD-CAD	5.25	1.29	1.22
18	A	9011	CLA	OBD-CAD	5.24	1.29	1.22
18	B	1239	CLA	O2A-CGA	5.24	1.48	1.33
18	B	1212	CLA	O2A-CGA	5.23	1.48	1.33
18	A	1126	CLA	O2A-CGA	5.22	1.48	1.33
18	I	1204	CLA	OBD-CAD	5.22	1.29	1.22
18	A	1140	CLA	O2A-CGA	5.21	1.48	1.33
20	B	6017	BCR	C10-C9	-5.20	1.28	1.35
18	J	2107	CLA	OBD-CAD	5.19	1.29	1.22
18	B	1205	CLA	O2D-CGD	5.19	1.45	1.33
18	B	1232	CLA	OBD-CAD	5.19	1.29	1.22
18	L	1502	CLA	OBD-CAD	5.19	1.29	1.22
18	B	1237	CLA	O2A-CGA	5.18	1.48	1.33
18	B	1202	CLA	OBD-CAD	5.18	1.29	1.22
18	A	1115	CLA	O2D-CGD	5.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1218	CLA	C4C-C3C	-5.17	1.36	1.45
18	B	1238	CLA	OBD-CAD	5.15	1.29	1.22
18	F	1302	CLA	O2D-CGD	5.15	1.45	1.33
18	L	1504	CLA	O2D-CGD	5.14	1.45	1.33
18	B	1235	CLA	OBD-CAD	5.14	1.29	1.22
18	A	1107	CLA	O2A-CGA	5.13	1.48	1.33
18	B	1227	CLA	CHC-C1C	5.13	1.48	1.35
18	A	1106	CLA	O2D-CGD	5.12	1.45	1.33
18	B	1212	CLA	C3B-CAB	-5.11	1.37	1.47
18	A	1129	CLA	O2D-CGD	5.10	1.45	1.33
18	L	1130	CLA	O2A-CGA	5.10	1.48	1.33
18	A	1137	CLA	O2D-CGD	5.08	1.45	1.33
18	2	2005	CLA	CHC-C1C	5.08	1.51	1.39
18	A	1106	CLA	OBD-CAD	5.08	1.29	1.22
18	A	1109	CLA	CHC-C1C	5.08	1.51	1.39
18	A	1115	CLA	O2A-CGA	5.07	1.48	1.33
18	B	1220	CLA	O2A-CGA	5.06	1.48	1.33
18	A	1108	CLA	O2A-CGA	5.05	1.48	1.33
18	A	1109	CLA	MG-NA	-5.05	1.94	2.06
18	B	1301	CLA	CHC-C1C	5.05	1.51	1.39
18	B	1138	CLA	O2A-CGA	5.05	1.48	1.33
18	L	1502	CLA	O2D-CGD	5.04	1.45	1.33
18	B	1221	CLA	CHC-C1C	5.01	1.47	1.35
18	I	1204	CLA	O2A-CGA	5.01	1.48	1.33
18	4	4012	CLA	CHC-C1C	5.01	1.51	1.39
18	4	1304	CLA	OBD-CAD	5.01	1.29	1.22
18	B	1203	CLA	OBD-CAD	5.01	1.29	1.22
18	B	1219	CLA	O2D-CGD	5.00	1.45	1.33
18	B	1216	CLA	O2A-CGA	4.99	1.47	1.33
18	B	1236	CLA	O2D-CGD	4.98	1.45	1.33
18	L	1130	CLA	O2D-CGD	4.97	1.45	1.33
18	B	1215	CLA	CHC-C1C	4.97	1.47	1.35
18	A	9013	CLA	CHC-C1C	4.96	1.47	1.35
18	A	1119	CLA	O2A-CGA	4.95	1.47	1.33
18	L	1504	CLA	OBD-CAD	4.94	1.29	1.22
18	B	1221	CLA	O2A-CGA	4.93	1.47	1.33
18	4	4006	CLA	CHC-C1C	4.93	1.51	1.39
18	B	1214	CLA	O2A-CGA	4.92	1.47	1.33
18	B	1221	CLA	OBD-CAD	4.91	1.29	1.22
18	B	1214	CLA	OBD-CAD	4.91	1.29	1.22
18	B	1205	CLA	OBD-CAD	4.90	1.29	1.22
18	A	1122	CLA	O2A-CGA	4.89	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	1306	CLA	CHC-C1C	4.89	1.51	1.39
18	B	1210	CLA	CHC-C1C	4.87	1.51	1.39
18	A	1136	CLA	OBD-CAD	4.87	1.29	1.22
18	A	1136	CLA	C4C-C3C	-4.85	1.36	1.45
18	H	1501	CLA	O2A-CGA	4.85	1.47	1.33
18	A	1146	CLA	CHC-C1C	4.85	1.51	1.39
18	3	3003	CLA	CHC-C1C	4.84	1.51	1.39
18	L	1503	CLA	O2A-CGA	4.82	1.47	1.33
18	L	1125	CLA	CHC-C1C	4.82	1.51	1.39
18	A	1113	CLA	OBD-CAD	4.82	1.29	1.22
18	3	3009	CLA	CHC-C1C	4.81	1.51	1.39
18	A	1117	CLA	CHC-C1C	4.81	1.51	1.39
18	B	9012	CLA	O2A-CGA	4.80	1.47	1.33
18	B	1238	CLA	O2A-CGA	4.79	1.47	1.33
18	B	1228	CLA	O2D-CGD	4.78	1.44	1.33
18	A	1143	CLA	CHC-C1C	4.78	1.51	1.39
18	B	1212	CLA	OBD-CAD	4.77	1.29	1.22
18	A	1107	CLA	C3B-C2B	-4.77	1.33	1.40
18	1	1014	CLA	CHC-C1C	4.77	1.51	1.39
18	A	1131	CLA	O2D-CGD	4.76	1.44	1.33
18	1	1004	CLA	CHC-C1C	4.76	1.51	1.39
18	B	9023	CLA	O2A-CGA	4.76	1.47	1.33
18	1	1010	CLA	CHC-C1C	4.75	1.51	1.39
18	3	3001	CLA	CHC-C1C	4.74	1.51	1.39
18	B	1239	CLA	OBD-CAD	4.73	1.28	1.22
18	4	4007	CLA	CHC-C1C	4.73	1.51	1.39
18	B	9010	CLA	O2A-CGA	4.73	1.47	1.33
18	A	1107	CLA	O2D-CGD	4.71	1.44	1.33
18	A	1129	CLA	O2A-CGA	4.71	1.47	1.33
18	A	1151	CLA	CHC-C1C	4.71	1.51	1.39
18	G	1233	CLA	OBD-CAD	4.71	1.28	1.22
18	A	1113	CLA	O2A-CGA	4.71	1.47	1.33
18	B	1234	CLA	OBD-CAD	4.71	1.28	1.22
18	A	1103	CLA	OBD-CAD	4.71	1.28	1.22
18	B	1239	CLA	O2D-CGD	4.70	1.44	1.33
18	4	4005	CLA	CHC-C1C	4.70	1.51	1.39
18	K	1150	CLA	CHC-C1C	4.69	1.51	1.39
18	1	1005	CLA	CHC-C1C	4.69	1.50	1.39
18	4	4013	CLA	CHC-C1C	4.69	1.50	1.39
18	A	9013	CLA	OBD-CAD	4.69	1.28	1.22
18	L	1503	CLA	MG-NA	-4.69	1.95	2.06
18	J	1307	CLA	CHC-C1C	4.67	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1142	CLA	CHC-C1C	4.67	1.50	1.39
18	B	1217	CLA	O2D-CGD	4.67	1.44	1.33
18	B	1218	CLA	O2A-CGA	4.67	1.47	1.33
18	4	4001	CLA	CHC-C1C	4.67	1.50	1.39
18	B	9022	CLA	O2D-CGD	4.66	1.44	1.33
18	B	1207	CLA	O2A-CGA	4.66	1.47	1.33
18	1	1001	CLA	CHC-C1C	4.66	1.50	1.39
18	4	1009	CLA	CHC-C1C	4.66	1.50	1.39
18	A	1126	CLA	OBD-CAD	4.65	1.28	1.22
18	1	1013	CLA	CHC-C1C	4.65	1.50	1.39
18	B	1235	CLA	O2A-CGA	4.65	1.46	1.33
18	B	1231	CLA	O2D-CGD	4.65	1.44	1.33
18	K	1141	CLA	CHC-C1C	4.65	1.50	1.39
18	B	1230	CLA	CHC-C1C	4.64	1.50	1.39
18	B	1215	CLA	C1C-C2C	-4.63	1.35	1.44
18	2	2001	CLA	CHC-C1C	4.63	1.50	1.39
18	A	1111	CLA	CHC-C1C	4.62	1.50	1.39
18	3	3012	CLA	CHC-C1C	4.62	1.50	1.39
18	F	1303	CLA	CHC-C1C	4.62	1.50	1.39
18	A	1152	CLA	CHC-C1C	4.61	1.50	1.39
18	B	1213	CLA	CHC-C1C	4.61	1.50	1.39
18	4	4008	CLA	CHC-C1C	4.61	1.50	1.39
18	1	1012	CLA	CHC-C1C	4.61	1.50	1.39
18	A	1113	CLA	C4C-C3C	-4.61	1.37	1.45
18	4	4003	CLA	CHC-C1C	4.61	1.50	1.39
18	L	1502	CLA	O2A-CGA	4.60	1.46	1.33
18	H	1505	CLA	CHC-C1C	4.60	1.50	1.39
20	A	6011	BCR	C10-C9	-4.60	1.29	1.35
18	2	2013	CLA	CHC-C1C	4.59	1.50	1.39
18	A	9011	CLA	O2A-CGA	4.59	1.46	1.33
18	L	1504	CLA	O2A-CGA	4.58	1.46	1.33
18	B	1201	CLA	CHC-C1C	4.58	1.50	1.39
18	B	9022	CLA	O2A-CGA	4.58	1.46	1.33
18	2	2012	CLA	CHC-C1C	4.58	1.50	1.39
18	A	1137	CLA	O2A-CGA	4.58	1.46	1.33
18	A	1102	CLA	CHC-C1C	4.58	1.50	1.39
18	G	1233	CLA	O2A-CGA	4.58	1.46	1.33
19	B	5002	PQN	C10-C5	4.57	1.48	1.40
18	B	1222	CLA	O2A-CGA	4.57	1.46	1.33
18	2	2015	CLA	CHC-C1C	4.57	1.50	1.39
18	1	1007	CLA	CHC-C1C	4.56	1.50	1.39
18	A	1118	CLA	CHC-C1C	4.56	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2004	CLA	CHC-C1C	4.55	1.50	1.39
18	H	1501	CLA	OBD-CAD	4.55	1.28	1.22
18	4	4009	CLA	CHC-C1C	4.54	1.50	1.39
18	A	1123	CLA	O2A-CGA	4.54	1.46	1.33
18	B	1241	CLA	CHC-C1C	4.54	1.50	1.39
18	F	1302	CLA	OBD-CAD	4.54	1.28	1.22
18	A	1101	CLA	CHC-C1C	4.54	1.50	1.39
18	3	3011	CLA	CHC-C1C	4.54	1.50	1.39
18	B	1212	CLA	C4C-C3C	-4.54	1.37	1.45
18	A	1124	CLA	CHC-C1C	4.53	1.50	1.39
18	B	1229	CLA	C4C-C3C	-4.53	1.37	1.45
18	B	1207	CLA	O2D-CGD	4.53	1.44	1.33
18	3	3002	CLA	CHC-C1C	4.52	1.50	1.39
18	3	2009	CLA	CHC-C1C	4.52	1.50	1.39
18	2	2010	CLA	CHC-C1C	4.52	1.50	1.39
18	2	2011	CLA	CHC-C1C	4.51	1.50	1.39
18	2	2007	CLA	CHC-C1C	4.51	1.50	1.39
18	A	1136	CLA	O2A-CGA	4.51	1.46	1.33
18	B	1242	CLA	OBD-CAD	4.51	1.28	1.22
18	1	1002	CLA	CHC-C1C	4.50	1.50	1.39
18	A	1110	CLA	CHC-C1C	4.50	1.50	1.39
18	A	1120	CLA	CHC-C1C	4.50	1.50	1.39
18	A	1148	CLA	CHC-C1C	4.50	1.50	1.39
18	A	1115	CLA	OBD-CAD	4.50	1.28	1.22
18	1	1011	CLA	CHC-C1C	4.49	1.50	1.39
18	A	1132	CLA	CHC-C1C	4.49	1.50	1.39
18	3	3006	CLA	CHC-C1C	4.49	1.50	1.39
18	B	1209	CLA	O2A-CGA	4.49	1.46	1.33
18	3	3008	CLA	CHC-C1C	4.49	1.50	1.39
18	A	1309	CLA	CHC-C1C	4.48	1.50	1.39
18	3	3010	CLA	CHC-C1C	4.47	1.50	1.39
18	A	9013	CLA	CHD-C4C	4.47	1.54	1.41
18	B	1223	CLA	CHC-C1C	4.47	1.50	1.39
18	B	1227	CLA	O2A-CGA	4.47	1.46	1.33
18	A	1147	CLA	CHC-C1C	4.46	1.50	1.39
18	F	1240	CLA	CHC-C1C	4.46	1.50	1.39
18	B	1242	CLA	O2A-CGA	4.46	1.46	1.33
18	B	1236	CLA	OBD-CAD	4.46	1.28	1.22
18	3	3004	CLA	CHC-C1C	4.46	1.50	1.39
18	1	1003	CLA	CHC-C1C	4.45	1.50	1.39
18	A	1103	CLA	O2A-CGA	4.44	1.46	1.33
18	B	1217	CLA	O2A-CGA	4.44	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4002	CLA	CHC-C1C	4.44	1.50	1.39
18	A	1133	CLA	CHC-C1C	4.44	1.50	1.39
18	2	2003	CLA	CHC-C1C	4.44	1.50	1.39
18	F	1305	CLA	CHC-C1C	4.43	1.50	1.39
18	3	3015	CLA	CHC-C1C	4.43	1.50	1.39
18	B	1211	CLA	CHC-C1C	4.42	1.50	1.39
18	B	1234	CLA	O2A-CGA	4.42	1.46	1.33
18	4	4010	CLA	CHC-C1C	4.41	1.50	1.39
18	A	1129	CLA	OBD-CAD	4.40	1.28	1.22
18	1	1006	CLA	CHC-C1C	4.39	1.50	1.39
18	4	4004	CLA	CHC-C1C	4.39	1.50	1.39
18	G	1248	CLA	CHC-C1C	4.39	1.50	1.39
18	A	1116	CLA	CHC-C1C	4.38	1.50	1.39
18	B	9012	CLA	OBD-CAD	4.38	1.28	1.22
18	B	1226	CLA	CHC-C1C	4.38	1.50	1.39
18	4	1304	CLA	O2A-CGA	4.37	1.46	1.33
18	A	1108	CLA	OBD-CAD	4.37	1.28	1.22
18	3	3005	CLA	CHC-C1C	4.36	1.50	1.39
18	A	1103	CLA	C1C-C2C	-4.36	1.36	1.44
18	1	1008	CLA	CHC-C1C	4.36	1.50	1.39
18	F	4015	CLA	CHC-C1C	4.36	1.50	1.39
18	B	1231	CLA	O2A-CGA	4.35	1.46	1.33
18	A	1127	CLA	CHC-C1C	4.35	1.50	1.39
18	B	1224	CLA	OBD-CAD	4.35	1.28	1.22
18	B	1219	CLA	CHD-C4C	4.34	1.53	1.41
18	B	1208	CLA	OBD-CAD	4.34	1.28	1.22
18	3	3013	CLA	CHC-C1C	4.34	1.50	1.39
18	4	4011	CLA	CHC-C1C	4.34	1.50	1.39
18	2	2002	CLA	CHC-C1C	4.34	1.50	1.39
18	B	1229	CLA	O2A-CGA	4.34	1.46	1.33
18	2	2006	CLA	CHC-C1C	4.34	1.50	1.39
18	B	1202	CLA	O2A-CGA	4.33	1.46	1.33
18	B	1232	CLA	O2A-CGA	4.33	1.46	1.33
18	B	1224	CLA	O2A-CGA	4.33	1.46	1.33
18	2	2008	CLA	CHC-C1C	4.33	1.50	1.39
18	B	1236	CLA	O2A-CGA	4.33	1.46	1.33
18	B	9022	CLA	OBD-CAD	4.32	1.28	1.22
18	B	1219	CLA	O2A-CGA	4.31	1.45	1.33
18	J	1308	CLA	CHC-C1C	4.30	1.50	1.39
18	A	1104	CLA	CHC-C1C	4.29	1.50	1.39
18	A	1134	CLA	CHC-C1C	4.29	1.50	1.39
18	A	1144	CLA	CHC-C1C	4.27	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1235	CLA	CHD-C4C	4.26	1.53	1.41
18	A	1105	CLA	CHC-C1C	4.25	1.49	1.39
18	B	1215	CLA	OBD-CAD	4.23	1.28	1.22
18	A	1131	CLA	CHD-C4C	4.20	1.53	1.41
18	B	9022	CLA	C3D-CAD	-4.19	1.35	1.46
18	L	1130	CLA	OBD-CAD	4.18	1.28	1.22
18	B	1229	CLA	OBD-CAD	4.18	1.28	1.22
18	B	1217	CLA	OBD-CAD	4.18	1.28	1.22
18	B	1209	CLA	OBD-CAD	4.17	1.28	1.22
18	F	1302	CLA	O2A-CGA	4.17	1.45	1.33
18	J	2107	CLA	O2A-CGA	4.17	1.45	1.33
18	K	1153	CLA	CHC-C1C	4.17	1.49	1.39
18	B	1203	CLA	O2A-CGA	4.16	1.45	1.33
18	B	1227	CLA	OBD-CAD	4.16	1.28	1.22
18	A	9013	CLA	O2A-CGA	4.15	1.46	1.33
18	B	1224	CLA	C4C-C3C	-4.13	1.37	1.45
18	B	1225	CLA	C4C-C3C	-4.13	1.37	1.45
18	B	1237	CLA	CHD-C4C	4.11	1.52	1.41
18	B	1225	CLA	C1C-C2C	-4.11	1.36	1.44
18	B	1228	CLA	C4C-C3C	-4.11	1.38	1.45
18	3	3007	CLA	CHC-C1C	4.09	1.49	1.39
18	B	1225	CLA	OBD-CAD	4.09	1.28	1.22
18	B	1207	CLA	OBD-CAD	4.09	1.28	1.22
18	B	9010	CLA	OBD-CAD	4.09	1.28	1.22
18	B	9010	CLA	C1C-C2C	-4.08	1.36	1.44
18	A	1109	CLA	C4C-CHD	4.08	1.51	1.41
18	B	1205	CLA	O2A-CGA	4.07	1.45	1.33
18	A	1129	CLA	CHD-C4C	4.06	1.52	1.41
18	B	1206	CLA	CHC-C1C	4.06	1.49	1.39
18	B	1231	CLA	CHD-C4C	4.05	1.52	1.41
18	B	1225	CLA	CHD-C4C	4.05	1.52	1.41
18	B	1235	CLA	O2D-CGD	4.04	1.43	1.33
18	B	1205	CLA	C4C-C3C	-4.03	1.38	1.45
18	B	1138	CLA	CHD-C4C	4.02	1.52	1.41
18	A	1126	CLA	CHD-C4C	4.00	1.52	1.41
18	A	1123	CLA	C1B-NB	-3.99	1.31	1.35
18	B	1215	CLA	CHD-C4C	3.99	1.52	1.41
18	B	1138	CLA	OBD-CAD	3.99	1.27	1.22
18	L	1502	CLA	CHD-C4C	3.98	1.52	1.41
18	A	1123	CLA	CHD-C4C	3.98	1.52	1.41
18	B	1202	CLA	CHD-C4C	3.97	1.52	1.41
18	A	1132	CLA	CHB-C4A	-3.97	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	1233	CLA	C4C-C3C	-3.95	1.38	1.45
18	B	1217	CLA	CHD-C4C	3.93	1.52	1.41
18	A	1111	CLA	CHD-C4C	3.92	1.52	1.41
18	A	1103	CLA	CHD-C4C	3.90	1.52	1.41
18	B	1203	CLA	CHD-C4C	3.88	1.52	1.41
18	A	1108	CLA	C4C-C3C	-3.88	1.38	1.45
18	A	1140	CLA	CHD-C4C	3.87	1.52	1.41
18	B	1218	CLA	C1C-C2C	-3.87	1.37	1.44
18	B	1239	CLA	CHD-C4C	3.86	1.52	1.41
18	G	1233	CLA	C4B-CHC	3.86	1.51	1.41
18	A	1106	CLA	C3A-C2A	-3.85	1.50	1.54
18	A	1107	CLA	CHD-C4C	3.84	1.52	1.41
18	A	9011	CLA	CHD-C4C	3.84	1.52	1.41
18	B	1208	CLA	C4B-CHC	3.83	1.51	1.41
18	F	1302	CLA	CHD-C4C	3.83	1.52	1.41
18	1	1007	CLA	CHD-C4C	3.83	1.52	1.41
18	B	9023	CLA	C4C-C3C	-3.83	1.38	1.45
18	B	1215	CLA	O2A-CGA	3.82	1.44	1.33
18	A	1122	CLA	CHD-C4C	3.82	1.52	1.41
18	A	1128	CLA	C1B-NB	-3.82	1.31	1.35
20	L	6020	BCR	C11-C12	-3.82	1.24	1.34
18	B	1208	CLA	CHD-C4C	3.82	1.52	1.41
18	B	1238	CLA	CHD-C4C	3.81	1.52	1.41
18	A	1101	CLA	CHD-C4C	3.80	1.52	1.41
18	B	1232	CLA	CHD-C4C	3.79	1.52	1.41
18	J	2107	CLA	CHD-C4C	3.79	1.52	1.41
18	B	9023	CLA	OBD-CAD	3.78	1.27	1.22
18	A	1128	CLA	CHD-C4C	3.78	1.52	1.41
18	I	1204	CLA	CHD-C4C	3.78	1.52	1.41
18	B	1228	CLA	CHD-C4C	3.77	1.52	1.41
18	B	1229	CLA	C4B-CHC	3.77	1.51	1.41
18	A	1129	CLA	C4B-CHC	3.77	1.51	1.41
18	A	1137	CLA	CHD-C4C	3.77	1.51	1.41
18	B	1222	CLA	CHD-C4C	3.76	1.51	1.41
18	A	1133	CLA	CHD-C4C	3.76	1.51	1.41
18	A	1128	CLA	OBD-CAD	3.76	1.27	1.22
18	A	1107	CLA	C4C-C3C	-3.75	1.38	1.45
18	L	1130	CLA	CHD-C4C	3.74	1.51	1.41
18	J	1308	CLA	CHD-C4C	3.74	1.51	1.41
18	B	1209	CLA	CHD-C4C	3.74	1.51	1.41
18	B	1201	CLA	MG-NA	-3.73	1.97	2.06
18	B	1207	CLA	CHD-C4C	3.73	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	1304	CLA	CHD-C4C	3.72	1.51	1.41
18	B	9012	CLA	CHD-C4C	3.71	1.51	1.41
18	A	1124	CLA	MG-NA	-3.71	1.97	2.06
18	A	1107	CLA	C1C-C2C	-3.70	1.37	1.44
19	A	5001	PQN	C10-C5	3.70	1.46	1.40
18	B	1301	CLA	C4B-CHC	3.69	1.51	1.43
18	2	2001	CLA	CHD-C4C	3.69	1.51	1.41
18	A	1119	CLA	CHD-C4C	3.69	1.51	1.41
18	B	1236	CLA	CHD-C4C	3.69	1.51	1.41
18	B	1205	CLA	CHD-C4C	3.69	1.51	1.41
18	B	1220	CLA	CHD-C4C	3.68	1.51	1.41
18	A	1120	CLA	CHD-C4C	3.68	1.51	1.41
18	3	3008	CLA	CHD-C4C	3.68	1.51	1.41
18	A	1119	CLA	C4B-CHC	3.67	1.51	1.41
18	B	1234	CLA	CHD-C4C	3.66	1.51	1.41
18	2	2005	CLA	CHD-C4C	3.66	1.51	1.41
18	H	1501	CLA	CHD-C4C	3.66	1.51	1.41
18	2	2008	CLA	CHD-C4C	3.65	1.51	1.41
18	B	1234	CLA	C4B-CHC	3.65	1.51	1.41
18	B	9022	CLA	CHD-C4C	3.65	1.51	1.41
18	B	1235	CLA	C1C-C2C	-3.65	1.37	1.44
18	A	1126	CLA	O2D-CGD	3.64	1.42	1.33
18	B	1201	CLA	CHD-C4C	3.64	1.51	1.41
18	F	1240	CLA	CHD-C4C	3.64	1.51	1.41
18	A	1102	CLA	CHD-C4C	3.64	1.51	1.41
18	B	1242	CLA	C4B-CHC	3.64	1.51	1.41
18	4	1009	CLA	C4B-CHC	3.63	1.51	1.43
18	F	1306	CLA	C4B-CHC	3.63	1.51	1.43
18	4	4006	CLA	MG-NA	-3.63	1.97	2.06
18	L	1502	CLA	C4B-CHC	3.63	1.51	1.41
18	1	1013	CLA	CHD-C4C	3.63	1.51	1.41
18	B	9010	CLA	C4C-C3C	-3.62	1.38	1.45
18	A	1109	CLA	C1D-CHD	3.62	1.49	1.41
18	B	1202	CLA	C3D-CAD	-3.62	1.36	1.46
18	L	1503	CLA	C3D-CAD	-3.62	1.36	1.46
18	2	2005	CLA	C4B-CHC	3.62	1.51	1.43
18	4	4012	CLA	CHD-C4C	3.62	1.51	1.41
18	2	2015	CLA	CHD-C4C	3.62	1.51	1.41
18	2	2006	CLA	CHD-C4C	3.61	1.51	1.41
18	B	1241	CLA	CHB-C4A	-3.61	1.32	1.34
18	A	1120	CLA	MG-NA	-3.61	1.97	2.06
18	B	1226	CLA	CHD-C4C	3.61	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1008	CLA	CHD-C4C	3.61	1.51	1.41
18	B	1216	CLA	CHD-C4C	3.61	1.51	1.41
18	4	4003	CLA	CHD-C4C	3.61	1.51	1.41
18	B	1237	CLA	OBD-CAD	3.61	1.27	1.22
18	4	4012	CLA	MG-NA	-3.60	1.97	2.06
18	G	1233	CLA	CHD-C4C	3.59	1.51	1.41
18	4	4008	CLA	CHD-C4C	3.58	1.51	1.41
18	L	1504	CLA	CHD-C4C	3.58	1.51	1.41
18	A	1118	CLA	CHD-C4C	3.58	1.51	1.41
18	A	1137	CLA	C4B-CHC	3.57	1.50	1.41
18	B	9010	CLA	CHD-C4C	3.57	1.51	1.41
18	B	1214	CLA	C4B-CHC	3.57	1.50	1.41
18	F	1305	CLA	CHD-C4C	3.57	1.51	1.41
18	B	1205	CLA	C1C-C2C	-3.57	1.37	1.44
18	4	4010	CLA	CHD-C4C	3.56	1.51	1.41
18	B	1221	CLA	CHD-C4C	3.56	1.51	1.41
18	1	1014	CLA	CHD-C4C	3.56	1.51	1.41
18	A	1135	CLA	C4C-C3C	-3.56	1.38	1.45
18	A	1119	CLA	C4C-C3C	-3.55	1.38	1.45
18	2	2010	CLA	CHD-C4C	3.54	1.51	1.41
18	B	1236	CLA	C4C-C3C	-3.54	1.38	1.45
18	B	1214	CLA	C4C-C3C	-3.54	1.38	1.45
18	B	1239	CLA	C1C-C2C	-3.54	1.37	1.44
18	A	1135	CLA	CHD-C4C	3.54	1.51	1.41
18	B	1223	CLA	MG-NA	-3.54	1.97	2.06
18	A	1132	CLA	C4B-CHC	3.53	1.51	1.43
18	B	1218	CLA	C4B-CHC	3.53	1.50	1.41
18	1	1001	CLA	C4B-CHC	3.53	1.51	1.43
18	1	1005	CLA	C4B-CHC	3.53	1.51	1.43
18	4	4009	CLA	CHD-C4C	3.53	1.51	1.41
18	3	3015	CLA	CHD-C4C	3.53	1.51	1.41
18	A	1115	CLA	CHD-C4C	3.53	1.51	1.41
18	B	1214	CLA	CHD-C4C	3.52	1.51	1.41
18	2	2012	CLA	MG-NA	-3.52	1.97	2.06
18	A	1144	CLA	CHD-C4C	3.52	1.51	1.41
18	A	1116	CLA	CHD-C4C	3.52	1.51	1.41
18	K	1153	CLA	CHD-C4C	3.52	1.51	1.41
18	A	1127	CLA	CHD-C4C	3.52	1.51	1.41
18	4	4006	CLA	C4B-CHC	3.52	1.50	1.43
18	3	3002	CLA	CHD-C4C	3.52	1.51	1.41
18	4	4001	CLA	CHD-C4C	3.51	1.51	1.41
18	3	3004	CLA	CHD-C4C	3.51	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1242	CLA	C4C-C3C	-3.51	1.39	1.45
18	A	1113	CLA	CHD-C4C	3.51	1.51	1.41
18	4	4006	CLA	CHD-C4C	3.51	1.51	1.41
18	3	3005	CLA	CHD-C4C	3.51	1.51	1.41
18	B	1210	CLA	C4B-CHC	3.51	1.50	1.43
18	4	4012	CLA	C4B-CHC	3.51	1.50	1.43
18	A	1309	CLA	CHD-C4C	3.50	1.51	1.41
18	A	1122	CLA	C4B-CHC	3.50	1.50	1.41
18	A	1128	CLA	O2A-CGA	3.50	1.43	1.33
18	2	2013	CLA	CHD-C4C	3.50	1.51	1.41
18	B	1236	CLA	C4B-CHC	3.50	1.50	1.41
18	F	1303	CLA	CHD-C4C	3.50	1.51	1.41
18	B	1228	CLA	OBD-CAD	3.50	1.27	1.22
18	F	1303	CLA	C4B-CHC	3.50	1.50	1.43
18	B	1227	CLA	CHD-C4C	3.49	1.51	1.41
18	J	1307	CLA	CHD-C4C	3.49	1.51	1.41
18	J	1307	CLA	C4B-CHC	3.48	1.50	1.43
18	3	3001	CLA	C4B-CHC	3.48	1.50	1.43
18	A	1106	CLA	CHD-C4C	3.48	1.51	1.41
18	A	1148	CLA	CHD-C4C	3.48	1.51	1.41
18	B	1222	CLA	C4B-CHC	3.48	1.50	1.41
18	B	1220	CLA	C4C-C3C	-3.48	1.39	1.45
18	1	1011	CLA	CHD-C4C	3.48	1.51	1.41
18	3	3001	CLA	CHD-C4C	3.47	1.51	1.41
18	A	1143	CLA	C4B-CHC	3.47	1.50	1.43
18	B	1212	CLA	CHD-C4C	3.47	1.51	1.41
18	B	1223	CLA	CHD-C4C	3.47	1.51	1.41
18	2	2004	CLA	CHD-C4C	3.47	1.51	1.41
18	K	1150	CLA	CHD-C4C	3.47	1.51	1.41
18	A	1146	CLA	C4B-CHC	3.47	1.50	1.43
18	B	1221	CLA	C1C-C2C	-3.47	1.37	1.44
18	A	9013	CLA	C1C-C2C	-3.46	1.37	1.44
18	2	2011	CLA	CHD-C4C	3.46	1.51	1.41
18	L	1130	CLA	C4B-CHC	3.46	1.50	1.41
18	4	4007	CLA	CHD-C4C	3.46	1.51	1.41
18	1	1002	CLA	CHD-C4C	3.46	1.51	1.41
18	4	4005	CLA	CHD-C4C	3.46	1.51	1.41
18	1	1001	CLA	CHD-C4C	3.46	1.51	1.41
18	B	1224	CLA	C4B-CHC	3.45	1.50	1.41
18	3	3011	CLA	CHD-C4C	3.45	1.51	1.41
18	B	1206	CLA	CHD-C4C	3.45	1.51	1.41
18	A	1106	CLA	C3B-C2B	-3.45	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1218	CLA	MG-NA	-3.45	1.98	2.06
18	1	1004	CLA	C4B-CHC	3.45	1.50	1.43
18	B	1301	CLA	CHD-C4C	3.44	1.51	1.41
18	J	2107	CLA	C4B-CHC	3.44	1.50	1.41
18	A	1142	CLA	C4B-CHC	3.44	1.50	1.43
18	F	1306	CLA	CHD-C4C	3.44	1.51	1.41
18	1	1010	CLA	CHD-C4C	3.44	1.51	1.41
18	L	1125	CLA	CHD-C4C	3.44	1.51	1.41
18	L	1503	CLA	C1C-C2C	-3.44	1.37	1.44
18	A	1109	CLA	C4B-CHC	3.44	1.50	1.43
18	B	1207	CLA	C4C-C3C	-3.43	1.39	1.45
18	B	1224	CLA	CHD-C4C	3.43	1.51	1.41
18	3	3013	CLA	CHD-C4C	3.43	1.51	1.41
18	A	1123	CLA	C4C-C3C	-3.43	1.39	1.45
18	2	2002	CLA	CHD-C4C	3.43	1.51	1.41
18	B	1237	CLA	C1C-C2C	-3.43	1.37	1.44
18	A	1146	CLA	CHD-C4C	3.43	1.51	1.41
18	A	1105	CLA	CHD-C4C	3.43	1.51	1.41
18	B	1216	CLA	C4B-CHC	3.43	1.50	1.41
18	1	1010	CLA	C4B-CHC	3.42	1.50	1.43
18	2	2004	CLA	C4B-CHC	3.42	1.50	1.43
18	F	4015	CLA	CHD-C4C	3.42	1.50	1.41
18	3	3007	CLA	CHD-C4C	3.42	1.50	1.41
18	A	1135	CLA	C4B-CHC	3.42	1.50	1.41
18	B	1235	CLA	C1B-NB	-3.41	1.32	1.35
18	G	1248	CLA	MG-NA	-3.41	1.98	2.06
18	1	1003	CLA	CHD-C4C	3.41	1.50	1.41
18	A	1132	CLA	CHD-C4C	3.41	1.50	1.41
18	1	1014	CLA	C4B-CHC	3.41	1.50	1.43
18	A	1108	CLA	CHD-C4C	3.41	1.50	1.41
18	1	1014	CLA	MG-NA	-3.40	1.98	2.06
18	3	3013	CLA	MG-NA	-3.40	1.98	2.06
18	2	2007	CLA	MG-NA	-3.40	1.98	2.06
18	4	4007	CLA	C4B-CHC	3.39	1.50	1.43
18	H	1501	CLA	C4C-C3C	-3.39	1.39	1.45
18	3	3009	CLA	CHD-C4C	3.39	1.50	1.41
18	B	1230	CLA	CHD-C4C	3.39	1.50	1.41
18	1	1005	CLA	CHD-C4C	3.39	1.50	1.41
18	4	1304	CLA	C4B-CHC	3.39	1.50	1.41
18	B	1207	CLA	C4B-CHC	3.39	1.50	1.41
18	A	1134	CLA	CHD-C4C	3.38	1.50	1.41
18	3	3010	CLA	CHD-C4C	3.38	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1123	CLA	C4B-CHC	3.38	1.50	1.41
18	B	1230	CLA	C4B-CHC	3.38	1.50	1.43
18	4	4004	CLA	CHD-C4C	3.38	1.50	1.41
18	B	1212	CLA	C4B-CHC	3.37	1.50	1.41
18	2	2012	CLA	CHD-C4C	3.37	1.50	1.41
18	B	1241	CLA	CHD-C4C	3.37	1.50	1.41
18	A	1143	CLA	CHD-C4C	3.37	1.50	1.41
18	A	1126	CLA	C4B-CHC	3.37	1.50	1.41
18	4	4005	CLA	MG-NA	-3.37	1.98	2.06
18	B	9023	CLA	C4B-CHC	3.36	1.50	1.41
18	B	1210	CLA	CHD-C4C	3.36	1.50	1.41
18	B	9012	CLA	C4C-C3C	-3.36	1.39	1.45
18	A	1131	CLA	C1C-C2C	-3.35	1.38	1.44
18	4	4003	CLA	C4B-CHC	3.35	1.50	1.43
18	3	3003	CLA	CHD-C4C	3.35	1.50	1.41
18	3	3008	CLA	MG-NA	-3.35	1.98	2.06
18	B	1232	CLA	C4B-CHC	3.35	1.50	1.41
18	4	4004	CLA	MG-NA	-3.35	1.98	2.06
18	F	1240	CLA	MG-NA	-3.35	1.98	2.06
18	B	1238	CLA	MG-NA	-3.35	1.98	2.06
18	B	1213	CLA	CHD-C4C	3.34	1.50	1.41
18	2	2003	CLA	MG-NA	-3.34	1.98	2.06
18	3	2009	CLA	CHD-C4C	3.34	1.50	1.41
18	4	4002	CLA	CHD-C4C	3.34	1.50	1.41
18	4	4011	CLA	CHD-C4C	3.34	1.50	1.41
18	B	9023	CLA	CHD-C4C	3.34	1.50	1.41
18	1	1002	CLA	MG-NA	-3.34	1.98	2.06
18	1	1003	CLA	MG-NA	-3.34	1.98	2.06
18	B	1226	CLA	CHB-C4A	-3.33	1.32	1.34
18	A	1152	CLA	C4B-CHC	3.33	1.50	1.43
18	K	1141	CLA	CHD-C4C	3.33	1.50	1.41
18	4	4005	CLA	C4B-CHC	3.33	1.50	1.43
18	B	1242	CLA	CHD-C4C	3.32	1.50	1.41
18	F	1302	CLA	C4B-CHC	3.32	1.50	1.41
18	3	3004	CLA	MG-NA	-3.32	1.98	2.06
18	1	1012	CLA	CHD-C4C	3.32	1.50	1.41
18	J	1308	CLA	MG-NA	-3.32	1.98	2.06
18	B	1220	CLA	C4B-CHC	3.32	1.50	1.41
18	A	1104	CLA	C4B-CHC	3.32	1.50	1.43
18	3	3001	CLA	MG-NA	-3.32	1.98	2.06
18	F	1305	CLA	C4B-CHC	3.32	1.50	1.43
18	B	1219	CLA	C4B-CHC	3.32	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1006	CLA	C4B-CHC	3.31	1.50	1.43
18	2	2003	CLA	CHD-C4C	3.31	1.50	1.41
18	B	9012	CLA	C4B-CHC	3.31	1.50	1.41
18	B	1241	CLA	C4B-CHC	3.31	1.50	1.43
18	2	2010	CLA	MG-NA	-3.31	1.98	2.06
18	A	1116	CLA	MG-NA	-3.31	1.98	2.06
18	2	2013	CLA	C4B-CHC	3.31	1.50	1.43
18	4	4010	CLA	C4B-CHC	3.31	1.50	1.43
18	F	4015	CLA	C4B-CHC	3.31	1.50	1.43
18	A	1134	CLA	C4B-CHC	3.31	1.50	1.43
18	F	1139	CLA	CHD-C4C	3.30	1.50	1.41
18	A	1142	CLA	CHD-C4C	3.30	1.50	1.41
18	A	1127	CLA	MG-NA	-3.30	1.98	2.06
18	B	1213	CLA	MG-NA	-3.29	1.98	2.06
18	A	1128	CLA	C4C-C3C	-3.29	1.39	1.45
18	2	2011	CLA	C4B-CHC	3.29	1.50	1.43
18	B	1211	CLA	CHD-C4C	3.29	1.50	1.41
18	1	1006	CLA	MG-NA	-3.29	1.98	2.06
18	A	1117	CLA	CHD-C4C	3.29	1.50	1.41
18	4	4001	CLA	C4B-CHC	3.29	1.50	1.43
18	B	9012	CLA	C3B-C2B	-3.29	1.35	1.40
18	A	1120	CLA	C4B-CHC	3.29	1.50	1.43
18	F	1240	CLA	C4B-CHC	3.29	1.50	1.43
18	L	1502	CLA	C4C-C3C	-3.28	1.39	1.45
18	B	1211	CLA	MG-NA	-3.28	1.98	2.06
18	B	1210	CLA	MG-NA	-3.28	1.98	2.06
18	B	9010	CLA	C4B-CHC	3.28	1.50	1.41
18	1	1007	CLA	MG-NA	-3.28	1.98	2.06
18	B	1238	CLA	C4B-CHC	3.28	1.50	1.41
18	4	4009	CLA	MG-NA	-3.28	1.98	2.06
18	B	1236	CLA	C3D-CAD	-3.28	1.37	1.46
18	L	1130	CLA	C4C-C3C	-3.27	1.39	1.45
18	3	3007	CLA	MG-NA	-3.27	1.98	2.06
18	A	1110	CLA	CHD-C4C	3.26	1.50	1.41
18	H	1505	CLA	CHD-C4C	3.26	1.50	1.41
18	A	1124	CLA	C4B-CHC	3.26	1.50	1.43
18	A	1104	CLA	CHD-C4C	3.26	1.50	1.41
18	B	1237	CLA	C4B-CHC	3.26	1.50	1.41
18	A	1118	CLA	MG-NA	-3.26	1.98	2.06
18	4	4010	CLA	MG-NA	-3.26	1.98	2.06
18	A	1148	CLA	MG-NA	-3.25	1.98	2.06
18	A	1144	CLA	MG-NA	-3.25	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1152	CLA	CHD-C4C	3.25	1.50	1.41
18	3	3006	CLA	CHD-C4C	3.25	1.50	1.41
18	4	4007	CLA	MG-NA	-3.25	1.98	2.06
18	A	1104	CLA	CHA-C1A	3.25	1.50	1.41
18	A	1116	CLA	C4B-CHC	3.25	1.50	1.43
18	B	1234	CLA	C4C-C3C	-3.25	1.39	1.45
18	1	1013	CLA	C4B-CHC	3.25	1.50	1.43
18	G	1248	CLA	CHD-C4C	3.25	1.50	1.41
18	F	1302	CLA	C4C-C3C	-3.25	1.39	1.45
18	3	3011	CLA	C4B-CHC	3.25	1.50	1.43
18	B	1231	CLA	C4B-CHC	3.24	1.50	1.41
18	A	1111	CLA	C4B-CHC	3.24	1.50	1.43
18	A	1147	CLA	CHD-C4C	3.24	1.50	1.41
18	K	1141	CLA	C4B-CHC	3.24	1.50	1.43
18	A	1118	CLA	C4B-CHC	3.24	1.50	1.43
18	B	9010	CLA	C3D-CAD	-3.24	1.37	1.46
18	A	1151	CLA	CHD-C4C	3.24	1.50	1.41
18	1	1005	CLA	MG-NA	-3.24	1.98	2.06
18	1	1011	CLA	MG-NA	-3.23	1.98	2.06
18	4	4013	CLA	CHD-C4C	3.23	1.50	1.41
18	B	1238	CLA	C1C-C2C	-3.23	1.38	1.44
18	2	2002	CLA	MG-NA	-3.23	1.98	2.06
18	B	1237	CLA	C4C-C3C	-3.23	1.39	1.45
18	A	1133	CLA	C4B-CHC	3.23	1.50	1.43
18	B	1202	CLA	C1C-C2C	-3.23	1.38	1.44
18	A	1102	CLA	C4B-CHC	3.23	1.50	1.43
18	1	1012	CLA	MG-NA	-3.23	1.98	2.06
18	B	1218	CLA	C1C-NC	-3.22	1.33	1.37
18	H	1501	CLA	C4B-CHC	3.22	1.50	1.41
18	3	3012	CLA	CHD-C4C	3.22	1.50	1.41
18	B	9022	CLA	C1C-C2C	-3.22	1.38	1.44
18	F	4015	CLA	MG-NA	-3.22	1.98	2.06
18	A	1147	CLA	MG-NA	-3.22	1.98	2.06
18	3	3010	CLA	C4B-CHC	3.22	1.50	1.43
18	K	1150	CLA	C4B-CHC	3.22	1.50	1.43
18	3	3015	CLA	C4B-CHC	3.21	1.50	1.43
18	A	1151	CLA	C4B-CHC	3.21	1.50	1.43
18	B	1206	CLA	C4B-CHC	3.21	1.50	1.43
18	1	1011	CLA	C4B-CHC	3.21	1.50	1.43
18	A	1101	CLA	C4B-CHC	3.21	1.50	1.43
18	L	1125	CLA	C4B-CHC	3.21	1.50	1.43
18	2	2007	CLA	C4B-CHC	3.21	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	1013	CLA	MG-NA	-3.21	1.98	2.06
18	3	3013	CLA	C4B-CHC	3.20	1.50	1.43
18	4	4002	CLA	C4B-CHC	3.20	1.50	1.43
18	3	3004	CLA	C4B-CHC	3.20	1.50	1.43
18	1	1008	CLA	C4B-CHC	3.19	1.50	1.43
18	3	3012	CLA	C4B-CHC	3.19	1.50	1.43
18	1	1008	CLA	MG-NA	-3.19	1.98	2.06
18	B	1223	CLA	C4B-CHC	3.19	1.50	1.43
18	B	1228	CLA	C4B-CHC	3.18	1.49	1.41
18	B	1205	CLA	C4B-CHC	3.18	1.49	1.41
18	A	1111	CLA	MG-NA	-3.18	1.98	2.06
18	4	4011	CLA	MG-NA	-3.17	1.98	2.06
18	2	2015	CLA	C4B-CHC	3.17	1.50	1.43
18	1	1006	CLA	CHD-C4C	3.17	1.50	1.41
18	2	2004	CLA	MG-NA	-3.17	1.98	2.06
18	3	3005	CLA	MG-NA	-3.17	1.98	2.06
18	2	2008	CLA	MG-NA	-3.17	1.98	2.06
18	2	2012	CLA	C4B-CHC	3.16	1.50	1.43
18	L	1504	CLA	C4B-CHC	3.16	1.49	1.41
18	B	1241	CLA	MG-NA	-3.16	1.98	2.06
18	3	3006	CLA	MG-NA	-3.16	1.98	2.06
18	2	2007	CLA	CHD-C4C	3.16	1.50	1.41
18	3	3006	CLA	C4B-CHC	3.16	1.50	1.43
18	A	1122	CLA	C1C-C2C	-3.16	1.38	1.44
18	3	3003	CLA	C4B-CHC	3.16	1.50	1.43
18	4	4013	CLA	MG-NA	-3.16	1.98	2.06
18	B	1229	CLA	C3D-CAD	-3.16	1.38	1.46
18	A	1143	CLA	MG-NA	-3.16	1.98	2.06
18	B	1138	CLA	C1C-C2C	-3.16	1.38	1.44
18	I	1204	CLA	C4B-CHC	3.16	1.49	1.41
18	2	2010	CLA	C4B-CHC	3.15	1.50	1.43
18	B	1206	CLA	MG-NA	-3.15	1.98	2.06
18	A	1128	CLA	C4B-CHC	3.15	1.49	1.41
18	3	2009	CLA	C4B-CHC	3.15	1.50	1.43
18	A	1136	CLA	C4B-CHC	3.15	1.49	1.41
18	B	1225	CLA	C4B-CHC	3.14	1.49	1.41
18	4	4004	CLA	C4B-CHC	3.14	1.50	1.43
18	3	3009	CLA	C4B-CHC	3.14	1.50	1.43
18	A	1148	CLA	C4B-CHC	3.14	1.50	1.43
18	B	9022	CLA	C4C-C3C	-3.14	1.39	1.45
18	A	1117	CLA	C4B-CHC	3.14	1.50	1.43
18	A	1309	CLA	MG-NA	-3.14	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	1306	CLA	MG-NA	-3.13	1.98	2.06
18	3	3002	CLA	C4B-CHC	3.13	1.50	1.43
18	A	1108	CLA	C4B-CHC	3.13	1.49	1.41
20	I	6018	BCR	C1-C6	-3.13	1.49	1.53
18	B	1301	CLA	MG-NA	-3.13	1.98	2.06
18	4	1009	CLA	CHD-C4C	3.13	1.50	1.41
18	B	1220	CLA	OBD-CAD	3.13	1.26	1.22
18	1	1003	CLA	C4B-CHC	3.12	1.50	1.43
18	J	1308	CLA	C4B-CHC	3.12	1.50	1.43
18	B	1218	CLA	CHD-C4C	3.12	1.50	1.41
18	A	1110	CLA	C4B-CHC	3.12	1.50	1.43
18	1	1001	CLA	MG-NA	-3.12	1.98	2.06
18	B	1225	CLA	MG-NA	-3.12	1.98	2.06
18	1	1004	CLA	CHD-C4C	3.11	1.50	1.41
18	4	4013	CLA	C4B-CHC	3.11	1.50	1.43
18	A	1105	CLA	MG-NA	-3.11	1.98	2.06
18	4	1304	CLA	C4C-C3C	-3.11	1.39	1.45
18	A	1140	CLA	C1B-CHB	3.11	1.49	1.41
18	A	1107	CLA	C4B-CHC	3.10	1.49	1.41
18	B	1201	CLA	C4B-CHC	3.10	1.50	1.43
18	B	1216	CLA	C4C-C3C	-3.10	1.39	1.45
18	A	1122	CLA	C4C-C3C	-3.10	1.39	1.45
18	A	1142	CLA	MG-NA	-3.09	1.98	2.06
18	B	1227	CLA	C1C-C2C	-3.09	1.38	1.44
18	B	1229	CLA	CHD-C4C	3.08	1.50	1.41
18	2	2003	CLA	C4B-CHC	3.08	1.50	1.43
18	2	2001	CLA	C4B-CHC	3.08	1.50	1.43
18	3	2009	CLA	MG-NA	-3.08	1.99	2.06
18	F	1303	CLA	MG-NA	-3.08	1.99	2.06
18	A	1147	CLA	C4B-CHC	3.08	1.50	1.43
18	1	1002	CLA	C4B-CHC	3.07	1.50	1.43
18	B	1213	CLA	C4B-CHC	3.07	1.50	1.43
18	B	1217	CLA	C4B-CHC	3.07	1.49	1.41
18	1	1007	CLA	C4B-CHC	3.07	1.50	1.43
18	A	1113	CLA	C1C-C2C	-3.07	1.38	1.44
18	2	2013	CLA	MG-NA	-3.07	1.99	2.06
18	B	9022	CLA	C3B-C2B	-3.06	1.36	1.40
18	A	1124	CLA	CHD-C4C	3.06	1.49	1.41
18	A	1136	CLA	CHD-C4C	3.06	1.49	1.41
18	B	9022	CLA	C4B-CHC	3.06	1.49	1.41
18	4	4001	CLA	MG-NA	-3.06	1.99	2.06
18	H	1505	CLA	MG-NA	-3.06	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1102	CLA	MG-NA	-3.06	1.99	2.06
18	B	1220	CLA	C3D-CAD	-3.05	1.38	1.46
18	A	1101	CLA	MG-NA	-3.05	1.99	2.06
18	2	2002	CLA	C4B-CHC	3.05	1.50	1.43
18	A	1309	CLA	C4B-CHC	3.05	1.50	1.43
18	A	1115	CLA	C4C-C3C	-3.05	1.39	1.45
18	3	3008	CLA	C4B-CHC	3.04	1.50	1.43
18	4	4008	CLA	C4B-CHC	3.04	1.50	1.43
18	B	1201	CLA	CHA-C1A	3.03	1.49	1.41
18	B	1216	CLA	C1C-C2C	-3.03	1.38	1.44
18	B	1209	CLA	C4B-CHC	3.03	1.49	1.41
18	B	1221	CLA	C4C-C3C	-3.03	1.39	1.45
18	K	1150	CLA	MG-NA	-3.03	1.99	2.06
18	B	1227	CLA	C4C-C3C	-3.02	1.39	1.45
18	A	1107	CLA	C1B-CHB	3.02	1.49	1.41
18	A	1144	CLA	C4B-CHC	3.02	1.49	1.43
18	B	1225	CLA	C3D-CAD	-3.01	1.38	1.46
18	B	1231	CLA	C1C-C2C	-3.01	1.38	1.44
18	B	1239	CLA	C4B-CHC	3.01	1.49	1.41
18	4	4008	CLA	MG-NA	-3.01	1.99	2.06
18	A	9013	CLA	C1C-NC	-3.00	1.33	1.37
18	A	1105	CLA	C4B-CHC	3.00	1.49	1.43
18	2	2006	CLA	C4B-CHC	3.00	1.49	1.43
18	L	1503	CLA	OBD-CAD	3.00	1.26	1.22
18	B	1222	CLA	C4C-C3C	-3.00	1.39	1.45
18	B	1239	CLA	C4C-C3C	-2.99	1.39	1.45
18	B	1202	CLA	C4B-CHC	2.99	1.49	1.41
18	3	3009	CLA	MG-NA	-2.99	1.99	2.06
18	H	1505	CLA	C4B-CHC	2.99	1.49	1.43
18	2	2011	CLA	MG-NA	-2.99	1.99	2.06
18	B	1202	CLA	C4C-C3C	-2.99	1.39	1.45
18	A	1140	CLA	C4C-C3C	-2.98	1.39	1.45
18	1	1010	CLA	MG-NA	-2.98	1.99	2.06
18	K	1153	CLA	C4B-CHC	2.98	1.49	1.43
18	B	1231	CLA	C4C-C3C	-2.98	1.39	1.45
18	A	1152	CLA	MG-NA	-2.98	1.99	2.06
18	L	1125	CLA	MG-NA	-2.98	1.99	2.06
18	F	1139	CLA	C4B-CHC	2.98	1.49	1.41
18	B	1232	CLA	C4C-C3C	-2.98	1.39	1.45
18	L	1503	CLA	CHD-C4C	2.97	1.49	1.41
18	B	1235	CLA	C4B-NB	-2.97	1.32	1.35
18	A	1134	CLA	CHA-C1A	2.97	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4009	CLA	C4B-CHC	2.96	1.49	1.43
18	L	1503	CLA	C4B-CHC	2.96	1.49	1.41
18	A	1135	CLA	C1C-C2C	-2.96	1.38	1.44
18	B	1241	CLA	C1B-NB	-2.96	1.32	1.35
18	1	1012	CLA	C4B-CHC	2.96	1.49	1.43
18	A	1110	CLA	MG-NA	-2.96	1.99	2.06
18	2	2005	CLA	CHA-C1A	2.96	1.49	1.41
18	4	4011	CLA	C4B-CHC	2.96	1.49	1.43
18	B	1235	CLA	C4B-CHC	2.96	1.49	1.41
18	A	9011	CLA	C1C-C2C	-2.96	1.38	1.44
18	B	1238	CLA	C4C-C3C	-2.95	1.40	1.45
18	3	3005	CLA	C4B-CHC	2.95	1.49	1.43
18	1	1004	CLA	MG-NA	-2.95	1.99	2.06
18	K	1153	CLA	CHB-C4A	-2.95	1.32	1.34
18	2	2006	CLA	MG-NA	-2.95	1.99	2.06
18	A	1131	CLA	C4B-CHC	2.95	1.49	1.41
18	L	1504	CLA	C4C-C3C	-2.94	1.40	1.45
18	A	1115	CLA	MG-NA	-2.94	1.99	2.06
18	A	1113	CLA	C3D-CAD	-2.94	1.38	1.46
18	B	1215	CLA	C4B-CHC	2.94	1.49	1.41
18	A	1128	CLA	C1C-C2C	-2.93	1.38	1.44
18	B	1242	CLA	C3D-CAD	-2.92	1.38	1.46
18	2	2001	CLA	MG-NA	-2.91	1.99	2.06
18	2	2008	CLA	C4B-CHC	2.91	1.49	1.43
18	A	1127	CLA	C4B-CHC	2.90	1.49	1.43
18	A	1140	CLA	C4B-CHC	2.90	1.49	1.41
18	3	3002	CLA	MG-NA	-2.90	1.99	2.06
18	A	1115	CLA	C1C-C2C	-2.90	1.39	1.44
18	B	1235	CLA	C1C-NC	-2.90	1.33	1.37
18	A	1133	CLA	MG-NA	-2.90	1.99	2.06
18	L	1130	CLA	C1C-C2C	-2.89	1.39	1.44
18	K	1141	CLA	MG-NA	-2.88	1.99	2.06
18	A	1137	CLA	C4C-C3C	-2.88	1.40	1.45
18	A	1131	CLA	MG-NA	-2.88	1.99	2.06
18	B	1226	CLA	C4B-CHC	2.87	1.49	1.43
18	B	1216	CLA	MG-NA	-2.87	1.99	2.06
18	A	1146	CLA	MG-NA	-2.87	1.99	2.06
18	J	1307	CLA	MG-NA	-2.87	1.99	2.06
18	2	2015	CLA	MG-NA	-2.86	1.99	2.06
18	K	1153	CLA	CHA-C1A	2.86	1.49	1.41
18	B	1232	CLA	C1B-NB	-2.86	1.32	1.35
18	1	1011	CLA	CHA-C1A	2.86	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1103	CLA	C4C-C3C	-2.84	1.40	1.45
18	A	1106	CLA	C4B-CHC	2.84	1.48	1.41
18	F	1305	CLA	CHA-C1A	2.84	1.49	1.41
18	B	1217	CLA	C1C-C2C	-2.84	1.39	1.44
18	G	1248	CLA	C4B-CHC	2.84	1.49	1.43
18	B	1242	CLA	C1C-C2C	-2.84	1.39	1.44
18	B	1208	CLA	C4C-C3C	-2.84	1.40	1.45
18	F	1139	CLA	C4C-C3C	-2.84	1.40	1.45
18	3	3007	CLA	C4B-CHC	2.83	1.49	1.43
18	A	1113	CLA	MG-NA	-2.83	1.99	2.06
18	A	1108	CLA	C3D-CAD	-2.83	1.38	1.46
18	3	3004	CLA	CHA-C1A	2.83	1.49	1.41
18	B	1226	CLA	MG-NA	-2.83	1.99	2.06
18	B	1205	CLA	C3D-CAD	-2.82	1.38	1.46
18	B	1224	CLA	C1C-C2C	-2.82	1.39	1.44
18	H	1501	CLA	C1C-C2C	-2.82	1.39	1.44
18	B	1228	CLA	C1C-C2C	-2.82	1.39	1.44
18	I	1204	CLA	C4C-C3C	-2.82	1.40	1.45
18	A	1136	CLA	C3D-CAD	-2.82	1.38	1.46
18	A	1113	CLA	C4B-CHC	2.81	1.48	1.41
18	3	3009	CLA	CHA-C1A	2.81	1.49	1.41
18	B	1138	CLA	C4B-CHC	2.80	1.48	1.41
18	F	1240	CLA	CHA-C1A	2.80	1.49	1.41
18	B	1220	CLA	C1B-CHB	2.80	1.48	1.41
18	B	1138	CLA	C3D-CAD	-2.80	1.39	1.46
18	A	1106	CLA	C1C-C2C	-2.79	1.39	1.44
18	A	1152	CLA	CHA-C1A	2.79	1.49	1.41
18	2	2013	CLA	C1B-NB	-2.79	1.32	1.35
18	A	1151	CLA	MG-NA	-2.79	1.99	2.06
18	4	4002	CLA	MG-NA	-2.79	1.99	2.06
18	B	1215	CLA	C1B-CHB	2.79	1.48	1.41
18	B	1230	CLA	MG-NA	-2.79	1.99	2.06
18	4	1304	CLA	C1C-C2C	-2.79	1.39	1.44
18	1	1006	CLA	CHA-C1A	2.78	1.49	1.41
18	A	1151	CLA	CHA-C1A	2.78	1.49	1.41
18	A	1137	CLA	MG-NA	-2.77	1.99	2.06
18	B	1138	CLA	C4C-C3C	-2.77	1.40	1.45
18	A	1110	CLA	CHA-C1A	2.77	1.49	1.41
18	B	1217	CLA	C4C-C3C	-2.77	1.40	1.45
18	B	1207	CLA	C3D-CAD	-2.76	1.39	1.46
18	B	1219	CLA	C4C-C3C	-2.76	1.40	1.45
18	A	1111	CLA	CHA-C1A	2.76	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1236	CLA	C3B-C2B	-2.76	1.36	1.40
18	B	1209	CLA	C3D-CAD	-2.75	1.39	1.46
18	B	1231	CLA	C3B-C2B	-2.75	1.36	1.40
18	B	1217	CLA	C3D-CAD	-2.75	1.39	1.46
18	A	1104	CLA	CHB-C4A	-2.75	1.32	1.34
18	B	1215	CLA	C4C-C3C	-2.75	1.40	1.45
18	B	1234	CLA	C1B-CHB	2.75	1.48	1.41
18	A	1126	CLA	C1B-NB	-2.75	1.32	1.35
18	A	1132	CLA	MG-NA	-2.75	1.99	2.06
18	3	3015	CLA	MG-NA	-2.75	1.99	2.06
18	A	9011	CLA	C4B-CHC	2.75	1.48	1.41
18	4	4003	CLA	MG-NA	-2.74	1.99	2.06
18	J	2107	CLA	C1C-C2C	-2.74	1.39	1.44
18	3	3008	CLA	CHA-C1A	2.74	1.49	1.41
18	B	1203	CLA	C4B-CHC	2.73	1.48	1.41
18	B	9023	CLA	C3B-C2B	-2.73	1.36	1.40
18	A	1123	CLA	C1C-C2C	-2.73	1.39	1.44
18	A	1137	CLA	C1C-C2C	-2.72	1.39	1.44
18	F	1305	CLA	MG-NA	-2.72	1.99	2.06
18	B	1229	CLA	C1B-CHB	2.72	1.48	1.41
18	3	3011	CLA	MG-NA	-2.72	1.99	2.06
18	L	1504	CLA	C1C-C2C	-2.72	1.39	1.44
18	3	3003	CLA	MG-NA	-2.72	1.99	2.06
18	1	1010	CLA	CHA-C1A	2.72	1.49	1.41
18	A	1107	CLA	C3D-CAD	-2.72	1.39	1.46
18	3	3012	CLA	CHA-C1A	2.72	1.49	1.41
18	B	1202	CLA	C3B-C2B	-2.72	1.36	1.40
18	A	1109	CLA	C4C-C3C	-2.71	1.37	1.45
18	B	1227	CLA	C3B-C2B	-2.71	1.36	1.40
18	B	1226	CLA	CHA-C1A	2.71	1.49	1.41
18	B	1221	CLA	C4B-CHC	2.71	1.48	1.41
18	B	1205	CLA	C1B-CHB	2.70	1.48	1.41
18	B	1212	CLA	C1C-C2C	-2.70	1.39	1.44
18	A	1103	CLA	C4B-CHC	2.69	1.48	1.41
18	4	4003	CLA	CHA-C1A	2.68	1.48	1.41
18	A	1140	CLA	MG-NA	-2.68	1.99	2.06
18	B	1206	CLA	CHA-C1A	2.68	1.48	1.41
18	3	3012	CLA	MG-NA	-2.68	1.99	2.06
18	4	4004	CLA	CHA-C1A	2.68	1.48	1.41
18	B	1232	CLA	C1C-C2C	-2.67	1.39	1.44
18	B	1218	CLA	C3D-CAD	-2.67	1.39	1.46
18	B	1220	CLA	C1C-C2C	-2.67	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1229	CLA	C1C-C2C	-2.66	1.39	1.44
18	3	3010	CLA	MG-NA	-2.66	2.00	2.06
18	A	1115	CLA	C3B-C2B	-2.66	1.36	1.40
18	2	2012	CLA	CHA-C1A	2.66	1.48	1.41
18	L	1503	CLA	C3D-C2D	-2.66	1.34	1.39
18	B	1234	CLA	C3D-CAD	-2.66	1.39	1.46
18	A	1107	CLA	C1C-NC	-2.65	1.33	1.37
18	B	9023	CLA	C1C-C2C	-2.65	1.39	1.44
18	A	1115	CLA	C4B-CHC	2.65	1.48	1.41
18	3	3015	CLA	CHA-C1A	2.65	1.48	1.41
18	4	4002	CLA	CHA-C1A	2.65	1.48	1.41
18	4	1009	CLA	MG-NA	-2.65	2.00	2.06
18	A	1103	CLA	MG-NA	-2.64	2.00	2.06
18	A	1147	CLA	CHA-C1A	2.64	1.48	1.41
20	B	6017	BCR	C8-C9	2.64	1.51	1.45
18	1	1001	CLA	CHA-C1A	2.64	1.48	1.41
18	H	1505	CLA	CHA-C1A	2.64	1.48	1.41
18	B	1227	CLA	C1B-CHB	2.64	1.48	1.41
18	3	3010	CLA	CHA-C1A	2.64	1.48	1.41
18	A	1129	CLA	C4C-C3C	-2.64	1.40	1.45
18	2	2007	CLA	CHA-C1A	2.63	1.48	1.41
18	A	1134	CLA	MG-NA	-2.63	2.00	2.06
18	J	1307	CLA	CHA-C1A	2.63	1.48	1.41
18	B	1207	CLA	MG-NA	-2.63	2.00	2.06
18	2	2013	CLA	CHA-C1A	2.63	1.48	1.41
18	4	4010	CLA	CHA-C1A	2.63	1.48	1.41
18	A	1126	CLA	C4C-C3C	-2.63	1.40	1.45
18	A	1142	CLA	CHA-C1A	2.63	1.48	1.41
18	3	3005	CLA	CHA-C1A	2.62	1.48	1.41
18	A	1127	CLA	CHA-C1A	2.62	1.48	1.41
18	4	4008	CLA	CHA-C1A	2.62	1.48	1.41
18	A	9011	CLA	C4C-C3C	-2.62	1.40	1.45
18	A	1118	CLA	CHA-C1A	2.62	1.48	1.41
18	1	1002	CLA	CHA-C1A	2.62	1.48	1.41
18	B	1212	CLA	C3D-CAD	-2.61	1.39	1.46
18	1	1008	CLA	CHA-C1A	2.61	1.48	1.41
18	A	1119	CLA	MG-NA	-2.61	2.00	2.06
18	2	2002	CLA	CHA-C1A	2.61	1.48	1.41
18	A	1143	CLA	CHA-C1A	2.61	1.48	1.41
18	A	1101	CLA	CHA-C1A	2.61	1.48	1.41
18	A	1146	CLA	CHA-C1A	2.60	1.48	1.41
18	B	9023	CLA	MG-NA	-2.60	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	2008	CLA	C1B-NB	-2.60	1.32	1.35
18	B	1207	CLA	C1C-C2C	-2.60	1.39	1.44
18	2	2005	CLA	MG-NA	-2.60	2.00	2.06
18	B	9023	CLA	C3D-CAD	-2.60	1.39	1.46
18	4	4007	CLA	CHA-C1A	2.60	1.48	1.41
18	3	3002	CLA	CHA-C1A	2.60	1.48	1.41
18	4	4013	CLA	CHA-C1A	2.59	1.48	1.41
18	B	9012	CLA	MG-NA	-2.59	2.00	2.06
18	2	2015	CLA	CHA-C1A	2.59	1.48	1.41
18	A	1140	CLA	C1C-C2C	-2.59	1.39	1.44
18	A	1117	CLA	CHA-C1A	2.59	1.48	1.41
18	1	1013	CLA	CHA-C1A	2.59	1.48	1.41
18	3	3003	CLA	CHA-C1A	2.59	1.48	1.41
18	A	1110	CLA	CHB-C4A	-2.59	1.32	1.34
18	3	3013	CLA	CHA-C1A	2.58	1.48	1.41
18	2	2011	CLA	CHA-C1A	2.58	1.48	1.41
18	4	4009	CLA	CHA-C1A	2.58	1.48	1.41
18	B	1228	CLA	C3D-CAD	-2.58	1.39	1.46
18	1	1007	CLA	CHA-C1A	2.58	1.48	1.41
18	A	1120	CLA	CHB-C4A	-2.58	1.32	1.34
18	A	1129	CLA	C3D-CAD	-2.58	1.39	1.46
18	B	1202	CLA	MG-NA	-2.57	2.00	2.06
18	2	2006	CLA	CHA-C1A	2.57	1.48	1.41
18	B	1222	CLA	C1B-CHB	2.57	1.48	1.41
18	B	1234	CLA	C1C-C2C	-2.57	1.39	1.44
18	A	1144	CLA	CHA-C1A	2.57	1.48	1.41
18	A	1128	CLA	C1B-CHB	2.57	1.48	1.41
18	A	1123	CLA	C3D-CAD	-2.57	1.39	1.46
18	K	1153	CLA	C1B-NB	-2.56	1.32	1.35
18	2	2001	CLA	CHA-C1A	2.56	1.48	1.41
18	A	1108	CLA	C1C-C2C	-2.56	1.39	1.44
18	A	1309	CLA	CHA-C1A	2.56	1.48	1.41
18	G	1248	CLA	CHA-C1A	2.56	1.48	1.41
18	B	1227	CLA	C4B-CHC	2.55	1.48	1.41
18	4	4005	CLA	CHA-C1A	2.55	1.48	1.41
18	2	2010	CLA	CHA-C1A	2.55	1.48	1.41
18	A	1147	CLA	C1B-NB	-2.55	1.32	1.35
18	A	1123	CLA	MG-NA	-2.55	2.00	2.06
18	I	1204	CLA	C3B-C2B	-2.55	1.36	1.40
18	A	1116	CLA	CHA-C1A	2.55	1.48	1.41
18	B	9010	CLA	C3B-C2B	-2.54	1.36	1.40
18	3	3011	CLA	CHA-C1A	2.54	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1237	CLA	C3D-CAD	-2.54	1.39	1.46
18	B	1212	CLA	MG-NA	-2.53	2.00	2.06
18	A	9013	CLA	C4C-C3C	-2.53	1.40	1.45
18	B	1230	CLA	CHA-C1A	2.53	1.48	1.41
18	A	1135	CLA	C3D-CAD	-2.53	1.39	1.46
18	F	1306	CLA	C1B-NB	-2.53	1.33	1.35
18	B	1210	CLA	CHA-C1A	2.52	1.48	1.41
18	A	1131	CLA	C1B-NB	-2.52	1.33	1.35
18	A	1117	CLA	MG-NA	-2.51	2.00	2.06
18	H	1505	CLA	CHB-C4A	-2.51	1.32	1.34
18	A	1102	CLA	CHA-C1A	2.51	1.48	1.41
18	F	1306	CLA	CHA-C1A	2.51	1.48	1.41
18	3	2009	CLA	CHA-C1A	2.51	1.48	1.41
18	B	1208	CLA	C3B-C2B	-2.51	1.36	1.40
18	A	1132	CLA	C4B-NB	-2.50	1.33	1.35
18	B	1205	CLA	MG-NA	-2.50	2.00	2.06
18	H	1501	CLA	MG-NA	-2.50	2.00	2.06
18	B	1213	CLA	CHA-C1A	2.50	1.48	1.41
18	F	1302	CLA	C1C-C2C	-2.49	1.39	1.44
18	I	1204	CLA	C1C-C2C	-2.49	1.39	1.44
18	2	2003	CLA	CHA-C1A	2.49	1.48	1.41
18	F	1139	CLA	C1B-CHB	2.49	1.47	1.41
18	A	1105	CLA	CHA-C1A	2.49	1.48	1.41
18	A	1131	CLA	C4C-C3C	-2.49	1.40	1.45
18	H	1501	CLA	C3D-CAD	-2.49	1.39	1.46
18	B	1203	CLA	C1B-CHB	2.49	1.47	1.41
18	K	1150	CLA	CHA-C1A	2.49	1.48	1.41
18	J	2107	CLA	C4C-C3C	-2.48	1.40	1.45
18	F	1303	CLA	CHA-C1A	2.48	1.48	1.41
18	J	1308	CLA	CHA-C1A	2.48	1.48	1.41
18	F	1139	CLA	C3D-CAD	-2.48	1.39	1.46
18	B	1211	CLA	CHA-C1A	2.47	1.48	1.41
18	K	1141	CLA	CHA-C1A	2.47	1.48	1.41
18	4	1304	CLA	C3D-CAD	-2.47	1.39	1.46
18	B	9010	CLA	C1B-NB	-2.47	1.33	1.35
18	G	1248	CLA	C3C-C4C	-2.47	1.37	1.43
18	F	4015	CLA	CHA-C1A	2.47	1.48	1.41
18	B	1211	CLA	C4B-CHC	2.46	1.48	1.43
18	A	1148	CLA	CHA-C1A	2.46	1.48	1.41
18	B	1227	CLA	C1B-NB	-2.46	1.33	1.35
18	A	1103	CLA	C3D-CAD	-2.46	1.39	1.46
18	A	1133	CLA	CHA-C1A	2.46	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	1125	CLA	CHA-C1A	2.46	1.48	1.41
18	A	1105	CLA	CHB-C4A	-2.46	1.32	1.34
18	B	1223	CLA	CHA-C1A	2.45	1.48	1.41
18	4	4011	CLA	CHA-C1A	2.45	1.48	1.41
18	3	3001	CLA	CHA-C1A	2.45	1.48	1.41
20	I	6018	BCR	C23-C22	2.45	1.51	1.45
18	B	1209	CLA	C1B-NB	-2.45	1.33	1.35
18	A	1136	CLA	C1C-C2C	-2.44	1.39	1.44
18	F	1302	CLA	C3D-CAD	-2.44	1.39	1.46
18	B	1229	CLA	C1C-NC	-2.44	1.34	1.37
18	4	4012	CLA	CHA-C1A	2.44	1.48	1.41
18	L	1130	CLA	C3D-CAD	-2.44	1.39	1.46
18	J	2107	CLA	C3D-CAD	-2.44	1.39	1.46
18	B	1221	CLA	C1B-CHB	2.44	1.47	1.41
18	A	1135	CLA	C1B-NB	-2.44	1.33	1.35
18	1	1001	CLA	CHB-C4A	-2.43	1.32	1.34
18	A	1113	CLA	C1B-CHB	2.43	1.47	1.41
18	B	1228	CLA	C1C-NC	-2.43	1.34	1.37
18	3	3003	CLA	CHB-C4A	-2.43	1.32	1.34
18	A	9013	CLA	C4B-CHC	2.43	1.47	1.41
18	1	1014	CLA	CHA-C1A	2.43	1.48	1.41
18	B	1225	CLA	C1C-NC	-2.42	1.34	1.37
18	A	1140	CLA	C3B-C2B	-2.42	1.37	1.40
18	B	1214	CLA	C1C-C2C	-2.42	1.39	1.44
18	B	1208	CLA	C1C-C2C	-2.42	1.39	1.44
18	B	1203	CLA	C1C-C2C	-2.42	1.39	1.44
18	J	2107	CLA	C1B-CHB	2.42	1.47	1.41
18	B	1221	CLA	C3D-CAD	-2.41	1.39	1.46
18	L	1502	CLA	C1C-C2C	-2.41	1.39	1.44
18	B	1235	CLA	C3B-C2B	-2.41	1.37	1.40
18	B	1239	CLA	MG-NA	-2.41	2.00	2.06
18	4	1009	CLA	C1B-NB	-2.41	1.33	1.35
18	4	4001	CLA	CHA-C1A	2.41	1.48	1.41
18	A	1122	CLA	C1C-NC	-2.41	1.34	1.37
18	G	1233	CLA	C1B-NB	-2.40	1.33	1.35
18	B	1236	CLA	C1C-C2C	-2.40	1.39	1.44
18	A	1140	CLA	C3D-CAD	-2.40	1.40	1.46
18	B	1217	CLA	C3B-C2B	-2.40	1.37	1.40
18	G	1248	CLA	C2C-C1C	-2.40	1.37	1.43
18	L	1502	CLA	C3D-CAD	-2.40	1.40	1.46
18	B	1209	CLA	C1C-C2C	-2.40	1.39	1.44
18	H	1501	CLA	C3B-C2B	-2.40	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	3013	CLA	CHB-C4A	-2.40	1.33	1.34
18	A	1120	CLA	CHA-C1A	2.39	1.48	1.41
18	B	1216	CLA	C3D-CAD	-2.38	1.40	1.46
18	A	1122	CLA	C3D-CAD	-2.38	1.40	1.46
18	B	1217	CLA	MG-NA	-2.38	2.00	2.06
18	L	1504	CLA	C1B-CHB	2.38	1.47	1.41
18	A	1126	CLA	MG-NA	-2.38	2.00	2.06
18	B	1222	CLA	C3D-CAD	-2.37	1.40	1.46
18	A	1122	CLA	C3B-C2B	-2.37	1.37	1.40
18	A	1128	CLA	C3D-CAD	-2.37	1.40	1.46
18	1	1005	CLA	CHA-C1A	2.37	1.48	1.41
18	A	1108	CLA	C1B-CHB	2.37	1.47	1.41
18	A	1129	CLA	C1C-C2C	-2.37	1.40	1.44
18	2	2008	CLA	CHA-C1A	2.36	1.48	1.41
18	3	3006	CLA	CHA-C1A	2.36	1.48	1.41
18	G	1233	CLA	C3D-CAD	-2.36	1.40	1.46
18	B	1239	CLA	C1B-CHB	2.36	1.47	1.41
18	3	3013	CLA	C1B-NB	-2.36	1.33	1.35
18	B	1222	CLA	C1C-C2C	-2.36	1.40	1.44
18	A	1135	CLA	C1C-NC	-2.36	1.34	1.37
18	A	1136	CLA	MG-NA	-2.36	2.00	2.06
18	B	1212	CLA	C1B-CHB	2.36	1.47	1.41
18	L	1130	CLA	C1B-CHB	2.35	1.47	1.41
18	B	9010	CLA	MG-NA	-2.35	2.00	2.06
18	B	9012	CLA	C1C-C2C	-2.35	1.40	1.44
18	B	1231	CLA	C1B-CHB	2.34	1.47	1.41
18	B	1219	CLA	C1B-CHB	2.34	1.47	1.41
18	A	1127	CLA	C1B-NB	-2.34	1.33	1.35
18	4	4002	CLA	CHB-C4A	-2.34	1.33	1.34
18	1	1007	CLA	C1B-NB	-2.34	1.33	1.35
18	4	4012	CLA	C3C-C4C	-2.34	1.37	1.43
18	A	1109	CLA	C2C-C1C	-2.34	1.37	1.43
18	A	1106	CLA	C3D-CAD	-2.33	1.40	1.46
18	4	4006	CLA	CHA-C1A	2.33	1.47	1.41
18	2	2002	CLA	C1B-NB	-2.33	1.33	1.35
18	3	3008	CLA	CHB-C4A	-2.33	1.33	1.34
18	B	1218	CLA	C2-C3	2.33	1.38	1.33
18	1	1004	CLA	CHA-C1A	2.32	1.47	1.41
18	B	1242	CLA	MG-NA	-2.32	2.00	2.06
18	A	1103	CLA	C1B-NB	-2.32	1.33	1.35
18	B	1138	CLA	MG-NA	-2.31	2.00	2.06
18	A	1115	CLA	C3D-CAD	-2.31	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	1136	CLA	C1B-CHB	2.31	1.47	1.41
18	K	1153	CLA	MG-NA	-2.31	2.00	2.06
18	1	1004	CLA	C1B-NB	-2.31	1.33	1.35
18	A	1116	CLA	CHB-C4A	-2.30	1.33	1.34
18	B	1227	CLA	C3D-CAD	-2.30	1.40	1.46
18	A	1106	CLA	C1B-CHB	2.30	1.47	1.41
18	2	2004	CLA	CHA-C1A	2.29	1.47	1.41
18	A	1104	CLA	MG-NA	-2.29	2.00	2.06
18	B	1202	CLA	C1B-CHB	2.29	1.47	1.41
18	B	1214	CLA	MG-NA	-2.29	2.00	2.06
18	I	1204	CLA	C1B-CHB	2.29	1.47	1.41
18	B	1203	CLA	C3B-C2B	-2.29	1.37	1.40
18	A	1126	CLA	C1C-C2C	-2.29	1.40	1.44
18	B	1301	CLA	CHA-C1A	2.28	1.47	1.41
20	A	6011	BCR	C27-C26	2.28	1.55	1.51
18	B	1210	CLA	CHB-C4A	-2.28	1.33	1.34
18	3	3007	CLA	CHA-C1A	2.28	1.47	1.41
18	1	1012	CLA	CHA-C1A	2.27	1.47	1.41
18	B	1237	CLA	MG-NA	-2.27	2.00	2.06
18	B	1201	CLA	CHB-C4A	-2.27	1.33	1.34
18	B	1203	CLA	MG-NA	-2.27	2.00	2.06
18	B	1208	CLA	C3D-CAD	-2.27	1.40	1.46
18	1	1003	CLA	CHA-C1A	2.27	1.47	1.41
18	B	1228	CLA	MG-NA	-2.27	2.00	2.06
18	B	1214	CLA	C1B-NB	-2.26	1.33	1.35
18	L	1504	CLA	C3D-CAD	-2.26	1.40	1.46
18	A	9011	CLA	MG-NA	-2.26	2.00	2.06
18	B	1239	CLA	C3D-CAD	-2.25	1.40	1.46
18	B	1215	CLA	C3B-C2B	-2.25	1.37	1.40
18	A	1127	CLA	C2C-C1C	-2.25	1.37	1.43
18	A	1137	CLA	C1C-NC	-2.25	1.34	1.37
18	A	1129	CLA	MG-NA	-2.25	2.00	2.06
18	B	1224	CLA	MG-NA	-2.25	2.00	2.06
18	G	1233	CLA	C1B-CHB	2.24	1.47	1.41
18	B	1241	CLA	CHA-C1A	2.24	1.47	1.41
18	B	1215	CLA	MG-NA	-2.24	2.01	2.06
18	B	9022	CLA	C1A-CHA	2.24	1.52	1.43
18	A	1135	CLA	C1B-CHB	2.23	1.47	1.41
18	B	1208	CLA	MG-NA	-2.23	2.01	2.06
18	3	3004	CLA	C3C-C4C	-2.23	1.38	1.43
18	4	1304	CLA	C1B-CHB	2.23	1.47	1.41
18	F	1302	CLA	C1B-CHB	2.23	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1138	CLA	C1B-CHB	2.22	1.47	1.41
18	B	1206	CLA	C2C-C1C	-2.22	1.38	1.43
18	A	1106	CLA	C4C-C3C	-2.22	1.41	1.45
18	4	4004	CLA	C3C-C4C	-2.22	1.38	1.43
18	B	1232	CLA	C3D-CAD	-2.22	1.40	1.46
18	L	1503	CLA	C2A-C1A	-2.22	1.47	1.52
18	A	9011	CLA	C1B-CHB	2.21	1.47	1.41
18	2	2003	CLA	C3C-C4C	-2.21	1.38	1.43
18	B	1235	CLA	MG-NA	-2.20	2.01	2.06
18	A	1135	CLA	MG-NA	-2.20	2.01	2.06
18	B	1212	CLA	CBB-CAB	2.20	1.43	1.29
18	A	1309	CLA	CHB-C4A	-2.20	1.33	1.34
18	2	2012	CLA	C3C-C4C	-2.20	1.38	1.43
18	4	4004	CLA	C2C-C1C	-2.20	1.38	1.43
18	G	1233	CLA	C1C-C2C	-2.20	1.40	1.44
18	2	2003	CLA	C2C-C1C	-2.20	1.38	1.43
18	L	1502	CLA	C1B-CHB	2.19	1.47	1.41
18	A	1148	CLA	CHB-C4A	-2.19	1.33	1.34
18	L	1130	CLA	MG-NA	-2.18	2.01	2.06
18	B	1238	CLA	C3D-CAD	-2.18	1.40	1.46
18	B	1211	CLA	C1B-NB	-2.17	1.33	1.35
18	B	1223	CLA	C2C-C1C	-2.17	1.38	1.43
18	B	1237	CLA	C3B-C2B	-2.17	1.37	1.40
18	B	1223	CLA	C1B-NB	-2.17	1.33	1.35
18	A	1128	CLA	MG-NA	-2.17	2.01	2.06
18	B	1207	CLA	C1C-NC	-2.17	1.34	1.37
18	A	1128	CLA	C3B-C2B	-2.17	1.37	1.40
18	B	1138	CLA	C3A-C2A	-2.16	1.48	1.54
18	A	1127	CLA	C3C-C4C	-2.16	1.38	1.43
18	2	2007	CLA	C1B-NB	-2.16	1.33	1.35
18	A	1146	CLA	CHB-C4A	-2.16	1.33	1.34
18	B	1238	CLA	C1B-NB	-2.16	1.33	1.35
18	A	1119	CLA	C3D-CAD	-2.16	1.40	1.46
18	B	1225	CLA	C1B-CHB	2.16	1.47	1.41
18	3	3012	CLA	C3C-C4C	-2.15	1.38	1.43
18	L	1502	CLA	MG-NA	-2.15	2.01	2.06
18	B	1218	CLA	C1-C2	2.15	1.55	1.49
18	B	9010	CLA	C1C-NC	-2.14	1.34	1.37
18	B	1224	CLA	C1B-CHB	2.14	1.46	1.41
18	A	1115	CLA	C1B-NB	-2.14	1.33	1.35
18	A	1132	CLA	C1B-NB	-2.14	1.33	1.35
18	B	1138	CLA	C3B-C2B	-2.13	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1217	CLA	C1B-NB	-2.13	1.33	1.35
18	B	9010	CLA	C1A-CHA	2.13	1.52	1.43
18	B	1231	CLA	C3D-CAD	-2.13	1.40	1.46
18	B	1209	CLA	C4C-C3C	-2.12	1.41	1.45
18	A	1119	CLA	C1C-C2C	-2.12	1.40	1.44
18	B	1227	CLA	MG-NA	-2.12	2.01	2.06
18	I	1204	CLA	MG-NA	-2.12	2.01	2.06
18	B	1234	CLA	MG-NA	-2.12	2.01	2.06
18	3	3005	CLA	C2C-C1C	-2.11	1.38	1.43
18	B	1242	CLA	C3B-C2B	-2.11	1.37	1.40
18	3	3009	CLA	C3C-C4C	-2.10	1.38	1.43
18	A	1129	CLA	C1B-CHB	2.10	1.46	1.41
18	A	1124	CLA	C1B-NB	-2.10	1.33	1.35
18	B	1224	CLA	C3B-C2B	-2.10	1.37	1.40
18	F	1240	CLA	CHB-C4A	-2.10	1.33	1.34
18	A	1126	CLA	C3D-CAD	-2.10	1.40	1.46
18	A	1116	CLA	C2C-C1C	-2.09	1.38	1.43
18	2	2012	CLA	C2C-C1C	-2.09	1.38	1.43
18	1	1007	CLA	CHB-C4A	-2.09	1.33	1.34
18	G	1233	CLA	MG-NA	-2.09	2.01	2.06
18	A	1118	CLA	C2C-C1C	-2.09	1.38	1.43
18	2	2004	CLA	C1B-NB	-2.09	1.33	1.35
18	B	1224	CLA	C3D-CAD	-2.09	1.40	1.46
18	H	1505	CLA	C3C-C4C	-2.08	1.38	1.43
18	3	3012	CLA	C2C-C1C	-2.08	1.38	1.43
18	A	1147	CLA	C3C-C4C	-2.07	1.38	1.43
18	3	3007	CLA	CHB-C4A	-2.07	1.33	1.34
18	2	2012	CLA	C1B-NB	-2.07	1.33	1.35
18	A	1119	CLA	C1B-CHB	2.07	1.46	1.41
18	A	1132	CLA	CHA-C1A	2.07	1.47	1.41
18	A	1118	CLA	C3C-C4C	-2.07	1.38	1.43
18	3	2009	CLA	C2C-C1C	-2.06	1.38	1.43
18	3	3005	CLA	CHB-C4A	-2.06	1.33	1.34
18	A	1151	CLA	C3C-C4C	-2.06	1.38	1.43
18	B	1223	CLA	C3C-C4C	-2.06	1.38	1.43
18	1	1002	CLA	CHB-C4A	-2.06	1.33	1.34
18	B	1214	CLA	C3D-CAD	-2.06	1.40	1.46
18	A	1105	CLA	C1B-NB	-2.06	1.33	1.35
18	B	9012	CLA	C3D-CAD	-2.05	1.40	1.46
18	4	4013	CLA	C3C-C4C	-2.05	1.38	1.43
18	A	1109	CLA	C1D-C2D	-2.05	1.39	1.45
18	A	1146	CLA	C1B-NB	-2.05	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	4007	CLA	C3C-C4C	-2.05	1.38	1.43
18	B	1226	CLA	C1B-CHB	2.05	1.48	1.43
18	4	4013	CLA	C1B-NB	-2.05	1.33	1.35
18	3	3004	CLA	C2C-C1C	-2.05	1.38	1.43
18	A	1134	CLA	C1B-CHB	2.04	1.48	1.43
18	B	1242	CLA	C1B-CHB	2.04	1.46	1.41
18	A	1126	CLA	C3B-C2B	-2.04	1.37	1.40
18	4	4011	CLA	C3C-C4C	-2.04	1.38	1.43
18	4	4007	CLA	CHB-C4A	-2.04	1.33	1.34
18	3	3002	CLA	C1B-CHB	2.03	1.48	1.43
18	1	1006	CLA	C3C-C4C	-2.03	1.38	1.43
18	3	3007	CLA	C2C-C1C	-2.03	1.38	1.43
18	1	1006	CLA	C2C-C1C	-2.03	1.38	1.43
18	A	1108	CLA	MG-NA	-2.03	2.01	2.06
18	3	2009	CLA	C3C-C4C	-2.02	1.38	1.43
18	A	1109	CLA	C1B-NB	-2.02	1.33	1.35
18	1	1004	CLA	C3C-C4C	-2.02	1.38	1.43
18	B	1231	CLA	C1B-NB	-2.02	1.33	1.35
18	A	1123	CLA	C3B-C2B	-2.02	1.37	1.40
18	B	9022	CLA	C1B-CHB	2.02	1.46	1.41
18	2	2011	CLA	C2C-C1C	-2.02	1.38	1.43
18	A	1152	CLA	CHB-C4A	-2.01	1.33	1.34
18	4	4012	CLA	C2C-C1C	-2.01	1.38	1.43
18	B	1211	CLA	C2C-C1C	-2.01	1.38	1.43
18	B	1230	CLA	C2C-C1C	-2.01	1.38	1.43
18	2	2002	CLA	C2C-C1C	-2.01	1.38	1.43
18	A	1122	CLA	C1B-CHB	2.00	1.46	1.41
18	F	1302	CLA	MG-NA	-2.00	2.01	2.06
18	B	1241	CLA	C3C-C4C	-2.00	1.38	1.43

All (3079) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	6011	BCR	C11-C10-C9	28.99	168.68	127.31
20	L	6020	BCR	C11-C10-C9	26.87	165.66	127.31
20	F	6016	BCR	C11-C10-C9	26.81	165.58	127.31
20	B	6017	BCR	C11-C10-C9	24.33	162.03	127.31
18	A	1126	CLA	OBD-CAD-CBD	-21.09	95.77	125.89
20	I	6018	BCR	C11-C10-C9	20.43	156.47	127.31
18	B	9022	CLA	OBD-CAD-C3D	-20.41	94.09	127.98
18	B	1209	CLA	OBD-CAD-CBD	-18.37	99.64	125.89
20	I	6018	BCR	C7-C8-C9	-17.05	100.47	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1231	CLA	OBD-CAD-CBD	-16.95	101.68	125.89
18	B	1207	CLA	OBD-CAD-C3D	-16.65	100.34	127.98
18	B	1229	CLA	OBD-CAD-C3D	-16.47	100.64	127.98
18	B	1229	CLA	OBD-CAD-CBD	-16.36	102.53	125.89
18	B	1236	CLA	OBD-CAD-C3D	-16.24	101.02	127.98
18	B	1227	CLA	OBD-CAD-CBD	-15.63	103.56	125.89
18	B	1207	CLA	OBD-CAD-CBD	-15.38	103.92	125.89
18	B	1202	CLA	OBD-CAD-C3D	-15.34	102.51	127.98
18	B	1203	CLA	OBD-CAD-C3D	-15.23	108.59	127.11
18	A	9011	CLA	OBD-CAD-CBD	-15.18	104.20	125.89
18	L	1503	CLA	OBD-CAD-CBD	-14.84	104.69	125.89
20	L	6020	BCR	C10-C11-C12	14.75	169.25	123.22
18	B	1237	CLA	OBD-CAD-C3D	-14.64	103.68	127.98
18	B	1217	CLA	OBD-CAD-C3D	-14.62	103.71	127.98
18	J	2107	CLA	OBD-CAD-CBD	-14.61	105.02	125.89
18	B	1227	CLA	OBD-CAD-C3D	-14.56	103.81	127.98
18	B	1220	CLA	OBD-CAD-C3D	-14.55	103.83	127.98
18	A	1129	CLA	OBD-CAD-C3D	-14.34	104.18	127.98
18	L	1503	CLA	C4D-C3D-CAD	14.30	116.45	108.47
18	A	1113	CLA	OBD-CAD-CBD	-14.30	105.46	125.89
18	J	2107	CLA	OBD-CAD-C3D	-14.24	104.34	127.98
18	B	1205	CLA	OBD-CAD-C3D	-14.09	104.59	127.98
18	A	1103	CLA	OBD-CAD-C3D	-14.08	104.60	127.98
18	A	1140	CLA	OBD-CAD-C3D	-13.99	104.75	127.98
18	G	1233	CLA	OBD-CAD-CBD	-13.98	105.92	125.89
18	B	1225	CLA	OBD-CAD-C3D	-13.96	104.80	127.98
18	B	1220	CLA	OBD-CAD-CBD	-13.88	106.07	125.89
18	L	1503	CLA	OBD-CAD-C3D	-13.80	105.08	127.98
18	B	1232	CLA	OBD-CAD-CBD	-13.75	106.25	125.89
18	B	1242	CLA	OBD-CAD-C3D	-13.65	105.32	127.98
18	A	1113	CLA	OBD-CAD-C3D	-13.65	105.32	127.98
18	B	1231	CLA	OBD-CAD-C3D	-13.58	105.43	127.98
18	B	1242	CLA	OBD-CAD-CBD	-13.42	106.72	125.89
18	B	1236	CLA	OBD-CAD-CBD	-13.36	106.81	125.89
18	A	1136	CLA	C4D-C3D-CAD	13.26	115.86	108.47
18	B	1205	CLA	OBD-CAD-CBD	-13.24	106.98	125.89
18	B	1217	CLA	OBD-CAD-CBD	-13.19	107.05	125.89
18	H	1501	CLA	OBD-CAD-C3D	-13.17	106.11	127.98
18	B	1235	CLA	OBD-CAD-CBD	-13.14	107.12	125.89
18	L	1503	CLA	CAB-C3B-C2B	-13.14	98.95	124.69
18	A	1140	CLA	OBD-CAD-CBD	-13.02	107.29	125.89
18	B	1236	CLA	C4D-C3D-CAD	13.02	115.73	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1238	CLA	OBD-CAD-CBD	-12.94	107.41	125.89
18	4	1304	CLA	OBD-CAD-CBD	-12.90	107.46	125.89
18	B	1237	CLA	OBD-CAD-CBD	-12.88	107.50	125.89
18	L	1504	CLA	OBD-CAD-C3D	-12.87	106.61	127.98
18	H	1501	CLA	OBD-CAD-CBD	-12.74	107.69	125.89
18	A	1123	CLA	OBD-CAD-C3D	-12.73	106.84	127.98
18	A	1108	CLA	OBD-CAD-CBD	-12.71	107.73	125.89
18	B	1232	CLA	OBD-CAD-C3D	-12.54	107.16	127.98
18	B	1228	CLA	OBD-CAD-C3D	-12.53	107.17	127.98
18	A	1108	CLA	OBD-CAD-C3D	-12.52	107.19	127.98
18	G	1233	CLA	OBD-CAD-C3D	-12.46	107.29	127.98
18	A	1107	CLA	OBD-CAD-C3D	-12.41	107.38	127.98
18	A	1119	CLA	OBD-CAD-CBD	-12.29	108.34	125.89
18	B	1228	CLA	OBD-CAD-CBD	-12.25	108.40	125.89
18	L	1504	CLA	OBD-CAD-CBD	-12.24	108.41	125.89
18	B	1216	CLA	OBD-CAD-C3D	-12.19	107.74	127.98
18	A	1129	CLA	OBD-CAD-CBD	-12.15	108.54	125.89
18	B	1225	CLA	C4D-C3D-CAD	12.14	115.24	108.47
18	F	1302	CLA	C4D-C3D-CAD	12.12	115.23	108.47
18	B	1202	CLA	C4D-C3D-CAD	12.04	115.18	108.47
18	B	1220	CLA	C4D-C3D-CAD	12.00	115.16	108.47
18	B	1212	CLA	C4D-C3D-CAD	11.98	115.15	108.47
18	A	1106	CLA	OBD-CAD-C3D	-11.97	108.11	127.98
18	A	1115	CLA	OBD-CAD-C3D	-11.96	108.13	127.98
18	B	1217	CLA	C4D-C3D-CAD	11.92	115.12	108.47
18	B	1208	CLA	C4D-C3D-CAD	11.91	115.11	108.47
18	B	1238	CLA	OBD-CAD-C3D	-11.85	108.30	127.98
18	A	1135	CLA	OBD-CAD-C3D	-11.80	108.39	127.98
18	B	1229	CLA	C4D-C3D-CAD	11.79	115.05	108.47
18	A	1107	CLA	C4D-C3D-CAD	11.79	115.04	108.47
18	F	1139	CLA	C4D-C3D-CAD	11.79	115.04	108.47
18	A	1123	CLA	C4D-C3D-CAD	11.73	115.01	108.47
20	I	6018	BCR	C10-C11-C12	11.62	159.48	123.22
18	A	1126	CLA	OBD-CAD-C3D	-11.54	108.81	127.98
18	B	1228	CLA	C4D-C3D-CAD	11.48	114.87	108.47
18	B	1229	CLA	CAB-C3B-C4B	-11.46	110.85	128.46
18	A	1103	CLA	OBD-CAD-CBD	-11.44	109.54	125.89
18	A	1128	CLA	C4D-C3D-CAD	11.43	114.85	108.47
18	A	1108	CLA	C4D-C3D-CAD	11.41	114.83	108.47
18	I	1204	CLA	OBD-CAD-C3D	-11.38	109.09	127.98
18	A	1126	CLA	C4D-C3D-CAD	11.32	114.78	108.47
20	F	6016	BCR	C10-C11-C12	11.29	158.47	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	1304	CLA	C4D-C3D-CAD	11.27	114.75	108.47
18	L	1130	CLA	OBD-CAD-C3D	-11.21	109.38	127.98
18	A	9011	CLA	C4D-C3D-CAD	11.17	114.70	108.47
18	A	1106	CLA	C4D-C3D-CAD	11.16	114.69	108.47
18	B	9022	CLA	C4D-C3D-CAD	11.16	114.69	108.47
18	A	1140	CLA	C4D-C3D-CAD	11.14	114.68	108.47
18	A	1122	CLA	C4D-C3D-CAD	11.13	114.67	108.47
18	B	9023	CLA	C4D-C3D-CAD	11.10	114.66	108.47
18	4	1304	CLA	OBD-CAD-C3D	-11.08	109.58	127.98
18	B	1212	CLA	OBD-CAD-C3D	-11.00	109.72	127.98
18	A	1119	CLA	OBD-CAD-C3D	-10.93	109.83	127.98
18	A	1131	CLA	C4D-C3D-CAD	10.92	114.56	108.47
18	B	1138	CLA	C4D-C3D-CAD	10.92	114.56	108.47
20	B	6017	BCR	C10-C11-C12	10.91	157.27	123.22
18	B	9023	CLA	OBD-CAD-C3D	-10.84	109.99	127.98
18	B	1138	CLA	OBD-CAD-C3D	-10.83	110.00	127.98
18	B	1239	CLA	OBD-CAD-C3D	-10.79	110.06	127.98
18	F	1302	CLA	OBD-CAD-CBD	-10.79	110.49	125.89
18	B	1218	CLA	OBD-CAD-C3D	-10.78	110.09	127.98
18	B	1216	CLA	OBD-CAD-CBD	-10.75	110.54	125.89
18	B	1208	CLA	OBD-CAD-C3D	-10.74	110.14	127.98
18	B	1207	CLA	C4D-C3D-CAD	10.72	114.45	108.47
18	A	1119	CLA	C4D-C3D-CAD	10.72	114.45	108.47
18	B	1205	CLA	C4D-C3D-CAD	10.68	114.43	108.47
18	F	1302	CLA	OBD-CAD-C3D	-10.66	110.28	127.98
18	B	9010	CLA	OBD-CAD-C3D	-10.66	110.28	127.98
18	B	1219	CLA	C4D-C3D-CAD	10.63	114.40	108.47
18	A	1129	CLA	C4D-C3D-CAD	10.59	114.38	108.47
18	A	1131	CLA	OBD-CAD-CBD	-10.59	110.76	125.89
18	B	1209	CLA	OBD-CAD-C3D	-10.55	110.46	127.98
18	B	1222	CLA	C4D-C3D-CAD	10.51	114.33	108.47
18	H	1501	CLA	C4D-C3D-CAD	10.51	114.33	108.47
18	A	9011	CLA	OBD-CAD-C3D	-10.51	110.54	127.98
18	B	1215	CLA	OBD-CAD-CBD	-10.48	110.92	125.89
18	A	1113	CLA	C4D-C3D-CAD	10.45	114.30	108.47
18	A	9013	CLA	OBD-CAD-CBD	-10.44	110.98	125.89
18	B	1237	CLA	C4D-C3D-CAD	10.44	114.29	108.47
18	B	1242	CLA	C4D-C3D-CAD	10.39	114.27	108.47
18	A	1123	CLA	OBD-CAD-CBD	-10.31	111.16	125.89
18	B	1216	CLA	C4D-C3D-CAD	10.27	114.20	108.47
18	B	1214	CLA	C4D-C3D-CAD	10.23	114.18	108.47
18	B	9012	CLA	OBD-CAD-CBD	-10.22	111.30	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	9012	CLA	C4D-C3D-CAD	10.16	114.14	108.47
18	B	1234	CLA	OBD-CAD-CBD	-10.10	111.47	125.89
18	A	1128	CLA	OBD-CAD-C3D	-10.09	111.23	127.98
18	I	1204	CLA	OBD-CAD-CBD	-10.08	111.49	125.89
18	A	1115	CLA	C4D-C3D-CAD	10.08	114.09	108.47
18	B	1227	CLA	C4D-C3D-CAD	10.07	114.09	108.47
18	L	1130	CLA	OBD-CAD-CBD	-10.06	111.52	125.89
18	B	9022	CLA	OBD-CAD-CBD	-10.03	111.57	125.89
18	B	1235	CLA	C4D-C3D-CAD	10.02	114.06	108.47
18	B	1209	CLA	C4D-C3D-CAD	10.01	114.05	108.47
18	A	1137	CLA	OBD-CAD-CBD	-9.99	111.62	125.89
18	A	1136	CLA	OBD-CAD-C3D	-9.98	111.41	127.98
18	A	1131	CLA	CAB-C3B-C4B	-9.97	113.14	128.46
20	A	6011	BCR	C10-C11-C12	9.94	154.22	123.22
18	B	1225	CLA	OBD-CAD-CBD	-9.84	111.84	125.89
18	A	1122	CLA	OBD-CAD-C3D	-9.83	111.66	127.98
18	A	1115	CLA	OBD-CAD-CBD	-9.80	111.90	125.89
18	L	1502	CLA	OBD-CAD-C3D	-9.74	111.82	127.98
18	B	9010	CLA	C4D-C3D-CAD	9.64	113.85	108.47
18	B	1232	CLA	C4D-C3D-CAD	9.58	113.81	108.47
18	A	9013	CLA	C4D-C3D-CAD	9.52	113.78	108.47
18	I	1204	CLA	C4D-C3D-CAD	9.51	113.77	108.47
18	B	1228	CLA	O2D-CGD-CBD	9.45	128.07	111.27
18	A	1137	CLA	C4D-C3D-CAD	9.45	113.74	108.47
18	B	1218	CLA	C4D-C3D-CAD	9.38	113.70	108.47
18	B	1234	CLA	OBD-CAD-C3D	-9.29	112.55	127.98
18	A	1107	CLA	OBD-CAD-CBD	-9.24	112.69	125.89
18	A	1135	CLA	C4D-C3D-CAD	9.17	113.59	108.47
18	A	1135	CLA	OBD-CAD-CBD	-9.09	112.90	125.89
18	B	1239	CLA	C4D-C3D-CAD	9.07	113.53	108.47
18	B	1234	CLA	O2D-CGD-CBD	9.06	127.37	111.27
18	L	1502	CLA	C4D-C3D-CAD	9.04	113.51	108.47
18	B	1231	CLA	C4D-C3D-CAD	9.04	113.51	108.47
18	B	1235	CLA	OBD-CAD-C3D	-9.03	112.99	127.98
18	L	1503	CLA	CAB-C3B-C4B	-8.98	114.67	128.46
18	G	1233	CLA	C4D-C3D-CAD	8.94	113.46	108.47
18	L	1504	CLA	C4D-C3D-CAD	8.93	113.45	108.47
18	L	1503	CLA	C1D-CHD-C4C	-8.90	110.81	122.56
18	A	1136	CLA	O2D-CGD-CBD	8.90	127.08	111.27
18	B	1138	CLA	OBD-CAD-CBD	-8.87	113.22	125.89
18	A	1103	CLA	C4D-C3D-CAD	8.83	113.39	108.47
18	L	1130	CLA	C4D-C3D-CAD	8.82	113.39	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1122	CLA	OBD-CAD-CBD	-8.81	113.31	125.89
18	B	1212	CLA	OBD-CAD-CBD	-8.76	113.38	125.89
18	B	1234	CLA	C4D-C3D-CAD	8.69	113.31	108.47
18	L	1502	CLA	OBD-CAD-CBD	-8.68	113.49	125.89
18	B	9023	CLA	OBD-CAD-CBD	-8.62	113.58	125.89
18	B	1239	CLA	OBD-CAD-CBD	-8.58	113.64	125.89
18	B	1229	CLA	C1D-CHD-C4C	-8.29	111.62	122.56
18	B	1218	CLA	C1D-CHD-C4C	-8.23	111.70	122.56
18	J	2107	CLA	C4D-C3D-CAD	8.22	113.05	108.47
18	B	9010	CLA	OBD-CAD-CBD	-8.22	114.16	125.89
20	I	6018	BCR	C16-C15-C14	-8.13	106.81	123.47
18	B	9012	CLA	OBD-CAD-C3D	-8.03	114.65	127.98
18	B	1214	CLA	OBD-CAD-CBD	-7.96	114.52	125.89
18	B	1222	CLA	OBD-CAD-C3D	-7.95	114.78	127.98
18	B	1238	CLA	C4D-C3D-CAD	7.91	112.88	108.47
18	B	1218	CLA	OBD-CAD-CBD	-7.80	114.75	125.89
18	B	1208	CLA	OBD-CAD-CBD	-7.77	114.80	125.89
18	B	1235	CLA	CAC-C3C-C4C	7.75	134.87	124.81
18	A	1113	CLA	C1D-CHD-C4C	-7.75	112.33	122.56
18	A	1135	CLA	O2D-CGD-CBD	7.60	124.77	111.27
20	I	6018	BCR	C30-C25-C26	-7.54	111.99	122.61
18	B	1221	CLA	OBD-CAD-C3D	-7.53	115.48	127.98
18	B	1219	CLA	OBD-CAD-C3D	-7.53	115.48	127.98
18	B	1242	CLA	C1D-CHD-C4C	-7.49	112.67	122.56
18	B	1221	CLA	C1D-CHD-C4C	-7.45	112.73	122.56
18	B	1202	CLA	OBD-CAD-CBD	-7.43	115.29	125.89
18	B	1220	CLA	C1D-CHD-C4C	-7.40	112.80	122.56
18	A	1131	CLA	CAB-C3B-C2B	-7.39	110.21	124.69
18	B	1229	CLA	CAB-C3B-C2B	-7.33	110.33	124.69
18	B	1235	CLA	O2D-CGD-CBD	7.30	124.24	111.27
18	B	1221	CLA	C4D-C3D-CAD	7.28	112.53	108.47
18	L	1503	CLA	CHD-C4C-NC	7.26	135.64	124.20
18	B	1202	CLA	C1D-CHD-C4C	-7.25	112.99	122.56
18	B	1218	CLA	O2D-CGD-CBD	7.24	124.13	111.27
18	A	1136	CLA	C1D-CHD-C4C	-7.20	113.05	122.56
18	B	1224	CLA	C4D-C3D-CAD	7.17	112.47	108.47
18	B	1228	CLA	C1D-CHD-C4C	-7.14	113.13	122.56
18	B	1225	CLA	C1D-CHD-C4C	-7.13	113.15	122.56
18	A	1137	CLA	OBD-CAD-C3D	-7.10	116.19	127.98
18	B	1205	CLA	C1D-CHD-C4C	-7.09	113.20	122.56
18	B	1222	CLA	OBD-CAD-CBD	-7.06	115.80	125.89
18	A	1108	CLA	C1D-CHD-C4C	-7.06	113.24	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	9010	CLA	C4A-NA-C1A	7.01	109.86	106.71
18	B	9022	CLA	C1D-CHD-C4C	-6.97	113.36	122.56
18	A	1135	CLA	C1D-CHD-C4C	-6.93	113.41	122.56
18	B	1212	CLA	C1D-CHD-C4C	-6.90	113.45	122.56
18	B	1216	CLA	C1D-CHD-C4C	-6.88	113.48	122.56
20	L	6020	BCR	C24-C23-C22	-6.87	115.86	126.23
18	J	2107	CLA	O2D-CGD-CBD	6.87	123.47	111.27
18	G	1233	CLA	C1D-CHD-C4C	-6.84	113.53	122.56
18	B	1239	CLA	C1D-CHD-C4C	-6.84	113.53	122.56
18	F	1139	CLA	OBD-CAD-CBD	-6.84	116.13	125.89
18	L	1502	CLA	C1D-CHD-C4C	-6.83	113.54	122.56
18	L	1130	CLA	O2D-CGD-CBD	6.81	123.37	111.27
18	B	1203	CLA	C1D-CHD-C4C	-6.76	113.64	122.56
18	B	1224	CLA	O2D-CGD-CBD	6.72	123.21	111.27
18	B	1232	CLA	O2D-CGD-CBD	6.70	123.18	111.27
18	B	1237	CLA	C1D-CHD-C4C	-6.70	113.72	122.56
18	A	1124	CLA	C2B-C1B-NB	6.70	115.97	110.11
18	B	1219	CLA	C1-C2-C3	-6.69	114.48	126.04
18	F	1240	CLA	C2B-C1B-NB	6.60	115.89	110.11
18	4	4012	CLA	C2B-C1B-NB	6.53	115.83	110.11
18	A	1119	CLA	C1D-CHD-C4C	-6.53	113.94	122.56
18	A	1136	CLA	C3D-CAD-CBD	-6.51	99.03	107.61
20	L	6020	BCR	C7-C8-C9	6.51	136.08	126.23
18	A	1116	CLA	C2B-C1B-NB	6.48	115.78	110.11
18	L	1504	CLA	C1D-CHD-C4C	-6.46	114.03	122.56
18	A	1134	CLA	C2B-C1B-NB	6.44	115.75	110.11
18	B	1210	CLA	C2B-C1B-NB	6.44	115.75	110.11
18	F	1302	CLA	C1D-CHD-C4C	-6.43	114.07	122.56
18	A	1131	CLA	C1D-CHD-C4C	-6.42	114.09	122.56
18	H	1501	CLA	C1D-CHD-C4C	-6.39	114.12	122.56
18	A	1126	CLA	O2D-CGD-CBD	6.39	122.63	111.27
18	A	1133	CLA	C2B-C1B-NB	6.39	115.70	110.11
18	A	1128	CLA	OBD-CAD-CBD	-6.37	116.79	125.89
18	B	1232	CLA	C1D-CHD-C4C	-6.37	114.15	122.56
18	2	2007	CLA	C2B-C1B-NB	6.37	115.69	110.11
18	L	1130	CLA	C1D-CHD-C4C	-6.36	114.16	122.56
18	B	1236	CLA	C1D-CHD-C4C	-6.34	114.19	122.56
18	A	1115	CLA	C1D-CHD-C4C	-6.33	114.20	122.56
18	1	1010	CLA	C2B-C1B-NB	6.32	115.64	110.11
18	B	1224	CLA	C1D-CHD-C4C	-6.29	114.25	122.56
18	B	1221	CLA	O2D-CGD-CBD	6.29	122.44	111.27
18	2	2012	CLA	C2B-C1B-NB	6.28	115.61	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1214	CLA	OBD-CAD-C3D	-6.28	117.56	127.98
18	A	1129	CLA	C1D-CHD-C4C	-6.26	114.30	122.56
18	L	1502	CLA	O2D-CGD-CBD	6.25	122.38	111.27
18	A	9013	CLA	OBD-CAD-C3D	-6.25	117.60	127.98
18	F	1306	CLA	C2B-C1B-NB	6.25	115.58	110.11
18	B	1207	CLA	C1D-CHD-C4C	-6.25	114.32	122.56
18	4	1304	CLA	C1D-CHD-C4C	-6.24	114.32	122.56
20	F	6016	BCR	C19-C18-C17	-6.24	109.36	118.94
18	A	1120	CLA	C2B-C1B-NB	6.24	115.58	110.11
18	A	1132	CLA	C2B-C1B-NB	6.24	115.57	110.11
18	B	9023	CLA	C1D-CHD-C4C	-6.22	114.35	122.56
18	B	1222	CLA	O2D-CGD-CBD	6.20	122.28	111.27
18	1	1001	CLA	C2B-C1B-NB	6.20	115.54	110.11
18	A	1113	CLA	CHD-C4C-NC	6.20	133.96	124.20
18	B	1237	CLA	C4-C3-C5	6.18	123.05	115.98
18	3	3005	CLA	C2B-C1B-NB	6.16	115.50	110.11
18	4	4012	CLA	C4A-NA-C1A	6.16	109.47	106.71
18	B	1138	CLA	C1D-CHD-C4C	-6.15	114.45	122.56
18	B	1205	CLA	O2D-CGD-CBD	6.14	122.19	111.27
18	A	1136	CLA	CHD-C4C-C3C	-6.14	115.82	124.84
20	F	6016	BCR	C23-C22-C21	-6.14	109.53	118.94
18	1	1011	CLA	C2B-C1B-NB	6.12	115.47	110.11
18	B	9022	CLA	O2D-CGD-CBD	6.11	122.13	111.27
18	A	1148	CLA	C2B-C1B-NB	6.11	115.46	110.11
18	4	4006	CLA	C2B-C1B-NB	6.10	115.45	110.11
18	A	1131	CLA	OBD-CAD-C3D	-6.09	117.86	127.98
18	4	4010	CLA	C2B-C1B-NB	6.09	115.45	110.11
18	L	1503	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
18	B	1219	CLA	OBD-CAD-CBD	-6.09	117.20	125.89
18	A	1104	CLA	C2B-C1B-NB	6.09	115.44	110.11
18	2	2003	CLA	C2B-C1B-NB	6.09	115.44	110.11
18	B	1201	CLA	C2B-C1B-NB	6.08	115.44	110.11
18	3	3013	CLA	C2B-C1B-NB	6.08	115.43	110.11
18	B	9010	CLA	C1D-CHD-C4C	-6.07	114.55	122.56
18	A	1126	CLA	O2D-CGD-O1D	-6.07	111.97	123.84
18	3	3004	CLA	C2B-C1B-NB	6.06	115.42	110.11
18	4	4001	CLA	C2B-C1B-NB	6.06	115.42	110.11
18	B	9010	CLA	O2D-CGD-CBD	6.06	122.03	111.27
18	B	1234	CLA	C1D-CHD-C4C	-6.05	114.57	122.56
18	I	1204	CLA	C1D-CHD-C4C	-6.05	114.58	122.56
18	A	1110	CLA	C2B-C1B-NB	6.04	115.40	110.11
18	B	1225	CLA	O2D-CGD-CBD	6.04	122.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4005	CLA	C2B-C1B-NB	6.04	115.40	110.11
18	3	3001	CLA	C2B-C1B-NB	6.03	115.39	110.11
18	J	1308	CLA	C2B-C1B-NB	6.02	115.38	110.11
18	B	9012	CLA	O2D-CGD-CBD	6.01	121.95	111.27
20	B	6017	BCR	C20-C21-C22	-6.00	118.74	127.31
18	1	1005	CLA	C2B-C1B-NB	6.00	115.36	110.11
18	A	1103	CLA	CHC-C1C-NC	5.99	133.29	124.20
18	B	1227	CLA	C1D-CHD-C4C	-5.98	114.67	122.56
18	B	1217	CLA	C1D-CHD-C4C	-5.97	114.68	122.56
18	2	2010	CLA	C2B-C1B-NB	5.97	115.33	110.11
18	A	1143	CLA	C2B-C1B-NB	5.96	115.33	110.11
18	F	4015	CLA	C2B-C1B-NB	5.96	115.33	110.11
18	3	3015	CLA	C2B-C1B-NB	5.95	115.32	110.11
18	3	3009	CLA	C2B-C1B-NB	5.95	115.32	110.11
18	2	2005	CLA	C2B-C1B-NB	5.94	115.32	110.11
18	B	1211	CLA	C2B-C1B-NB	5.94	115.31	110.11
18	2	2011	CLA	C2B-C1B-NB	5.93	115.30	110.11
18	B	1212	CLA	CHD-C4C-NC	5.92	133.53	124.20
18	J	1307	CLA	C2B-C1B-NB	5.91	115.28	110.11
18	A	1123	CLA	C1D-CHD-C4C	-5.90	114.77	122.56
19	B	5002	PQN	C11-C12-C13	-5.90	116.97	126.79
18	1	1003	CLA	C2B-C1B-NB	5.89	115.27	110.11
18	B	1215	CLA	C4A-NA-C1A	5.87	109.34	106.71
18	B	1215	CLA	O2D-CGD-CBD	5.86	121.69	111.27
18	A	1152	CLA	C2B-C1B-NB	5.86	115.24	110.11
18	1	1006	CLA	C2B-C1B-NB	5.86	115.24	110.11
18	A	1109	CLA	C2B-C1B-NB	5.86	115.24	110.11
18	B	1221	CLA	OBD-CAD-CBD	-5.85	117.53	125.89
18	4	4007	CLA	C2B-C1B-NB	5.85	115.23	110.11
18	B	1212	CLA	C3D-CAD-CBD	-5.85	99.91	107.61
20	F	6016	BCR	C24-C23-C22	-5.84	117.41	126.23
18	B	1209	CLA	C1D-CHD-C4C	-5.84	114.85	122.56
18	F	1302	CLA	C3D-CAD-CBD	-5.83	99.92	107.61
18	2	2002	CLA	C2B-C1B-NB	5.83	115.21	110.11
18	B	1202	CLA	O2D-CGD-CBD	5.82	121.61	111.27
18	H	1505	CLA	C2B-C1B-NB	5.82	115.21	110.11
18	L	1504	CLA	O2D-CGD-CBD	5.82	121.61	111.27
18	B	1301	CLA	C2B-C1B-NB	5.81	115.20	110.11
18	F	1303	CLA	C2B-C1B-NB	5.81	115.20	110.11
18	A	1131	CLA	C4A-NA-C1A	5.81	109.32	106.71
18	B	1214	CLA	C1D-CHD-C4C	-5.80	114.91	122.56
18	K	1150	CLA	C2B-C1B-NB	5.79	115.18	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	6020	BCR	C37-C22-C21	-5.79	114.81	122.92
18	1	1013	CLA	C2B-C1B-NB	5.78	115.17	110.11
18	4	4011	CLA	C2B-C1B-NB	5.77	115.16	110.11
18	A	1140	CLA	C1D-CHD-C4C	-5.76	114.95	122.56
18	A	1122	CLA	C1D-CHD-C4C	-5.76	114.96	122.56
18	G	1248	CLA	C2B-C1B-NB	5.75	115.14	110.11
18	1	1007	CLA	C2B-C1B-NB	5.75	115.14	110.11
18	B	1222	CLA	C1D-CHD-C4C	-5.74	114.99	122.56
18	A	1124	CLA	C1D-CHD-C4C	-5.74	111.90	126.10
18	4	4009	CLA	C2B-C1B-NB	5.73	115.13	110.11
18	B	1242	CLA	O2D-CGD-CBD	5.73	121.45	111.27
20	L	6020	BCR	C8-C7-C6	-5.72	111.13	127.20
18	A	9011	CLA	C1D-CHD-C4C	-5.72	115.01	122.56
18	B	1229	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
18	A	1111	CLA	C2B-C1B-NB	5.72	115.12	110.11
18	J	2107	CLA	C1D-CHD-C4C	-5.71	115.02	122.56
18	B	1202	CLA	CMD-C2D-C3D	-5.71	114.00	124.68
18	A	1105	CLA	C2B-C1B-NB	5.71	115.11	110.11
18	B	1225	CLA	CHD-C4C-NC	5.70	133.18	124.20
18	A	1113	CLA	O2D-CGD-CBD	5.69	121.38	111.27
18	A	1103	CLA	C1D-CHD-C4C	-5.68	115.06	122.56
18	2	2004	CLA	C2B-C1B-NB	5.67	115.08	110.11
18	B	1238	CLA	O2D-CGD-CBD	5.67	121.34	111.27
18	A	1132	CLA	C3A-C4A-CHB	-5.67	116.97	123.91
18	A	1109	CLA	C1D-CHD-C4C	-5.67	112.92	128.75
18	A	1123	CLA	C3D-CAD-CBD	-5.66	100.15	107.61
18	2	2015	CLA	C2B-C1B-NB	5.65	115.06	110.11
18	3	3007	CLA	C2B-C1B-NB	5.65	115.06	110.11
18	F	1305	CLA	C2B-C1B-NB	5.65	115.05	110.11
18	A	1144	CLA	C2B-C1B-NB	5.64	115.05	110.11
18	B	1241	CLA	C2B-C1B-NB	5.64	115.05	110.11
18	A	1117	CLA	C2B-C1B-NB	5.63	115.04	110.11
18	A	1146	CLA	C2B-C1B-NB	5.63	115.04	110.11
18	3	3003	CLA	C2B-C1B-NB	5.61	115.03	110.11
18	A	1309	CLA	C2B-C1B-NB	5.60	115.02	110.11
18	B	1203	CLA	OBD-CAD-CBD	-5.59	117.90	125.89
18	1	1014	CLA	C2B-C1B-NB	5.58	115.00	110.11
18	B	1229	CLA	C3D-CAD-CBD	-5.58	100.26	107.61
18	1	1012	CLA	C2B-C1B-NB	5.58	115.00	110.11
18	F	1139	CLA	C1D-CHD-C4C	-5.57	115.20	122.56
18	A	1113	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
18	4	4008	CLA	C2B-C1B-NB	5.56	114.98	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	6016	BCR	C11-C12-C13	-5.56	110.81	126.42
18	B	1212	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
18	2	2001	CLA	C2B-C1B-NB	5.55	114.97	110.11
18	B	1208	CLA	CAC-C3C-C4C	5.54	132.00	124.81
18	1	1002	CLA	C2B-C1B-NB	5.54	114.96	110.11
18	B	1203	CLA	C1-C2-C3	-5.54	117.79	126.75
18	K	1141	CLA	C2B-C1B-NB	5.54	114.96	110.11
18	1	1008	CLA	C2B-C1B-NB	5.53	114.95	110.11
18	A	1136	CLA	CHD-C4C-NC	5.52	132.91	124.20
18	A	1101	CLA	C2B-C1B-NB	5.52	114.94	110.11
18	F	1139	CLA	OBD-CAD-C3D	-5.52	118.82	127.98
18	B	1215	CLA	OBD-CAD-C3D	-5.52	118.82	127.98
18	A	1147	CLA	C2B-C1B-NB	5.51	114.93	110.11
18	4	4004	CLA	C2B-C1B-NB	5.51	114.93	110.11
18	3	3008	CLA	C2B-C1B-NB	5.50	114.93	110.11
18	B	1215	CLA	C4D-C3D-CAD	5.49	111.53	108.47
18	B	1223	CLA	CHC-C1C-NC	5.49	132.34	124.23
18	A	1102	CLA	C2B-C1B-NB	5.49	114.91	110.11
18	A	1137	CLA	O2D-CGD-CBD	5.48	121.01	111.27
18	B	1239	CLA	O2D-CGD-CBD	5.47	120.98	111.27
18	B	1207	CLA	CAA-C2A-C3A	-5.46	97.83	112.78
18	A	1122	CLA	O2D-CGD-CBD	5.45	120.96	111.27
18	L	1503	CLA	CHC-C1C-NC	5.45	132.48	124.20
18	A	1128	CLA	O2D-CGD-CBD	5.45	120.96	111.27
18	B	1236	CLA	O2D-CGD-CBD	5.45	120.95	111.27
20	A	6011	BCR	C38-C26-C25	-5.45	118.41	124.53
18	A	1126	CLA	C1D-CHD-C4C	-5.44	115.37	122.56
18	A	1119	CLA	O2D-CGD-CBD	5.44	120.94	111.27
18	3	2009	CLA	C2B-C1B-NB	5.44	114.88	110.11
18	G	1248	CLA	CHD-C4C-NC	5.44	132.60	124.21
18	2	2008	CLA	C2B-C1B-NB	5.44	114.87	110.11
18	B	1231	CLA	O2D-CGD-CBD	5.44	120.93	111.27
18	A	1134	CLA	C3B-C2B-C1B	-5.43	101.64	106.29
18	A	1127	CLA	C2B-C1B-NB	5.43	114.86	110.11
18	A	1142	CLA	C2B-C1B-NB	5.43	114.86	110.11
18	A	9011	CLA	C3D-CAD-CBD	-5.43	100.46	107.61
18	1	1006	CLA	C3A-C4A-CHB	-5.43	117.27	123.91
18	4	4005	CLA	C2D-C3D-C4D	-5.42	101.63	106.30
18	4	4013	CLA	C2B-C1B-NB	5.42	114.86	110.11
18	A	9013	CLA	C1D-CHD-C4C	-5.42	115.41	122.56
18	B	1234	CLA	O2D-CGD-O1D	-5.41	113.27	123.84
20	F	6016	BCR	C21-C20-C19	-5.41	106.34	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3005	CLA	C3B-C2B-C1B	-5.39	101.67	106.29
18	2	2013	CLA	C2B-C1B-NB	5.39	114.83	110.11
18	3	3011	CLA	C2B-C1B-NB	5.39	114.83	110.11
18	A	1116	CLA	C3A-C4A-CHB	-5.38	117.32	123.91
18	B	1208	CLA	C1-O2A-CGA	5.38	130.56	116.44
18	A	1118	CLA	C2B-C1B-NB	5.38	114.82	110.11
18	4	1304	CLA	O2D-CGD-CBD	5.37	120.82	111.27
18	B	1218	CLA	CED-O2D-CGD	5.35	128.04	115.94
18	B	1238	CLA	CAA-C2A-C1A	-5.35	94.44	111.97
18	A	1120	CLA	C3A-C4A-CHB	-5.34	117.37	123.91
18	A	1136	CLA	O1D-CGD-CBD	-5.33	113.58	124.48
18	A	1131	CLA	C3D-CAD-CBD	-5.33	100.59	107.61
18	G	1233	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
18	G	1233	CLA	CHD-C4C-NC	5.31	132.57	124.20
18	F	1139	CLA	C3D-CAD-CBD	-5.31	100.61	107.61
20	L	6020	BCR	C23-C22-C21	5.31	127.09	118.94
18	B	1217	CLA	CMD-C2D-C3D	-5.31	114.75	124.68
18	B	1230	CLA	C2B-C1B-NB	5.30	114.75	110.11
18	3	3006	CLA	C2B-C1B-NB	5.30	114.75	110.11
18	B	1209	CLA	CGD-CBD-CAD	-5.30	93.57	110.73
18	B	1207	CLA	C4A-NA-C1A	5.30	109.09	106.71
18	A	1134	CLA	C3A-C4A-CHB	-5.29	117.43	123.91
18	A	1104	CLA	C3A-C4A-CHB	-5.29	117.44	123.91
18	A	1106	CLA	C1D-CHD-C4C	-5.29	115.58	122.56
18	A	1110	CLA	C3B-C2B-C1B	-5.28	101.77	106.29
18	4	4002	CLA	C2B-C1B-NB	5.28	114.73	110.11
18	B	1223	CLA	C2B-C1B-NB	5.27	114.72	110.11
18	A	1103	CLA	O2D-CGD-CBD	5.26	120.62	111.27
20	B	6017	BCR	C21-C20-C19	-5.26	106.81	123.22
18	A	1133	CLA	C3B-C2B-C1B	-5.26	101.79	106.29
18	3	3010	CLA	C2B-C1B-NB	5.25	114.71	110.11
18	A	1124	CLA	C2A-C1A-CHA	-5.24	113.69	122.63
18	G	1248	CLA	C1D-CHD-C4C	-5.24	113.14	126.10
18	A	1122	CLA	C3D-CAD-CBD	-5.23	100.72	107.61
18	1	1012	CLA	C4A-NA-C1A	5.23	109.06	106.71
18	A	1118	CLA	C4A-NA-C1A	5.23	109.06	106.71
18	A	1108	CLA	CHD-C4C-NC	5.23	132.44	124.20
18	1	1004	CLA	C2B-C1B-NB	5.22	114.69	110.11
18	A	1103	CLA	C4A-NA-C1A	5.22	109.05	106.71
18	B	9022	CLA	O2D-CGD-O1D	-5.22	113.64	123.84
18	1	1010	CLA	C3A-C4A-CHB	-5.21	117.53	123.91
18	B	1213	CLA	C2B-C1B-NB	5.21	114.67	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1215	CLA	CHC-C1C-NC	5.21	132.10	124.20
18	B	1206	CLA	C3D-C2D-C1D	5.21	110.79	106.30
18	A	1119	CLA	CHD-C4C-NC	5.20	132.40	124.20
18	B	1229	CLA	CHD-C4C-NC	5.19	132.38	124.20
18	G	1248	CLA	CHC-C1C-NC	5.18	131.88	124.23
18	B	1216	CLA	O2D-CGD-CBD	5.18	120.47	111.27
18	A	1148	CLA	C3A-C4A-CHB	-5.17	117.58	123.91
18	4	1304	CLA	C3D-CAD-CBD	-5.17	100.80	107.61
18	B	1206	CLA	C2D-C3D-C4D	-5.17	101.85	106.30
18	A	1128	CLA	C1D-CHD-C4C	-5.16	115.75	122.56
18	B	1208	CLA	C1D-CHD-C4C	-5.16	115.75	122.56
18	G	1233	CLA	O2D-CGD-CBD	5.16	120.43	111.27
18	B	1201	CLA	C3A-C4A-CHB	-5.16	117.60	123.91
18	L	1503	CLA	O2D-CGD-CBD	5.15	120.42	111.27
20	F	6016	BCR	C33-C5-C6	-5.15	118.74	124.53
18	B	1219	CLA	O2D-CGD-CBD	5.15	120.41	111.27
18	4	4009	CLA	C3A-C4A-CHB	-5.14	117.61	123.91
18	B	1229	CLA	C1B-C2B-C3B	-5.14	102.14	106.92
18	B	1217	CLA	O2D-CGD-CBD	5.14	120.40	111.27
18	A	1115	CLA	CHC-C1C-NC	5.14	132.00	124.20
18	A	1151	CLA	C2B-C1B-NB	5.11	114.59	110.11
18	4	4011	CLA	C3A-C4A-CHB	-5.11	117.65	123.91
18	4	4007	CLA	C3A-C4A-CHB	-5.11	117.65	123.91
20	I	6018	BCR	C38-C26-C27	5.11	123.43	113.62
18	B	1224	CLA	OBD-CAD-C3D	-5.11	119.50	127.98
18	B	9012	CLA	C4A-NA-C1A	5.11	109.00	106.71
18	L	1502	CLA	CHD-C4C-NC	5.10	132.24	124.20
18	F	1240	CLA	C3B-C2B-C1B	-5.10	101.92	106.29
18	B	1225	CLA	CAA-C2A-C1A	-5.10	95.27	111.97
18	F	4015	CLA	C3B-C2B-C1B	-5.09	101.93	106.29
18	B	1220	CLA	CHD-C4C-NC	5.09	132.23	124.20
18	B	1218	CLA	CHD-C4C-NC	5.09	132.23	124.20
18	A	1101	CLA	C4A-NA-C1A	5.09	109.00	106.71
18	1	1013	CLA	C3A-C4A-CHB	-5.09	117.68	123.91
18	2	2015	CLA	C3A-C4A-CHB	-5.08	117.69	123.91
18	L	1503	CLA	C3D-CAD-CBD	-5.08	100.92	107.61
18	B	9023	CLA	C4A-NA-C1A	5.08	108.99	106.71
18	4	4005	CLA	C1D-CHD-C4C	-5.08	113.54	126.10
18	3	3002	CLA	C2B-C1B-NB	5.07	114.55	110.11
18	B	9012	CLA	C1D-CHD-C4C	-5.06	115.88	122.56
18	2	2003	CLA	CHD-C4C-NC	5.06	132.01	124.21
18	1	1008	CLA	C1D-CHD-C4C	-5.05	113.59	126.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1123	CLA	CHD-C4C-NC	5.05	132.17	124.20
18	B	1203	CLA	C4A-NA-C1A	5.05	108.97	106.71
18	B	1223	CLA	CHD-C4C-NC	5.04	131.99	124.21
18	A	1104	CLA	C3B-C2B-C1B	-5.04	101.97	106.29
18	1	1012	CLA	C2A-C1A-CHA	-5.04	114.03	122.63
18	4	4003	CLA	C2B-C1B-NB	5.03	114.52	110.11
18	A	1136	CLA	C4A-NA-C1A	5.03	108.97	106.71
18	2	2003	CLA	C4A-NA-C1A	5.03	108.97	106.71
18	4	4005	CLA	C3D-C2D-C1D	5.02	110.63	106.30
18	3	3001	CLA	C3A-C4A-CHB	-5.02	117.76	123.91
18	2	2005	CLA	C3A-C4A-CHB	-5.01	117.77	123.91
18	A	1137	CLA	C1D-CHD-C4C	-5.01	115.94	122.56
18	J	1307	CLA	C3A-C4A-CHB	-5.01	117.78	123.91
18	B	1235	CLA	O2D-CGD-O1D	-5.00	114.06	123.84
18	F	1240	CLA	C2D-C3D-C4D	-5.00	101.99	106.30
18	L	1503	CLA	CMD-C2D-C3D	-5.00	115.33	124.68
18	B	1235	CLA	C1D-CHD-C4C	-5.00	115.96	122.56
18	A	1151	CLA	C1D-CHD-C4C	-4.99	113.76	126.10
18	A	1135	CLA	CHD-C4C-NC	4.99	132.06	124.20
18	3	3007	CLA	C3A-C4A-CHB	-4.99	117.81	123.91
18	A	1135	CLA	CHD-C4C-C3C	-4.98	117.51	124.84
18	I	1204	CLA	O2D-CGD-CBD	4.98	120.12	111.27
18	A	1148	CLA	C1D-CHD-C4C	-4.98	113.78	126.10
18	A	1124	CLA	C3B-C2B-C1B	-4.98	102.03	106.29
18	3	2009	CLA	C1D-CHD-C4C	-4.97	113.80	126.10
18	J	1308	CLA	C3A-C4A-CHB	-4.96	117.83	123.91
18	B	1226	CLA	C2A-C1A-CHA	-4.96	114.17	122.63
18	B	1238	CLA	C1D-CHD-C4C	-4.96	116.01	122.56
18	B	1239	CLA	CHC-C1C-NC	4.96	131.72	124.20
18	A	1119	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
18	A	9011	CLA	C4A-NA-C1A	4.96	108.93	106.71
18	K	1153	CLA	C2B-C1B-NB	4.95	114.45	110.11
18	B	1220	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
18	1	1008	CLA	C3A-C4A-CHB	-4.95	117.85	123.91
18	F	1240	CLA	C3A-C4A-CHB	-4.94	117.86	123.91
18	B	1234	CLA	C3D-CAD-CBD	-4.94	101.09	107.61
20	B	6017	BCR	C15-C16-C17	-4.94	113.35	123.47
18	3	3012	CLA	C2B-C1B-NB	4.94	114.44	110.11
18	B	1242	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
18	L	1503	CLA	CAA-C2A-C3A	4.94	126.30	112.78
18	3	2009	CLA	C3A-C4A-CHB	-4.94	117.87	123.91
18	B	1224	CLA	CHD-C4C-NC	4.93	131.98	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3012	CLA	C1D-CHD-C4C	-4.93	113.90	126.10
18	A	1108	CLA	O2D-CGD-CBD	4.93	120.02	111.27
18	A	1108	CLA	CHD-C4C-C3C	-4.93	117.60	124.84
18	4	4006	CLA	C2A-C1A-CHA	-4.92	114.24	122.63
18	B	1301	CLA	C2A-C1A-CHA	-4.92	114.24	122.63
18	4	4013	CLA	C1D-CHD-C4C	-4.92	113.92	126.10
18	A	1147	CLA	C1D-CHD-C4C	-4.92	113.93	126.10
18	4	4002	CLA	C1D-CHD-C4C	-4.92	113.93	126.10
18	3	3008	CLA	C3A-C4A-CHB	-4.92	117.89	123.91
18	B	1203	CLA	O2D-CGD-O1D	-4.91	114.23	123.84
18	1	1003	CLA	C3A-C4A-CHB	-4.91	117.89	123.91
18	A	1142	CLA	C1D-CHD-C4C	-4.91	113.94	126.10
18	3	3008	CLA	C4A-NA-C1A	4.91	108.91	106.71
18	F	1240	CLA	C2A-C1A-CHA	-4.91	114.27	122.63
18	4	4007	CLA	C1D-CHD-C4C	-4.91	113.96	126.10
18	F	1305	CLA	C3A-C4A-CHB	-4.90	117.91	123.91
18	3	3004	CLA	C3A-C4A-CHB	-4.90	117.91	123.91
18	B	1207	CLA	CHD-C4C-C3C	-4.90	117.63	124.84
18	3	3002	CLA	C1D-CHD-C4C	-4.90	113.98	126.10
18	3	2009	CLA	CHD-C4C-NC	4.90	131.76	124.21
18	3	3005	CLA	C1D-CHD-C4C	-4.89	113.99	126.10
18	A	1152	CLA	C3A-C4A-CHB	-4.89	117.92	123.91
18	B	1202	CLA	CAA-C2A-C3A	-4.89	99.40	112.78
18	A	1110	CLA	C3D-C2D-C1D	4.89	110.51	106.30
18	B	1205	CLA	C4A-NA-C1A	4.88	108.90	106.71
18	A	1146	CLA	C3A-C4A-CHB	-4.88	117.93	123.91
18	A	1132	CLA	C3B-C2B-C1B	-4.88	102.11	106.29
18	B	1205	CLA	CHD-C4C-NC	4.88	131.89	124.20
20	F	6016	BCR	C23-C24-C25	-4.88	113.50	127.20
18	2	2006	CLA	C2B-C1B-NB	4.88	114.38	110.11
18	L	1503	CLA	C4A-NA-C1A	4.88	108.90	106.71
18	2	2001	CLA	C1D-CHD-C4C	-4.87	114.04	126.10
18	B	1226	CLA	C2B-C1B-NB	4.87	114.38	110.11
18	4	1009	CLA	C1C-NC-C4C	-4.87	104.52	106.71
18	B	1213	CLA	C3A-C4A-CHB	-4.87	117.94	123.91
18	4	4005	CLA	C2A-C1A-CHA	-4.87	114.33	122.63
18	4	4004	CLA	C3A-C4A-CHB	-4.87	117.95	123.91
18	B	1207	CLA	CHB-C4A-NA	4.87	131.24	124.51
18	H	1505	CLA	C4A-NA-C1A	4.87	108.89	106.71
18	A	1111	CLA	C3A-C4A-CHB	-4.87	117.95	123.91
18	2	2012	CLA	C3A-C4A-CHB	-4.87	117.95	123.91
18	B	1201	CLA	C4A-NA-C1A	4.86	108.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1101	CLA	C2A-C1A-CHA	-4.86	114.34	122.63
18	1	1011	CLA	C3A-C4A-CHB	-4.86	117.95	123.91
18	B	1225	CLA	C3D-CAD-CBD	-4.86	101.21	107.61
18	F	4015	CLA	C3A-C4A-CHB	-4.86	117.96	123.91
18	B	1202	CLA	CHC-C1C-NC	4.86	131.57	124.20
18	K	1150	CLA	C3A-C4A-CHB	-4.86	117.96	123.91
18	A	1102	CLA	C2A-C1A-CHA	-4.86	114.35	122.63
18	A	1137	CLA	C4-C3-C5	4.85	123.44	115.27
18	A	1129	CLA	O2D-CGD-CBD	4.85	119.89	111.27
18	A	1135	CLA	O2D-CGD-O1D	-4.85	114.35	123.84
18	2	2004	CLA	C2A-C1A-CHA	-4.85	114.36	122.63
20	I	6018	BCR	C15-C16-C17	4.85	133.41	123.47
18	H	1505	CLA	C3A-C4A-CHB	-4.84	117.98	123.91
18	1	1002	CLA	C3A-C4A-CHB	-4.84	117.98	123.91
18	B	1236	CLA	CHD-C4C-NC	4.84	131.83	124.20
18	1	1002	CLA	C1D-CHD-C4C	-4.83	114.14	126.10
18	2	2003	CLA	C1D-CHD-C4C	-4.83	114.14	126.10
18	G	1248	CLA	C4A-NA-C1A	4.83	108.88	106.71
18	A	1142	CLA	CHD-C4C-NC	4.83	131.66	124.21
18	4	4010	CLA	C3A-C4A-CHB	-4.83	118.00	123.91
18	A	1126	CLA	CGD-CBD-CAD	-4.83	95.10	110.73
18	3	3005	CLA	C3A-C4A-CHB	-4.82	118.00	123.91
18	B	1206	CLA	C3A-C4A-CHB	-4.82	118.00	123.91
18	4	4012	CLA	C3A-C4A-CHB	-4.82	118.00	123.91
18	1	1001	CLA	C3B-C2B-C1B	-4.82	102.16	106.29
18	B	1231	CLA	C1D-CHD-C4C	-4.82	116.20	122.56
18	B	1220	CLA	O2D-CGD-CBD	4.82	119.83	111.27
18	A	1108	CLA	C4A-NA-C1A	4.81	108.87	106.71
18	B	1216	CLA	CHD-C4C-NC	4.81	131.78	124.20
18	L	1125	CLA	C2B-C1B-NB	4.81	114.32	110.11
18	1	1011	CLA	C1D-CHD-C4C	-4.81	114.20	126.10
18	B	1238	CLA	CHD-C4C-NC	4.81	131.78	124.20
18	A	1127	CLA	CHD-C4C-NC	4.81	131.62	124.21
18	B	1242	CLA	CHD-C4C-NC	4.80	131.77	124.20
18	3	3004	CLA	C4A-NA-C1A	4.80	108.86	106.71
18	1	1014	CLA	C2A-C1A-CHA	-4.80	114.44	122.63
18	3	3013	CLA	C3A-C4A-CHB	-4.80	118.03	123.91
18	A	1101	CLA	CHD-C4C-NC	4.80	131.61	124.21
18	A	1111	CLA	C1D-CHD-C4C	-4.79	114.23	126.10
18	A	1109	CLA	CHC-C1C-NC	4.79	131.46	124.29
18	B	9023	CLA	CHD-C4C-NC	4.79	131.75	124.20
18	A	1137	CLA	C3D-CAD-CBD	-4.79	101.30	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1150	CLA	C2A-C1A-CHA	-4.78	114.48	122.63
18	B	1207	CLA	O2D-CGD-O1D	-4.78	114.49	123.84
18	B	9012	CLA	C1-C2-C3	4.78	134.31	126.04
18	3	3009	CLA	C1D-CHD-C4C	-4.78	114.28	126.10
18	3	3012	CLA	CHD-C4C-NC	4.78	131.57	124.21
18	A	1147	CLA	CHD-C4C-NC	4.78	131.57	124.21
18	2	2001	CLA	CHD-C4C-NC	4.77	131.57	124.21
18	1	1004	CLA	C1D-CHD-C4C	-4.77	114.29	126.10
18	A	1101	CLA	CHC-C1C-NC	4.77	131.27	124.23
18	B	1208	CLA	C3D-CAD-CBD	-4.77	101.33	107.61
18	A	1151	CLA	CHD-C4C-NC	4.77	131.56	124.21
18	2	2006	CLA	C2A-C1A-CHA	-4.77	114.50	122.63
18	B	1205	CLA	C3D-CAD-CBD	-4.77	101.33	107.61
18	A	1110	CLA	C2D-C3D-C4D	-4.76	102.20	106.30
18	4	1009	CLA	C1D-CHD-C4C	-4.76	114.32	126.10
18	4	4010	CLA	C1D-CHD-C4C	-4.76	114.32	126.10
18	A	1152	CLA	C1D-CHD-C4C	-4.76	114.32	126.10
18	A	1105	CLA	C3A-C4A-CHB	-4.76	118.08	123.91
18	B	1202	CLA	CHD-C4C-NC	4.75	131.69	124.20
18	A	1146	CLA	C1D-CHD-C4C	-4.75	114.34	126.10
18	B	1210	CLA	C3A-C4A-CHB	-4.75	118.09	123.91
18	B	1206	CLA	C2A-C1A-CHA	-4.75	114.53	122.63
18	B	9023	CLA	CHB-C4A-NA	4.75	131.08	124.51
18	4	4005	CLA	CHD-C4C-NC	4.74	131.53	124.21
18	K	1150	CLA	C1D-CHD-C4C	-4.74	114.36	126.10
18	3	3006	CLA	C2A-C1A-CHA	-4.74	114.55	122.63
18	2	2003	CLA	CHC-C1C-NC	4.74	131.23	124.23
18	3	3003	CLA	C1D-CHD-C4C	-4.74	114.37	126.10
18	A	1309	CLA	C3A-C4A-CHB	-4.74	118.11	123.91
18	A	1105	CLA	C1D-CHD-C4C	-4.74	114.38	126.10
18	B	1223	CLA	C1D-CHD-C4C	-4.74	114.38	126.10
18	B	1224	CLA	OBD-CAD-CBD	-4.74	119.13	125.89
18	2	2007	CLA	C3A-C4A-CHB	-4.73	118.12	123.91
18	B	9010	CLA	CHD-C4C-C3C	-4.73	117.89	124.84
18	4	4004	CLA	C1D-CHD-C4C	-4.73	114.41	126.10
18	3	3015	CLA	C3A-C4A-CHB	-4.73	118.12	123.91
18	F	1139	CLA	O2D-CGD-CBD	4.73	119.67	111.27
20	L	6020	BCR	C15-C14-C13	-4.72	120.57	127.31
18	J	1307	CLA	C3B-C2B-C1B	-4.72	102.25	106.29
18	1	1005	CLA	C2A-C1A-CHA	-4.72	114.58	122.63
18	3	3002	CLA	C3A-C4A-CHB	-4.72	118.13	123.91
18	K	1153	CLA	C3A-C4A-CHB	-4.72	118.13	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2007	CLA	CHD-C4C-NC	4.72	131.49	124.21
18	2	2010	CLA	C3A-C4A-CHB	-4.72	118.13	123.91
18	4	4013	CLA	CHD-C4C-NC	4.71	131.48	124.21
18	4	4006	CLA	C3A-C4A-CHB	-4.71	118.14	123.91
18	B	1229	CLA	CAA-CBA-CGA	-4.71	99.49	113.25
18	2	2002	CLA	C3A-C4A-CHB	-4.71	118.14	123.91
18	A	1115	CLA	C3D-CAD-CBD	-4.71	101.41	107.61
18	4	1009	CLA	C2A-C1A-CHA	-4.71	114.61	122.63
18	1	1005	CLA	C3A-C4A-CHB	-4.71	118.15	123.91
18	A	1132	CLA	C1D-CHD-C4C	-4.71	114.45	126.10
18	2	2002	CLA	C1D-CHD-C4C	-4.71	114.46	126.10
18	B	1228	CLA	CHD-C4C-NC	4.71	131.62	124.20
18	B	1232	CLA	CHD-C4C-NC	4.70	131.61	124.20
18	3	3003	CLA	C3A-C4A-CHB	-4.70	118.15	123.91
18	3	3005	CLA	CHD-C4C-NC	4.70	131.46	124.21
18	A	1147	CLA	C3A-C4A-CHB	-4.70	118.15	123.91
18	B	1242	CLA	C3D-CAD-CBD	-4.70	101.41	107.61
18	F	1302	CLA	CHD-C4C-NC	4.70	131.61	124.20
18	A	1106	CLA	CAA-C2A-C3A	-4.70	105.13	116.10
18	4	4001	CLA	C2A-C1A-CHA	-4.70	114.62	122.63
18	B	1206	CLA	C2B-C1B-NB	4.70	114.22	110.11
18	4	4011	CLA	C3B-C2B-C1B	-4.70	102.27	106.29
18	A	1118	CLA	C3A-C4A-CHB	-4.70	118.16	123.91
18	B	1202	CLA	O2D-CGD-O1D	-4.70	114.65	123.84
18	L	1130	CLA	CHD-C4C-NC	4.70	131.60	124.20
18	A	1113	CLA	C4A-NA-C1A	4.70	108.82	106.71
18	A	1123	CLA	CHD-C4C-C3C	-4.69	117.94	124.84
18	4	4001	CLA	C3B-C2B-C1B	-4.69	102.27	106.29
18	3	3009	CLA	CHD-C4C-NC	4.69	131.45	124.21
18	1	1008	CLA	CHD-C4C-NC	4.69	131.44	124.21
18	A	1137	CLA	CHD-C4C-C3C	-4.68	117.95	124.84
18	3	3007	CLA	C2A-C1A-CHA	-4.68	114.65	122.63
18	A	1147	CLA	C4A-NA-C1A	4.68	108.81	106.71
18	A	1116	CLA	C3B-C2B-C1B	-4.68	102.29	106.29
18	3	3011	CLA	C3A-C4A-CHB	-4.67	118.19	123.91
18	A	1144	CLA	CHD-C4C-NC	4.67	131.41	124.21
18	A	1131	CLA	CHC-C1C-NC	4.67	131.29	124.20
18	1	1011	CLA	CHD-C4C-NC	4.66	131.40	124.21
18	L	1125	CLA	C2A-C1A-CHA	-4.66	114.68	122.63
18	A	1107	CLA	C1D-CHD-C4C	-4.66	116.40	122.56
18	B	1214	CLA	CHD-C4C-NC	4.66	131.55	124.20
18	F	1240	CLA	C3D-C2D-C1D	4.66	110.32	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	1303	CLA	C2A-C1A-CHA	-4.66	114.68	122.63
18	1	1010	CLA	C3B-C2B-C1B	-4.66	102.30	106.29
18	4	4012	CLA	CHD-C4C-NC	4.66	131.40	124.21
18	B	1225	CLA	CHD-C4C-C3C	-4.66	117.99	124.84
18	B	9023	CLA	C3D-CAD-CBD	-4.66	101.47	107.61
18	B	1219	CLA	C1D-CHD-C4C	-4.66	116.41	122.56
18	B	1210	CLA	C3B-C2B-C1B	-4.66	102.30	106.29
18	H	1501	CLA	C3D-CAD-CBD	-4.66	101.47	107.61
18	B	1220	CLA	C3D-CAD-CBD	-4.65	101.48	107.61
18	B	1218	CLA	CHD-C4C-C3C	-4.65	118.00	124.84
18	3	3007	CLA	C4A-NA-C1A	4.65	108.80	106.71
18	F	4015	CLA	C1D-CHD-C4C	-4.65	114.59	126.10
18	2	2008	CLA	C2A-C1A-CHA	-4.65	114.70	122.63
18	3	3007	CLA	CHD-C4C-NC	4.65	131.38	124.21
18	A	1110	CLA	C3A-C4A-CHB	-4.65	118.22	123.91
18	4	4002	CLA	CHD-C4C-NC	4.65	131.38	124.21
18	B	1224	CLA	CHD-C4C-C3C	-4.65	118.01	124.84
18	A	1143	CLA	C3A-C4A-CHB	-4.65	118.22	123.91
18	3	3002	CLA	CHD-C4C-NC	4.65	131.38	124.21
18	B	1211	CLA	CHD-C4C-NC	4.64	131.37	124.21
18	2	2010	CLA	CHD-C4C-NC	4.64	131.37	124.21
18	F	1305	CLA	CHD-C4C-NC	4.64	131.37	124.21
18	3	2009	CLA	CHC-C1C-NC	4.64	131.09	124.23
18	A	1123	CLA	O2D-CGD-CBD	4.64	119.52	111.27
18	4	4007	CLA	CHD-C4C-NC	4.64	131.37	124.21
18	3	3008	CLA	C2A-C1A-CHA	-4.64	114.72	122.63
18	A	1127	CLA	CHC-C1C-NC	4.64	131.08	124.23
18	B	1236	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
18	B	9022	CLA	CHC-C1C-NC	4.63	131.23	124.20
18	A	1120	CLA	C2A-C1A-CHA	-4.63	114.74	122.63
18	3	3011	CLA	C1D-CHD-C4C	-4.63	114.65	126.10
18	1	1013	CLA	C1D-CHD-C4C	-4.63	114.66	126.10
18	J	1308	CLA	C2A-C1A-CHA	-4.62	114.75	122.63
18	B	1213	CLA	C1D-CHD-C4C	-4.62	114.66	126.10
18	B	1235	CLA	CAC-C3C-C2C	-4.62	119.62	127.53
18	3	3008	CLA	CHC-C1C-NC	4.62	131.05	124.23
18	1	1012	CLA	CHC-C1C-NC	4.62	131.05	124.23
18	A	1110	CLA	C1D-CHD-C4C	-4.62	114.68	126.10
18	3	3004	CLA	CHC-C1C-NC	4.62	131.05	124.23
18	2	2004	CLA	C1D-CHD-C4C	-4.61	114.69	126.10
18	A	1108	CLA	C3D-CAD-CBD	-4.61	101.53	107.61
18	1	1006	CLA	CHD-C4C-NC	4.61	131.32	124.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	9010	CLA	CHD-C4C-NC	4.61	131.47	124.20
18	A	1118	CLA	CHC-C1C-NC	4.61	131.04	124.23
18	3	3013	CLA	C1D-CHD-C4C	-4.61	114.69	126.10
18	2	2010	CLA	C1D-CHD-C4C	-4.61	114.70	126.10
18	1	1007	CLA	C3A-C4A-CHB	-4.61	118.27	123.91
20	I	6018	BCR	C20-C19-C18	-4.60	113.48	126.42
18	A	1140	CLA	O2A-CGA-CBA	4.60	126.35	111.91
18	4	4013	CLA	CHC-C1C-NC	4.60	131.02	124.23
20	B	6017	BCR	C28-C27-C26	-4.60	105.86	114.08
18	2	2007	CLA	C1D-CHD-C4C	-4.60	114.73	126.10
18	4	4008	CLA	C1D-CHD-C4C	-4.59	114.73	126.10
18	A	1148	CLA	CHD-C4C-NC	4.59	131.29	124.21
18	1	1002	CLA	CHD-C4C-NC	4.59	131.29	124.21
18	4	4012	CLA	C1D-CHD-C4C	-4.59	114.74	126.10
18	A	1119	CLA	C3D-CAD-CBD	-4.59	101.56	107.61
18	2	2003	CLA	C2A-C1A-CHA	-4.59	114.81	122.63
18	2	2001	CLA	CHC-C1C-NC	4.59	131.01	124.23
18	A	1117	CLA	C1D-CHD-C4C	-4.59	114.75	126.10
18	1	1003	CLA	C1D-CHD-C4C	-4.59	114.75	126.10
18	B	1216	CLA	CHD-C4C-C3C	-4.58	118.10	124.84
18	B	1217	CLA	C3D-CAD-CBD	-4.58	101.57	107.61
18	1	1011	CLA	C3B-C2B-C1B	-4.58	102.37	106.29
18	F	1306	CLA	C2A-C1A-CHA	-4.58	114.82	122.63
18	A	1143	CLA	C2A-C1A-CHA	-4.58	114.82	122.63
18	B	1237	CLA	O2D-CGD-CBD	4.58	119.40	111.27
18	A	1120	CLA	C3B-C2B-C1B	-4.58	102.37	106.29
18	B	1234	CLA	CHD-C4C-NC	4.58	131.41	124.20
18	3	3008	CLA	CHD-C4C-NC	4.57	131.26	124.21
18	H	1505	CLA	CHD-C4C-NC	4.57	131.26	124.21
18	B	1241	CLA	C1D-CHD-C4C	-4.57	114.79	126.10
18	L	1503	CLA	C2A-C1A-CHA	-4.57	115.87	123.86
18	J	1308	CLA	C3B-C2B-C1B	-4.57	102.38	106.29
18	H	1501	CLA	CHD-C4C-NC	4.57	131.40	124.20
18	A	1151	CLA	C3A-C4A-CHB	-4.57	118.31	123.91
18	2	2008	CLA	C1D-CHD-C4C	-4.57	114.79	126.10
18	H	1505	CLA	C1D-CHD-C4C	-4.57	114.80	126.10
18	F	1240	CLA	C1D-CHD-C4C	-4.57	114.80	126.10
18	B	1225	CLA	CHC-C1C-NC	4.57	131.13	124.20
18	A	1144	CLA	CHC-C1C-NC	4.57	130.97	124.23
18	2	2011	CLA	C3A-C4A-CHB	-4.56	118.32	123.91
18	4	4005	CLA	C3D-C4D-ND	4.56	114.11	110.14
18	A	1111	CLA	CHD-C4C-NC	4.56	131.25	124.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1115	CLA	O2D-CGD-CBD	4.56	119.37	111.27
18	4	4003	CLA	C1D-CHD-C4C	-4.56	114.82	126.10
18	A	1140	CLA	O2D-CGD-CBD	4.56	119.36	111.27
18	B	1211	CLA	C1D-CHD-C4C	-4.56	114.83	126.10
18	F	1303	CLA	C1D-CHD-C4C	-4.56	114.83	126.10
18	B	1216	CLA	CHC-C1C-NC	4.55	131.11	124.20
18	A	1133	CLA	C1D-CHD-C4C	-4.55	114.84	126.10
18	1	1001	CLA	C3A-C4A-CHB	-4.55	118.34	123.91
18	3	3013	CLA	C3B-C2B-C1B	-4.55	102.39	106.29
18	B	1234	CLA	CHD-C4C-C3C	-4.55	118.15	124.84
18	A	1110	CLA	C2A-C1A-CHA	-4.55	114.88	122.63
18	B	1228	CLA	CHB-C4A-NA	4.55	130.80	124.51
18	A	1106	CLA	C3D-CAD-CBD	-4.54	101.62	107.61
18	B	1241	CLA	C3B-C2B-C1B	-4.54	102.40	106.29
18	B	1211	CLA	C2A-C1A-CHA	-4.54	114.89	122.63
18	H	1501	CLA	C4A-NA-C1A	4.54	108.75	106.71
18	2	2011	CLA	C1D-CHD-C4C	-4.54	114.87	126.10
18	B	1226	CLA	C1D-CHD-C4C	-4.53	114.88	126.10
18	A	1101	CLA	C1D-CHD-C4C	-4.53	114.88	126.10
18	2	2007	CLA	CHC-C1C-NC	4.53	130.92	124.23
18	B	1215	CLA	CHD-C4C-NC	4.53	131.34	124.20
18	B	1201	CLA	C1D-CHD-C4C	-4.53	114.89	126.10
18	H	1505	CLA	CHC-C1C-NC	4.53	130.91	124.23
18	K	1141	CLA	C2A-C1A-CHA	-4.53	114.91	122.63
18	A	1116	CLA	CHD-C4C-NC	4.53	131.19	124.21
18	B	1214	CLA	CHD-C4C-C3C	-4.52	118.19	124.84
18	3	3002	CLA	CHC-C1C-NC	4.52	130.91	124.23
18	B	1235	CLA	C3D-CAD-CBD	-4.52	101.65	107.61
18	A	1116	CLA	C1D-CHD-C4C	-4.52	114.92	126.10
18	B	1241	CLA	C3A-C4A-CHB	-4.52	118.38	123.91
18	A	1116	CLA	C4A-NA-C1A	4.52	108.74	106.71
18	2	2015	CLA	C1D-CHD-C4C	-4.52	114.92	126.10
18	3	3001	CLA	C2A-C1A-CHA	-4.51	114.94	122.63
18	1	1001	CLA	C2A-C1A-CHA	-4.51	114.94	122.63
18	1	1006	CLA	C1D-CHD-C4C	-4.51	114.94	126.10
18	B	1238	CLA	CHC-C1C-NC	4.51	131.04	124.20
18	A	1118	CLA	C1D-CHD-C4C	-4.51	114.94	126.10
18	2	2011	CLA	C3B-C2B-C1B	-4.51	102.43	106.29
18	3	3004	CLA	CHD-C4C-NC	4.51	131.16	124.21
18	B	1214	CLA	O2D-CGD-CBD	4.51	119.28	111.27
18	F	1303	CLA	C4A-NA-C1A	4.51	108.73	106.71
18	F	1306	CLA	C3A-C4A-CHB	-4.50	118.39	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1228	CLA	C4A-NA-C1A	4.50	108.73	106.71
18	1	1012	CLA	CHD-C4C-NC	4.50	131.16	124.21
18	2	2010	CLA	C2A-C1A-CHA	-4.50	114.95	122.63
18	4	1009	CLA	C2B-C1B-NB	4.50	114.05	110.11
18	B	1225	CLA	C4A-NA-C1A	4.50	108.73	106.71
18	2	2011	CLA	CHC-C1C-NC	4.50	130.88	124.23
18	A	1127	CLA	C2A-C1A-CHA	-4.50	114.96	122.63
18	3	3006	CLA	C1D-CHD-C4C	-4.50	114.96	126.10
18	2	2013	CLA	C1D-CHD-C4C	-4.50	114.96	126.10
18	A	1309	CLA	C1D-CHD-C4C	-4.50	114.96	126.10
18	4	4012	CLA	C2A-C1A-CHA	-4.50	114.96	122.63
18	B	1211	CLA	CHC-C1C-NC	4.50	130.87	124.23
18	F	1303	CLA	C3B-C2B-C1B	-4.50	102.44	106.29
18	3	3010	CLA	C1D-CHD-C4C	-4.50	114.97	126.10
18	A	1148	CLA	C3B-C2B-C1B	-4.50	102.44	106.29
18	4	4002	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	A	1120	CLA	C1D-CHD-C4C	-4.49	114.98	126.10
18	A	1142	CLA	CHC-C1C-NC	4.49	130.87	124.23
18	A	1144	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	A	1144	CLA	C2A-C1A-CHA	-4.49	114.97	122.63
18	F	1303	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	A	1101	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	4	1304	CLA	CHD-C4C-NC	4.49	131.28	124.20
18	1	1014	CLA	C4A-NA-C1A	4.49	108.72	106.71
18	4	4001	CLA	C3A-C4A-CHB	-4.49	118.41	123.91
18	4	4009	CLA	C1D-CHD-C4C	-4.49	114.99	126.10
18	F	1305	CLA	C1D-CHD-C4C	-4.49	115.00	126.10
18	B	1227	CLA	CHC-C1C-NC	4.49	131.01	124.20
18	A	1118	CLA	CHD-C4C-NC	4.49	131.13	124.21
18	3	3001	CLA	C1D-CHD-C4C	-4.49	115.00	126.10
18	3	3007	CLA	CHC-C1C-NC	4.48	130.85	124.23
18	F	4015	CLA	CHD-C4C-NC	4.48	131.13	124.21
18	2	2007	CLA	C4A-NA-C1A	4.48	108.72	106.71
18	2	2010	CLA	CHC-C1C-NC	4.48	130.85	124.23
18	B	1215	CLA	C1D-CHD-C4C	-4.48	116.64	122.56
18	J	1308	CLA	C1D-CHD-C4C	-4.48	115.01	126.10
18	A	1118	CLA	C2A-C1A-CHA	-4.48	114.99	122.63
18	A	1134	CLA	C1D-CHD-C4C	-4.48	115.01	126.10
18	1	1012	CLA	C3A-C4A-CHB	-4.48	118.42	123.91
18	B	1222	CLA	CHD-C4C-NC	4.48	131.26	124.20
18	4	4004	CLA	CHD-C4C-NC	4.48	131.12	124.21
18	4	4010	CLA	CHD-C4C-NC	4.48	131.12	124.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3015	CLA	C1D-CHD-C4C	-4.48	115.02	126.10
18	1	1002	CLA	CHC-C1C-NC	4.48	130.84	124.23
18	A	1144	CLA	C1D-CHD-C4C	-4.48	115.02	126.10
18	A	1143	CLA	C1D-CHD-C4C	-4.47	115.03	126.10
18	A	1111	CLA	C2A-C1A-CHA	-4.47	115.00	122.63
18	B	1230	CLA	C2A-C1A-CHA	-4.47	115.01	122.63
18	B	1228	CLA	O2D-CGD-O1D	-4.47	115.10	123.84
18	4	4012	CLA	C3B-C2B-C1B	-4.47	102.46	106.29
18	A	1128	CLA	CHD-C4C-NC	4.47	131.24	124.20
18	L	1504	CLA	CHD-C4C-NC	4.46	131.23	124.20
18	1	1006	CLA	C3B-C2B-C1B	-4.46	102.47	106.29
18	B	1212	CLA	O2D-CGD-CBD	4.46	119.19	111.27
18	A	1106	CLA	CMB-C2B-C1B	4.46	135.32	128.46
18	4	4009	CLA	C3B-C2B-C1B	-4.46	102.47	106.29
18	3	3007	CLA	C1D-CHD-C4C	-4.46	115.07	126.10
18	F	4015	CLA	C2A-C1A-CHA	-4.46	115.03	122.63
18	B	1241	CLA	C2A-C1A-CHA	-4.46	115.03	122.63
18	3	3007	CLA	C3B-C2B-C1B	-4.46	102.47	106.29
18	J	1307	CLA	C1D-CHD-C4C	-4.46	115.07	126.10
18	1	1004	CLA	C2A-C1A-CHA	-4.45	115.04	122.63
18	B	1222	CLA	C3D-CAD-CBD	-4.45	101.74	107.61
18	4	4008	CLA	C3A-C4A-CHB	-4.45	118.46	123.91
18	B	1213	CLA	C2A-C1A-CHA	-4.45	115.05	122.63
18	B	1211	CLA	C4A-NA-C1A	4.45	108.70	106.71
18	B	1202	CLA	C3D-CAD-CBD	-4.44	101.75	107.61
18	B	1214	CLA	C3D-CAD-CBD	-4.44	101.75	107.61
18	A	1147	CLA	CHC-C1C-NC	4.44	130.79	124.23
18	4	4009	CLA	CHD-C4C-NC	4.44	131.06	124.21
18	F	1240	CLA	C3D-C4D-ND	4.44	114.00	110.14
18	A	1127	CLA	C1D-CHD-C4C	-4.44	115.12	126.10
18	A	1152	CLA	CHD-C4C-NC	4.44	131.05	124.21
18	3	3008	CLA	C1D-CHD-C4C	-4.44	115.12	126.10
18	2	2004	CLA	C3A-C4A-CHB	-4.43	118.48	123.91
18	A	1135	CLA	C3D-CAD-CBD	-4.43	101.77	107.61
18	4	4013	CLA	C2A-C1A-CHA	-4.43	115.07	122.63
18	B	1230	CLA	C1D-CHD-C4C	-4.43	115.13	126.10
18	B	1236	CLA	C3D-CAD-CBD	-4.43	101.77	107.61
18	F	1305	CLA	CHC-C1C-NC	4.43	130.77	124.23
19	A	5001	PQN	O4-C4-C5	-4.43	114.39	121.56
18	A	1102	CLA	C4A-NA-C1A	4.43	108.70	106.71
18	B	1223	CLA	C3A-C4A-CHB	-4.43	118.49	123.91
20	I	6018	BCR	C27-C26-C25	-4.43	116.31	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1012	CLA	C1D-CHD-C4C	-4.42	115.15	126.10
18	4	4010	CLA	C3B-C2B-C1B	-4.42	102.50	106.29
18	B	1221	CLA	C4A-NA-C1A	4.42	108.69	106.71
18	A	1133	CLA	C2A-C1A-CHA	-4.42	115.09	122.63
18	2	2003	CLA	C3A-C4A-CHB	-4.42	118.49	123.91
18	I	1204	CLA	C3D-CAD-CBD	-4.42	101.78	107.61
18	B	9010	CLA	CHC-C1C-NC	4.42	130.91	124.20
18	3	3009	CLA	C3A-C4A-CHB	-4.42	118.50	123.91
18	4	4009	CLA	C4A-NA-C1A	4.42	108.69	106.71
18	2	2013	CLA	CHD-C4C-NC	4.42	131.03	124.21
18	B	1208	CLA	CHC-C1C-NC	4.42	130.91	124.20
18	A	1129	CLA	CHD-C4C-NC	4.42	131.16	124.20
18	K	1150	CLA	CHD-C4C-NC	4.42	131.02	124.21
18	B	1210	CLA	CHD-C4C-NC	4.42	131.02	124.21
18	A	1105	CLA	C2A-C1A-CHA	-4.41	115.10	122.63
18	3	3010	CLA	CHD-C4C-NC	4.41	131.02	124.21
18	L	1502	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
18	B	1201	CLA	CHD-C4C-NC	4.41	131.01	124.21
18	3	3003	CLA	CHD-C4C-NC	4.41	131.01	124.21
18	F	1139	CLA	CED-O2D-CGD	4.41	125.90	115.94
18	A	1111	CLA	C4A-NA-C1A	4.41	108.69	106.71
18	B	1221	CLA	CHD-C4C-NC	4.41	131.15	124.20
18	1	1014	CLA	CHC-C1C-NC	4.40	130.73	124.23
18	B	1238	CLA	O2D-CGD-O1D	-4.40	115.23	123.84
18	B	1206	CLA	C1D-CHD-C4C	-4.40	115.21	126.10
18	2	2007	CLA	C3B-C2B-C1B	-4.40	102.53	106.29
18	2	2008	CLA	CHD-C4C-NC	4.40	130.99	124.21
18	3	3004	CLA	C3B-C2B-C1B	-4.40	102.53	106.29
20	F	6016	BCR	C37-C22-C21	4.40	129.08	122.92
18	B	1237	CLA	C3D-CAD-CBD	-4.40	101.82	107.61
18	3	3015	CLA	C3B-C2B-C1B	-4.40	102.53	106.29
18	A	1117	CLA	C3B-C2B-C1B	-4.40	102.53	106.29
18	3	3001	CLA	C3B-C2B-C1B	-4.39	102.53	106.29
18	A	1128	CLA	O2D-CGD-O1D	-4.39	115.25	123.84
18	G	1233	CLA	C3D-CAD-CBD	-4.39	101.83	107.61
18	3	3005	CLA	CHC-C1C-NC	4.39	130.71	124.23
18	A	1120	CLA	C2D-C3D-C4D	-4.39	102.52	106.30
18	A	1117	CLA	C2A-C1A-CHA	-4.38	115.16	122.63
18	2	2012	CLA	C3B-C2B-C1B	-4.38	102.54	106.29
18	I	1204	CLA	CHD-C4C-C3C	-4.38	118.39	124.84
18	2	2013	CLA	C2A-C1A-CHA	-4.38	115.16	122.63
18	B	1237	CLA	CHD-C4C-NC	4.38	131.10	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1201	CLA	C2A-C1A-CHA	-4.38	115.16	122.63
18	2	2012	CLA	CHC-C1C-NC	4.38	130.70	124.23
18	B	1217	CLA	CHD-C4C-NC	4.38	131.10	124.20
20	I	6018	BCR	C8-C9-C10	4.38	125.66	118.94
18	K	1141	CLA	C3A-C4A-CHB	-4.38	118.55	123.91
18	I	1204	CLA	CHD-C4C-NC	4.38	131.10	124.20
20	F	6016	BCR	C33-C5-C4	4.37	122.02	113.62
18	2	2002	CLA	C2A-C1A-CHA	-4.37	115.18	122.63
18	A	1137	CLA	CHD-C4C-NC	4.37	131.09	124.20
18	B	1203	CLA	O2D-CGD-CBD	4.37	119.03	111.27
18	3	3012	CLA	C3A-C4A-CHB	-4.36	118.57	123.91
18	4	4001	CLA	C1D-CHD-C4C	-4.36	115.30	126.10
20	A	6011	BCR	C1-C6-C5	-4.36	116.47	122.61
18	A	1105	CLA	C2D-C3D-C4D	-4.36	102.54	106.30
18	A	1148	CLA	C2A-C1A-CHA	-4.36	115.20	122.63
18	1	1005	CLA	C3B-C2B-C1B	-4.36	102.56	106.29
18	4	4003	CLA	C3A-C4A-CHB	-4.36	118.57	123.91
18	1	1003	CLA	C3B-C2B-C1B	-4.36	102.56	106.29
18	A	1113	CLA	C3D-CAD-CBD	-4.36	101.87	107.61
18	3	3009	CLA	C3B-C2B-C1B	-4.36	102.56	106.29
18	4	4003	CLA	C2A-C1A-CHA	-4.36	115.21	122.63
18	2	2002	CLA	CHD-C4C-NC	4.35	130.93	124.21
18	A	1105	CLA	CHD-C4C-NC	4.35	130.93	124.21
18	4	4005	CLA	CHC-C1C-NC	4.35	130.66	124.23
18	2	2011	CLA	CHD-C4C-NC	4.35	130.93	124.21
18	2	2005	CLA	C1D-CHD-C4C	-4.35	115.33	126.10
18	A	1107	CLA	CHC-C1C-NC	4.35	130.81	124.20
18	H	1505	CLA	C3B-C2B-C1B	-4.35	102.56	106.29
18	B	1301	CLA	C3A-C4A-CHB	-4.35	118.58	123.91
18	3	3009	CLA	CHC-C1C-NC	4.35	130.65	124.23
18	A	1309	CLA	C2A-C1A-CHA	-4.35	115.22	122.63
18	B	1210	CLA	CHC-C1C-NC	4.34	130.65	124.23
18	A	1142	CLA	C3A-C4A-CHB	-4.34	118.59	123.91
18	4	4013	CLA	C3A-C4A-CHB	-4.34	118.59	123.91
18	2	2001	CLA	C3A-C4A-CHB	-4.34	118.59	123.91
18	3	3010	CLA	CHC-C1C-NC	4.34	130.64	124.23
18	A	9013	CLA	C3D-CAD-CBD	-4.34	101.89	107.61
18	4	4009	CLA	C2A-C1A-CHA	-4.34	115.23	122.63
18	A	1104	CLA	C1D-CHD-C4C	-4.34	115.36	126.10
18	1	1010	CLA	C4A-NA-C1A	4.34	108.66	106.71
18	K	1150	CLA	C4A-NA-C1A	4.34	108.66	106.71
18	4	4010	CLA	C2A-C1A-CHA	-4.34	115.24	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	1306	CLA	C1D-CHD-C4C	-4.33	115.38	126.10
18	2	2006	CLA	C3A-C4A-CHB	-4.33	118.61	123.91
18	4	4002	CLA	C2D-C3D-C4D	-4.33	102.57	106.30
18	3	3005	CLA	C2A-C1A-CHA	-4.33	115.25	122.63
18	4	4006	CLA	CHC-C1C-NC	4.33	130.62	124.23
18	L	1125	CLA	CHC-C1C-NC	4.33	130.62	124.23
18	2	2008	CLA	C4A-NA-C1A	4.33	108.65	106.71
18	2	2008	CLA	CHC-C1C-NC	4.33	130.62	124.23
18	1	1014	CLA	C3A-C4A-CHB	-4.32	118.62	123.91
18	4	4008	CLA	C2A-C1A-CHA	-4.32	115.26	122.63
18	1	1003	CLA	CHD-C4C-NC	4.32	130.88	124.21
18	L	1502	CLA	C3D-CAD-CBD	-4.32	101.91	107.61
18	4	4002	CLA	CHC-C1C-NC	4.32	130.61	124.23
18	A	1122	CLA	CHD-C4C-C3C	-4.32	118.49	124.84
18	2	2015	CLA	CHD-C4C-NC	4.32	130.88	124.21
18	B	1226	CLA	CHD-C4C-NC	4.32	130.87	124.21
18	2	2004	CLA	C2D-C3D-C4D	-4.32	102.58	106.30
18	G	1248	CLA	C2A-C1A-CHA	-4.32	115.27	122.63
18	A	1127	CLA	C4A-NA-C1A	4.32	108.65	106.71
18	2	2007	CLA	C2A-C1A-CHA	-4.31	115.28	122.63
18	A	1102	CLA	C1D-CHD-C4C	-4.31	115.43	126.10
18	3	3012	CLA	CHC-C1C-NC	4.31	130.60	124.23
18	F	1303	CLA	CHD-C4C-NC	4.31	130.86	124.21
18	4	4007	CLA	C2A-C1A-CHA	-4.31	115.28	122.63
18	K	1153	CLA	C1D-CHD-C4C	-4.31	115.44	126.10
18	2	2013	CLA	C3A-C4A-CHB	-4.31	118.63	123.91
18	2	2005	CLA	CHC-C1C-NC	4.31	130.59	124.23
18	B	1218	CLA	C1-C2-C3	-4.31	118.59	126.04
18	3	3004	CLA	C2A-C1A-CHA	-4.31	115.29	122.63
18	2	2012	CLA	CHD-C4C-NC	4.31	130.85	124.21
18	4	4004	CLA	C4A-NA-C1A	4.31	108.64	106.71
18	B	1138	CLA	C3D-CAD-CBD	-4.31	101.94	107.61
18	1	1008	CLA	CHC-C1C-NC	4.30	130.59	124.23
18	B	1239	CLA	CHD-C4C-NC	4.30	130.99	124.20
18	2	2008	CLA	C3A-C4A-CHB	-4.30	118.64	123.91
18	A	1151	CLA	CHC-C1C-NC	4.30	130.58	124.23
18	A	1115	CLA	CHD-C4C-NC	4.30	130.98	124.20
18	A	9011	CLA	CED-O2D-CGD	4.30	125.67	115.94
18	A	1117	CLA	C3A-C4A-CHB	-4.30	118.64	123.91
18	1	1005	CLA	C4A-NA-C1A	4.30	108.64	106.71
18	B	1221	CLA	CHC-C1C-NC	4.30	130.72	124.20
18	J	1307	CLA	C2A-C1A-CHA	-4.30	115.31	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1225	CLA	CAA-CBA-CGA	-4.30	104.36	113.59
18	B	1227	CLA	O2D-CGD-CBD	4.30	118.90	111.27
18	4	4006	CLA	C3B-C2B-C1B	-4.29	102.61	106.29
18	2	2004	CLA	CHD-C4C-NC	4.29	130.83	124.21
18	3	3010	CLA	C3A-C4A-CHB	-4.29	118.66	123.91
18	1	1004	CLA	C3A-C4A-CHB	-4.29	118.66	123.91
18	B	1230	CLA	CHC-C1C-NC	4.29	130.57	124.23
18	3	3009	CLA	C2A-C1A-CHA	-4.29	115.32	122.63
18	1	1007	CLA	C1D-CHD-C4C	-4.29	115.49	126.10
18	F	1139	CLA	CHD-C4C-C3C	-4.29	118.54	124.84
18	A	1134	CLA	C2A-C1A-CHA	-4.29	115.33	122.63
18	B	1206	CLA	C4A-NA-C1A	4.28	108.63	106.71
18	3	3006	CLA	C3A-C4A-CHB	-4.28	118.67	123.91
18	A	1131	CLA	CHD-C4C-NC	4.28	130.95	124.20
18	1	1010	CLA	C1D-CHD-C4C	-4.28	115.51	126.10
18	2	2015	CLA	C4A-NA-C1A	4.28	108.63	106.71
18	3	2009	CLA	C4A-NA-C1A	4.28	108.63	106.71
18	1	1002	CLA	C2A-C1A-CHA	-4.27	115.34	122.63
18	A	1134	CLA	CHD-C4C-NC	4.27	130.80	124.21
18	3	3011	CLA	CHD-C4C-NC	4.27	130.80	124.21
18	1	1013	CLA	CHD-C4C-NC	4.27	130.80	124.21
18	2	2011	CLA	C2A-C1A-CHA	-4.27	115.35	122.63
18	B	1207	CLA	CHD-C4C-NC	4.27	130.93	124.20
18	A	1140	CLA	C3D-CAD-CBD	-4.27	101.98	107.61
18	B	1138	CLA	CHC-C1C-NC	4.27	130.68	124.20
18	J	1308	CLA	CHD-C4C-NC	4.27	130.79	124.21
18	B	1227	CLA	CHD-C4C-NC	4.27	130.93	124.20
18	L	1125	CLA	C3A-C4A-CHB	-4.27	118.69	123.91
18	J	1308	CLA	C4A-NA-C1A	4.26	108.62	106.71
18	B	1205	CLA	O2A-CGA-CBA	4.26	125.29	111.91
18	2	2013	CLA	CHC-C1C-NC	4.26	130.53	124.23
18	3	3001	CLA	C4A-NA-C1A	4.26	108.62	106.71
18	F	1302	CLA	CHD-C4C-C3C	-4.26	118.57	124.84
20	B	6017	BCR	C1-C6-C5	-4.26	116.61	122.61
18	1	1007	CLA	C2A-C1A-CHA	-4.26	115.37	122.63
18	A	1152	CLA	C3B-C2B-C1B	-4.26	102.64	106.29
20	I	6018	BCR	C11-C12-C13	-4.26	114.45	126.42
18	1	1014	CLA	C1D-CHD-C4C	-4.26	115.56	126.10
18	1	1010	CLA	CHD-C4C-NC	4.26	130.78	124.21
18	4	4007	CLA	CHC-C1C-NC	4.26	130.51	124.23
18	4	1304	CLA	CHD-C4C-C3C	-4.25	118.59	124.84
18	2	2003	CLA	C3B-C2B-C1B	-4.25	102.65	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1208	CLA	O2D-CGD-CBD	4.25	118.81	111.27
18	4	4009	CLA	CHC-C1C-NC	4.25	130.50	124.23
20	A	6011	BCR	C31-C1-C6	-4.25	103.41	110.30
18	A	1107	CLA	O2A-C1-C2	4.25	119.79	108.64
18	4	4012	CLA	CHC-C1C-NC	4.25	130.50	124.23
18	B	9012	CLA	CHD-C4C-NC	4.25	130.89	124.20
18	2	2005	CLA	CHD-C4C-NC	4.24	130.76	124.21
18	G	1248	CLA	C3A-C4A-CHB	-4.24	118.71	123.91
18	3	3013	CLA	CHD-C4C-NC	4.24	130.75	124.21
18	1	1012	CLA	C3B-C2B-C1B	-4.24	102.66	106.29
18	A	1107	CLA	C3D-CAD-CBD	-4.24	102.02	107.61
18	2	2012	CLA	C2A-C1A-CHA	-4.23	115.41	122.63
18	B	1210	CLA	C2A-C1A-CHA	-4.23	115.41	122.63
18	1	1011	CLA	CHC-C1C-NC	4.23	130.48	124.23
18	B	9023	CLA	CHD-C4C-C3C	-4.23	118.61	124.84
18	2	2006	CLA	CHC-C1C-NC	4.23	130.48	124.23
18	F	1240	CLA	CHD-C4C-NC	4.23	130.74	124.21
18	1	1014	CLA	CHD-C4C-NC	4.23	130.74	124.21
18	A	1151	CLA	C2A-C1A-CHA	-4.23	115.42	122.63
18	1	1011	CLA	C2A-C1A-CHA	-4.23	115.42	122.63
18	B	9012	CLA	CHD-C4C-C3C	-4.23	118.62	124.84
18	B	1212	CLA	C4A-NA-C1A	4.23	108.61	106.71
18	3	3004	CLA	C1D-CHD-C4C	-4.23	115.64	126.10
18	B	1301	CLA	C3B-C2B-C1B	-4.23	102.67	106.29
18	A	1124	CLA	CHD-C4C-NC	4.23	130.73	124.21
18	B	1205	CLA	CHC-C1C-NC	4.23	130.62	124.20
18	B	1226	CLA	C3A-C4A-CHB	-4.22	118.74	123.91
18	B	1230	CLA	CHD-C4C-NC	4.22	130.72	124.21
18	A	1127	CLA	C3A-C4A-CHB	-4.22	118.74	123.91
19	A	5001	PQN	C11-C3-C4	4.22	123.02	118.50
18	B	1301	CLA	C1D-CHD-C4C	-4.22	115.67	126.10
18	4	4002	CLA	C2A-C1A-CHA	-4.22	115.44	122.63
18	4	4013	CLA	C4A-NA-C1A	4.22	108.60	106.71
18	2	2003	CLA	C2D-C3D-C4D	-4.21	102.67	106.30
18	1	1004	CLA	CHD-C4C-NC	4.21	130.71	124.21
18	4	4001	CLA	CHC-C1C-NC	4.21	130.45	124.23
18	A	1126	CLA	CHD-C4C-NC	4.21	130.84	124.20
18	A	1102	CLA	CHD-C4C-NC	4.21	130.71	124.21
18	B	1209	CLA	CHD-C4C-NC	4.21	130.84	124.20
18	F	1305	CLA	C3B-C2B-C1B	-4.21	102.69	106.29
18	1	1001	CLA	C1D-CHD-C4C	-4.21	115.68	126.10
18	B	1216	CLA	C3D-CAD-CBD	-4.21	102.06	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1106	CLA	CMD-C2D-C3D	-4.21	116.80	124.68
18	A	1144	CLA	C4A-NA-C1A	4.21	108.60	106.71
18	F	1139	CLA	CHD-C4C-NC	4.21	130.83	124.20
18	A	1110	CLA	CHC-C1C-NC	4.21	130.44	124.23
18	4	4010	CLA	CHC-C1C-NC	4.20	130.44	124.23
18	1	1007	CLA	CHD-C4C-NC	4.20	130.69	124.21
18	L	1125	CLA	C1D-CHD-C4C	-4.20	115.70	126.10
18	A	1122	CLA	CHD-C4C-NC	4.20	130.82	124.20
18	3	3010	CLA	C2A-C1A-CHA	-4.20	115.47	122.63
18	F	1139	CLA	CMD-C2D-C3D	-4.20	116.82	124.68
18	3	3001	CLA	CHD-C4C-NC	4.20	130.69	124.21
18	A	1105	CLA	CHC-C1C-NC	4.19	130.42	124.23
18	2	2015	CLA	C3B-C2B-C1B	-4.19	102.70	106.29
18	1	1007	CLA	CHC-C1C-NC	4.19	130.42	124.23
18	3	3013	CLA	C2A-C1A-CHA	-4.19	115.49	122.63
18	4	4006	CLA	C1D-CHD-C4C	-4.19	115.74	126.10
18	F	1302	CLA	CHC-C1C-NC	4.18	130.55	124.20
18	3	3006	CLA	CHD-C4C-NC	4.18	130.66	124.21
18	H	1501	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
18	2	2006	CLA	C1D-CHD-C4C	-4.18	115.75	126.10
18	H	1505	CLA	C2A-C1A-CHA	-4.18	115.50	122.63
18	F	4015	CLA	CHC-C1C-NC	4.18	130.40	124.23
18	B	1225	CLA	CMD-C2D-C3D	-4.18	116.86	124.68
18	K	1150	CLA	CHC-C1C-NC	4.18	130.40	124.23
18	B	1212	CLA	C1-O2A-CGA	4.18	127.41	116.44
18	B	1213	CLA	C4A-NA-C1A	4.18	108.58	106.71
18	4	4011	CLA	C2A-C1A-CHA	-4.18	115.51	122.63
18	B	1228	CLA	C3D-CAD-CBD	-4.17	102.11	107.61
18	B	1201	CLA	C2D-C3D-C4D	-4.17	102.71	106.30
18	2	2006	CLA	C2D-C3D-C4D	-4.17	102.71	106.30
18	A	1152	CLA	CHC-C1C-NC	4.17	130.39	124.23
18	B	1208	CLA	CMD-C2D-C3D	-4.17	116.88	124.68
18	A	1116	CLA	C2A-C1A-CHA	-4.17	115.52	122.63
18	3	3006	CLA	CHC-C1C-NC	4.17	130.38	124.23
18	A	9011	CLA	CHB-C4A-NA	4.17	130.27	124.51
18	A	1102	CLA	CHC-C1C-NC	4.16	130.38	124.23
18	1	1006	CLA	CHC-C1C-NC	4.16	130.38	124.23
18	A	1309	CLA	CHD-C4C-NC	4.16	130.63	124.21
18	3	3011	CLA	C2A-C1A-CHA	-4.16	115.54	122.63
18	B	9023	CLA	CHC-C1C-NC	4.16	130.51	124.20
18	2	2005	CLA	C3B-C2B-C1B	-4.16	102.73	106.29
18	3	3002	CLA	C2A-C1A-CHA	-4.16	115.54	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1138	CLA	CHD-C4C-NC	4.16	130.75	124.20
18	B	1218	CLA	C3D-CAD-CBD	-4.16	102.13	107.61
20	F	6016	BCR	C36-C18-C19	4.16	124.62	118.08
18	B	9022	CLA	C4A-NA-C1A	4.15	108.57	106.71
18	A	1143	CLA	C3B-C2B-C1B	-4.15	102.73	106.29
18	3	3010	CLA	C4A-NA-C1A	4.15	108.57	106.71
18	2	2012	CLA	C1D-CHD-C4C	-4.15	115.83	126.10
18	L	1130	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
18	B	1205	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
18	L	1504	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
18	B	1222	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
18	K	1141	CLA	C3B-C2B-C1B	-4.15	102.74	106.29
18	B	1229	CLA	C4A-NA-C1A	4.15	108.57	106.71
18	1	1006	CLA	C4A-NA-C1A	4.14	108.57	106.71
18	A	1107	CLA	O2D-CGD-CBD	4.14	118.62	111.27
18	K	1141	CLA	C1D-CHD-C4C	-4.14	115.86	126.10
18	I	1204	CLA	O2A-CGA-CBA	4.14	124.89	111.91
18	1	1011	CLA	C4A-NA-C1A	4.13	108.56	106.71
18	A	1143	CLA	CHD-C4C-NC	4.13	130.59	124.21
18	4	4004	CLA	CHC-C1C-NC	4.13	130.33	124.23
18	J	1308	CLA	C2D-C3D-C4D	-4.13	102.74	106.30
18	B	1211	CLA	C3B-C2B-C1B	-4.13	102.75	106.29
18	1	1013	CLA	C2A-C1A-CHA	-4.13	115.59	122.63
18	B	1231	CLA	O2D-CGD-O1D	-4.13	115.77	123.84
18	4	4011	CLA	CHD-C4C-NC	4.13	130.57	124.21
18	4	4002	CLA	C3D-C2D-C1D	4.13	109.86	106.30
18	F	1306	CLA	CHC-C1C-NC	4.13	130.32	124.23
18	2	2004	CLA	C3D-C2D-C1D	4.12	109.86	106.30
18	3	2009	CLA	C2A-C1A-CHA	-4.12	115.60	122.63
18	B	1220	CLA	CAA-C2A-C3A	-4.12	101.49	112.78
18	A	1110	CLA	CHD-C4C-NC	4.12	130.57	124.21
18	F	1306	CLA	C3B-C2B-C1B	-4.12	102.76	106.29
18	A	1148	CLA	C4A-NA-C1A	4.12	108.56	106.71
18	A	1131	CLA	CMD-C2D-C3D	-4.11	116.98	124.68
18	F	1306	CLA	CHD-C4C-NC	4.11	130.56	124.21
18	A	1120	CLA	CHD-C4C-NC	4.11	130.55	124.21
18	A	1107	CLA	CHD-C4C-C3C	-4.10	118.81	124.84
18	3	3015	CLA	C2A-C1A-CHA	-4.10	115.63	122.63
18	B	1215	CLA	CHC-C1C-C2C	-4.10	115.37	126.72
18	1	1003	CLA	C2A-C1A-CHA	-4.10	115.64	122.63
18	A	1116	CLA	CHC-C1C-NC	4.10	130.29	124.23
18	B	1232	CLA	CHD-C4C-C3C	-4.10	118.81	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1205	CLA	O2A-CGA-O1A	-4.10	113.24	123.59
18	4	4006	CLA	CHD-C4C-NC	4.10	130.53	124.21
18	J	1308	CLA	CHC-C1C-NC	4.10	130.28	124.23
18	3	3003	CLA	CHC-C1C-NC	4.10	130.28	124.23
18	B	1220	CLA	O2A-CGA-CBA	4.10	124.77	111.91
18	B	1203	CLA	CHC-C1C-NC	4.10	130.42	124.20
18	B	1230	CLA	C3A-C4A-CHB	-4.10	118.89	123.91
18	B	1208	CLA	CHD-C4C-NC	4.09	130.65	124.20
18	2	2010	CLA	C3B-C2B-C1B	-4.09	102.79	106.29
18	A	1107	CLA	CHD-C4C-NC	4.09	130.65	124.20
18	A	1147	CLA	C2A-C1A-CHA	-4.09	115.66	122.63
18	1	1007	CLA	C4A-NA-C1A	4.09	108.54	106.71
18	1	1005	CLA	C1D-CHD-C4C	-4.09	115.98	126.10
18	B	1221	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
18	1	1013	CLA	C3B-C2B-C1B	-4.09	102.79	106.29
18	4	4008	CLA	CHD-C4C-NC	4.09	130.51	124.21
18	B	1232	CLA	C3D-CAD-CBD	-4.08	102.23	107.61
18	A	1134	CLA	CHC-C1C-NC	4.08	130.26	124.23
18	K	1150	CLA	C3B-C2B-C1B	-4.08	102.79	106.29
18	A	1105	CLA	C3B-C2B-C1B	-4.08	102.79	106.29
18	4	4006	CLA	C3D-C4D-ND	4.08	113.69	110.14
18	A	1148	CLA	CHC-C1C-NC	4.08	130.26	124.23
18	B	9022	CLA	CHB-C4A-NA	4.08	130.15	124.51
18	A	1106	CLA	OBD-CAD-CBD	-4.08	120.07	125.89
18	B	1215	CLA	CHD-C4C-C3C	-4.07	118.85	124.84
18	A	1142	CLA	C2A-C1A-CHA	-4.07	115.69	122.63
18	2	2001	CLA	C2A-C1A-CHA	-4.07	115.69	122.63
18	B	1239	CLA	C3D-CAD-CBD	-4.07	102.24	107.61
18	4	4011	CLA	C1D-CHD-C4C	-4.07	116.02	126.10
18	1	1006	CLA	C2A-C1A-CHA	-4.07	115.69	122.63
18	1	1010	CLA	CHC-C1C-NC	4.07	130.24	124.23
18	A	1140	CLA	CHD-C4C-NC	4.07	130.62	124.20
18	A	1146	CLA	C2A-C1A-CHA	-4.07	115.69	122.63
18	K	1153	CLA	C2A-C1A-CHA	-4.07	115.70	122.63
18	4	4005	CLA	C3A-C4A-CHB	-4.07	118.93	123.91
18	4	4004	CLA	C2A-C1A-CHA	-4.06	115.70	122.63
18	F	1303	CLA	CHC-C1C-NC	4.06	130.23	124.23
18	B	1218	CLA	CHC-C1C-NC	4.06	130.37	124.20
18	4	4001	CLA	CHD-C4C-NC	4.06	130.47	124.21
18	2	2008	CLA	C2D-C3D-C4D	-4.06	102.80	106.30
18	A	1140	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
18	B	1203	CLA	CAC-C3C-C4C	4.06	131.22	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	2006	CLA	C3D-C2D-C1D	4.06	109.80	106.30
18	B	1226	CLA	CHC-C1C-NC	4.06	130.22	124.23
18	3	3011	CLA	C3B-C2B-C1B	-4.06	102.82	106.29
18	B	1237	CLA	CHC-C1C-NC	4.06	130.36	124.20
18	F	1305	CLA	C2A-C1A-CHA	-4.05	115.72	122.63
18	1	1013	CLA	CHC-C1C-NC	4.05	130.21	124.23
18	A	1136	CLA	CGD-CBD-CAD	4.05	123.85	110.73
18	A	1102	CLA	C3A-C4A-CHB	-4.05	118.95	123.91
18	B	1203	CLA	C3D-CAD-CBD	-4.05	102.11	107.60
18	A	1140	CLA	CHC-C1C-NC	4.05	130.34	124.20
18	L	1130	CLA	O2D-CGD-O1D	-4.05	115.93	123.84
18	B	1236	CLA	CMD-C2D-C3D	-4.04	117.11	124.68
18	3	3001	CLA	C2D-C3D-C4D	-4.04	102.82	106.30
18	2	2004	CLA	CHC-C1C-NC	4.04	130.20	124.23
18	K	1141	CLA	C4A-NA-C1A	4.04	108.52	106.71
18	4	4007	CLA	C4A-NA-C1A	4.04	108.52	106.71
18	B	1213	CLA	CHD-C4C-NC	4.04	130.44	124.21
18	B	1221	CLA	C3D-CAD-CBD	-4.04	102.29	107.61
18	B	1201	CLA	CHC-C1C-NC	4.03	130.19	124.23
18	2	2015	CLA	CHC-C1C-NC	4.03	130.19	124.23
18	L	1125	CLA	CHD-C4C-NC	4.03	130.43	124.21
18	B	9010	CLA	C3D-CAD-CBD	-4.03	102.30	107.61
18	3	3011	CLA	CHC-C1C-NC	4.03	130.18	124.23
18	B	1235	CLA	CHC-C1C-NC	4.03	130.31	124.20
18	F	1305	CLA	C4A-NA-C1A	4.03	108.52	106.71
18	A	9013	CLA	O2D-CGD-CBD	4.03	118.42	111.27
18	A	1146	CLA	C3B-C2B-C1B	-4.02	102.84	106.29
18	A	1132	CLA	C2A-C1A-CHA	-4.02	115.77	122.63
18	2	2006	CLA	C4A-NA-C1A	4.02	108.52	106.71
18	4	4011	CLA	CHC-C1C-NC	4.02	130.17	124.23
18	B	1202	CLA	C5-C3-C4	4.02	123.49	114.60
18	B	1301	CLA	CHD-C4C-NC	4.02	130.41	124.21
18	A	1309	CLA	C3B-C2B-C1B	-4.02	102.85	106.29
18	A	1105	CLA	C3D-C2D-C1D	4.02	109.76	106.30
18	F	1240	CLA	C4A-NA-C1A	4.02	108.51	106.71
18	B	1210	CLA	C4A-NA-C1A	4.02	108.51	106.71
18	4	4003	CLA	CHD-C4C-NC	4.02	130.40	124.21
18	3	3012	CLA	C2A-C1A-CHA	-4.01	115.79	122.63
18	2	2006	CLA	CHD-C4C-NC	4.01	130.40	124.21
18	A	1113	CLA	CHC-C1C-NC	4.01	130.29	124.20
18	A	1109	CLA	C3B-C2B-C1B	-4.01	102.86	106.29
18	4	4007	CLA	C3B-C2B-C1B	-4.01	102.86	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1146	CLA	CHD-C4C-NC	4.01	130.40	124.21
18	1	1001	CLA	CHD-C4C-NC	4.01	130.39	124.21
18	4	4004	CLA	C3B-C2B-C1B	-4.01	102.86	106.29
18	4	4008	CLA	C4A-NA-C1A	4.01	108.51	106.71
20	B	6017	BCR	C34-C9-C10	-4.01	117.31	122.92
18	A	1106	CLA	C4A-NA-C1A	4.01	108.51	106.71
18	A	1144	CLA	C2D-C3D-C4D	-4.00	102.85	106.30
18	A	1133	CLA	C3A-C4A-CHB	-4.00	119.01	123.91
20	I	6018	BCR	C38-C26-C25	-4.00	120.04	124.53
18	F	1240	CLA	CHC-C1C-NC	4.00	130.13	124.23
18	4	4003	CLA	C3D-C2D-C1D	3.99	109.74	106.30
18	B	9022	CLA	CHD-C4C-NC	3.99	130.49	124.20
18	A	1126	CLA	O2A-C1-C2	3.99	119.12	108.64
18	A	9013	CLA	CMD-C2D-C3D	-3.99	117.22	124.68
18	4	1009	CLA	C3A-C4A-CHB	-3.98	119.03	123.91
18	B	1214	CLA	CAA-CBA-CGA	3.98	124.89	113.25
18	A	1143	CLA	CHC-C1C-NC	3.98	130.11	124.23
18	A	9013	CLA	CHD-C4C-NC	3.98	130.47	124.20
18	4	4005	CLA	C3B-C2B-C1B	-3.98	102.89	106.29
18	1	1010	CLA	C2A-C1A-CHA	-3.98	115.85	122.63
18	L	1125	CLA	C4A-NA-C1A	3.97	108.49	106.71
18	1	1001	CLA	C2D-C3D-C4D	-3.97	102.88	106.30
18	2	2002	CLA	C3B-C2B-C1B	-3.97	102.89	106.29
18	3	3005	CLA	C2D-C3D-C4D	-3.97	102.88	106.30
18	B	1219	CLA	CHD-C4C-NC	3.97	130.46	124.20
18	2	2002	CLA	C4A-NA-C1A	3.97	108.49	106.71
18	B	1217	CLA	CHC-C1C-NC	3.97	130.22	124.20
18	B	1210	CLA	C1D-CHD-C4C	-3.97	116.28	126.10
18	1	1002	CLA	C3B-C2B-C1B	-3.97	102.89	106.29
18	4	4006	CLA	C2D-C3D-C4D	-3.97	102.89	106.30
18	4	4001	CLA	C2D-C3D-C4D	-3.96	102.89	106.30
18	B	1237	CLA	CMD-C2D-C3D	-3.96	117.27	124.68
18	A	1152	CLA	C2A-C1A-CHA	-3.96	115.88	122.63
18	B	1238	CLA	CMB-C2B-C3B	3.96	132.09	124.68
18	A	1113	CLA	CED-O2D-CGD	3.96	124.90	115.94
18	A	1101	CLA	C2D-C3D-C4D	-3.96	102.89	106.30
18	2	2004	CLA	C3B-C2B-C1B	-3.96	102.90	106.29
18	A	1111	CLA	C3B-C2B-C1B	-3.96	102.90	106.29
18	B	1219	CLA	C3D-CAD-CBD	-3.96	102.39	107.61
18	A	1111	CLA	CHC-C1C-NC	3.96	130.07	124.23
18	B	1221	CLA	O2D-CGD-O1D	-3.96	116.10	123.84
18	1	1003	CLA	CHC-C1C-NC	3.96	130.07	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1103	CLA	CHD-C4C-NC	3.95	130.43	124.20
18	B	1241	CLA	CHD-C4C-NC	3.95	130.30	124.21
18	L	1130	CLA	CHC-C1C-NC	3.95	130.19	124.20
18	I	1204	CLA	CHC-C1C-NC	3.95	130.19	124.20
18	B	1232	CLA	CHC-C1C-NC	3.95	130.19	124.20
18	B	1228	CLA	CHD-C4C-C3C	-3.94	119.04	124.84
18	3	3001	CLA	CHC-C1C-NC	3.94	130.06	124.23
18	B	1223	CLA	C2A-C1A-CHA	-3.94	115.91	122.63
18	1	1008	CLA	C2A-C1A-CHA	-3.94	115.91	122.63
18	B	1236	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
18	A	1134	CLA	C2D-C3D-C4D	-3.94	102.91	106.30
18	B	1216	CLA	C4A-NA-C1A	3.94	108.48	106.71
18	A	1143	CLA	C4A-NA-C1A	3.94	108.48	106.71
20	F	6016	BCR	C35-C13-C14	-3.94	117.40	122.92
18	4	4010	CLA	C4A-NA-C1A	3.94	108.48	106.71
18	K	1153	CLA	CHD-C4C-NC	3.94	130.29	124.21
18	B	1209	CLA	CHC-C1C-NC	3.94	130.18	124.20
18	F	1306	CLA	C2D-C3D-C4D	-3.94	102.91	106.30
18	1	1001	CLA	C3D-C4D-ND	3.93	113.56	110.14
18	F	1302	CLA	C1-O2A-CGA	3.93	126.76	116.44
18	3	3003	CLA	C2A-C1A-CHA	-3.93	115.93	122.63
18	F	4015	CLA	C4A-NA-C1A	3.93	108.47	106.71
18	A	1129	CLA	O2A-CGA-CBA	3.93	124.23	111.91
18	B	1201	CLA	C3D-C4D-ND	3.92	113.55	110.14
18	2	2015	CLA	C2A-C1A-CHA	-3.92	115.94	122.63
18	A	1117	CLA	CHD-C4C-NC	3.92	130.26	124.21
18	4	4008	CLA	C3B-C2B-C1B	-3.92	102.93	106.29
18	1	1008	CLA	C3B-C2B-C1B	-3.92	102.93	106.29
18	2	2012	CLA	C4A-NA-C1A	3.92	108.47	106.71
18	A	1309	CLA	CHC-C1C-NC	3.92	130.02	124.23
18	B	9010	CLA	CHB-C4A-NA	3.92	129.93	124.51
18	A	1120	CLA	C3D-C4D-ND	3.92	113.54	110.14
18	3	3009	CLA	C4A-NA-C1A	3.91	108.47	106.71
18	K	1153	CLA	CHC-C1C-NC	3.91	130.01	124.23
18	J	1308	CLA	C3D-C2D-C1D	3.91	109.67	106.30
18	3	3013	CLA	CHC-C1C-NC	3.91	130.00	124.23
18	4	4003	CLA	C2D-C3D-C4D	-3.91	102.93	106.30
18	A	1140	CLA	C4A-NA-C1A	3.91	108.46	106.71
18	A	1129	CLA	CMD-C2D-C3D	-3.91	117.36	124.68
18	A	1124	CLA	C3A-C4A-CHB	-3.91	119.13	123.91
18	3	3003	CLA	C3B-C2B-C1B	-3.90	102.95	106.29
18	2	2003	CLA	C3D-C4D-ND	3.90	113.53	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3015	CLA	CHD-C4C-NC	3.90	130.23	124.21
20	I	6018	BCR	C30-C25-C24	3.90	126.81	115.78
18	A	1103	CLA	CHB-C4A-NA	3.89	129.90	124.51
18	A	1107	CLA	O2D-CGD-O1D	-3.89	116.22	123.84
18	B	9022	CLA	O2A-CGA-O1A	-3.89	113.77	123.59
18	B	1241	CLA	CHC-C1C-NC	3.89	129.98	124.23
18	A	1144	CLA	C3B-C2B-C1B	-3.89	102.96	106.29
18	H	1501	CLA	CHC-C1C-NC	3.89	130.10	124.20
18	A	1103	CLA	CHC-C1C-C2C	-3.89	115.97	126.72
18	B	9022	CLA	CHD-C4C-C3C	-3.89	119.12	124.84
18	A	1133	CLA	CHD-C4C-NC	3.89	130.21	124.21
18	B	1201	CLA	C3D-C2D-C1D	3.89	109.65	106.30
18	A	1151	CLA	C4A-NA-C1A	3.89	108.45	106.71
18	B	1212	CLA	CHC-C1C-NC	3.88	130.09	124.20
18	2	2013	CLA	C4A-NA-C1A	3.88	108.45	106.71
18	B	1219	CLA	O2A-C1-C2	3.88	118.83	108.64
18	A	1106	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
18	A	1120	CLA	CHC-C1C-NC	3.88	129.96	124.23
18	B	9012	CLA	CHB-C4A-NA	3.88	129.87	124.51
18	4	4003	CLA	CHC-C1C-NC	3.88	129.96	124.23
18	A	1128	CLA	C3D-CAD-CBD	-3.88	102.50	107.61
18	A	1120	CLA	C3D-C2D-C1D	3.87	109.64	106.30
18	1	1008	CLA	C4A-NA-C1A	3.87	108.44	106.71
18	B	1209	CLA	CHD-C4C-C3C	-3.87	119.15	124.84
18	A	9013	CLA	C2C-C1C-NC	3.86	113.59	109.97
18	A	1104	CLA	CHD-C4C-NC	3.86	130.17	124.21
18	A	1106	CLA	CHD-C4C-NC	3.86	130.29	124.20
18	4	4001	CLA	C3D-C2D-C1D	3.86	109.63	106.30
18	H	1501	CLA	O2D-CGD-CBD	3.86	118.13	111.27
18	2	2010	CLA	C2D-C3D-C4D	-3.86	102.98	106.30
18	4	4011	CLA	C4A-NA-C1A	3.86	108.44	106.71
18	A	1107	CLA	C2A-C1A-CHA	-3.86	117.12	123.86
18	B	1226	CLA	C4A-NA-C1A	3.85	108.44	106.71
18	1	1003	CLA	C2D-C3D-C4D	-3.85	102.98	106.30
18	B	1219	CLA	CHD-C4C-C3C	-3.85	119.18	124.84
18	F	1139	CLA	CHC-C1C-NC	3.85	130.04	124.20
18	K	1141	CLA	CHD-C4C-NC	3.85	130.14	124.21
18	B	1242	CLA	CHC-C1C-NC	3.84	130.04	124.20
18	1	1004	CLA	CHC-C1C-NC	3.84	129.91	124.23
18	B	1213	CLA	C3B-C2B-C1B	-3.84	103.00	106.29
18	B	1228	CLA	CHC-C1C-NC	3.84	130.03	124.20
18	A	1131	CLA	CHB-C4A-NA	3.84	129.82	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1207	CLA	C1-O2A-CGA	3.84	126.51	116.44
20	B	6017	BCR	C16-C17-C18	-3.84	121.83	127.31
18	B	9012	CLA	C3D-CAD-CBD	-3.84	102.56	107.61
18	A	1122	CLA	C4-C3-C5	3.83	121.72	115.27
18	A	1129	CLA	CHD-C4C-C3C	-3.83	119.21	124.84
18	A	1146	CLA	CHC-C1C-NC	3.83	129.88	124.23
18	J	1307	CLA	C3D-C2D-C1D	3.83	109.60	106.30
18	2	2008	CLA	C3D-C2D-C1D	3.83	109.60	106.30
18	3	3015	CLA	CHC-C1C-NC	3.83	129.88	124.23
18	B	1228	CLA	O2A-CGA-CBA	3.83	123.91	111.91
18	3	3005	CLA	C4A-NA-C1A	3.82	108.42	106.71
18	B	1203	CLA	CHD-C4C-NC	3.82	130.22	124.20
18	A	1129	CLA	C3D-CAD-CBD	-3.82	102.58	107.61
18	B	1231	CLA	CHD-C4C-NC	3.81	130.21	124.20
18	A	1135	CLA	CHC-C1C-NC	3.81	129.99	124.20
18	A	1107	CLA	C1-O2A-CGA	3.81	126.44	116.44
18	2	2007	CLA	C2D-C3D-C4D	-3.81	103.02	106.30
18	B	1242	CLA	C4A-NA-C1A	3.81	108.42	106.71
18	2	2005	CLA	C2A-C1A-CHA	-3.81	116.14	122.63
18	F	1306	CLA	C4A-NA-C1A	3.80	108.41	106.71
18	J	2107	CLA	CAC-C3C-C4C	3.80	129.74	124.81
18	B	1201	CLA	C3B-C2B-C1B	-3.80	103.04	106.29
18	4	4002	CLA	C4A-NA-C1A	3.79	108.41	106.71
18	2	2002	CLA	CHC-C1C-NC	3.79	129.82	124.23
18	K	1141	CLA	CHC-C1C-NC	3.79	129.82	124.23
18	4	4008	CLA	C2D-C3D-C4D	-3.79	103.04	106.30
18	A	1101	CLA	C3D-C2D-C1D	3.79	109.56	106.30
18	3	3002	CLA	C3B-C2B-C1B	-3.78	103.05	106.29
18	3	2009	CLA	C3B-C2B-C1B	-3.78	103.05	106.29
18	B	1301	CLA	CHC-C1C-NC	3.78	129.81	124.23
18	2	2005	CLA	C2D-C3D-C4D	-3.78	103.05	106.30
18	B	1211	CLA	C3A-C4A-CHB	-3.77	119.29	123.91
18	4	4006	CLA	C4A-NA-C1A	3.77	108.40	106.71
18	A	1128	CLA	CHD-C4C-C3C	-3.77	119.29	124.84
18	B	1231	CLA	CHC-C1C-NC	3.77	129.93	124.20
18	A	1124	CLA	C4A-NA-C1A	3.77	108.40	106.71
18	L	1504	CLA	C3D-CAD-CBD	-3.77	102.64	107.61
18	4	1304	CLA	CHC-C1C-NC	3.76	129.91	124.20
18	A	1104	CLA	C3D-C2D-C1D	3.76	109.54	106.30
18	A	1126	CLA	CMD-C2D-C3D	-3.76	117.65	124.68
18	A	1126	CLA	C3D-CAD-CBD	-3.76	102.66	107.61
18	A	1119	CLA	CMD-C2D-C3D	-3.76	117.65	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1309	CLA	C4A-NA-C1A	3.76	108.39	106.71
20	F	6016	BCR	C15-C16-C17	-3.75	115.78	123.47
18	L	1504	CLA	CHC-C1C-NC	3.75	129.90	124.20
18	A	1136	CLA	OBD-CAD-CBD	-3.75	120.53	125.89
18	B	1224	CLA	CHC-C1C-NC	3.75	129.89	124.20
18	4	4013	CLA	C3B-C2B-C1B	-3.75	103.08	106.29
18	1	1005	CLA	CHD-C4C-NC	3.74	129.98	124.21
18	1	1001	CLA	CHC-C1C-NC	3.74	129.76	124.23
18	B	1221	CLA	CMD-C2D-C3D	-3.74	117.69	124.68
18	B	1228	CLA	O1D-CGD-CBD	-3.74	116.84	124.48
18	3	3001	CLA	C3D-C2D-C1D	3.74	109.52	106.30
18	B	1213	CLA	CHC-C1C-NC	3.73	129.74	124.23
18	4	4008	CLA	CHC-C1C-NC	3.73	129.74	124.23
18	3	3013	CLA	C2D-C3D-C4D	-3.73	103.09	106.30
18	3	3008	CLA	C2D-C3D-C4D	-3.73	103.09	106.30
18	4	1009	CLA	CHD-C4C-NC	3.73	129.96	124.21
18	B	1138	CLA	O2D-CGD-CBD	3.73	117.89	111.27
18	B	1206	CLA	C3D-C4D-ND	3.73	113.38	110.14
18	B	1221	CLA	C1-O2A-CGA	3.73	126.22	116.44
18	A	1118	CLA	C2D-C3D-C4D	-3.73	103.09	106.30
18	A	1108	CLA	CHC-C1C-NC	3.73	129.85	124.20
18	B	1203	CLA	CED-O2D-CGD	3.72	124.36	115.94
18	B	1230	CLA	C2D-C3D-C4D	-3.72	103.09	106.30
18	A	1124	CLA	C3D-C2D-C1D	3.72	109.51	106.30
18	1	1005	CLA	CHC-C1C-NC	3.72	129.73	124.23
18	A	1107	CLA	CMB-C2B-C1B	3.72	134.18	128.46
18	A	1137	CLA	CMD-C2D-C3D	-3.72	117.72	124.68
18	A	1148	CLA	C2D-C3D-C4D	-3.72	103.10	106.30
18	3	3006	CLA	C4A-NA-C1A	3.71	108.38	106.71
18	3	3005	CLA	C3D-C2D-C1D	3.71	109.50	106.30
18	3	3010	CLA	C3B-C2B-C1B	-3.71	103.11	106.29
18	B	1211	CLA	C2D-C3D-C4D	-3.71	103.11	106.30
18	F	1306	CLA	C3D-C4D-ND	3.70	113.36	110.14
18	A	1113	CLA	CBC-CAC-C3C	-3.70	102.22	112.43
18	1	1007	CLA	C3B-C2B-C1B	-3.70	103.12	106.29
18	A	1106	CLA	CHB-C4A-NA	3.70	129.63	124.51
18	2	2010	CLA	C3D-C2D-C1D	3.70	109.49	106.30
18	A	9013	CLA	CHC-C1C-NC	3.70	129.81	124.20
18	B	1208	CLA	C1-C2-C3	3.69	132.43	126.04
18	3	3001	CLA	C3D-C4D-ND	3.69	113.35	110.14
18	B	1235	CLA	C6-C5-C3	-3.69	103.78	113.45
18	B	1230	CLA	C3B-C2B-C1B	-3.69	103.13	106.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1142	CLA	C4A-NA-C1A	3.69	108.36	106.71
18	2	2004	CLA	C3D-C4D-ND	3.68	113.34	110.14
18	1	1012	CLA	C2D-C3D-C4D	-3.68	103.13	106.30
18	3	3006	CLA	C3B-C2B-C1B	-3.68	103.14	106.29
18	3	3002	CLA	C3D-C2D-C1D	3.68	109.47	106.30
18	A	1108	CLA	C1-O2A-CGA	3.68	126.09	116.44
20	L	6020	BCR	C40-C30-C25	-3.67	104.34	110.30
18	1	1005	CLA	C2D-C3D-C4D	-3.67	103.14	106.30
18	B	1236	CLA	CHC-C1C-NC	3.67	129.77	124.20
18	B	1224	CLA	C4A-NA-C1A	3.67	108.36	106.71
18	2	2011	CLA	C2D-C3D-C4D	-3.67	103.14	106.30
18	3	3015	CLA	C2D-C3D-C4D	-3.66	103.15	106.30
18	B	1220	CLA	C1-C2-C3	-3.66	119.71	126.04
18	A	9011	CLA	O2A-CGA-CBA	3.66	123.40	111.91
18	B	1224	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
18	A	1105	CLA	C3D-C4D-ND	3.66	113.32	110.14
18	A	9013	CLA	CHC-C1C-C2C	-3.66	116.60	126.72
18	J	1308	CLA	C3D-C4D-ND	3.66	113.32	110.14
18	B	1218	CLA	C2A-C1A-CHA	-3.66	117.47	123.86
18	3	3008	CLA	C3D-C2D-C1D	3.66	109.45	106.30
18	B	9012	CLA	CHC-C1C-NC	3.66	129.75	124.20
18	A	1107	CLA	C6-C5-C3	-3.65	103.88	113.45
18	A	1106	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
18	1	1014	CLA	C2D-C3D-C4D	-3.65	103.16	106.30
18	A	1132	CLA	CHD-C4C-NC	3.64	129.83	124.21
18	G	1248	CLA	C3B-C2B-C1B	-3.64	103.17	106.29
18	A	1117	CLA	CHC-C1C-NC	3.64	129.60	124.23
18	A	1120	CLA	C4A-NA-C1A	3.63	108.34	106.71
18	B	1213	CLA	C2D-C3D-C4D	-3.63	103.17	106.30
18	B	1209	CLA	O2A-CGA-CBA	3.63	123.31	111.91
18	2	2011	CLA	C3D-C2D-C1D	3.63	109.43	106.30
18	B	1227	CLA	CHD-C4C-C3C	-3.63	119.50	124.84
18	A	1103	CLA	C3D-CAD-CBD	-3.63	102.83	107.61
18	F	1139	CLA	C4A-NA-C1A	3.63	108.34	106.71
18	1	1005	CLA	C3D-C2D-C1D	3.62	109.42	106.30
18	B	1219	CLA	CHC-C1C-NC	3.62	129.70	124.20
18	4	4013	CLA	C2D-C3D-C4D	-3.62	103.18	106.30
18	2	2010	CLA	C4A-NA-C1A	3.61	108.33	106.71
18	K	1153	CLA	C3D-C2D-C1D	3.61	109.41	106.30
18	2	2001	CLA	C4A-NA-C1A	3.61	108.33	106.71
18	A	1107	CLA	CMD-C2D-C3D	-3.60	117.94	124.68
18	4	4007	CLA	C2D-C3D-C4D	-3.60	103.20	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3013	CLA	C4A-NA-C1A	3.60	108.33	106.71
18	B	9023	CLA	CBC-CAC-C3C	-3.60	102.51	112.43
18	B	1223	CLA	C4A-NA-C1A	3.60	108.32	106.71
18	B	9022	CLA	CMD-C2D-C3D	-3.60	117.95	124.68
18	2	2003	CLA	C3D-C2D-C1D	3.60	109.40	106.30
18	L	1503	CLA	O2A-CGA-CBA	3.60	123.19	111.91
18	B	1219	CLA	CMD-C2D-C3D	-3.59	117.95	124.68
18	B	1216	CLA	C1-O2A-CGA	3.59	125.87	116.44
18	2	2013	CLA	C2D-C3D-C4D	-3.59	103.21	106.30
18	J	1307	CLA	C2D-C3D-C4D	-3.59	103.21	106.30
18	3	3012	CLA	C3B-C2B-C1B	-3.59	103.22	106.29
18	A	1148	CLA	C3D-C2D-C1D	3.59	109.39	106.30
18	1	1013	CLA	C4A-NA-C1A	3.59	108.32	106.71
18	B	1209	CLA	CMD-C2D-C3D	-3.58	117.97	124.68
18	A	1144	CLA	C3D-C2D-C1D	3.58	109.39	106.30
18	L	1125	CLA	C2D-C3D-C4D	-3.58	103.22	106.30
18	A	1309	CLA	C2D-C3D-C4D	-3.58	103.22	106.30
18	B	1238	CLA	CHD-C4C-C3C	-3.58	119.58	124.84
18	A	9011	CLA	CMA-C3A-C4A	-3.58	102.15	111.77
18	B	1221	CLA	CHC-C1C-C2C	-3.58	116.82	126.72
18	A	1144	CLA	C3D-C4D-ND	3.58	113.25	110.14
18	A	1133	CLA	CHC-C1C-NC	3.57	129.51	124.23
18	3	3007	CLA	C2D-C3D-C4D	-3.57	103.22	106.30
18	A	1101	CLA	C3D-C4D-ND	3.57	113.24	110.14
18	A	1151	CLA	C3B-C2B-C1B	-3.57	103.23	106.29
18	A	1129	CLA	O2A-C1-C2	3.57	118.01	108.64
18	4	4002	CLA	C3B-C2B-C1B	-3.57	103.24	106.29
18	2	2008	CLA	C3B-C2B-C1B	-3.57	103.24	106.29
18	A	1123	CLA	CMD-C2D-C3D	-3.56	118.01	124.68
18	B	1231	CLA	CMD-C2D-C3D	-3.56	118.01	124.68
18	B	1211	CLA	C3D-C2D-C1D	3.56	109.37	106.30
18	B	1224	CLA	C3D-CAD-CBD	-3.56	102.92	107.61
20	I	6018	BCR	C23-C24-C25	-3.56	117.20	127.20
18	2	2011	CLA	C4A-NA-C1A	3.56	108.31	106.71
18	A	1126	CLA	O2A-CGA-CBA	3.56	123.06	111.91
18	A	1102	CLA	C3B-C2B-C1B	-3.55	103.25	106.29
18	1	1004	CLA	C2D-C3D-C4D	-3.55	103.24	106.30
18	A	1134	CLA	C3D-C2D-C1D	3.55	109.36	106.30
18	B	1212	CLA	O2A-CGA-CBA	3.55	123.04	111.91
18	A	1122	CLA	CMB-C2B-C3B	3.55	131.32	124.68
18	J	2107	CLA	CHD-C4C-NC	3.55	129.79	124.20
18	B	1208	CLA	CHD-C4C-C3C	-3.55	119.62	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1209	CLA	O2D-CGD-CBD	3.55	117.57	111.27
18	A	1128	CLA	CHC-C1C-NC	3.55	129.58	124.20
18	B	1301	CLA	C4A-NA-C1A	3.54	108.30	106.71
18	1	1002	CLA	C4A-NA-C1A	3.54	108.30	106.71
18	B	9010	CLA	CHC-C1C-C2C	-3.54	116.93	126.72
18	A	9013	CLA	CHD-C4C-C3C	-3.54	119.64	124.84
18	B	1209	CLA	C3D-CAD-CBD	-3.54	102.95	107.61
18	3	3011	CLA	C4A-NA-C1A	3.53	108.30	106.71
18	B	1206	CLA	CHD-C4C-NC	3.53	129.66	124.21
18	J	1307	CLA	CHD-C4C-NC	3.53	129.66	124.21
18	3	3013	CLA	C3D-C2D-C1D	3.53	109.34	106.30
18	B	1209	CLA	CMB-C2B-C3B	3.53	131.28	124.68
18	A	1129	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
18	B	1239	CLA	CHD-C4C-C3C	-3.53	119.65	124.84
18	F	1302	CLA	CAA-C2A-C1A	3.53	123.54	111.97
18	B	1228	CLA	CAA-C2A-C3A	-3.53	103.12	112.78
18	L	1503	CLA	O1D-CGD-CBD	-3.52	117.28	124.48
18	L	1502	CLA	CHC-C1C-NC	3.52	129.55	124.20
18	A	1133	CLA	C4A-NA-C1A	3.52	108.29	106.71
18	B	1224	CLA	CHB-C4A-NA	3.52	129.38	124.51
18	B	9022	CLA	C1-O2A-CGA	3.52	125.67	116.44
18	A	1126	CLA	CAA-C2A-C3A	-3.52	103.15	112.78
18	A	1137	CLA	CAA-C2A-C1A	3.51	123.49	111.97
18	2	2010	CLA	C3D-C4D-ND	3.51	113.19	110.14
18	A	1147	CLA	C3B-C2B-C1B	-3.51	103.28	106.29
18	A	1107	CLA	C4A-NA-C1A	3.51	108.28	106.71
18	1	1014	CLA	C3D-C4D-ND	3.51	113.19	110.14
18	B	1207	CLA	C3D-CAD-CBD	-3.51	102.98	107.61
18	K	1153	CLA	C3B-C2B-C1B	-3.51	103.29	106.29
18	K	1153	CLA	C4A-NA-C1A	3.51	108.28	106.71
18	2	2005	CLA	C3D-C4D-ND	3.50	113.19	110.14
20	F	6016	BCR	C8-C7-C6	-3.50	117.37	127.20
18	B	1228	CLA	CMB-C2B-C3B	3.50	131.23	124.68
18	A	1115	CLA	CHD-C4C-C3C	-3.50	119.69	124.84
18	1	1007	CLA	C2D-C3D-C4D	-3.50	103.29	106.30
18	F	1302	CLA	O2D-CGD-CBD	3.50	117.49	111.27
18	F	1306	CLA	C3D-C2D-C1D	3.50	109.32	106.30
18	A	9013	CLA	O1D-CGD-CBD	-3.50	117.33	124.48
18	2	2002	CLA	C2D-C3D-C4D	-3.49	103.29	106.30
18	L	1502	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
18	B	1226	CLA	C3D-C2D-C1D	3.49	109.31	106.30
18	B	1237	CLA	CHD-C4C-C3C	-3.49	119.71	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1237	CLA	C1-C2-C3	-3.49	120.01	126.04
18	2	2007	CLA	C3D-C2D-C1D	3.48	109.30	106.30
18	A	1104	CLA	CHC-C1C-NC	3.48	129.38	124.23
18	3	3008	CLA	C3B-C2B-C1B	-3.48	103.31	106.29
18	B	1230	CLA	C3D-C2D-C1D	3.48	109.30	106.30
18	2	2001	CLA	C2D-C3D-C4D	-3.48	103.30	106.30
18	B	1227	CLA	CED-O2D-CGD	3.48	123.81	115.94
18	3	3002	CLA	C2D-C3D-C4D	-3.48	103.30	106.30
18	L	1130	CLA	O2A-CGA-CBA	3.48	122.83	111.91
20	L	6020	BCR	C1-C6-C5	-3.48	117.71	122.61
18	A	1137	CLA	CHC-C1C-NC	3.48	129.48	124.20
18	B	1214	CLA	CHC-C1C-NC	3.47	129.47	124.20
18	B	1221	CLA	O2A-CGA-CBA	3.47	122.81	111.91
18	B	1205	CLA	CMD-C2D-C3D	-3.47	118.18	124.68
18	B	1237	CLA	O2A-CGA-CBA	3.47	122.80	111.91
18	3	3015	CLA	C3D-C2D-C1D	3.47	109.29	106.30
18	B	1239	CLA	CHC-C1C-C2C	-3.47	117.13	126.72
18	B	1238	CLA	CMD-C2D-C3D	-3.47	118.19	124.68
18	3	3006	CLA	C2D-C3D-C4D	-3.47	103.31	106.30
18	A	9011	CLA	CHD-C4C-NC	3.47	129.67	124.20
18	B	1206	CLA	C1C-NC-C4C	-3.47	105.15	106.71
18	J	2107	CLA	CHD-C4C-C3C	-3.46	119.75	124.84
18	B	1222	CLA	CHC-C1C-NC	3.46	129.46	124.20
18	A	1133	CLA	C3D-C4D-ND	3.46	113.15	110.14
18	B	1301	CLA	C2D-C3D-C4D	-3.46	103.32	106.30
18	B	1301	CLA	C3D-C4D-ND	3.46	113.14	110.14
18	A	1118	CLA	C3D-C4D-ND	3.46	113.14	110.14
18	3	3005	CLA	C2B-C3B-C4B	3.46	109.25	106.29
18	4	4007	CLA	C3D-C2D-C1D	3.45	109.28	106.30
18	B	1231	CLA	C3D-CAD-CBD	-3.45	103.06	107.61
18	B	1239	CLA	C1-O2A-CGA	3.45	125.49	116.44
18	A	1116	CLA	C2D-C3D-C4D	-3.45	103.33	106.30
18	A	1126	CLA	CHB-C4A-NA	3.45	129.28	124.51
18	2	2001	CLA	C3D-C2D-C1D	3.45	109.27	106.30
18	4	4003	CLA	C3B-C2B-C1B	-3.45	103.34	106.29
18	B	1226	CLA	C2D-C3D-C4D	-3.45	103.33	106.30
18	4	4008	CLA	C3D-C4D-ND	3.45	113.13	110.14
18	A	1117	CLA	C4A-NA-C1A	3.44	108.25	106.71
20	I	6018	BCR	C24-C23-C22	3.44	131.44	126.23
18	3	3012	CLA	C4A-NA-C1A	3.44	108.25	106.71
18	B	1218	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
18	2	2005	CLA	C3D-C2D-C1D	3.43	109.26	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	1233	CLA	CHC-C1C-NC	3.43	129.41	124.20
18	2	2001	CLA	C3B-C2B-C1B	-3.43	103.35	106.29
18	4	1009	CLA	C3D-C2D-C1D	3.43	109.26	106.30
18	1	1001	CLA	C3D-C2D-C1D	3.43	109.26	106.30
18	B	1235	CLA	CHC-C1C-C2C	-3.43	117.23	126.72
20	F	6016	BCR	C12-C13-C14	3.43	124.20	118.94
18	3	3012	CLA	C3D-C2D-C1D	3.43	109.25	106.30
18	B	1213	CLA	C3D-C2D-C1D	3.43	109.25	106.30
18	J	2107	CLA	C3D-CAD-CBD	-3.43	103.09	107.61
18	3	3002	CLA	C4A-NA-C1A	3.43	108.25	106.71
18	B	1214	CLA	CMD-C2D-C3D	-3.42	118.27	124.68
18	1	1007	CLA	C3D-C4D-ND	3.42	113.11	110.14
18	1	1012	CLA	C3D-C4D-ND	3.42	113.11	110.14
18	L	1502	CLA	C4-C3-C5	3.42	119.89	115.98
18	1	1004	CLA	C3D-C2D-C1D	3.41	109.24	106.30
18	A	1117	CLA	C3D-C2D-C1D	3.41	109.24	106.30
18	B	1216	CLA	CED-O2D-CGD	3.41	123.65	115.94
18	3	3006	CLA	C3D-C2D-C1D	3.41	109.24	106.30
18	A	1106	CLA	O2D-CGD-CBD	3.41	117.32	111.27
18	K	1150	CLA	C2D-C3D-C4D	-3.41	103.37	106.30
18	1	1003	CLA	C3D-C2D-C1D	3.41	109.24	106.30
18	1	1014	CLA	C3B-C2B-C1B	-3.40	103.38	106.29
18	B	1222	CLA	C4A-NA-C1A	3.40	108.24	106.71
18	A	1137	CLA	CBC-CAC-C3C	3.40	121.81	112.43
18	2	2006	CLA	C3D-C4D-ND	3.40	113.09	110.14
18	4	1304	CLA	O2A-CGA-CBA	3.40	122.57	111.91
18	B	1232	CLA	CED-O2D-CGD	3.40	123.62	115.94
18	A	1118	CLA	C3B-C2B-C1B	-3.40	103.38	106.29
18	A	1133	CLA	C2D-C3D-C4D	-3.39	103.38	106.30
18	A	1106	CLA	CHC-C1C-NC	3.39	129.35	124.20
18	B	1301	CLA	C3D-C2D-C1D	3.39	109.22	106.30
18	A	1102	CLA	C3D-C2D-C1D	3.39	109.22	106.30
18	G	1248	CLA	C3C-C4C-CHD	-3.39	117.79	125.22
18	A	9013	CLA	C4A-NA-C1A	3.39	108.23	106.71
18	3	3013	CLA	C3D-C4D-ND	3.39	113.08	110.14
18	K	1141	CLA	C2D-C3D-C4D	-3.39	103.38	106.30
18	B	1212	CLA	CMD-C2D-C3D	-3.38	118.35	124.68
18	4	4013	CLA	C3D-C2D-C1D	3.38	109.22	106.30
18	F	4015	CLA	C2B-C3B-C4B	3.38	109.18	106.29
18	A	1134	CLA	C3D-C4D-ND	3.38	113.08	110.14
18	2	2013	CLA	C3D-C2D-C1D	3.38	109.21	106.30
18	A	9011	CLA	O2D-CGD-CBD	3.38	117.27	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4002	CLA	C3D-C4D-ND	3.38	113.07	110.14
18	A	1115	CLA	CHC-C1C-C2C	-3.37	117.39	126.72
18	3	3010	CLA	C2D-C3D-C4D	-3.37	103.40	106.30
18	3	3012	CLA	C2D-C3D-C4D	-3.37	103.40	106.30
18	L	1130	CLA	C3D-CAD-CBD	-3.37	103.17	107.61
18	A	1132	CLA	C1C-NC-C4C	-3.37	105.19	106.71
18	3	3009	CLA	C2D-C3D-C4D	-3.37	103.40	106.30
20	F	6016	BCR	C1-C6-C7	3.37	125.31	115.78
18	B	1227	CLA	CHC-C1C-C2C	-3.37	117.41	126.72
18	4	4001	CLA	C3D-C4D-ND	3.36	113.06	110.14
18	B	1214	CLA	C1-O2A-CGA	3.36	125.27	116.44
18	A	1116	CLA	C3D-C2D-C1D	3.36	109.20	106.30
18	B	1214	CLA	CAA-C2A-C3A	-3.36	103.57	112.78
18	4	4009	CLA	C2D-C3D-C4D	-3.36	103.41	106.30
18	B	1227	CLA	C4A-NA-C1A	3.36	108.22	106.71
18	B	1219	CLA	C4-C3-C5	3.36	119.83	115.98
18	B	1205	CLA	O1D-CGD-CBD	-3.36	117.61	124.48
18	B	1222	CLA	CMD-C2D-C3D	-3.36	118.39	124.68
18	A	1104	CLA	C2A-C3A-C4A	-3.36	98.91	104.18
18	A	1123	CLA	CHC-C1C-NC	3.36	129.30	124.20
18	G	1248	CLA	C2D-C3D-C4D	-3.35	103.41	106.30
18	A	1102	CLA	C2D-C3D-C4D	-3.35	103.41	106.30
18	B	1219	CLA	CAA-C2A-C3A	-3.35	103.60	112.78
18	4	4011	CLA	C2A-C3A-C4A	-3.35	98.92	104.18
18	A	1143	CLA	C2D-C3D-C4D	-3.35	103.42	106.30
18	A	1134	CLA	C2B-C3B-C4B	3.35	109.15	106.29
18	A	1126	CLA	CHD-C4C-C3C	-3.35	119.92	124.84
18	A	1146	CLA	C2D-C3D-C4D	-3.35	103.42	106.30
18	2	2004	CLA	C4A-NA-C1A	3.35	108.21	106.71
18	B	1227	CLA	C3D-CAD-CBD	-3.34	103.20	107.61
20	L	6020	BCR	C15-C16-C17	-3.34	116.63	123.47
18	A	1152	CLA	C2D-C3D-C4D	-3.34	103.42	106.30
18	A	1113	CLA	O1D-CGD-CBD	-3.34	117.65	124.48
18	3	3007	CLA	C3D-C2D-C1D	3.34	109.18	106.30
18	A	1146	CLA	C4A-NA-C1A	3.33	108.20	106.71
18	F	4015	CLA	C3D-C2D-C1D	3.33	109.17	106.30
18	A	1131	CLA	CHC-C1C-C2C	-3.33	117.50	126.72
18	G	1233	CLA	O2A-CGA-CBA	3.33	122.37	111.91
18	B	1211	CLA	C3D-C4D-ND	3.33	113.03	110.14
18	A	1140	CLA	C1-O2A-CGA	3.33	125.18	116.44
20	L	6020	BCR	C30-C25-C26	-3.33	117.92	122.61
18	B	1217	CLA	CHD-C4C-C3C	-3.33	119.95	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1129	CLA	CAA-C2A-C1A	-3.33	101.08	111.97
18	A	1103	CLA	CMD-C2D-C3D	-3.32	118.46	124.68
18	B	1234	CLA	CMD-C2D-C3D	-3.32	118.46	124.68
18	1	1004	CLA	C3B-C2B-C1B	-3.32	103.44	106.29
18	B	1203	CLA	O2A-CGA-CBA	3.32	122.33	111.91
18	3	3009	CLA	C3D-C4D-ND	3.32	113.03	110.14
18	J	1307	CLA	CHC-C1C-NC	3.32	129.13	124.23
18	B	9022	CLA	O2A-CGA-CBA	3.32	122.32	111.91
18	2	2001	CLA	C3D-C4D-ND	3.32	113.02	110.14
18	A	1143	CLA	C3D-C2D-C1D	3.32	109.16	106.30
18	J	2107	CLA	O2D-CGD-O1D	-3.32	117.36	123.84
20	I	6018	BCR	C28-C27-C26	-3.31	108.16	114.08
18	A	1110	CLA	C3D-C4D-ND	3.31	113.02	110.14
18	3	3010	CLA	C3D-C2D-C1D	3.31	109.16	106.30
18	F	4015	CLA	C2D-C3D-C4D	-3.31	103.45	106.30
18	B	1223	CLA	C3C-C4C-CHD	-3.31	117.97	125.22
18	B	9023	CLA	CMA-C3A-C4A	-3.31	102.88	111.77
18	3	3005	CLA	C3D-C4D-ND	3.31	113.02	110.14
18	1	1005	CLA	C3D-C4D-ND	3.31	113.01	110.14
18	B	1241	CLA	C2D-C3D-C4D	-3.31	103.45	106.30
18	A	1309	CLA	C3D-C2D-C1D	3.30	109.15	106.30
18	A	1146	CLA	C3D-C2D-C1D	3.30	109.15	106.30
18	B	1202	CLA	CHD-C4C-C3C	-3.30	119.99	124.84
18	2	2012	CLA	C3D-C4D-ND	3.30	113.00	110.14
18	1	1008	CLA	C3D-C2D-C1D	3.29	109.14	106.30
18	B	1227	CLA	CMB-C2B-C1B	3.29	133.52	128.46
18	A	1123	CLA	O2A-CGA-CBA	3.29	122.23	111.91
18	1	1004	CLA	C4A-NA-C1A	3.29	108.18	106.71
18	A	1142	CLA	C3B-C2B-C1B	-3.29	103.48	106.29
18	B	1218	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
18	A	1148	CLA	C3D-C4D-ND	3.28	112.99	110.14
18	B	1225	CLA	CHB-C4A-NA	3.28	129.05	124.51
18	B	1207	CLA	CHC-C1C-NC	3.28	129.18	124.20
18	4	1304	CLA	C4A-NA-C1A	3.28	108.18	106.71
18	A	1104	CLA	C2A-C1A-CHA	-3.27	117.05	122.63
18	B	1206	CLA	CHC-C1C-NC	3.27	129.06	124.23
18	1	1003	CLA	C3D-C4D-ND	3.27	112.98	110.14
18	4	4008	CLA	C3D-C2D-C1D	3.27	109.12	106.30
18	A	1151	CLA	C3C-C4C-CHD	-3.27	118.06	125.22
18	G	1233	CLA	CMB-C2B-C3B	3.27	130.79	124.68
18	B	1229	CLA	CHC-C1C-NC	3.27	129.16	124.20
18	2	2008	CLA	C3D-C4D-ND	3.27	112.98	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	2107	CLA	CHC-C1C-NC	3.27	129.16	124.20
18	K	1150	CLA	C3D-C2D-C1D	3.27	109.12	106.30
18	J	1307	CLA	C1C-NC-C4C	-3.27	105.24	106.71
18	A	1126	CLA	C4A-NA-C1A	3.27	108.17	106.71
18	A	1124	CLA	CHC-C1C-NC	3.26	129.05	124.23
18	A	1124	CLA	C2D-C3D-C4D	-3.26	103.49	106.30
18	B	1215	CLA	C2A-C1A-CHA	-3.26	118.16	123.86
18	B	1202	CLA	CAC-C3C-C4C	3.26	129.04	124.81
18	B	1234	CLA	CHC-C1C-NC	3.26	129.15	124.20
20	B	6017	BCR	C30-C25-C24	3.26	124.99	115.78
20	F	6016	BCR	C16-C15-C14	-3.26	116.80	123.47
18	3	3009	CLA	C3D-C2D-C1D	3.26	109.11	106.30
18	A	1101	CLA	C3B-C2B-C1B	-3.26	103.50	106.29
18	2	2002	CLA	C3D-C2D-C1D	3.25	109.11	106.30
18	A	1118	CLA	C3D-C2D-C1D	3.25	109.11	106.30
18	B	1138	CLA	CAA-C2A-C3A	-3.25	103.87	112.78
18	A	1129	CLA	C2A-C1A-CHA	-3.25	118.17	123.86
18	B	1222	CLA	C4-C3-C5	3.25	120.74	115.27
18	2	2012	CLA	C2D-C3D-C4D	-3.25	103.51	106.30
18	B	1212	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
18	A	1137	CLA	CHB-C4A-NA	3.24	128.99	124.51
18	4	4003	CLA	C4A-NA-C1A	3.24	108.16	106.71
18	2	2015	CLA	C2D-C3D-C4D	-3.24	103.51	106.30
18	A	1137	CLA	CMB-C2B-C3B	3.24	130.74	124.68
18	1	1003	CLA	C2A-C3A-C4A	-3.24	99.10	104.18
18	B	1225	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
18	G	1248	CLA	C3D-C4D-ND	3.23	112.95	110.14
18	B	1202	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
18	2	2007	CLA	C3C-C4C-CHD	-3.23	118.14	125.22
18	4	4012	CLA	CHB-C4A-NA	3.23	129.29	124.34
20	I	6018	BCR	C33-C5-C6	-3.23	120.90	124.53
18	K	1153	CLA	C2D-C3D-C4D	-3.23	103.52	106.30
18	A	1116	CLA	C3D-C4D-ND	3.23	112.94	110.14
18	B	1234	CLA	O2A-CGA-CBA	3.23	122.03	111.91
18	B	1203	CLA	CHB-C4A-NA	3.22	128.97	124.51
18	B	1138	CLA	CHD-C4C-C3C	-3.22	120.10	124.84
18	L	1125	CLA	C3D-C2D-C1D	3.22	109.08	106.30
18	B	1241	CLA	C3D-C2D-C1D	3.22	109.08	106.30
18	B	1239	CLA	C4A-NA-C1A	3.22	108.15	106.71
18	A	1147	CLA	C3C-C4C-CHD	-3.22	118.17	125.22
20	A	6011	BCR	C3-C4-C5	-3.22	108.33	114.08
18	1	1013	CLA	C2D-C3D-C4D	-3.22	103.53	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1222	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
18	A	1119	CLA	O2A-CGA-CBA	3.22	122.00	111.91
18	4	4007	CLA	C3D-C4D-ND	3.21	112.93	110.14
18	A	1115	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
18	1	1008	CLA	C2D-C3D-C4D	-3.21	103.53	106.30
18	A	1137	CLA	C4-C3-C2	-3.21	115.44	123.68
18	A	1127	CLA	C3B-C2B-C1B	-3.21	103.54	106.29
18	B	1138	CLA	C4-C3-C5	3.21	120.67	115.27
18	B	1222	CLA	O2A-CGA-CBA	3.21	121.98	111.91
18	A	1126	CLA	CAA-C2A-C1A	-3.21	101.46	111.97
18	B	1223	CLA	C2C-C1C-CHC	-3.21	117.99	125.67
18	B	1226	CLA	C3D-C4D-ND	3.21	112.93	110.14
18	4	4013	CLA	C3C-C4C-CHD	-3.21	118.20	125.22
18	A	9011	CLA	CHC-C1C-NC	3.21	129.07	124.20
20	B	6017	BCR	C29-C30-C25	3.21	115.42	110.48
18	A	1142	CLA	C3C-C4C-CHD	-3.20	118.21	125.22
20	B	6017	BCR	C23-C22-C21	3.20	123.85	118.94
18	4	4001	CLA	C4A-NA-C1A	3.20	108.14	106.71
18	L	1125	CLA	C3B-C2B-C1B	-3.20	103.55	106.29
18	1	1006	CLA	C2A-C3A-C4A	-3.20	99.16	104.18
18	2	2013	CLA	C3D-C4D-ND	3.20	112.92	110.14
18	2	2013	CLA	C3B-C2B-C1B	-3.20	103.55	106.29
18	B	1226	CLA	C3B-C2B-C1B	-3.20	103.55	106.29
18	B	9022	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
18	B	9022	CLA	C4-C3-C5	3.20	120.65	115.27
18	B	9022	CLA	CAA-C2A-C1A	3.19	122.44	111.97
18	F	1302	CLA	CMD-C2D-C3D	-3.19	118.71	124.68
20	F	6016	BCR	C34-C9-C8	3.19	123.10	118.08
18	A	1136	CLA	CHC-C1C-NC	3.19	129.04	124.20
18	1	1006	CLA	C3C-C4C-CHD	-3.19	118.25	125.22
18	2	2007	CLA	C3D-C4D-ND	3.18	112.91	110.14
20	B	6017	BCR	C16-C15-C14	3.18	130.00	123.47
18	1	1003	CLA	C4A-NA-C1A	3.18	108.14	106.71
18	A	9011	CLA	CHD-C4C-C3C	-3.18	120.16	124.84
18	B	9012	CLA	C4-C3-C2	-3.18	115.52	123.68
18	L	1125	CLA	C3D-C4D-ND	3.18	112.90	110.14
18	B	1227	CLA	CMD-C2D-C3D	-3.17	118.74	124.68
18	B	1138	CLA	C4-C3-C2	-3.17	115.54	123.68
18	3	3015	CLA	C4A-NA-C1A	3.17	108.13	106.71
18	2	2005	CLA	C4A-NA-C1A	3.17	108.13	106.71
20	I	6018	BCR	C2-C1-C6	-3.17	105.60	110.48
18	K	1141	CLA	C3D-C4D-ND	3.16	112.89	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1222	CLA	O2A-CGA-O1A	-3.16	115.61	123.59
18	A	9011	CLA	CMD-C2D-C3D	-3.16	118.76	124.68
18	A	1110	CLA	C2B-C3B-C4B	3.16	108.99	106.29
18	A	1103	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
18	4	4006	CLA	C3D-C2D-C1D	3.16	109.02	106.30
18	L	1504	CLA	CMD-C2D-C3D	-3.16	118.77	124.68
18	3	3008	CLA	C3D-C4D-ND	3.16	112.88	110.14
18	A	1131	CLA	CHD-C4C-C3C	-3.15	120.21	124.84
20	A	6011	BCR	C8-C7-C6	-3.15	118.36	127.20
18	B	1223	CLA	C3D-C4D-ND	3.15	112.87	110.14
18	1	1013	CLA	C3D-C2D-C1D	3.15	109.01	106.30
18	3	2009	CLA	C3C-C4C-CHD	-3.14	118.33	125.22
18	A	1111	CLA	C3D-C2D-C1D	3.14	109.01	106.30
18	1	1012	CLA	C3D-C2D-C1D	3.14	109.01	106.30
18	3	3003	CLA	C3C-C4C-CHD	-3.14	118.33	125.22
18	A	1117	CLA	C2D-C3D-C4D	-3.14	103.59	106.30
18	3	3004	CLA	C2D-C3D-C4D	-3.14	103.59	106.30
18	A	1133	CLA	C3D-C2D-C1D	3.14	109.01	106.30
18	F	1305	CLA	C2D-C3D-C4D	-3.14	103.60	106.30
18	B	1220	CLA	CHC-C1C-NC	3.14	128.96	124.20
18	B	1208	CLA	CAC-C3C-C2C	-3.14	122.17	127.53
18	A	1115	CLA	CAC-C3C-C4C	3.14	128.88	124.81
18	2	2002	CLA	C3D-C4D-ND	3.13	112.86	110.14
18	4	4003	CLA	C3D-C4D-ND	3.13	112.86	110.14
18	H	1505	CLA	C3C-C4C-CHD	-3.13	118.36	125.22
18	A	1123	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
20	L	6020	BCR	C34-C9-C8	3.13	123.01	118.08
18	B	1229	CLA	CHB-C4A-NA	3.13	128.84	124.51
18	4	4013	CLA	C3D-C4D-ND	3.13	112.86	110.14
18	A	1115	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
18	A	1151	CLA	C2D-C3D-C4D	-3.13	103.61	106.30
18	B	1209	CLA	C4A-NA-C1A	3.13	108.11	106.71
18	B	1215	CLA	CAA-C2A-C3A	-3.12	104.22	112.78
18	A	1119	CLA	CED-O2D-CGD	3.12	123.00	115.94
20	I	6018	BCR	C33-C5-C4	3.12	119.61	113.62
18	B	1208	CLA	C4-C3-C2	-3.12	115.67	123.68
18	A	1134	CLA	C3C-C4C-CHD	-3.12	118.39	125.22
18	B	9023	CLA	CED-O2D-CGD	3.12	123.00	115.94
18	4	4012	CLA	C3C-C4C-CHD	-3.12	118.39	125.22
18	H	1501	CLA	O2A-CGA-CBA	3.12	121.69	111.91
18	B	1207	CLA	O2D-CGD-CBD	3.12	116.81	111.27
18	A	1108	CLA	O2A-CGA-CBA	3.12	121.69	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	4004	CLA	C3C-C4C-CHD	-3.12	118.39	125.22
18	3	3003	CLA	C2D-C3D-C4D	-3.12	103.62	106.30
18	B	1231	CLA	CHD-C4C-C3C	-3.12	120.26	124.84
18	A	1129	CLA	CHC-C1C-NC	3.11	128.93	124.20
18	B	1220	CLA	C1-O2A-CGA	3.11	124.61	116.44
18	3	3011	CLA	C2D-C3D-C4D	-3.11	103.62	106.30
18	2	2011	CLA	C3D-C4D-ND	3.11	112.84	110.14
18	B	1213	CLA	C3D-C4D-ND	3.11	112.84	110.14
18	B	1232	CLA	CMB-C2B-C3B	3.11	130.50	124.68
18	B	1216	CLA	O2A-CGA-CBA	3.11	121.67	111.91
18	3	3004	CLA	C3D-C4D-ND	3.11	112.84	110.14
18	A	1106	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
18	2	2015	CLA	C3D-C2D-C1D	3.10	108.97	106.30
18	3	3011	CLA	C3D-C2D-C1D	3.10	108.97	106.30
20	F	6016	BCR	C30-C25-C26	-3.10	118.25	122.61
18	3	2009	CLA	C2D-C3D-C4D	-3.10	103.63	106.30
18	B	1232	CLA	O2A-CGA-CBA	3.10	121.63	111.91
18	A	1122	CLA	CHC-C1C-NC	3.10	128.90	124.20
18	4	4005	CLA	C4A-NA-C1A	3.10	108.10	106.71
18	1	1011	CLA	C3D-C2D-C1D	3.10	108.97	106.30
18	B	1217	CLA	CAA-C2A-C3A	-3.09	104.30	112.78
18	K	1150	CLA	C3D-C4D-ND	3.09	112.82	110.14
18	B	9012	CLA	C1-O2A-CGA	3.09	124.55	116.44
18	4	1009	CLA	C2D-C3D-C4D	-3.09	103.64	106.30
18	A	1132	CLA	C2D-C3D-C4D	-3.09	103.64	106.30
18	B	1232	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	L	1130	CLA	O2A-C1-C2	3.09	116.75	108.64
18	B	1219	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
18	4	4007	CLA	C3C-C4C-CHD	-3.08	118.47	125.22
18	A	1132	CLA	CHC-C1C-NC	3.08	128.78	124.23
18	L	1504	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
20	L	6020	BCR	C20-C21-C22	3.08	131.70	127.31
18	4	4009	CLA	C3D-C4D-ND	3.08	112.81	110.14
18	A	1151	CLA	C3D-C2D-C1D	3.08	108.95	106.30
18	A	1127	CLA	C3C-C4C-CHD	-3.08	118.48	125.22
18	A	1152	CLA	C4A-NA-C1A	3.07	108.09	106.71
18	3	3012	CLA	C3C-C4C-CHD	-3.07	118.50	125.22
18	A	1129	CLA	CAC-C3C-C4C	3.07	128.79	124.81
18	3	3006	CLA	C3D-C4D-ND	3.07	112.81	110.14
18	3	3009	CLA	C3C-C4C-CHD	-3.07	118.50	125.22
18	4	4002	CLA	C3C-C4C-CHD	-3.07	118.50	125.22
20	L	6020	BCR	C21-C20-C19	-3.07	113.64	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1148	CLA	C3C-C4C-CHD	-3.07	118.50	125.22
18	K	1150	CLA	C3C-C4C-CHD	-3.07	118.50	125.22
18	L	1130	CLA	CMD-C2D-C3D	-3.07	118.94	124.68
18	F	1303	CLA	C2D-C3D-C4D	-3.07	103.66	106.30
18	A	1124	CLA	C3C-C4C-CHD	-3.06	118.51	125.22
18	1	1012	CLA	C3C-C4C-CHD	-3.06	118.52	125.22
18	1	1011	CLA	C3C-C4C-CHD	-3.06	118.52	125.22
18	A	1126	CLA	CHC-C1C-NC	3.05	128.83	124.20
18	A	1105	CLA	C4A-NA-C1A	3.05	108.08	106.71
18	A	1142	CLA	C3D-C2D-C1D	3.05	108.93	106.30
18	1	1004	CLA	C3D-C4D-ND	3.05	112.79	110.14
18	B	1230	CLA	C3D-C4D-ND	3.05	112.79	110.14
18	B	1138	CLA	CMD-C2D-C3D	-3.05	118.97	124.68
18	B	1218	CLA	CAA-C2A-C1A	-3.05	101.98	111.97
18	H	1505	CLA	C2D-C3D-C4D	-3.05	103.67	106.30
18	B	9022	CLA	C3D-CAD-CBD	-3.05	103.59	107.61
18	A	1152	CLA	C3D-C2D-C1D	3.04	108.92	106.30
18	A	1122	CLA	C1-O2A-CGA	3.04	124.43	116.44
18	B	1239	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
18	4	4009	CLA	C3D-C2D-C1D	3.04	108.92	106.30
18	B	1216	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
20	A	6011	BCR	C38-C26-C27	3.04	119.46	113.62
18	F	1303	CLA	C3D-C4D-ND	3.04	112.78	110.14
18	1	1002	CLA	C2D-C3D-C4D	-3.04	103.69	106.30
18	1	1002	CLA	C3C-C4C-CHD	-3.04	118.57	125.22
18	A	1142	CLA	C2D-C3D-C4D	-3.04	103.69	106.30
18	A	1110	CLA	C3C-C4C-CHD	-3.03	118.58	125.22
18	A	1119	CLA	CHC-C1C-NC	3.03	128.81	124.20
18	A	9011	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
20	I	6018	BCR	C8-C7-C6	3.03	135.71	127.20
18	4	4012	CLA	C3D-C4D-ND	3.03	112.77	110.14
18	A	1132	CLA	C4A-NA-C1A	3.03	108.07	106.71
18	B	1209	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
18	B	1214	CLA	O2A-CGA-CBA	3.03	121.41	111.91
18	A	1108	CLA	CMD-C2D-C3D	-3.02	119.02	124.68
18	A	1113	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
18	3	3015	CLA	C3D-C4D-ND	3.02	112.76	110.14
18	B	1215	CLA	CMD-C2D-C3D	-3.02	119.03	124.68
18	1	1004	CLA	C3C-C4C-CHD	-3.02	118.61	125.22
18	A	1152	CLA	C3C-C4C-CHD	-3.02	118.61	125.22
18	1	1012	CLA	CHB-C4A-NA	3.01	128.96	124.34
18	A	1104	CLA	C1C-NC-C4C	-3.01	105.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1109	CLA	C2A-C3A-C4A	-3.01	100.46	104.70
18	B	9010	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	4	1009	CLA	CHC-C1C-NC	3.01	128.68	124.23
18	4	4010	CLA	C3D-C4D-ND	3.01	112.75	110.14
18	4	4006	CLA	C3C-C4C-CHD	-3.01	118.63	125.22
18	A	1111	CLA	C2D-C3D-C4D	-3.01	103.71	106.30
18	B	1216	CLA	CHB-C4A-NA	3.01	128.67	124.51
18	A	1127	CLA	C2C-C1C-CHC	-3.01	118.47	125.67
18	B	1214	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
18	L	1503	CLA	CAC-C3C-C4C	-3.01	120.91	124.81
18	4	4004	CLA	C3D-C4D-ND	3.00	112.75	110.14
18	A	1134	CLA	C4A-NA-C1A	3.00	108.06	106.71
18	2	2015	CLA	C3D-C4D-ND	3.00	112.74	110.14
18	A	1104	CLA	C2D-C3D-C4D	-3.00	103.72	106.30
18	3	3003	CLA	C3D-C2D-C1D	3.00	108.88	106.30
18	A	1140	CLA	CMD-C2D-C3D	-3.00	119.07	124.68
18	A	1102	CLA	C3D-C4D-ND	2.99	112.74	110.14
18	A	1124	CLA	C3D-C4D-ND	2.99	112.74	110.14
18	L	1503	CLA	CED-O2D-CGD	2.99	122.71	115.94
18	A	1309	CLA	C3D-C4D-ND	2.99	112.74	110.14
18	2	2003	CLA	C3C-C4C-CHD	-2.99	118.67	125.22
18	A	1104	CLA	C2B-C3B-C4B	2.99	108.85	106.29
20	L	6020	BCR	C28-C27-C26	-2.99	108.74	114.08
19	B	5002	PQN	C2M-C2-C1	2.99	121.22	116.27
18	F	1305	CLA	C3D-C4D-ND	2.99	112.74	110.14
18	B	1228	CLA	CMA-C3A-C4A	-2.99	103.74	111.77
18	1	1013	CLA	C3D-C4D-ND	2.98	112.73	110.14
18	1	1008	CLA	C3D-C4D-ND	2.98	112.73	110.14
18	A	1128	CLA	C4-C3-C5	2.98	120.28	115.27
18	B	1218	CLA	C6-C5-C3	-2.98	99.04	113.58
18	A	1126	CLA	C1-O2A-CGA	2.98	124.26	116.44
18	K	1141	CLA	C3D-C2D-C1D	2.98	108.87	106.30
18	B	9023	CLA	O2A-CGA-CBA	2.98	121.25	111.91
18	A	1107	CLA	CED-O2D-CGD	2.98	122.67	115.94
18	B	1215	CLA	O2A-CGA-CBA	2.98	121.25	111.91
18	A	1111	CLA	C3D-C4D-ND	2.98	112.72	110.14
18	A	1146	CLA	C3D-C4D-ND	2.98	112.72	110.14
18	L	1504	CLA	C1-O2A-CGA	2.98	124.25	116.44
18	A	1103	CLA	CAC-C3C-C4C	2.97	128.67	124.81
18	A	1108	CLA	O1D-CGD-CBD	-2.97	118.40	124.48
20	F	6016	BCR	C34-C9-C10	-2.97	118.76	122.92
18	A	1144	CLA	C2C-C1C-CHC	-2.97	118.55	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1203	CLA	CHD-C4C-C3C	-2.97	120.34	124.98
18	4	4010	CLA	C3C-C4C-CHD	-2.97	118.72	125.22
20	I	6018	BCR	C19-C18-C17	-2.97	114.38	118.94
18	3	3007	CLA	C3D-C4D-ND	2.97	112.72	110.14
18	A	1126	CLA	CMC-C2C-C1C	2.97	129.56	125.04
18	2	2008	CLA	C2C-C1C-CHC	-2.97	118.56	125.67
18	3	3002	CLA	C3C-C4C-CHD	-2.97	118.72	125.22
18	A	1143	CLA	C3D-C4D-ND	2.96	112.72	110.14
18	F	1139	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
20	F	6016	BCR	C27-C26-C25	-2.96	118.43	122.73
18	1	1006	CLA	C3D-C2D-C1D	2.96	108.85	106.30
18	3	3007	CLA	C2C-C1C-CHC	-2.96	118.58	125.67
18	2	2001	CLA	C3C-C4C-CHD	-2.96	118.73	125.22
18	A	1108	CLA	CHB-C4A-NA	2.96	128.60	124.51
18	B	1138	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
18	F	1305	CLA	C2C-C1C-CHC	-2.96	118.59	125.67
18	B	1220	CLA	CMD-C2D-C3D	-2.96	119.15	124.68
20	I	6018	BCR	C40-C30-C25	-2.96	105.50	110.30
18	1	1002	CLA	C3D-C4D-ND	2.96	112.71	110.14
18	B	1206	CLA	CHB-C4A-NA	2.95	128.86	124.34
20	B	6017	BCR	C23-C24-C25	-2.95	118.91	127.20
18	B	9023	CLA	O2D-CGD-CBD	2.95	116.51	111.27
18	B	1238	CLA	C2A-C1A-CHA	-2.95	118.70	123.86
18	B	1218	CLA	O1D-CGD-CBD	-2.95	118.45	124.48
19	B	5002	PQN	C17-C16-C15	-2.95	105.35	113.36
18	3	2009	CLA	C3D-C2D-C1D	2.95	108.84	106.30
20	B	6017	BCR	C33-C5-C6	-2.95	121.22	124.53
18	F	1303	CLA	C3C-C4C-CHD	-2.95	118.77	125.22
18	H	1501	CLA	CED-O2D-CGD	2.95	122.60	115.94
18	B	9012	CLA	CED-O2D-CGD	2.95	122.60	115.94
18	B	1215	CLA	CED-O2D-CGD	2.94	122.60	115.94
18	B	1138	CLA	C1-O2A-CGA	2.94	124.17	116.44
18	2	2010	CLA	C3C-C4C-CHD	-2.94	118.78	125.22
18	J	1307	CLA	C3D-C4D-ND	2.94	112.69	110.14
19	B	5002	PQN	O1-C1-C10	-2.94	116.80	121.56
18	B	1225	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
18	4	1304	CLA	CMD-C2D-C3D	-2.93	119.19	124.68
18	2	2011	CLA	C3C-C4C-CHD	-2.93	118.80	125.22
18	B	1222	CLA	C4-C3-C2	-2.93	116.16	123.68
18	B	1228	CLA	O2A-CGA-O1A	-2.93	116.20	123.59
18	3	3004	CLA	C3C-C4C-CHD	-2.93	118.80	125.22
18	F	1305	CLA	C3D-C2D-C1D	2.93	108.83	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1107	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
18	B	9012	CLA	CMA-C3A-C4A	-2.93	103.91	111.77
18	B	1201	CLA	CHB-C4A-NA	2.93	128.82	124.34
18	3	3011	CLA	C3C-C4C-CHD	-2.92	118.82	125.22
18	G	1248	CLA	C2C-C1C-CHC	-2.92	118.67	125.67
18	B	1226	CLA	C3C-C4C-CHD	-2.92	118.82	125.22
18	B	1238	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
18	F	1302	CLA	O2A-CGA-CBA	2.92	121.07	111.91
18	A	1133	CLA	C3C-C4C-CHD	-2.92	118.83	125.22
18	A	1143	CLA	C3C-C4C-CHD	-2.92	118.83	125.22
18	B	9010	CLA	CMB-C2B-C3B	2.92	130.14	124.68
18	F	1302	CLA	C4A-NA-C1A	2.92	108.02	106.71
18	H	1501	CLA	C1-O2A-CGA	2.92	124.10	116.44
18	B	1210	CLA	C3D-C4D-ND	2.92	112.67	110.14
18	B	1234	CLA	C2A-C1A-CHA	-2.92	118.76	123.86
18	F	1139	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
18	4	4010	CLA	C2D-C3D-C4D	-2.91	103.79	106.30
18	A	9013	CLA	CHB-C4A-NA	2.91	128.54	124.51
18	B	1236	CLA	C4A-NA-C1A	2.91	108.01	106.71
18	1	1006	CLA	C2D-C3D-C4D	-2.91	103.80	106.30
18	A	1136	CLA	O2A-CGA-CBA	2.91	121.03	111.91
18	A	1111	CLA	C3C-C4C-CHD	-2.91	118.86	125.22
18	B	1241	CLA	C3C-C4C-CHD	-2.91	118.86	125.22
18	2	2012	CLA	C3C-C4C-CHD	-2.91	118.86	125.22
18	L	1503	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
18	B	1219	CLA	O2A-CGA-CBA	2.91	121.03	111.91
18	A	1132	CLA	C3D-C2D-C1D	2.90	108.80	106.30
18	4	1304	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
18	4	4011	CLA	C3C-C4C-CHD	-2.90	118.87	125.22
18	B	1205	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
20	B	6017	BCR	C24-C25-C26	-2.90	114.44	121.46
18	4	1009	CLA	C3C-C4C-CHD	-2.90	118.88	125.22
18	K	1150	CLA	CHB-C4A-NA	2.89	128.77	124.34
18	B	1239	CLA	O2A-CGA-CBA	2.89	120.99	111.91
18	A	1115	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	3	3005	CLA	C3C-C4C-CHD	-2.89	118.89	125.22
18	L	1502	CLA	C4-C3-C2	-2.89	116.26	123.68
18	B	1220	CLA	C4A-NA-C1A	2.89	108.01	106.71
18	4	4005	CLA	C3C-C4C-CHD	-2.89	118.89	125.22
18	A	1128	CLA	CMD-C2D-C3D	-2.88	119.29	124.68
18	F	1302	CLA	CHB-C4A-NA	2.88	128.49	124.51
18	A	1101	CLA	C2C-C1C-CHC	-2.88	118.78	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	1125	CLA	C3C-C4C-CHD	-2.88	118.92	125.22
18	A	1105	CLA	C3C-C4C-CHD	-2.88	118.92	125.22
18	B	1228	CLA	C1-O2A-CGA	2.88	124.00	116.44
18	B	1203	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
18	B	1224	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
18	L	1503	CLA	CGD-CBD-CAD	-2.88	101.42	110.73
18	3	3003	CLA	C4A-NA-C1A	2.88	108.00	106.71
18	1	1008	CLA	C3C-C4C-CHD	-2.88	118.92	125.22
18	A	1117	CLA	C3C-C4C-CHD	-2.87	118.93	125.22
18	B	9012	CLA	C5-C3-C2	2.87	126.93	121.12
18	2	2005	CLA	C3C-C4C-CHD	-2.87	118.93	125.22
18	B	1230	CLA	C3C-C4C-CHD	-2.87	118.93	125.22
18	A	1113	CLA	O2A-CGA-CBA	2.87	120.91	111.91
18	A	1113	CLA	CHB-C4A-NA	2.87	128.48	124.51
18	3	3007	CLA	C3C-C4C-CHD	-2.87	118.94	125.22
18	B	1232	CLA	CMD-C2D-C3D	-2.87	119.32	124.68
18	2	2002	CLA	C3C-C4C-CHD	-2.86	118.95	125.22
18	A	1115	CLA	O2A-CGA-CBA	2.86	120.89	111.91
18	3	3008	CLA	C3C-C4C-CHD	-2.86	118.95	125.22
18	1	1013	CLA	C3C-C4C-CHD	-2.86	118.95	125.22
18	A	1117	CLA	C1C-NC-C4C	-2.86	105.42	106.71
18	2	2006	CLA	C3B-C2B-C1B	-2.86	103.84	106.29
18	A	1107	CLA	O2A-CGA-CBA	2.86	120.88	111.91
18	1	1002	CLA	C2C-C1C-CHC	-2.86	118.83	125.67
18	B	1203	CLA	C5-C3-C4	2.86	120.92	114.60
18	A	1140	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
18	B	1237	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
18	3	3002	CLA	C3D-C4D-ND	2.86	112.62	110.14
18	F	4015	CLA	C2C-C1C-CHC	-2.86	118.83	125.67
18	F	1240	CLA	CHB-C4A-NA	2.86	128.71	124.34
18	A	1104	CLA	C3A-C4A-NA	2.85	115.90	109.92
18	3	3002	CLA	C2C-C1C-CHC	-2.85	118.84	125.67
18	3	2009	CLA	C2C-C1C-CHC	-2.85	118.84	125.67
18	L	1130	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
18	1	1011	CLA	C2D-C3D-C4D	-2.85	103.85	106.30
18	A	1118	CLA	C3C-C4C-CHD	-2.85	118.99	125.22
18	B	1226	CLA	C2C-C1C-CHC	-2.85	118.85	125.67
18	3	3010	CLA	C3C-C4C-CHD	-2.85	118.99	125.22
18	A	1147	CLA	C2C-C1C-CHC	-2.85	118.86	125.67
18	A	9011	CLA	C1-O2A-CGA	2.85	123.91	116.44
18	A	1107	CLA	CHC-C1C-C2C	-2.84	118.85	126.72
18	3	3008	CLA	C2C-C1C-CHC	-2.84	118.86	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3001	CLA	CHB-C4A-NA	2.84	128.69	124.34
18	B	1211	CLA	C3C-C4C-CHD	-2.84	119.00	125.22
18	1	1014	CLA	C3C-C4C-CHD	-2.84	119.00	125.22
18	A	1144	CLA	C3C-C4C-CHD	-2.84	119.00	125.22
18	2	2013	CLA	C2C-C1C-CHC	-2.84	118.87	125.67
20	I	6018	BCR	C35-C13-C12	2.84	122.55	118.08
18	B	1225	CLA	CBC-CAC-C3C	-2.84	104.61	112.43
18	B	9012	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
18	3	3006	CLA	C3C-C4C-CHD	-2.84	119.01	125.22
18	A	1113	CLA	CMB-C2B-C3B	2.83	129.98	124.68
18	B	1229	CLA	C4-C3-C2	-2.83	114.46	122.65
18	B	1242	CLA	O1D-CGD-CBD	-2.83	118.69	124.48
18	K	1153	CLA	C2C-C1C-CHC	-2.83	118.89	125.67
18	B	1239	CLA	CMD-C2D-C3D	-2.83	119.38	124.68
18	H	1501	CLA	C6-C5-C3	-2.83	106.03	113.45
18	A	1151	CLA	C3D-C4D-ND	2.83	112.60	110.14
18	4	4004	CLA	C2D-C3D-C4D	-2.83	103.87	106.30
18	B	1224	CLA	C4-C3-C5	2.83	119.21	115.98
18	F	4015	CLA	C3C-C4C-CHD	-2.82	119.03	125.22
18	B	1207	CLA	CMD-C2D-C3D	-2.82	119.39	124.68
18	G	1233	CLA	C1-C2-C3	-2.82	121.16	126.04
18	3	3008	CLA	CHB-C4A-NA	2.82	128.66	124.34
18	A	1146	CLA	C3C-C4C-CHD	-2.82	119.04	125.22
18	B	1206	CLA	C3B-C2B-C1B	-2.82	103.87	106.29
18	A	1122	CLA	C5-C3-C2	-2.82	115.41	121.12
18	4	4009	CLA	C3C-C4C-CHD	-2.82	119.04	125.22
18	B	1212	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	A	1118	CLA	CHB-C4A-NA	2.82	128.65	124.34
18	B	1225	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
18	B	1217	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
18	2	2010	CLA	C2C-C1C-CHC	-2.81	118.93	125.67
18	H	1501	CLA	CMD-C2D-C3D	-2.81	119.41	124.68
18	A	1102	CLA	C3C-C4C-CHD	-2.81	119.06	125.22
18	3	3005	CLA	C2C-C1C-CHC	-2.81	118.94	125.67
20	F	6016	BCR	C32-C1-C6	-2.81	105.74	110.30
18	A	1101	CLA	CHB-C4A-NA	2.81	128.64	124.34
19	B	5002	PQN	C16-C17-C18	-2.81	106.84	115.92
18	F	1305	CLA	C3C-C4C-CHD	-2.80	119.08	125.22
18	3	3011	CLA	C3D-C4D-ND	2.80	112.58	110.14
18	A	1128	CLA	CED-O2D-CGD	2.80	122.28	115.94
18	B	1138	CLA	O2A-CGA-CBA	2.80	120.70	111.91
18	A	1115	CLA	CGD-CBD-CAD	2.80	119.81	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1221	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
18	A	1132	CLA	C2A-C3A-C4A	-2.80	99.78	104.18
18	A	9011	CLA	C2C-C1C-NC	2.80	112.60	109.97
18	2	2003	CLA	C2C-C1C-CHC	-2.80	118.97	125.67
18	1	1010	CLA	C2D-C3D-C4D	-2.80	103.89	106.30
18	2	2006	CLA	C2C-C1C-CHC	-2.80	118.97	125.67
18	1	1010	CLA	C3D-C4D-ND	2.80	112.57	110.14
18	B	1238	CLA	C4-C3-C5	2.80	119.97	115.27
18	1	1003	CLA	C3C-C4C-CHD	-2.79	119.10	125.22
18	A	1126	CLA	CMB-C2B-C3B	2.79	129.90	124.68
18	G	1248	CLA	C3D-C2D-C1D	2.79	108.71	106.30
18	1	1010	CLA	C3C-C4C-CHD	-2.79	119.11	125.22
18	A	1110	CLA	C4A-NA-C1A	2.79	107.96	106.71
18	I	1204	CLA	C4A-NA-C1A	2.79	107.96	106.71
18	4	4011	CLA	C2C-C1C-CHC	-2.79	118.99	125.67
18	A	1129	CLA	CED-O2D-CGD	2.79	122.24	115.94
18	H	1501	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
18	J	2107	CLA	C5-C3-C2	-2.79	115.48	121.12
18	A	1135	CLA	CAC-C3C-C4C	2.79	128.42	124.81
18	1	1006	CLA	C2C-C1C-CHC	-2.78	119.00	125.67
18	B	1214	CLA	CBA-CAA-C2A	2.78	122.08	113.86
18	4	4001	CLA	C3C-C4C-CHD	-2.78	119.12	125.22
18	1	1014	CLA	CHB-C4A-NA	2.78	128.60	124.34
18	J	2107	CLA	C4-C3-C5	2.78	119.95	115.27
18	A	1105	CLA	C2C-C1C-CHC	-2.78	119.01	125.67
18	B	1222	CLA	CED-O2D-CGD	2.78	122.23	115.94
18	A	1135	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
18	3	3004	CLA	C3D-C2D-C1D	2.78	108.69	106.30
18	A	1115	CLA	CED-O2D-CGD	2.78	122.22	115.94
18	F	1306	CLA	C3C-C4C-CHD	-2.78	119.14	125.22
18	3	3012	CLA	C2C-C1C-CHC	-2.78	119.02	125.67
18	B	1239	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
18	B	1220	CLA	CAA-C2A-C1A	-2.77	102.89	111.97
18	3	3015	CLA	C3C-C4C-CHD	-2.77	119.15	125.22
18	F	1303	CLA	C3D-C2D-C1D	2.77	108.69	106.30
18	B	9010	CLA	CAA-CBA-CGA	2.77	121.35	113.25
18	A	1132	CLA	C2B-C3B-C4B	2.77	108.66	106.29
18	B	1237	CLA	C1-O2A-CGA	2.77	123.70	116.44
18	2	2008	CLA	C3C-C4C-CHD	-2.77	119.16	125.22
18	J	1308	CLA	C2C-C1C-CHC	-2.77	119.04	125.67
18	L	1504	CLA	O2A-CGA-CBA	2.77	120.59	111.91
18	3	3010	CLA	C3D-C4D-ND	2.77	112.54	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1207	CLA	C4-C3-C5	2.76	119.92	115.27
18	A	1116	CLA	C2A-C3A-C4A	-2.76	99.84	104.18
18	B	1241	CLA	C3D-C4D-ND	2.76	112.54	110.14
18	3	3010	CLA	C2C-C1C-CHC	-2.76	119.06	125.67
18	B	1231	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
18	B	1215	CLA	CMA-C3A-C2A	-2.76	102.70	113.83
18	B	1238	CLA	C4A-NA-C1A	2.76	107.95	106.71
18	3	3012	CLA	C3D-C4D-ND	2.76	112.53	110.14
18	3	3003	CLA	C3D-C4D-ND	2.76	112.53	110.14
18	2	2004	CLA	C2C-C1C-CHC	-2.76	119.07	125.67
18	B	1230	CLA	C4A-NA-C1A	2.76	107.94	106.71
18	1	1013	CLA	C2A-C3A-C4A	-2.75	99.86	104.18
18	1	1007	CLA	C3D-C2D-C1D	2.75	108.67	106.30
18	K	1141	CLA	C3C-C4C-CHD	-2.75	119.19	125.22
18	B	1220	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
18	4	4009	CLA	C2C-C1C-CHC	-2.75	119.08	125.67
18	L	1502	CLA	CMD-C2D-C3D	-2.75	119.53	124.68
18	2	2003	CLA	CHB-C4A-NA	2.75	128.55	124.34
18	B	1223	CLA	C2A-C3A-C4A	-2.75	99.87	104.18
18	B	1237	CLA	CMB-C2B-C3B	2.75	129.82	124.68
18	1	1001	CLA	C3C-C4C-CHD	-2.75	119.20	125.22
18	A	1101	CLA	C3C-C4C-CHD	-2.75	119.20	125.22
18	B	1232	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
18	B	9022	CLA	CAC-C3C-C4C	2.74	128.37	124.81
18	F	1303	CLA	CHB-C4A-NA	2.74	128.54	124.34
18	A	1152	CLA	C3D-C4D-ND	2.74	112.52	110.14
18	B	1201	CLA	C2C-C1C-CHC	-2.74	119.11	125.67
18	B	1223	CLA	C2D-C3D-C4D	-2.74	103.94	106.30
18	2	2001	CLA	C2C-C1C-CHC	-2.74	119.12	125.67
18	A	1136	CLA	CED-O2D-CGD	2.74	122.12	115.94
18	3	3001	CLA	C3C-C4C-CHD	-2.74	119.23	125.22
18	F	4015	CLA	C3D-C4D-ND	2.74	112.52	110.14
18	B	1217	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
18	I	1204	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
18	B	1242	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	3	3006	CLA	C2C-C1C-CHC	-2.73	119.12	125.67
18	A	1309	CLA	C3C-C4C-CHD	-2.73	119.23	125.22
18	B	1209	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	H	1505	CLA	C3D-C4D-ND	2.73	112.51	110.14
18	A	1122	CLA	C7-C6-C5	2.73	120.77	113.36
18	B	1208	CLA	O2A-CGA-CBA	2.73	120.48	111.91
18	4	4005	CLA	C2C-C1C-CHC	-2.73	119.14	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1129	CLA	C1-C2-C3	-2.73	121.33	126.04
18	A	1134	CLA	C2C-C1C-CHC	-2.73	119.14	125.67
18	B	1239	CLA	C4-C3-C5	2.72	119.86	115.27
18	4	1009	CLA	C3B-C2B-C1B	-2.72	103.96	106.29
18	B	1215	CLA	C2C-C1C-NC	2.72	112.52	109.97
18	B	1301	CLA	C3C-C4C-CHD	-2.72	119.27	125.22
18	K	1153	CLA	C1C-NC-C4C	-2.72	105.48	106.71
18	B	1206	CLA	C2C-C1C-CHC	-2.72	119.17	125.67
20	A	6011	BCR	C20-C21-C22	-2.71	123.44	127.31
18	A	1106	CLA	C2C-C1C-NC	2.71	112.51	109.97
18	A	1109	CLA	C3A-C4A-CHB	-2.71	120.59	123.91
18	A	1115	CLA	CMD-C2D-C3D	-2.71	119.61	124.68
18	A	1111	CLA	CHB-C4A-NA	2.71	128.49	124.34
18	4	4009	CLA	CHB-C4A-NA	2.71	128.49	124.34
18	A	1148	CLA	C2A-C3A-C4A	-2.71	99.93	104.18
18	4	1009	CLA	C2C-C1C-CHC	-2.71	119.19	125.67
18	A	1104	CLA	C3C-C4C-CHD	-2.71	119.29	125.22
18	2	2013	CLA	C3C-C4C-CHD	-2.70	119.30	125.22
18	A	1151	CLA	C2C-C1C-CHC	-2.70	119.20	125.67
18	4	4008	CLA	C3C-C4C-CHD	-2.70	119.31	125.22
18	A	1116	CLA	C3C-C4C-CHD	-2.70	119.31	125.22
18	1	1007	CLA	C2C-C1C-CHC	-2.70	119.20	125.67
18	1	1014	CLA	C3D-C2D-C1D	2.70	108.63	106.30
18	G	1233	CLA	CED-O2D-CGD	2.70	122.04	115.94
18	2	2004	CLA	C3C-C4C-CHD	-2.70	119.31	125.22
18	1	1010	CLA	C2C-C1C-CHC	-2.70	119.21	125.67
18	B	1210	CLA	C2C-C1C-CHC	-2.70	119.21	125.67
18	B	1202	CLA	CAC-C3C-C2C	-2.70	122.92	127.53
18	A	1136	CLA	CMD-C2D-C3D	-2.70	119.64	124.68
18	A	9013	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
18	B	1215	CLA	CMB-C2B-C1B	2.69	132.61	128.46
18	A	1120	CLA	C2C-C1C-CHC	-2.69	119.22	125.67
18	A	9013	CLA	CMB-C2B-C3B	2.69	129.72	124.68
18	B	1230	CLA	C2C-C1C-CHC	-2.69	119.22	125.67
18	4	4002	CLA	C2C-C1C-CHC	-2.69	119.22	125.67
18	3	2009	CLA	C3D-C4D-ND	2.69	112.48	110.14
18	J	1308	CLA	CHB-C4A-NA	2.69	128.46	124.34
18	1	1012	CLA	C2C-C1C-CHC	-2.69	119.23	125.67
18	A	1120	CLA	CHB-C4A-NA	2.69	128.46	124.34
18	A	1116	CLA	C2C-C1C-CHC	-2.69	119.23	125.67
20	B	6017	BCR	C19-C18-C17	2.69	123.07	118.94
18	A	1140	CLA	CED-O2D-CGD	2.69	122.01	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1008	CLA	C2C-C1C-CHC	-2.69	119.24	125.67
18	B	1202	CLA	CHB-C4A-NA	2.69	128.22	124.51
18	A	1132	CLA	C3C-C4C-CHD	-2.68	119.34	125.22
18	A	1122	CLA	O1D-CGD-CBD	-2.68	118.99	124.48
18	2	2015	CLA	C2C-C1C-CHC	-2.68	119.24	125.67
18	A	1116	CLA	CHB-C4A-NA	2.68	128.45	124.34
18	A	1152	CLA	C2C-C1C-CHC	-2.68	119.25	125.67
18	F	1240	CLA	C3C-C4C-CHD	-2.68	119.36	125.22
18	B	1242	CLA	O2A-CGA-CBA	2.68	120.31	111.91
18	3	3013	CLA	C2C-C1C-CHC	-2.68	119.26	125.67
18	A	1309	CLA	C2C-C1C-CHC	-2.68	119.26	125.67
18	B	1213	CLA	C3C-C4C-CHD	-2.68	119.36	125.22
18	4	4010	CLA	C3D-C2D-C1D	2.68	108.61	106.30
18	A	1124	CLA	CHB-C4A-NA	2.68	128.44	124.34
18	B	1218	CLA	CMB-C2B-C3B	2.68	129.68	124.68
18	B	1232	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
18	K	1153	CLA	C3C-C4C-CHD	-2.67	119.37	125.22
18	B	1232	CLA	O1D-CGD-CBD	-2.67	119.02	124.48
18	B	1211	CLA	C2C-C1C-CHC	-2.67	119.28	125.67
18	B	9012	CLA	CAA-C2A-C1A	2.67	120.72	111.97
18	A	1142	CLA	C3D-C4D-ND	2.67	112.46	110.14
18	A	1137	CLA	C4A-NA-C1A	2.67	107.91	106.71
18	1	1010	CLA	C2A-C3A-C4A	-2.67	99.99	104.18
18	I	1204	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
18	3	3004	CLA	C2C-C1C-CHC	-2.67	119.28	125.67
20	F	6016	BCR	C39-C30-C25	2.67	114.62	110.30
18	J	1307	CLA	C2B-C3B-C4B	2.67	108.57	106.29
19	B	5002	PQN	C14-C13-C15	2.66	119.75	115.27
18	I	1204	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
18	A	1123	CLA	CED-O2D-CGD	2.66	121.96	115.94
18	2	2012	CLA	C2C-C1C-CHC	-2.66	119.29	125.67
18	B	1205	CLA	C4-C3-C5	2.66	119.75	115.27
18	H	1501	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	A	1142	CLA	C2C-C1C-CHC	-2.66	119.31	125.67
18	2	2015	CLA	C2A-C3A-C4A	-2.66	100.01	104.18
18	1	1013	CLA	C2C-C1C-CHC	-2.66	119.31	125.67
18	2	2005	CLA	C2A-C3A-C4A	-2.65	100.01	104.18
18	B	1215	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
18	F	1302	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
18	2	2015	CLA	C3C-C4C-CHD	-2.65	119.41	125.22
18	L	1503	CLA	C4B-C3B-C2B	-2.65	104.45	106.92
18	B	1208	CLA	CMB-C2B-C3B	2.65	129.64	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1228	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
18	A	1126	CLA	CAC-C3C-C4C	2.65	128.25	124.81
18	B	1201	CLA	C3C-C4C-CHD	-2.65	119.42	125.22
18	B	1221	CLA	C2C-C1C-NC	2.65	112.45	109.97
18	B	1235	CLA	C2C-C1C-NC	2.65	112.45	109.97
18	A	1129	CLA	CAA-CBA-CGA	-2.65	105.52	113.25
18	J	1307	CLA	C3C-C4C-CHD	-2.65	119.43	125.22
18	B	1222	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	A	1135	CLA	CMD-C2D-C3D	-2.65	119.73	124.68
18	1	1014	CLA	C2C-C1C-CHC	-2.64	119.34	125.67
20	L	6020	BCR	C34-C9-C10	-2.64	119.22	122.92
18	1	1003	CLA	C2C-C1C-CHC	-2.64	119.34	125.67
18	2	2007	CLA	C2C-C1C-CHC	-2.64	119.34	125.67
18	1	1004	CLA	C2C-C1C-CHC	-2.64	119.34	125.67
18	2	2012	CLA	C2A-C3A-C4A	-2.64	100.03	104.18
18	3	3013	CLA	C3C-C4C-CHD	-2.64	119.44	125.22
18	B	1138	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	B	1207	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
18	A	1118	CLA	C2C-C1C-CHC	-2.64	119.35	125.67
18	4	1304	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
18	4	1304	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	A	1128	CLA	O2A-CGA-CBA	2.63	120.17	111.91
18	3	3011	CLA	C2C-C1C-CHC	-2.63	119.37	125.67
18	4	4003	CLA	C3C-C4C-CHD	-2.63	119.47	125.22
18	4	4010	CLA	C2C-C1C-CHC	-2.63	119.38	125.67
18	A	1137	CLA	C6-C5-C3	2.62	120.34	113.45
18	B	1220	CLA	O1D-CGD-CBD	-2.62	119.11	124.48
18	B	1210	CLA	C3C-C4C-CHD	-2.62	119.47	125.22
20	A	6011	BCR	C4-C5-C6	-2.62	118.92	122.73
18	B	1208	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
18	4	1304	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
18	F	1302	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
18	B	1210	CLA	C2D-C3D-C4D	-2.62	104.05	106.30
18	A	1147	CLA	C3D-C2D-C1D	2.62	108.56	106.30
18	A	1127	CLA	C3D-C4D-ND	2.62	112.41	110.14
18	A	1134	CLA	C2A-C3A-C4A	-2.61	100.08	104.18
18	B	1235	CLA	C1-O2A-CGA	2.61	123.30	116.44
18	2	2002	CLA	C2C-C1C-CHC	-2.61	119.42	125.67
18	3	3009	CLA	C2C-C1C-CHC	-2.61	119.42	125.67
18	3	3003	CLA	C2C-C1C-CHC	-2.61	119.42	125.67
18	A	1113	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
18	J	1307	CLA	C4A-NA-C1A	2.61	107.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1120	CLA	C3C-C4C-CHD	-2.61	119.51	125.22
18	L	1504	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
18	A	1148	CLA	C2C-C1C-CHC	-2.60	119.43	125.67
20	I	6018	BCR	C3-C4-C5	-2.60	109.43	114.08
18	1	1004	CLA	C1C-NC-C4C	-2.60	105.54	106.71
18	A	1105	CLA	C2A-C3A-C4A	-2.60	100.10	104.18
18	4	4004	CLA	C2C-C1C-CHC	-2.60	119.45	125.67
18	2	2005	CLA	C2C-C1C-CHC	-2.60	119.45	125.67
18	J	2107	CLA	O1D-CGD-CBD	-2.60	119.17	124.48
18	L	1125	CLA	C2C-C1C-CHC	-2.60	119.45	125.67
18	K	1153	CLA	C2A-C3A-C4A	-2.59	100.11	104.18
18	B	1238	CLA	CED-O2D-CGD	2.59	121.80	115.94
18	H	1505	CLA	C2C-C1C-CHC	-2.59	119.47	125.67
18	1	1005	CLA	C3C-C4C-CHD	-2.59	119.55	125.22
18	1	1005	CLA	CHB-C4A-NA	2.59	128.31	124.34
18	A	1137	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
18	A	1110	CLA	C2C-C1C-CHC	-2.59	119.48	125.67
18	A	1113	CLA	CMD-C2D-C3D	-2.59	119.84	124.68
18	A	1148	CLA	CHB-C4A-NA	2.58	128.30	124.34
18	A	1123	CLA	CMB-C2B-C3B	2.58	129.51	124.68
18	B	1203	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
18	4	4001	CLA	C2C-C1C-CHC	-2.58	119.49	125.67
18	H	1505	CLA	C3D-C2D-C1D	2.58	108.53	106.30
18	B	9010	CLA	CED-O2D-CGD	2.58	121.77	115.94
18	3	3004	CLA	CHB-C4A-NA	2.58	128.29	124.34
18	4	4011	CLA	C1C-NC-C4C	-2.58	105.55	106.71
18	4	4003	CLA	C2C-C1C-CHC	-2.58	119.50	125.67
18	2	2011	CLA	C2C-C1C-CHC	-2.58	119.50	125.67
18	B	1216	CLA	CAC-C3C-C4C	2.57	128.15	124.81
18	B	1212	CLA	CGD-CBD-CAD	-2.57	102.40	110.73
18	B	1212	CLA	CED-O2D-CGD	2.57	121.76	115.94
18	J	2107	CLA	C6-C7-C8	-2.57	107.61	115.92
18	A	1117	CLA	C2C-C1C-CHC	-2.57	119.51	125.67
18	F	1240	CLA	C2B-C3B-C4B	2.57	108.49	106.29
18	A	1133	CLA	C2B-C3B-C4B	2.57	108.48	106.29
18	B	1208	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
18	4	4007	CLA	C2A-C3A-C4A	-2.57	100.15	104.18
18	A	1152	CLA	C2A-C3A-C4A	-2.57	100.15	104.18
18	1	1002	CLA	C3D-C2D-C1D	2.57	108.51	106.30
20	F	6016	BCR	C7-C6-C5	-2.56	115.25	121.46
18	4	4013	CLA	C2C-C1C-CHC	-2.56	119.53	125.67
20	F	6016	BCR	C20-C21-C22	2.56	130.97	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3007	CLA	CHB-C4A-NA	2.56	128.26	124.34
18	A	1102	CLA	C2C-C1C-CHC	-2.56	119.54	125.67
18	B	1208	CLA	C5-C3-C2	2.56	126.30	121.12
18	L	1130	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
18	A	1115	CLA	C4A-NA-C1A	2.56	107.86	106.71
18	1	1011	CLA	C2C-C1C-CHC	-2.56	119.55	125.67
18	F	1240	CLA	C2C-C1C-CHC	-2.56	119.55	125.67
18	1	1007	CLA	C3C-C4C-CHD	-2.56	119.62	125.22
18	B	1238	CLA	C3D-CAD-CBD	-2.56	104.24	107.61
19	B	5002	PQN	C11-C3-C4	-2.55	115.77	118.50
18	4	4009	CLA	C2A-C3A-C4A	-2.55	100.17	104.18
18	B	1237	CLA	C4A-NA-C1A	2.55	107.85	106.71
20	A	6011	BCR	C24-C23-C22	-2.55	122.38	126.23
18	A	1131	CLA	CAA-CBA-CGA	-2.55	108.11	113.59
20	L	6020	BCR	C11-C12-C13	-2.55	119.26	126.42
19	B	5002	PQN	C19-C18-C17	-2.55	102.07	111.29
18	B	9023	CLA	CHC-C1C-C2C	-2.55	119.68	126.72
18	F	1303	CLA	C2B-C3B-C4B	2.55	108.47	106.29
18	F	1306	CLA	C2C-C1C-CHC	-2.54	119.58	125.67
18	B	1207	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
18	2	2012	CLA	C3D-C2D-C1D	2.54	108.49	106.30
18	1	1001	CLA	C4A-NA-C1A	2.54	107.85	106.71
18	3	3015	CLA	C2A-C3A-C4A	-2.54	100.19	104.18
18	4	4004	CLA	CHB-C4A-NA	2.54	128.23	124.34
18	1	1001	CLA	C2B-C3B-C4B	2.54	108.46	106.29
18	3	3015	CLA	C2C-C1C-CHC	-2.54	119.59	125.67
18	4	4007	CLA	C2C-C1C-CHC	-2.54	119.59	125.67
20	L	6020	BCR	C39-C30-C25	2.54	114.42	110.30
20	A	6011	BCR	C29-C28-C27	2.54	117.05	111.38
18	1	1008	CLA	C2A-C3A-C4A	-2.54	100.20	104.18
18	B	1237	CLA	CHB-C4A-NA	2.53	128.02	124.51
18	F	1305	CLA	CHB-C4A-NA	2.53	128.22	124.34
18	2	2006	CLA	C3C-C4C-CHD	-2.53	119.67	125.22
18	B	1209	CLA	O2A-C1-C2	2.53	115.29	108.64
18	A	1143	CLA	CHB-C4A-NA	2.53	128.21	124.34
18	I	1204	CLA	CAA-C2A-C1A	-2.53	103.69	111.97
18	B	1241	CLA	C2B-C3B-C4B	2.53	108.45	106.29
18	4	4008	CLA	C2C-C1C-CHC	-2.53	119.61	125.67
18	B	1301	CLA	CHB-C4A-NA	2.52	128.21	124.34
18	2	2001	CLA	C2A-C3A-C4A	-2.52	100.22	104.18
18	B	1209	CLA	C4-C3-C5	2.52	119.52	115.27
18	B	1235	CLA	CMB-C2B-C3B	2.52	129.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	1130	CLA	C1-O2A-CGA	2.52	123.06	116.44
18	A	1132	CLA	C2C-C1C-CHC	-2.52	119.63	125.67
18	J	1308	CLA	C3C-C4C-CHD	-2.52	119.70	125.22
18	3	3013	CLA	C2A-C3A-C4A	-2.52	100.23	104.18
18	B	1213	CLA	CHB-C4A-NA	2.52	128.20	124.34
18	B	1241	CLA	C2A-C3A-C4A	-2.52	100.23	104.18
18	A	1102	CLA	CHB-C4A-NA	2.52	128.19	124.34
18	F	4015	CLA	CHB-C4A-NA	2.52	128.19	124.34
18	A	1136	CLA	CHB-C4A-NA	2.52	127.99	124.51
18	A	1104	CLA	C2C-C1C-CHC	-2.51	119.65	125.67
18	4	4007	CLA	CHB-C4A-NA	2.51	128.19	124.34
18	B	1238	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	L	1130	CLA	C4A-NA-C1A	2.51	107.83	106.71
18	2	2011	CLA	C2A-C3A-C4A	-2.51	100.24	104.18
18	3	2009	CLA	C2A-C3A-C4A	-2.51	100.24	104.18
18	3	3003	CLA	C2A-C3A-C4A	-2.51	100.25	104.18
18	B	1241	CLA	C1C-NC-C4C	-2.50	105.58	106.71
18	B	1234	CLA	O1D-CGD-CBD	-2.50	119.36	124.48
18	J	1307	CLA	C2A-C3A-C4A	-2.50	100.26	104.18
18	K	1150	CLA	C2C-C1C-CHC	-2.50	119.68	125.67
18	B	1241	CLA	C2C-C1C-CHC	-2.50	119.68	125.67
18	A	1137	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
18	B	1219	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
18	B	1229	CLA	C5-C3-C4	2.50	120.11	114.60
18	4	4010	CLA	CHB-C4A-NA	2.49	128.16	124.34
18	1	1010	CLA	CHB-C4A-NA	2.49	128.16	124.34
18	G	1233	CLA	CMD-C2D-C3D	-2.49	120.01	124.68
18	A	1111	CLA	C2C-C1C-CHC	-2.49	119.71	125.67
18	B	1236	CLA	CHB-C4A-NA	2.49	127.95	124.51
18	4	4006	CLA	C2C-C1C-CHC	-2.49	119.71	125.67
18	B	1237	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
18	B	1235	CLA	CMD-C2D-C3D	-2.49	120.02	124.68
18	H	1501	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
18	A	1136	CLA	CMC-C2C-C1C	2.49	128.83	125.04
18	B	1224	CLA	CMD-C2D-C3D	-2.49	120.03	124.68
18	2	2015	CLA	CHB-C4A-NA	2.49	128.15	124.34
18	B	1214	CLA	C4A-NA-C1A	2.48	107.82	106.71
18	A	1137	CLA	O2A-CGA-CBA	2.48	119.69	111.91
18	B	9022	CLA	O2A-C1-C2	2.48	115.14	108.64
18	A	1134	CLA	CHB-C4A-NA	2.48	128.13	124.34
18	B	1222	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
18	A	1108	CLA	CHC-C1C-C2C	-2.48	119.87	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	1001	CLA	C2C-C1C-CHC	-2.48	119.74	125.67
18	3	3001	CLA	C2C-C1C-CHC	-2.47	119.75	125.67
18	B	1242	CLA	CED-O2D-CGD	2.47	121.53	115.94
18	2	2011	CLA	C2B-C3B-C4B	2.47	108.40	106.29
18	B	1227	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
18	F	1303	CLA	C2C-C1C-CHC	-2.47	119.75	125.67
18	3	2009	CLA	CHB-C4A-NA	2.47	128.12	124.34
18	B	1213	CLA	C2C-C1C-CHC	-2.47	119.76	125.67
18	3	3007	CLA	C2A-C3A-C4A	-2.47	100.31	104.18
18	3	3005	CLA	CHB-C4A-NA	2.47	128.12	124.34
18	2	2002	CLA	CHB-C4A-NA	2.47	128.12	124.34
18	L	1504	CLA	C4-C3-C5	2.47	119.42	115.27
18	A	1132	CLA	C3D-C4D-ND	2.47	112.28	110.14
18	B	9022	CLA	CAA-C2A-C3A	-2.46	106.03	112.78
18	A	1136	CLA	CMB-C2B-C3B	2.46	129.28	124.68
18	B	1215	CLA	CHB-C4A-NA	2.46	127.91	124.51
18	B	1219	CLA	CHC-C1C-C2C	-2.46	119.93	126.72
18	B	1138	CLA	C1-C2-C3	2.46	130.29	126.04
20	F	6016	BCR	C29-C30-C25	-2.45	106.70	110.48
18	A	1146	CLA	C2A-C3A-C4A	-2.45	100.33	104.18
18	B	1234	CLA	CHC-C1C-C2C	-2.45	119.93	126.72
18	A	1115	CLA	C1-O2A-CGA	2.45	123.86	116.73
18	A	1147	CLA	C2D-C3D-C4D	-2.45	104.19	106.30
18	B	1225	CLA	CMB-C2B-C3B	2.45	129.26	124.68
18	B	1241	CLA	C4A-NA-C1A	2.45	107.81	106.71
18	A	1128	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
20	I	6018	BCR	C34-C9-C8	-2.45	114.22	118.08
18	A	1140	CLA	CMB-C2B-C1B	2.45	132.23	128.46
18	A	1151	CLA	CHB-C4A-NA	2.45	128.09	124.34
18	2	2005	CLA	CHB-C4A-NA	2.45	128.09	124.34
18	I	1204	CLA	CMD-C2D-C3D	-2.45	120.10	124.68
18	H	1505	CLA	CHB-C4A-NA	2.44	128.08	124.34
18	A	1136	CLA	C4-C3-C5	2.44	119.38	115.27
18	4	4006	CLA	CHB-C4A-NA	2.44	128.08	124.34
18	B	9012	CLA	CMD-C2D-C3D	-2.44	120.11	124.68
18	F	1302	CLA	C1-C2-C3	2.44	130.26	126.04
18	B	1216	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
18	A	1122	CLA	O2A-CGA-CBA	2.43	119.55	111.91
18	A	1132	CLA	C3A-C4A-NA	2.43	115.03	109.92
18	A	1108	CLA	CGD-CBD-CAD	-2.43	102.85	110.73
18	B	1217	CLA	CMB-C2B-C3B	2.43	129.23	124.68
18	B	1210	CLA	C2A-C3A-C4A	-2.43	100.37	104.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	1304	CLA	C4-C3-C5	2.43	119.36	115.27
18	B	1226	CLA	CHB-C4A-NA	2.43	128.06	124.34
18	A	1122	CLA	CMD-C2D-C3D	-2.42	120.14	124.68
18	2	2007	CLA	CHB-C4A-NA	2.42	128.05	124.34
18	B	1238	CLA	CAC-C3C-C4C	2.42	127.95	124.81
18	B	1215	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
18	4	1009	CLA	C3D-C4D-ND	2.42	112.24	110.14
18	3	3015	CLA	C1C-NC-C4C	-2.42	105.62	106.71
18	B	1228	CLA	CMD-C2D-C3D	-2.42	120.15	124.68
18	L	1503	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
18	B	1202	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
18	A	1144	CLA	CHB-C4A-NA	2.42	128.04	124.34
18	2	2007	CLA	C2A-C3A-C4A	-2.42	100.39	104.18
18	L	1130	CLA	CHB-C4A-NA	2.41	127.85	124.51
18	1	1011	CLA	CHB-C4A-NA	2.41	128.03	124.34
18	A	1127	CLA	C2D-C3D-C4D	-2.41	104.23	106.30
20	F	6016	BCR	C4-C5-C6	-2.41	119.24	122.73
18	F	1139	CLA	CAA-C2A-C1A	2.41	119.86	111.97
18	K	1141	CLA	CHB-C4A-NA	2.41	128.02	124.34
18	A	1147	CLA	CHB-C4A-NA	2.41	128.02	124.34
18	B	1208	CLA	C3A-C2A-C1A	2.40	104.94	101.34
18	1	1005	CLA	C2C-C1C-CHC	-2.40	119.91	125.67
18	1	1002	CLA	CHB-C4A-NA	2.40	128.02	124.34
18	L	1125	CLA	CHB-C4A-NA	2.40	128.02	124.34
18	B	1231	CLA	CHB-C4A-NA	2.40	127.84	124.51
18	1	1008	CLA	CHB-C4A-NA	2.40	128.02	124.34
18	A	1113	CLA	CBA-CAA-C2A	2.40	120.95	113.86
18	B	1231	CLA	CMA-C3A-C4A	-2.40	105.32	111.77
18	B	1301	CLA	C2C-C1C-CHC	-2.40	119.92	125.67
18	A	1147	CLA	C2A-C3A-C4A	-2.40	100.41	104.18
18	B	1235	CLA	CHD-C4C-NC	2.40	127.98	124.20
18	B	1205	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	4	4001	CLA	C2B-C3B-C4B	2.40	108.34	106.29
18	H	1505	CLA	C2A-C3A-C4A	-2.40	100.42	104.18
18	A	9011	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
18	2	2006	CLA	CHB-C4A-NA	2.39	128.00	124.34
18	A	1132	CLA	CHB-C4A-NA	2.39	128.00	124.34
18	A	1309	CLA	CHB-C4A-NA	2.39	128.00	124.34
18	B	1206	CLA	C3C-C4C-CHD	-2.39	119.98	125.22
18	2	2005	CLA	C2B-C3B-C4B	2.39	108.33	106.29
18	B	1138	CLA	CAA-C2A-C1A	-2.39	104.14	111.97
18	A	1146	CLA	C2C-C1C-CHC	-2.39	119.95	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1239	CLA	CHB-C4A-NA	2.39	127.81	124.51
18	K	1141	CLA	C2C-C1C-CHC	-2.39	119.95	125.67
18	A	1115	CLA	C3A-C2A-C1A	2.39	104.91	101.34
18	B	1207	CLA	CMA-C3A-C4A	-2.39	105.36	111.77
18	F	1139	CLA	CMA-C3A-C4A	2.39	118.19	111.77
18	B	1231	CLA	CAC-C3C-C4C	2.39	127.91	124.81
18	A	1117	CLA	C3D-C4D-ND	2.38	112.21	110.14
18	B	1242	CLA	CHC-C1C-C2C	-2.38	120.13	126.72
18	A	1128	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
18	2	2010	CLA	C2A-C3A-C4A	-2.38	100.44	104.18
18	A	1109	CLA	CHB-C4A-NA	2.38	127.99	124.34
18	L	1503	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
18	1	1006	CLA	CHB-C4A-NA	2.38	127.98	124.34
18	A	1143	CLA	C2C-C1C-CHC	-2.38	119.97	125.67
18	A	1128	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
18	L	1504	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
18	A	1127	CLA	CHB-C4A-NA	2.38	127.98	124.34
18	B	1232	CLA	C4-C3-C5	2.38	119.27	115.27
20	L	6020	BCR	C31-C1-C6	-2.38	106.44	110.30
18	3	3004	CLA	C2A-C3A-C4A	-2.38	100.45	104.18
18	L	1502	CLA	O2A-CGA-CBA	2.38	119.37	111.91
18	F	1305	CLA	C2B-C3B-C4B	2.38	108.32	106.29
18	A	1122	CLA	CBC-CAC-C3C	2.38	118.98	112.43
20	A	6011	BCR	C19-C18-C17	2.38	122.59	118.94
18	4	4011	CLA	C3A-C4A-NA	2.38	114.91	109.92
18	B	1213	CLA	C2A-C3A-C4A	-2.37	100.46	104.18
18	B	1224	CLA	O2A-CGA-CBA	2.37	119.35	111.91
18	A	1126	CLA	CMA-C3A-C4A	-2.37	105.40	111.77
18	B	1219	CLA	CHB-C4A-NA	2.37	127.79	124.51
18	B	1205	CLA	CED-O2D-CGD	2.37	121.30	115.94
18	4	4009	CLA	C2B-C3B-C4B	2.37	108.31	106.29
18	B	1209	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
18	B	1223	CLA	C3B-C2B-C1B	-2.37	104.26	106.29
18	B	1218	CLA	CGD-CBD-CAD	2.37	118.40	110.73
18	B	1222	CLA	C1-O2A-CGA	2.37	122.65	116.44
18	L	1502	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
18	4	4002	CLA	CHB-C4A-NA	2.36	127.96	124.34
18	A	1120	CLA	C2A-C3A-C4A	-2.36	100.47	104.18
18	A	1131	CLA	C1B-C2B-C3B	-2.36	104.72	106.92
18	A	9013	CLA	O2A-CGA-CBA	2.36	121.57	112.23
18	A	1117	CLA	CHB-C4A-NA	2.36	127.95	124.34
18	4	4013	CLA	CHB-C4A-NA	2.36	127.95	124.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	1248	CLA	CHB-C4A-NA	2.36	127.95	124.34
18	B	1215	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
18	3	3002	CLA	C2A-C3A-C4A	-2.35	100.48	104.18
18	A	1122	CLA	C6-C5-C3	2.35	119.63	113.45
18	B	9012	CLA	CHC-C1C-C2C	-2.35	120.21	126.72
18	4	4004	CLA	C2A-C3A-C4A	-2.35	100.49	104.18
18	A	1103	CLA	C3B-C4B-NB	2.35	112.25	109.21
18	B	1202	CLA	CED-O2D-CGD	2.35	121.25	115.94
20	B	6017	BCR	C34-C9-C8	2.35	121.78	118.08
18	A	1135	CLA	C4A-NA-C1A	2.35	107.76	106.71
18	B	1207	CLA	CAC-C3C-C2C	2.35	131.54	127.53
18	B	1207	CLA	C3A-C2A-C1A	2.35	104.86	101.34
18	B	1228	CLA	C3A-C2A-C1A	2.35	104.86	101.34
18	3	3011	CLA	C2A-C3A-C4A	-2.35	100.50	104.18
18	A	1103	CLA	CED-O2D-CGD	2.34	121.24	115.94
18	B	1214	CLA	CHB-C4A-NA	2.34	127.75	124.51
18	A	1122	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
19	A	5001	PQN	C14-C13-C15	2.34	119.21	115.27
18	A	1103	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
18	A	1140	CLA	CAC-C3C-C4C	2.34	127.85	124.81
18	A	1128	CLA	C4A-NA-C1A	2.34	107.76	106.71
18	B	9010	CLA	C2C-C1C-NC	2.34	112.16	109.97
19	A	5001	PQN	O4-C4-C3	2.34	124.32	120.56
18	A	1123	CLA	CHC-C1C-C2C	-2.34	120.26	126.72
18	1	1011	CLA	C3D-C4D-ND	2.34	112.17	110.14
18	B	1209	CLA	C1-C2-C3	2.34	130.09	126.04
18	2	2010	CLA	CHB-C4A-NA	2.34	127.92	124.34
18	4	4011	CLA	C2B-C3B-C4B	2.33	108.28	106.29
18	L	1502	CLA	CMB-C2B-C3B	2.33	129.04	124.68
18	B	1238	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	F	1139	CLA	CGD-CBD-CAD	-2.33	103.19	110.73
18	A	1140	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
18	J	2107	CLA	CHC-C1C-C2C	-2.33	120.29	126.72
18	A	1136	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
18	B	1208	CLA	CED-O2D-CGD	2.33	121.20	115.94
18	3	3010	CLA	CHB-C4A-NA	2.32	127.90	124.34
18	B	1216	CLA	CMD-C2D-C3D	-2.32	120.33	124.68
18	J	2107	CLA	CMB-C2B-C3B	2.32	129.02	124.68
18	A	1123	CLA	C4-C3-C5	2.32	119.17	115.27
18	F	1305	CLA	C2A-C3A-C4A	-2.32	100.54	104.18
18	1	1013	CLA	CHB-C4A-NA	2.32	127.89	124.34
18	A	1119	CLA	O1D-CGD-CBD	-2.32	119.74	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	1304	CLA	C4-C3-C2	-2.32	117.73	123.68
20	F	6016	BCR	C29-C28-C27	2.32	116.56	111.38
18	A	1117	CLA	C2B-C3B-C4B	2.32	108.27	106.29
18	A	1142	CLA	C2A-C3A-C4A	-2.32	100.54	104.18
18	A	1134	CLA	C1C-NC-C4C	-2.32	105.67	106.71
18	4	4005	CLA	CHB-C4A-NA	2.32	127.88	124.34
18	B	9012	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
18	F	1306	CLA	C2A-C3A-C4A	-2.31	100.55	104.18
18	A	1119	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
20	L	6020	BCR	C16-C15-C14	2.31	128.21	123.47
18	B	1202	CLA	C1-O2A-CGA	2.31	122.51	116.44
18	B	1207	CLA	CMB-C2B-C3B	2.31	129.00	124.68
18	A	1126	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
18	3	3009	CLA	CHB-C4A-NA	2.31	127.87	124.34
18	A	1146	CLA	CHB-C4A-NA	2.31	127.87	124.34
18	2	2008	CLA	CHB-C4A-NA	2.31	127.87	124.34
18	A	1136	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
18	B	1227	CLA	C5-C3-C4	2.30	119.69	114.60
18	B	1205	CLA	CMB-C2B-C3B	2.30	128.99	124.68
18	B	1205	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
18	A	1136	CLA	C4-C3-C2	-2.30	117.77	123.68
18	B	1212	CLA	CHC-C1C-C2C	-2.30	120.35	126.72
18	1	1006	CLA	C3A-C4A-NA	2.30	114.75	109.92
18	A	1131	CLA	CED-O2D-CGD	2.30	121.14	115.94
20	I	6018	BCR	C1-C6-C5	-2.30	119.38	122.61
18	A	1106	CLA	CGD-CBD-CAD	2.30	118.18	110.73
18	A	1119	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
18	B	1225	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
18	B	1234	CLA	C5-C3-C4	2.30	119.67	114.60
18	L	1130	CLA	CMA-C3A-C2A	-2.30	104.57	113.83
18	B	1217	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
18	J	1307	CLA	C2C-C1C-CHC	-2.29	120.18	125.67
18	A	1140	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
18	2	2004	CLA	CHB-C4A-NA	2.29	127.85	124.34
18	A	1103	CLA	CHD-C4C-C3C	-2.29	121.47	124.84
18	F	1302	CLA	CED-O2D-CGD	2.29	121.12	115.94
18	1	1011	CLA	C2A-C3A-C4A	-2.29	100.59	104.18
18	B	1215	CLA	C3B-C4B-NB	2.29	112.17	109.21
18	B	9010	CLA	O2A-CGA-CBA	2.29	119.09	111.91
18	B	1220	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
18	B	1205	CLA	C5-C3-C2	-2.29	116.49	121.12
18	B	1238	CLA	O2A-CGA-CBA	2.29	119.08	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1138	CLA	C3A-C2A-C1A	2.28	104.76	101.34
18	A	1129	CLA	CBA-CAA-C2A	2.28	120.60	113.86
18	4	4008	CLA	CHB-C4A-NA	2.28	127.83	124.34
18	B	1210	CLA	C2B-C3B-C4B	2.28	108.24	106.29
18	F	4015	CLA	C2A-C3A-C4A	-2.28	100.61	104.18
18	B	1242	CLA	CMD-C2D-C3D	-2.27	120.42	124.68
18	1	1006	CLA	C3D-C4D-ND	2.27	112.11	110.14
18	A	1140	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
18	B	1224	CLA	C1-C2-C3	-2.27	122.12	126.04
18	1	1012	CLA	C2B-C3B-C4B	2.27	108.23	106.29
20	F	6016	BCR	C1-C6-C5	-2.27	119.42	122.61
18	1	1010	CLA	C2B-C3B-C4B	2.27	108.23	106.29
18	3	3006	CLA	CHB-C4A-NA	2.27	127.81	124.34
18	A	1123	CLA	CHB-C4A-NA	2.26	127.64	124.51
18	B	1229	CLA	C4B-C3B-C2B	2.26	109.03	106.92
18	1	1007	CLA	CHB-C4A-NA	2.26	127.80	124.34
18	A	1309	CLA	C2A-C3A-C4A	-2.26	100.63	104.18
18	B	1224	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	B	1207	CLA	CAA-C2A-C1A	-2.26	104.57	111.97
18	G	1233	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
18	B	1138	CLA	CAC-C3C-C4C	2.26	127.74	124.81
18	B	1208	CLA	CHB-C4A-NA	2.26	127.63	124.51
18	B	1216	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
18	3	3012	CLA	C2A-C3A-C4A	-2.26	100.64	104.18
18	1	1007	CLA	C2A-C3A-C4A	-2.26	100.64	104.18
18	B	1239	CLA	CAC-C3C-C4C	2.26	127.74	124.81
18	B	9010	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
20	I	6018	BCR	C4-C5-C6	-2.25	119.46	122.73
18	3	3001	CLA	C2B-C3B-C4B	2.25	108.22	106.29
18	4	4010	CLA	C2A-C3A-C4A	-2.25	100.65	104.18
18	B	9010	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
18	B	1138	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
20	B	6017	BCR	C1-C6-C7	2.25	122.14	115.78
18	A	1129	CLA	C4-C3-C5	2.25	119.06	115.27
20	I	6018	BCR	C37-C22-C21	-2.25	119.77	122.92
18	B	1228	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
18	H	1501	CLA	CAA-C2A-C3A	2.25	118.93	112.78
18	B	1235	CLA	CBC-CAC-C3C	2.25	118.62	112.43
18	H	1501	CLA	CMB-C2B-C3B	2.24	128.87	124.68
18	B	1217	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
18	A	1123	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
18	B	1224	CLA	CED-O2D-CGD	2.24	121.01	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1119	CLA	C1-O2A-CGA	2.24	122.32	116.44
18	B	1218	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
18	3	3011	CLA	CHB-C4A-NA	2.24	127.76	124.34
20	B	6017	BCR	C12-C13-C14	-2.24	115.51	118.94
20	I	6018	BCR	C23-C22-C21	2.24	122.37	118.94
18	3	3002	CLA	CHB-C4A-NA	2.24	127.76	124.34
18	B	1215	CLA	CMC-C2C-C3C	2.23	132.18	126.12
18	B	1221	CLA	CAA-C2A-C3A	2.23	118.89	112.78
18	4	4012	CLA	C2C-C1C-CHC	-2.23	120.33	125.67
20	A	6011	BCR	C33-C5-C4	2.23	117.90	113.62
18	B	1217	CLA	CHB-C4A-NA	2.23	127.59	124.51
18	B	1214	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
20	B	6017	BCR	C33-C5-C4	2.23	117.89	113.62
18	B	1218	CLA	O2A-CGA-CBA	2.23	118.90	111.91
18	A	1136	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
20	B	6017	BCR	C31-C1-C6	-2.22	106.69	110.30
18	1	1003	CLA	C3A-C4A-NA	2.22	114.58	109.92
18	B	1210	CLA	CHB-C4A-NA	2.22	127.74	124.34
18	A	1147	CLA	C3D-C4D-ND	2.22	112.07	110.14
18	A	1123	CLA	C4A-NA-C1A	2.22	107.70	106.71
18	J	1308	CLA	C2B-C3B-C4B	2.22	108.19	106.29
18	B	1138	CLA	O2A-C1-C2	2.22	114.47	108.64
18	A	1126	CLA	C3A-C2A-C1A	2.22	104.66	101.34
18	K	1153	CLA	C3A-C4A-NA	2.22	114.57	109.92
18	B	1241	CLA	C3A-C4A-NA	2.22	114.57	109.92
18	A	1135	CLA	CHB-C4A-NA	2.22	127.58	124.51
18	B	1236	CLA	CMA-C3A-C2A	-2.21	104.89	113.83
18	4	4001	CLA	C2A-C3A-C4A	-2.21	100.71	104.18
18	B	1208	CLA	CBC-CAC-C3C	2.21	118.53	112.43
18	1	1010	CLA	C3D-C2D-C1D	2.21	108.21	106.30
18	1	1002	CLA	C2A-C3A-C4A	-2.21	100.71	104.18
18	A	1107	CLA	CHB-C4A-NA	2.21	127.57	124.51
18	F	1302	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
18	J	1308	CLA	C2A-C3A-C4A	-2.21	100.71	104.18
18	B	1221	CLA	C3B-C4B-NB	2.21	112.07	109.21
18	A	1103	CLA	C3C-C4C-NC	-2.21	108.10	110.57
18	B	9010	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
18	B	9022	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
18	B	1217	CLA	C5-C3-C4	2.20	119.47	114.60
18	1	1005	CLA	C2B-C3B-C4B	2.20	108.17	106.29
18	B	1202	CLA	O2A-CGA-CBA	2.20	118.82	111.91
18	A	1126	CLA	CHC-C1C-C2C	-2.20	120.64	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1120	CLA	C2B-C3B-C4B	2.20	108.17	106.29
18	L	1502	CLA	C4A-NA-C1A	2.20	107.69	106.71
18	4	4003	CLA	CHB-C4A-NA	2.20	127.70	124.34
18	A	1124	CLA	C3A-C2A-C1A	-2.20	100.73	104.18
18	J	1307	CLA	CHB-C4A-NA	2.20	127.70	124.34
18	B	9023	CLA	CMD-C2D-C3D	-2.20	120.57	124.68
18	B	1208	CLA	CHC-C1C-C2C	-2.20	120.65	126.72
18	A	1119	CLA	CHB-C4A-NA	2.19	127.55	124.51
18	J	1307	CLA	C3A-C4A-NA	2.19	114.52	109.92
18	A	9011	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
18	B	1232	CLA	CHB-C4A-NA	2.19	127.54	124.51
18	A	1110	CLA	CHB-C4A-NA	2.19	127.69	124.34
18	3	3005	CLA	C2A-C3A-C4A	-2.19	100.75	104.18
18	B	1205	CLA	C1-O2A-CGA	2.19	122.18	116.44
18	A	1113	CLA	O2A-C1-C2	2.19	114.38	108.64
18	K	1141	CLA	C2B-C3B-C4B	2.19	108.16	106.29
18	L	1502	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
20	L	6020	BCR	C35-C13-C12	-2.18	114.64	118.08
18	B	1214	CLA	O2A-C1-C2	2.18	114.07	108.97
18	B	1228	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
18	4	4011	CLA	C3D-C2D-C1D	2.18	108.18	106.30
18	4	4006	CLA	C2A-C3A-C4A	-2.18	100.76	104.18
18	2	2012	CLA	CHB-C4A-NA	2.18	127.68	124.34
18	B	1203	CLA	CAC-C3C-C2C	-2.18	122.23	126.75
18	3	3015	CLA	CHB-C4A-NA	2.18	127.67	124.34
18	B	1238	CLA	CMB-C2B-C1B	-2.18	125.12	128.46
18	A	9011	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
18	J	2107	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
18	B	1217	CLA	O2A-CGA-CBA	2.18	118.74	111.91
18	B	1217	CLA	C1-O2A-CGA	2.18	122.15	116.44
18	2	2002	CLA	C2A-C3A-C4A	-2.17	100.77	104.18
18	A	1131	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
20	B	6017	BCR	C35-C13-C12	2.17	121.50	118.08
20	L	6020	BCR	C29-C28-C27	2.17	116.22	111.38
18	J	2107	CLA	O2A-CGA-CBA	2.17	118.71	111.91
18	A	1116	CLA	C2B-C3B-C4B	2.17	108.14	106.29
18	B	1208	CLA	C4A-NA-C1A	2.17	107.68	106.71
20	I	6018	BCR	C21-C20-C19	2.17	129.97	123.22
18	A	1105	CLA	C3A-C4A-NA	2.16	114.46	109.92
18	B	1138	CLA	CBA-CAA-C2A	2.16	120.25	113.86
18	3	3007	CLA	C2B-C3B-C4B	2.16	108.14	106.29
18	A	1133	CLA	CHB-C4A-NA	2.16	127.64	124.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3013	CLA	CHB-C4A-NA	2.16	127.64	124.34
18	A	1152	CLA	CHB-C4A-NA	2.16	127.64	124.34
18	A	1134	CLA	C3A-C4A-NA	2.16	114.44	109.92
18	1	1006	CLA	C2B-C3B-C4B	2.15	108.13	106.29
18	F	1306	CLA	CHB-C4A-NA	2.15	127.64	124.34
18	3	3003	CLA	C3A-C4A-NA	2.15	114.44	109.92
18	4	4003	CLA	C1C-NC-C4C	-2.15	105.74	106.71
18	A	1152	CLA	C3A-C4A-NA	2.15	114.43	109.92
18	B	1224	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
20	L	6020	BCR	C1-C6-C7	2.15	121.85	115.78
18	G	1233	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
18	1	1013	CLA	C3A-C4A-NA	2.15	114.43	109.92
18	B	9012	CLA	C6-C5-C3	-2.15	107.82	113.45
18	H	1501	CLA	C4-C3-C5	2.15	118.88	115.27
18	A	1103	CLA	O2A-CGA-CBA	2.14	118.64	111.91
18	A	1131	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
18	B	1238	CLA	CMC-C2C-C1C	2.14	128.30	125.04
18	A	1109	CLA	C2C-C1C-CHC	-2.14	120.54	125.67
18	4	1304	CLA	C1-O2A-CGA	2.14	122.06	116.44
18	4	4004	CLA	C3D-C2D-C1D	2.14	108.15	106.30
18	B	1234	CLA	C4A-NA-C1A	2.14	107.67	106.71
18	B	1218	CLA	C1-O2A-CGA	2.14	122.06	116.44
18	4	4011	CLA	C2D-C3D-C4D	-2.14	104.46	106.30
18	A	1128	CLA	C5-C3-C2	-2.14	116.79	121.12
18	3	3015	CLA	C2B-C3B-C4B	2.14	108.12	106.29
18	3	3012	CLA	CHB-C4A-NA	2.14	127.61	124.34
18	B	1224	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
20	I	6018	BCR	C15-C14-C13	2.13	130.36	127.31
18	2	2013	CLA	CHB-C4A-NA	2.13	127.61	124.34
18	B	1224	CLA	CMC-C2C-C1C	2.13	128.29	125.04
20	F	6016	BCR	C30-C25-C24	2.13	121.81	115.78
18	B	1211	CLA	CHB-C4A-NA	2.13	127.60	124.34
18	B	9023	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
18	B	1227	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
18	B	1202	CLA	CMB-C2B-C1B	2.13	131.73	128.46
18	4	4001	CLA	CHB-C4A-NA	2.13	127.59	124.34
18	2	2011	CLA	CHB-C4A-NA	2.12	127.59	124.34
18	B	1205	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
18	2	2015	CLA	C2B-C3B-C4B	2.12	108.11	106.29
18	1	1011	CLA	C2B-C3B-C4B	2.12	108.11	106.29
18	1	1001	CLA	CHB-C4A-NA	2.12	127.59	124.34
18	B	1236	CLA	CHC-C1C-C2C	-2.12	120.85	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	3004	CLA	C2B-C3B-C4B	2.12	108.10	106.29
18	B	1226	CLA	C1C-NC-C4C	-2.12	105.75	106.71
18	2	2012	CLA	C3A-C4A-NA	2.12	114.37	109.92
18	B	1217	CLA	O2A-C1-C2	2.12	114.21	108.64
18	1	1004	CLA	CHB-C4A-NA	2.12	127.58	124.34
18	A	1129	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
18	A	1103	CLA	CMB-C2B-C3B	2.11	128.63	124.68
18	B	1229	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
18	F	1302	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
20	F	6016	BCR	C36-C18-C17	2.11	125.88	122.92
18	A	1129	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
18	B	1237	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
18	B	1209	CLA	C1-O2A-CGA	2.11	121.97	116.44
18	B	1222	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
18	1	1004	CLA	C2A-C3A-C4A	-2.11	100.88	104.18
18	B	1207	CLA	CBC-CAC-C3C	2.10	118.23	112.43
18	L	1502	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
18	B	1236	CLA	CED-O2D-CGD	2.10	120.69	115.94
18	B	1232	CLA	C1-O2A-CGA	2.10	121.95	116.44
18	B	1138	CLA	C4A-NA-C1A	2.10	107.65	106.71
18	3	3013	CLA	C3A-C4A-NA	2.10	114.32	109.92
18	1	1010	CLA	C3A-C4A-NA	2.10	114.32	109.92
18	A	1131	CLA	O2D-CGD-CBD	2.09	114.99	111.27
18	A	1113	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
18	A	1108	CLA	CED-O2D-CGD	2.09	120.67	115.94
18	B	1206	CLA	C2D-C1D-ND	-2.09	108.32	110.14
18	A	1131	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
18	B	1223	CLA	C3A-C4A-NA	2.09	114.30	109.92
20	I	6018	BCR	C36-C18-C19	2.09	121.37	118.08
20	A	6011	BCR	C29-C30-C25	2.09	113.69	110.48
18	B	1231	CLA	C1-O2A-CGA	2.09	122.98	116.11
18	G	1233	CLA	O2A-C1-C2	2.08	114.11	108.64
18	A	1137	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
18	I	1204	CLA	C3A-C2A-C1A	2.08	104.46	101.34
18	B	1229	CLA	O2A-CGA-CBA	2.08	118.44	111.91
18	L	1502	CLA	C3A-C2A-C1A	2.08	104.45	101.34
18	1	1003	CLA	CHB-C4A-NA	2.08	127.52	124.34
18	B	1215	CLA	CMA-C3A-C4A	2.08	117.36	111.77
18	A	1111	CLA	C2A-C3A-C4A	-2.08	100.92	104.18
18	3	3001	CLA	C2A-C3A-C4A	-2.08	100.92	104.18
18	B	9012	CLA	CAA-CBA-CGA	2.08	119.32	113.25
18	B	1230	CLA	CHB-C4A-NA	2.08	127.52	124.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1301	CLA	C2B-C3B-C4B	2.07	108.06	106.29
18	A	1142	CLA	CHB-C4A-NA	2.07	127.51	124.34
20	F	6016	BCR	C37-C22-C23	2.07	121.34	118.08
20	B	6017	BCR	C20-C19-C18	2.07	132.24	126.42
18	B	1227	CLA	O2A-CGA-CBA	2.07	118.41	111.91
18	3	3002	CLA	C2B-C3B-C4B	2.07	108.06	106.29
18	H	1501	CLA	CAA-CBA-CGA	-2.07	107.20	113.25
18	4	4003	CLA	C2A-C3A-C4A	-2.07	100.93	104.18
18	B	1208	CLA	C3B-C4B-NB	-2.07	106.53	109.21
18	A	1137	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
18	B	1138	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
18	4	4008	CLA	C2A-C3A-C4A	-2.06	100.94	104.18
18	B	1219	CLA	C4-C3-C2	-2.06	118.38	123.68
20	L	6020	BCR	C36-C18-C19	2.06	121.32	118.08
18	L	1130	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
18	B	9010	CLA	CMD-C2D-C3D	-2.06	120.83	124.68
18	B	1220	CLA	CHB-C4A-NA	2.06	127.36	124.51
18	A	1128	CLA	CMA-C3A-C2A	-2.06	105.52	113.83
18	B	1208	CLA	CAA-C2A-C1A	-2.06	105.23	111.97
18	B	1207	CLA	O1D-CGD-CBD	2.06	128.70	124.48
18	B	1213	CLA	C1C-NC-C4C	-2.06	105.78	106.71
18	A	1116	CLA	C3A-C4A-NA	2.05	114.23	109.92
18	I	1204	CLA	CHB-C4A-NA	2.05	127.35	124.51
18	J	2107	CLA	CBC-CAC-C3C	2.05	118.09	112.43
18	1	1001	CLA	C1C-NC-C4C	-2.05	105.78	106.71
18	A	1123	CLA	C1-O2A-CGA	2.05	121.82	116.44
20	I	6018	BCR	C34-C9-C10	-2.05	120.05	122.92
18	B	1230	CLA	C1C-NC-C4C	-2.05	105.78	106.71
18	B	1234	CLA	CGD-CBD-CAD	-2.05	104.10	110.73
18	3	3003	CLA	C1C-NC-C4C	-2.05	105.79	106.71
18	B	1214	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
18	1	1005	CLA	C2A-C3A-C4A	-2.04	100.97	104.18
18	B	9010	CLA	CGD-CBD-CAD	-2.04	104.11	110.73
18	4	4010	CLA	C2B-C3B-C4B	2.04	108.04	106.29
18	A	1119	CLA	CMA-C3A-C2A	-2.04	105.59	113.83
18	3	3015	CLA	C3A-C4A-NA	2.04	114.20	109.92
18	3	3013	CLA	C2B-C3B-C4B	2.04	108.03	106.29
18	B	1238	CLA	C3A-C2A-C1A	2.04	104.39	101.34
18	B	1209	CLA	C7-C6-C5	-2.04	107.82	113.36
18	1	1005	CLA	C1C-NC-C4C	-2.04	105.79	106.71
18	A	1152	CLA	C2B-C3B-C4B	2.04	108.03	106.29
18	B	1229	CLA	C1B-CHB-C4A	-2.04	126.08	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1146	CLA	C3A-C4A-NA	2.04	114.19	109.92
18	A	1105	CLA	CHB-C4A-NA	2.04	127.45	124.34
18	B	1242	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
18	B	9023	CLA	C1-O2A-CGA	2.03	122.63	116.73
18	B	1219	CLA	CMB-C2B-C3B	2.03	128.48	124.68
18	3	3011	CLA	C1C-NC-C4C	-2.03	105.79	106.71
18	A	1120	CLA	C3A-C4A-NA	2.03	114.18	109.92
18	4	4011	CLA	CHB-C4A-NA	2.03	127.44	124.34
18	2	2004	CLA	C2A-C3A-C4A	-2.03	101.00	104.18
18	L	1502	CLA	CAA-C2A-C1A	-2.03	105.33	111.97
18	B	1212	CLA	CMB-C2B-C3B	2.03	128.47	124.68
18	A	1140	CLA	O1A-CGA-CBA	-2.02	115.83	123.73
18	B	1210	CLA	C3D-C2D-C1D	2.02	108.05	106.30
18	A	1118	CLA	C2A-C3A-C4A	-2.02	101.00	104.18
18	2	2008	CLA	C2A-C3A-C4A	-2.02	101.00	104.18
18	B	1221	CLA	CMC-C2C-C3C	2.02	131.61	126.12
18	A	1144	CLA	C2A-C3A-C4A	-2.02	101.00	104.18
18	2	2015	CLA	C3A-C4A-NA	2.02	114.17	109.92
18	3	3011	CLA	C2B-C3B-C4B	2.02	108.02	106.29
18	4	4007	CLA	C3A-C4A-NA	2.02	114.17	109.92
18	B	1210	CLA	C3A-C4A-NA	2.02	114.17	109.92
18	A	1133	CLA	C2C-C1C-CHC	-2.02	120.83	125.67
18	B	1238	CLA	C5-C3-C2	-2.02	117.03	121.12
18	4	4006	CLA	C2B-C3B-C4B	2.02	108.02	106.29
18	2	2001	CLA	C3A-C4A-NA	2.02	114.16	109.92
18	B	1236	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
18	K	1141	CLA	C2A-C3A-C4A	-2.02	101.01	104.18
18	A	9011	CLA	CAC-C3C-C4C	2.02	127.43	124.81
18	B	1225	CLA	CED-O2D-CGD	2.02	120.50	115.94
18	2	2005	CLA	C3A-C4A-NA	2.01	114.14	109.92
18	A	1124	CLA	C2B-C3B-C4B	2.01	108.01	106.29
18	B	1235	CLA	C6-C7-C8	-2.01	106.50	115.98
18	B	1209	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
18	B	1227	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
18	B	1202	CLA	C3C-C4C-NC	-2.01	108.32	110.57
18	B	1229	CLA	CMD-C2D-C3D	-2.01	120.92	124.68
18	H	1501	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
18	3	3003	CLA	CHB-C4A-NA	2.01	127.41	124.34
18	1	1008	CLA	C3A-C4A-NA	2.01	114.13	109.92
18	A	1148	CLA	C3A-C4A-NA	2.00	114.13	109.92
18	F	1139	CLA	CHB-C4A-NA	2.00	127.28	124.51
18	A	1106	CLA	CED-O2D-CGD	2.00	120.47	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	1143	CLA	C2A-C3A-C4A	-2.00	101.03	104.18
18	B	1216	CLA	C4-C3-C2	-2.00	118.54	123.68
18	J	2107	CLA	CED-O2D-CGD	2.00	120.47	115.94
18	L	1502	CLA	CHB-C4A-NA	2.00	127.28	124.51

All (537) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	H	1501	CLA	C8
18	H	1501	CLA	NC
18	H	1501	CLA	ND
18	H	1501	CLA	NA
18	4	1009	CLA	NC
18	4	1009	CLA	ND
18	4	1009	CLA	NA
18	1	1002	CLA	NC
18	1	1002	CLA	ND
18	1	1002	CLA	NA
18	J	1308	CLA	NC
18	J	1308	CLA	ND
18	J	1308	CLA	NA
18	3	3006	CLA	NC
18	3	3006	CLA	ND
18	3	3006	CLA	NA
18	A	1133	CLA	NC
18	A	1133	CLA	ND
18	A	1133	CLA	NA
18	A	1140	CLA	C8
18	A	1140	CLA	NC
18	A	1140	CLA	ND
18	A	1140	CLA	NA
18	A	1122	CLA	C8
18	A	1122	CLA	NC
18	A	1122	CLA	ND
18	A	1122	CLA	NA
18	A	1152	CLA	NC
18	A	1152	CLA	ND
18	A	1152	CLA	NA
18	1	1001	CLA	NC
18	1	1001	CLA	ND
18	1	1001	CLA	NA
18	3	3012	CLA	NC

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Mol	Chain	Res	Type	Atom
18	3	3012	CLA	ND
18	3	3012	CLA	NA
18	B	1237	CLA	NC
18	B	1237	CLA	ND
18	B	1237	CLA	NA
18	4	4005	CLA	NC
18	4	4005	CLA	ND
18	4	4005	CLA	NA
18	3	3002	CLA	NC
18	3	3002	CLA	ND
18	3	3002	CLA	NA
18	B	1211	CLA	NC
18	B	1211	CLA	ND
18	B	1211	CLA	NA
18	A	1106	CLA	NC
18	A	1106	CLA	ND
18	A	1106	CLA	NA
18	B	1216	CLA	C8
18	B	1216	CLA	NC
18	B	1216	CLA	ND
18	B	1216	CLA	NA
18	3	3015	CLA	NC
18	3	3015	CLA	ND
18	3	3015	CLA	NA
18	1	1003	CLA	NC
18	1	1003	CLA	ND
18	1	1003	CLA	NA
18	1	1006	CLA	NC
18	1	1006	CLA	ND
18	1	1006	CLA	NA
18	A	1309	CLA	NC
18	A	1309	CLA	ND
18	A	1309	CLA	NA
18	B	9010	CLA	NC
18	B	9010	CLA	ND
18	B	9010	CLA	NA
18	A	1107	CLA	C8
18	A	1107	CLA	NC
18	A	1107	CLA	ND
18	A	1107	CLA	NA
18	A	1108	CLA	NC
18	A	1108	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	1108	CLA	NA
18	B	1238	CLA	NC
18	B	1238	CLA	ND
18	B	1238	CLA	NA
18	B	1215	CLA	NC
18	B	1215	CLA	ND
18	B	1215	CLA	NA
18	4	4010	CLA	NC
18	4	4010	CLA	ND
18	4	4010	CLA	NA
18	3	3013	CLA	NC
18	3	3013	CLA	ND
18	3	3013	CLA	NA
18	1	1005	CLA	NC
18	1	1005	CLA	ND
18	1	1005	CLA	NA
18	A	1127	CLA	NC
18	A	1127	CLA	ND
18	A	1127	CLA	NA
18	3	3010	CLA	NC
18	3	3010	CLA	ND
18	3	3010	CLA	NA
18	2	2004	CLA	NC
18	2	2004	CLA	ND
18	2	2004	CLA	NA
18	3	3001	CLA	NC
18	3	3001	CLA	ND
18	3	3001	CLA	NA
18	B	1202	CLA	NC
18	B	1202	CLA	ND
18	B	1202	CLA	NA
18	B	1224	CLA	NC
18	B	1224	CLA	ND
18	B	1224	CLA	NA
18	1	1010	CLA	NC
18	1	1010	CLA	ND
18	1	1010	CLA	NA
18	K	1141	CLA	NC
18	K	1141	CLA	ND
18	K	1141	CLA	NA
18	B	1212	CLA	C8
18	B	1212	CLA	NC

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Mol	Chain	Res	Type	Atom
18	B	1212	CLA	ND
18	B	1212	CLA	NA
18	A	1111	CLA	NC
18	A	1111	CLA	ND
18	A	1111	CLA	NA
18	B	1213	CLA	NC
18	B	1213	CLA	ND
18	B	1213	CLA	NA
18	2	2006	CLA	NC
18	2	2006	CLA	ND
18	2	2006	CLA	NA
18	4	4008	CLA	NC
18	4	4008	CLA	ND
18	4	4008	CLA	NA
18	B	1208	CLA	C8
18	B	1208	CLA	NC
18	B	1208	CLA	ND
18	B	1208	CLA	NA
18	A	1104	CLA	NC
18	A	1104	CLA	ND
18	A	1104	CLA	NA
18	A	1142	CLA	NC
18	A	1142	CLA	ND
18	A	1142	CLA	NA
18	F	1139	CLA	NC
18	F	1139	CLA	ND
18	F	1139	CLA	NA
19	B	5002	PQN	C23
18	3	3008	CLA	NC
18	3	3008	CLA	ND
18	3	3008	CLA	NA
18	A	1110	CLA	NC
18	A	1110	CLA	ND
18	A	1110	CLA	NA
18	4	4006	CLA	NC
18	4	4006	CLA	ND
18	4	4006	CLA	NA
18	L	1502	CLA	NC
18	L	1502	CLA	ND
18	L	1502	CLA	NA
18	B	1220	CLA	C8
18	B	1220	CLA	NC

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Mol	Chain	Res	Type	Atom
18	B	1220	CLA	ND
18	B	1220	CLA	NA
18	A	1134	CLA	NC
18	A	1134	CLA	ND
18	A	1134	CLA	NA
18	L	1125	CLA	NC
18	L	1125	CLA	ND
18	L	1125	CLA	NA
18	B	1206	CLA	NC
18	B	1206	CLA	ND
18	B	1206	CLA	NA
18	B	1232	CLA	C8
18	B	1232	CLA	NC
18	B	1232	CLA	ND
18	B	1232	CLA	NA
18	4	4012	CLA	NC
18	4	4012	CLA	ND
18	4	4012	CLA	NA
18	B	9023	CLA	NC
18	B	9023	CLA	ND
18	B	9023	CLA	NA
18	L	1130	CLA	NC
18	L	1130	CLA	ND
18	L	1130	CLA	NA
18	2	2002	CLA	NC
18	2	2002	CLA	ND
18	2	2002	CLA	NA
18	B	9012	CLA	C8
18	B	9012	CLA	NC
18	B	9012	CLA	ND
18	B	9012	CLA	NA
18	2	2003	CLA	NC
18	2	2003	CLA	ND
18	2	2003	CLA	NA
18	B	1218	CLA	NC
18	B	1218	CLA	ND
18	B	1218	CLA	NA
18	F	1306	CLA	NC
18	F	1306	CLA	ND
18	F	1306	CLA	NA
18	A	1109	CLA	NC
18	A	1109	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	1109	CLA	NA
18	2	2015	CLA	NC
18	2	2015	CLA	ND
18	2	2015	CLA	NA
18	A	1120	CLA	NC
18	A	1120	CLA	ND
18	A	1120	CLA	NA
18	4	4011	CLA	NC
18	4	4011	CLA	ND
18	4	4011	CLA	NA
18	3	2009	CLA	NC
18	3	2009	CLA	ND
18	3	2009	CLA	NA
18	2	2010	CLA	NC
18	2	2010	CLA	ND
18	2	2010	CLA	NA
18	4	1304	CLA	C8
18	4	1304	CLA	NC
18	4	1304	CLA	ND
18	4	1304	CLA	NA
18	L	1503	CLA	NC
18	L	1503	CLA	ND
18	L	1503	CLA	NA
18	1	1012	CLA	NC
18	1	1012	CLA	ND
18	1	1012	CLA	NA
18	4	4013	CLA	NC
18	4	4013	CLA	ND
18	4	4013	CLA	NA
18	A	1117	CLA	NC
18	A	1117	CLA	ND
18	A	1117	CLA	NA
18	B	1219	CLA	NC
18	B	1219	CLA	ND
18	B	1219	CLA	NA
18	F	1303	CLA	NC
18	F	1303	CLA	ND
18	F	1303	CLA	NA
18	H	1505	CLA	NC
18	H	1505	CLA	ND
18	H	1505	CLA	NA
18	A	1118	CLA	NC

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Mol	Chain	Res	Type	Atom
18	A	1118	CLA	ND
18	A	1118	CLA	NA
18	A	1144	CLA	NC
18	A	1144	CLA	ND
18	A	1144	CLA	NA
18	B	9022	CLA	NC
18	B	9022	CLA	ND
18	B	9022	CLA	NA
18	F	4015	CLA	NC
18	F	4015	CLA	ND
18	F	4015	CLA	NA
18	B	1301	CLA	NC
18	B	1301	CLA	ND
18	B	1301	CLA	NA
18	A	1147	CLA	NC
18	A	1147	CLA	ND
18	A	1147	CLA	NA
18	4	4001	CLA	NC
18	4	4001	CLA	ND
18	4	4001	CLA	NA
18	F	1302	CLA	C8
18	F	1302	CLA	NC
18	F	1302	CLA	ND
18	F	1302	CLA	NA
18	A	1128	CLA	C8
18	A	1128	CLA	NC
18	A	1128	CLA	ND
18	A	1128	CLA	NA
18	A	1136	CLA	C8
18	A	1136	CLA	NC
18	A	1136	CLA	ND
18	A	1136	CLA	NA
18	3	3009	CLA	NC
18	3	3009	CLA	ND
18	3	3009	CLA	NA
18	B	1205	CLA	C8
18	B	1205	CLA	NC
18	B	1205	CLA	ND
18	B	1205	CLA	NA
18	1	1007	CLA	NC
18	1	1007	CLA	ND
18	1	1007	CLA	NA

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Mol	Chain	Res	Type	Atom
18	4	4002	CLA	NC
18	4	4002	CLA	ND
18	4	4002	CLA	NA
18	A	1123	CLA	C8
18	A	1123	CLA	NC
18	A	1123	CLA	ND
18	A	1123	CLA	NA
19	A	5001	PQN	C23
18	I	1204	CLA	C8
18	I	1204	CLA	NC
18	I	1204	CLA	ND
18	I	1204	CLA	NA
18	A	1135	CLA	NC
18	A	1135	CLA	ND
18	A	1135	CLA	NA
18	B	1229	CLA	NC
18	B	1229	CLA	ND
18	B	1229	CLA	NA
18	B	1225	CLA	NC
18	B	1225	CLA	ND
18	B	1225	CLA	NA
18	B	1241	CLA	NC
18	B	1241	CLA	ND
18	B	1241	CLA	NA
18	B	1214	CLA	NC
18	B	1214	CLA	ND
18	B	1214	CLA	NA
18	2	2012	CLA	NC
18	2	2012	CLA	ND
18	2	2012	CLA	NA
18	4	4007	CLA	NC
18	4	4007	CLA	ND
18	4	4007	CLA	NA
18	1	1008	CLA	NC
18	1	1008	CLA	ND
18	1	1008	CLA	NA
18	A	1151	CLA	NC
18	A	1151	CLA	ND
18	A	1151	CLA	NA
18	F	1305	CLA	NC
18	F	1305	CLA	ND
18	F	1305	CLA	NA

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Mol	Chain	Res	Type	Atom
18	A	1102	CLA	NC
18	A	1102	CLA	ND
18	A	1102	CLA	NA
18	B	1231	CLA	NC
18	B	1231	CLA	ND
18	B	1231	CLA	NA
18	3	3005	CLA	NC
18	3	3005	CLA	ND
18	3	3005	CLA	NA
18	A	1132	CLA	NC
18	A	1132	CLA	ND
18	A	1132	CLA	NA
18	F	1240	CLA	NC
18	F	1240	CLA	ND
18	F	1240	CLA	NA
18	A	9011	CLA	C8
18	A	9011	CLA	NC
18	A	9011	CLA	ND
18	A	9011	CLA	NA
18	2	2011	CLA	NC
18	2	2011	CLA	ND
18	2	2011	CLA	NA
18	1	1004	CLA	NC
18	1	1004	CLA	ND
18	1	1004	CLA	NA
18	A	1131	CLA	NC
18	A	1131	CLA	ND
18	A	1131	CLA	NA
18	1	1013	CLA	NC
18	1	1013	CLA	ND
18	1	1013	CLA	NA
18	A	1143	CLA	NC
18	A	1143	CLA	ND
18	A	1143	CLA	NA
18	B	1242	CLA	NC
18	B	1242	CLA	ND
18	B	1242	CLA	NA
18	2	2013	CLA	NC
18	2	2013	CLA	ND
18	2	2013	CLA	NA
18	B	1236	CLA	NC
18	B	1236	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	1236	CLA	NA
18	B	1221	CLA	NC
18	B	1221	CLA	ND
18	B	1221	CLA	NA
18	G	1233	CLA	NC
18	G	1233	CLA	ND
18	G	1233	CLA	NA
18	K	1153	CLA	NC
18	K	1153	CLA	ND
18	K	1153	CLA	NA
18	2	2001	CLA	NC
18	2	2001	CLA	ND
18	2	2001	CLA	NA
18	A	1124	CLA	NC
18	A	1124	CLA	ND
18	A	1124	CLA	NA
18	J	1307	CLA	NC
18	J	1307	CLA	ND
18	J	1307	CLA	NA
18	B	1223	CLA	NC
18	B	1223	CLA	ND
18	B	1223	CLA	NA
18	A	1115	CLA	NC
18	A	1115	CLA	ND
18	A	1115	CLA	NA
18	B	1207	CLA	C8
18	B	1207	CLA	NC
18	B	1207	CLA	ND
18	B	1207	CLA	NA
18	4	4009	CLA	NC
18	4	4009	CLA	ND
18	4	4009	CLA	NA
18	L	1504	CLA	C8
18	L	1504	CLA	NC
18	L	1504	CLA	ND
18	L	1504	CLA	NA
18	A	9013	CLA	NC
18	A	9013	CLA	ND
18	A	9013	CLA	NA
18	2	2007	CLA	NC
18	2	2007	CLA	ND
18	2	2007	CLA	NA

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Mol	Chain	Res	Type	Atom
18	B	1201	CLA	NC
18	B	1201	CLA	ND
18	B	1201	CLA	NA
18	2	2005	CLA	NC
18	2	2005	CLA	ND
18	2	2005	CLA	NA
18	4	4003	CLA	NC
18	4	4003	CLA	ND
18	4	4003	CLA	NA
18	A	1148	CLA	NC
18	A	1148	CLA	ND
18	A	1148	CLA	NA
18	J	2107	CLA	C8
18	J	2107	CLA	NC
18	J	2107	CLA	ND
18	J	2107	CLA	NA
18	3	3004	CLA	NC
18	3	3004	CLA	ND
18	3	3004	CLA	NA
18	B	1203	CLA	NC
18	B	1203	CLA	ND
18	B	1203	CLA	NA
18	A	1101	CLA	NC
18	A	1101	CLA	ND
18	A	1101	CLA	NA
18	3	3011	CLA	NC
18	3	3011	CLA	ND
18	3	3011	CLA	NA
18	B	1138	CLA	C8
18	B	1138	CLA	NC
18	B	1138	CLA	ND
18	B	1138	CLA	NA
18	A	1137	CLA	C8
18	A	1137	CLA	NC
18	A	1137	CLA	ND
18	A	1137	CLA	NA
18	B	1227	CLA	NC
18	B	1227	CLA	ND
18	B	1227	CLA	NA
18	B	1226	CLA	NC
18	B	1226	CLA	ND
18	B	1226	CLA	NA

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Mol	Chain	Res	Type	Atom
18	B	1230	CLA	NC
18	B	1230	CLA	ND
18	B	1230	CLA	NA
18	B	1217	CLA	NC
18	B	1217	CLA	ND
18	B	1217	CLA	NA
18	A	1119	CLA	C8
18	A	1119	CLA	NC
18	A	1119	CLA	ND
18	A	1119	CLA	NA
18	A	1113	CLA	NC
18	A	1113	CLA	ND
18	A	1113	CLA	NA
18	1	1011	CLA	NC
18	1	1011	CLA	ND
18	1	1011	CLA	NA
18	A	1146	CLA	NC
18	A	1146	CLA	ND
18	A	1146	CLA	NA
18	1	1014	CLA	NC
18	1	1014	CLA	ND
18	1	1014	CLA	NA
18	B	1239	CLA	C8
18	B	1239	CLA	NC
18	B	1239	CLA	ND
18	B	1239	CLA	NA
18	K	1150	CLA	NC
18	K	1150	CLA	ND
18	K	1150	CLA	NA
18	A	1129	CLA	C8
18	A	1129	CLA	NC
18	A	1129	CLA	ND
18	A	1129	CLA	NA
18	A	1126	CLA	C8
18	A	1126	CLA	NC
18	A	1126	CLA	ND
18	A	1126	CLA	NA
18	A	1105	CLA	NC
18	A	1105	CLA	ND
18	A	1105	CLA	NA
18	A	1116	CLA	NC
18	A	1116	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	1116	CLA	NA
18	B	1210	CLA	NC
18	B	1210	CLA	ND
18	B	1210	CLA	NA
18	G	1248	CLA	NC
18	G	1248	CLA	ND
18	G	1248	CLA	NA
18	B	1228	CLA	C8
18	B	1228	CLA	NC
18	B	1228	CLA	ND
18	B	1228	CLA	NA
18	3	3003	CLA	NC
18	3	3003	CLA	ND
18	3	3003	CLA	NA
18	A	1103	CLA	NC
18	A	1103	CLA	ND
18	A	1103	CLA	NA
18	4	4004	CLA	NC
18	4	4004	CLA	ND
18	4	4004	CLA	NA
18	B	1234	CLA	NC
18	B	1234	CLA	ND
18	B	1234	CLA	NA
18	3	3007	CLA	NC
18	3	3007	CLA	ND
18	3	3007	CLA	NA
18	B	1235	CLA	C8
18	B	1235	CLA	NC
18	B	1235	CLA	ND
18	B	1235	CLA	NA
18	B	1209	CLA	C8
18	B	1209	CLA	NC
18	B	1209	CLA	ND
18	B	1209	CLA	NA
18	2	2008	CLA	NC
18	2	2008	CLA	ND
18	2	2008	CLA	NA
18	B	1222	CLA	C8
18	B	1222	CLA	NC
18	B	1222	CLA	ND
18	B	1222	CLA	NA

All (736) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	H	1501	CLA	C3A-C2A-CAA-CBA
18	A	1140	CLA	C1A-C2A-CAA-CBA
18	A	1140	CLA	C3A-C2A-CAA-CBA
18	A	1122	CLA	C1A-C2A-CAA-CBA
18	A	1122	CLA	C3A-C2A-CAA-CBA
18	A	1122	CLA	CBD-CGD-O2D-CED
20	F	6016	BCR	C10-C11-C12-C13
20	F	6016	BCR	C17-C18-C19-C20
20	F	6016	BCR	C36-C18-C19-C20
20	F	6016	BCR	C21-C22-C23-C24
20	F	6016	BCR	C37-C22-C23-C24
20	F	6016	BCR	C23-C24-C25-C26
20	F	6016	BCR	C23-C24-C25-C30
18	B	1237	CLA	C2-C1-O2A-CGA
18	B	1237	CLA	C2-C3-C5-C6
18	B	1237	CLA	C4-C3-C5-C6
18	B	1216	CLA	C1A-C2A-CAA-CBA
18	B	1216	CLA	CBA-CGA-O2A-C1
18	B	1216	CLA	O1A-CGA-O2A-C1
18	B	9010	CLA	C1A-C2A-CAA-CBA
18	B	9010	CLA	C3A-C2A-CAA-CBA
18	B	9010	CLA	CHA-CBD-CGD-O1D
18	B	9010	CLA	CHA-CBD-CGD-O2D
18	B	9010	CLA	CBD-CGD-O2D-CED
18	A	1107	CLA	C2-C1-O2A-CGA
18	A	1107	CLA	CBD-CGD-O2D-CED
18	A	1108	CLA	C1A-C2A-CAA-CBA
18	B	1238	CLA	C3A-C2A-CAA-CBA
18	B	1238	CLA	O1A-CGA-O2A-C1
18	B	1238	CLA	CBD-CGD-O2D-CED
18	B	1215	CLA	CBD-CGD-O2D-CED
18	B	1202	CLA	C1A-C2A-CAA-CBA
18	B	1202	CLA	CBA-CGA-O2A-C1
18	B	1202	CLA	O1A-CGA-O2A-C1
18	B	1202	CLA	CHA-CBD-CGD-O1D
18	B	1202	CLA	CHA-CBD-CGD-O2D
18	B	1212	CLA	C2-C1-O2A-CGA
18	B	1212	CLA	CHA-CBD-CGD-O1D
18	B	1212	CLA	CHA-CBD-CGD-O2D
18	B	1208	CLA	C1A-C2A-CAA-CBA
18	B	1208	CLA	CBA-CGA-O2A-C1
18	B	1208	CLA	O1A-CGA-O2A-C1
18	F	1139	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	F	1139	CLA	O1D-CGD-O2D-CED
18	L	1502	CLA	CAD-CBD-CGD-O1D
18	L	1502	CLA	CAD-CBD-CGD-O2D
18	L	1502	CLA	C2-C3-C5-C6
18	L	1502	CLA	C4-C3-C5-C6
18	B	1220	CLA	CHA-CBD-CGD-O1D
18	B	1220	CLA	CHA-CBD-CGD-O2D
18	B	1220	CLA	C6-C7-C8-C10
18	B	1232	CLA	CBD-CGD-O2D-CED
18	B	9023	CLA	CBD-CGD-O2D-CED
18	L	1130	CLA	CBA-CGA-O2A-C1
18	L	1130	CLA	O1A-CGA-O2A-C1
18	L	1130	CLA	O2A-C1-C2-C3
18	B	9012	CLA	CBA-CGA-O2A-C1
18	B	9012	CLA	O1A-CGA-O2A-C1
18	B	9012	CLA	CAD-CBD-CGD-O1D
18	B	9012	CLA	CAD-CBD-CGD-O2D
18	B	9012	CLA	CBD-CGD-O2D-CED
18	B	1218	CLA	CHA-CBD-CGD-O1D
18	B	1218	CLA	CHA-CBD-CGD-O2D
18	B	1218	CLA	CAD-CBD-CGD-O1D
18	B	1218	CLA	CBD-CGD-O2D-CED
18	4	1304	CLA	C1A-C2A-CAA-CBA
18	4	1304	CLA	CHA-CBD-CGD-O1D
18	4	1304	CLA	CHA-CBD-CGD-O2D
18	4	1304	CLA	CAD-CBD-CGD-O1D
18	4	1304	CLA	CAD-CBD-CGD-O2D
18	4	1304	CLA	CBD-CGD-O2D-CED
18	L	1503	CLA	C1A-C2A-CAA-CBA
18	B	1219	CLA	C1A-C2A-CAA-CBA
18	B	1219	CLA	C3A-C2A-CAA-CBA
18	B	1219	CLA	C2-C3-C5-C6
18	B	9022	CLA	CBD-CGD-O2D-CED
18	B	9022	CLA	C2-C3-C5-C6
18	B	9022	CLA	C4-C3-C5-C6
18	F	1302	CLA	CBD-CGD-O2D-CED
18	A	1123	CLA	C1A-C2A-CAA-CBA
18	I	1204	CLA	C1A-C2A-CAA-CBA
18	I	1204	CLA	CBA-CGA-O2A-C1
18	I	1204	CLA	O1A-CGA-O2A-C1
18	I	1204	CLA	CBD-CGD-O2D-CED
18	A	1135	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	A	1135	CLA	C3A-C2A-CAA-CBA
18	A	1135	CLA	C2A-CAA-CBA-CGA
18	A	1135	CLA	CBD-CGD-O2D-CED
18	B	1229	CLA	CBD-CGD-O2D-CED
18	B	1229	CLA	O1D-CGD-O2D-CED
18	B	1229	CLA	O2A-C1-C2-C3
18	B	1225	CLA	C2A-CAA-CBA-CGA
18	B	1225	CLA	CBD-CGD-O2D-CED
18	B	1214	CLA	C1A-C2A-CAA-CBA
20	I	6018	BCR	C11-C10-C9-C8
20	I	6018	BCR	C11-C10-C9-C34
20	I	6018	BCR	C17-C18-C19-C20
20	I	6018	BCR	C36-C18-C19-C20
20	I	6018	BCR	C21-C22-C23-C24
20	I	6018	BCR	C37-C22-C23-C24
18	B	1231	CLA	C3A-C2A-CAA-CBA
18	B	1231	CLA	CBA-CGA-O2A-C1
18	B	1231	CLA	CHA-CBD-CGD-O1D
18	B	1231	CLA	CHA-CBD-CGD-O2D
18	B	1231	CLA	CBD-CGD-O2D-CED
20	A	6011	BCR	C7-C8-C9-C10
20	A	6011	BCR	C7-C8-C9-C34
20	A	6011	BCR	C11-C10-C9-C34
20	A	6011	BCR	C10-C11-C12-C13
20	A	6011	BCR	C15-C16-C17-C18
18	A	9011	CLA	C1A-C2A-CAA-CBA
18	A	9011	CLA	CBD-CGD-O2D-CED
18	A	1131	CLA	C1A-C2A-CAA-CBA
18	A	1131	CLA	CBD-CGD-O2D-CED
18	A	1131	CLA	O1D-CGD-O2D-CED
18	B	1242	CLA	C1A-C2A-CAA-CBA
18	B	1236	CLA	CHA-CBD-CGD-O1D
18	B	1236	CLA	CHA-CBD-CGD-O2D
18	B	1221	CLA	C3A-C2A-CAA-CBA
18	B	1221	CLA	CBA-CGA-O2A-C1
18	B	1221	CLA	O1A-CGA-O2A-C1
18	G	1233	CLA	C3A-C2A-CAA-CBA
18	G	1233	CLA	CHA-CBD-CGD-O1D
18	G	1233	CLA	CBD-CGD-O2D-CED
18	G	1233	CLA	C2-C3-C5-C6
18	B	1207	CLA	C3A-C2A-CAA-CBA
20	L	6020	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	L	6020	BCR	C7-C8-C9-C34
20	L	6020	BCR	C11-C10-C9-C8
20	L	6020	BCR	C11-C10-C9-C34
20	L	6020	BCR	C10-C11-C12-C13
20	L	6020	BCR	C37-C22-C23-C24
20	L	6020	BCR	C23-C24-C25-C26
20	L	6020	BCR	C23-C24-C25-C30
18	J	2107	CLA	C1A-C2A-CAA-CBA
18	J	2107	CLA	C3A-C2A-CAA-CBA
18	B	1203	CLA	C1A-C2A-CAA-CBA
18	B	1203	CLA	CBD-CGD-O2D-CED
18	B	1138	CLA	CBD-CGD-O2D-CED
18	B	1138	CLA	O1D-CGD-O2D-CED
18	B	1138	CLA	C2-C3-C5-C6
18	B	1138	CLA	C4-C3-C5-C6
18	A	1137	CLA	C1A-C2A-CAA-CBA
18	A	1137	CLA	C2-C3-C5-C6
18	A	1137	CLA	C4-C3-C5-C6
18	B	1227	CLA	C1A-C2A-CAA-CBA
18	B	1227	CLA	C3A-C2A-CAA-CBA
18	B	1227	CLA	CHA-CBD-CGD-O1D
18	B	1227	CLA	CHA-CBD-CGD-O2D
18	B	1227	CLA	CBD-CGD-O2D-CED
18	B	1217	CLA	C1A-C2A-CAA-CBA
18	A	1119	CLA	CBD-CGD-O2D-CED
18	A	1113	CLA	CBD-CGD-O2D-CED
18	B	1239	CLA	C2-C3-C5-C6
18	B	1239	CLA	C4-C3-C5-C6
18	A	1126	CLA	CBD-CGD-O2D-CED
20	B	6017	BCR	C7-C8-C9-C10
20	B	6017	BCR	C7-C8-C9-C34
20	B	6017	BCR	C11-C10-C9-C8
20	B	6017	BCR	C11-C10-C9-C34
20	B	6017	BCR	C23-C24-C25-C26
18	B	1228	CLA	CBA-CGA-O2A-C1
18	B	1228	CLA	O1A-CGA-O2A-C1
18	B	1228	CLA	O2A-C1-C2-C3
18	A	1103	CLA	C1A-C2A-CAA-CBA
18	B	1234	CLA	C1A-C2A-CAA-CBA
18	B	1235	CLA	C2C-C3C-CAC-CBC
18	B	1235	CLA	C4C-C3C-CAC-CBC
18	B	1235	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	B	1235	CLA	CAD-CBD-CGD-O2D
18	B	1235	CLA	C2-C3-C5-C6
18	B	1235	CLA	C4-C3-C5-C6
18	B	1209	CLA	C1A-C2A-CAA-CBA
18	B	1209	CLA	O2A-C1-C2-C3
18	B	1209	CLA	C2-C3-C5-C6
18	B	1209	CLA	C4-C3-C5-C6
18	B	1222	CLA	C2-C1-O2A-CGA
18	B	1222	CLA	CBD-CGD-O2D-CED
18	B	1207	CLA	C4C-C3C-CAC-CBC
18	B	1238	CLA	O1D-CGD-O2D-CED
18	B	1212	CLA	O1D-CGD-O2D-CED
18	F	1302	CLA	O1D-CGD-O2D-CED
18	G	1233	CLA	O1D-CGD-O2D-CED
18	B	1207	CLA	O1D-CGD-O2D-CED
18	A	1129	CLA	O1D-CGD-O2D-CED
18	B	1138	CLA	C5-C6-C7-C8
18	B	1221	CLA	C2C-C3C-CAC-CBC
18	B	1221	CLA	C4C-C3C-CAC-CBC
18	B	1207	CLA	C2C-C3C-CAC-CBC
18	B	9010	CLA	O1D-CGD-O2D-CED
18	4	1304	CLA	O1D-CGD-O2D-CED
18	B	1225	CLA	O1D-CGD-O2D-CED
18	A	9011	CLA	O1D-CGD-O2D-CED
18	B	1221	CLA	O1D-CGD-O2D-CED
18	A	1119	CLA	O1D-CGD-O2D-CED
18	A	1103	CLA	O1D-CGD-O2D-CED
18	B	1222	CLA	O1D-CGD-O2D-CED
18	B	1237	CLA	CBD-CGD-O2D-CED
18	A	1108	CLA	CBD-CGD-O2D-CED
18	B	1212	CLA	CBD-CGD-O2D-CED
18	B	1208	CLA	CBD-CGD-O2D-CED
18	B	1220	CLA	CBD-CGD-O2D-CED
18	A	1128	CLA	CBD-CGD-O2D-CED
18	B	1214	CLA	CBD-CGD-O2D-CED
18	B	1236	CLA	CBD-CGD-O2D-CED
18	B	1221	CLA	CBD-CGD-O2D-CED
18	B	1207	CLA	CBD-CGD-O2D-CED
18	L	1504	CLA	CBD-CGD-O2D-CED
18	A	9013	CLA	CBD-CGD-O2D-CED
18	B	1239	CLA	CBD-CGD-O2D-CED
18	A	1129	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	1103	CLA	CBD-CGD-O2D-CED
18	B	1212	CLA	O1A-CGA-O2A-C1
18	B	1218	CLA	O1A-CGA-O2A-C1
18	B	1227	CLA	O1A-CGA-O2A-C1
18	B	1231	CLA	O1A-CGA-O2A-C1
18	A	1108	CLA	O1D-CGD-O2D-CED
18	A	1128	CLA	O1D-CGD-O2D-CED
18	B	1231	CLA	O1D-CGD-O2D-CED
18	B	1236	CLA	O1D-CGD-O2D-CED
18	A	1113	CLA	O1D-CGD-O2D-CED
18	B	1236	CLA	CBA-CGA-O2A-C1
18	L	1503	CLA	C2C-C3C-CAC-CBC
18	I	1204	CLA	C4C-C3C-CAC-CBC
18	A	1122	CLA	O1D-CGD-O2D-CED
18	A	1107	CLA	O1D-CGD-O2D-CED
18	B	1215	CLA	O1D-CGD-O2D-CED
18	B	1232	CLA	O1D-CGD-O2D-CED
18	B	9012	CLA	O1D-CGD-O2D-CED
18	B	1218	CLA	O1D-CGD-O2D-CED
18	B	9022	CLA	O1D-CGD-O2D-CED
18	I	1204	CLA	O1D-CGD-O2D-CED
18	B	1203	CLA	O1D-CGD-O2D-CED
18	B	1227	CLA	O1D-CGD-O2D-CED
18	B	1218	CLA	CBA-CGA-O2A-C1
18	B	1227	CLA	CBA-CGA-O2A-C1
18	A	1136	CLA	CBD-CGD-O2D-CED
18	B	1234	CLA	CBD-CGD-O2D-CED
18	B	1220	CLA	C2C-C3C-CAC-CBC
18	I	1204	CLA	C2C-C3C-CAC-CBC
18	A	1137	CLA	C2C-C3C-CAC-CBC
18	B	1237	CLA	O1A-CGA-O2A-C1
18	B	1224	CLA	O1A-CGA-O2A-C1
18	L	1502	CLA	O1A-CGA-O2A-C1
18	B	1220	CLA	O1A-CGA-O2A-C1
18	4	1304	CLA	O1A-CGA-O2A-C1
18	F	1302	CLA	O1A-CGA-O2A-C1
18	B	1214	CLA	O1A-CGA-O2A-C1
18	L	1504	CLA	O1A-CGA-O2A-C1
18	A	1103	CLA	O1A-CGA-O2A-C1
18	B	1209	CLA	O1A-CGA-O2A-C1
18	A	1135	CLA	O1D-CGD-O2D-CED
18	A	1126	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	1137	CLA	C4C-C3C-CAC-CBC
18	B	9023	CLA	O1D-CGD-O2D-CED
18	B	1215	CLA	C2C-C3C-CAC-CBC
18	B	1215	CLA	C4C-C3C-CAC-CBC
18	L	1503	CLA	C4C-C3C-CAC-CBC
18	A	1115	CLA	CBD-CGD-O2D-CED
19	B	5002	PQN	C20-C21-C22-C23
18	L	1504	CLA	O1D-CGD-O2D-CED
18	A	9011	CLA	O1A-CGA-O2A-C1
18	A	1140	CLA	C3-C5-C6-C7
18	A	1128	CLA	C3-C5-C6-C7
18	A	1136	CLA	C3-C5-C6-C7
18	B	1205	CLA	C3-C5-C6-C7
19	A	5001	PQN	C13-C15-C16-C17
18	A	1119	CLA	C3-C5-C6-C7
18	A	1126	CLA	C3-C5-C6-C7
18	A	1140	CLA	CBA-CGA-O2A-C1
18	B	1238	CLA	CBA-CGA-O2A-C1
18	B	1212	CLA	CBA-CGA-O2A-C1
18	L	1502	CLA	CBA-CGA-O2A-C1
18	B	1220	CLA	CBA-CGA-O2A-C1
18	4	1304	CLA	CBA-CGA-O2A-C1
18	B	1229	CLA	CBA-CGA-O2A-C1
18	B	1214	CLA	CBA-CGA-O2A-C1
18	L	1504	CLA	CBA-CGA-O2A-C1
18	A	1113	CLA	CBA-CGA-O2A-C1
18	A	1103	CLA	CBA-CGA-O2A-C1
18	B	1209	CLA	CBA-CGA-O2A-C1
18	B	1220	CLA	C4C-C3C-CAC-CBC
18	B	1219	CLA	CBD-CGD-O2D-CED
18	A	1131	CLA	C2C-C3C-CAC-CBC
18	A	9013	CLA	O1A-CGA-O2A-C1
18	A	9013	CLA	CBA-CGA-O2A-C1
18	A	1126	CLA	C4-C3-C5-C6
18	A	1126	CLA	C2-C3-C5-C6
18	B	1216	CLA	C2A-CAA-CBA-CGA
18	4	1304	CLA	C2A-CAA-CBA-CGA
18	B	1231	CLA	C2A-CAA-CBA-CGA
18	B	1207	CLA	C2A-CAA-CBA-CGA
18	B	1234	CLA	C2A-CAA-CBA-CGA
18	B	1209	CLA	C2A-CAA-CBA-CGA
18	A	1140	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	1103	CLA	C2-C1-O2A-CGA
18	B	1236	CLA	O1A-CGA-O2A-C1
18	A	1107	CLA	C3-C5-C6-C7
18	B	1237	CLA	CBA-CGA-O2A-C1
18	B	1224	CLA	CBA-CGA-O2A-C1
18	B	9022	CLA	CBA-CGA-O2A-C1
18	F	1302	CLA	CBA-CGA-O2A-C1
18	B	1237	CLA	O1D-CGD-O2D-CED
18	B	1208	CLA	O1D-CGD-O2D-CED
18	B	1220	CLA	O1D-CGD-O2D-CED
18	A	1107	CLA	O1A-CGA-O2A-C1
18	B	1229	CLA	O1A-CGA-O2A-C1
18	B	1203	CLA	O1A-CGA-O2A-C1
18	A	9011	CLA	C2C-C3C-CAC-CBC
18	A	1131	CLA	C4C-C3C-CAC-CBC
18	B	1239	CLA	O1D-CGD-O2D-CED
20	F	6016	BCR	C9-C10-C11-C12
20	F	6016	BCR	C19-C20-C21-C22
20	I	6018	BCR	C9-C10-C11-C12
20	A	6011	BCR	C9-C10-C11-C12
20	A	6011	BCR	C13-C14-C15-C16
20	L	6020	BCR	C13-C14-C15-C16
20	L	6020	BCR	C15-C16-C17-C18
20	B	6017	BCR	C9-C10-C11-C12
20	B	6017	BCR	C13-C14-C15-C16
20	B	6017	BCR	C19-C20-C21-C22
18	A	1140	CLA	C2C-C3C-CAC-CBC
18	H	1501	CLA	CBD-CGD-O2D-CED
18	B	1224	CLA	CBD-CGD-O2D-CED
18	A	9013	CLA	O1D-CGD-O2D-CED
18	B	1232	CLA	C3-C5-C6-C7
18	J	2107	CLA	C3-C5-C6-C7
18	A	1137	CLA	C3-C5-C6-C7
18	B	1203	CLA	CBA-CGA-O2A-C1
18	A	1129	CLA	CBA-CGA-O2A-C1
18	B	9022	CLA	O1A-CGA-O2A-C1
18	A	1113	CLA	O1A-CGA-O2A-C1
18	B	1237	CLA	C2C-C3C-CAC-CBC
18	F	1139	CLA	C2C-C3C-CAC-CBC
18	B	1219	CLA	C2C-C3C-CAC-CBC
18	A	1123	CLA	C3-C5-C6-C7
18	A	1107	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	9011	CLA	CBA-CGA-O2A-C1
19	B	5002	PQN	C14-C13-C15-C16
18	A	9011	CLA	C4-C3-C5-C6
19	B	5002	PQN	C12-C13-C15-C16
18	A	9011	CLA	C2-C3-C5-C6
18	A	1119	CLA	C2A-CAA-CBA-CGA
18	A	1129	CLA	C2A-CAA-CBA-CGA
18	B	1222	CLA	C2A-CAA-CBA-CGA
18	B	9010	CLA	CBA-CGA-O2A-C1
18	B	1214	CLA	O1D-CGD-O2D-CED
18	B	1234	CLA	O1D-CGD-O2D-CED
18	B	1232	CLA	O1A-CGA-O2A-C1
18	A	1136	CLA	O1D-CGD-O2D-CED
18	A	1122	CLA	O1A-CGA-O2A-C1
18	B	9010	CLA	O1A-CGA-O2A-C1
18	A	1129	CLA	O1A-CGA-O2A-C1
18	B	9022	CLA	C3-C5-C6-C7
18	A	1122	CLA	CBA-CGA-O2A-C1
18	B	1232	CLA	CBA-CGA-O2A-C1
18	A	1136	CLA	CBA-CGA-O2A-C1
18	A	1123	CLA	CBA-CGA-O2A-C1
18	B	1242	CLA	CBA-CGA-O2A-C1
18	G	1233	CLA	CBA-CGA-O2A-C1
18	A	1115	CLA	CBA-CGA-O2A-C1
18	A	1137	CLA	CBA-CGA-O2A-C1
18	A	1126	CLA	CBA-CGA-O2A-C1
18	B	1235	CLA	CBA-CGA-O2A-C1
18	A	1123	CLA	CBD-CGD-O2D-CED
18	B	1215	CLA	C3-C5-C6-C7
18	A	1115	CLA	O1A-CGA-O2A-C1
18	A	1126	CLA	O1A-CGA-O2A-C1
19	A	5001	PQN	C19-C18-C20-C21
18	B	1222	CLA	C11-C10-C8-C9
18	A	1126	CLA	C2A-CAA-CBA-CGA
20	A	6011	BCR	C36-C18-C19-C20
18	A	1136	CLA	O1A-CGA-O2A-C1
18	B	1235	CLA	O1A-CGA-O2A-C1
18	A	1140	CLA	C5-C6-C7-C8
18	B	1216	CLA	CBD-CGD-O2D-CED
18	A	1107	CLA	C2C-C3C-CAC-CBC
18	B	1138	CLA	C3-C5-C6-C7
18	A	1107	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	J	2107	CLA	CBA-CGA-O2A-C1
18	A	9011	CLA	C4C-C3C-CAC-CBC
18	A	1123	CLA	C5-C6-C7-C8
19	A	5001	PQN	C18-C20-C21-C22
18	A	1123	CLA	C2C-C3C-CAC-CBC
18	B	1219	CLA	C4C-C3C-CAC-CBC
18	A	1129	CLA	C5-C6-C7-C8
18	B	1217	CLA	C2-C1-O2A-CGA
18	B	1209	CLA	C2-C1-O2A-CGA
18	A	1140	CLA	C4C-C3C-CAC-CBC
18	B	1232	CLA	C5-C6-C7-C8
18	A	1137	CLA	C5-C6-C7-C8
19	A	5001	PQN	C22-C23-C25-C26
18	B	1238	CLA	C3-C5-C6-C7
18	B	1242	CLA	O1A-CGA-O2A-C1
18	G	1233	CLA	O1A-CGA-O2A-C1
18	J	2107	CLA	O1A-CGA-O2A-C1
20	I	6018	BCR	C19-C20-C21-C22
20	A	6011	BCR	C19-C20-C21-C22
18	B	9010	CLA	C2A-CAA-CBA-CGA
18	B	9022	CLA	C2A-CAA-CBA-CGA
18	B	9012	CLA	C5-C6-C7-C8
18	A	1137	CLA	O1A-CGA-O2A-C1
20	I	6018	BCR	C10-C11-C12-C13
20	B	6017	BCR	C10-C11-C12-C13
19	A	5001	PQN	C23-C25-C26-C27
18	A	1123	CLA	O1A-CGA-O2A-C1
18	B	1208	CLA	C5-C6-C7-C8
18	B	1205	CLA	C5-C6-C7-C8
18	F	1139	CLA	C4C-C3C-CAC-CBC
18	B	1216	CLA	C5-C6-C7-C8
18	J	2107	CLA	C8-C10-C11-C12
18	H	1501	CLA	C4-C3-C5-C6
18	B	1212	CLA	C4-C3-C5-C6
18	B	1220	CLA	C5-C6-C7-C8
18	B	1235	CLA	C5-C6-C7-C8
18	A	1140	CLA	C2A-CAA-CBA-CGA
18	B	9012	CLA	C2A-CAA-CBA-CGA
18	F	1302	CLA	C2A-CAA-CBA-CGA
18	A	1137	CLA	C6-C7-C8-C10
18	B	1234	CLA	CBA-CGA-O2A-C1
18	B	1219	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	B	1208	CLA	C6-C7-C8-C10
18	B	9012	CLA	C6-C7-C8-C9
18	A	1128	CLA	C6-C7-C8-C9
18	A	1123	CLA	C6-C7-C8-C9
18	B	1228	CLA	C6-C7-C8-C10
18	B	1209	CLA	C6-C7-C8-C10
18	A	1115	CLA	O1D-CGD-O2D-CED
20	A	6011	BCR	C11-C10-C9-C8
18	A	1136	CLA	C6-C7-C8-C9
18	A	1119	CLA	C4-C3-C5-C6
18	B	1212	CLA	C2-C3-C5-C6
18	B	1220	CLA	C6-C7-C8-C9
20	B	6017	BCR	C11-C12-C13-C35
20	A	6011	BCR	C17-C18-C19-C20
20	L	6020	BCR	C21-C22-C23-C24
20	B	6017	BCR	C21-C22-C23-C24
18	H	1501	CLA	O1D-CGD-O2D-CED
18	B	1237	CLA	C4C-C3C-CAC-CBC
18	A	1119	CLA	C6-C7-C8-C9
18	A	1128	CLA	C5-C6-C7-C8
18	B	1224	CLA	O1D-CGD-O2D-CED
18	A	1108	CLA	C3A-C2A-CAA-CBA
18	B	1232	CLA	C3A-C2A-CAA-CBA
18	4	1304	CLA	C3A-C2A-CAA-CBA
18	L	1503	CLA	C3A-C2A-CAA-CBA
18	A	1123	CLA	C3A-C2A-CAA-CBA
18	I	1204	CLA	C3A-C2A-CAA-CBA
18	B	1214	CLA	C3A-C2A-CAA-CBA
18	A	9011	CLA	C3A-C2A-CAA-CBA
18	A	1131	CLA	C3A-C2A-CAA-CBA
18	B	1242	CLA	C3A-C2A-CAA-CBA
18	A	1137	CLA	C3A-C2A-CAA-CBA
18	B	1234	CLA	C3A-C2A-CAA-CBA
18	H	1501	CLA	C6-C7-C8-C9
18	B	1208	CLA	C6-C7-C8-C9
18	A	1119	CLA	C6-C7-C8-C10
18	B	1209	CLA	C6-C7-C8-C9
18	B	1221	CLA	O2A-C1-C2-C3
18	F	1139	CLA	C2A-CAA-CBA-CGA
18	B	1242	CLA	C2C-C3C-CAC-CBC
18	B	1205	CLA	C4-C3-C5-C6
18	A	1119	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	B	1234	CLA	O1A-CGA-O2A-C1
18	A	1137	CLA	C6-C7-C8-C9
18	B	1228	CLA	C6-C7-C8-C9
18	B	1238	CLA	C5-C6-C7-C8
18	B	9012	CLA	C6-C7-C8-C10
18	A	1123	CLA	C6-C7-C8-C10
20	B	6017	BCR	C23-C24-C25-C30
18	A	1123	CLA	C4C-C3C-CAC-CBC
18	B	1215	CLA	C4-C3-C5-C6
18	B	1222	CLA	C12-C13-C15-C16
18	A	1129	CLA	C3-C5-C6-C7
18	A	1136	CLA	C6-C7-C8-C10
18	B	1205	CLA	CBA-CGA-O2A-C1
18	B	1207	CLA	C5-C6-C7-C8
18	A	1107	CLA	C4C-C3C-CAC-CBC
18	B	1215	CLA	C2-C3-C5-C6
19	A	5001	PQN	C24-C23-C25-C26
18	B	1216	CLA	O1D-CGD-O2D-CED
18	J	2107	CLA	C2A-CAA-CBA-CGA
18	B	1203	CLA	C2A-CAA-CBA-CGA
20	B	6017	BCR	C37-C22-C23-C24
20	B	6017	BCR	C11-C12-C13-C14
18	H	1501	CLA	C1A-C2A-CAA-CBA
18	B	1238	CLA	C1A-C2A-CAA-CBA
18	B	1232	CLA	C1A-C2A-CAA-CBA
18	B	1218	CLA	C1A-C2A-CAA-CBA
18	A	1128	CLA	C1A-C2A-CAA-CBA
18	B	1231	CLA	C1A-C2A-CAA-CBA
18	B	1221	CLA	C1A-C2A-CAA-CBA
18	G	1233	CLA	C1A-C2A-CAA-CBA
18	B	1207	CLA	C1A-C2A-CAA-CBA
18	A	1119	CLA	C1A-C2A-CAA-CBA
18	A	1128	CLA	C6-C7-C8-C10
20	I	6018	BCR	C13-C14-C15-C16
18	B	1222	CLA	C15-C16-C17-C18
18	B	1205	CLA	O1A-CGA-O2A-C1
18	B	1222	CLA	C13-C15-C16-C17
18	A	1126	CLA	C6-C7-C8-C10
18	H	1501	CLA	C6-C7-C8-C10
18	B	1217	CLA	CBD-CGD-O2D-CED
18	B	1222	CLA	C8-C10-C11-C12
18	B	9022	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
18	A	1137	CLA	C2A-CAA-CBA-CGA
18	B	9022	CLA	C2-C1-O2A-CGA
18	J	2107	CLA	C2-C1-O2A-CGA
19	B	5002	PQN	C18-C20-C21-C22
18	A	1119	CLA	C2C-C3C-CAC-CBC
18	B	1220	CLA	C11-C10-C8-C7
19	A	5001	PQN	C17-C18-C20-C21
18	B	1216	CLA	C3-C5-C6-C7
18	A	1107	CLA	C11-C10-C8-C9
18	B	1212	CLA	C11-C10-C8-C9
18	B	1220	CLA	C11-C10-C8-C9
18	B	1222	CLA	C14-C13-C15-C16
18	A	1126	CLA	C5-C6-C7-C8
18	A	1123	CLA	O1D-CGD-O2D-CED
20	L	6020	BCR	C11-C12-C13-C35
20	B	6017	BCR	C17-C18-C19-C20
19	B	5002	PQN	C15-C16-C17-C18
18	B	1212	CLA	C2C-C3C-CAC-CBC
18	B	1205	CLA	C2-C3-C5-C6
18	I	1204	CLA	C6-C7-C8-C10
18	A	1119	CLA	CBA-CGA-O2A-C1
18	B	1212	CLA	CAA-CBA-CGA-O2A
18	B	1216	CLA	C3A-C2A-CAA-CBA
18	B	1212	CLA	C3A-C2A-CAA-CBA
18	B	1208	CLA	C3A-C2A-CAA-CBA
18	B	9012	CLA	C3A-C2A-CAA-CBA
18	B	1218	CLA	C3A-C2A-CAA-CBA
18	A	1103	CLA	C3A-C2A-CAA-CBA
18	B	1209	CLA	C3A-C2A-CAA-CBA
20	F	6016	BCR	C15-C16-C17-C18
18	B	1208	CLA	C3-C5-C6-C7
18	B	9012	CLA	C4-C3-C5-C6
18	H	1501	CLA	C2-C3-C5-C6
18	B	1208	CLA	C2A-CAA-CBA-CGA
18	A	1103	CLA	C2A-CAA-CBA-CGA
18	B	1208	CLA	C2-C1-O2A-CGA
18	B	1234	CLA	C2-C1-O2A-CGA
18	B	1219	CLA	C4-C3-C5-C6
18	G	1233	CLA	C4-C3-C5-C6
18	I	1204	CLA	C3-C5-C6-C7
19	B	5002	PQN	C25-C26-C27-C28
20	L	6020	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
18	B	1212	CLA	C11-C10-C8-C7
18	J	2107	CLA	C11-C12-C13-C15
18	B	1138	CLA	C6-C7-C8-C10
18	B	1222	CLA	C3-C5-C6-C7
20	L	6020	BCR	C9-C10-C11-C12
18	B	1239	CLA	C6-C7-C8-C10
18	I	1204	CLA	C2A-CAA-CBA-CGA
20	F	6016	BCR	C11-C10-C9-C34
18	B	1227	CLA	C2C-C3C-CAC-CBC
18	B	1202	CLA	O1D-CGD-O2D-CED
19	B	5002	PQN	C23-C25-C26-C27
18	B	1218	CLA	CAD-CBD-CGD-O2D
18	B	1217	CLA	CAD-CBD-CGD-O2D
18	J	2107	CLA	C10-C11-C12-C13
18	B	1220	CLA	C2A-CAA-CBA-CGA
19	B	5002	PQN	C26-C27-C28-C29
18	F	1139	CLA	CHA-CBD-CGD-O1D
18	F	1139	CLA	CHA-CBD-CGD-O2D
18	L	1502	CLA	CHA-CBD-CGD-O2D
18	B	1221	CLA	CHA-CBD-CGD-O1D
18	B	1221	CLA	CHA-CBD-CGD-O2D
18	G	1233	CLA	CHA-CBD-CGD-O2D
18	B	1228	CLA	CHA-CBD-CGD-O1D
18	B	1228	CLA	CHA-CBD-CGD-O2D
18	A	1119	CLA	O1A-CGA-O2A-C1
18	B	1239	CLA	C6-C7-C8-C9
18	G	1233	CLA	C2C-C3C-CAC-CBC
18	B	1235	CLA	C3-C5-C6-C7
18	J	2107	CLA	C11-C12-C13-C14
18	A	1126	CLA	C6-C7-C8-C9
20	B	6017	BCR	C36-C18-C19-C20
18	L	1502	CLA	C1A-C2A-CAA-CBA
18	A	1126	CLA	C2-C1-O2A-CGA
18	L	1504	CLA	C3-C5-C6-C7
18	B	1238	CLA	C2C-C3C-CAC-CBC
18	B	1215	CLA	C2A-CAA-CBA-CGA
18	A	1107	CLA	CAD-CBD-CGD-O1D
18	F	1139	CLA	CAD-CBD-CGD-O1D
18	F	1302	CLA	CAD-CBD-CGD-O1D
18	A	1136	CLA	CAD-CBD-CGD-O1D
18	B	1221	CLA	CAD-CBD-CGD-O1D
18	B	1203	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	B	1138	CLA	CAD-CBD-CGD-O1D
18	B	9012	CLA	C3-C5-C6-C7
18	A	1107	CLA	C6-C7-C8-C10
18	B	1222	CLA	C11-C10-C8-C7
18	B	1242	CLA	C4C-C3C-CAC-CBC
18	I	1204	CLA	C6-C7-C8-C9
18	B	1220	CLA	C10-C11-C12-C13
18	B	1215	CLA	CBA-CGA-O2A-C1
18	A	1107	CLA	C6-C7-C8-C9
18	B	1222	CLA	C11-C12-C13-C14
18	B	1207	CLA	C6-C7-C8-C10
18	A	1108	CLA	CAA-CBA-CGA-O2A
18	B	1209	CLA	C3-C5-C6-C7
18	B	1219	CLA	C2-C1-O2A-CGA
18	B	1214	CLA	O2A-C1-C2-C3
20	B	6017	BCR	C5-C6-C7-C8
18	B	1207	CLA	CAA-CBA-CGA-O2A
18	L	1504	CLA	C6-C7-C8-C10
18	B	1222	CLA	C11-C12-C13-C15
18	B	1231	CLA	C2C-C3C-CAC-CBC
20	B	6017	BCR	C15-C16-C17-C18
19	A	5001	PQN	C26-C27-C28-C29
18	B	1228	CLA	C3-C5-C6-C7
18	B	1202	CLA	CBD-CGD-O2D-CED
20	I	6018	BCR	C15-C16-C17-C18
18	B	1215	CLA	O1A-CGA-O2A-C1
18	B	1232	CLA	C2-C1-O2A-CGA
18	A	1136	CLA	C2-C1-O2A-CGA
18	B	1205	CLA	C2-C1-O2A-CGA
18	B	1212	CLA	C5-C6-C7-C8
18	B	1220	CLA	C3A-C2A-CAA-CBA
18	B	1229	CLA	C3A-C2A-CAA-CBA
18	A	1115	CLA	C3A-C2A-CAA-CBA
18	B	1203	CLA	C3A-C2A-CAA-CBA
18	B	1203	CLA	CAA-CBA-CGA-O2A
20	F	6016	BCR	C35-C13-C14-C15
20	A	6011	BCR	C16-C17-C18-C36
20	L	6020	BCR	C20-C21-C22-C37
18	A	1136	CLA	C2A-CAA-CBA-CGA
18	B	1208	CLA	C2C-C3C-CAC-CBC
18	I	1204	CLA	C4-C3-C5-C6
18	B	1212	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	F	1139	CLA	C1A-C2A-CAA-CBA
18	B	1229	CLA	C1A-C2A-CAA-CBA
19	A	5001	PQN	C21-C22-C23-C25
18	B	1205	CLA	C2A-CAA-CBA-CGA
19	A	5001	PQN	C25-C26-C27-C28
18	B	1227	CLA	C4C-C3C-CAC-CBC
18	A	1119	CLA	C4C-C3C-CAC-CBC
20	F	6016	BCR	C12-C13-C14-C15
20	A	6011	BCR	C16-C17-C18-C19
20	L	6020	BCR	C20-C21-C22-C23
18	B	1217	CLA	O1D-CGD-O2D-CED
18	B	1212	CLA	C4C-C3C-CAC-CBC
18	H	1501	CLA	C2-C1-O2A-CGA
18	B	9012	CLA	C2-C1-O2A-CGA
18	B	1218	CLA	C2-C1-O2A-CGA
18	B	1138	CLA	C2-C1-O2A-CGA
18	B	1222	CLA	O1A-CGA-O2A-C1
18	L	1503	CLA	C2-C1-O2A-CGA
20	I	6018	BCR	C23-C24-C25-C26
20	B	6017	BCR	C1-C6-C7-C8
18	B	9023	CLA	C2-C1-O2A-CGA
18	J	2107	CLA	C2C-C3C-CAC-CBC
18	L	1504	CLA	C6-C7-C8-C9
18	B	1242	CLA	C2-C1-O2A-CGA
18	B	1221	CLA	C2A-CAA-CBA-CGA
18	B	1229	CLA	CAA-CBA-CGA-O2A
18	B	1222	CLA	CBA-CGA-O2A-C1
18	A	1107	CLA	C5-C6-C7-C8
18	J	2107	CLA	C5-C6-C7-C8
18	G	1233	CLA	CAA-CBA-CGA-O2A
18	I	1204	CLA	C2-C3-C5-C6
18	B	1242	CLA	O1D-CGD-O2D-CED
18	B	1205	CLA	CAA-CBA-CGA-O2A
18	B	9012	CLA	C2-C3-C5-C6
18	B	1222	CLA	C2C-C3C-CAC-CBC
18	B	1217	CLA	C3A-C2A-CAA-CBA
18	B	1138	CLA	O1A-CGA-O2A-C1
18	A	1122	CLA	CAD-CBD-CGD-O2D
18	B	1242	CLA	CAD-CBD-CGD-O2D
18	B	1209	CLA	CAD-CBD-CGD-O2D
18	B	1242	CLA	CBD-CGD-O2D-CED
18	A	1107	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	A	5001	PQN	C26-C27-C28-C30
18	B	1220	CLA	CAA-CBA-CGA-O2A
18	L	1502	CLA	C2C-C3C-CAC-CBC
18	A	1128	CLA	O1A-CGA-O2A-C1
20	A	6011	BCR	C21-C22-C23-C24
18	A	1107	CLA	O2A-C1-C2-C3
18	A	1123	CLA	O2A-C1-C2-C3
18	B	1234	CLA	O2A-C1-C2-C3
18	B	1218	CLA	C2A-CAA-CBA-CGA
18	B	1237	CLA	CHA-CBD-CGD-O2D
18	A	1106	CLA	CHA-CBD-CGD-O1D
18	A	1106	CLA	CHA-CBD-CGD-O2D
18	B	1216	CLA	CHA-CBD-CGD-O1D
18	B	1208	CLA	CHA-CBD-CGD-O1D
18	B	1208	CLA	CHA-CBD-CGD-O2D
18	L	1502	CLA	CHA-CBD-CGD-O1D
18	B	1219	CLA	CHA-CBD-CGD-O1D
18	B	1219	CLA	CHA-CBD-CGD-O2D
18	B	9022	CLA	CHA-CBD-CGD-O1D
18	B	9022	CLA	CHA-CBD-CGD-O2D
18	A	1136	CLA	CHA-CBD-CGD-O1D
18	A	1136	CLA	CHA-CBD-CGD-O2D
18	B	1205	CLA	CHA-CBD-CGD-O1D
18	B	1205	CLA	CHA-CBD-CGD-O2D
18	A	1123	CLA	CHA-CBD-CGD-O2D
18	B	1242	CLA	CHA-CBD-CGD-O2D
18	A	1115	CLA	CAA-CBA-CGA-O2A
18	B	1215	CLA	CAA-CBA-CGA-O2A
18	B	1242	CLA	CAA-CBA-CGA-O2A
18	A	1128	CLA	CBA-CGA-O2A-C1
18	L	1503	CLA	CAA-CBA-CGA-O2A
18	B	1212	CLA	CAA-CBA-CGA-O1A
18	B	1205	CLA	CAA-CBA-CGA-O1A
18	B	1222	CLA	C10-C11-C12-C13
20	A	6011	BCR	C37-C22-C23-C24
18	B	1207	CLA	C6-C7-C8-C9
18	B	1138	CLA	CBA-CGA-O2A-C1
18	L	1504	CLA	C1A-C2A-CAA-CBA
18	A	1113	CLA	C1A-C2A-CAA-CBA
18	B	1212	CLA	C11-C12-C13-C15
18	A	1107	CLA	CAA-CBA-CGA-O1A
18	A	9011	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	A	1119	CLA	C2-C1-O2A-CGA
18	B	1220	CLA	CAA-CBA-CGA-O1A
18	B	1228	CLA	C5-C6-C7-C8
18	A	1115	CLA	CAA-CBA-CGA-O1A
18	B	1215	CLA	CAA-CBA-CGA-O1A
18	B	1242	CLA	CAA-CBA-CGA-O1A
18	A	1140	CLA	C6-C7-C8-C9
18	B	1222	CLA	CAA-CBA-CGA-O2A
18	A	1129	CLA	CAD-CBD-CGD-O1D
18	B	9023	CLA	CAA-CBA-CGA-O2A
18	B	1138	CLA	C6-C7-C8-C9
18	B	1237	CLA	CAA-CBA-CGA-O2A
18	A	1129	CLA	C2C-C3C-CAC-CBC
18	A	1140	CLA	CAA-CBA-CGA-O2A
18	B	1235	CLA	CAA-CBA-CGA-O2A
18	B	1202	CLA	C3A-C2A-CAA-CBA
18	L	1504	CLA	C3A-C2A-CAA-CBA
18	A	1140	CLA	CAA-CBA-CGA-O1A
18	B	9023	CLA	CAA-CBA-CGA-O1A
18	B	1222	CLA	CAA-CBA-CGA-O1A
18	B	1221	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

131 monomers are involved in 1354 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	H	1501	CLA	13	0
21	C	3102	SF4	8	0
18	3	3006	CLA	1	0
18	A	1133	CLA	2	0
18	A	1140	CLA	25	0
18	A	1122	CLA	4	0
20	F	6016	BCR	15	0
18	H	1505	CLA	2	0
18	4	4005	CLA	1	0
18	A	1101	CLA	4	0
18	3	3002	CLA	2	0
18	B	1211	CLA	7	0
18	A	1106	CLA	13	0
18	B	1216	CLA	23	0
18	1	1006	CLA	2	0
18	B	9010	CLA	29	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	1248	CLA	4	0
18	A	1107	CLA	16	0
18	A	1108	CLA	13	0
18	B	1238	CLA	23	0
18	B	1215	CLA	23	0
18	4	4010	CLA	1	0
18	A	1127	CLA	6	0
18	3	3010	CLA	1	0
18	2	2004	CLA	3	0
18	B	1202	CLA	42	0
18	B	1224	CLA	14	0
18	K	1141	CLA	5	0
18	B	1212	CLA	13	0
18	A	1111	CLA	2	0
18	B	1213	CLA	1	0
18	2	2006	CLA	2	0
18	B	1208	CLA	13	0
18	F	1139	CLA	21	0
18	A	1110	CLA	4	0
18	L	1502	CLA	18	0
18	B	1220	CLA	26	0
18	A	1134	CLA	7	0
18	B	1206	CLA	5	0
18	B	1232	CLA	6	0
18	4	4012	CLA	1	0
21	C	3103	SF4	7	0
18	B	9023	CLA	17	0
18	1	1003	CLA	3	0
18	2	2002	CLA	2	0
18	B	9012	CLA	20	0
18	2	2003	CLA	1	0
18	B	1218	CLA	44	0
18	A	1109	CLA	11	0
18	F	1303	CLA	2	0
18	4	4011	CLA	1	0
18	L	1503	CLA	59	0
18	1	1012	CLA	3	0
18	4	4013	CLA	1	0
18	B	1219	CLA	13	0
18	A	1118	CLA	7	0
18	B	9022	CLA	17	0
18	F	4015	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1301	CLA	3	0
18	A	1147	CLA	6	0
18	F	1302	CLA	16	0
18	A	1128	CLA	16	0
18	4	1304	CLA	11	0
18	B	1205	CLA	14	0
18	A	1123	CLA	24	0
19	A	5001	PQN	30	0
18	I	1204	CLA	11	0
18	A	1135	CLA	7	0
18	B	1229	CLA	13	0
21	B	3101	SF4	4	0
18	B	1225	CLA	43	0
18	B	1241	CLA	6	0
18	A	1136	CLA	26	0
18	2	2012	CLA	5	0
18	1	1008	CLA	1	0
20	I	6018	BCR	13	0
18	B	1231	CLA	3	0
18	B	1237	CLA	13	0
18	3	3005	CLA	5	0
18	A	1132	CLA	9	0
20	A	6011	BCR	17	0
18	F	1240	CLA	2	0
18	A	9011	CLA	24	0
18	2	2011	CLA	1	0
18	A	1131	CLA	10	0
18	1	1013	CLA	3	0
18	B	1242	CLA	19	0
18	B	1236	CLA	11	0
18	A	1120	CLA	1	0
18	B	1221	CLA	23	0
18	G	1233	CLA	8	0
18	A	1124	CLA	14	0
18	B	1223	CLA	5	0
18	A	1115	CLA	8	0
18	B	1207	CLA	16	0
18	L	1504	CLA	13	0
18	A	9013	CLA	19	0
20	L	6020	BCR	17	0
18	4	4001	CLA	2	0
18	2	2005	CLA	1	0

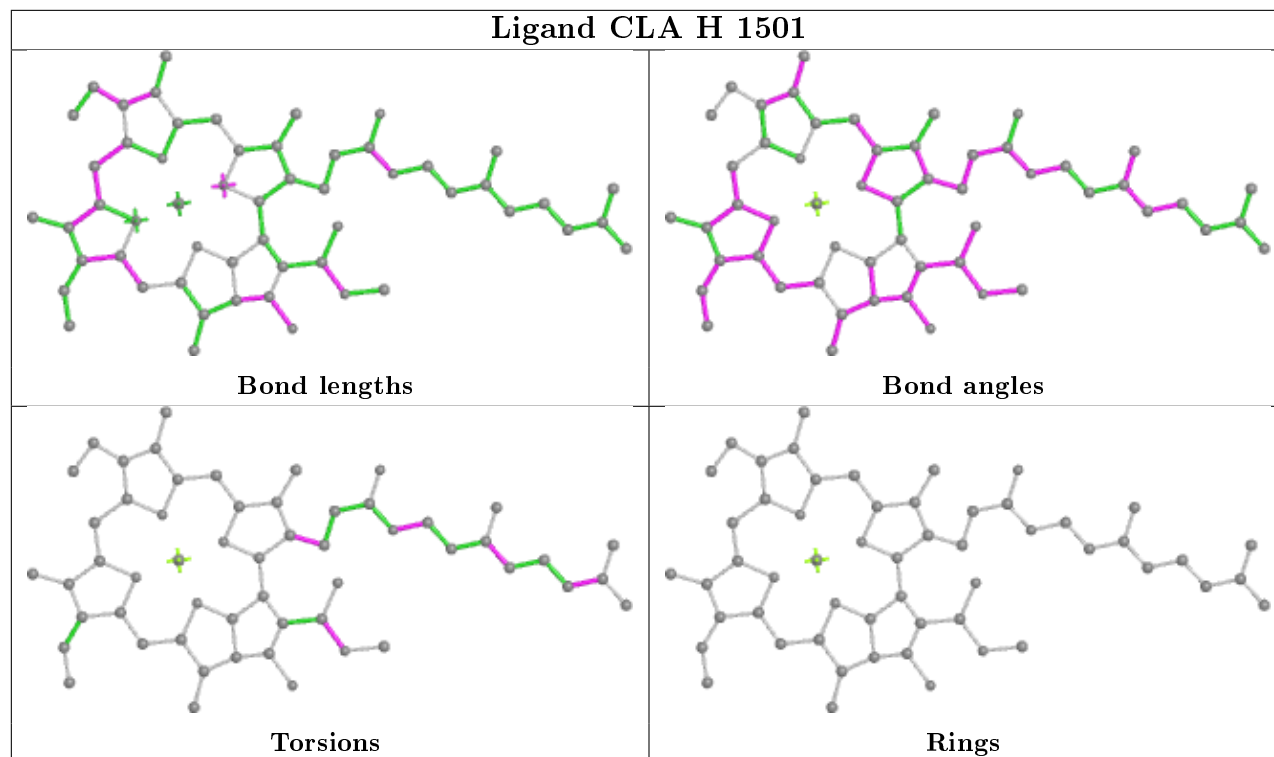
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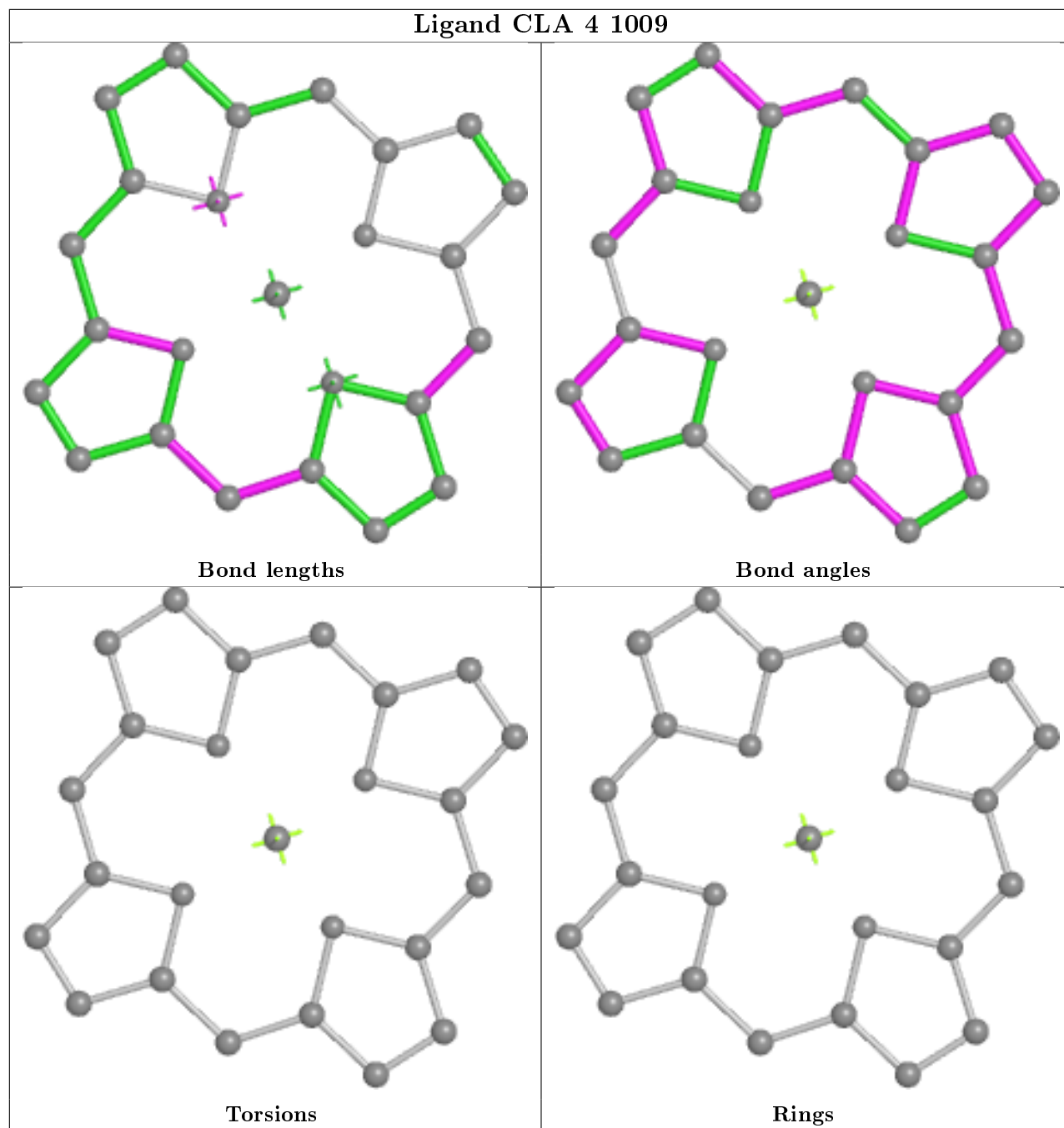
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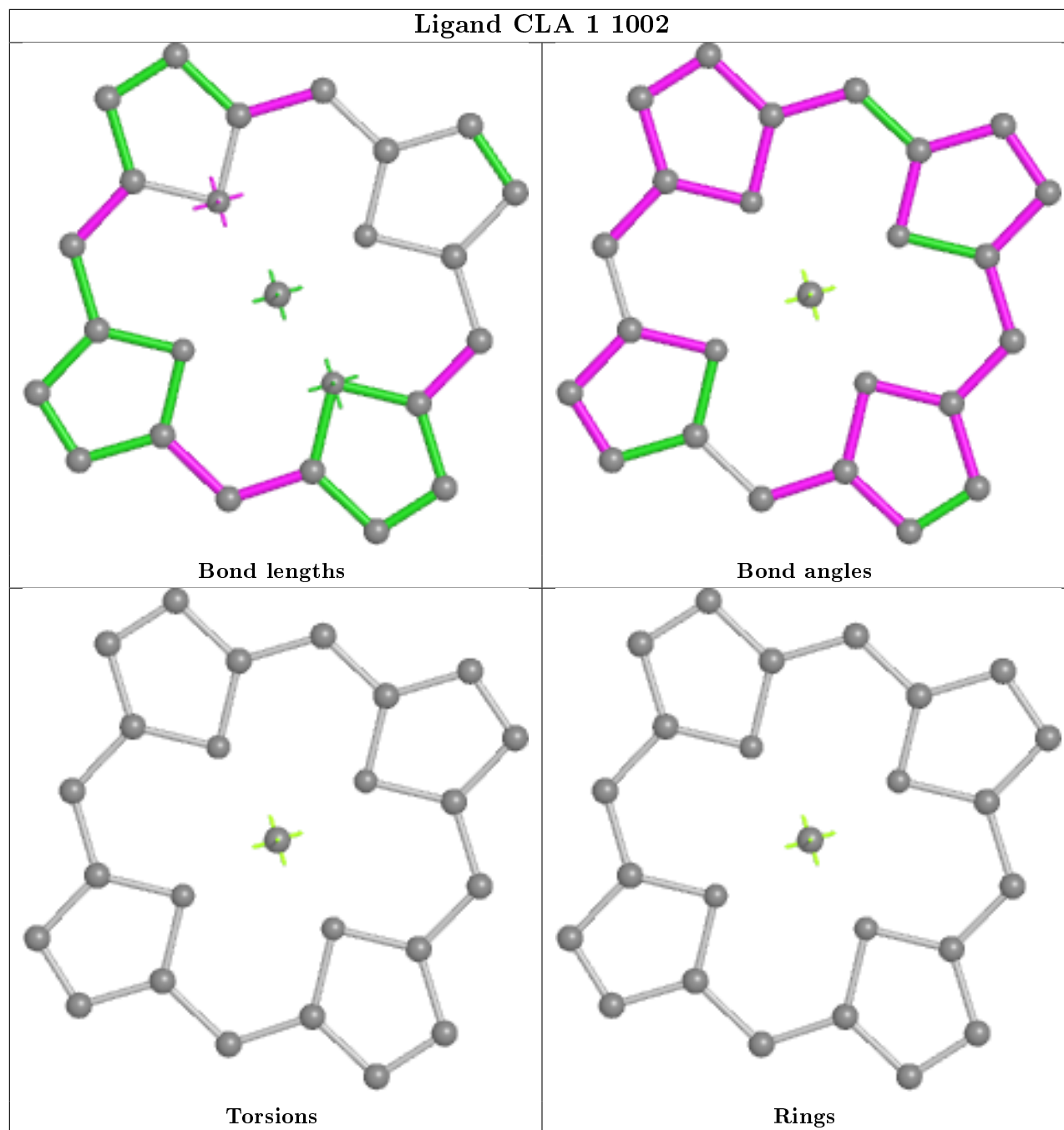
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	2007	CLA	2	0
18	B	1214	CLA	32	0
18	J	2107	CLA	8	0
18	3	3004	CLA	2	0
18	B	1203	CLA	14	0
18	A	1148	CLA	4	0
18	B	1138	CLA	28	0
18	A	1137	CLA	20	0
18	B	1227	CLA	23	0
18	B	1226	CLA	4	0
18	B	1230	CLA	6	0
18	B	1217	CLA	14	0
18	A	1119	CLA	7	0
18	A	1113	CLA	6	0
18	A	1146	CLA	1	0
18	B	1239	CLA	33	0
19	B	5002	PQN	20	0
18	A	1129	CLA	17	0
18	A	1126	CLA	23	0
18	A	1105	CLA	3	0
18	A	1116	CLA	5	0
18	B	1210	CLA	15	0
20	B	6017	BCR	20	0
18	B	1209	CLA	36	0
18	B	1228	CLA	27	0
18	A	1103	CLA	19	0
18	B	1234	CLA	25	0
18	3	3007	CLA	1	0
18	B	1235	CLA	20	0
18	L	1130	CLA	23	0
18	B	1222	CLA	13	0

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

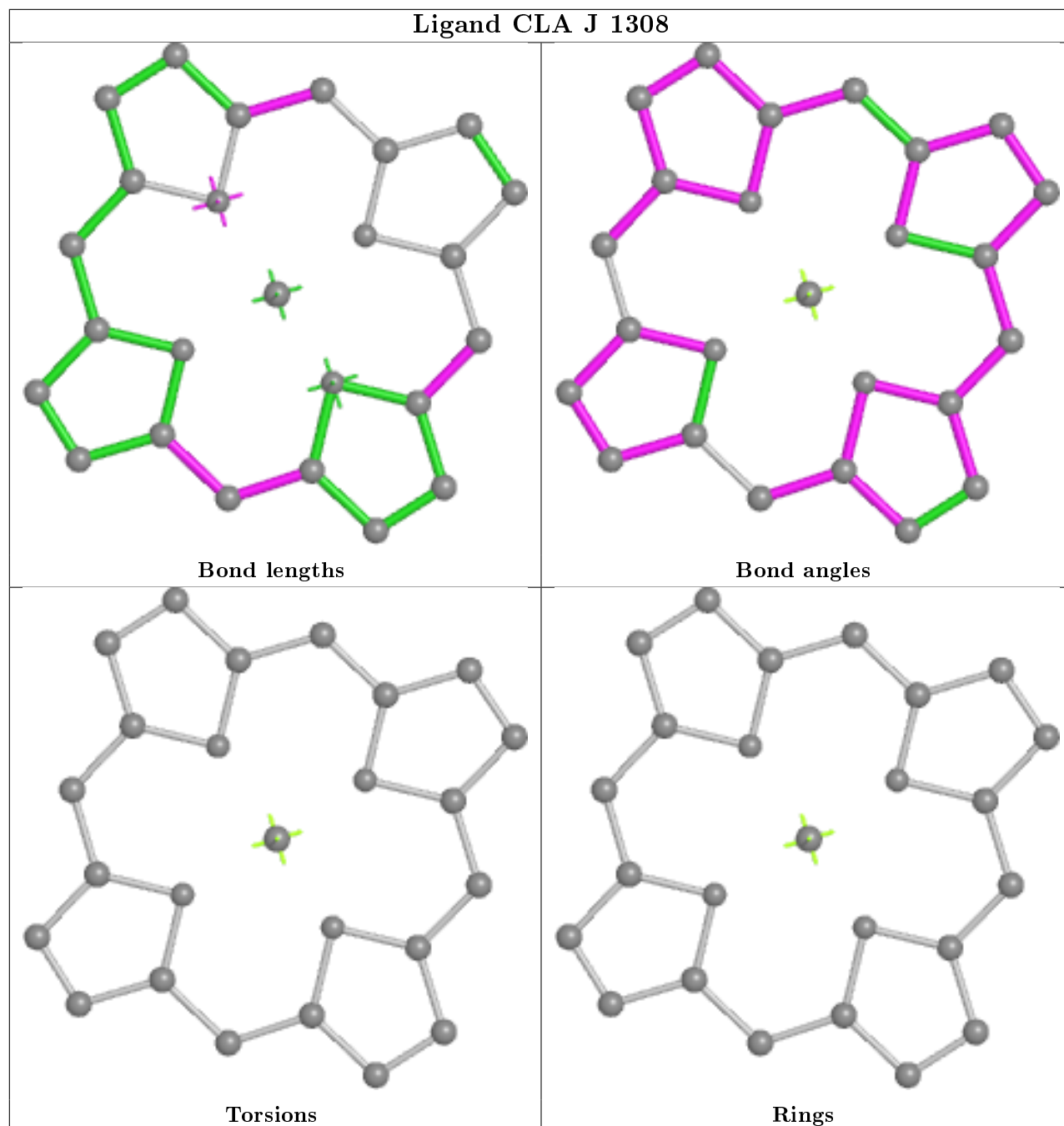
equivalents in the CSD to analyse the geometry.

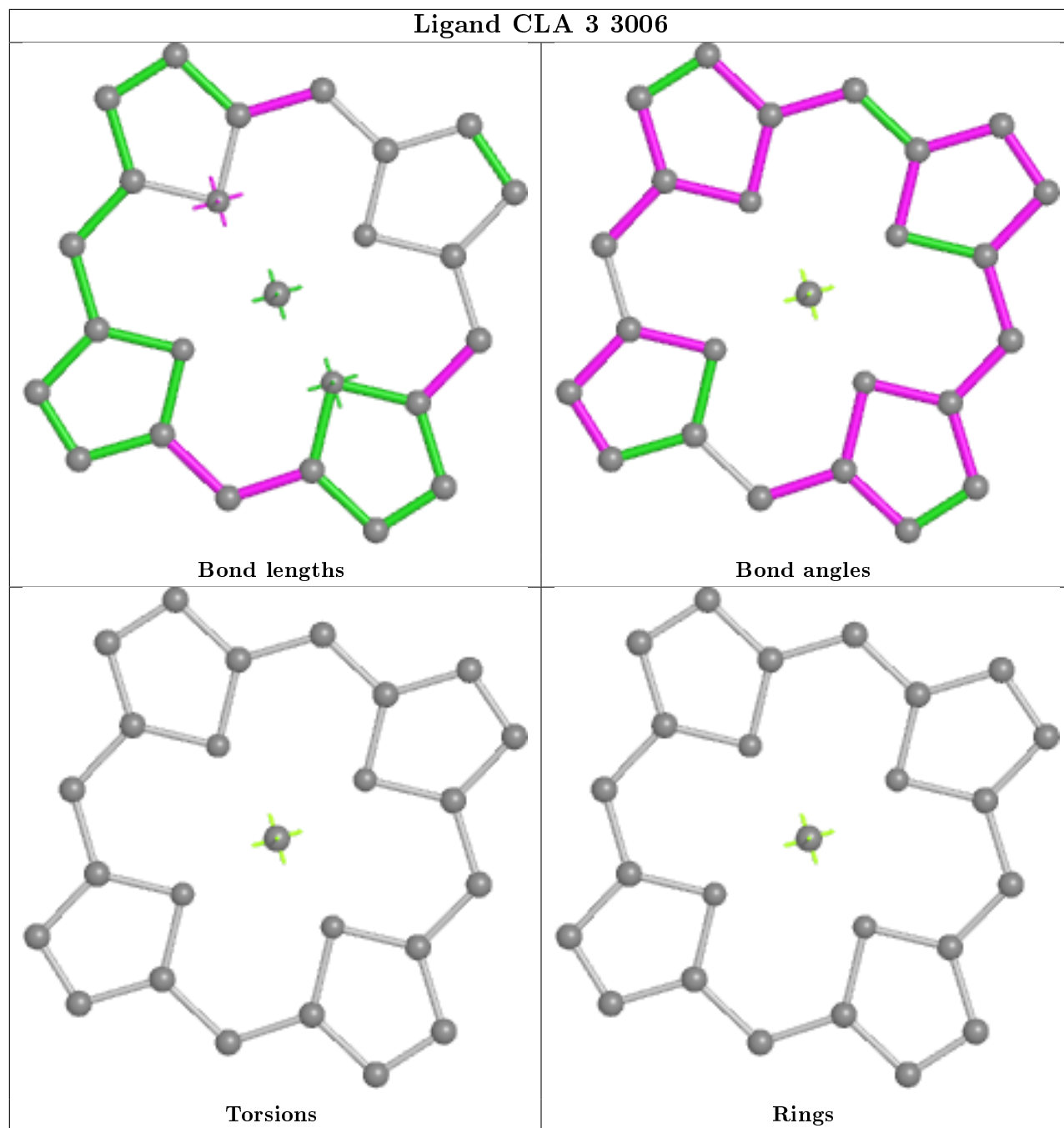




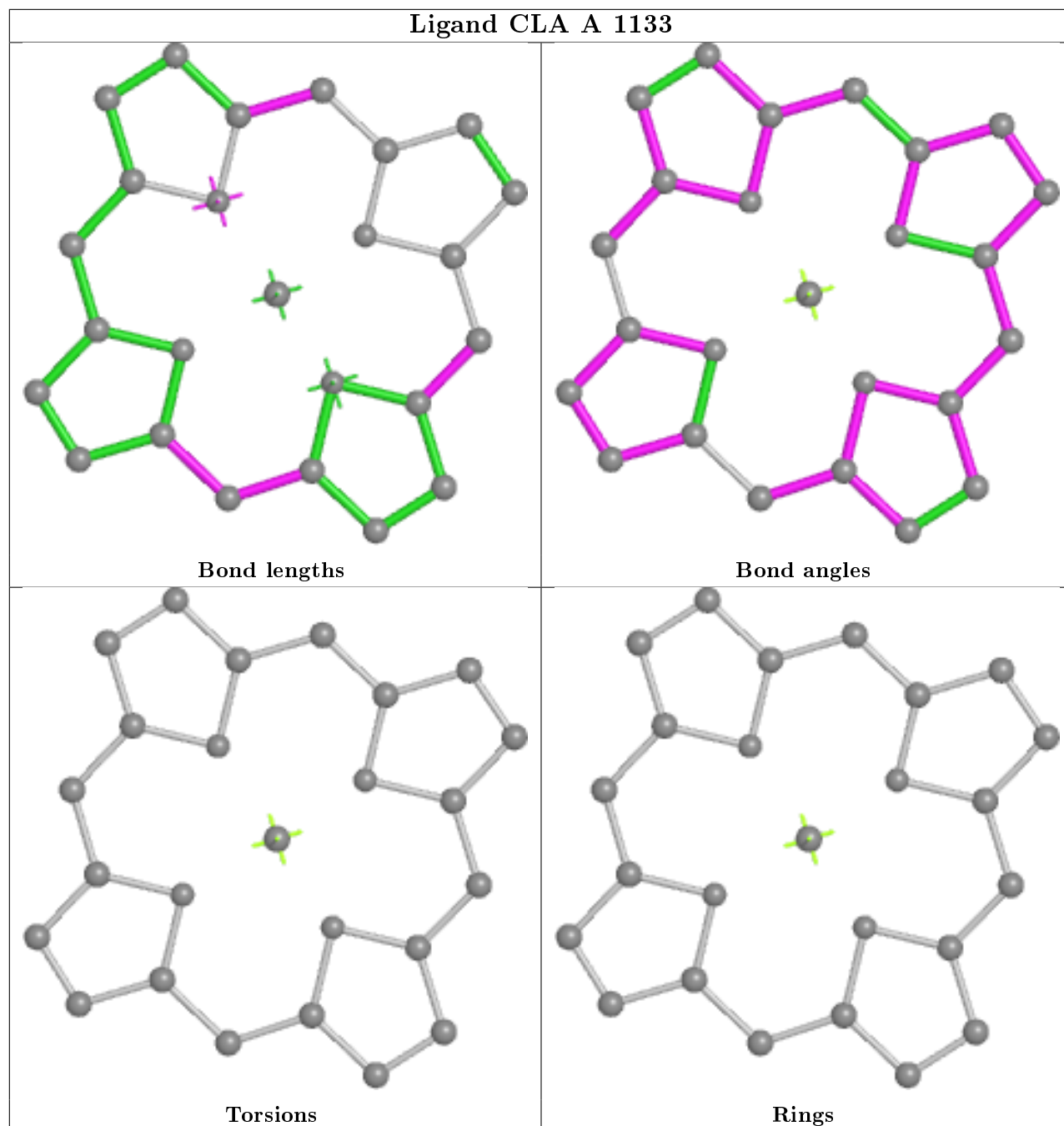


Ligand CLA J 1308

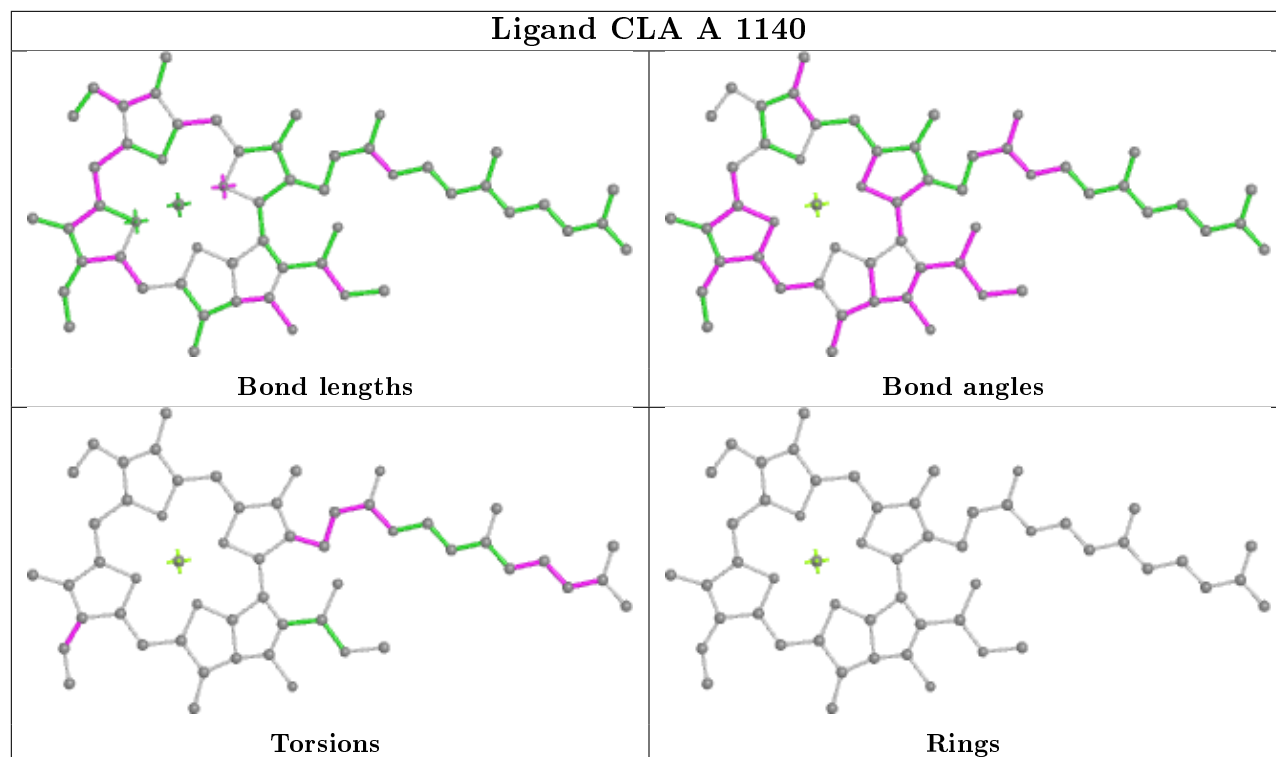




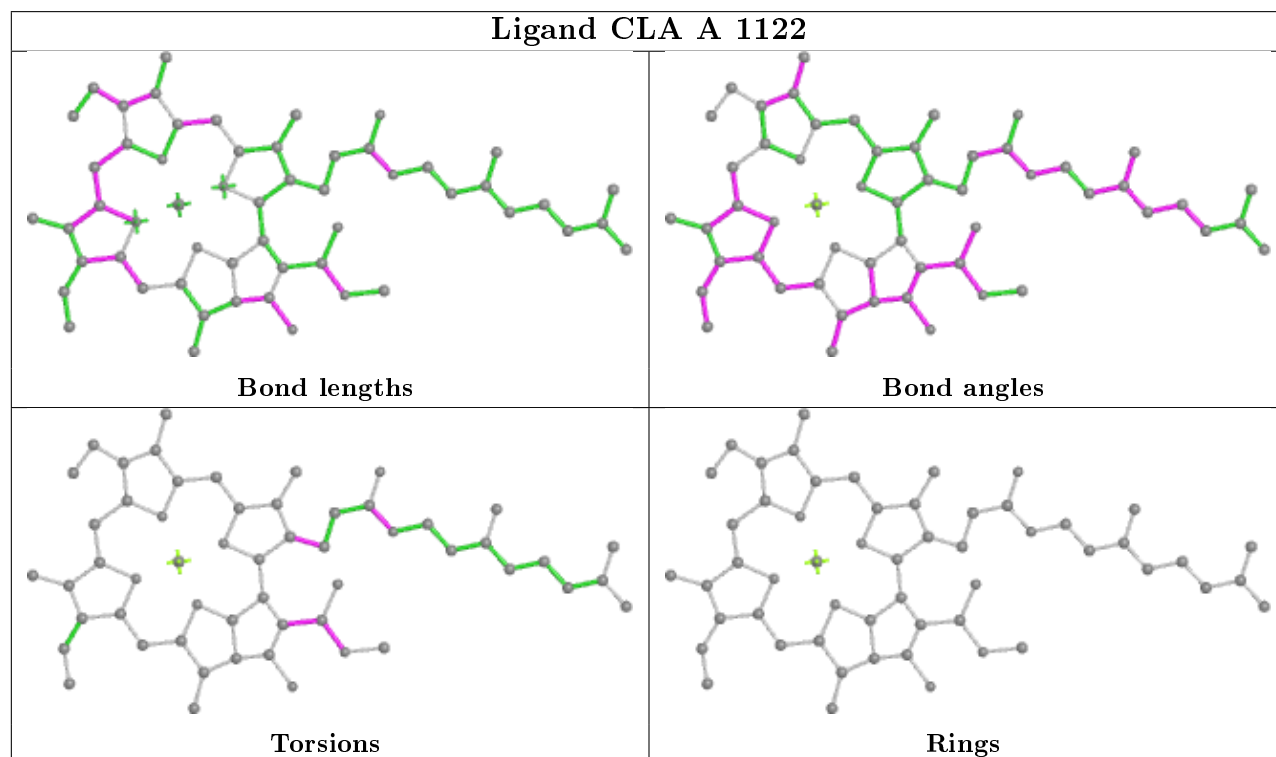
Ligand CLA A 1133



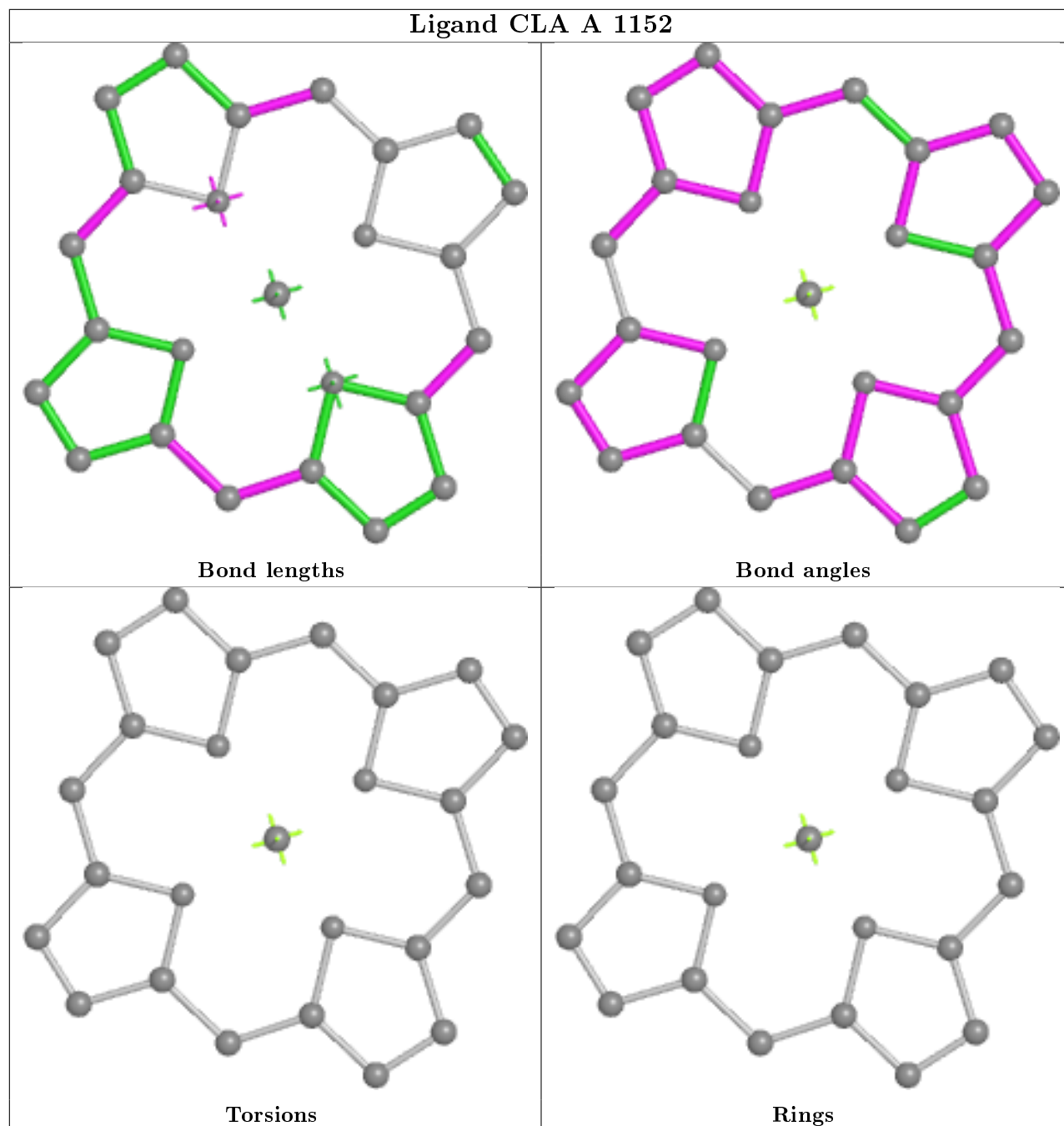
Ligand CLA A 1140

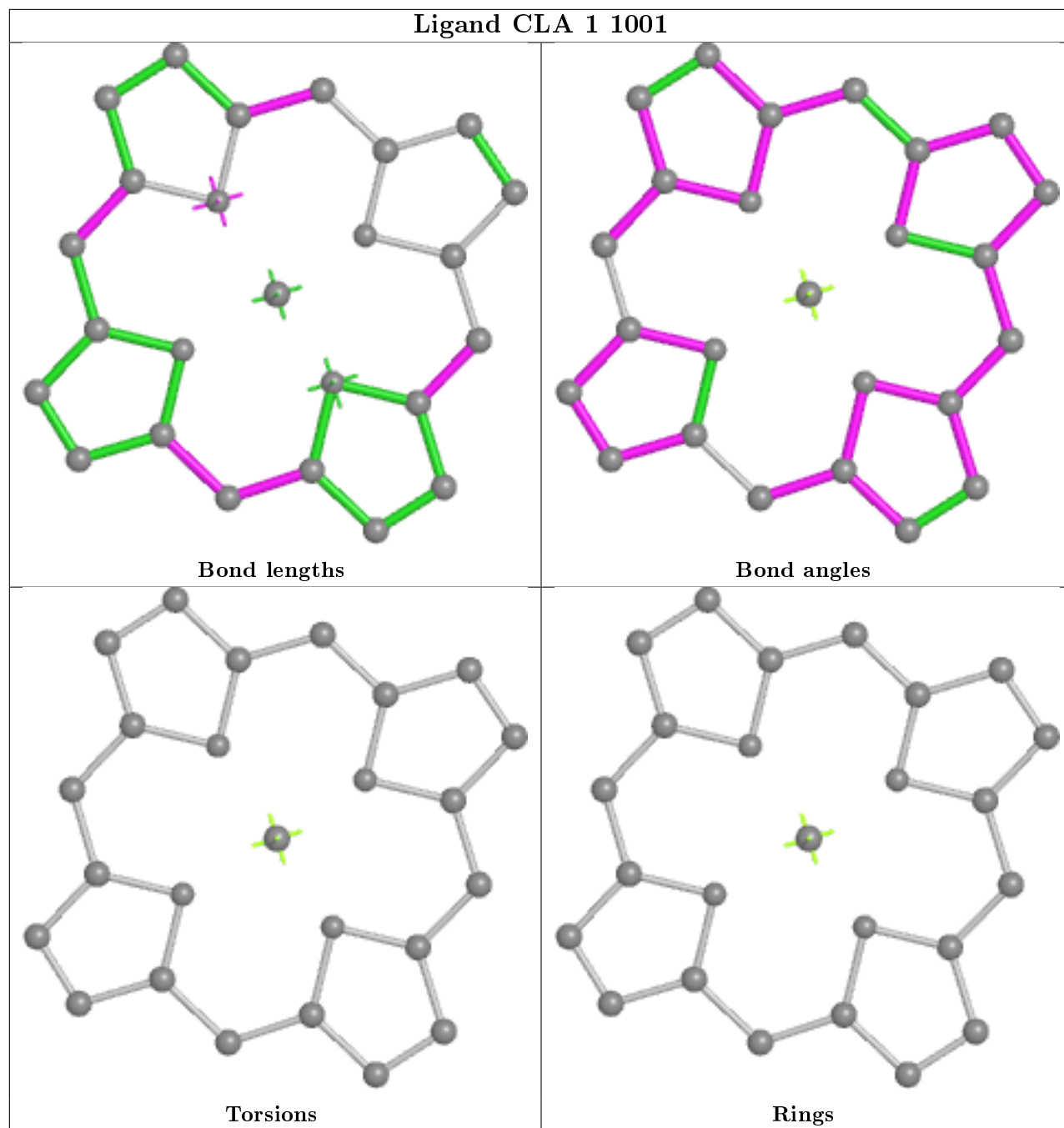


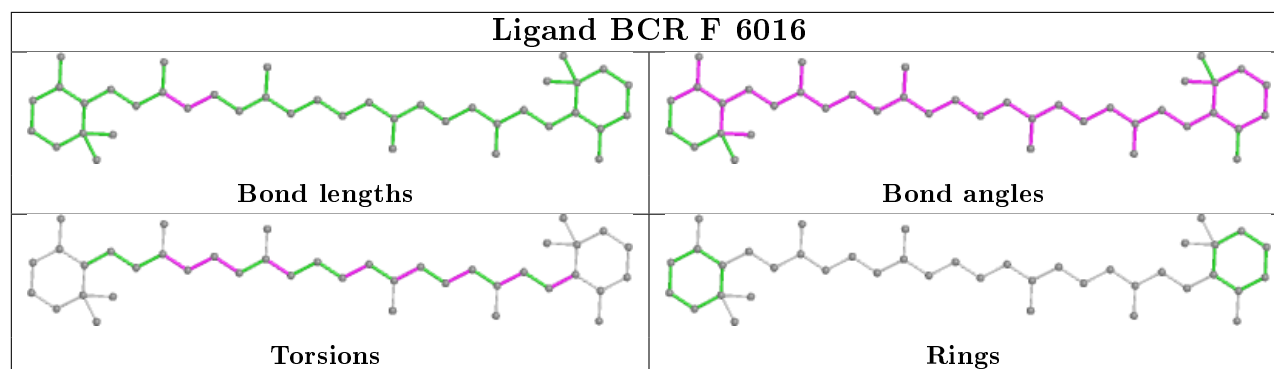
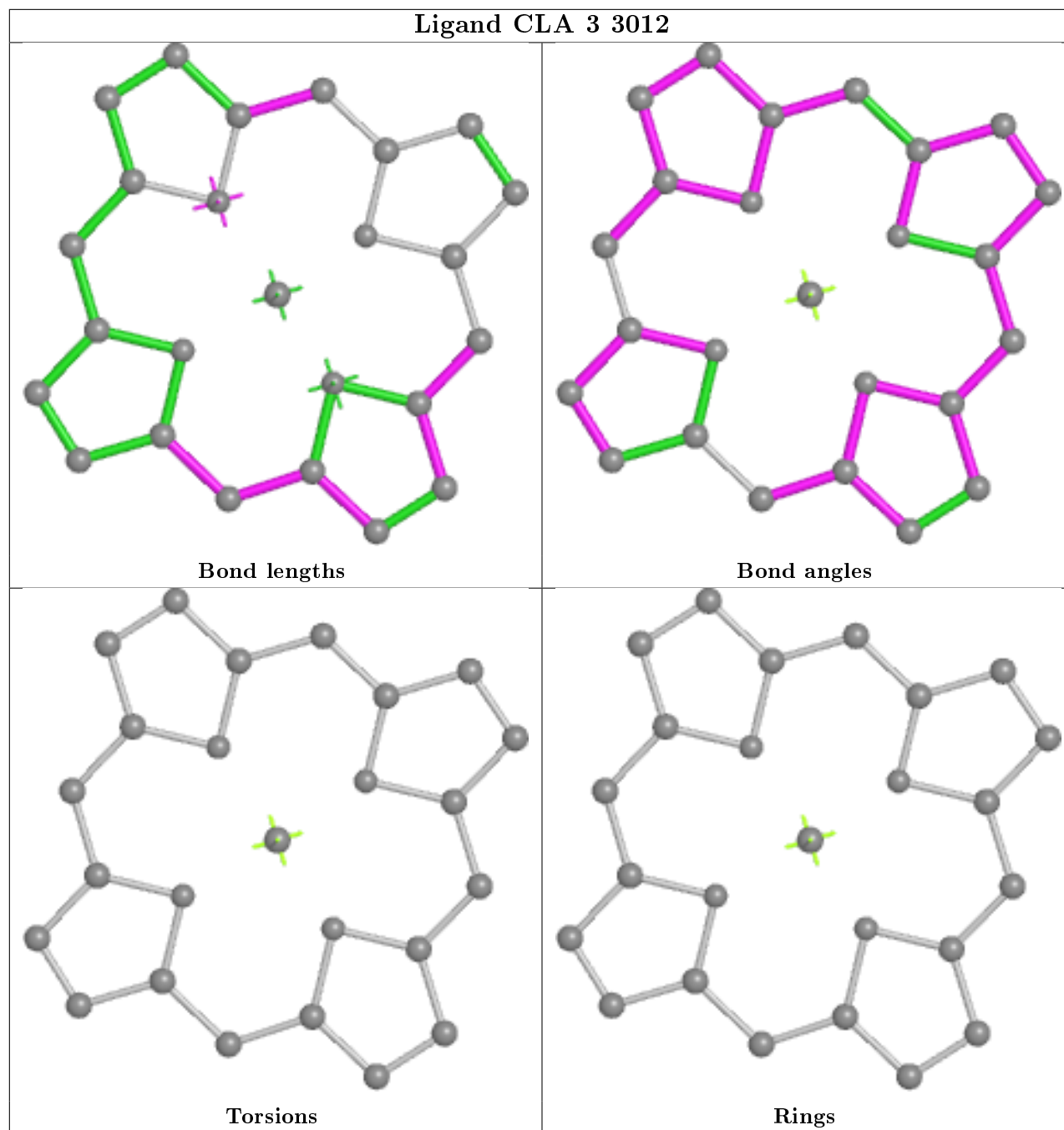
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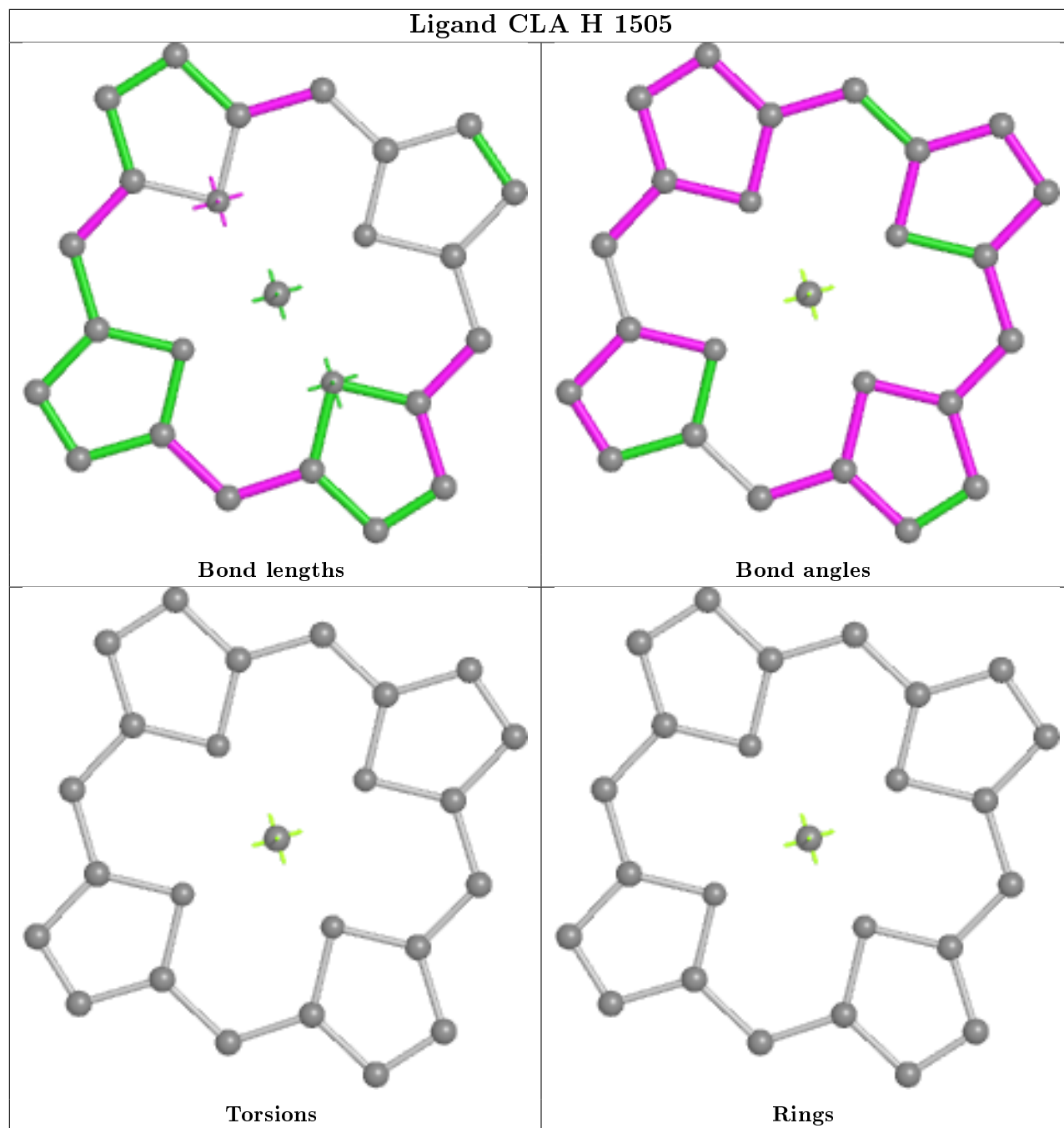
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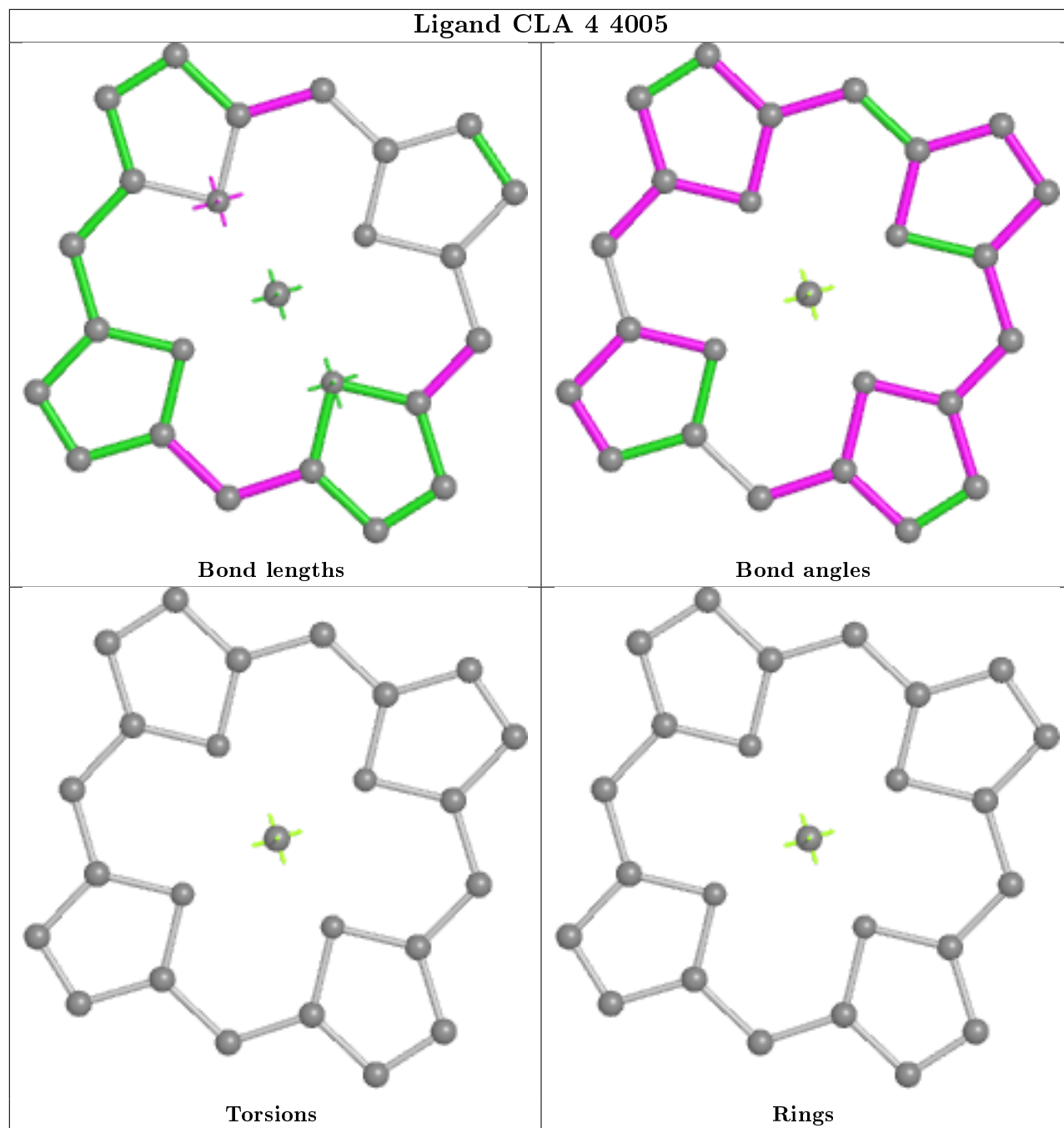




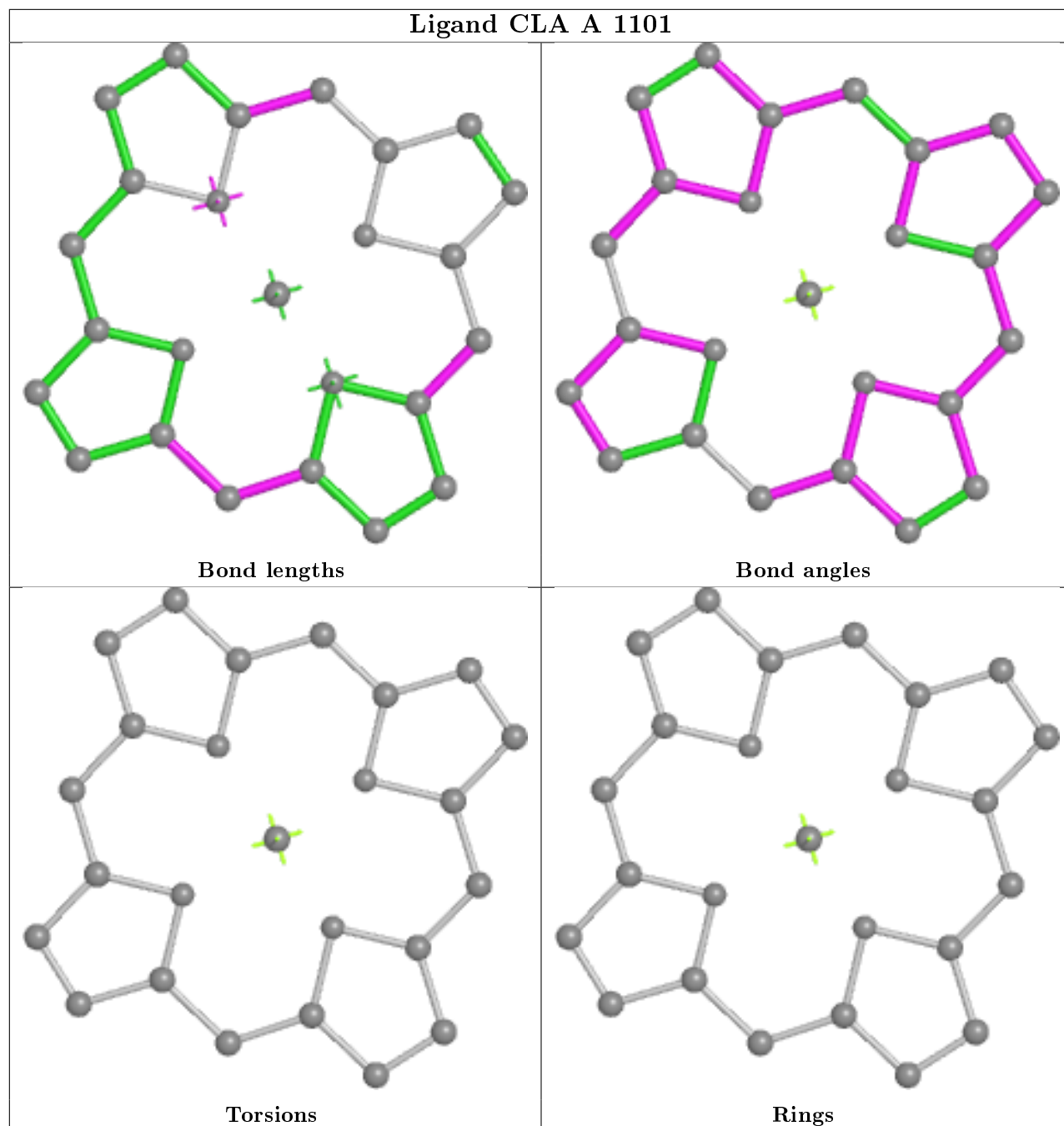


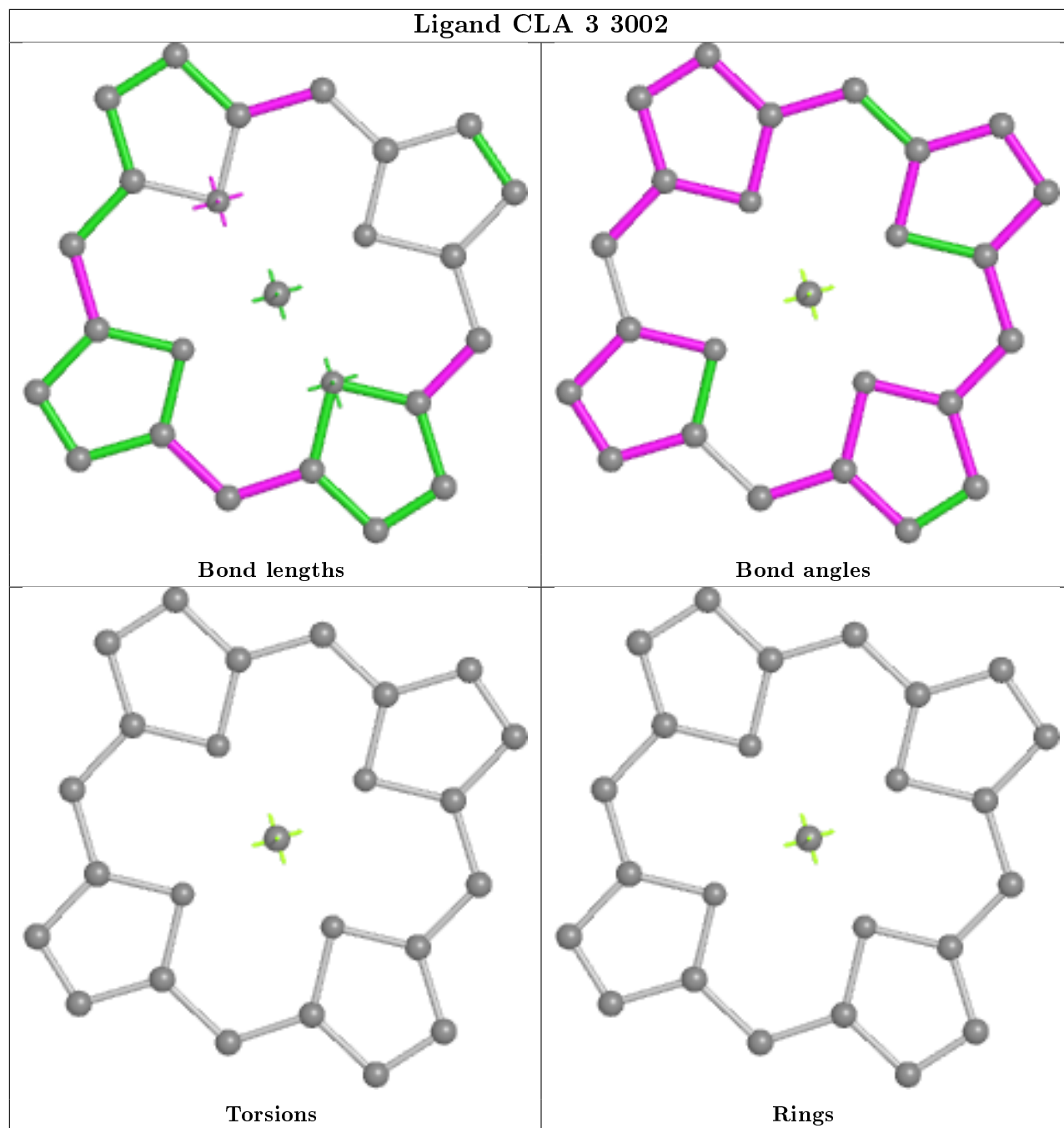
Ligand CLA H 1505



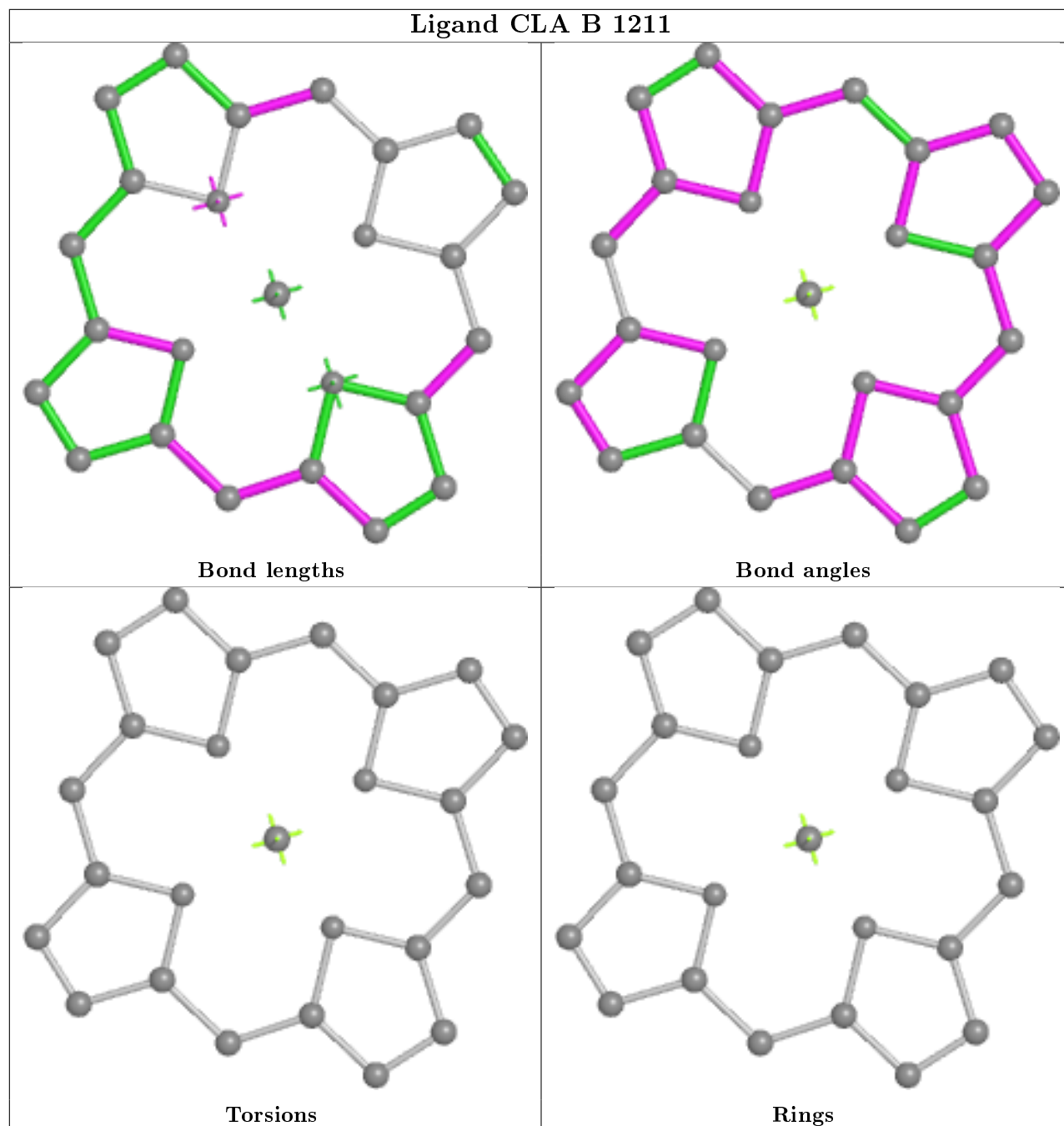


Ligand CLA A 1101

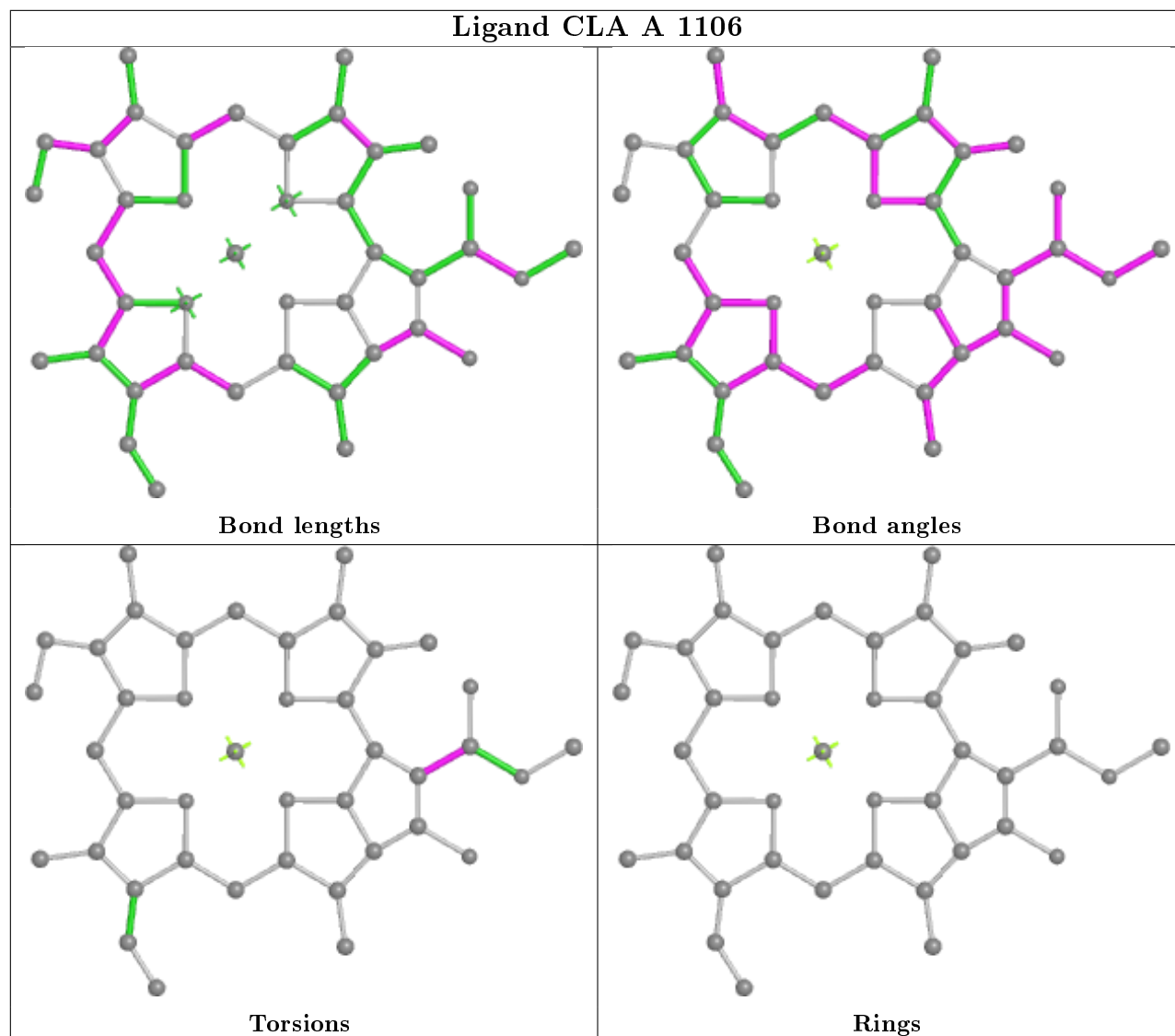


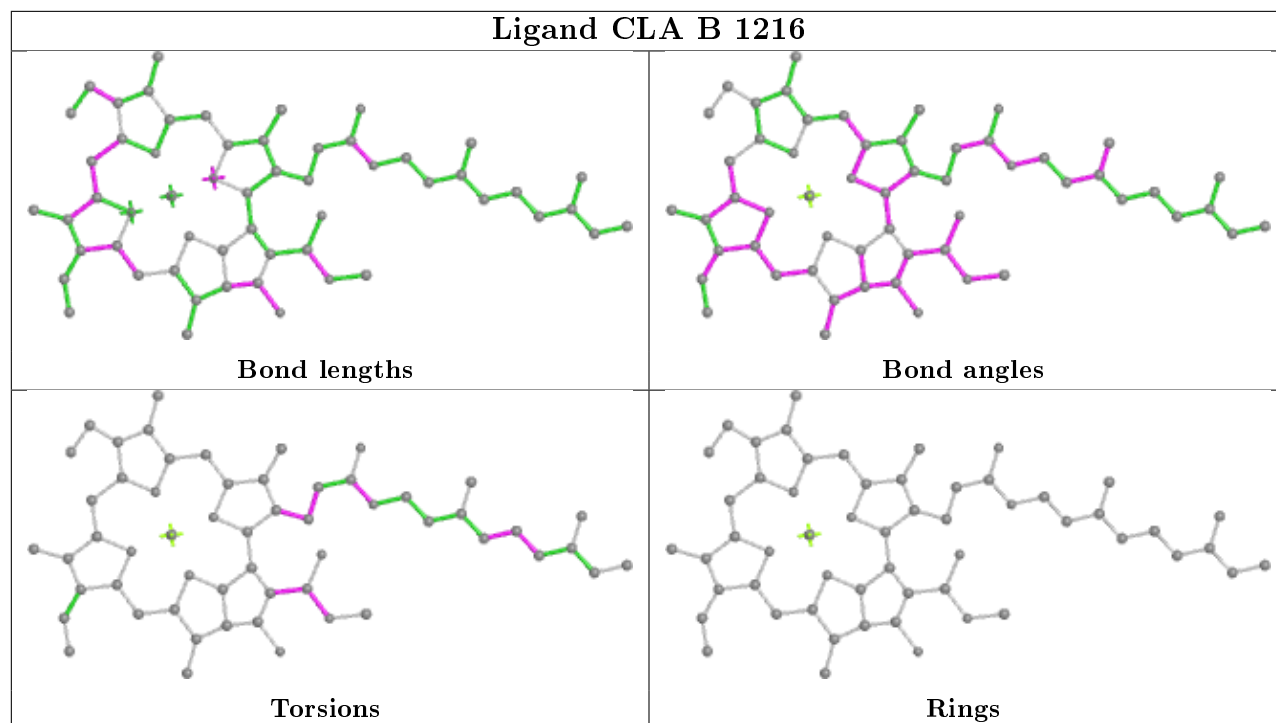


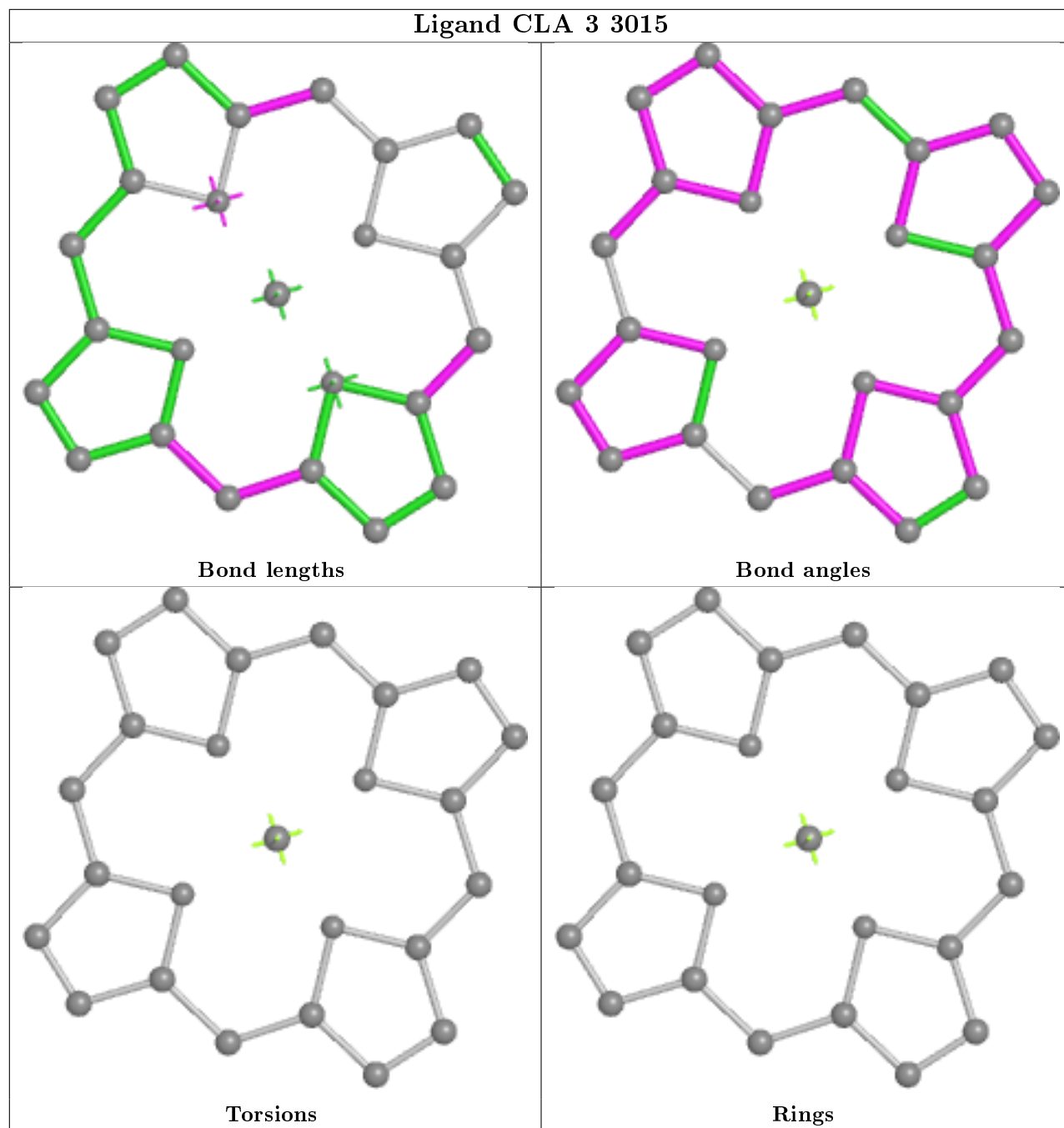
Ligand CLA B 1211

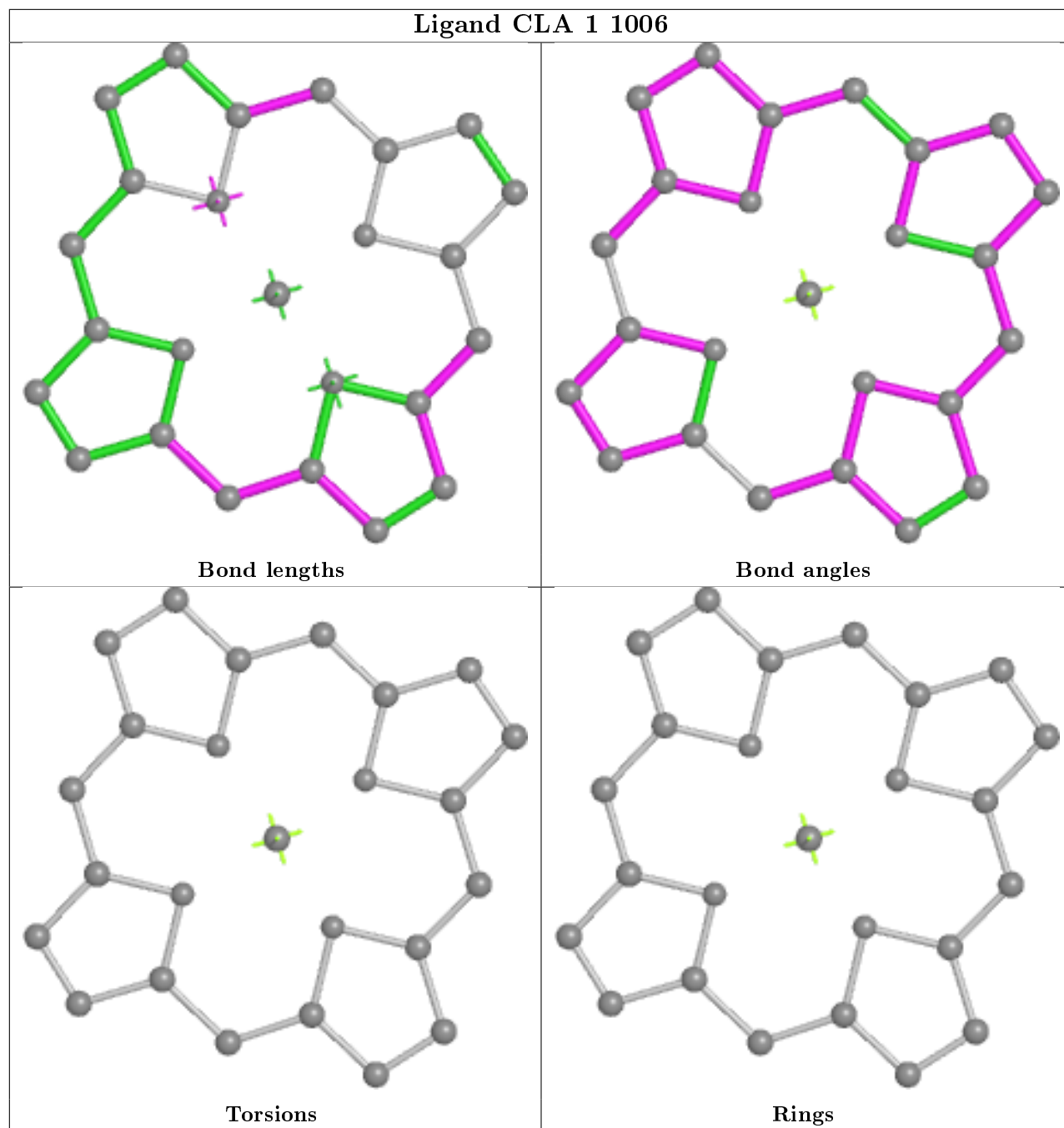


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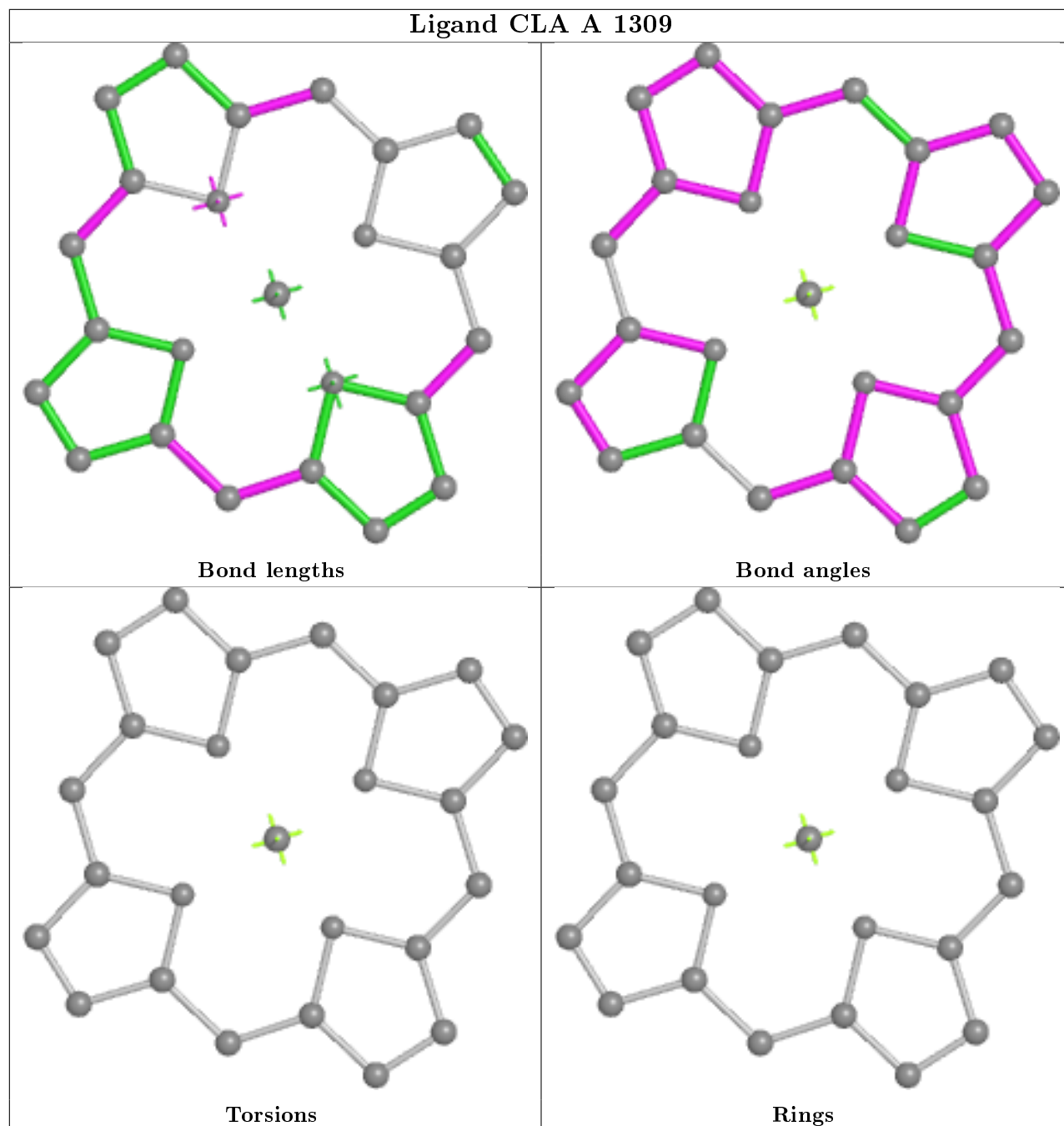


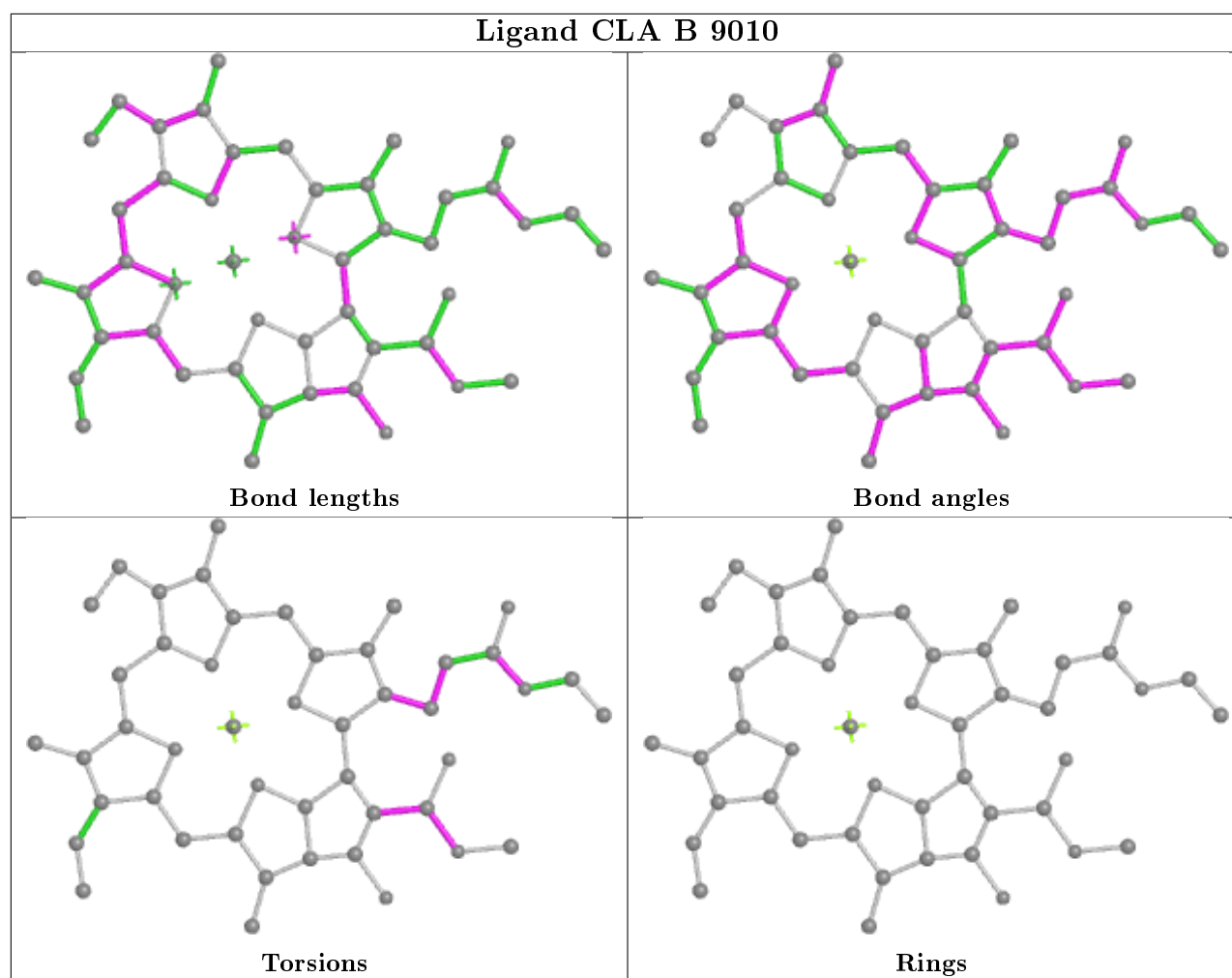




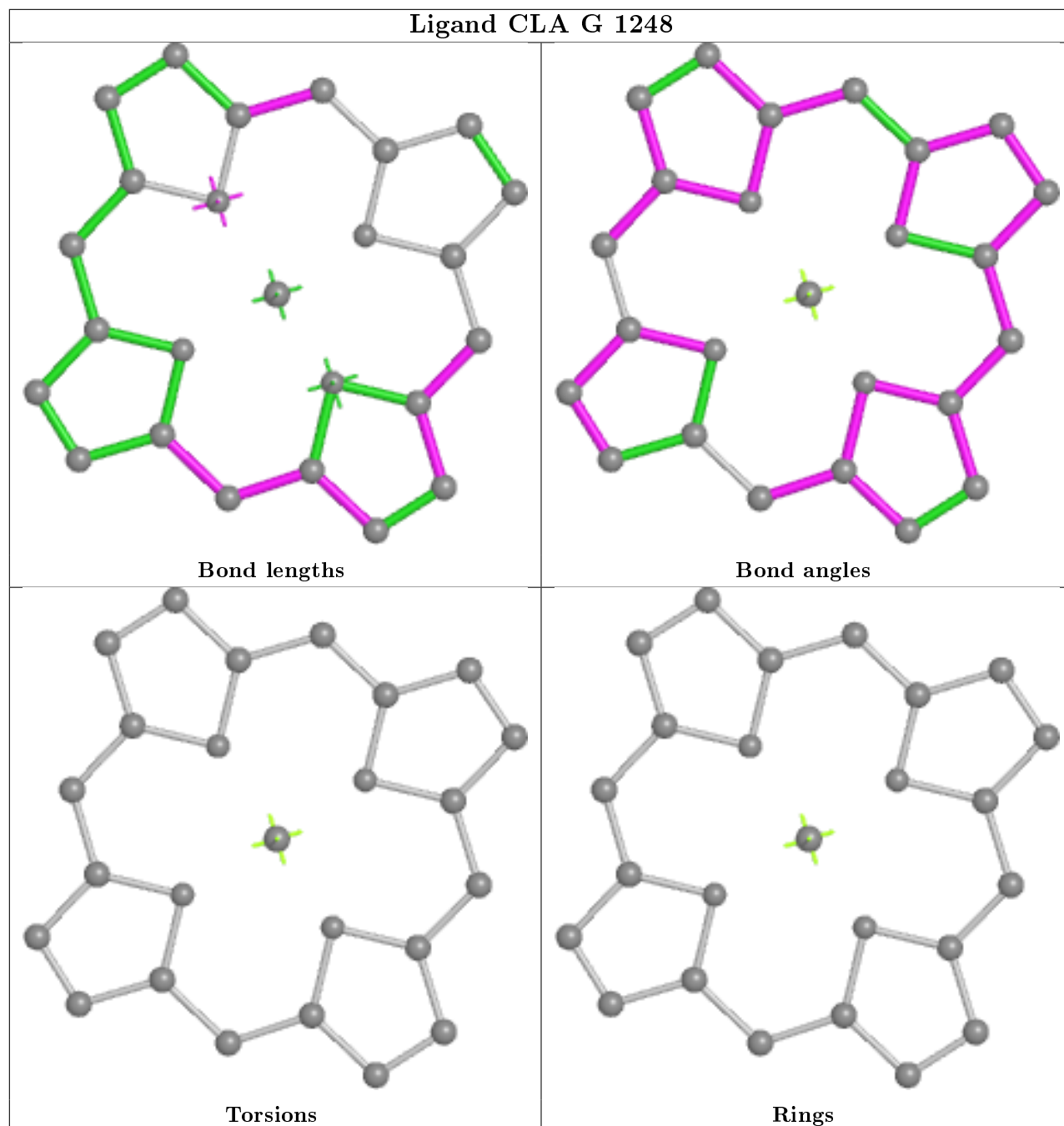


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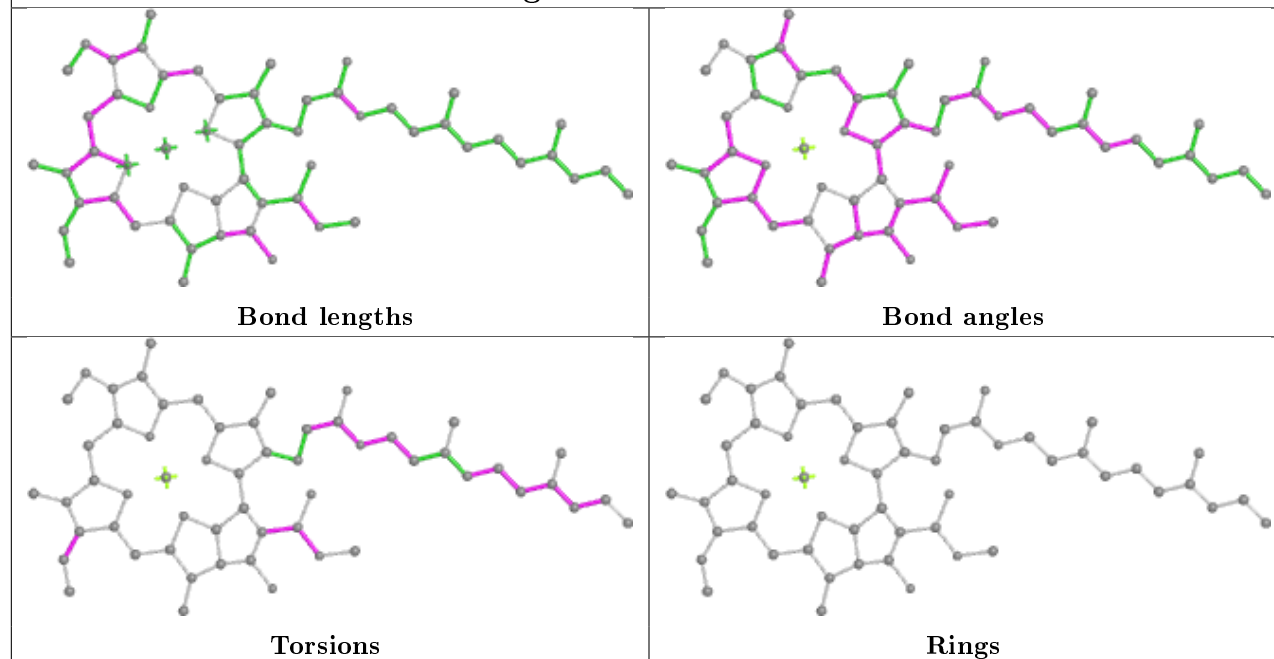




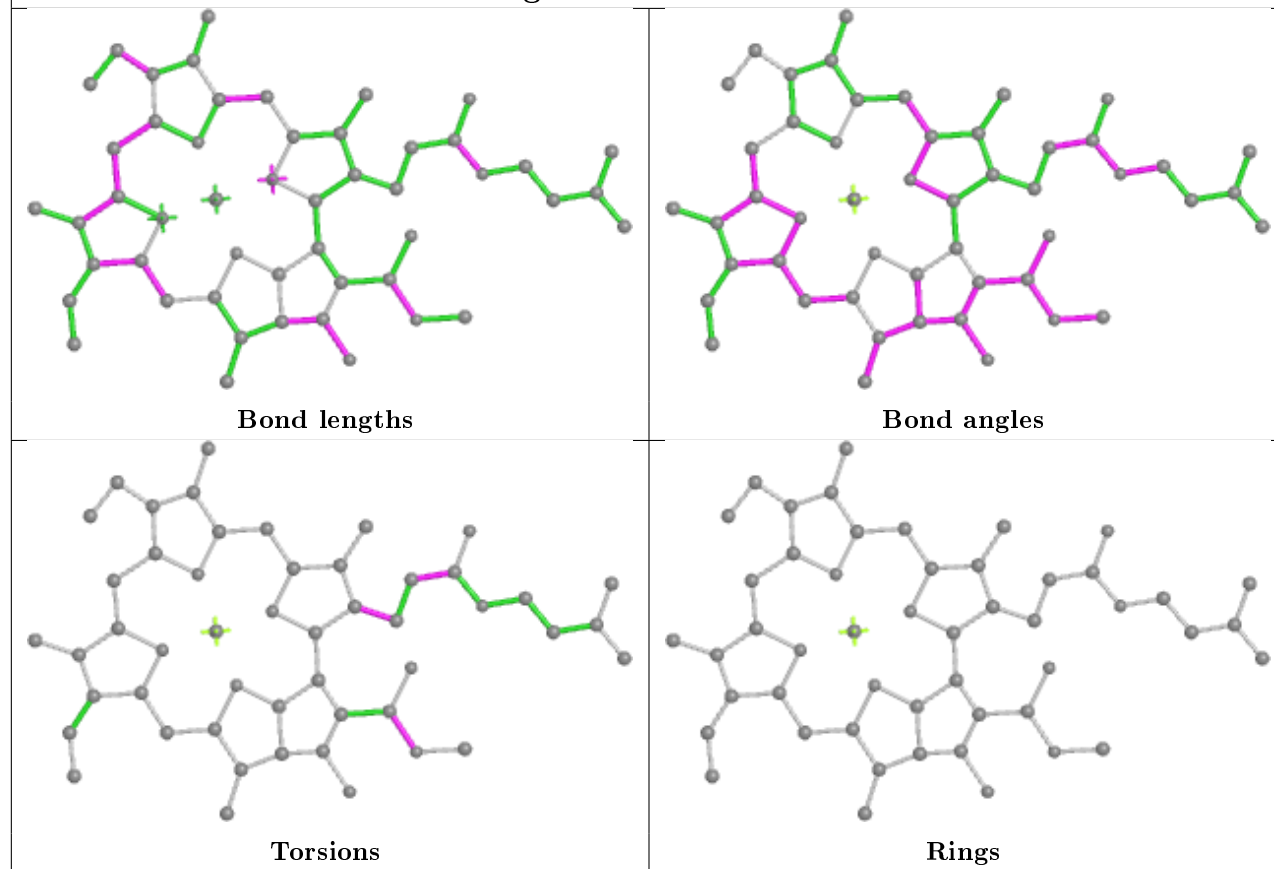
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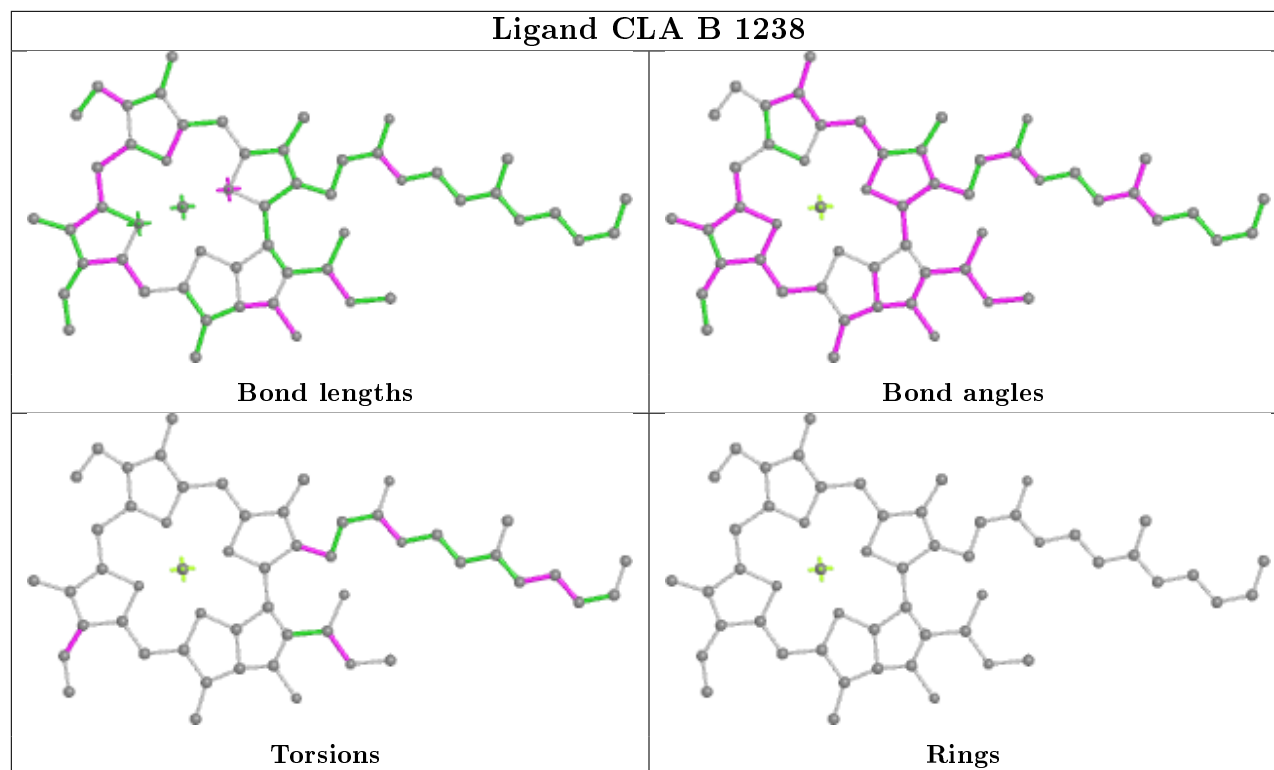
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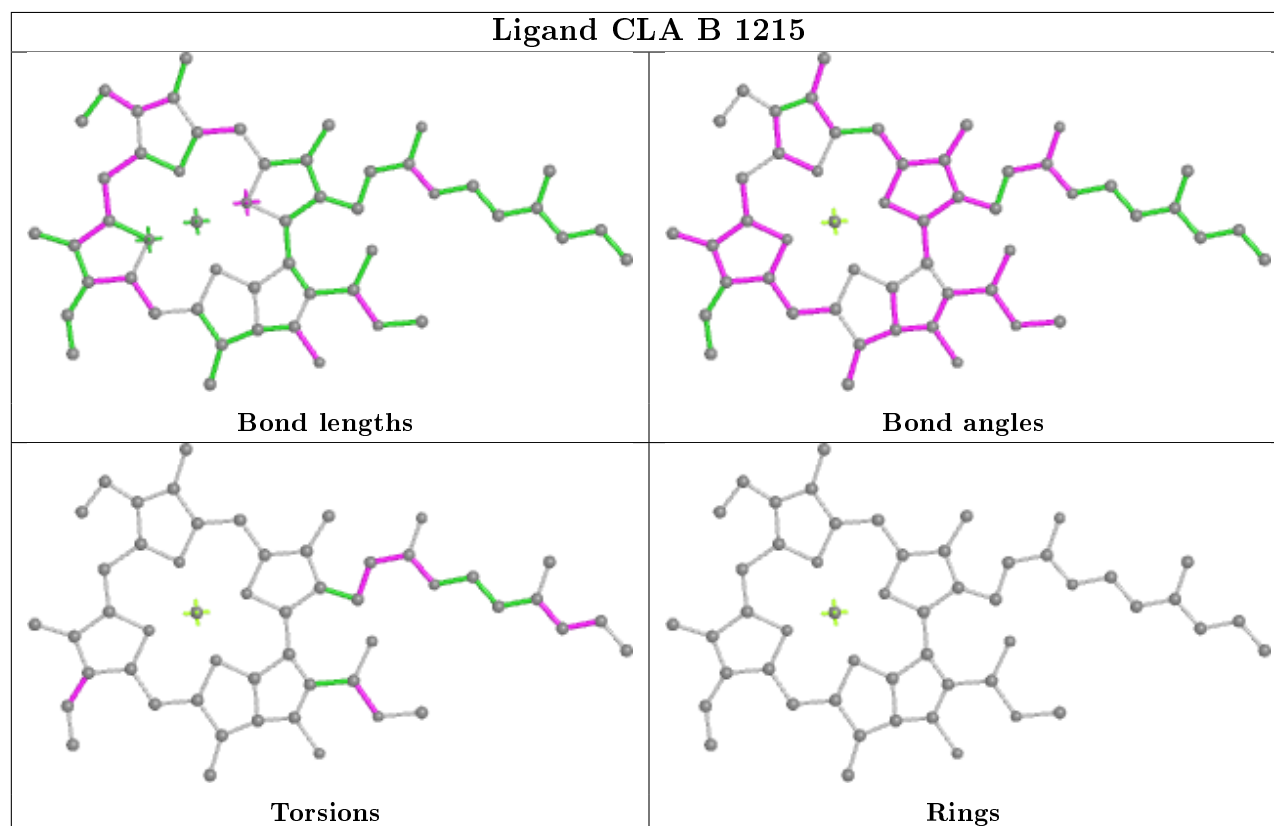
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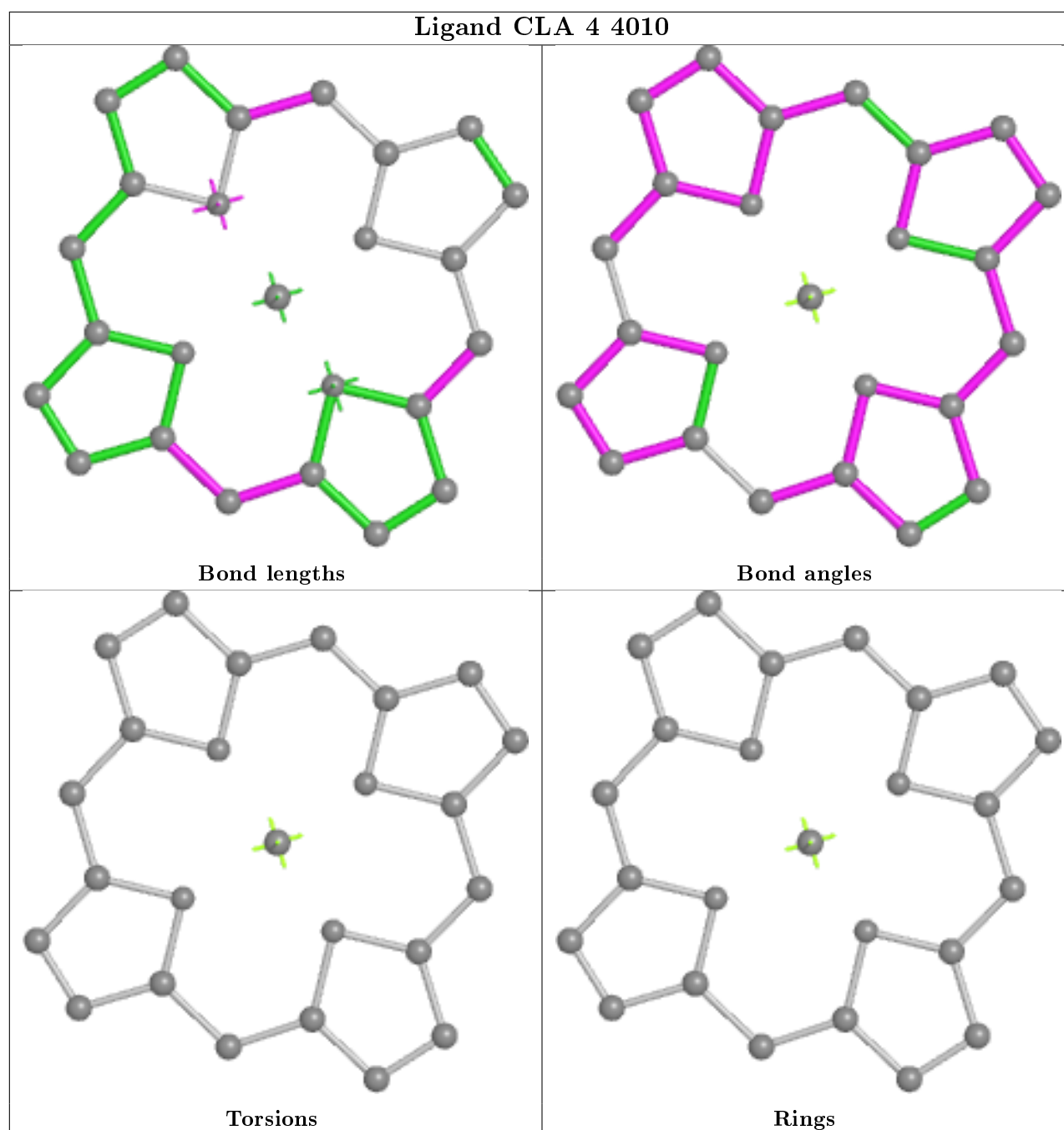


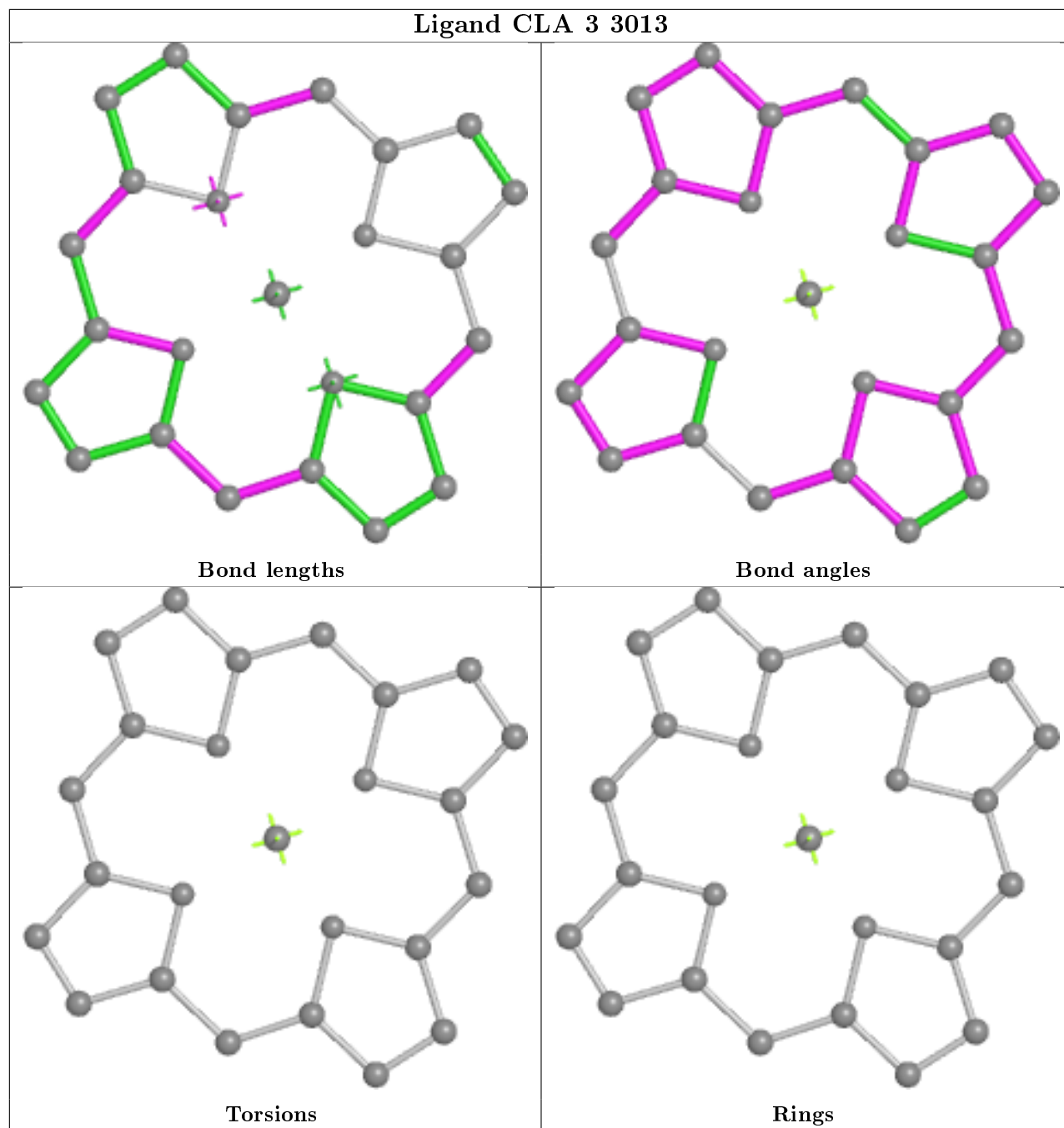
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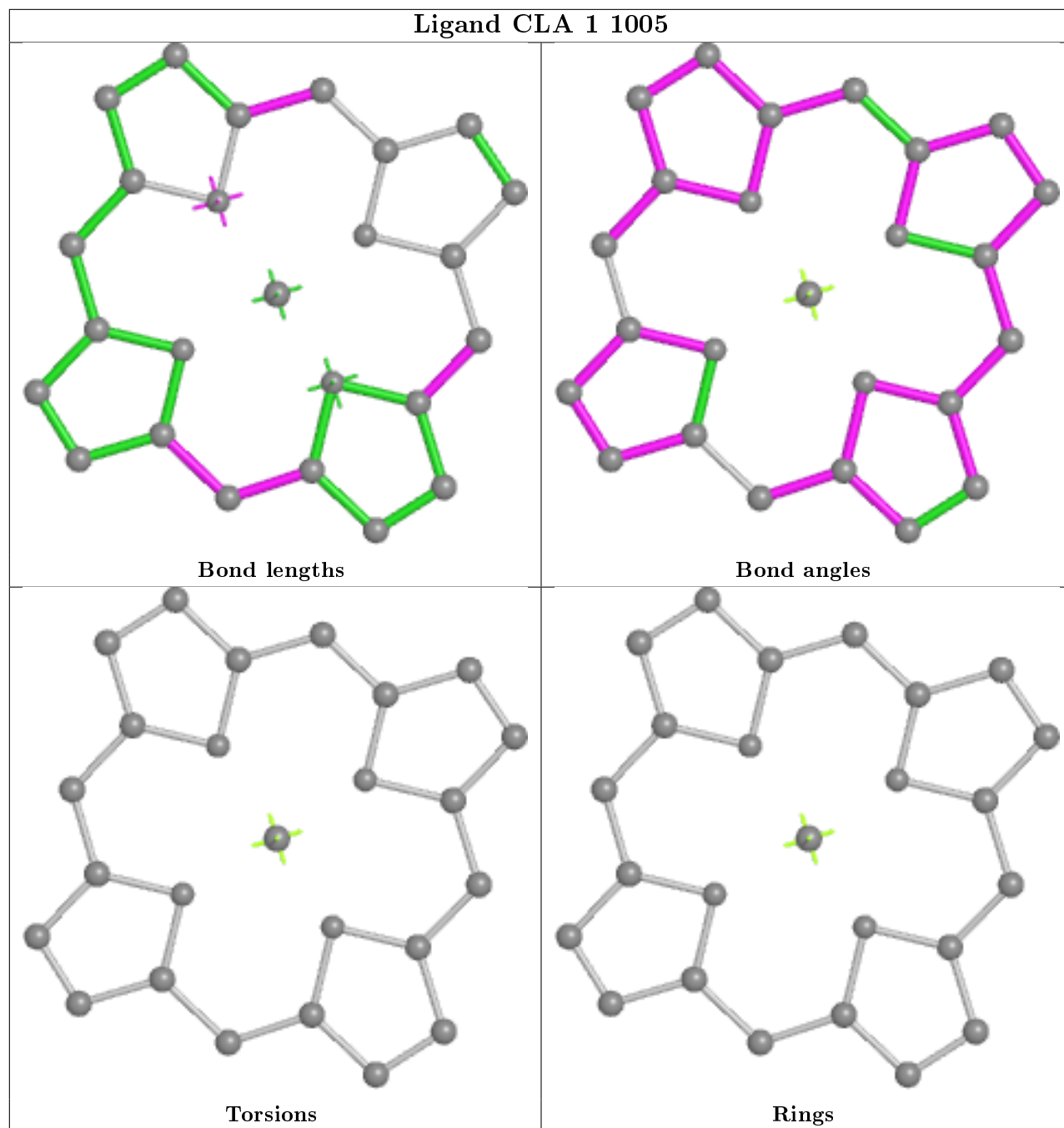


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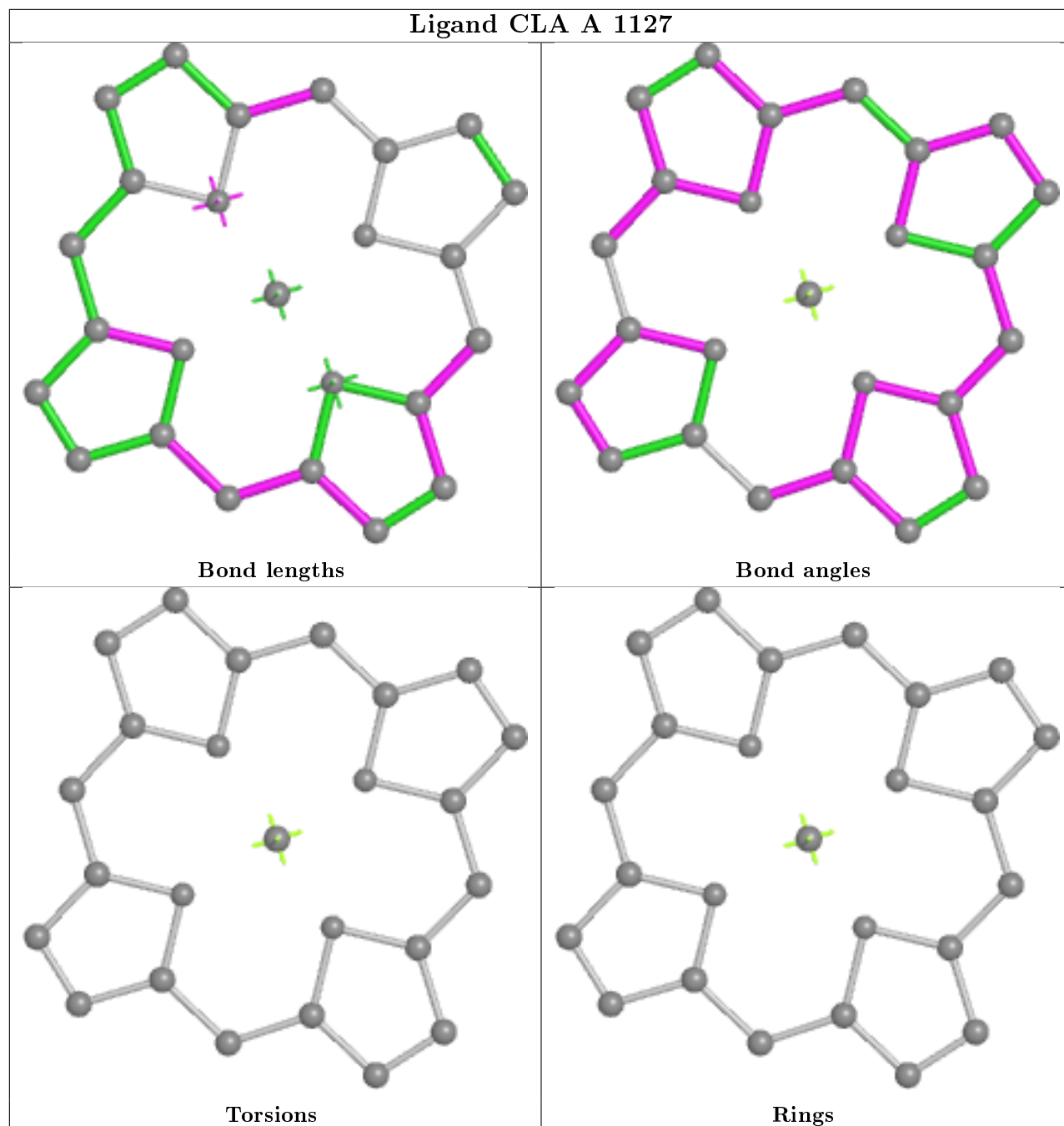


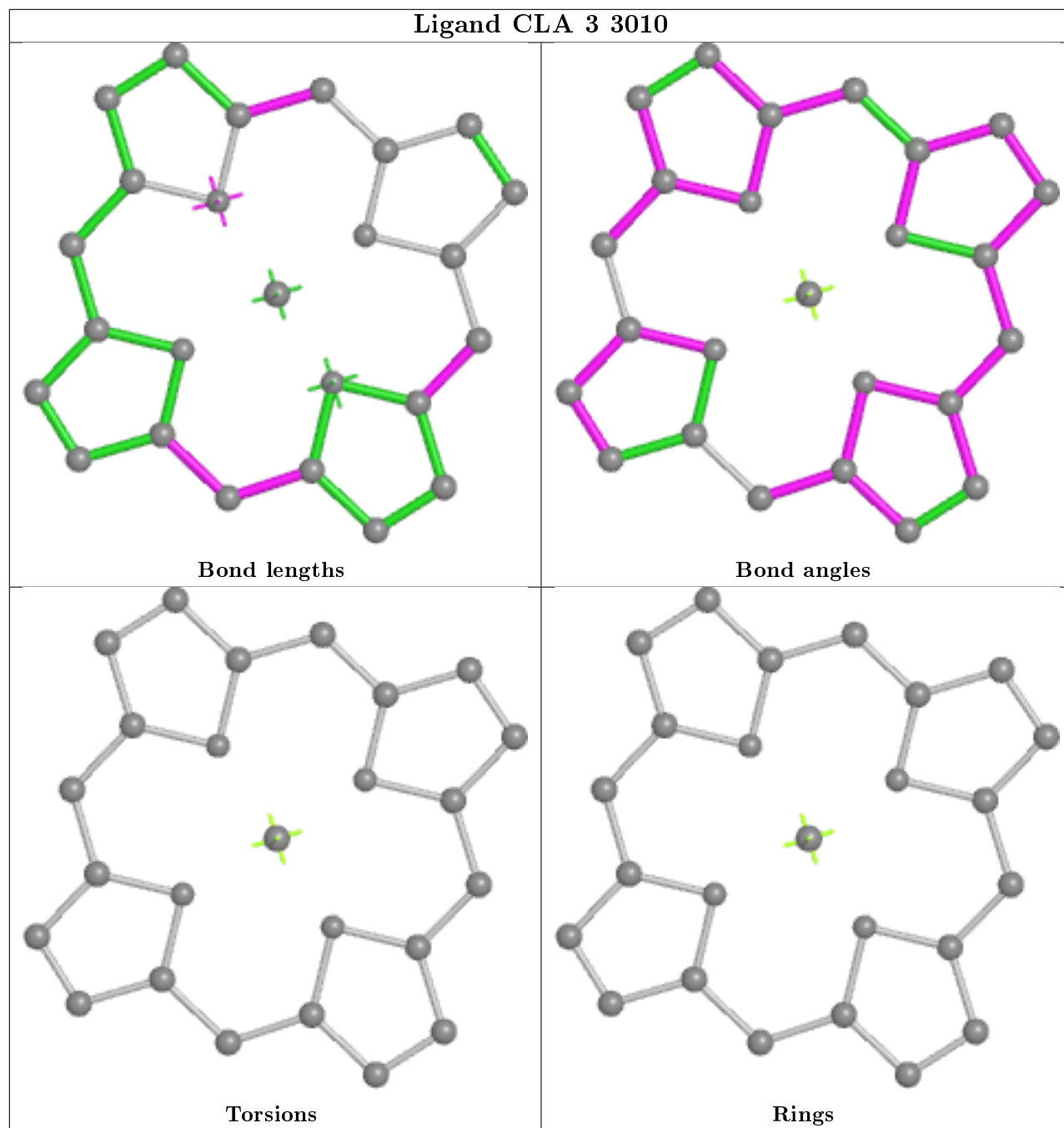


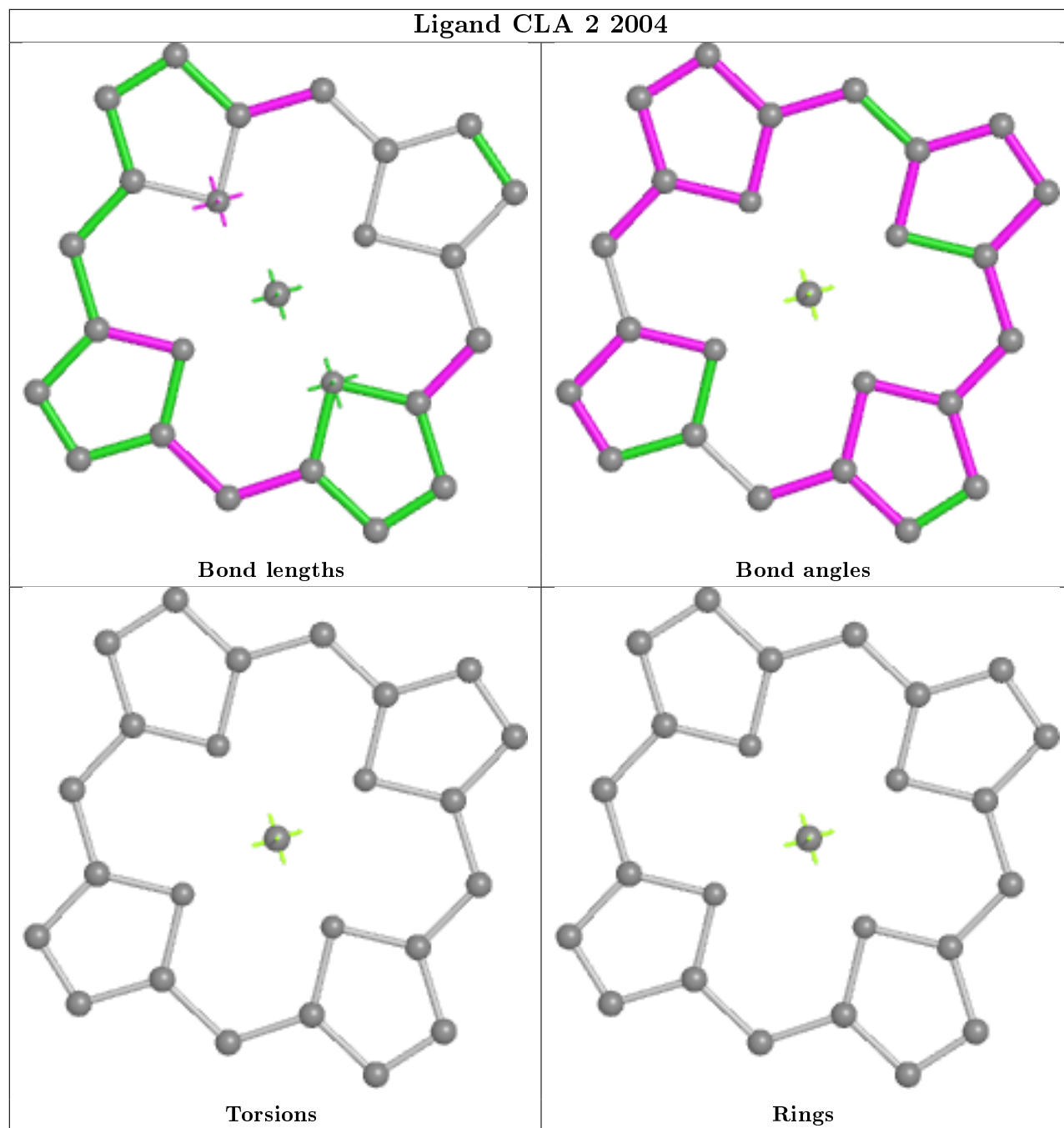


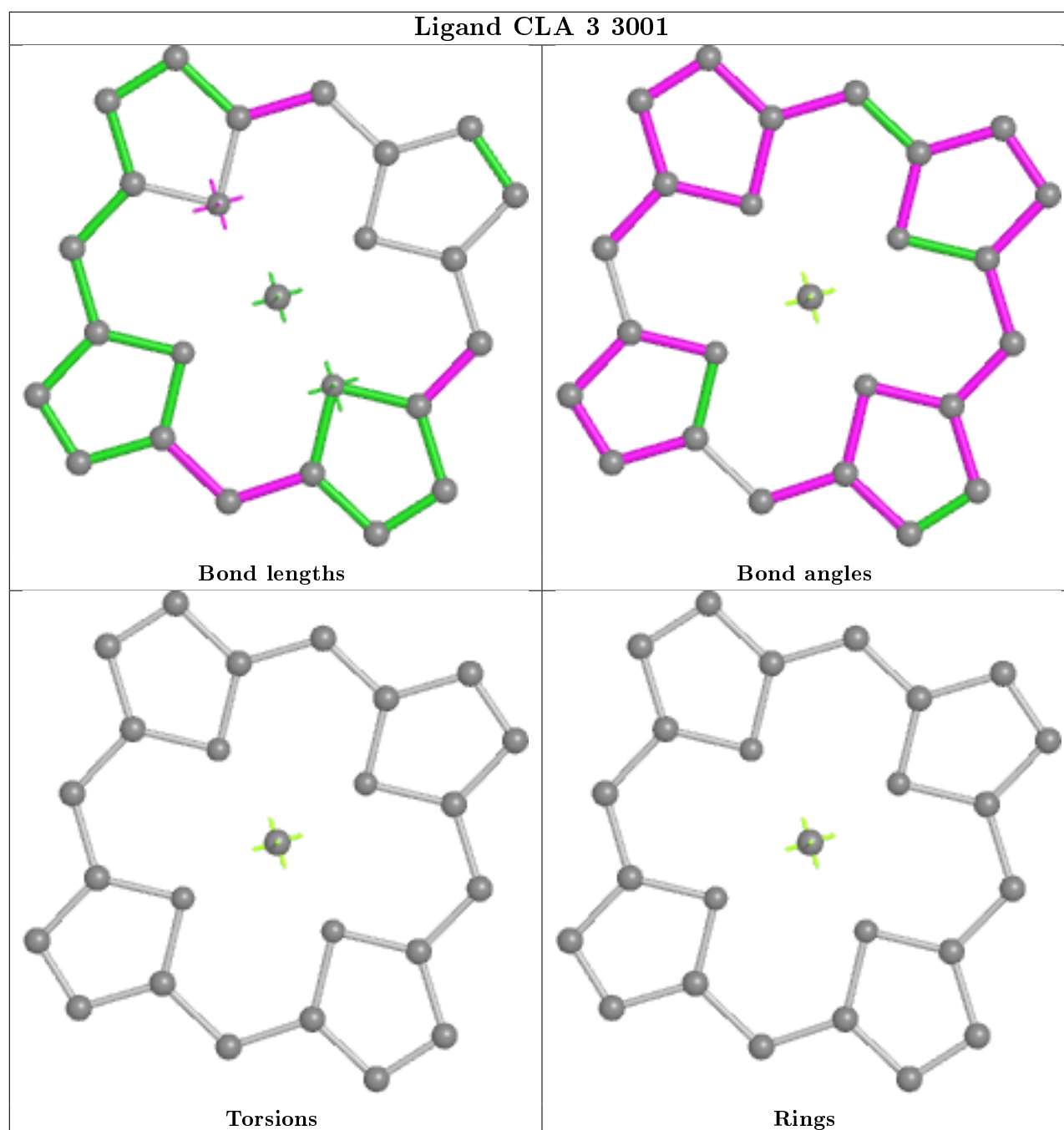


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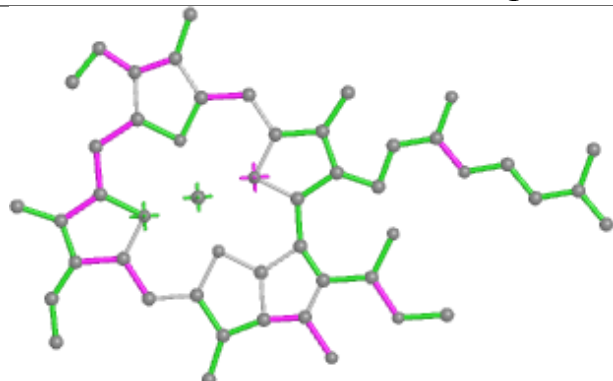




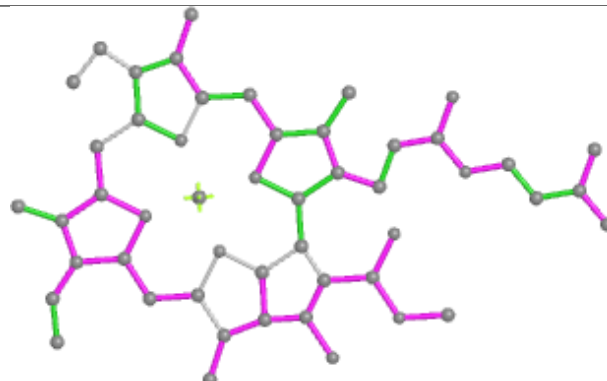




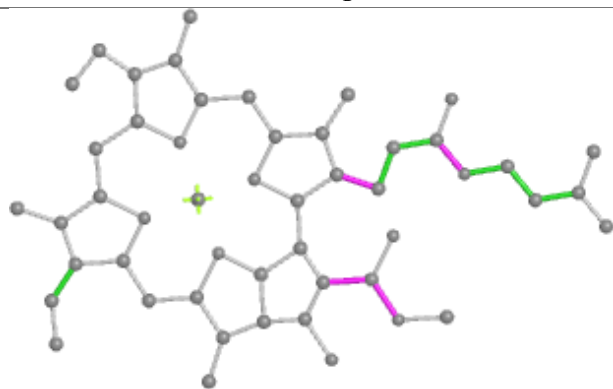
Ligand CLA B 1202



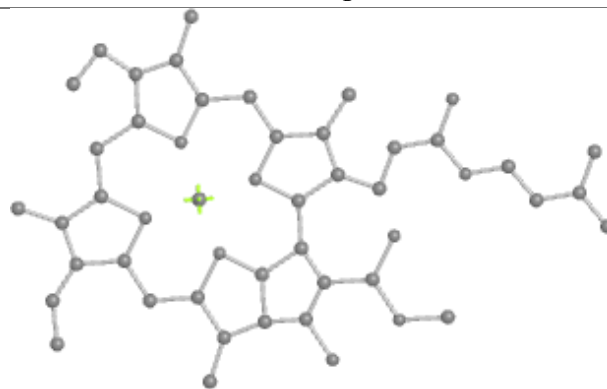
Bond lengths



Bond angles

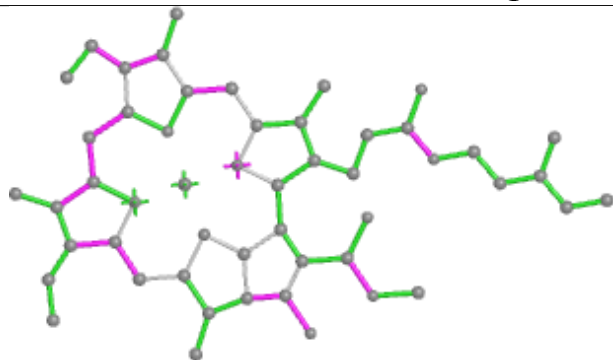


Torsions

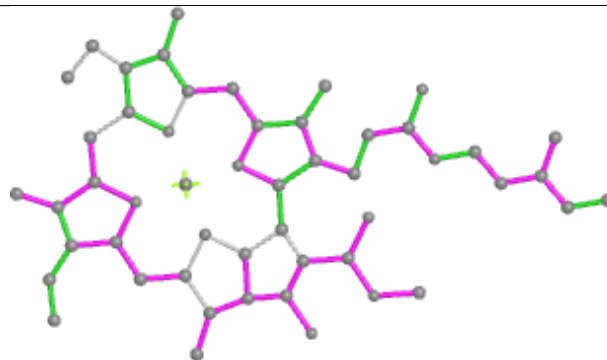


Rings

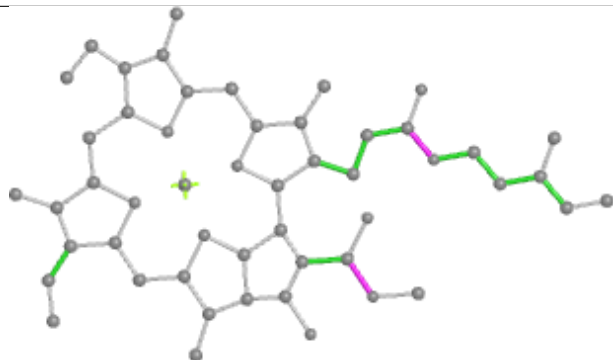
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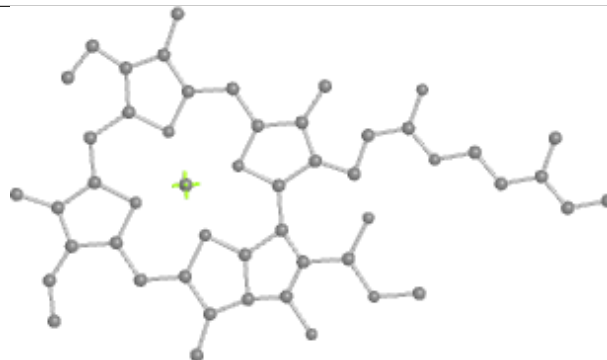
Bond lengths



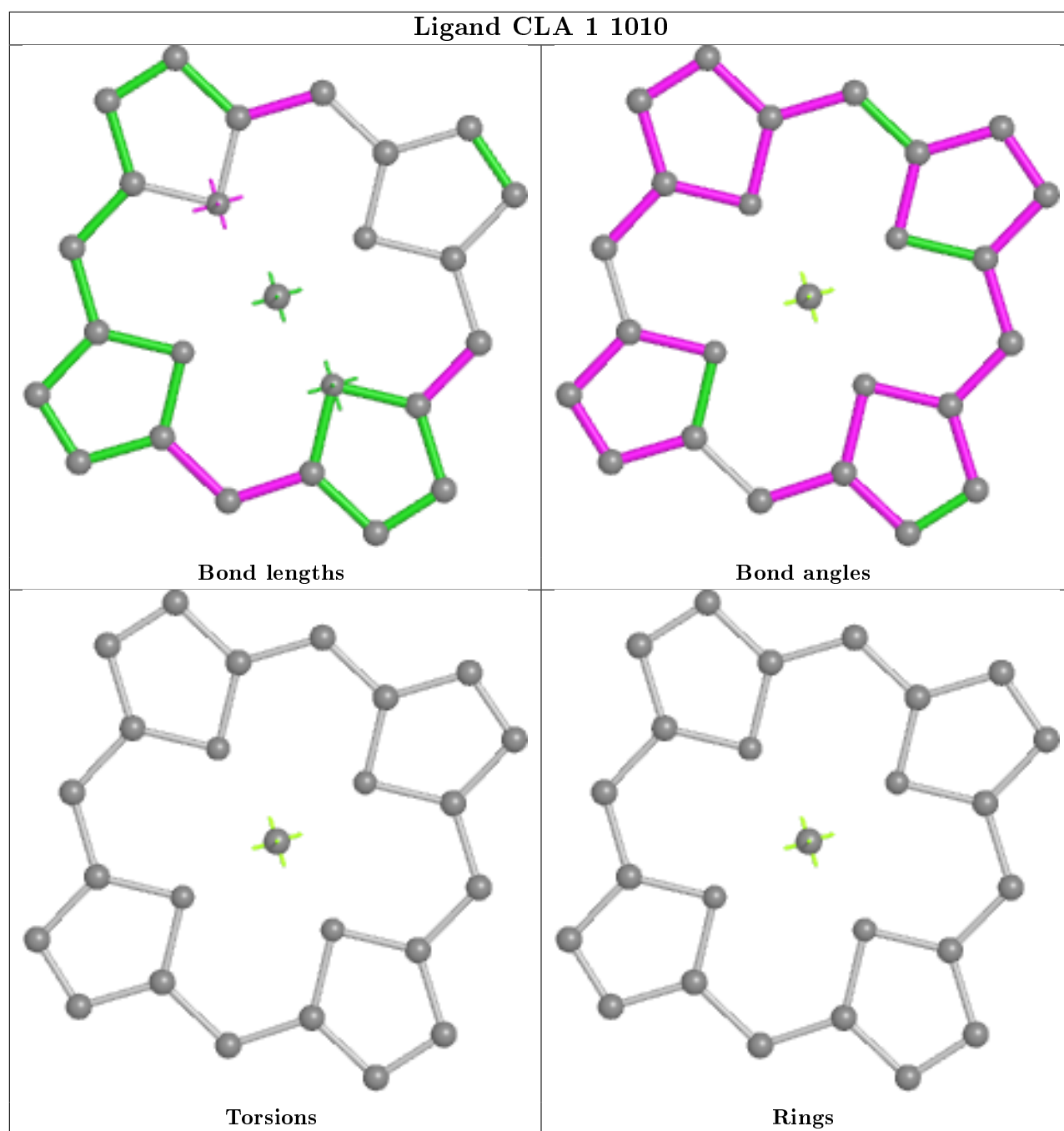
Bond angles



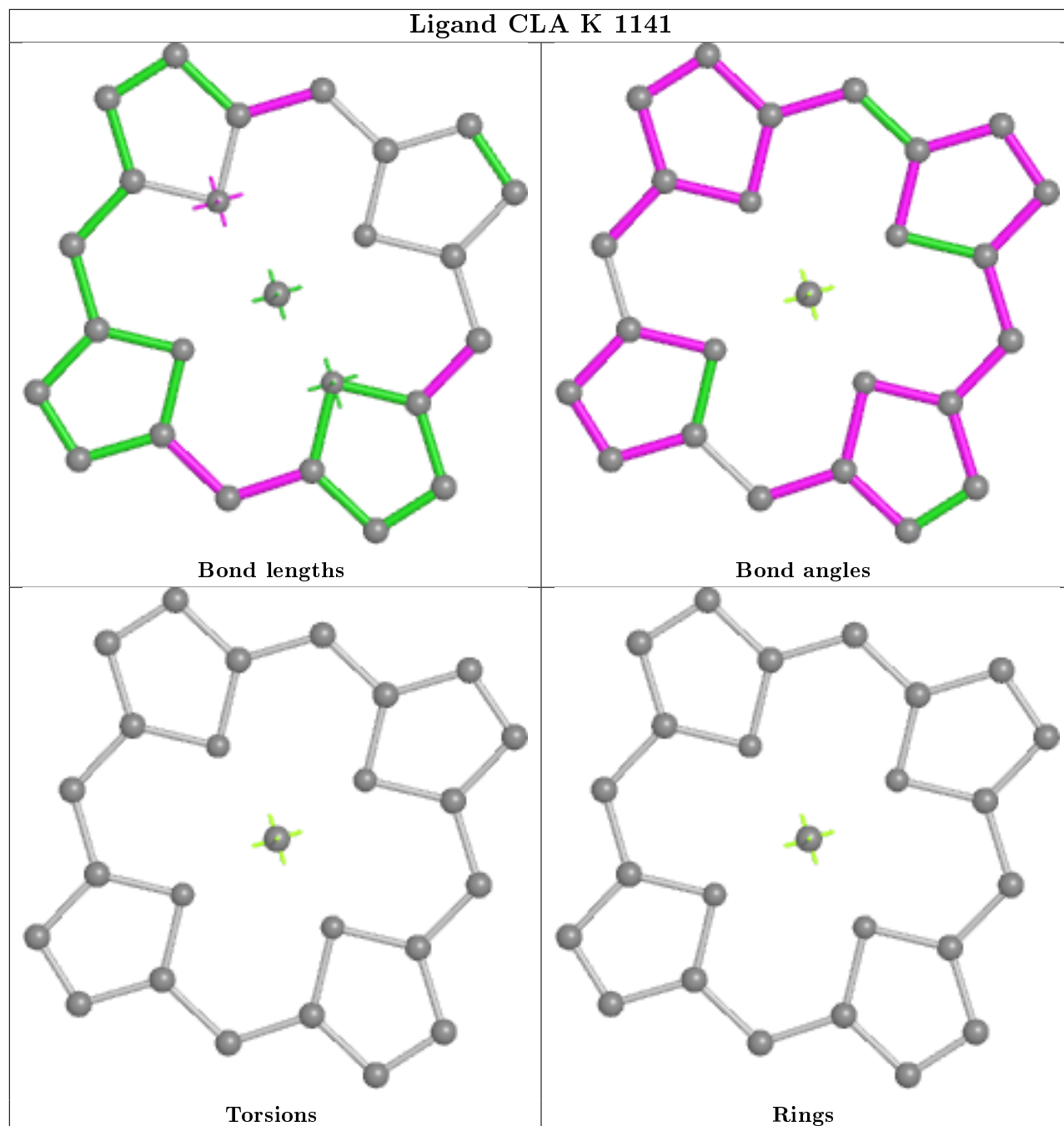
Torsions

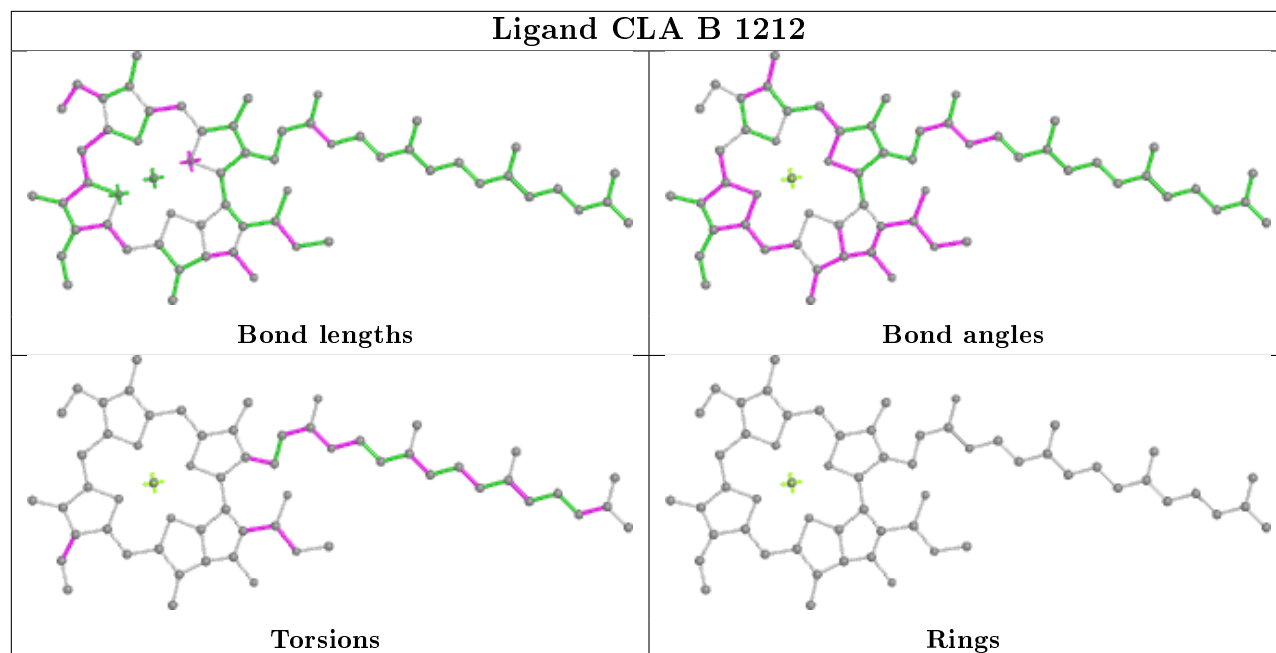


Rings

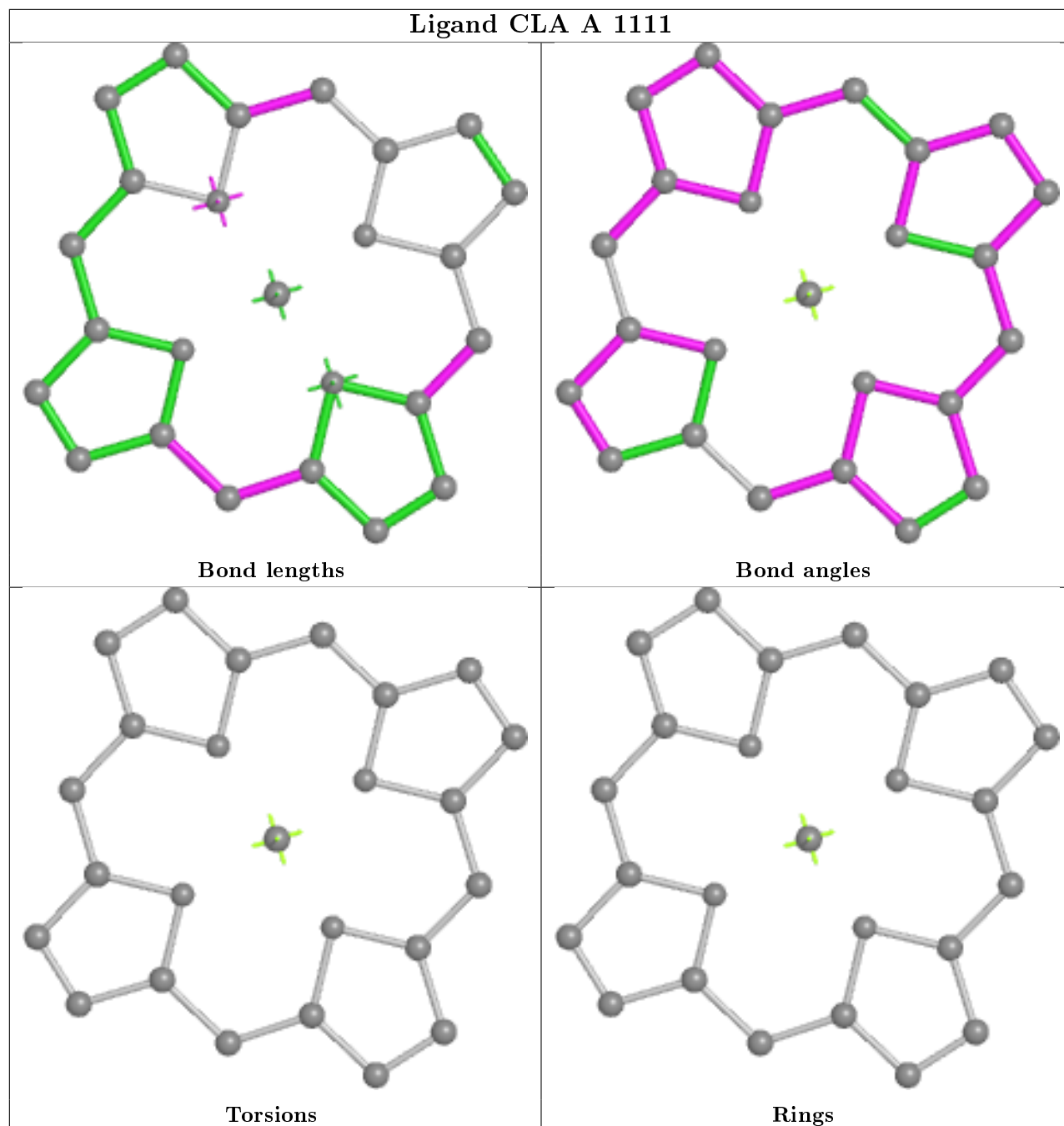


Ligand CLA K 1141

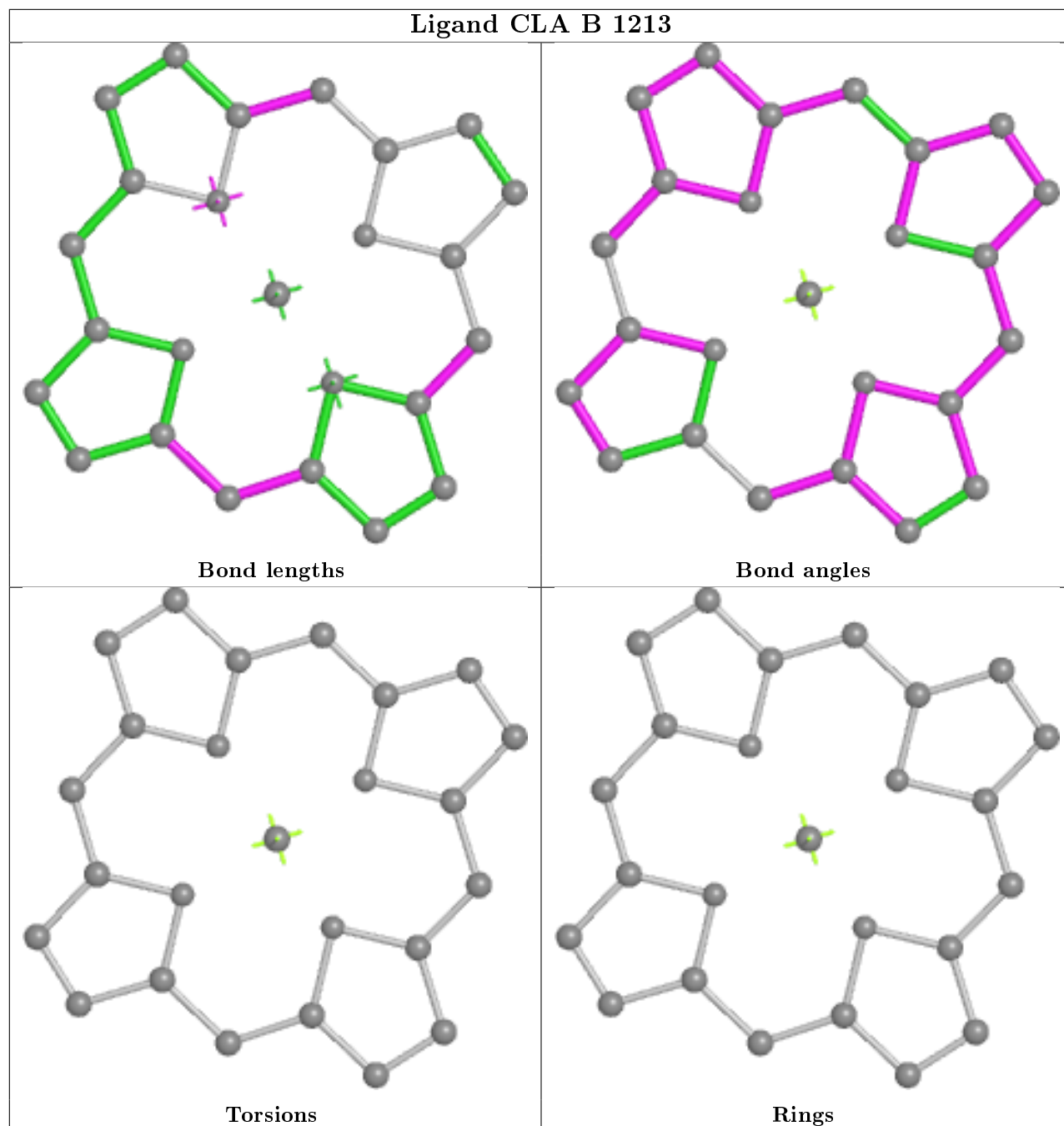


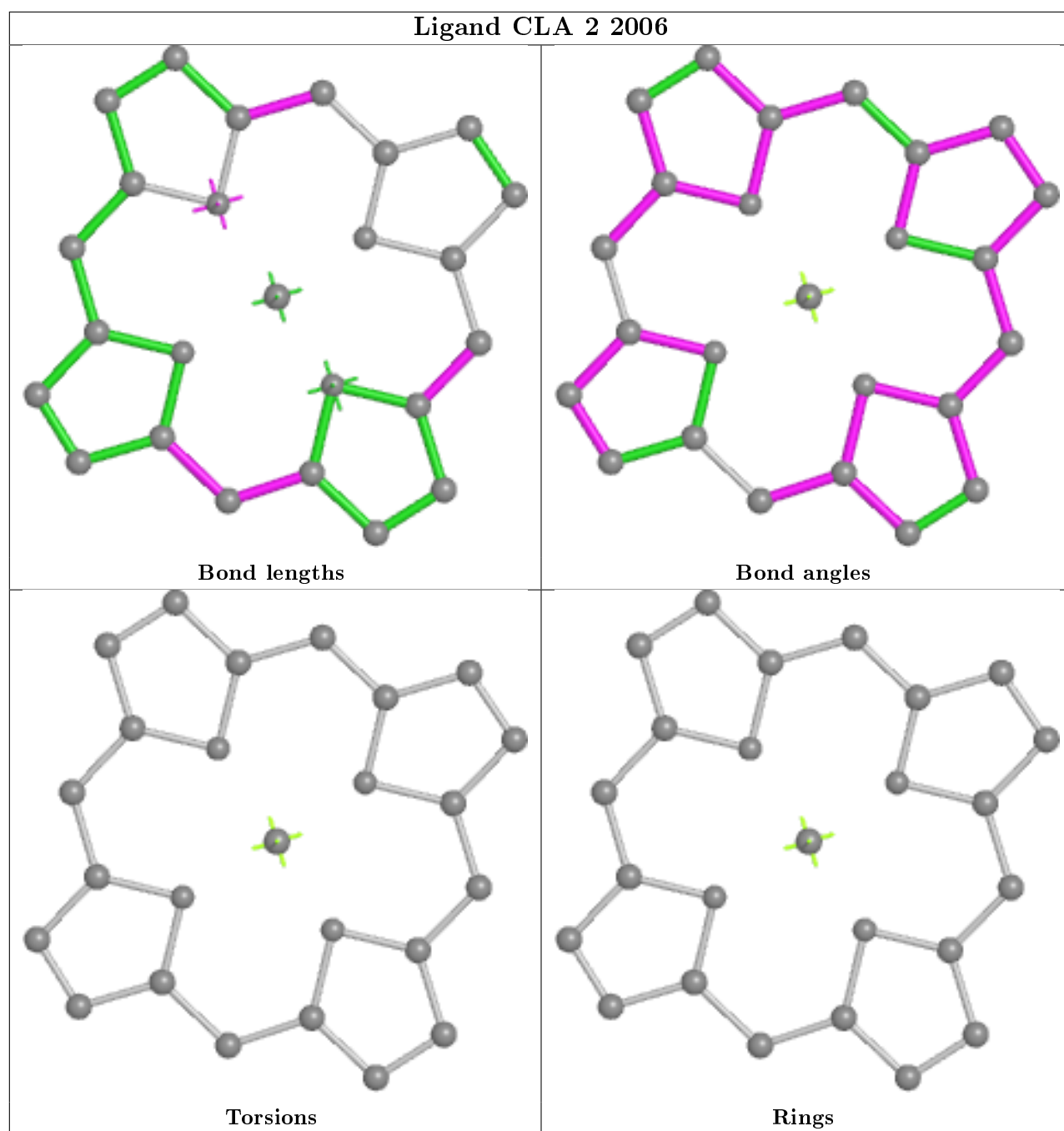


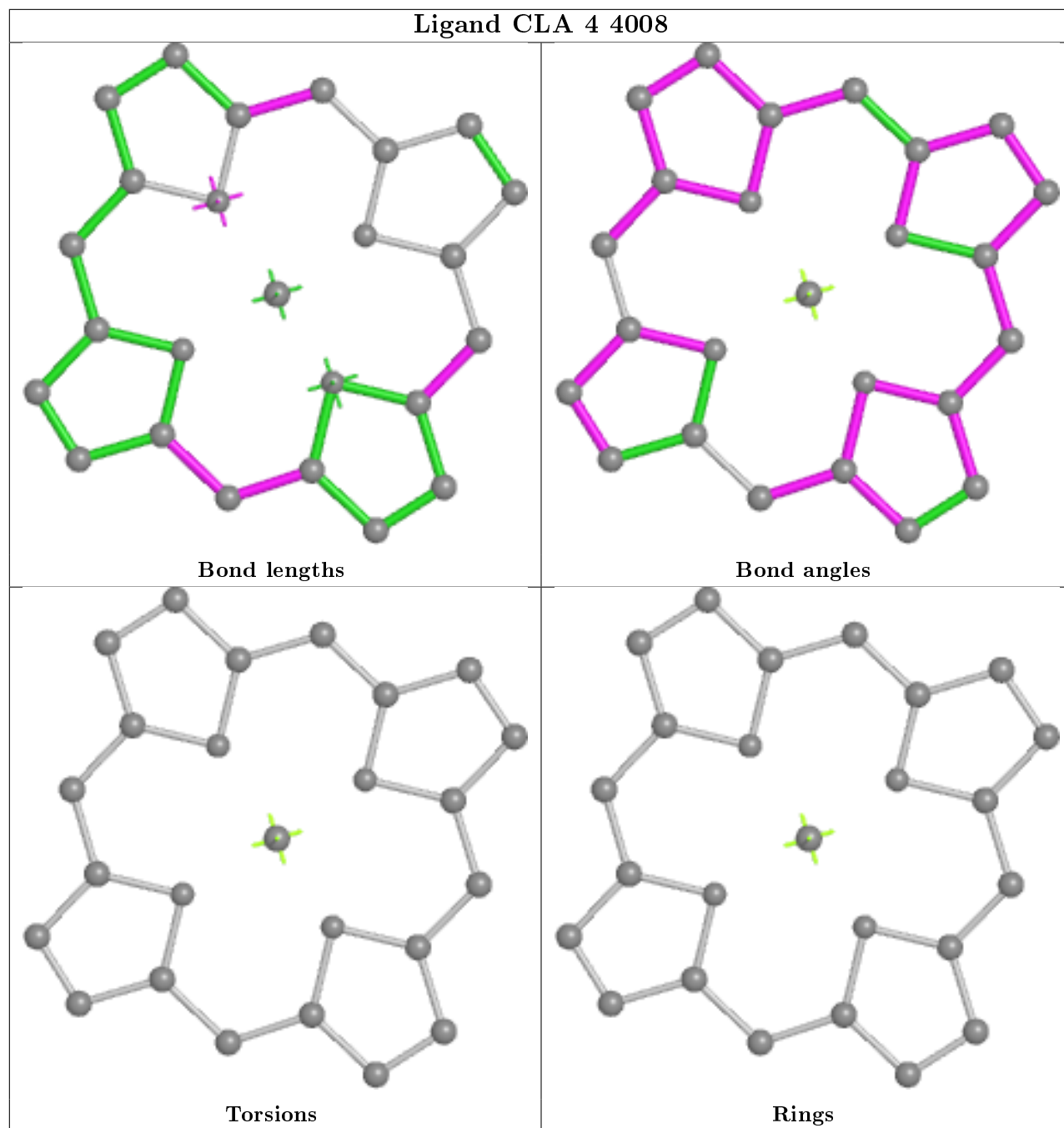
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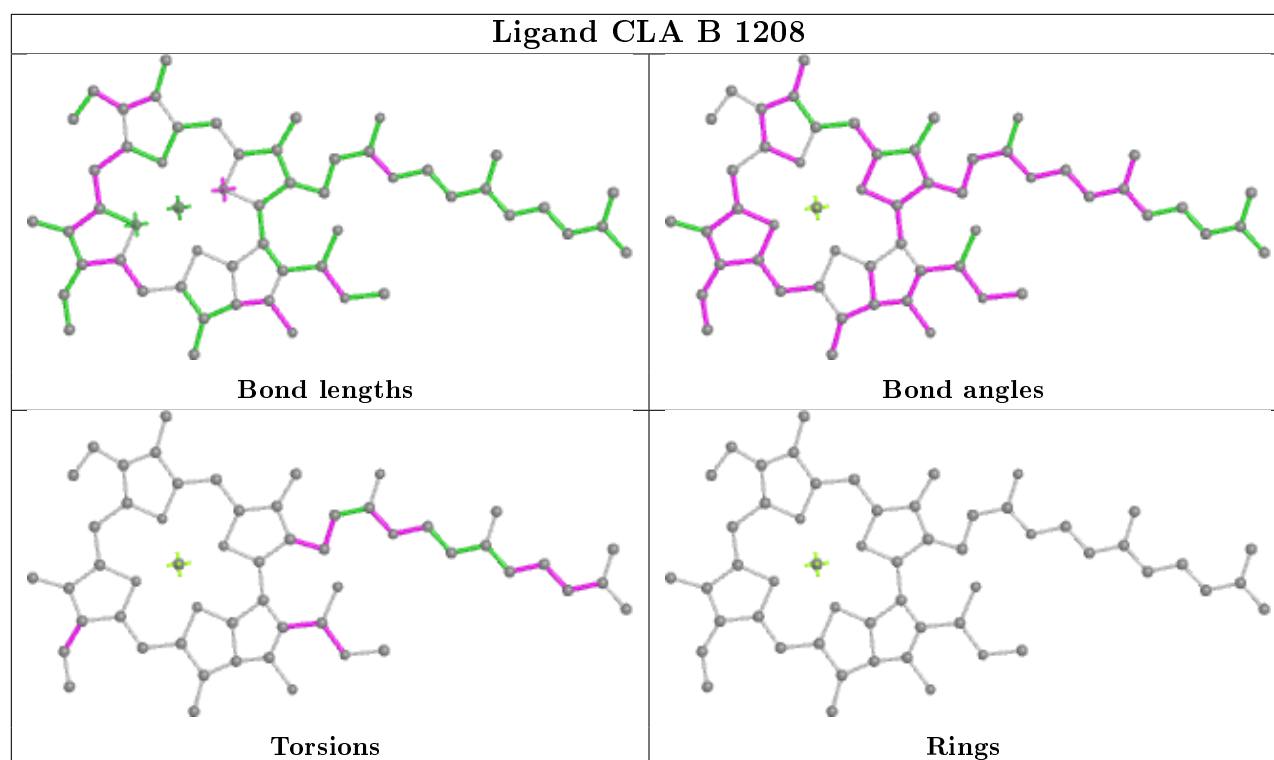


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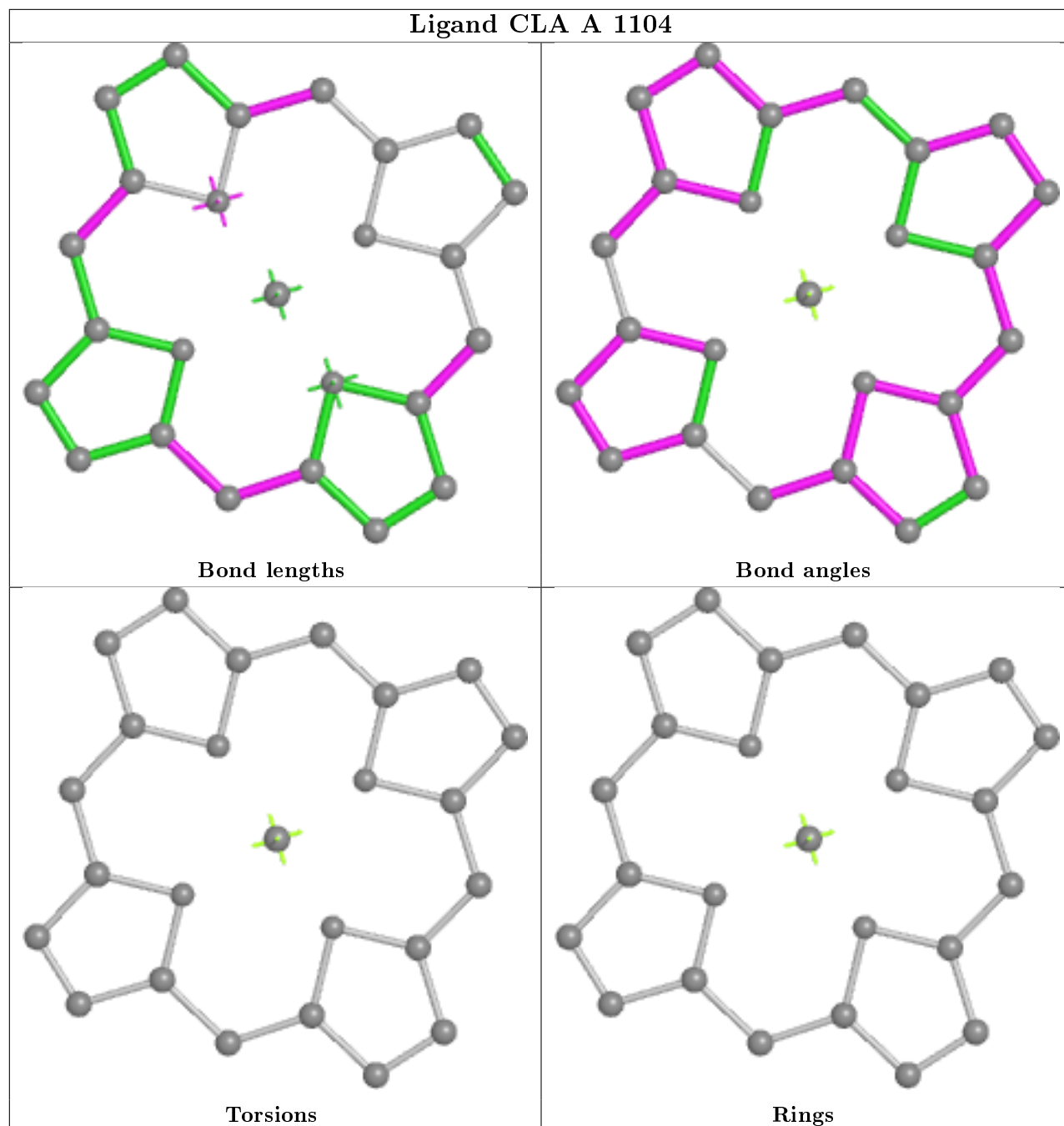




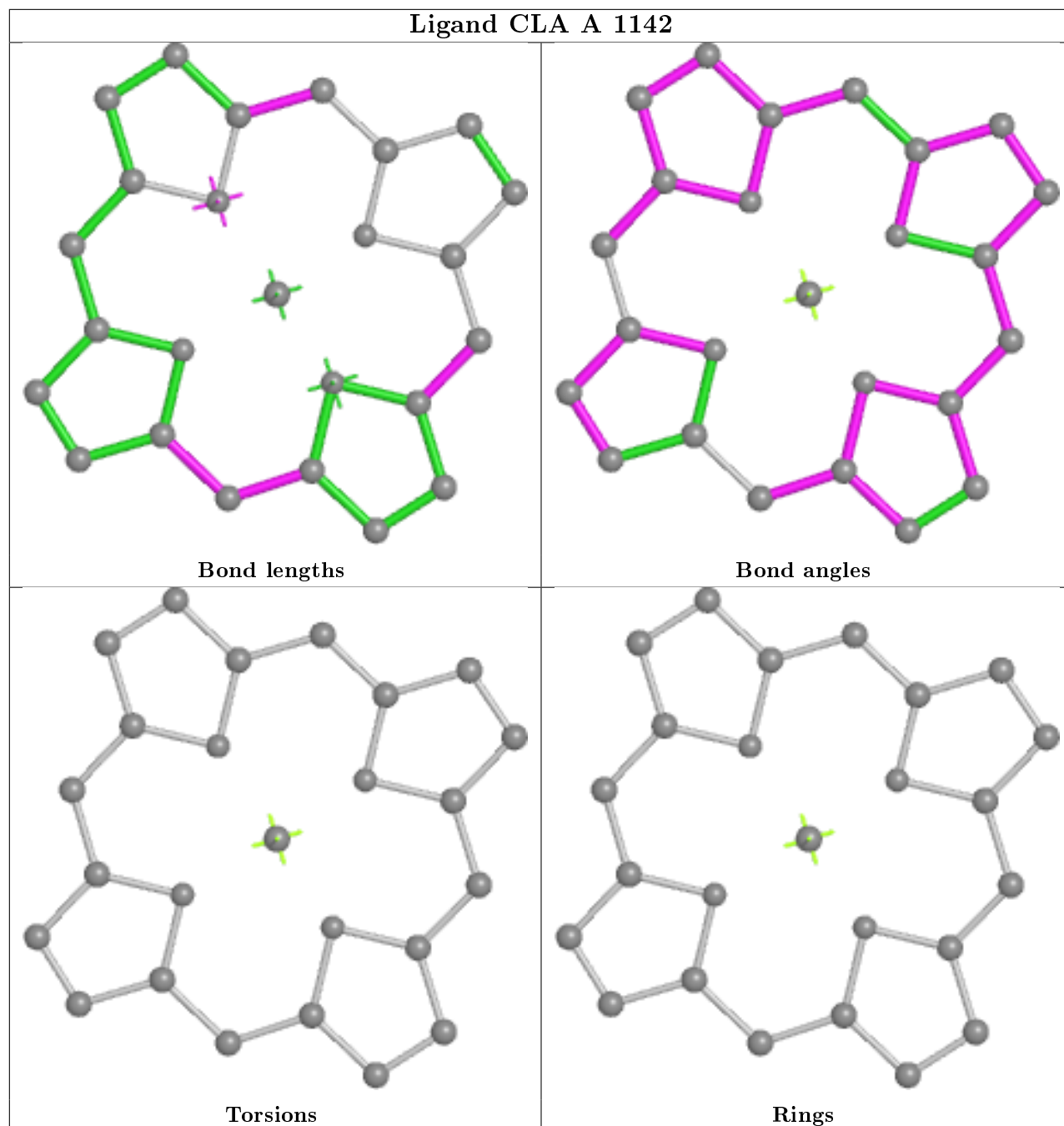


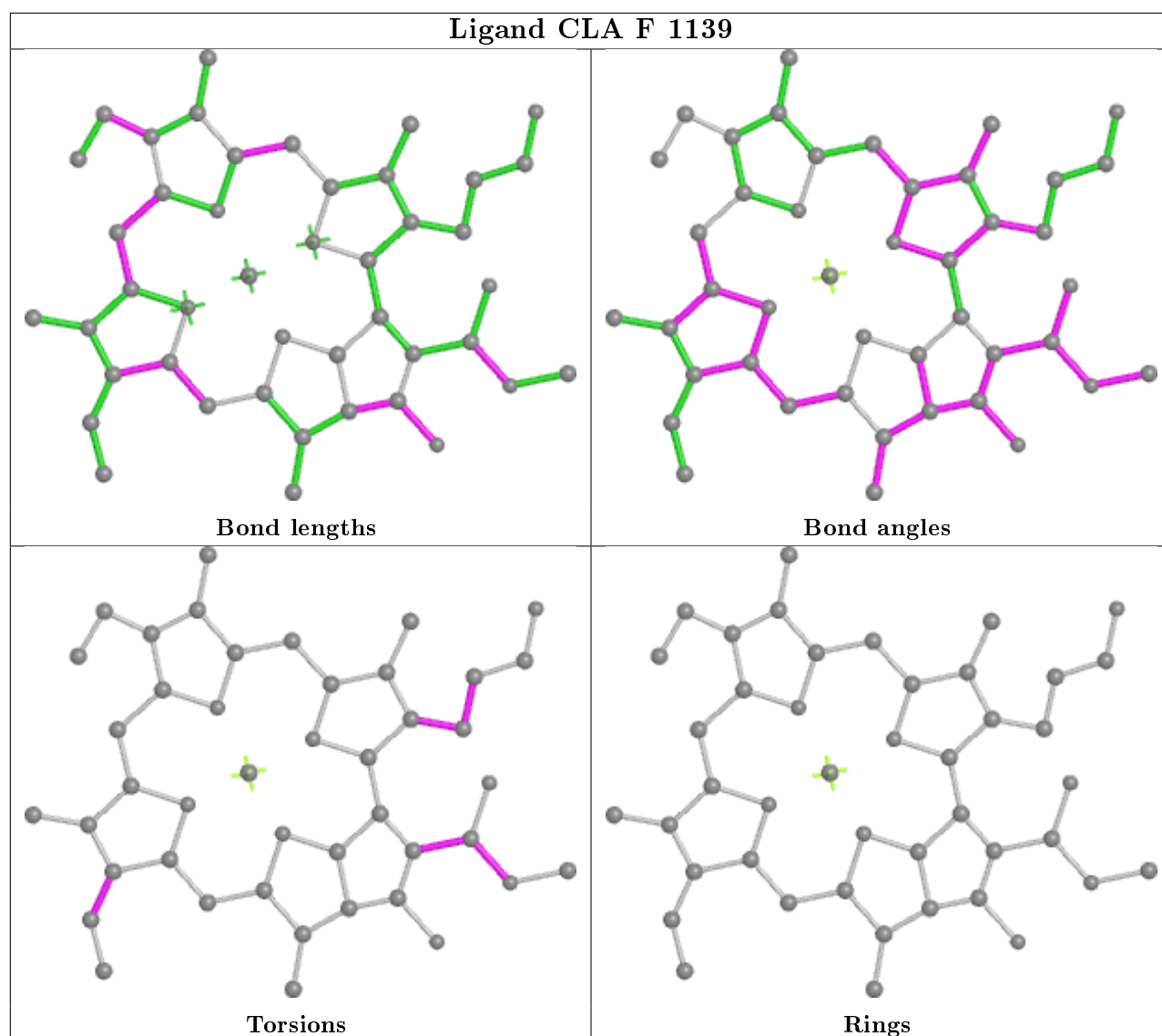


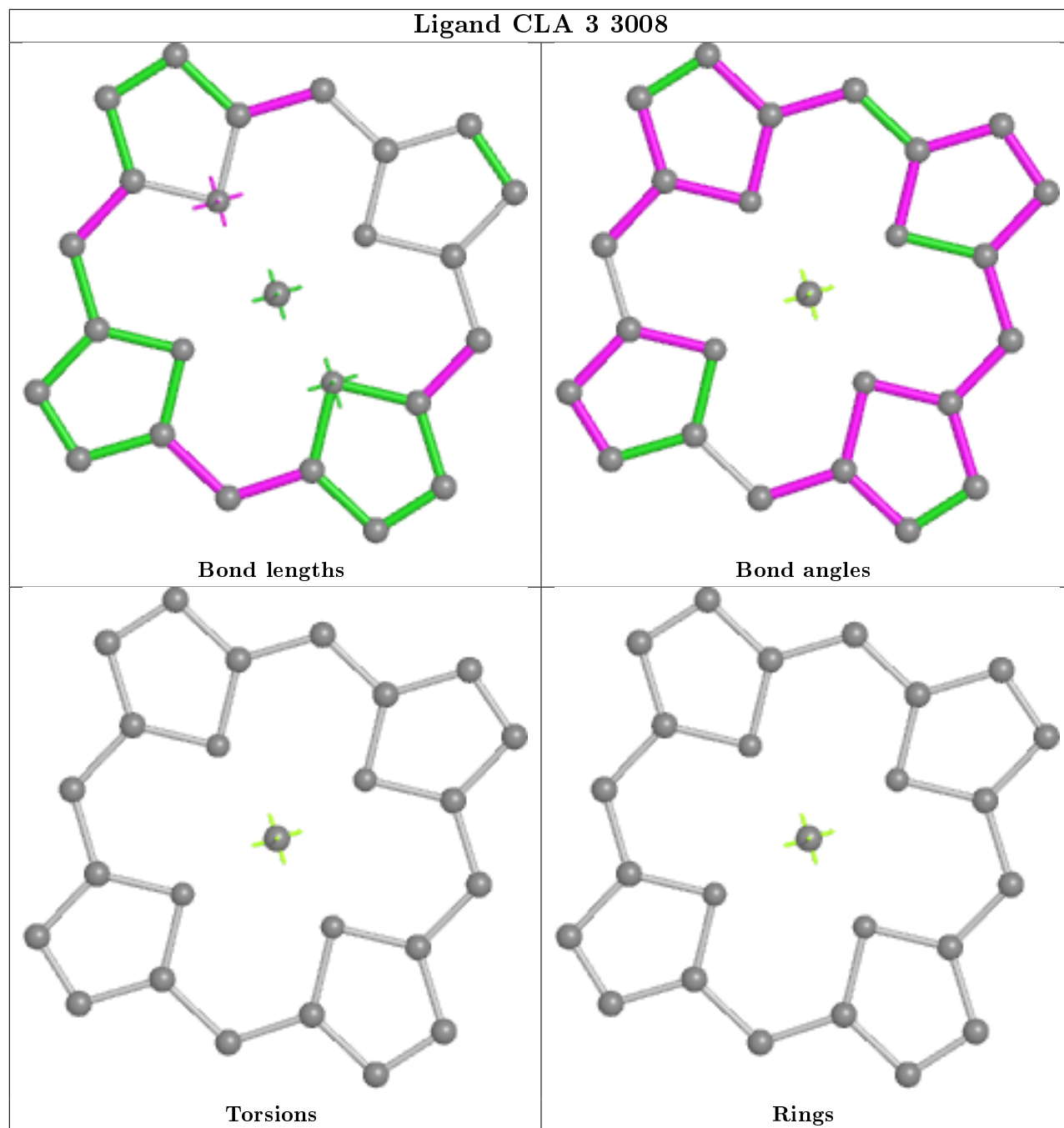
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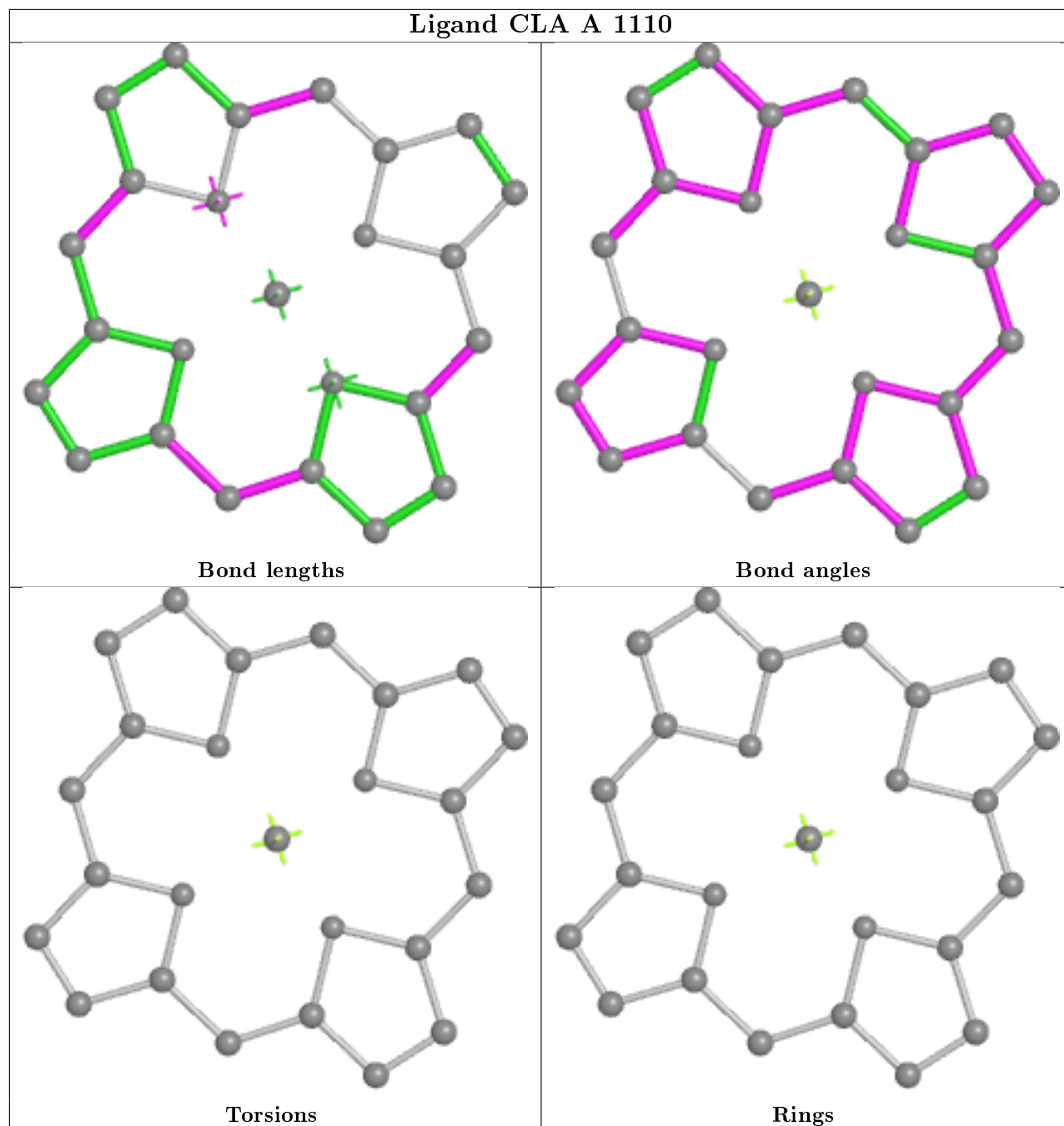
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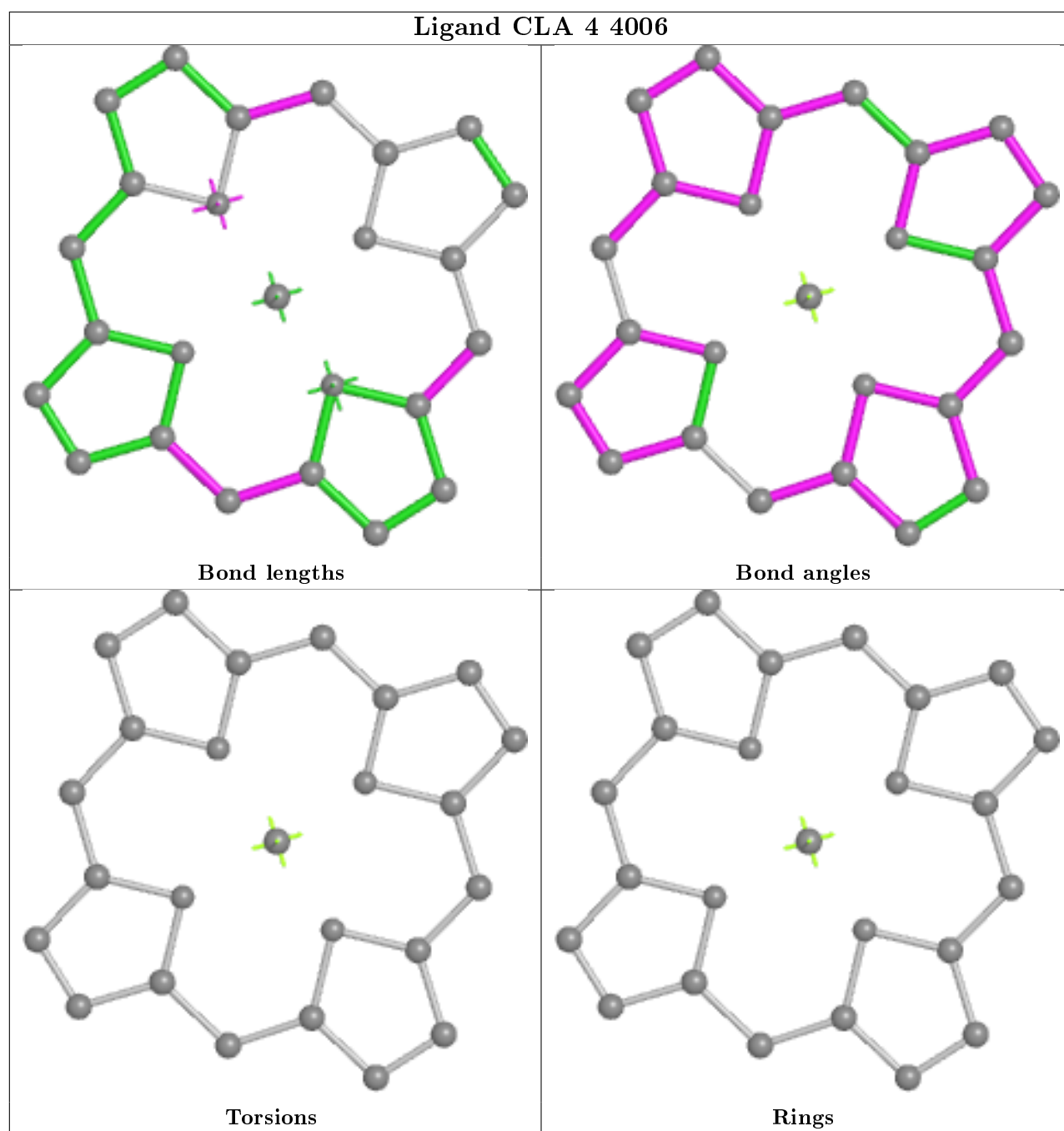


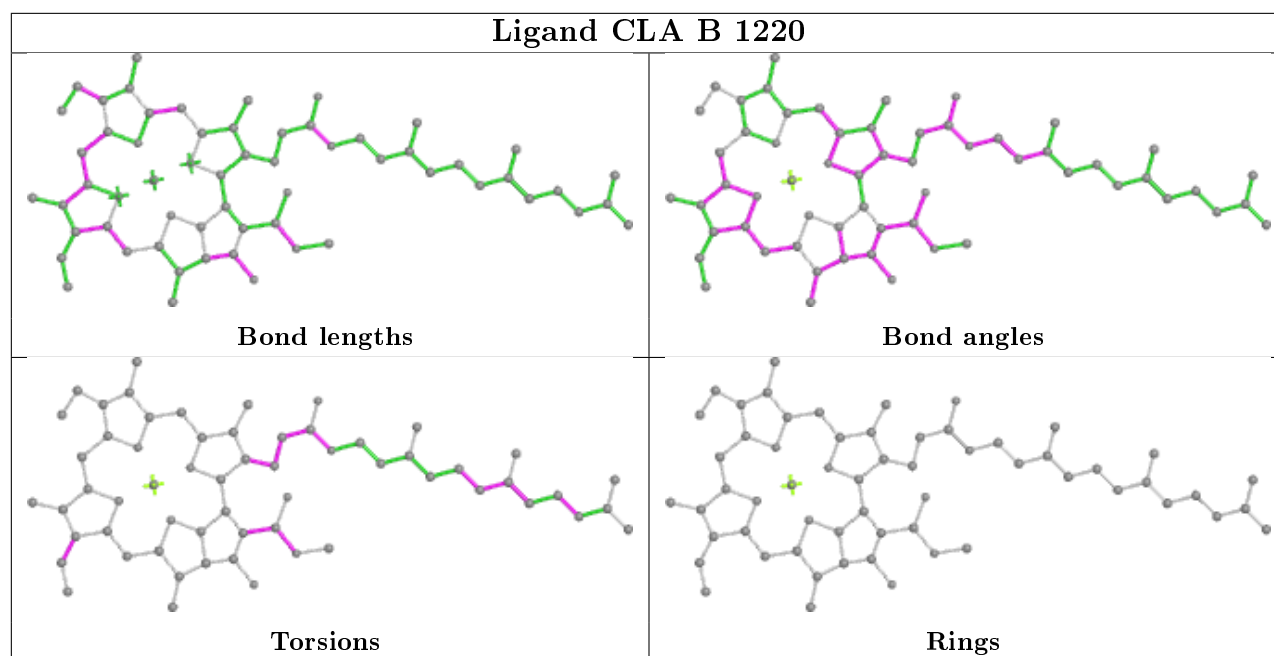
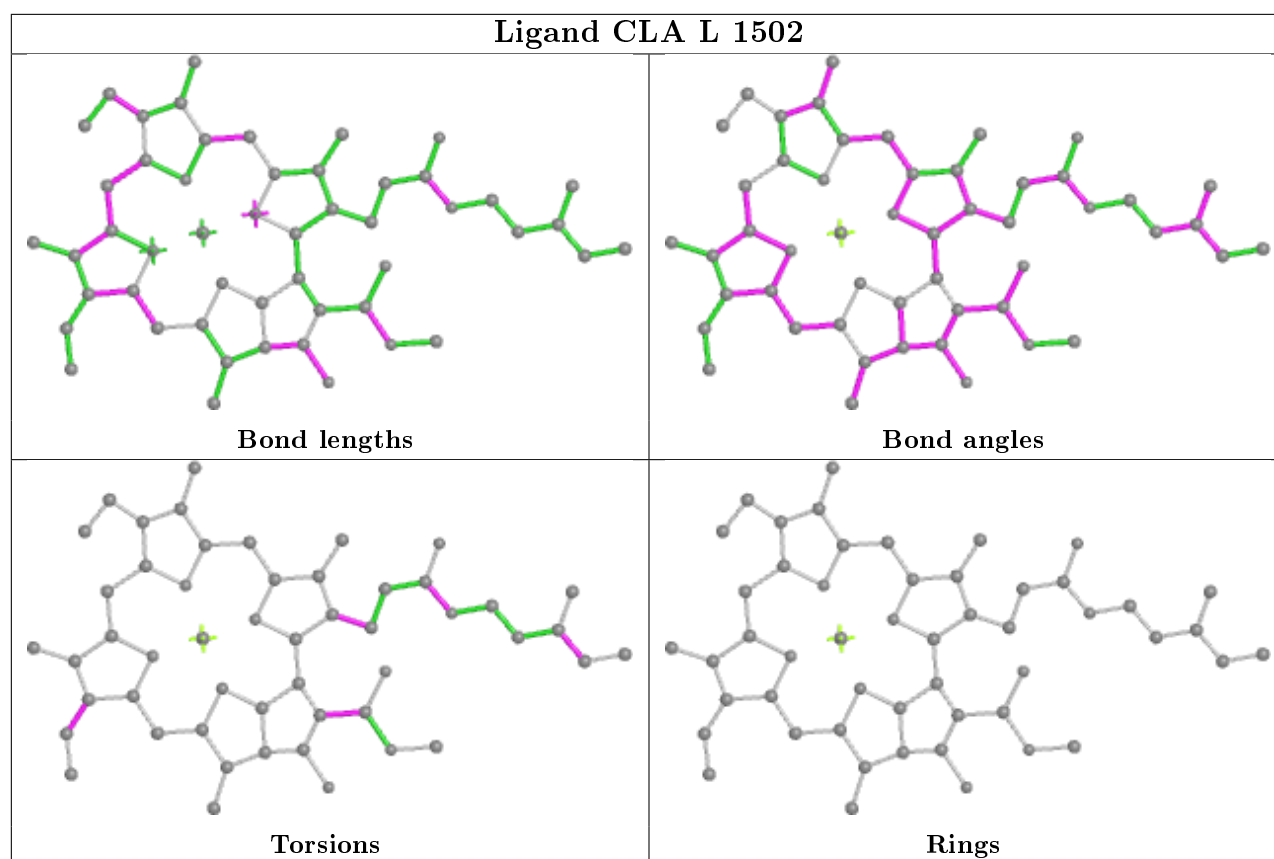




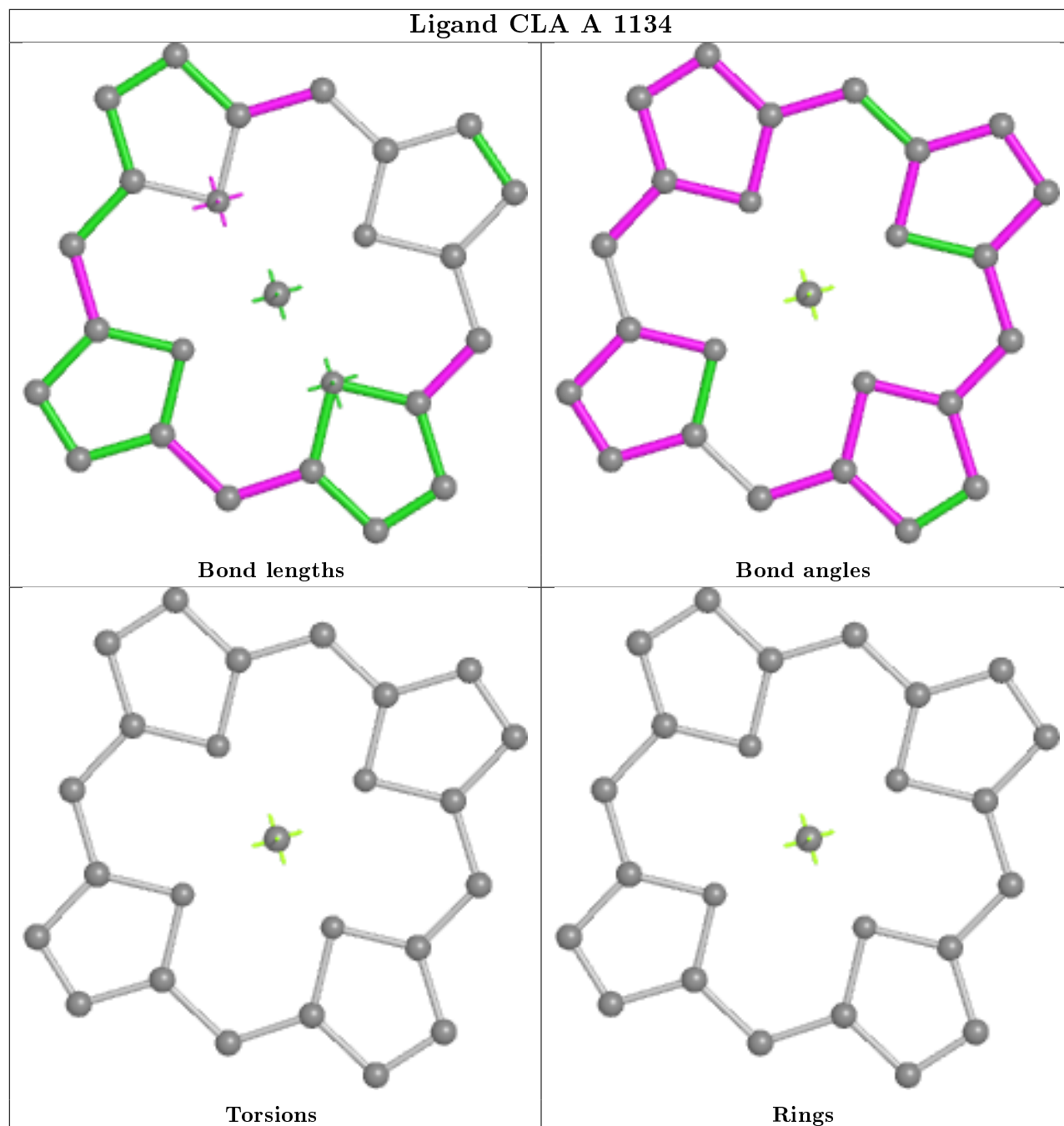
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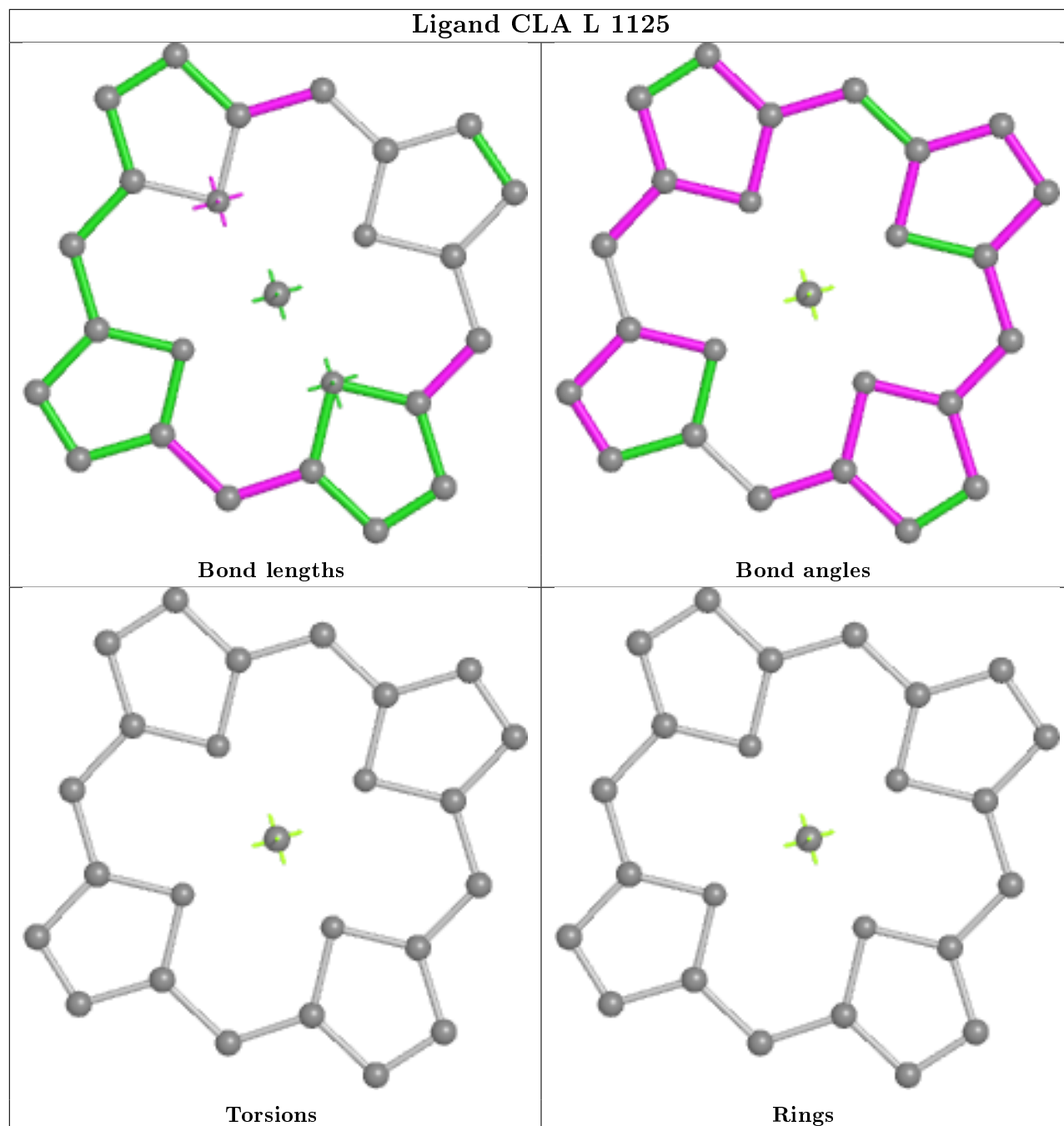




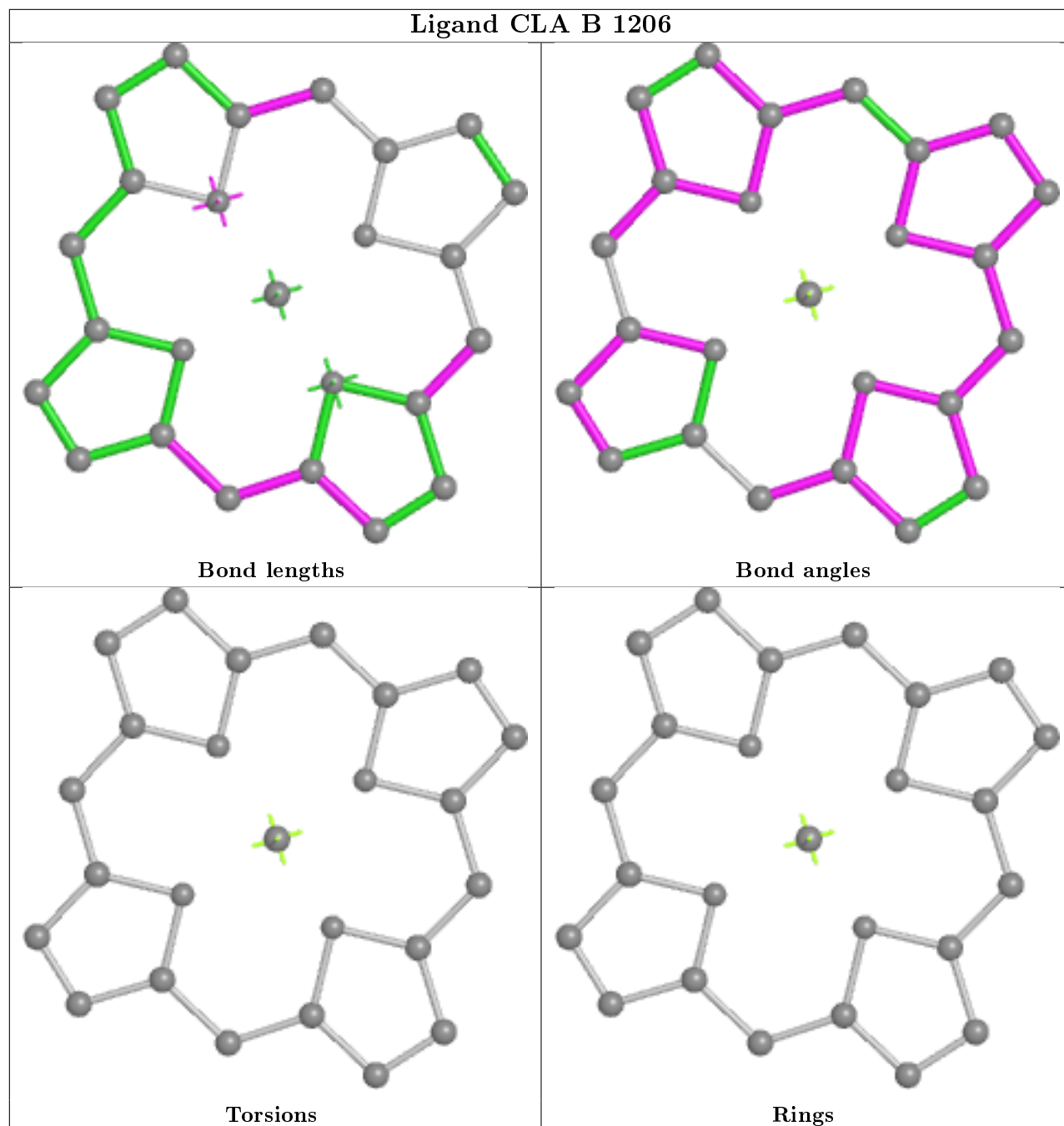
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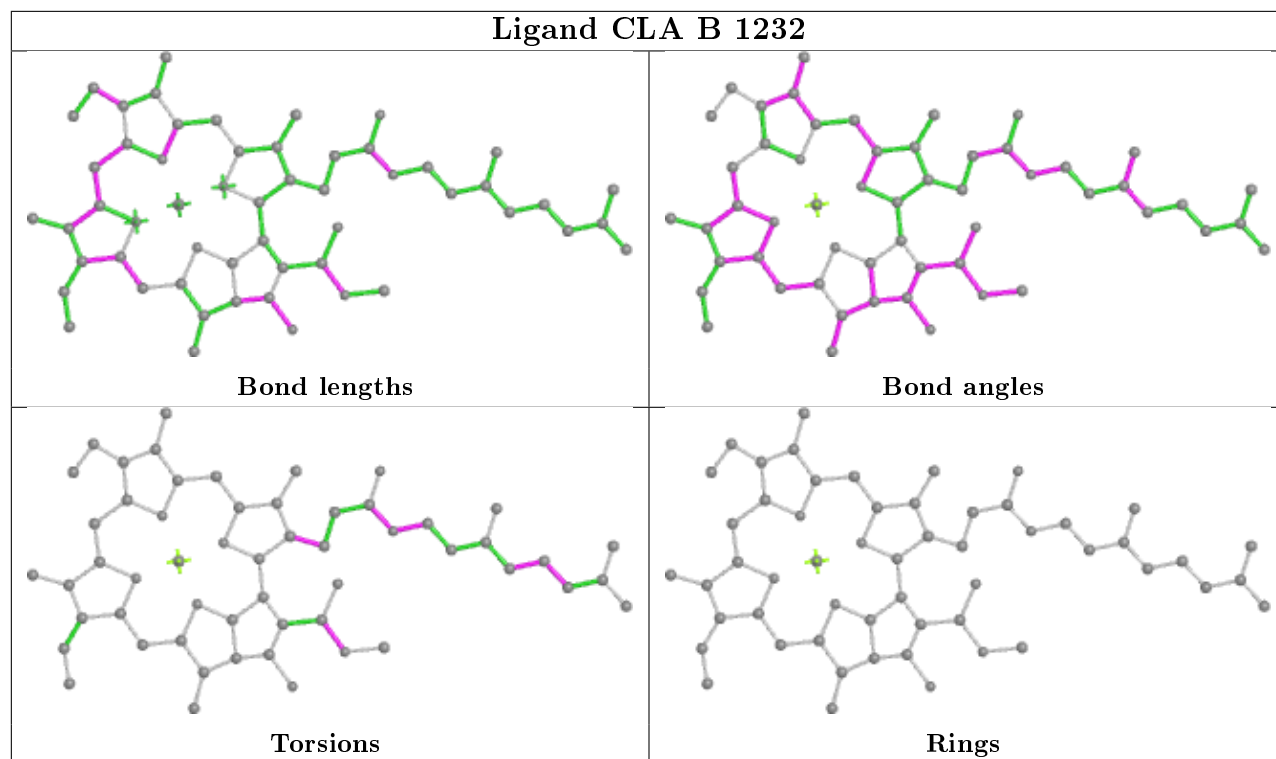


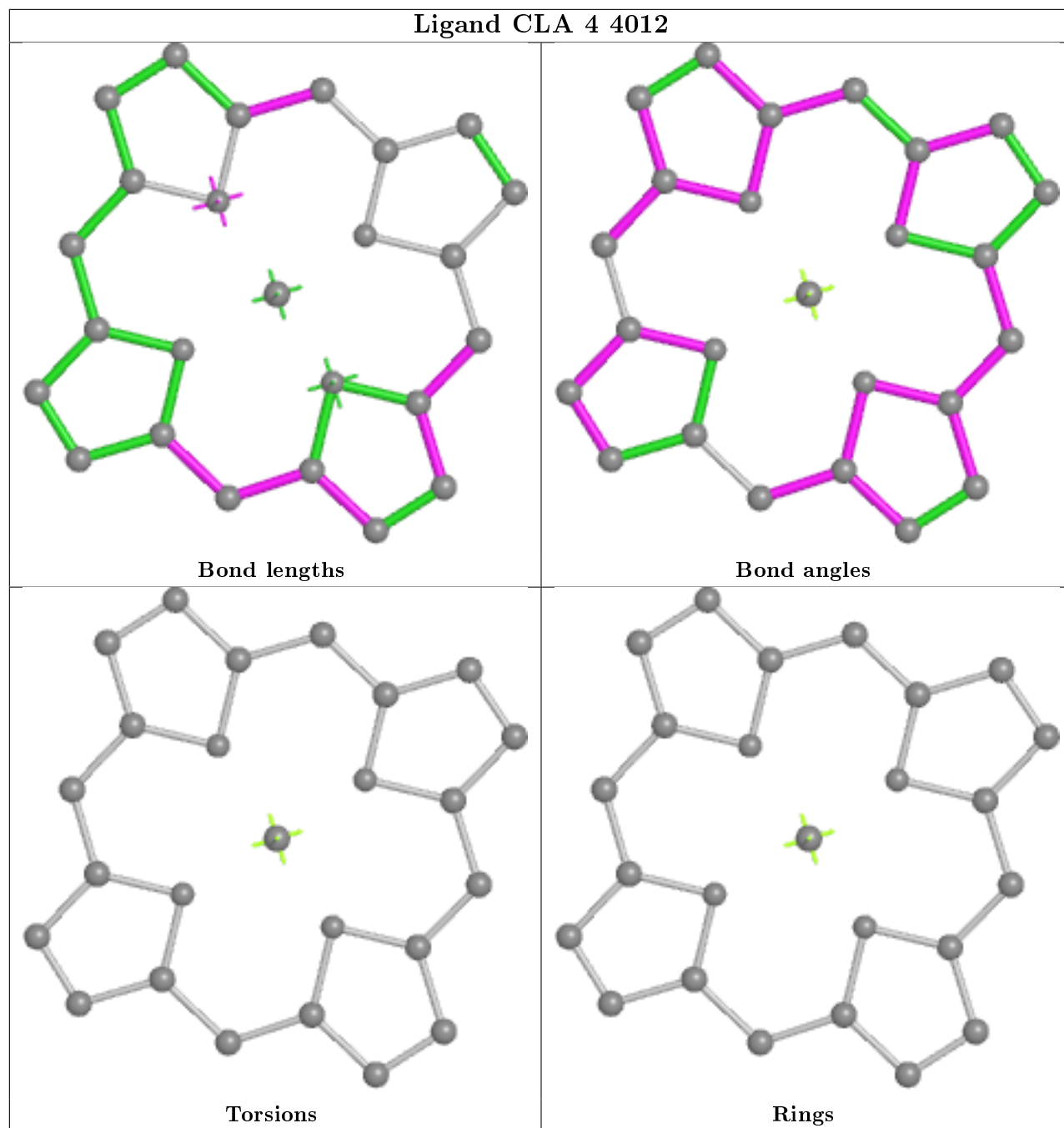
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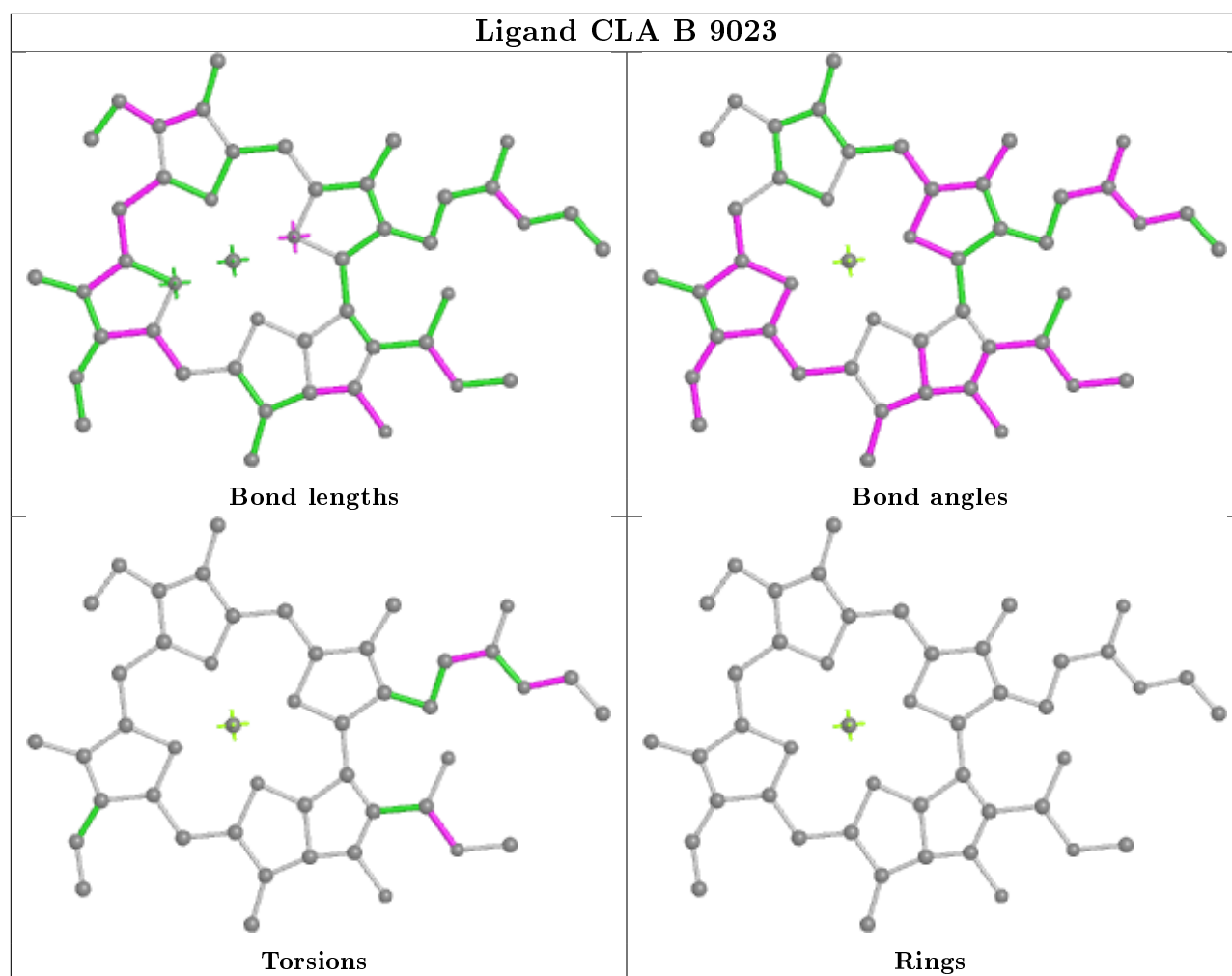


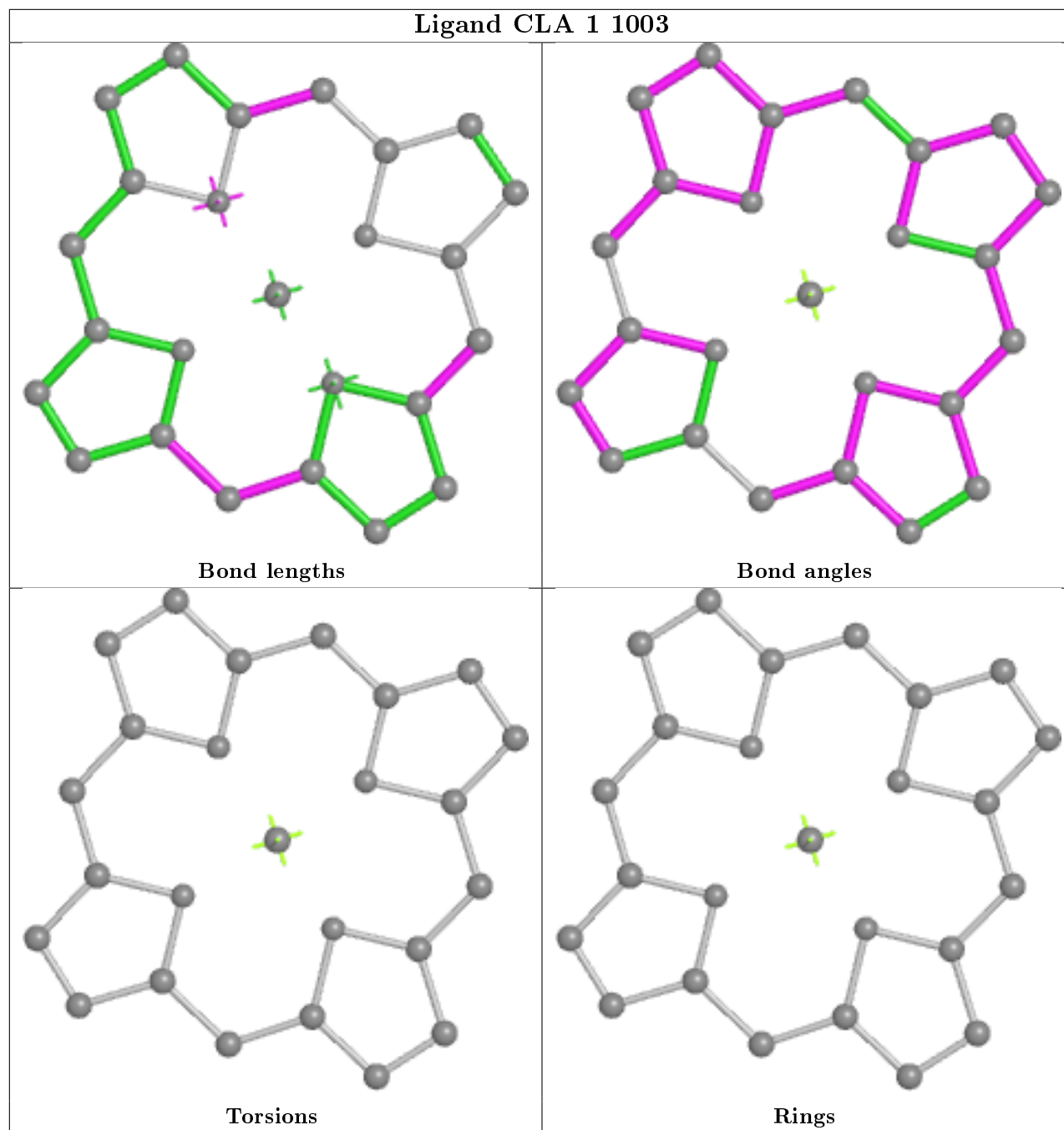
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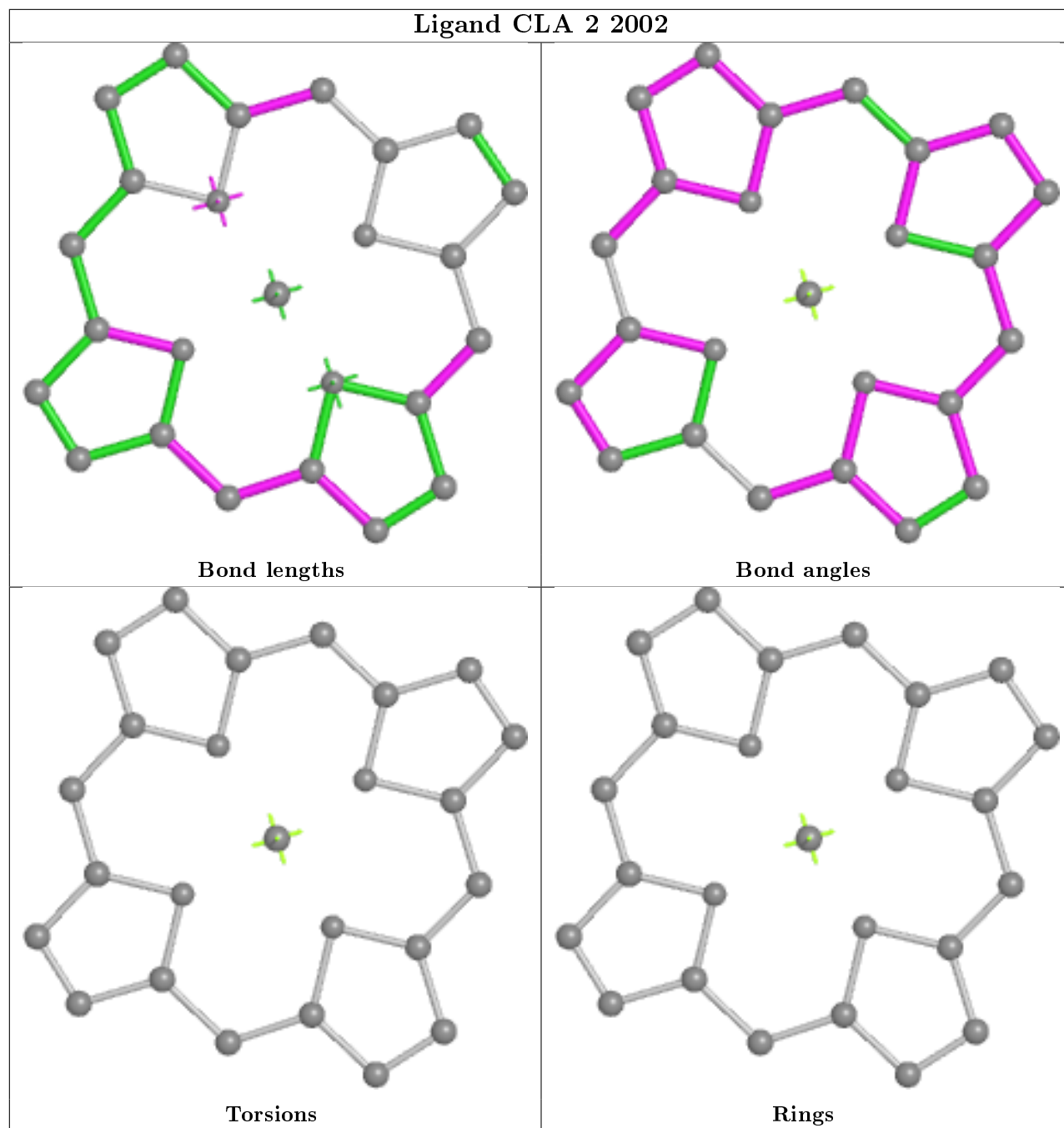


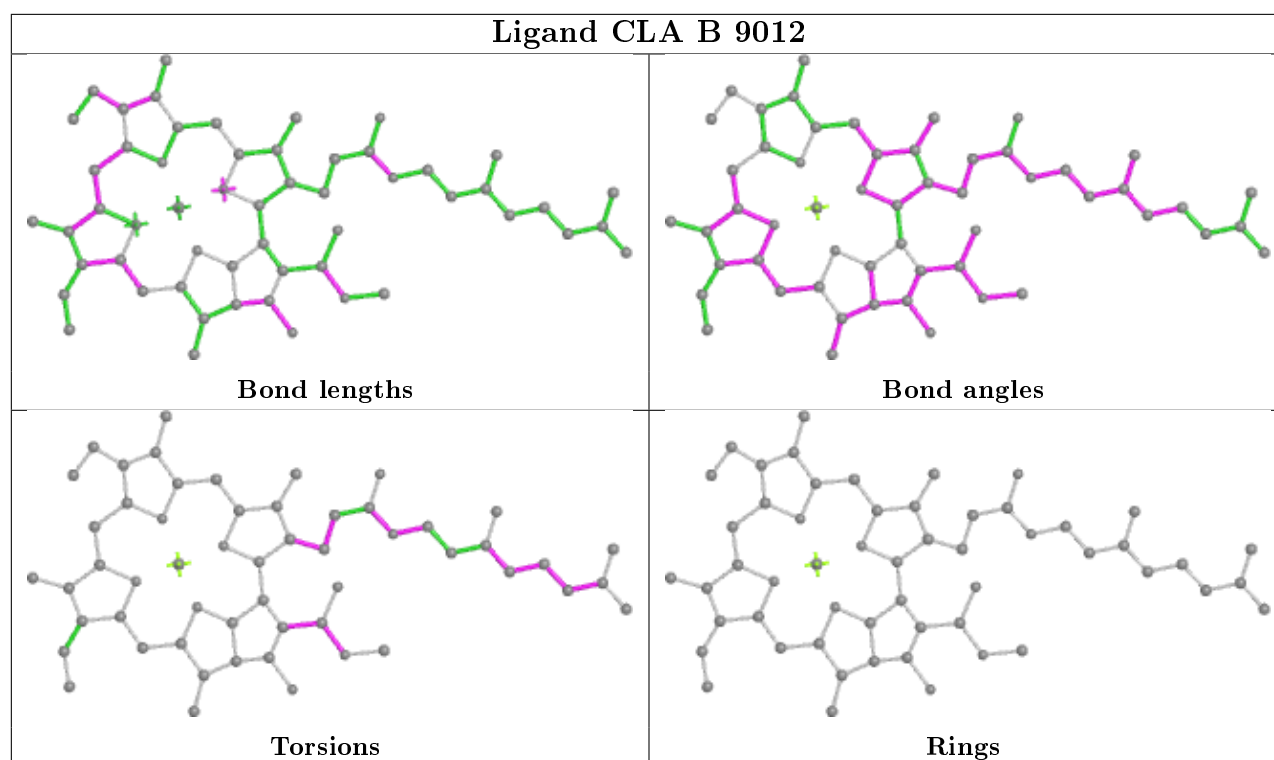


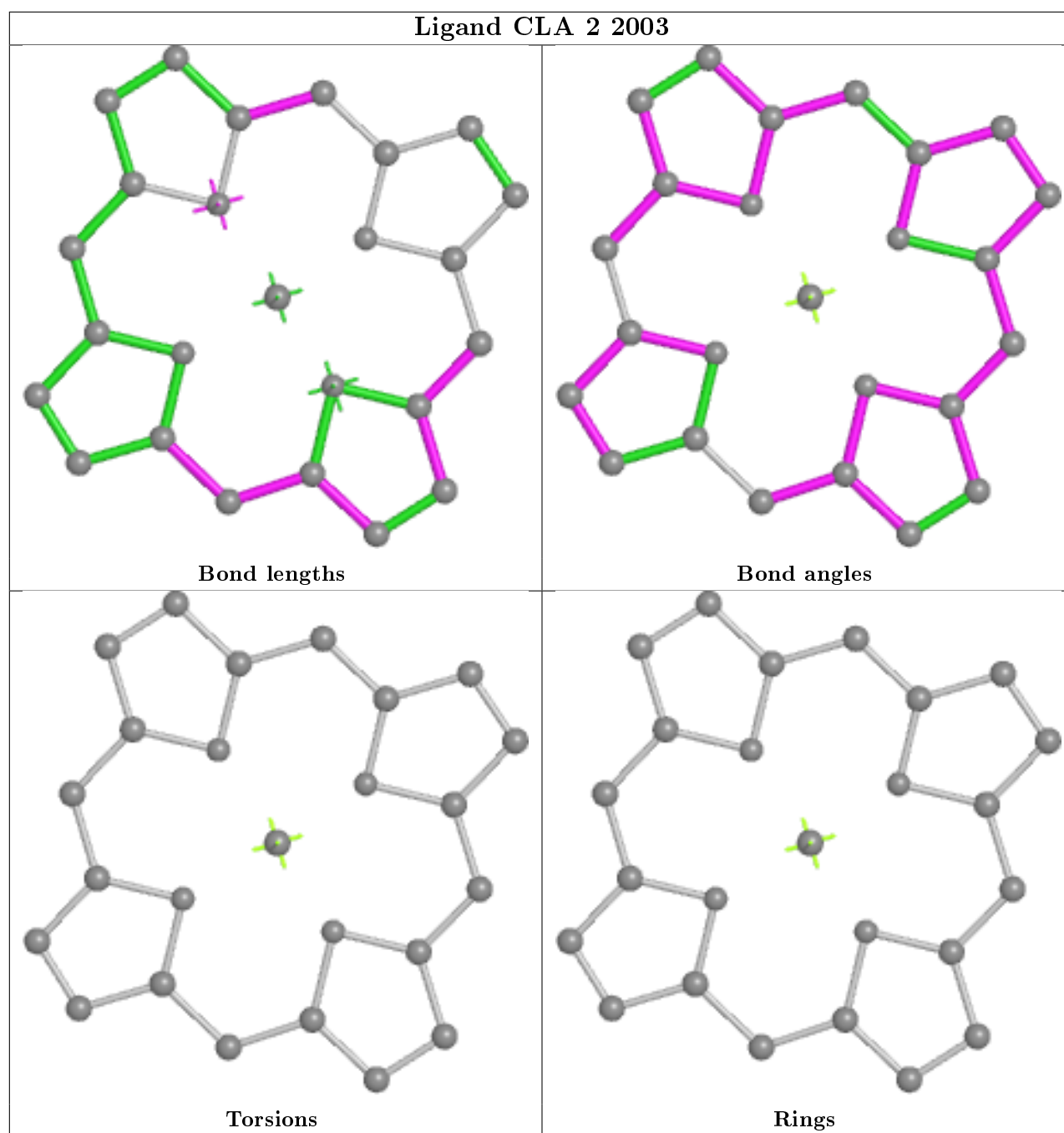


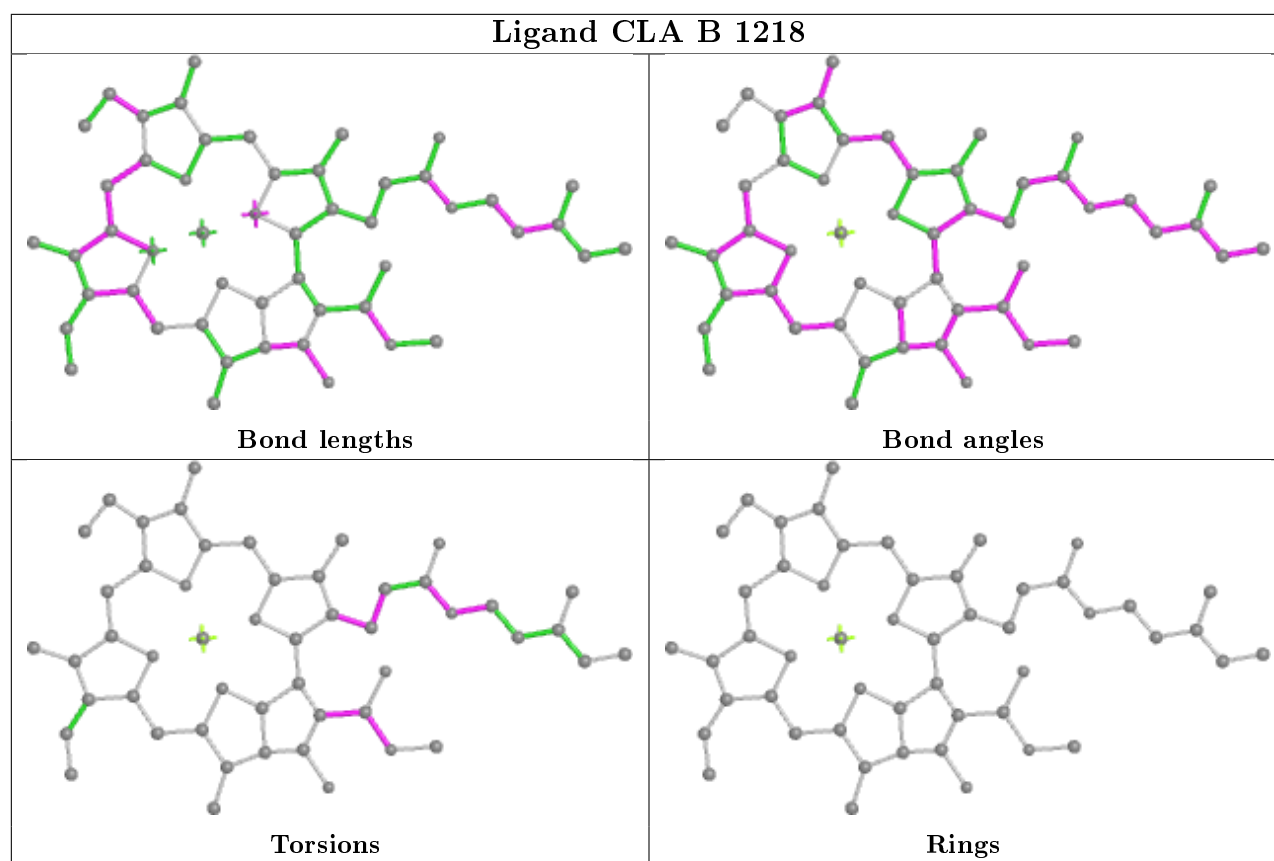




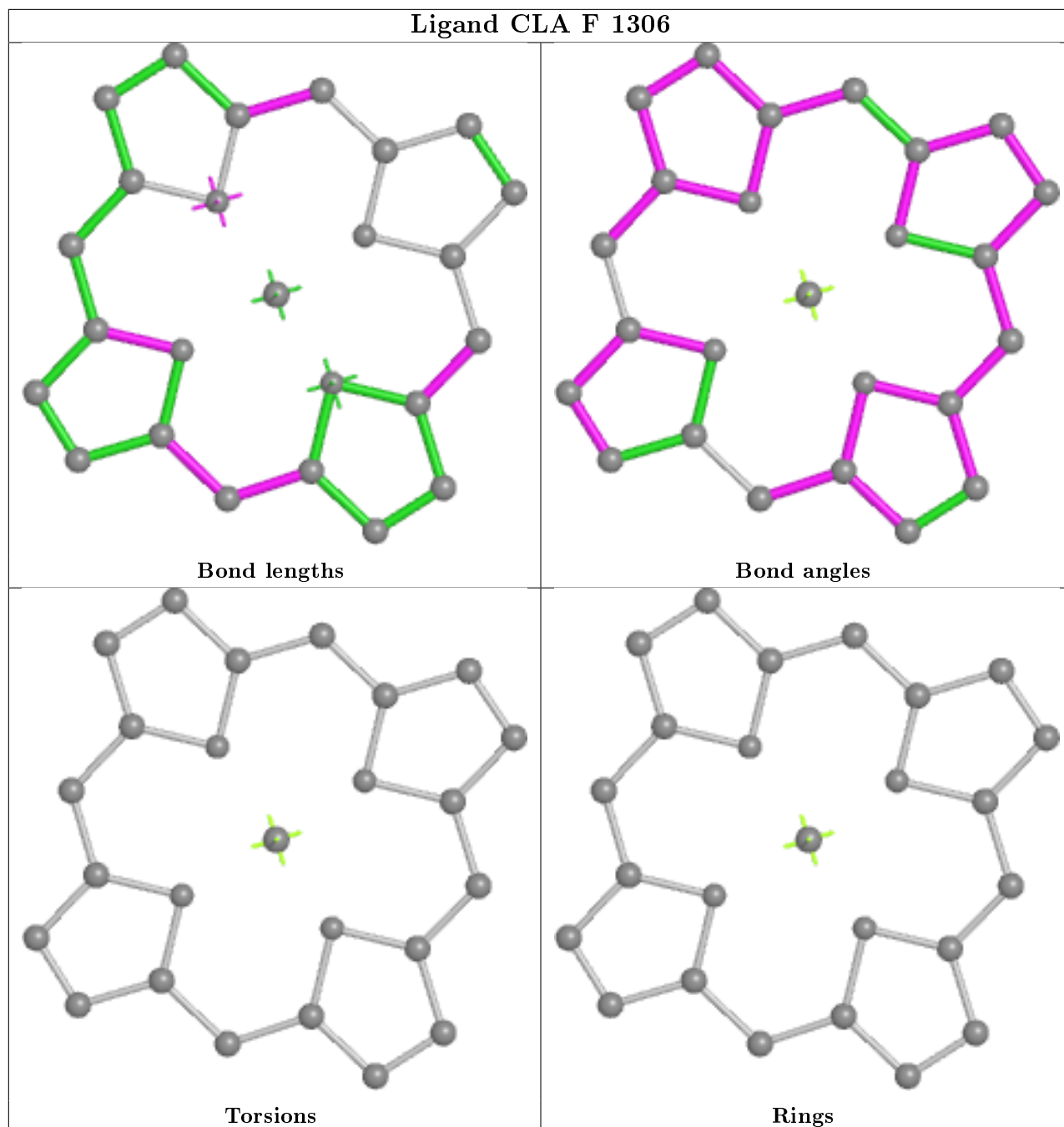


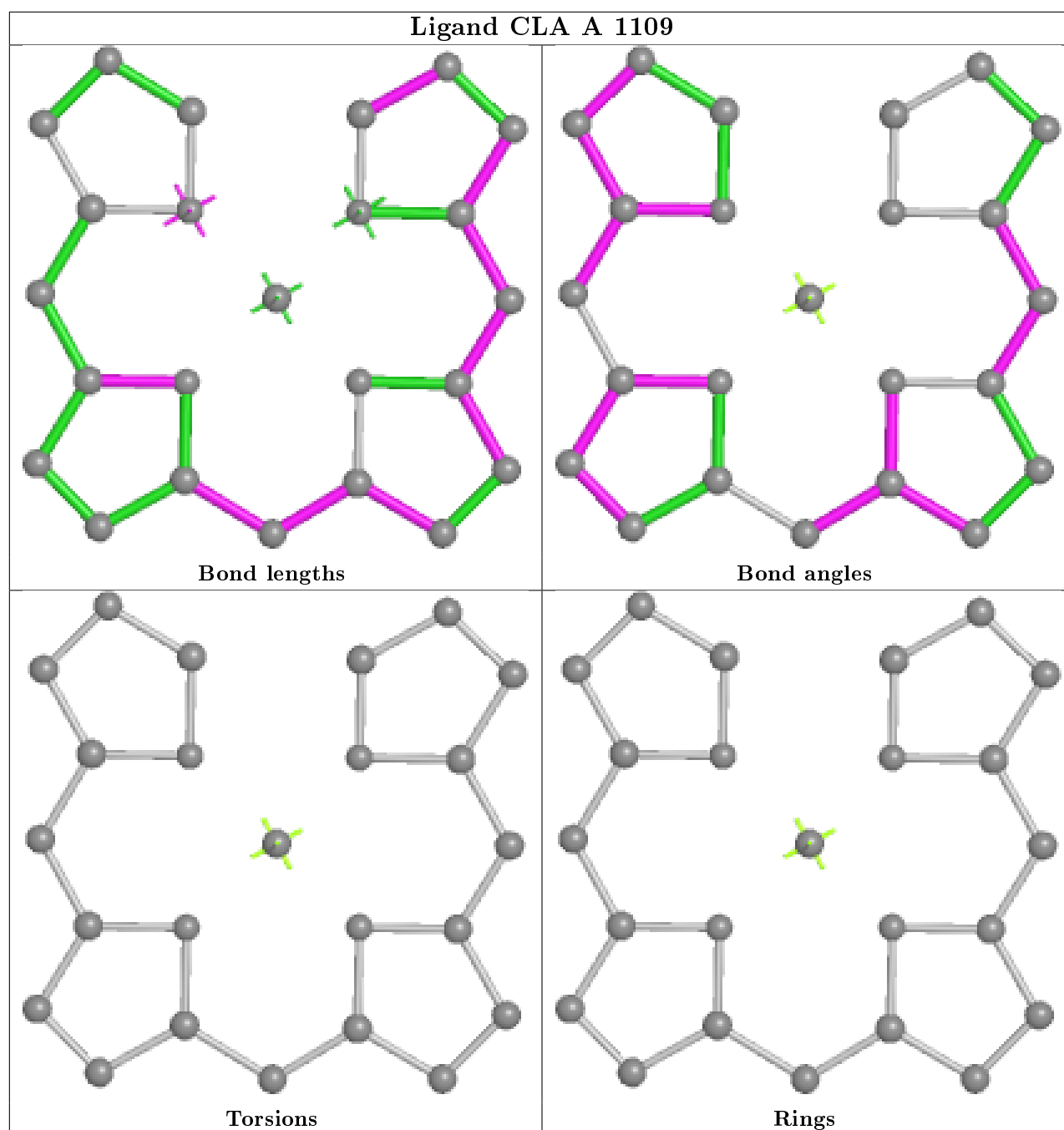


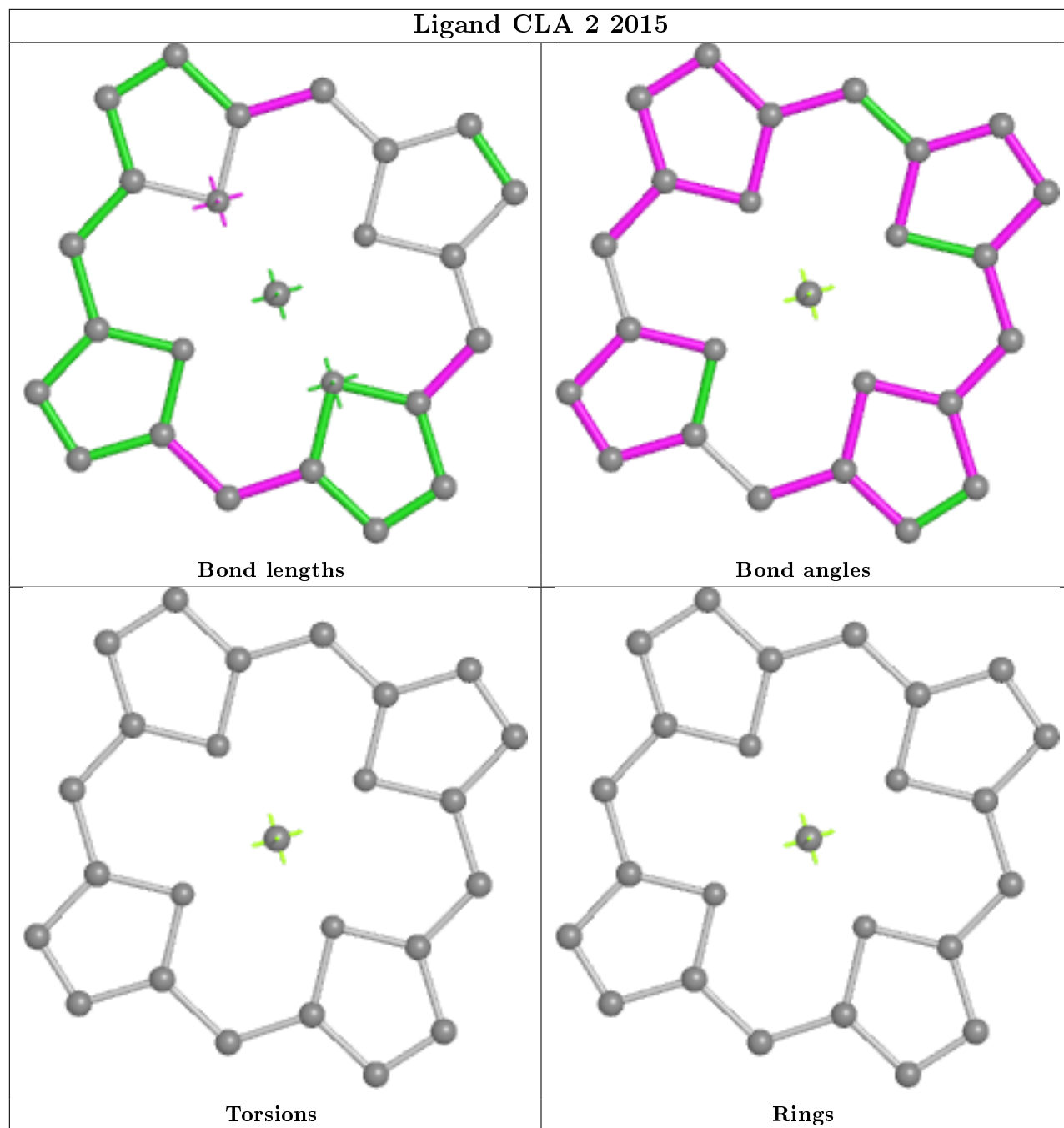




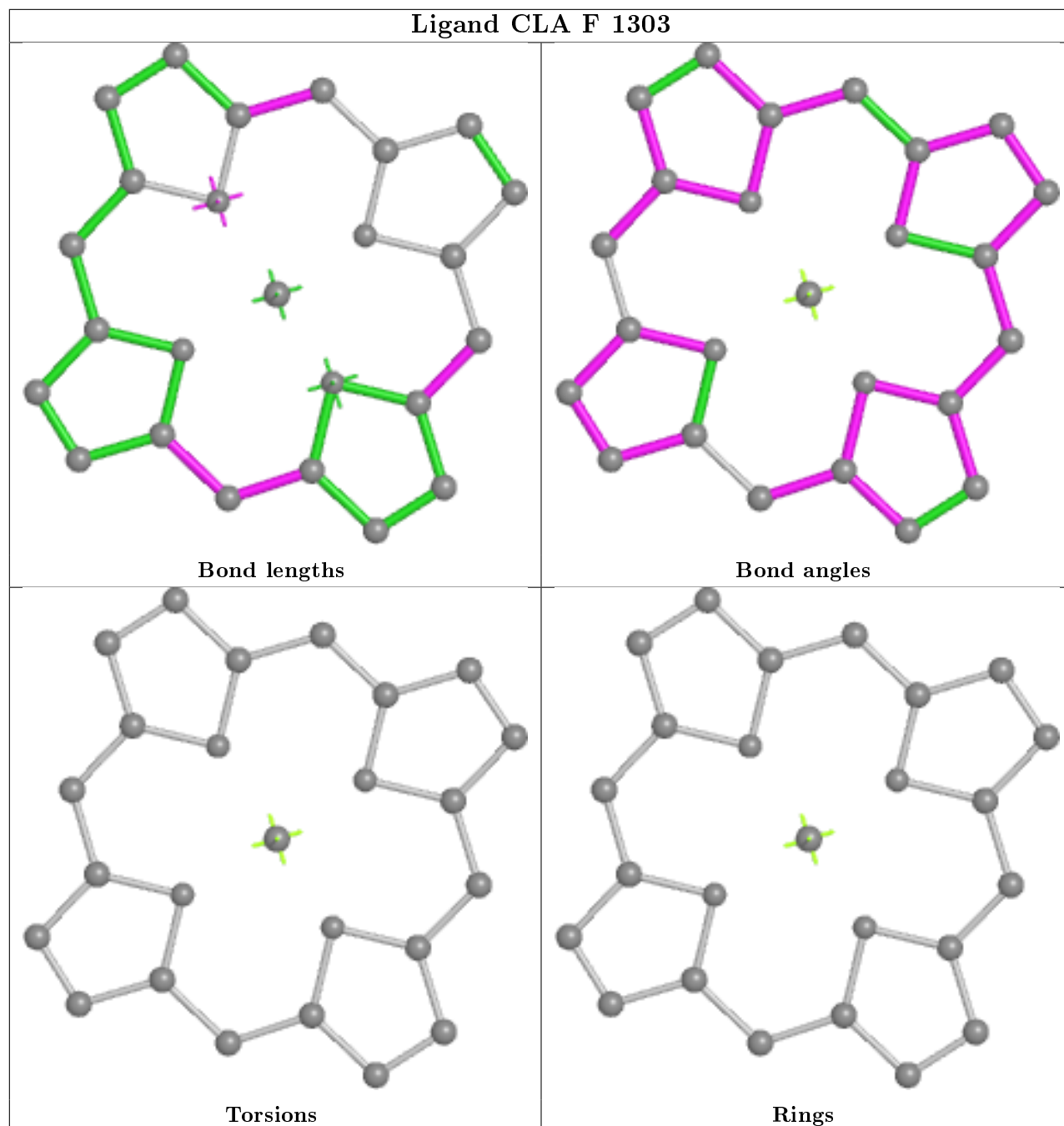
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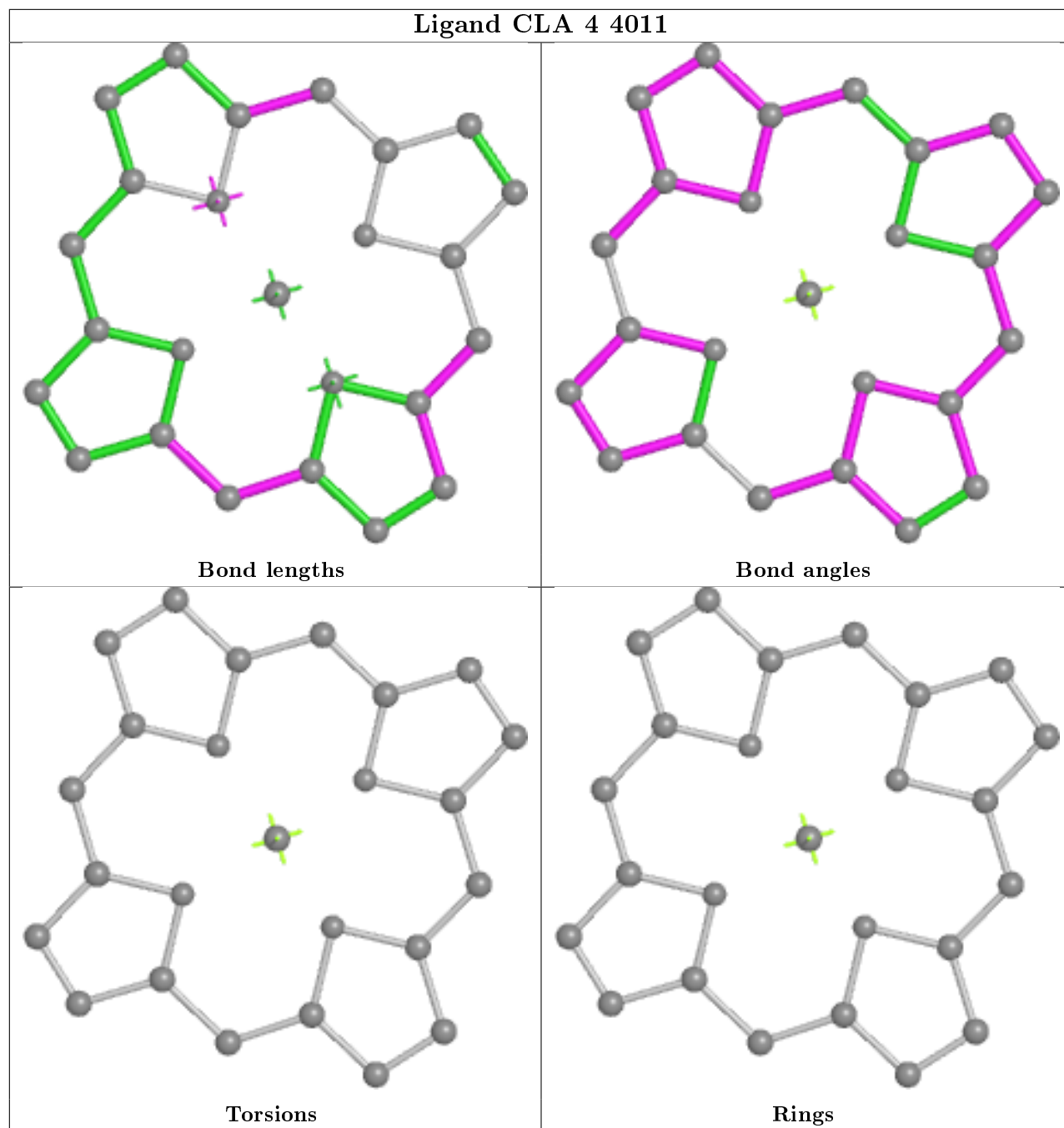


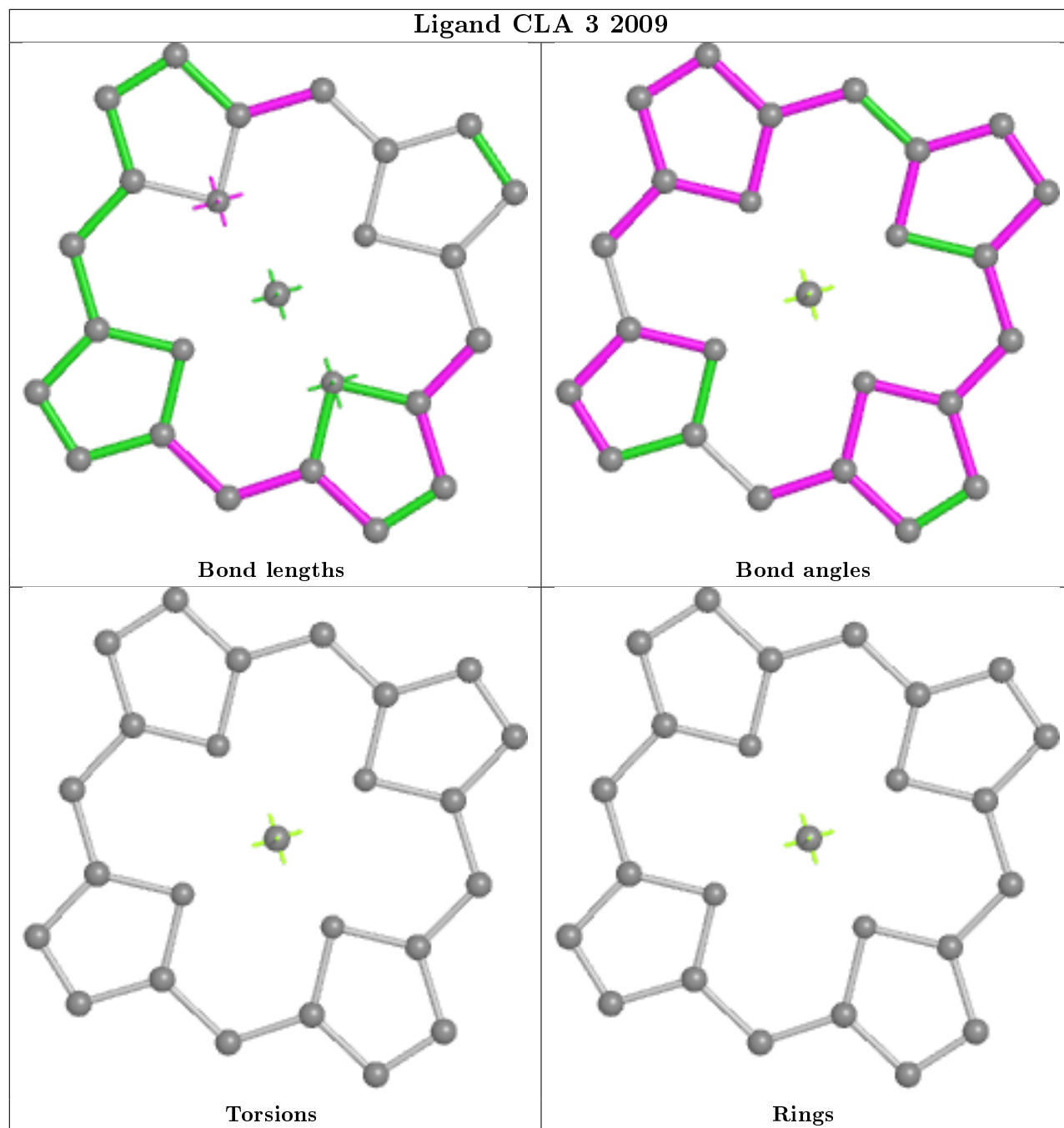


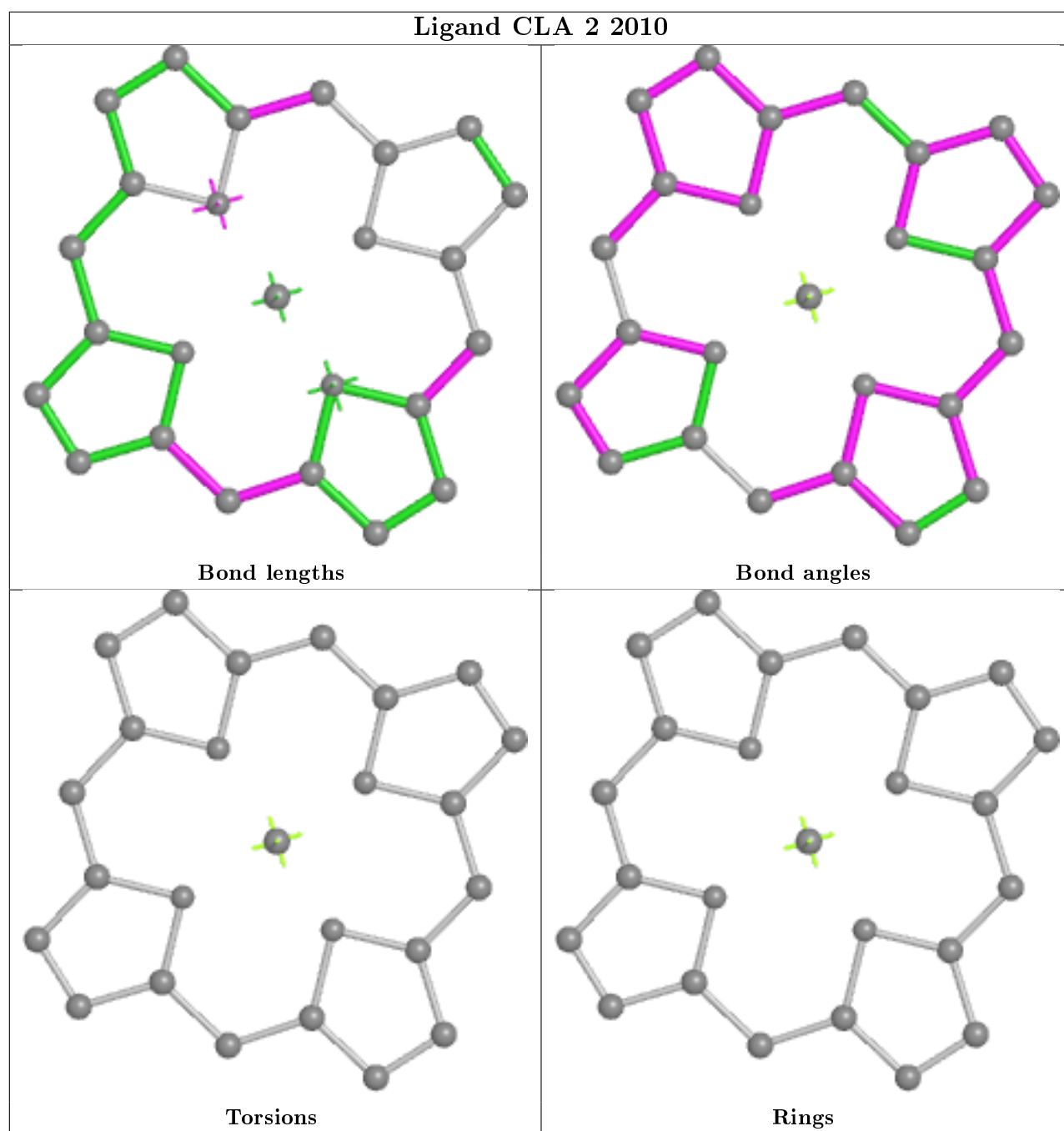


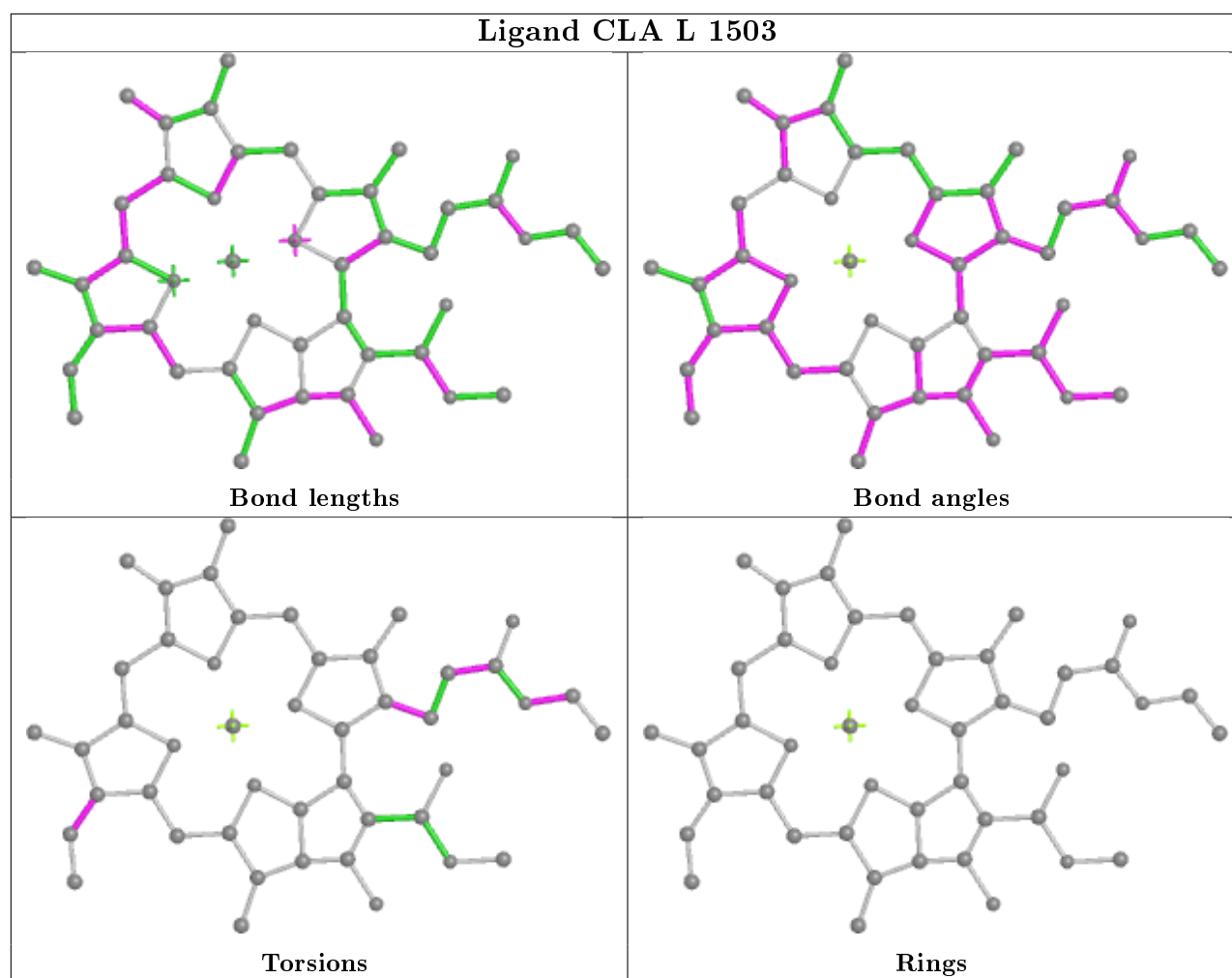
Ligand CLA F 1303

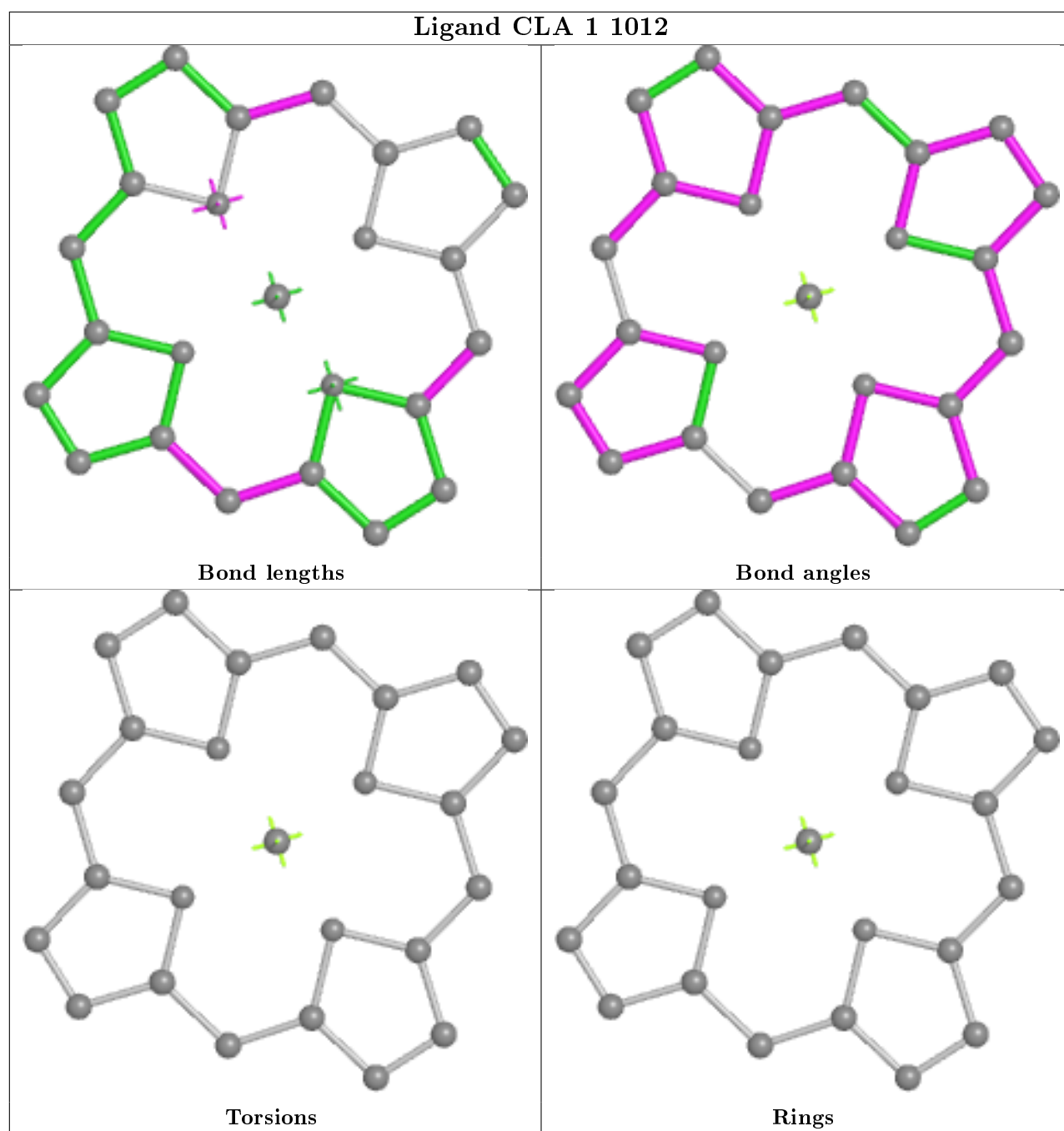


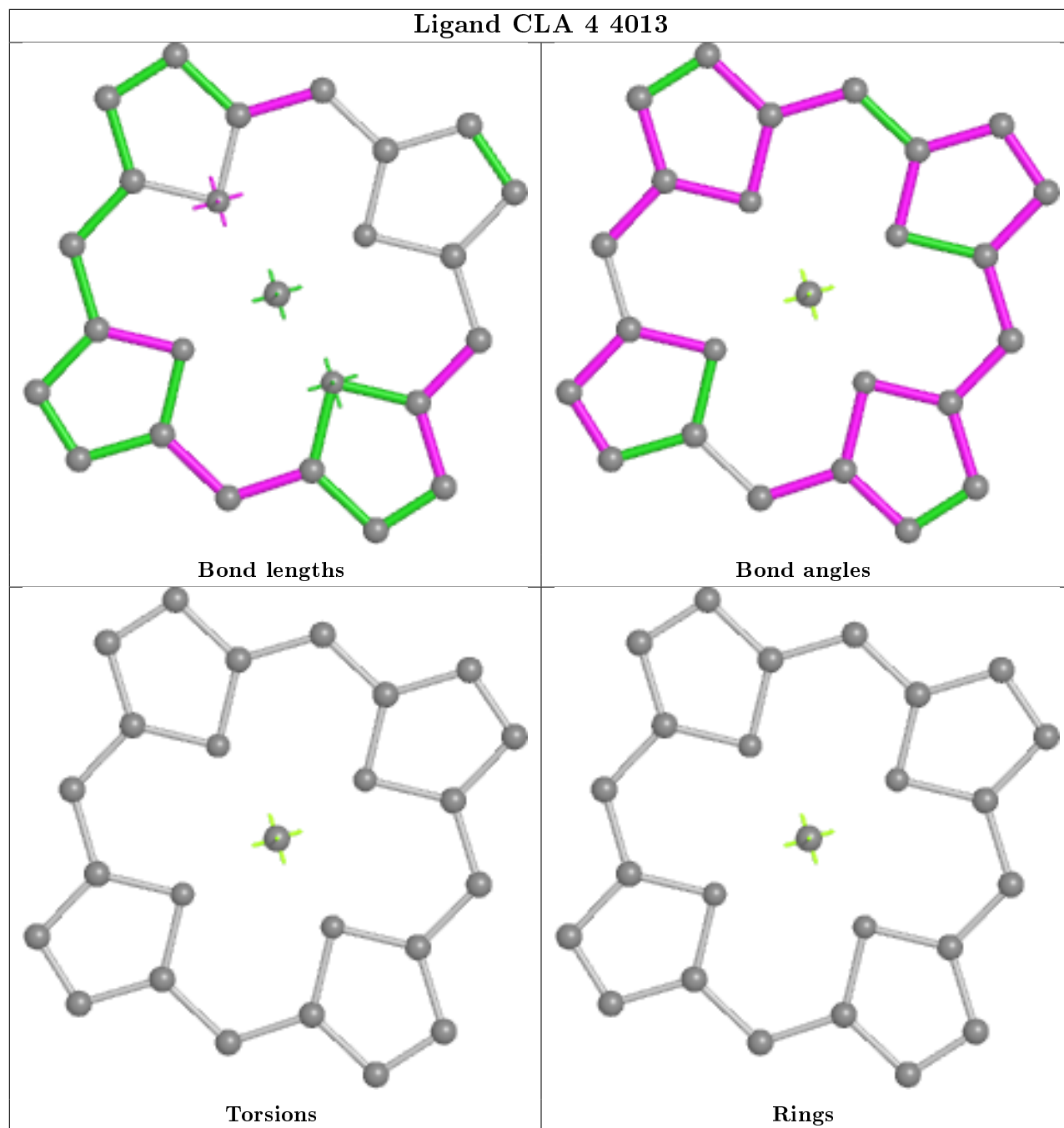




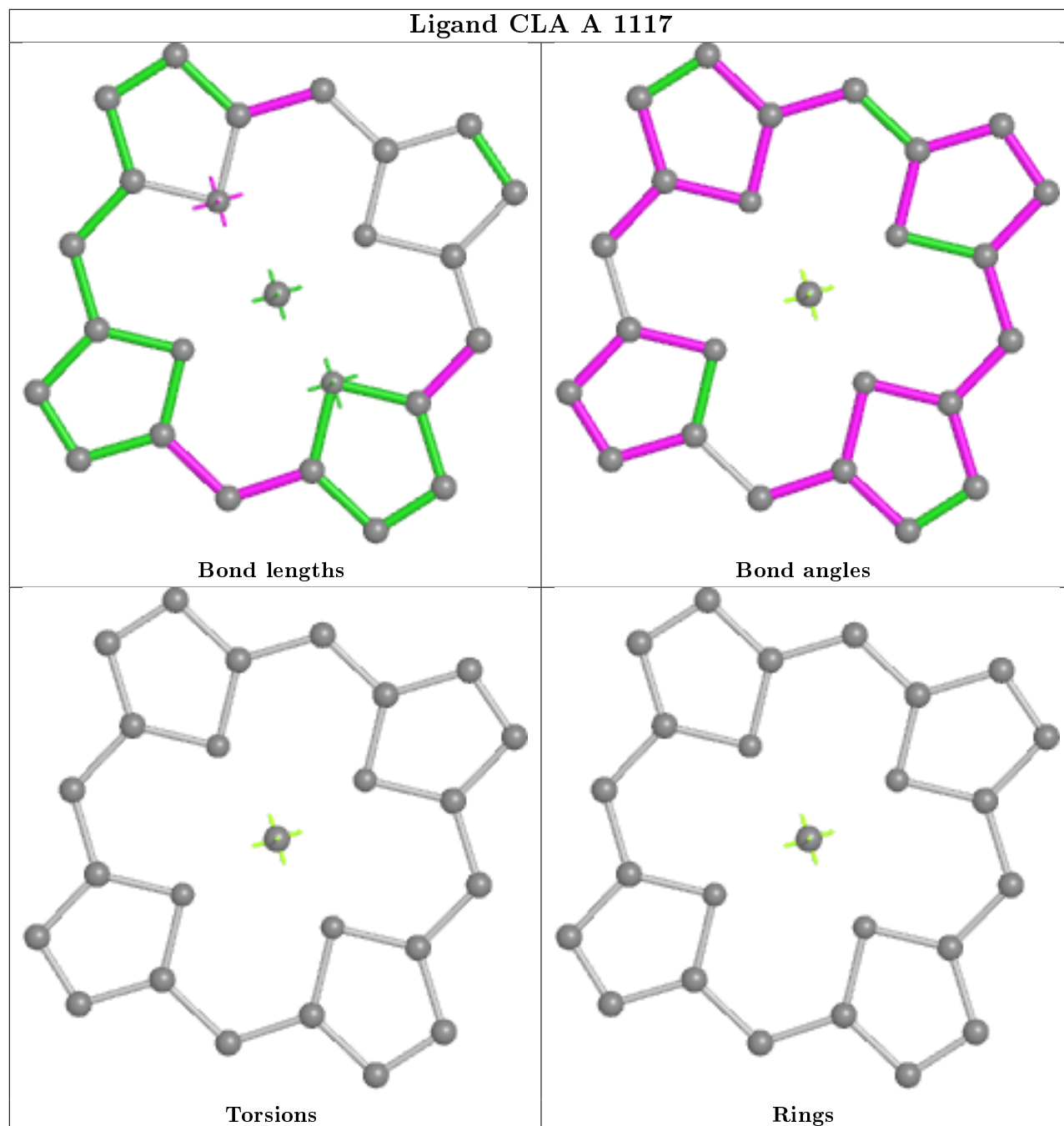


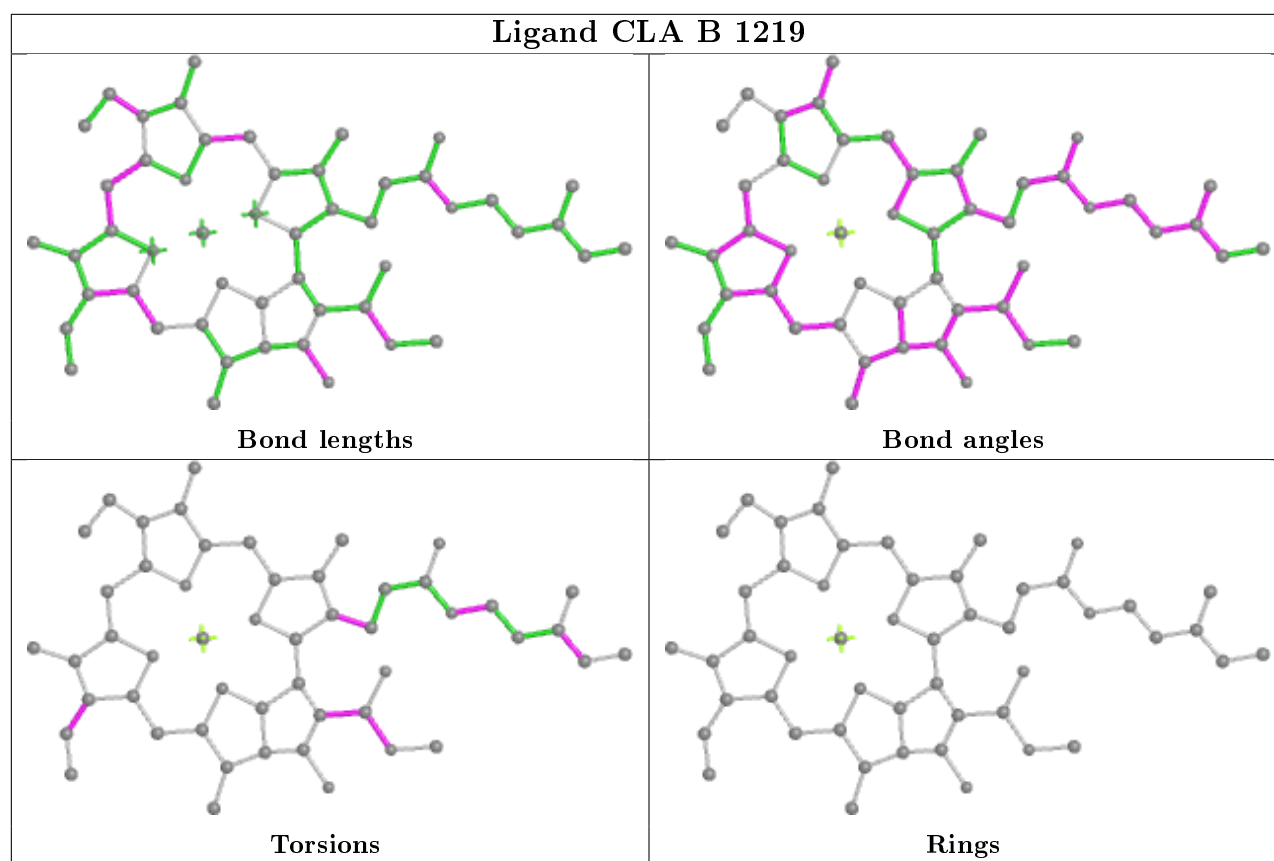




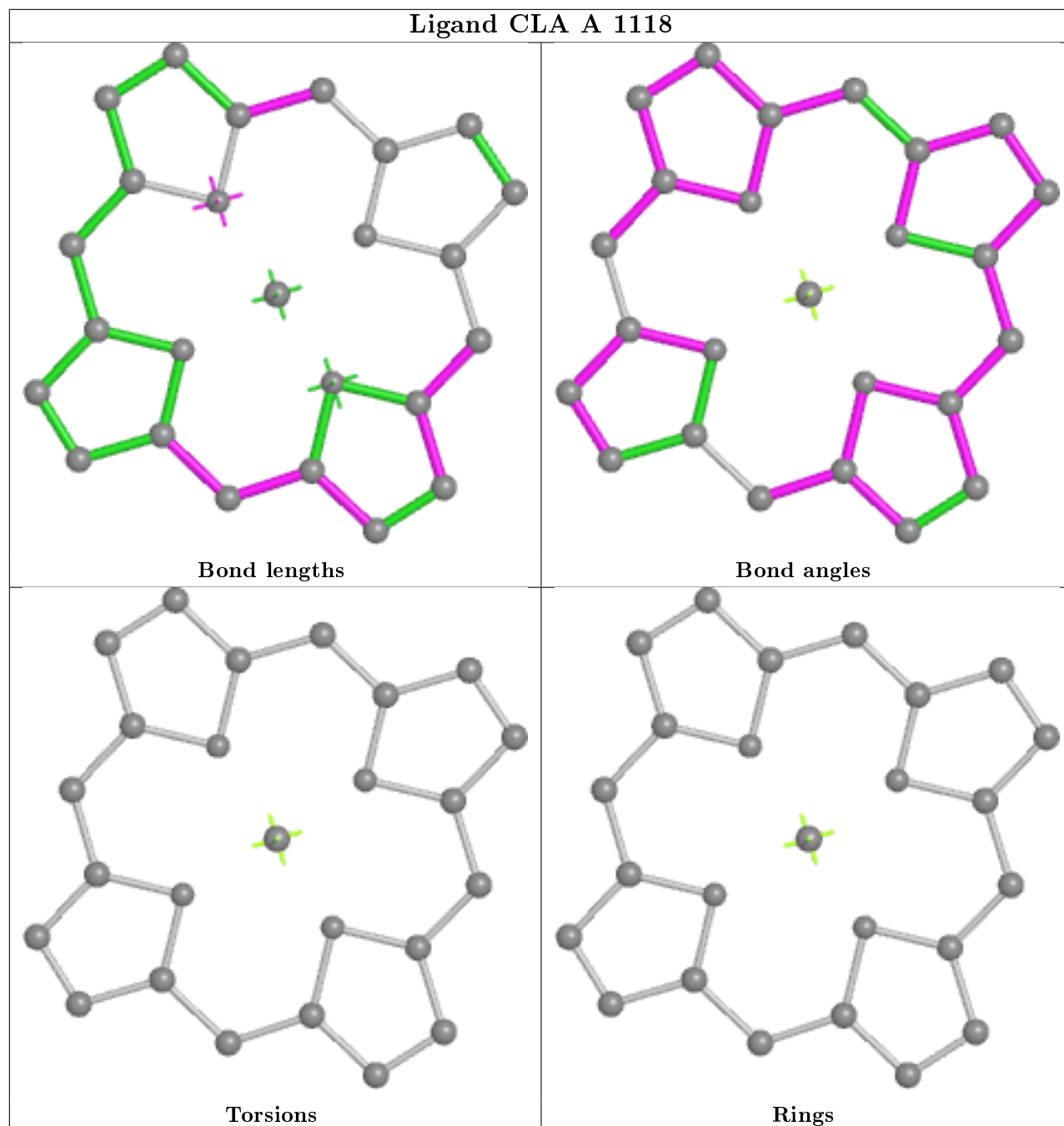


Ligand CLA A 1117

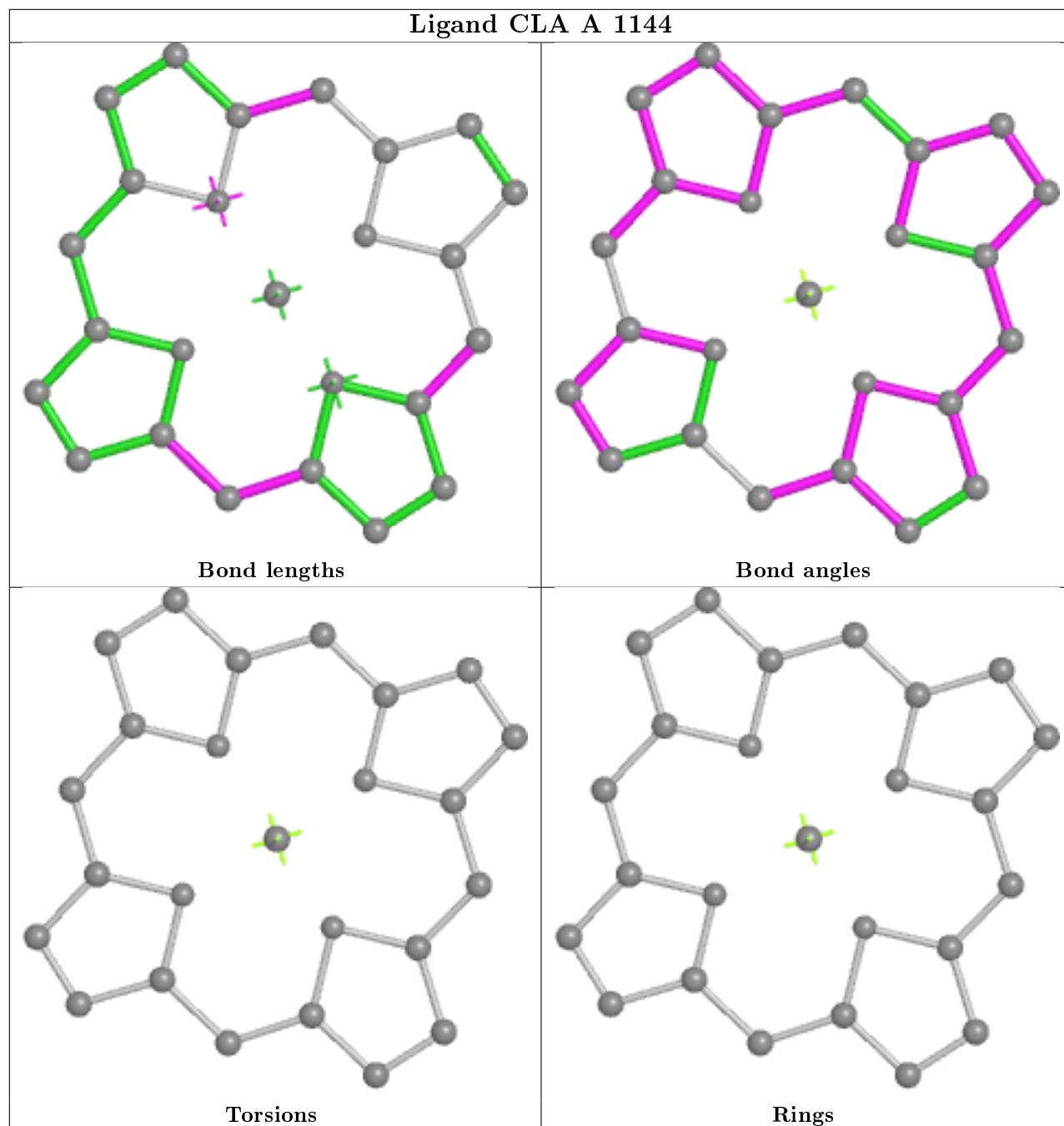


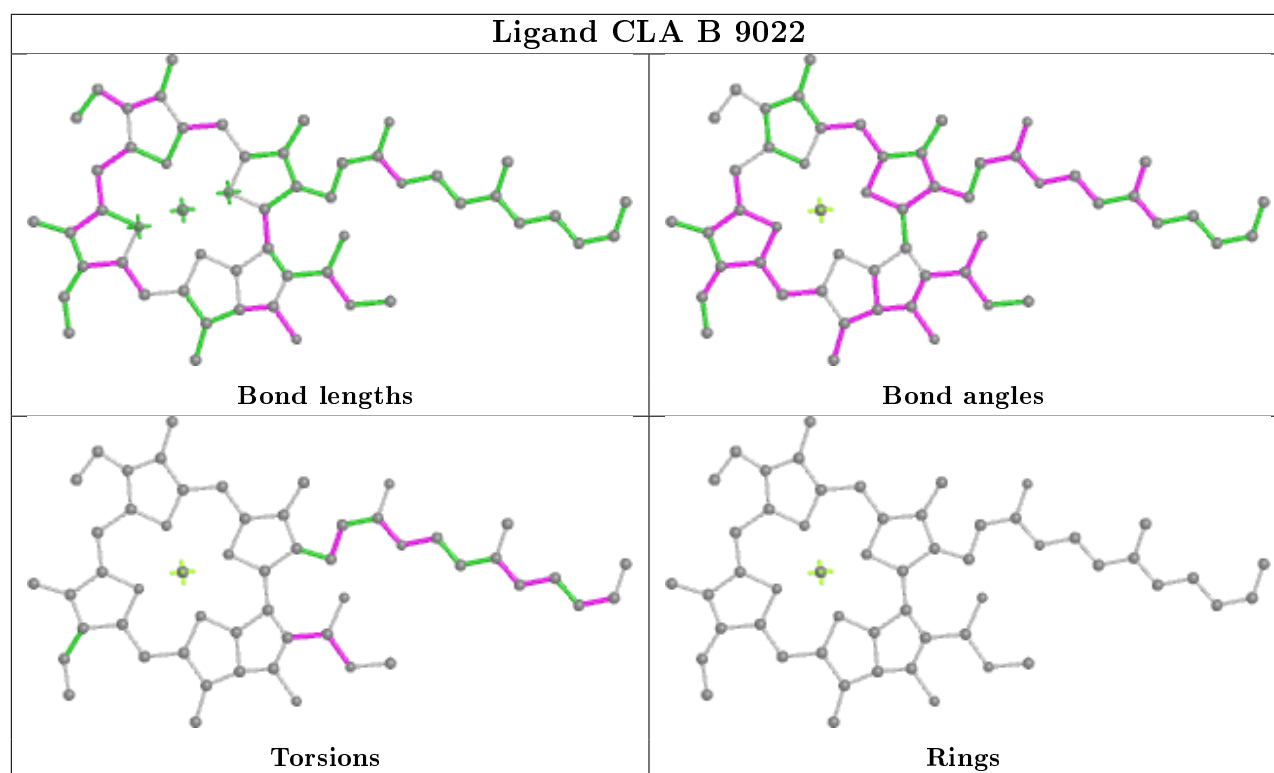


Ligand CLA A 1118

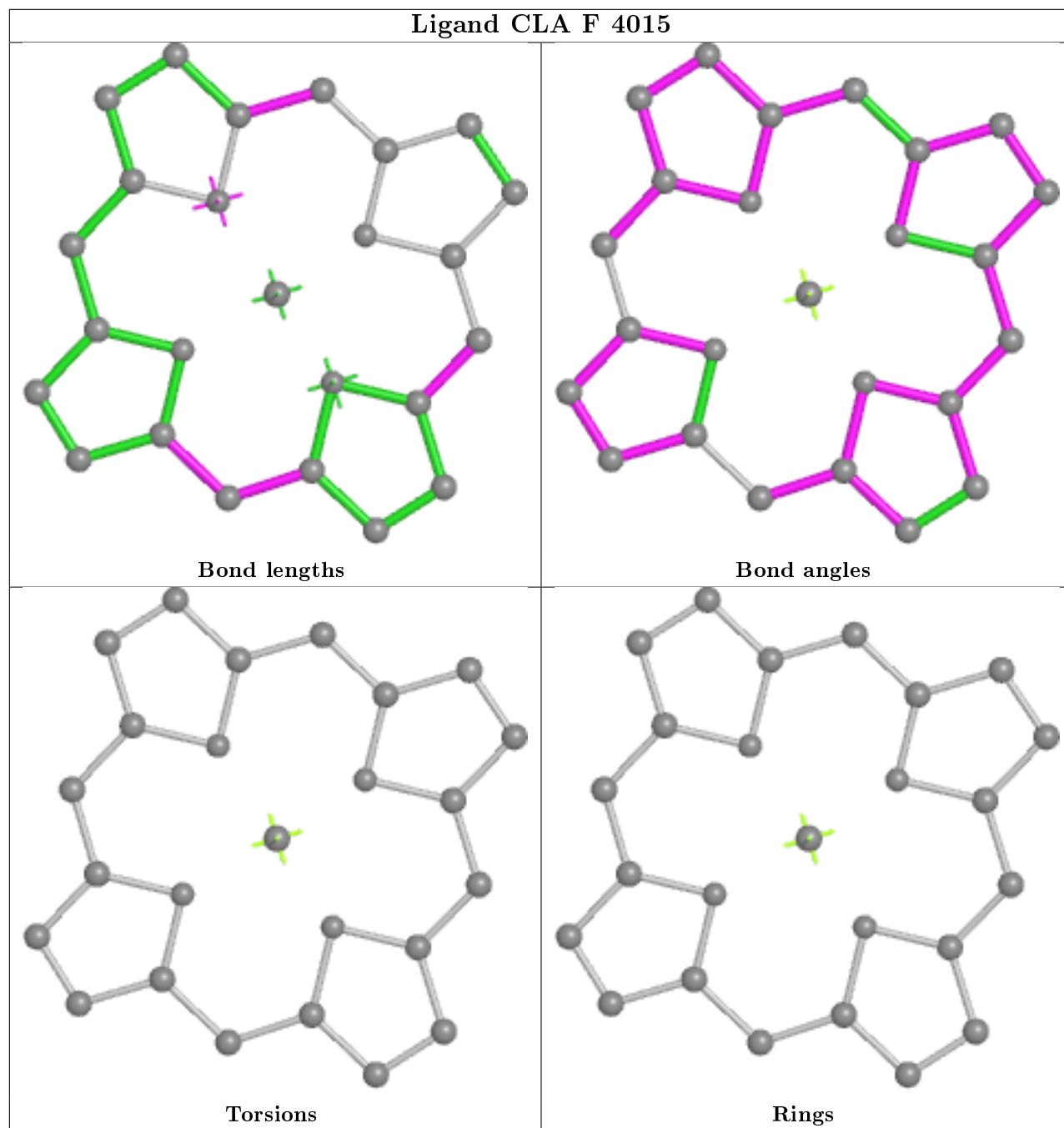


Ligand CLA A 1144

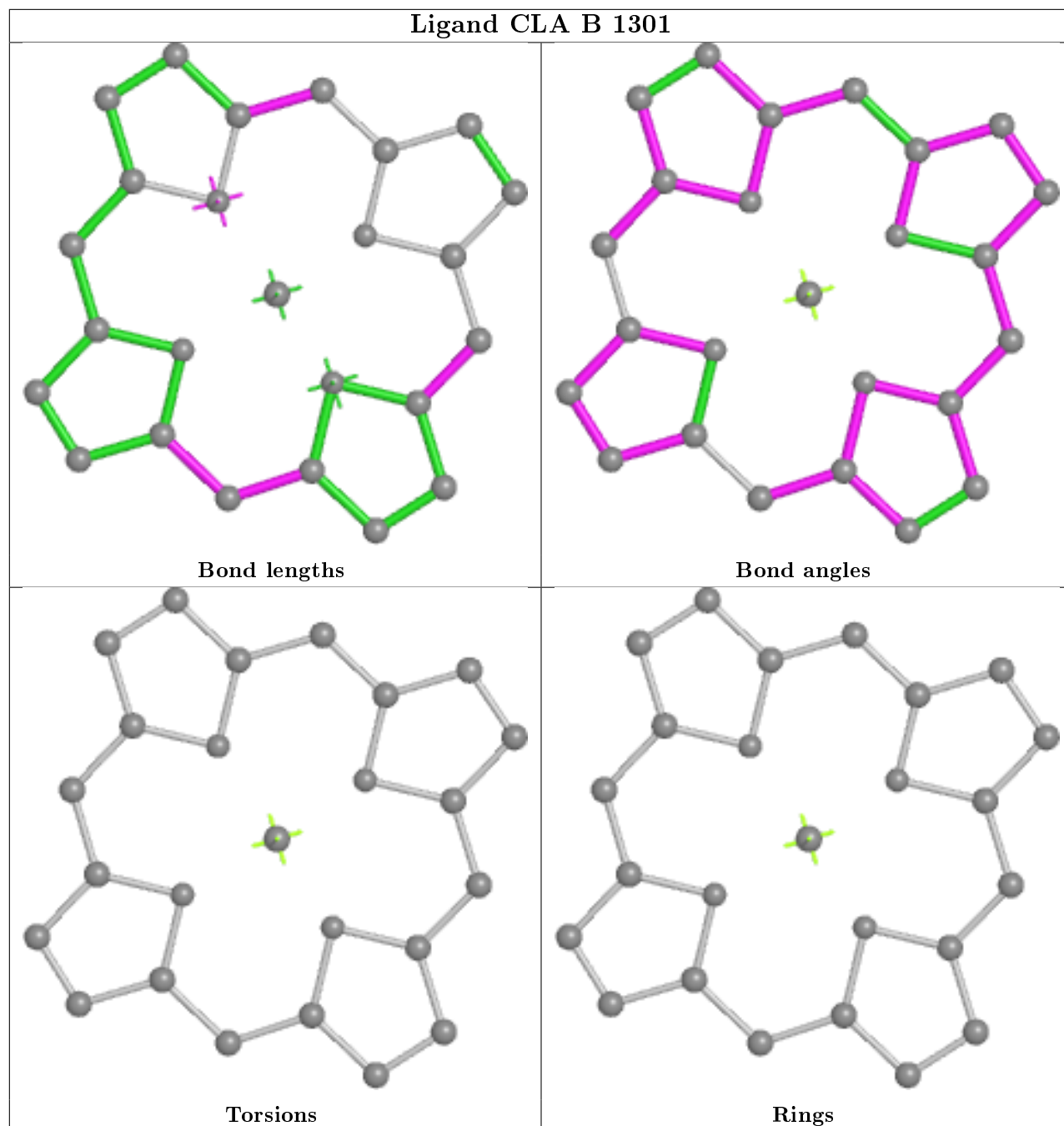




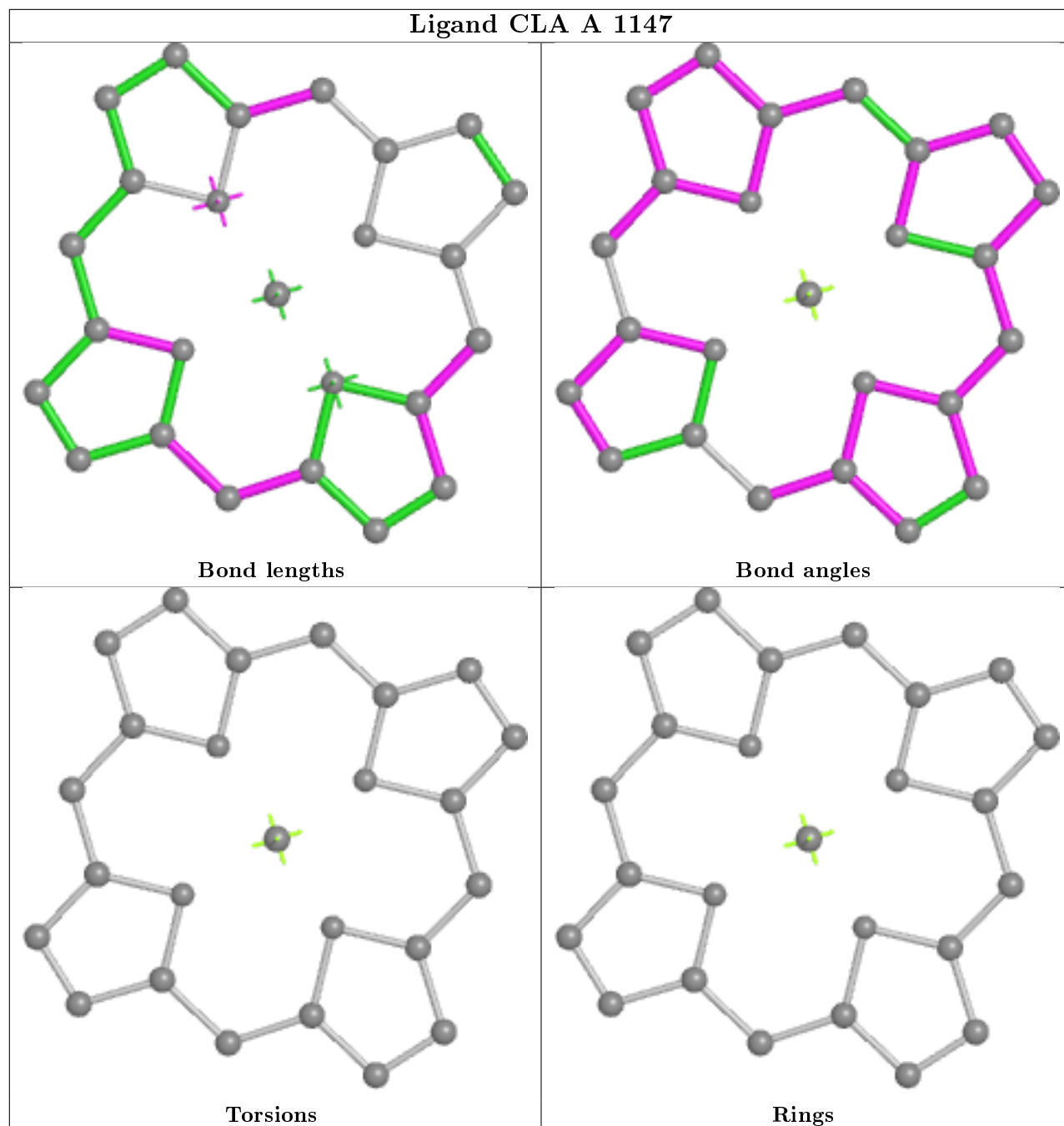
Ligand CLA F 4015



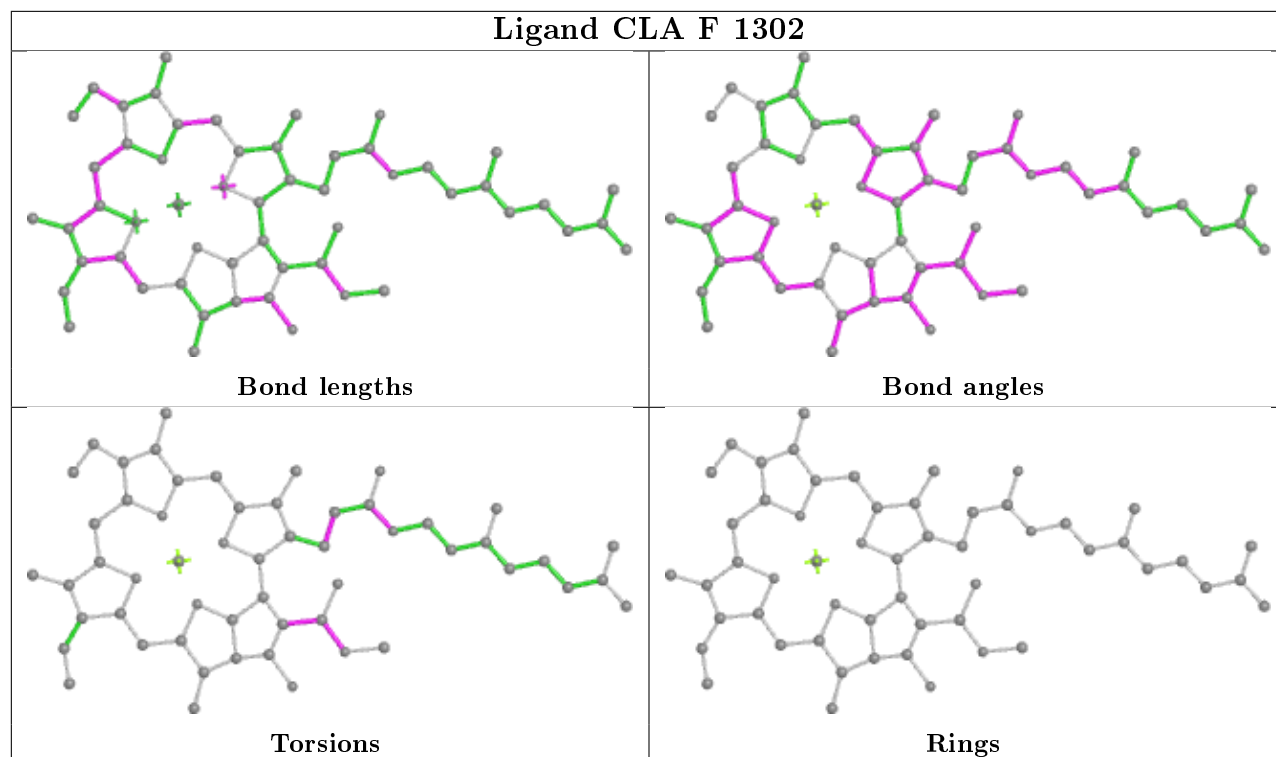
Ligand CLA B 1301



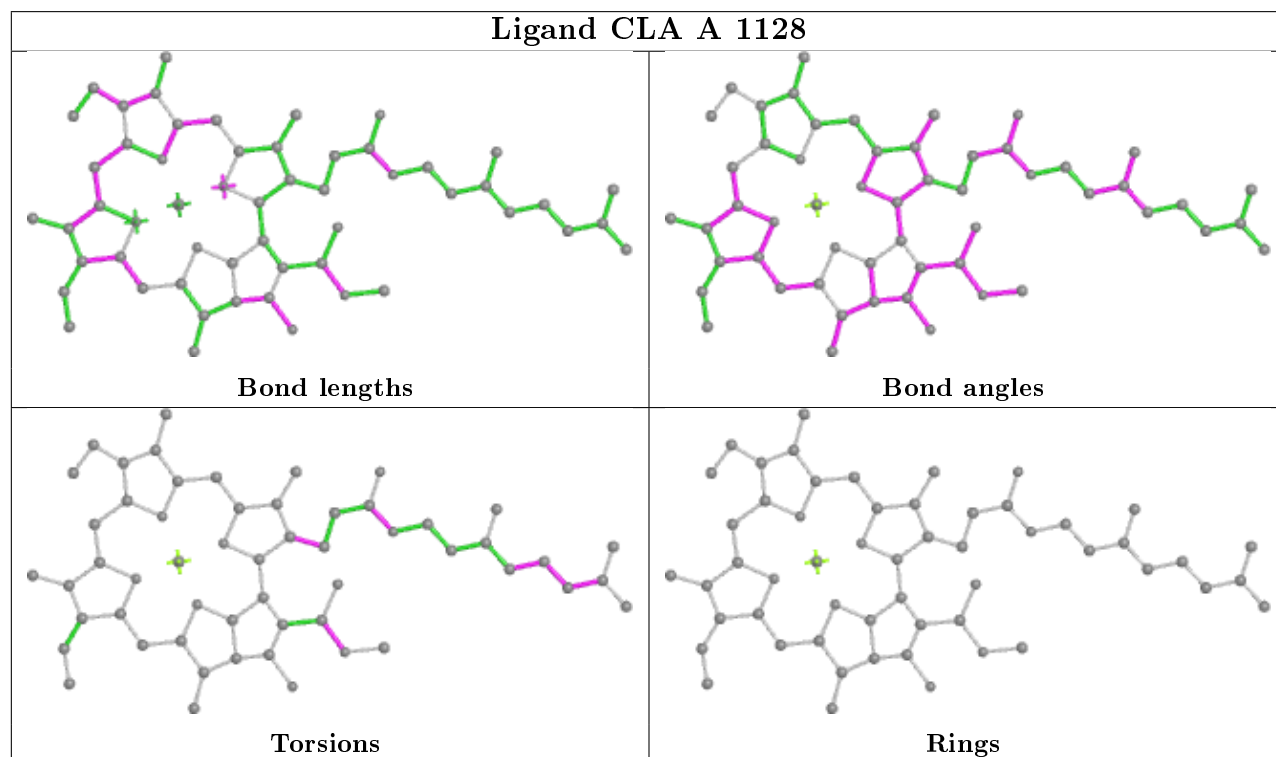
Ligand CLA A 1147

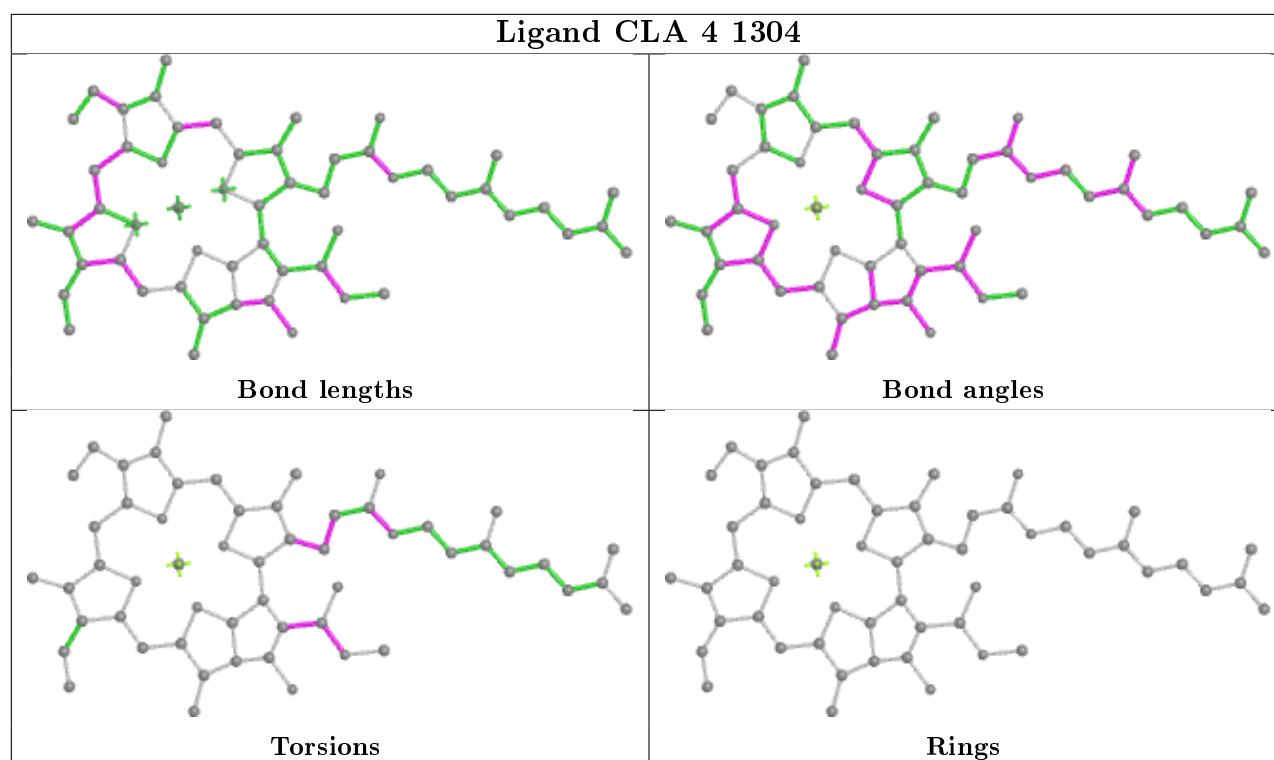


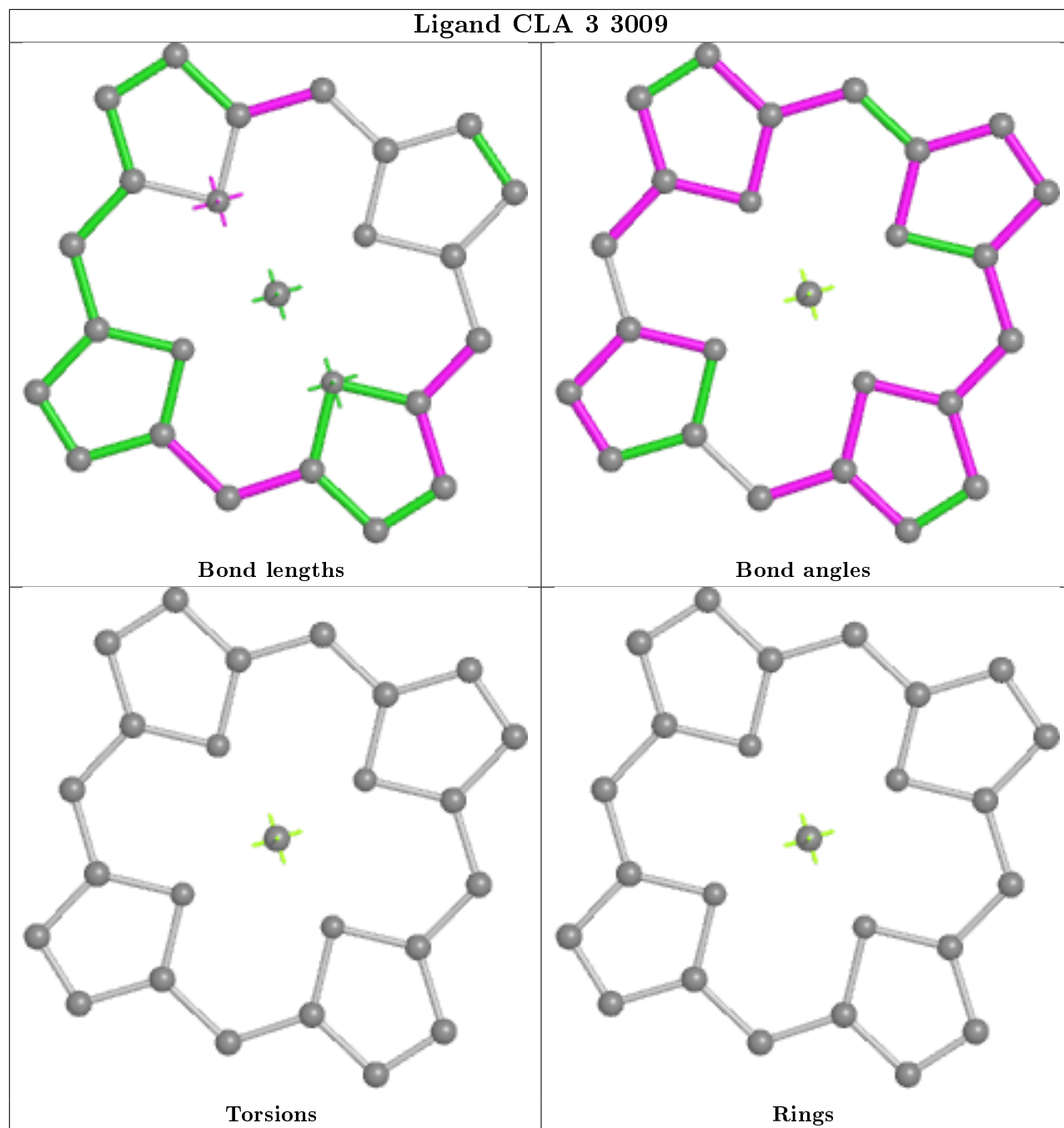
Ligand CLA F 1302

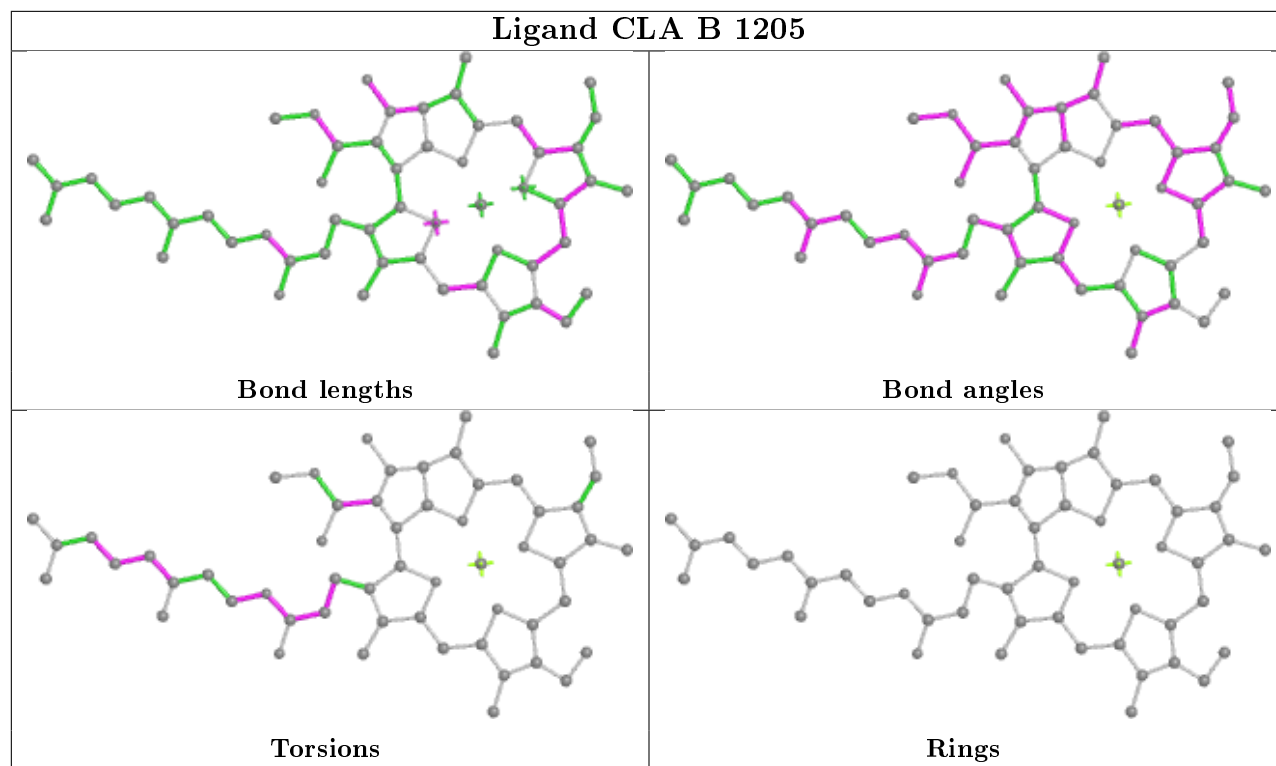


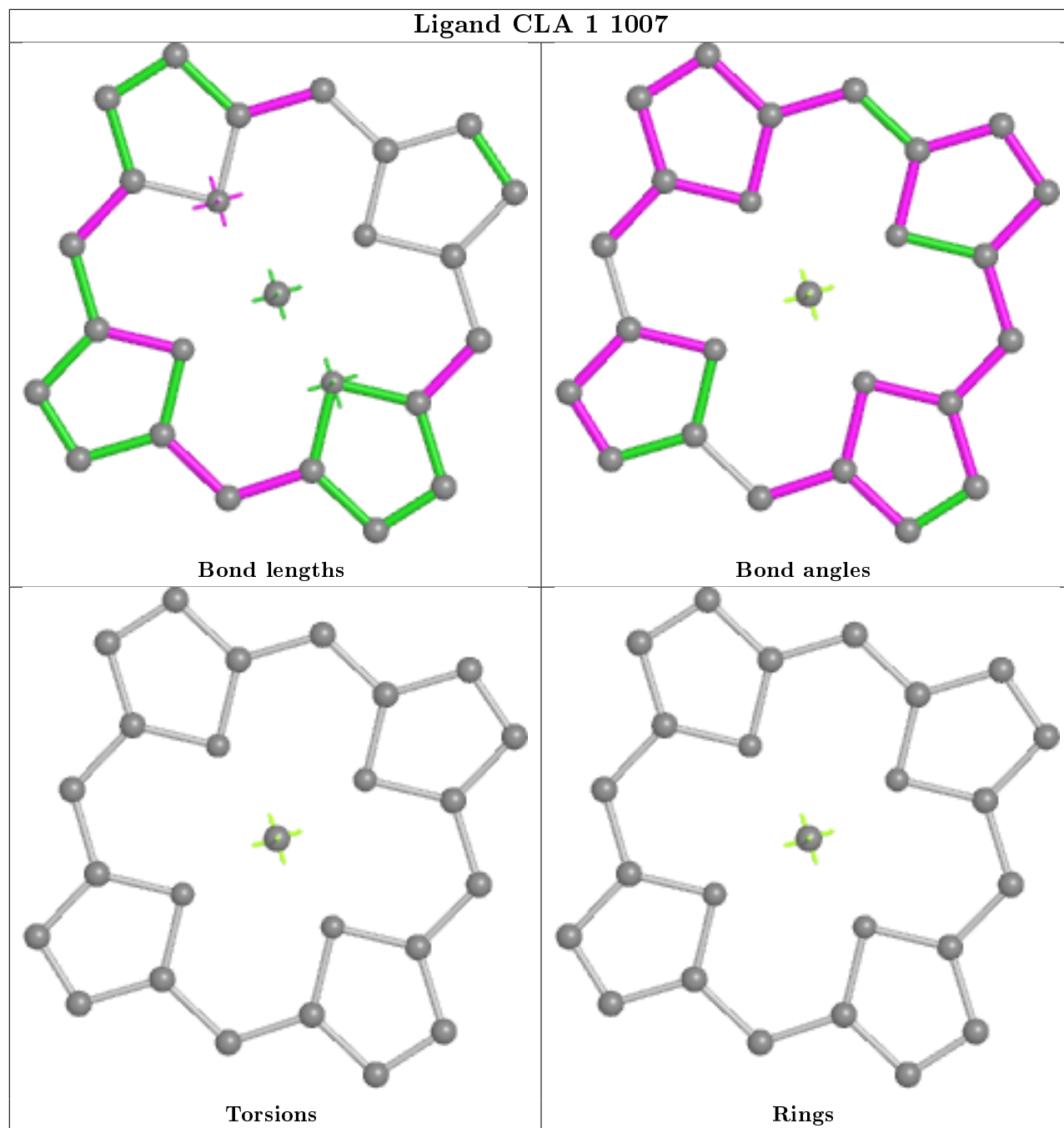
Ligand CLA A 1128

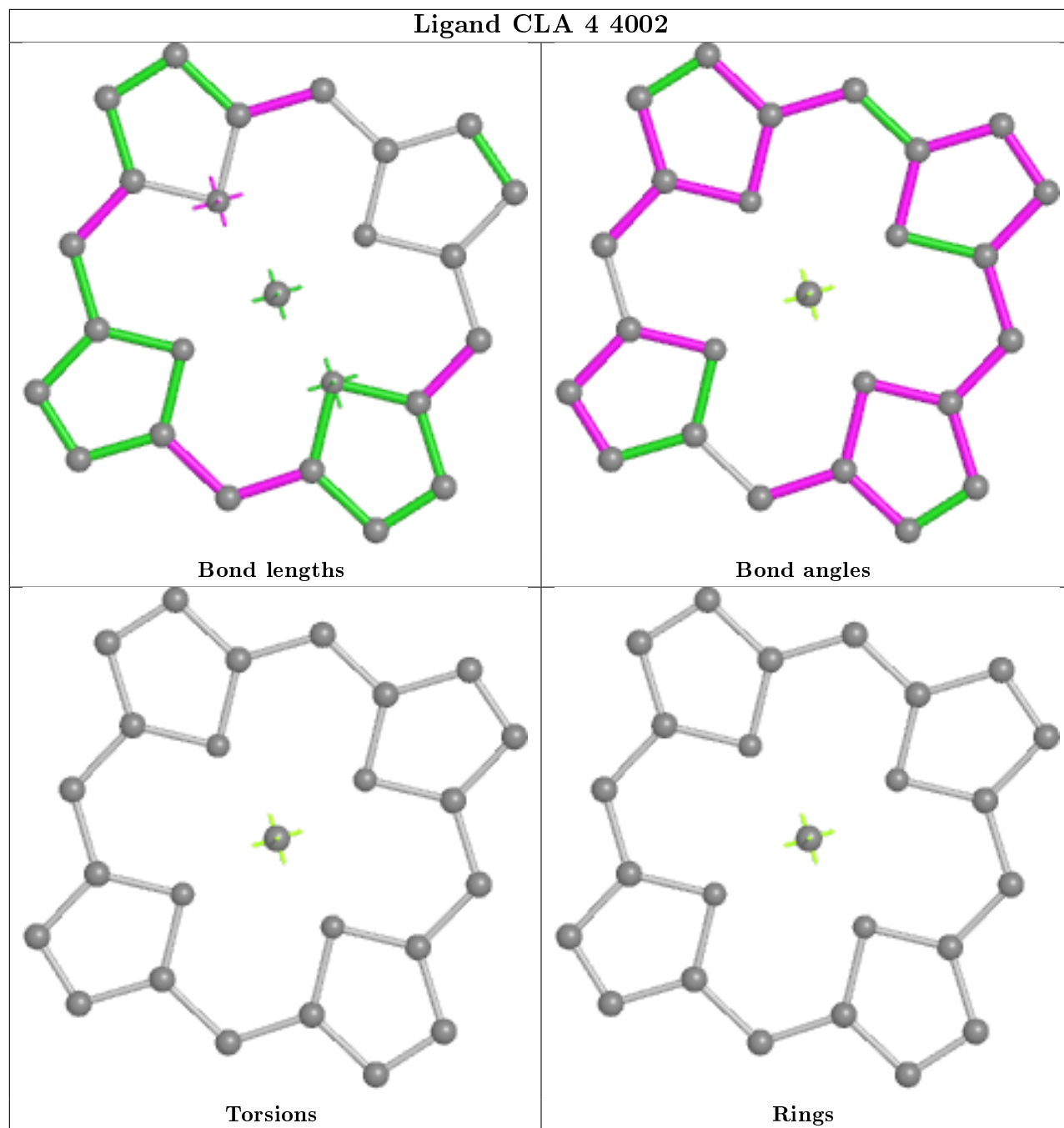


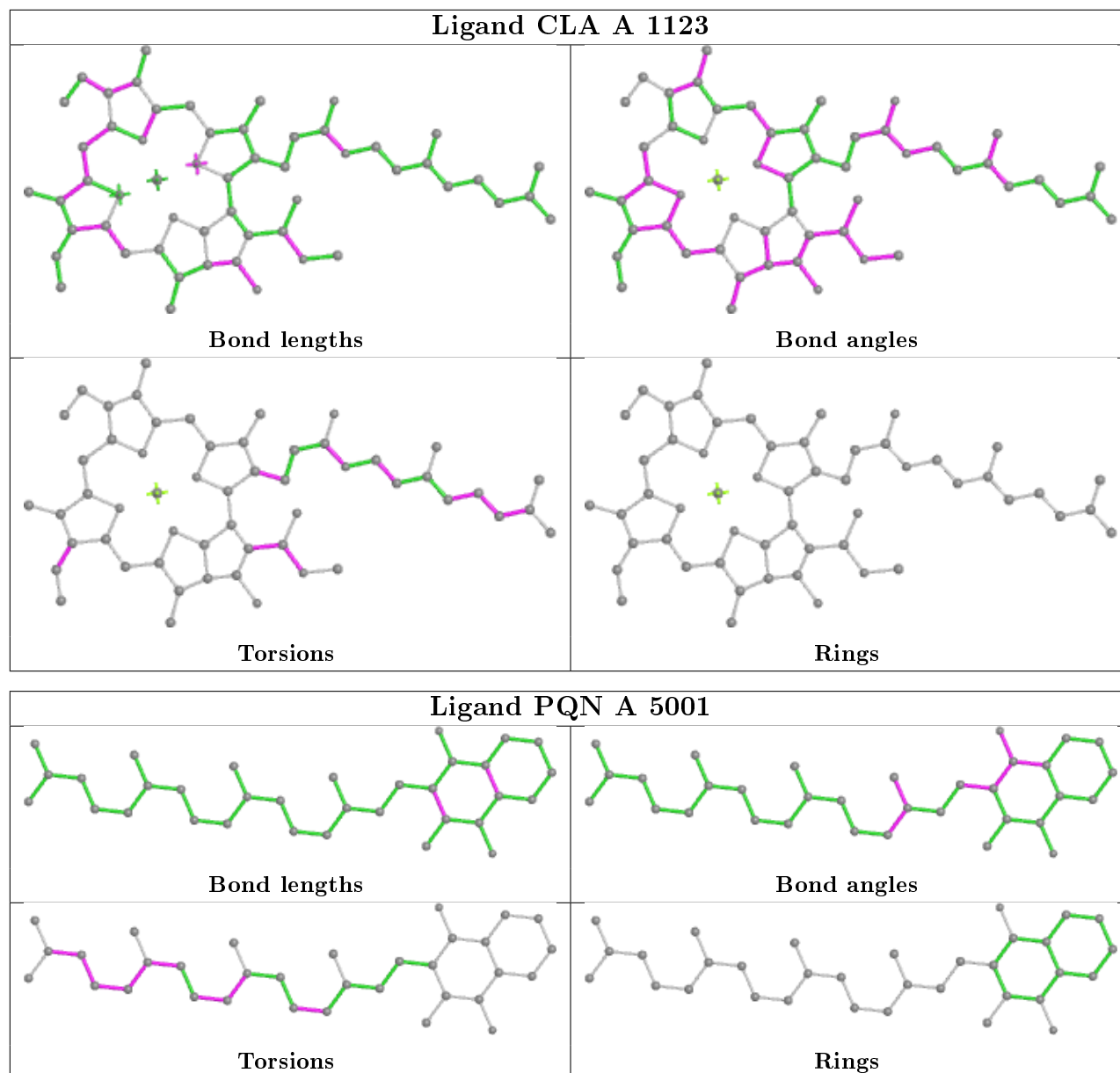


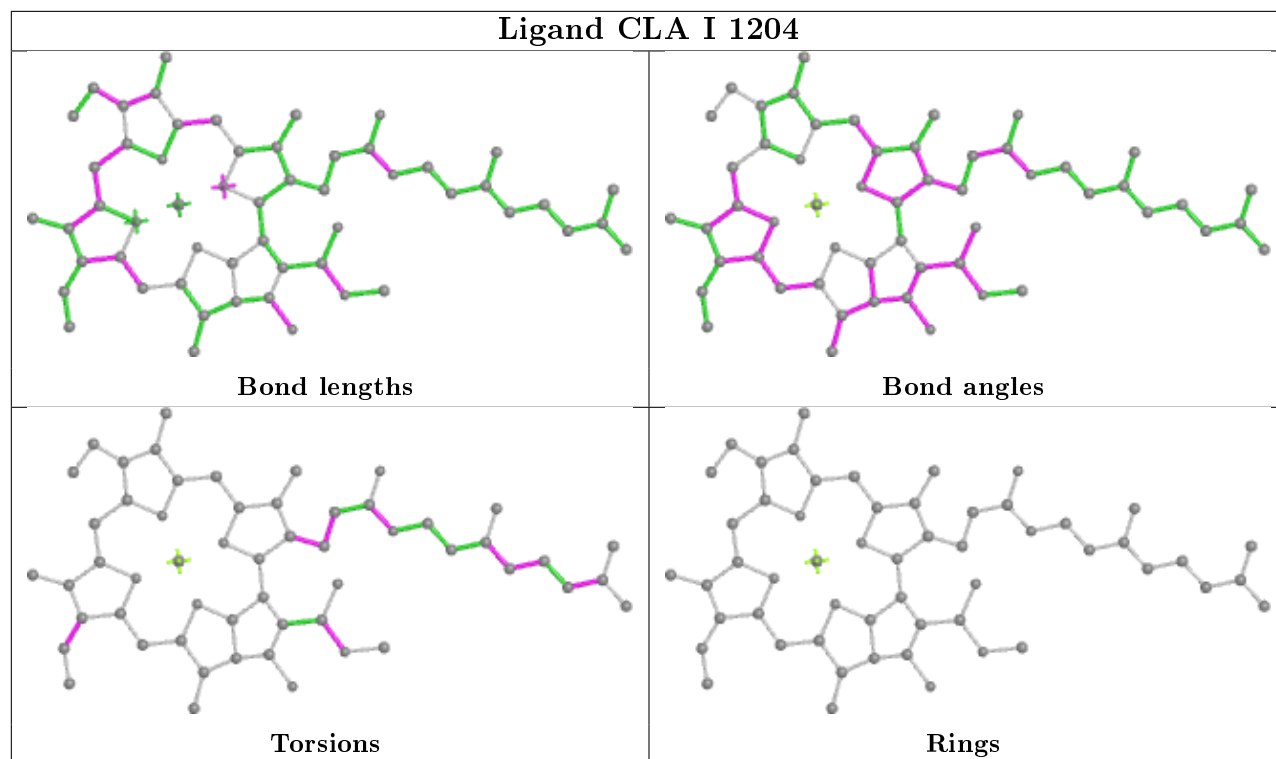




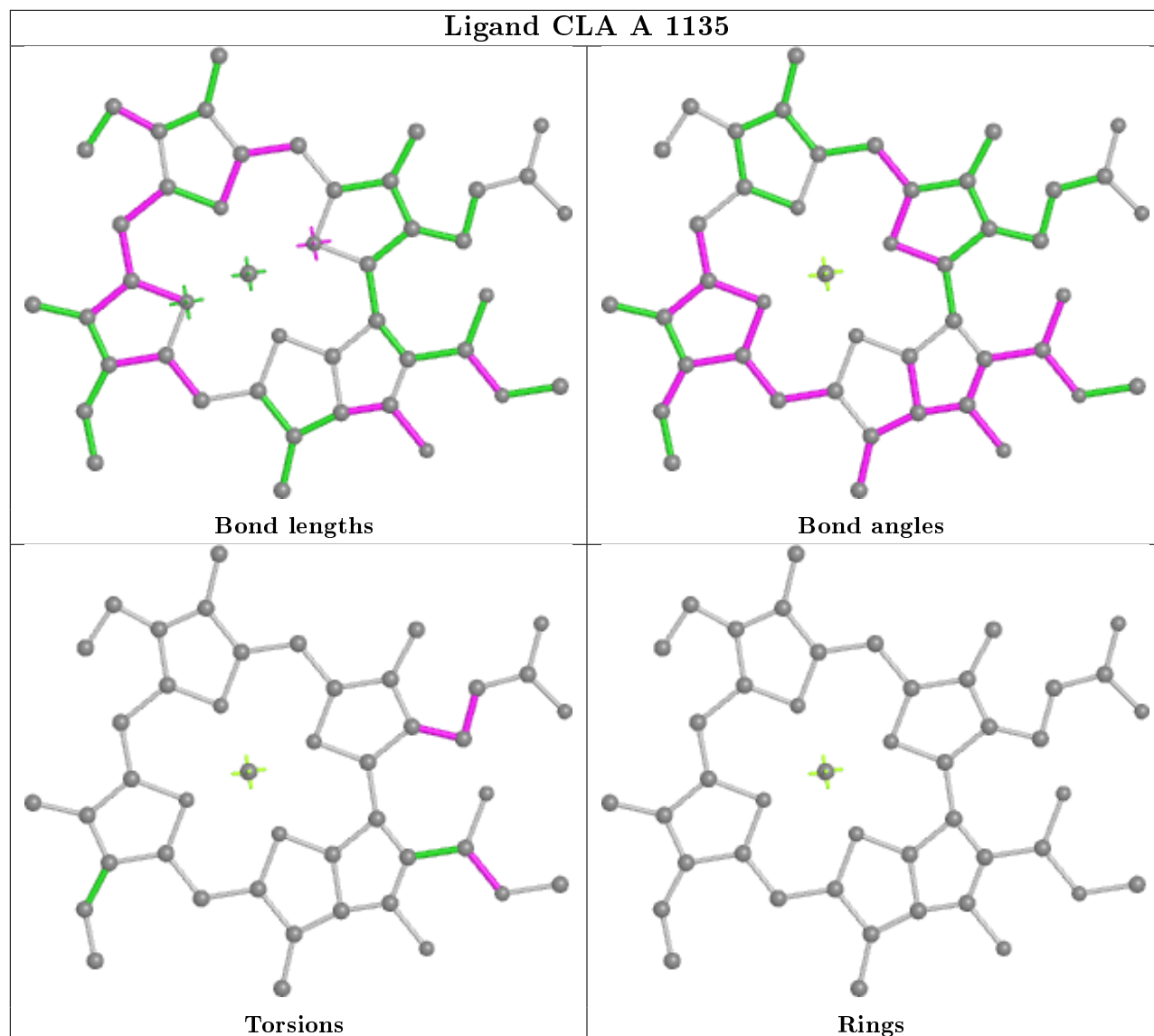


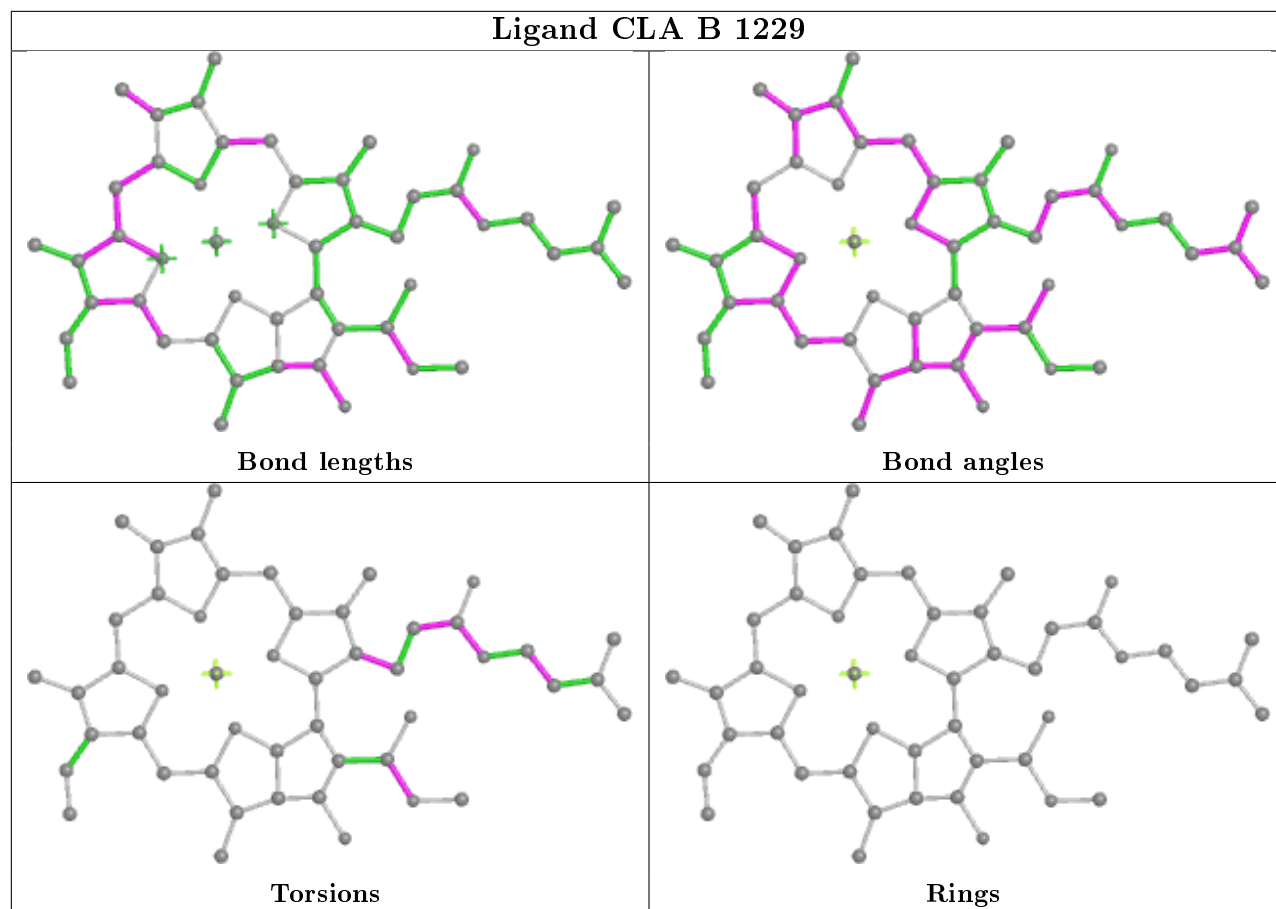




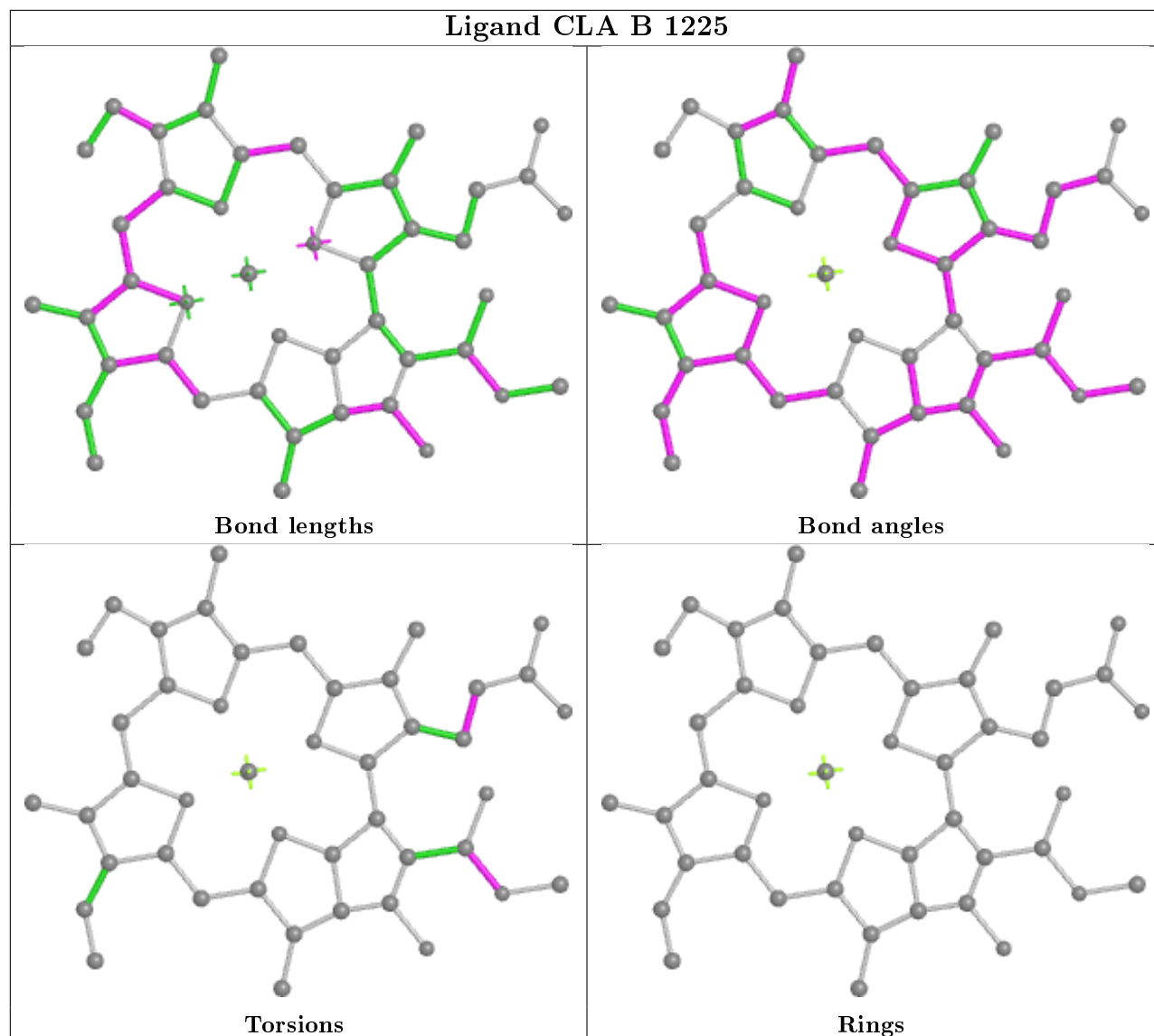


Ligand CLA A 1135

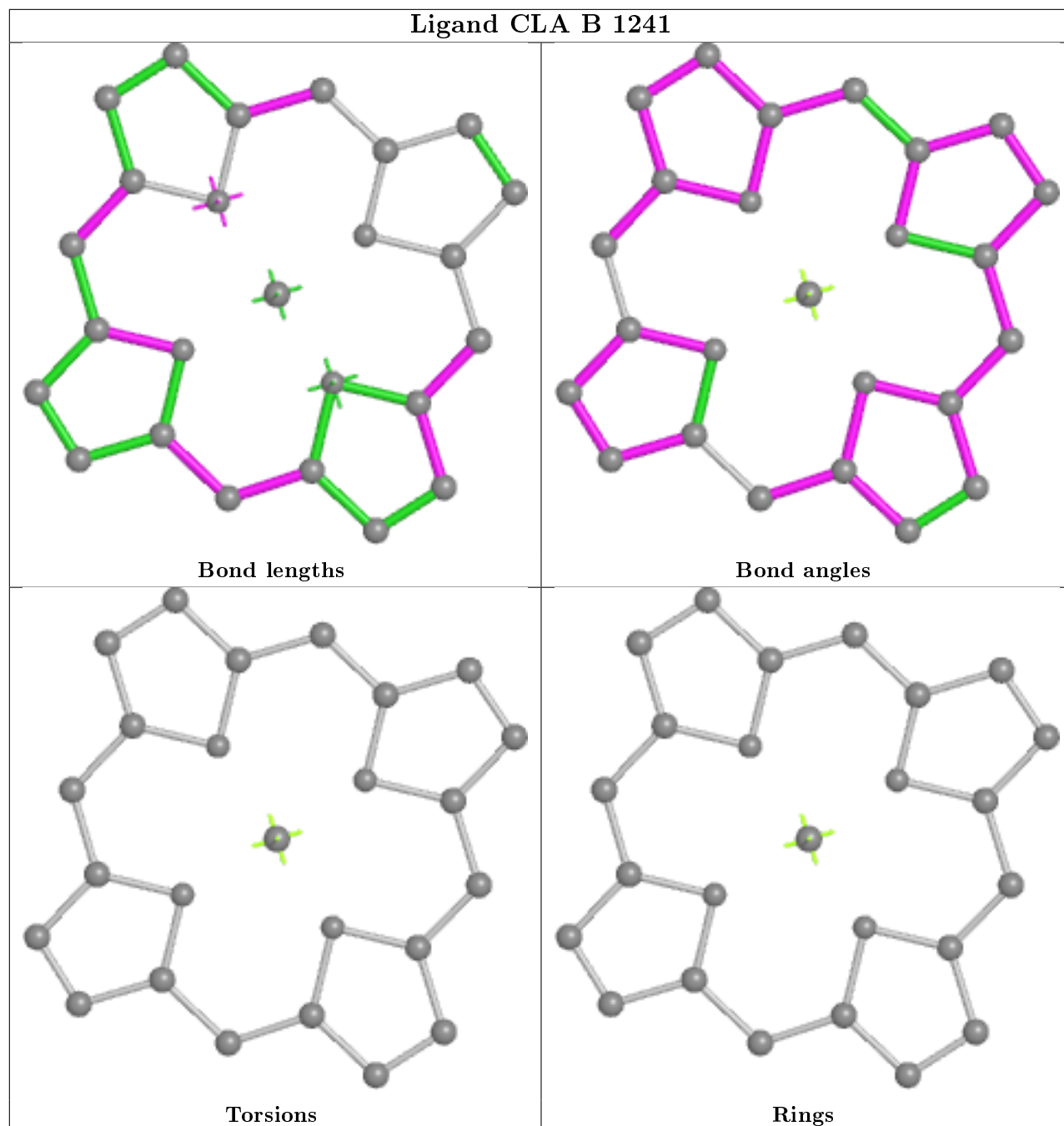


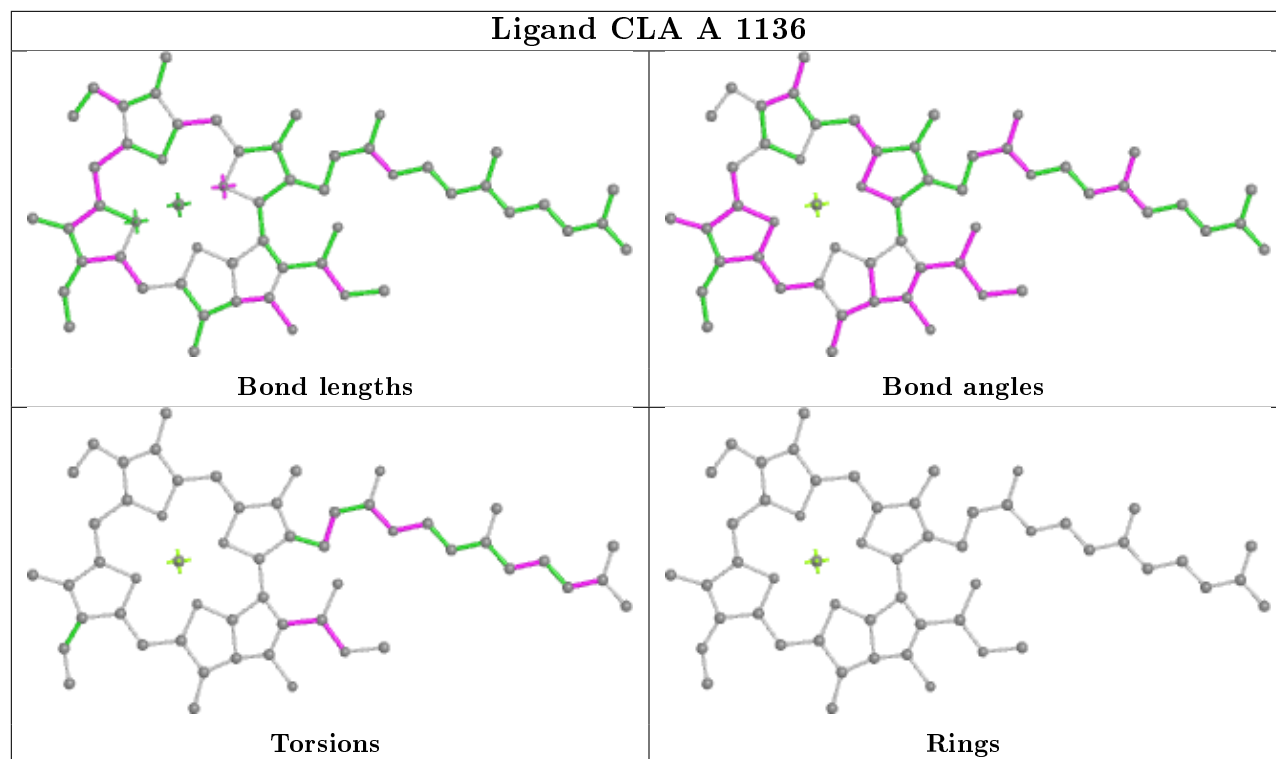


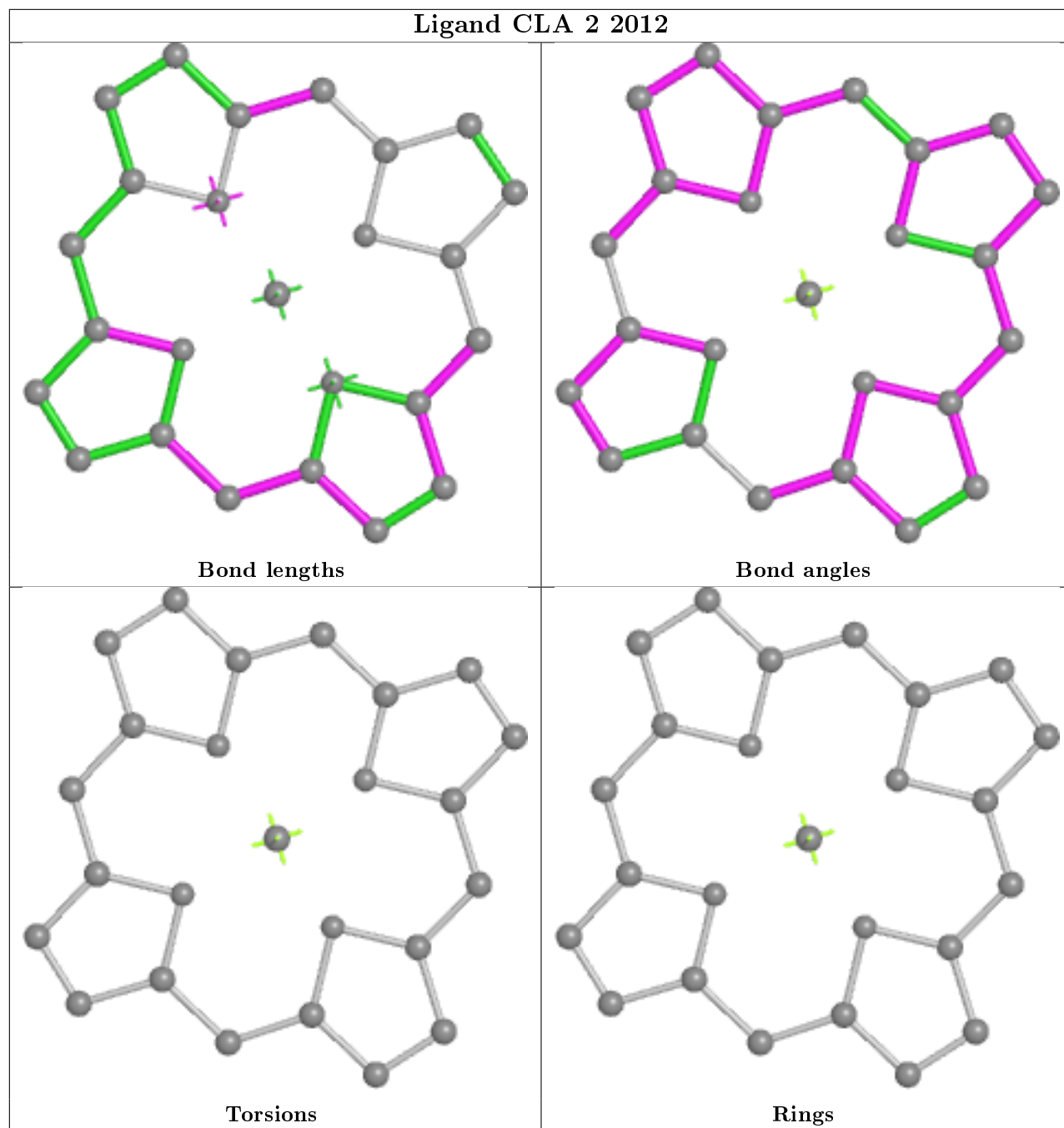
Ligand CLA B 1225

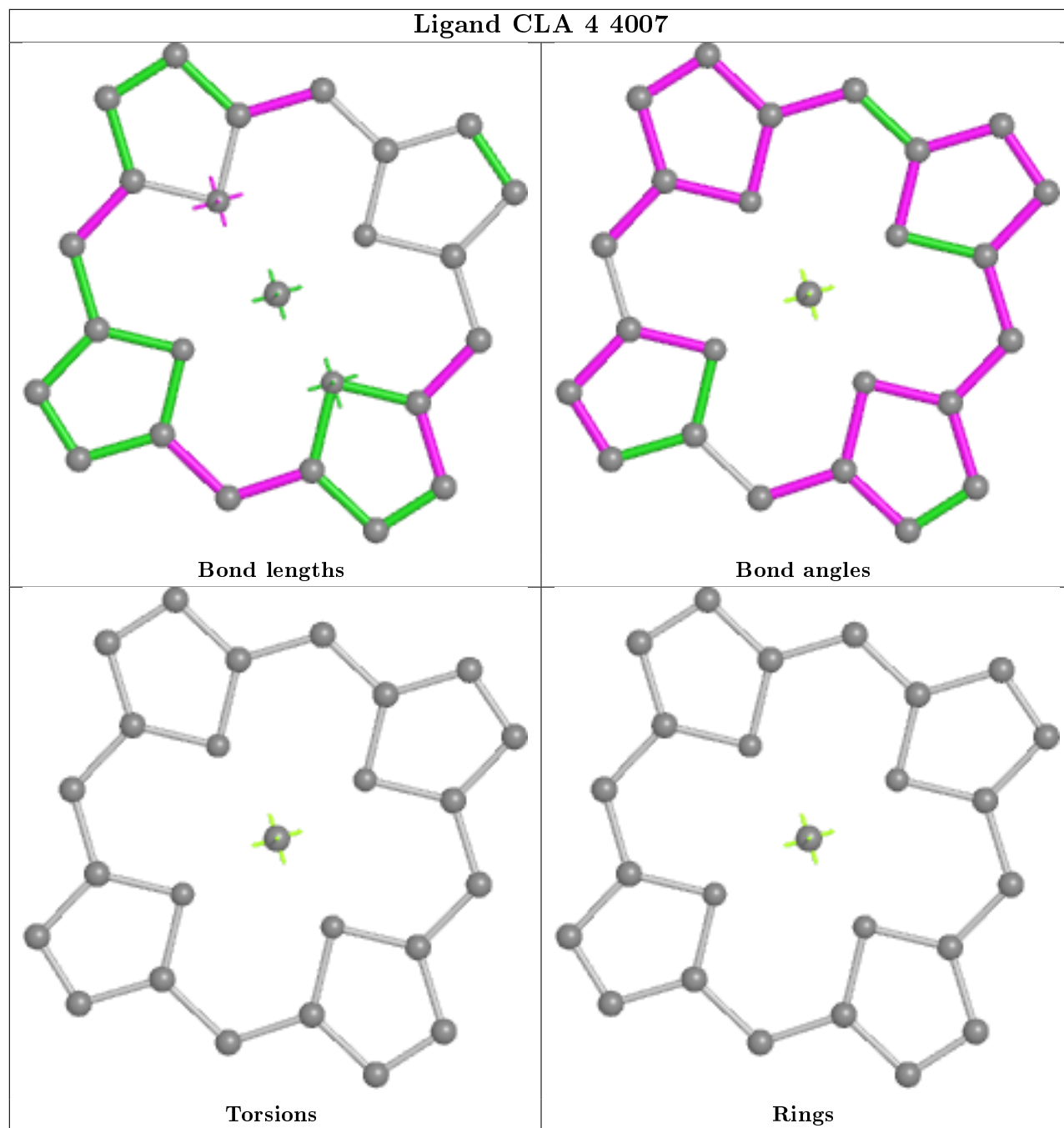


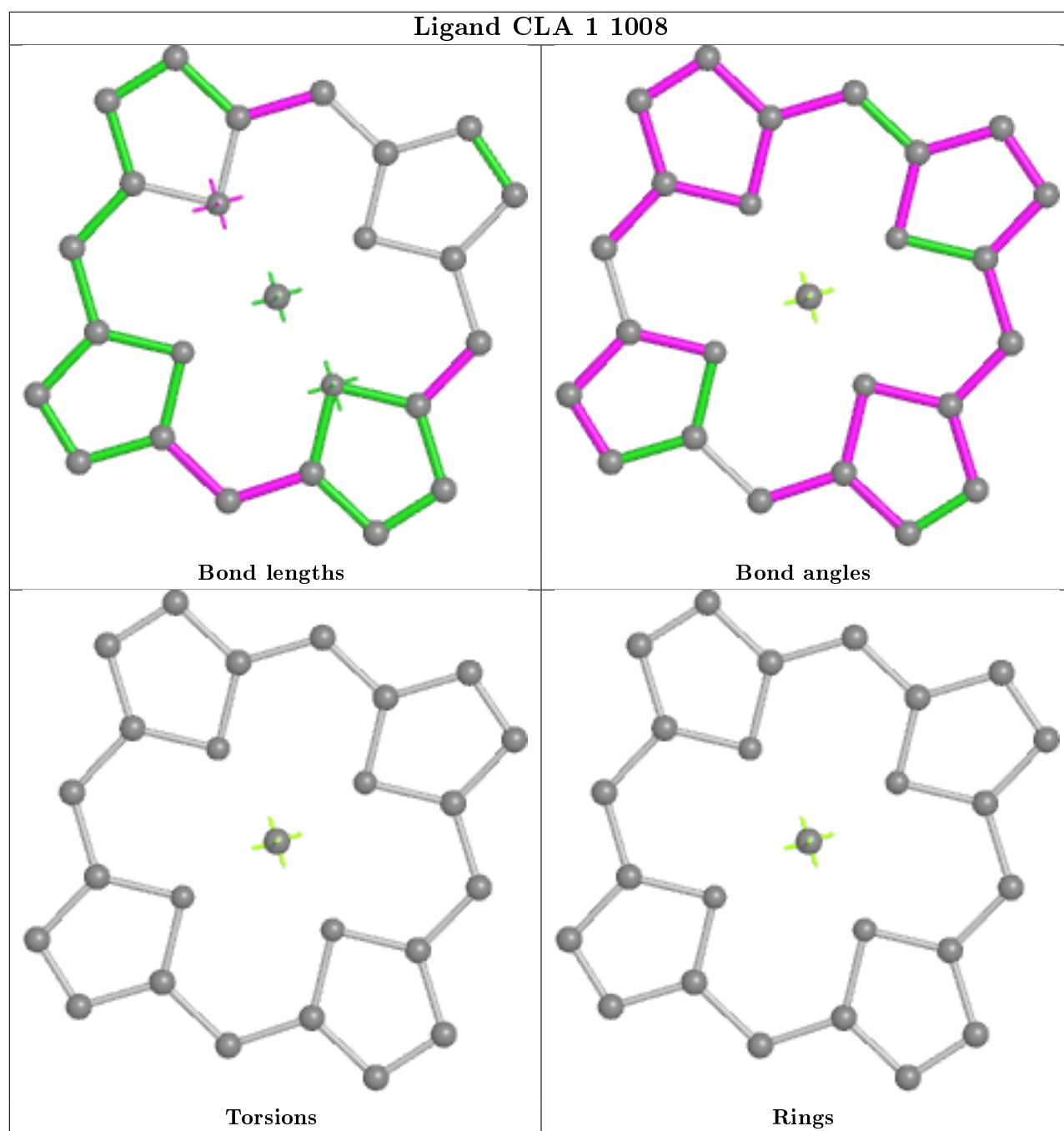
Ligand CLA B 1241



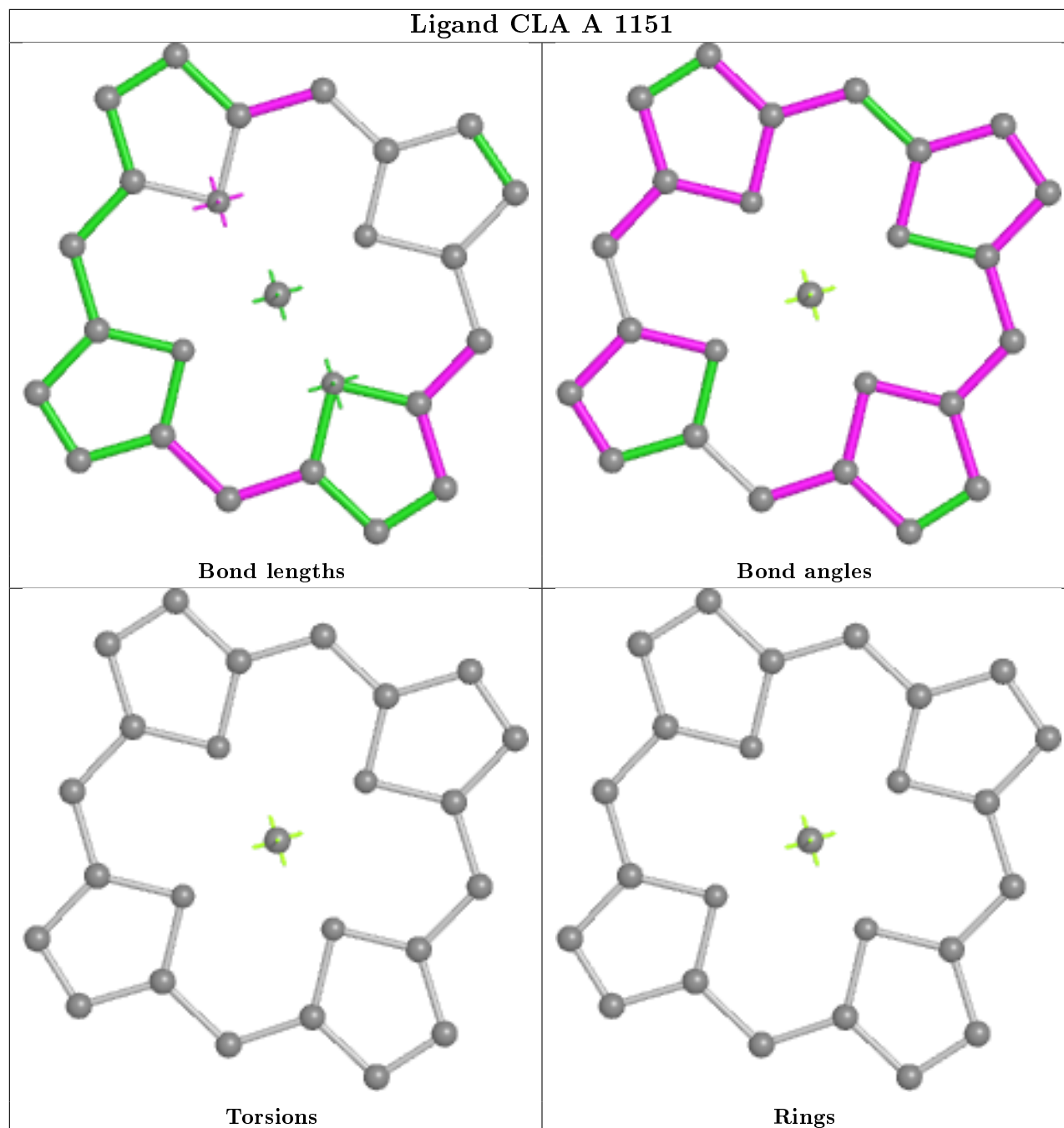




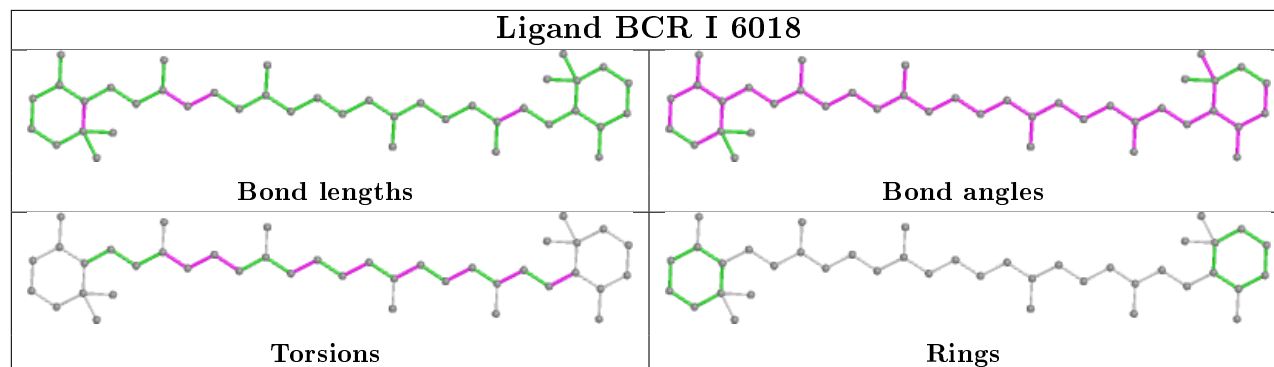




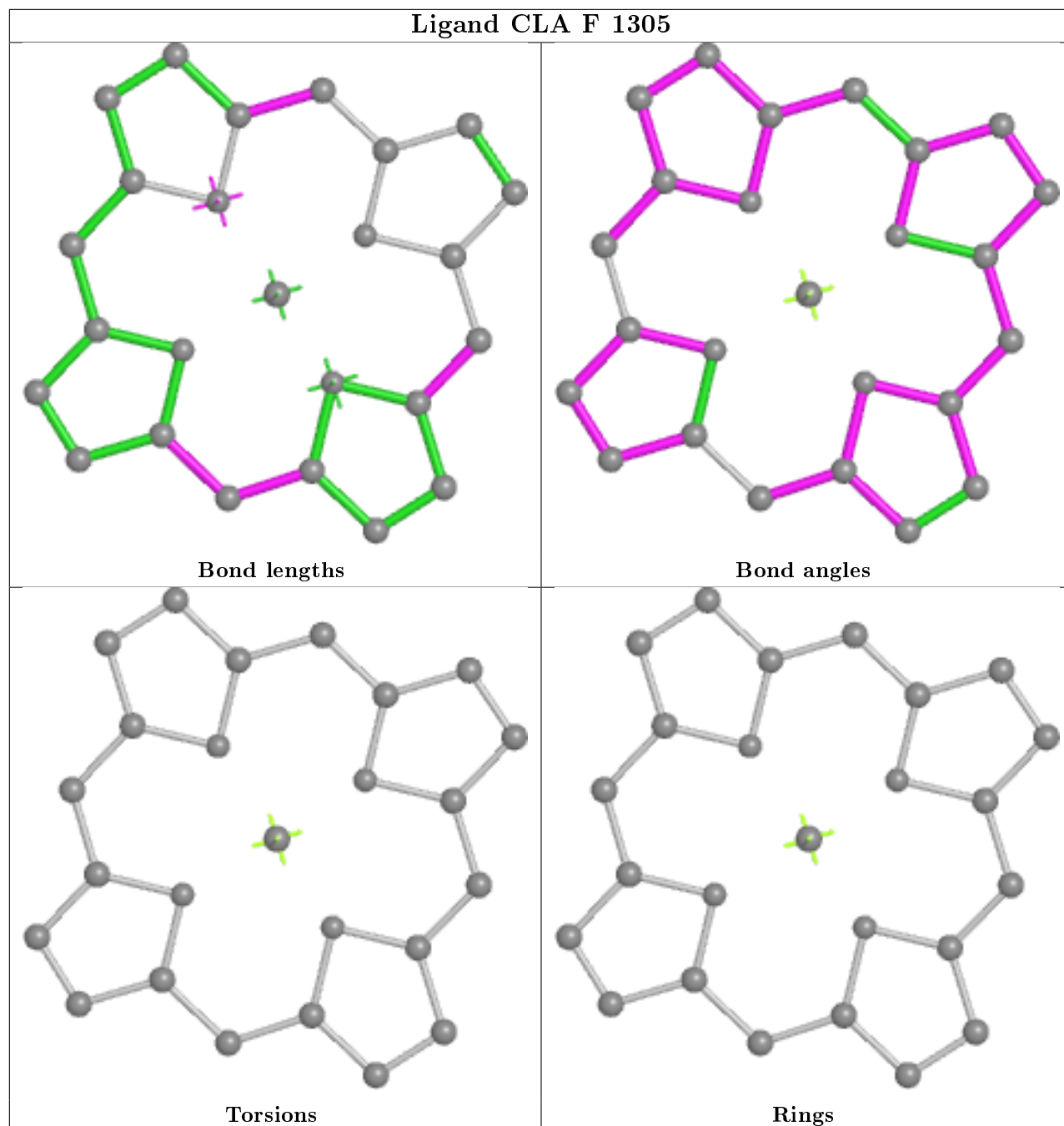
Ligand CLA A 1151



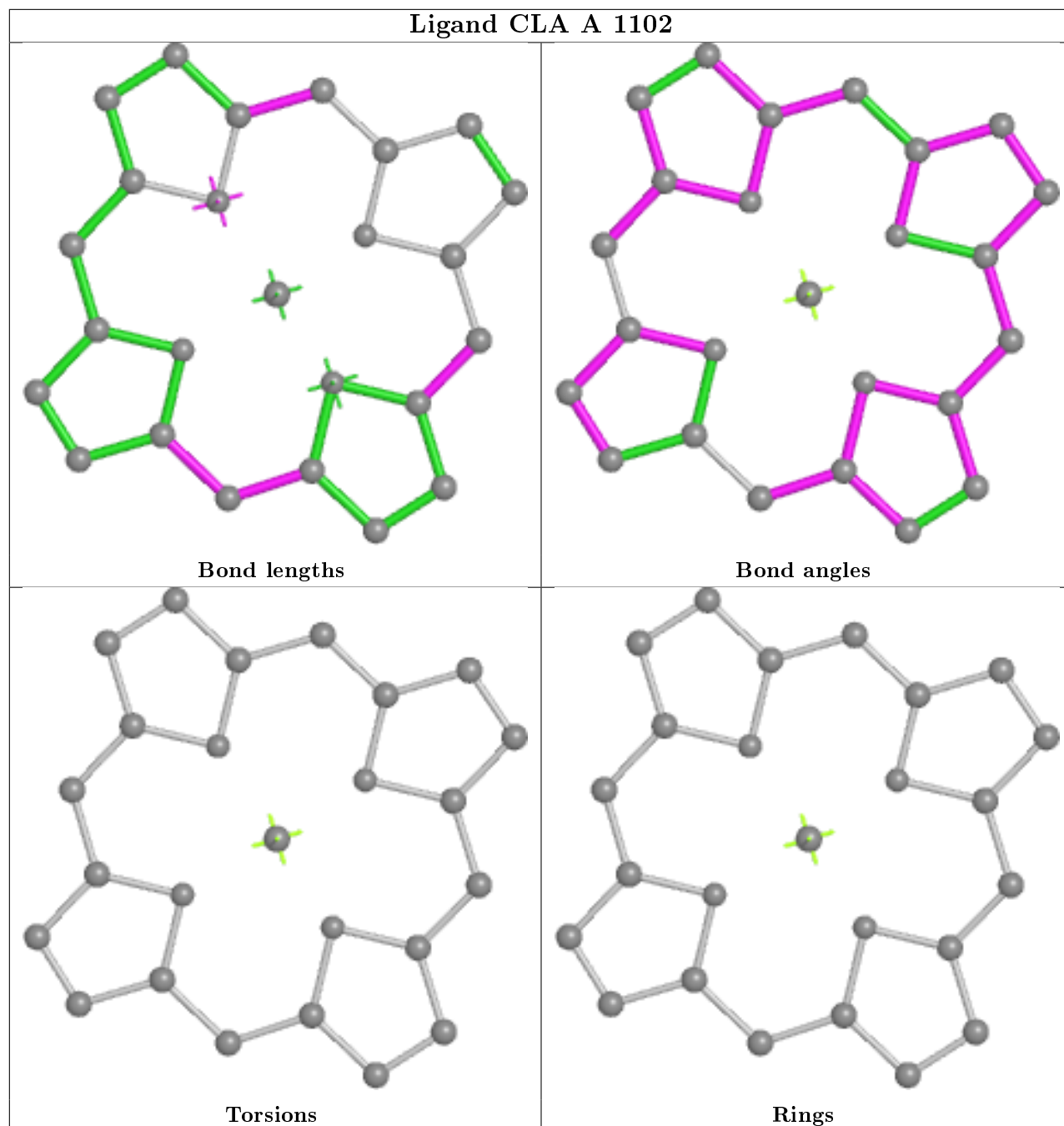
Ligand BCR I 6018



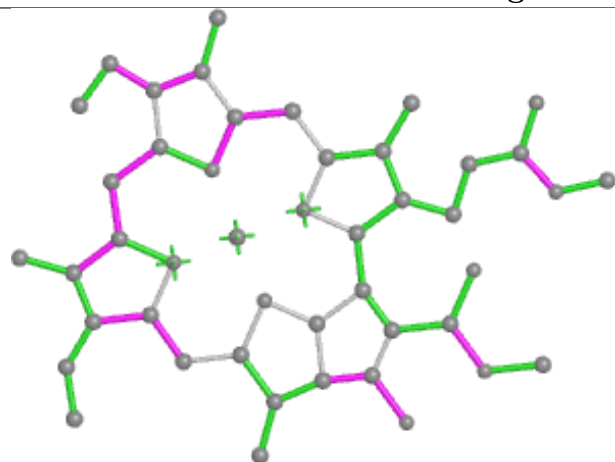
Ligand CLA F 1305



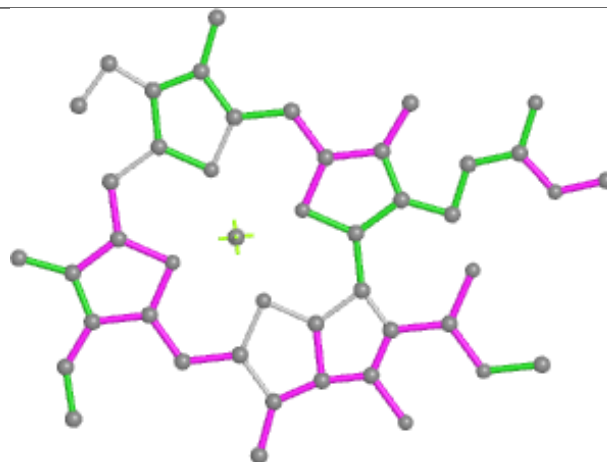
Ligand CLA A 1102



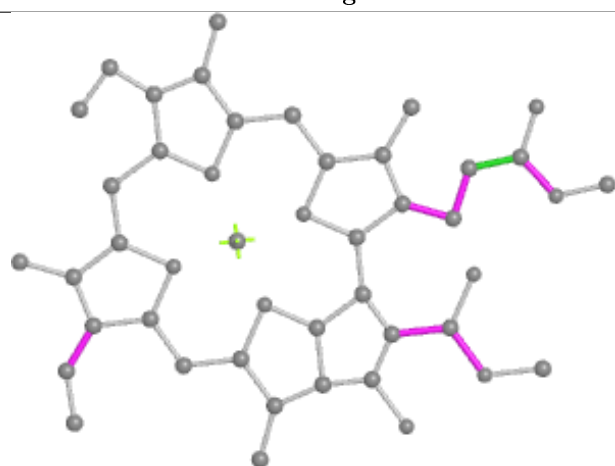
Ligand CLA B 1231



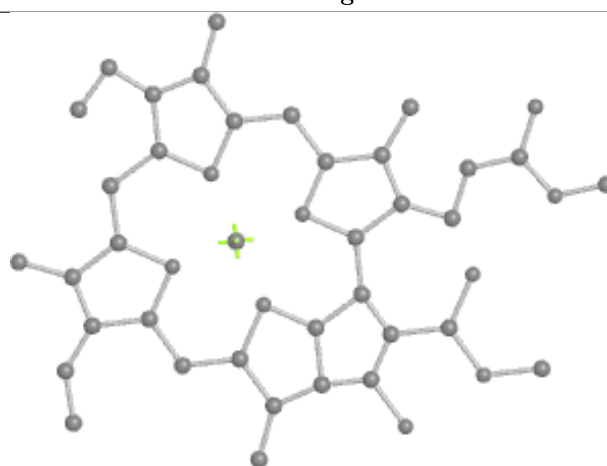
Bond lengths



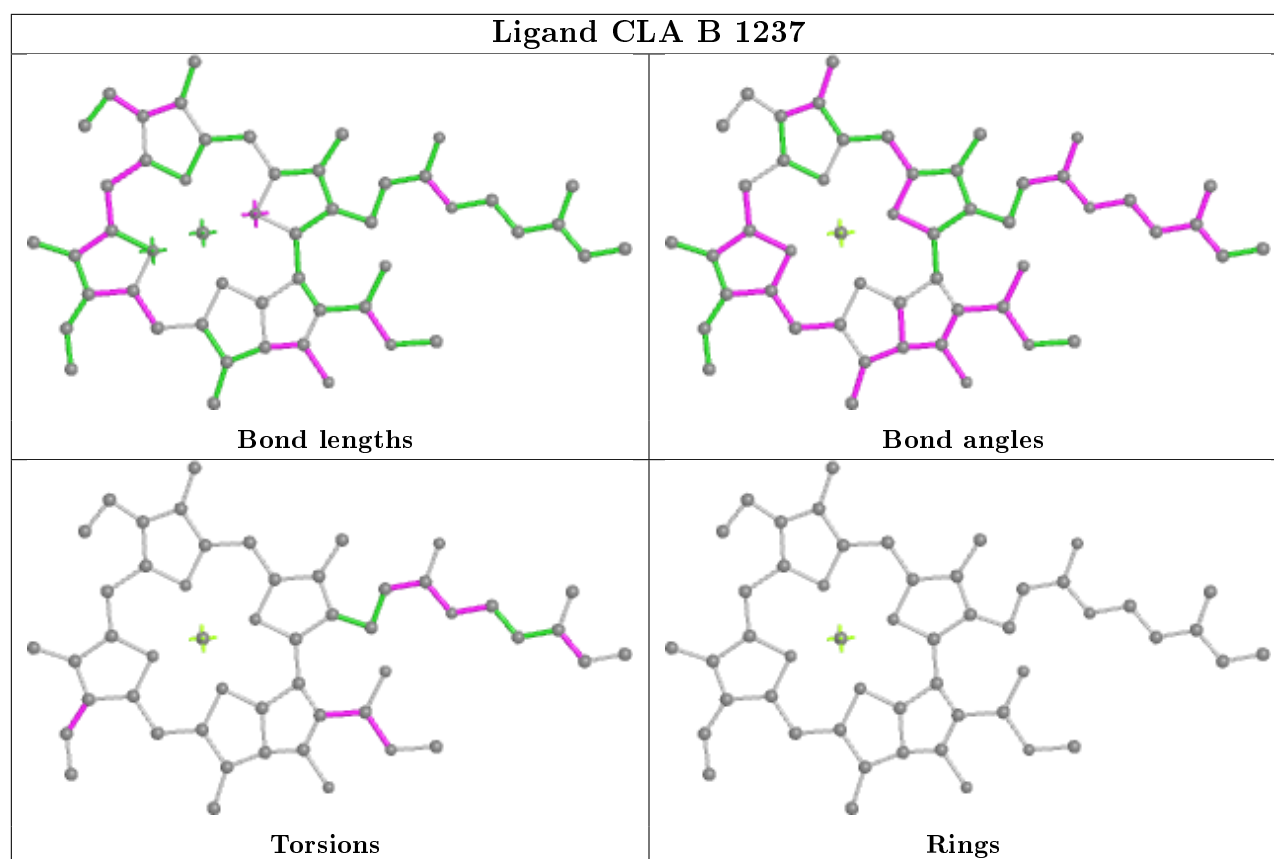
Bond angles

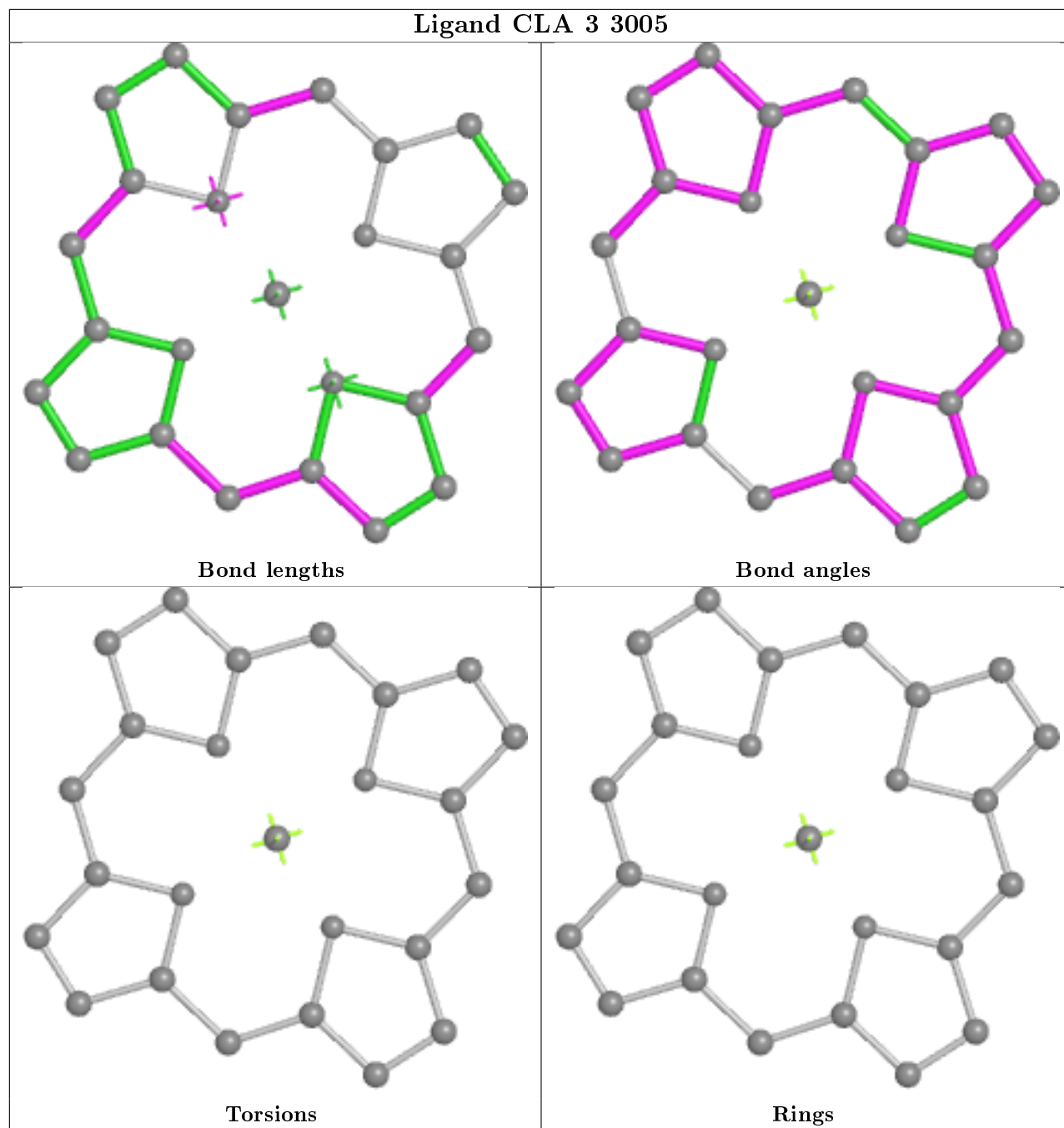


Torsions

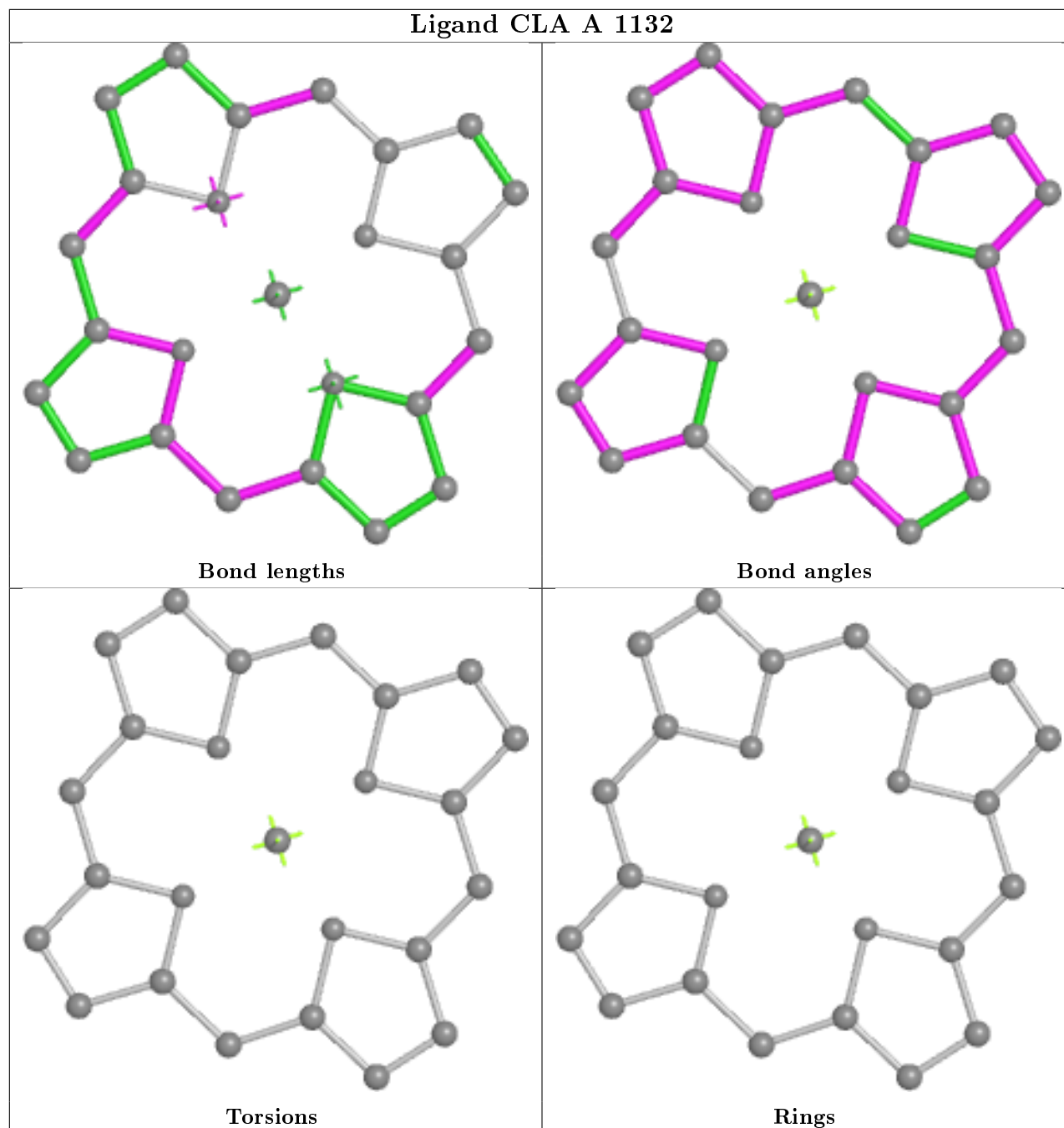


Rings

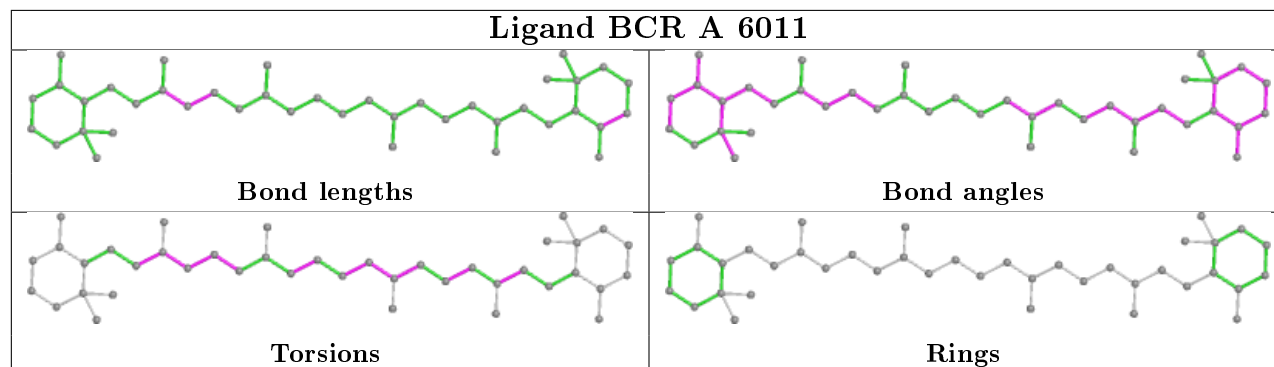




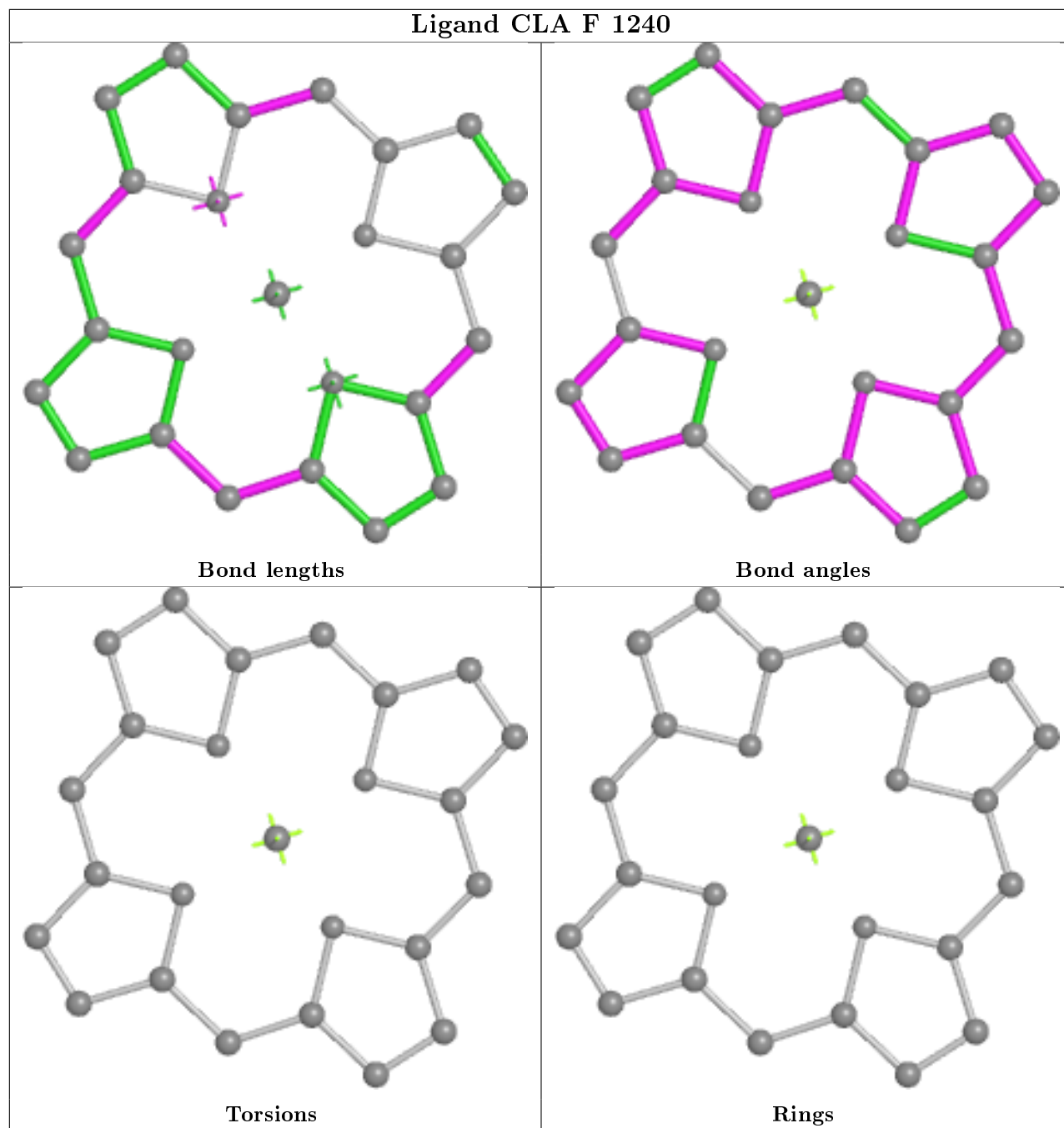
Ligand CLA A 1132

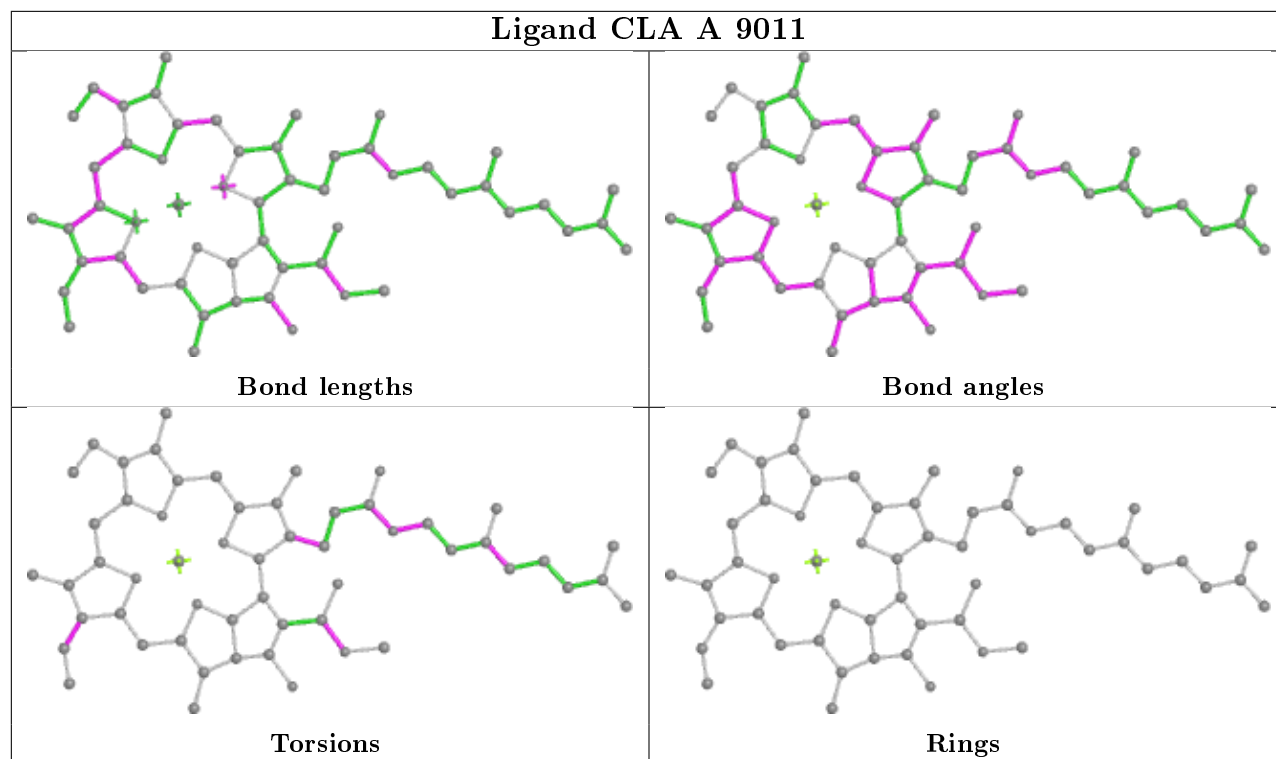


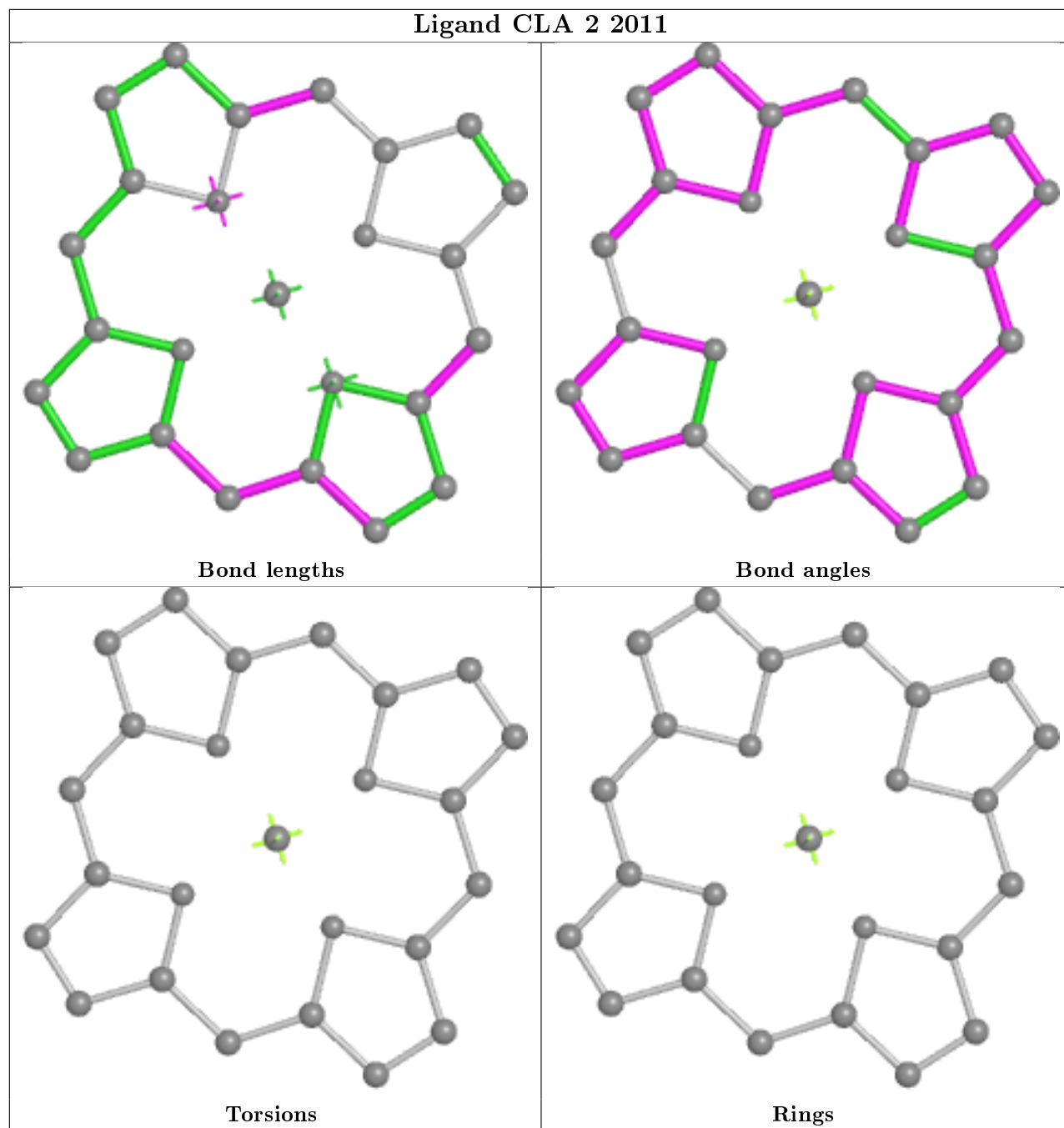
Ligand BCR A 6011

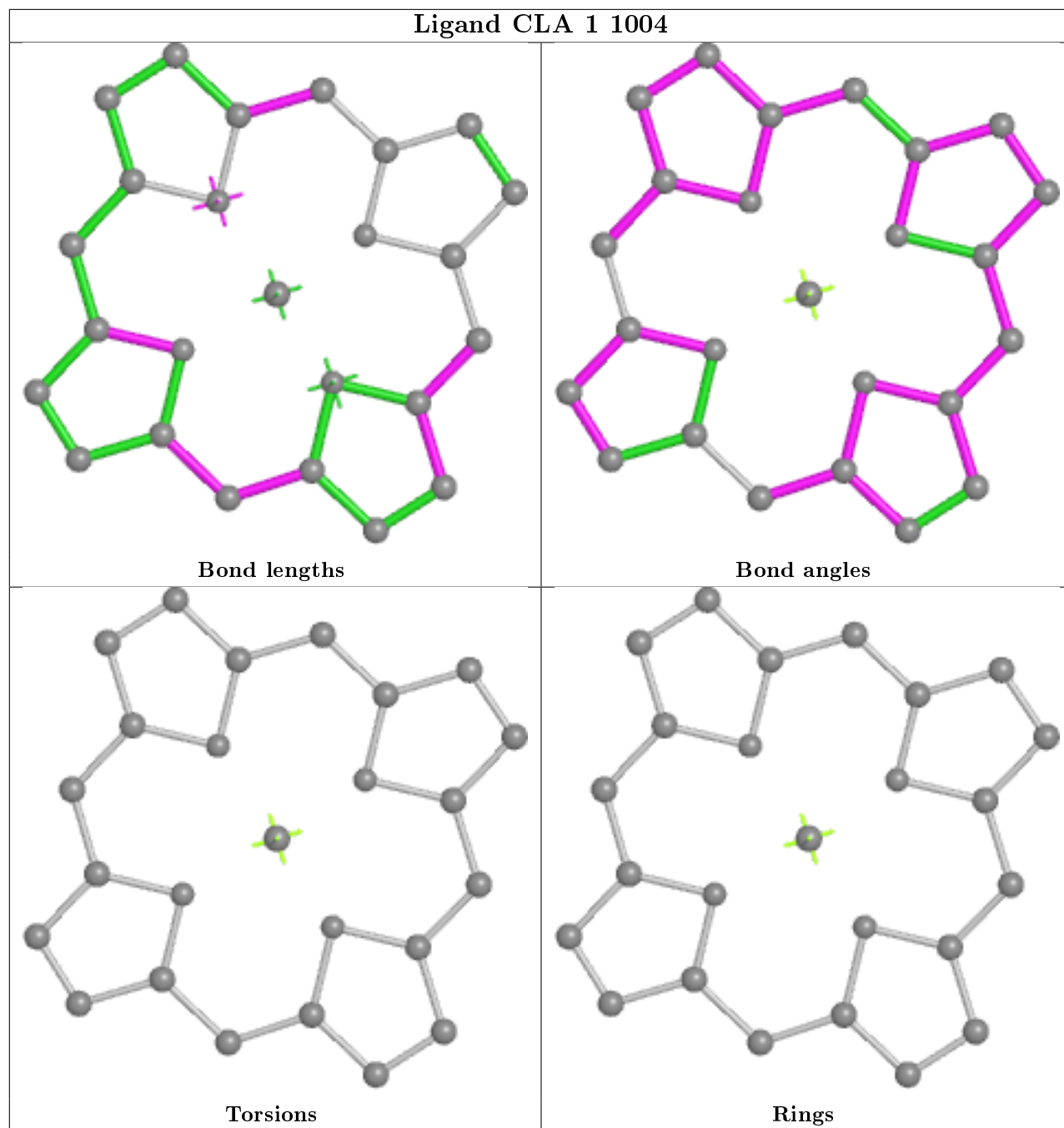


Ligand CLA F 1240

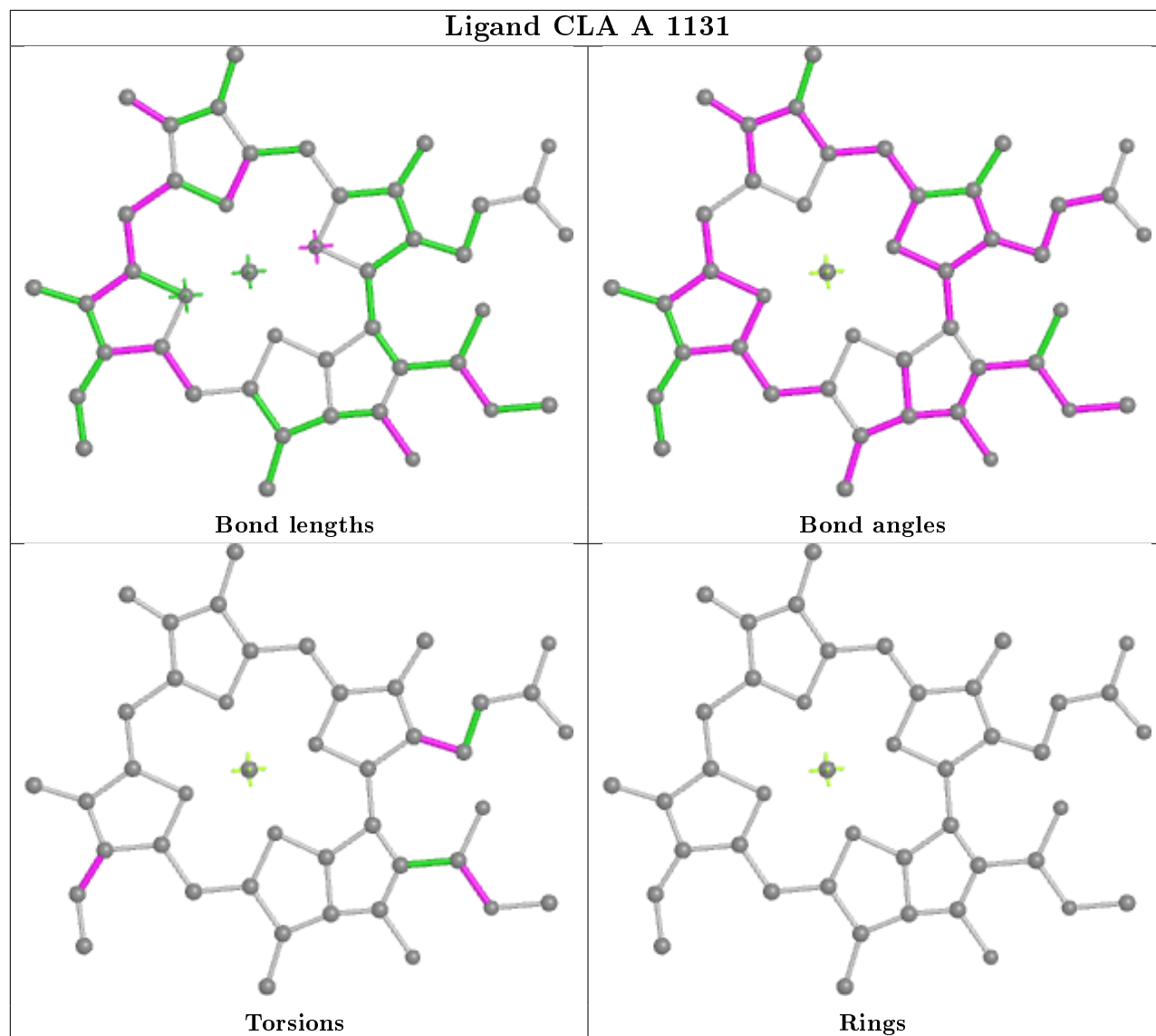


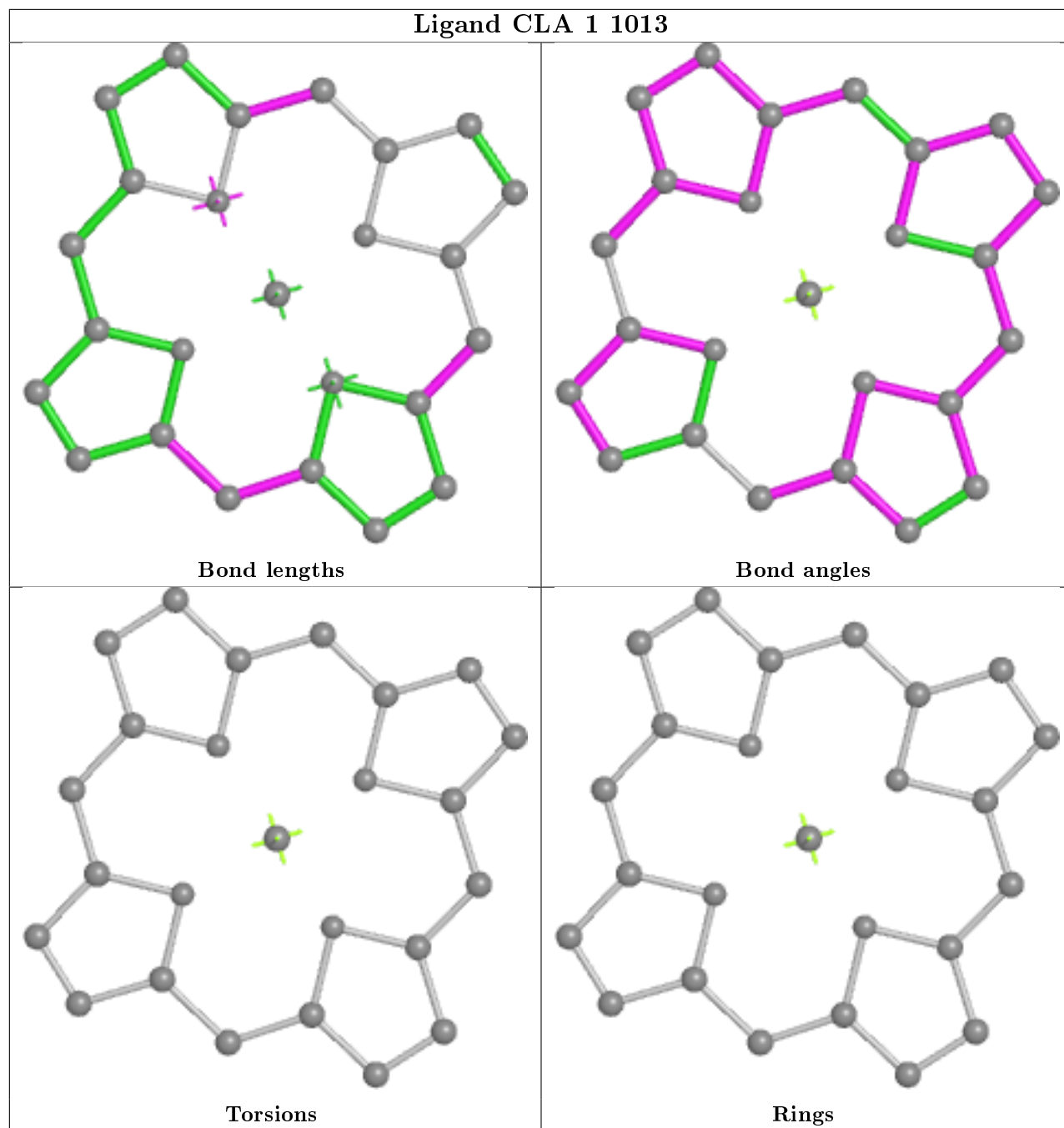




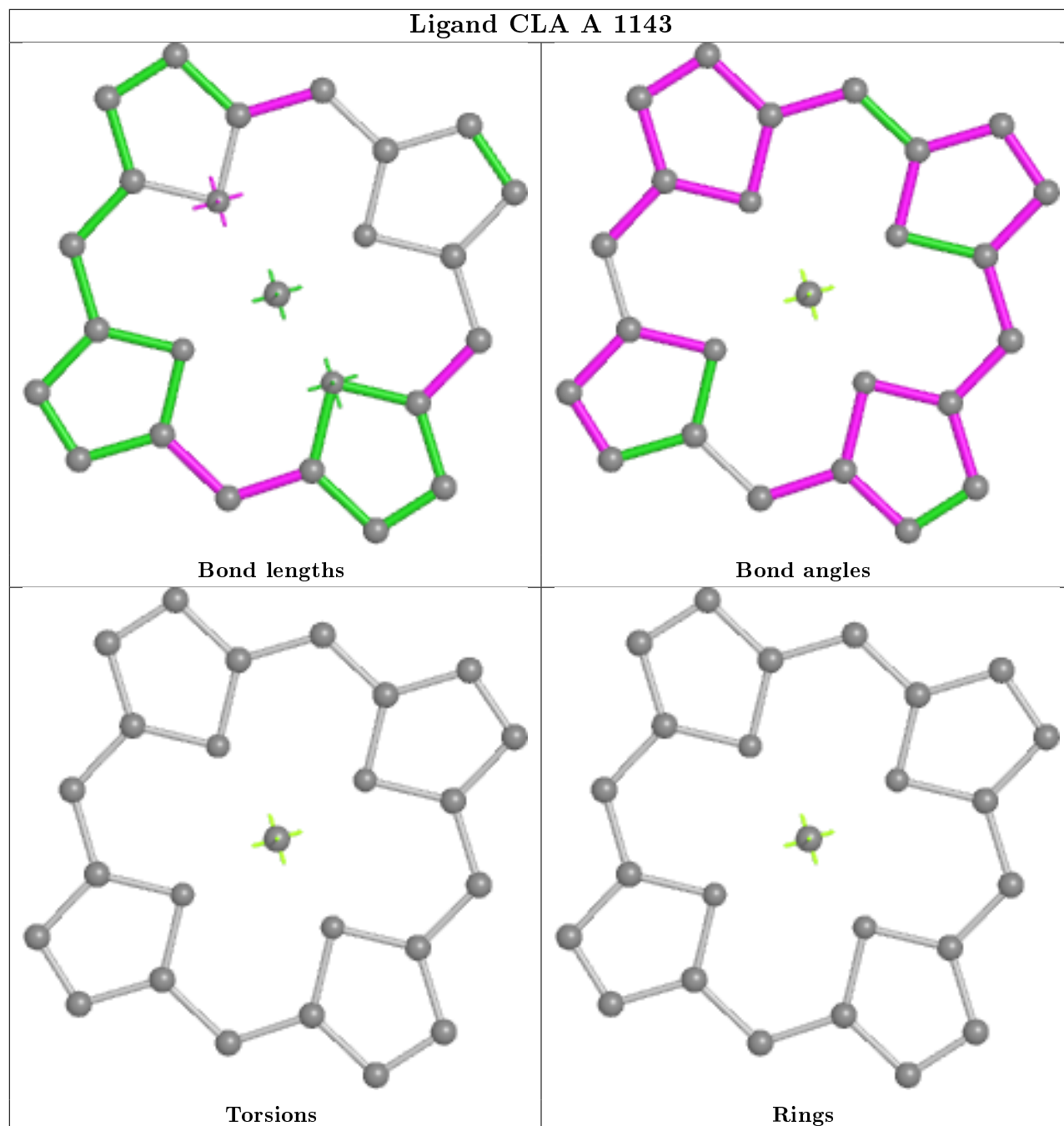


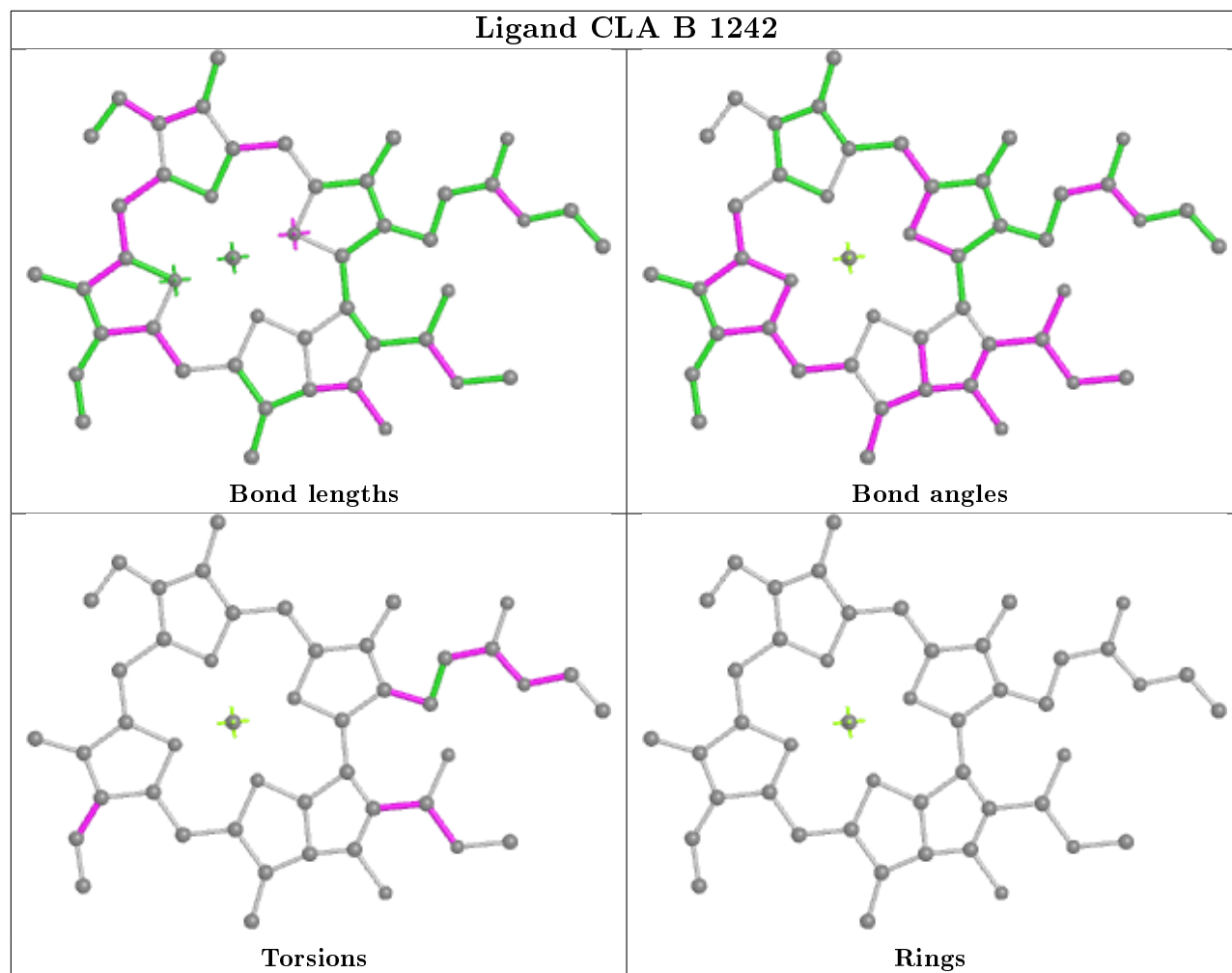
Ligand CLA A 1131

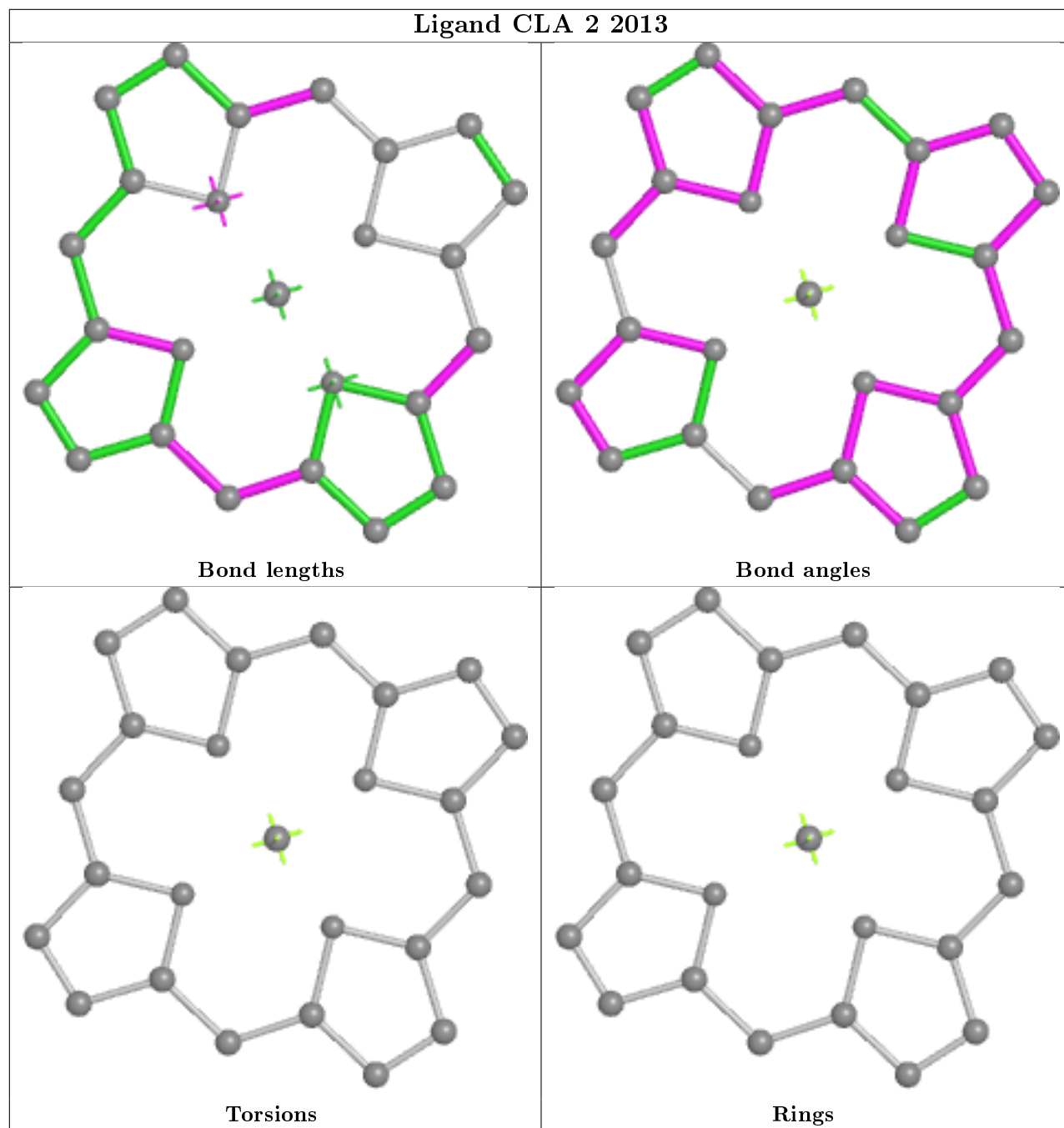




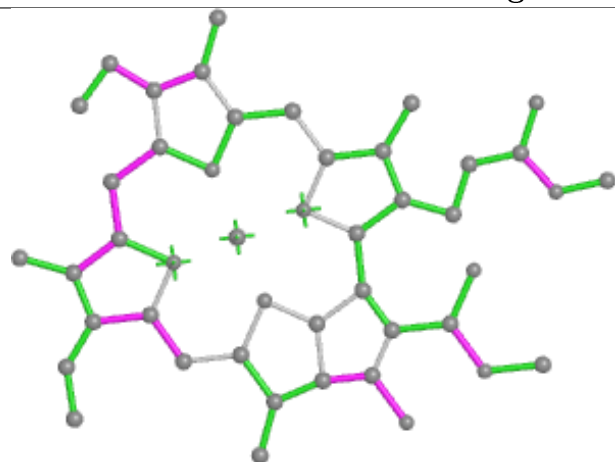
Ligand CLA A 1143



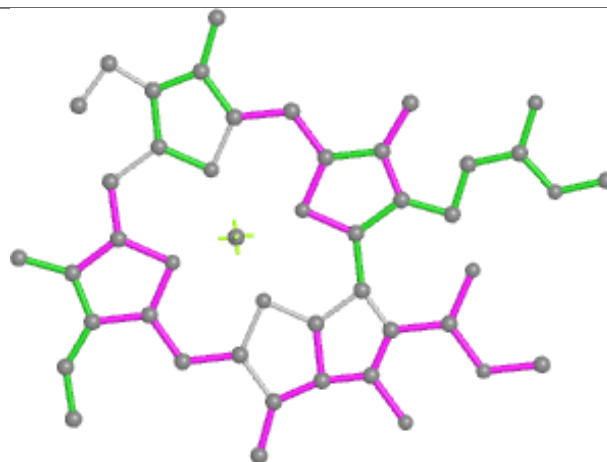




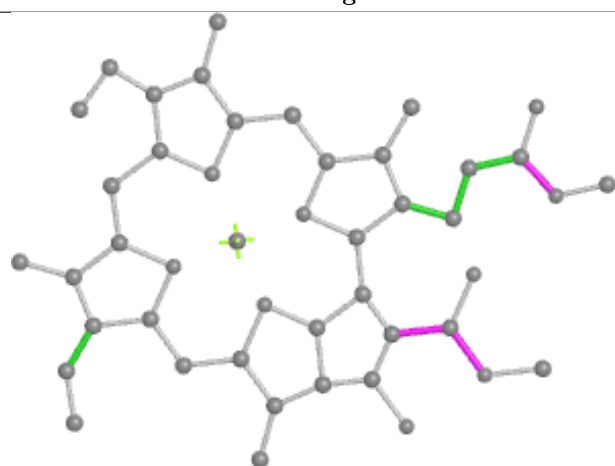
Ligand CLA B 1236



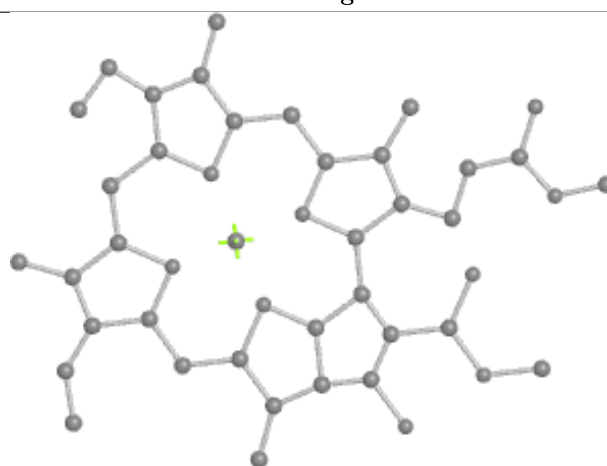
Bond lengths



Bond angles

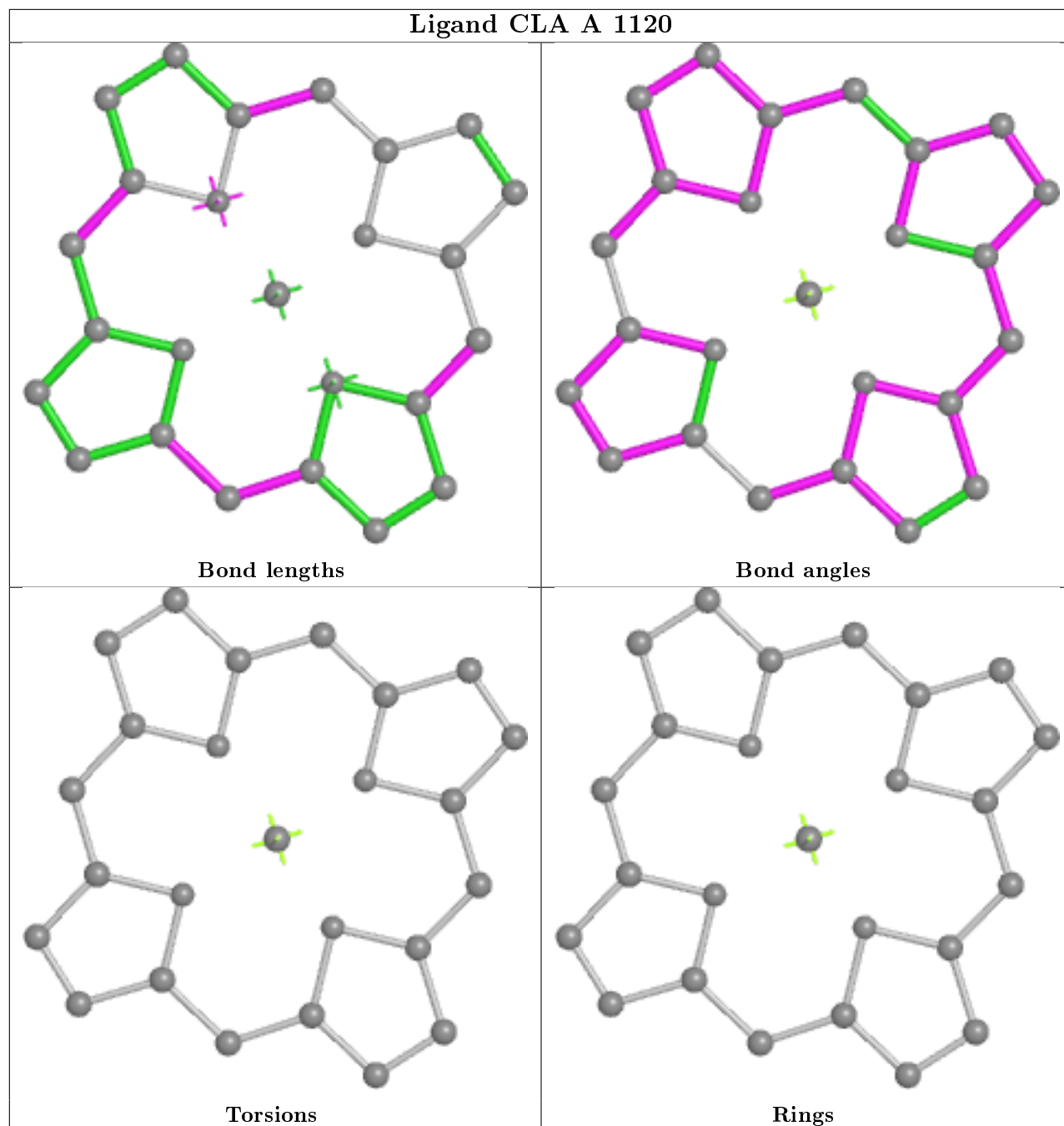


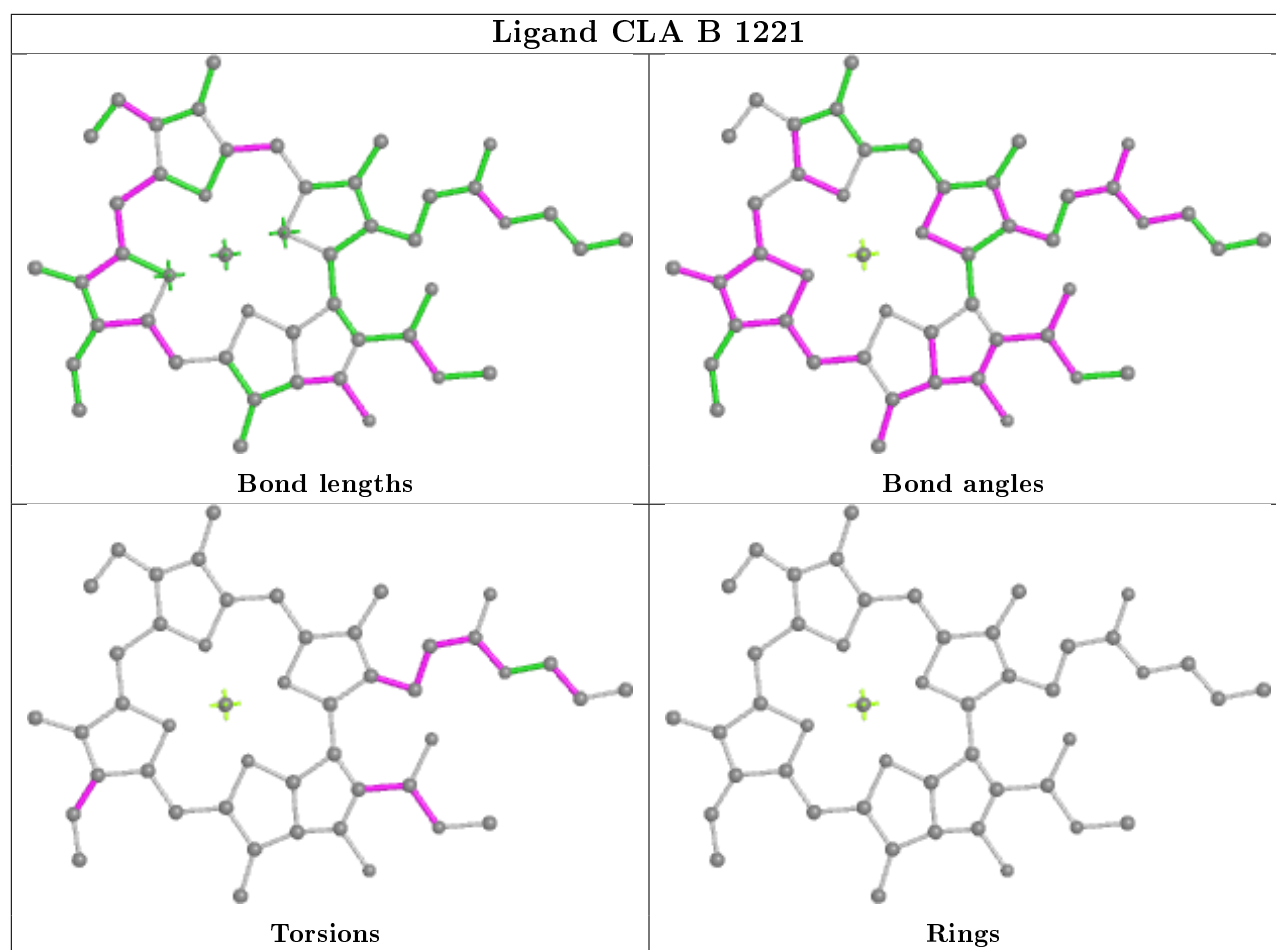
Torsions

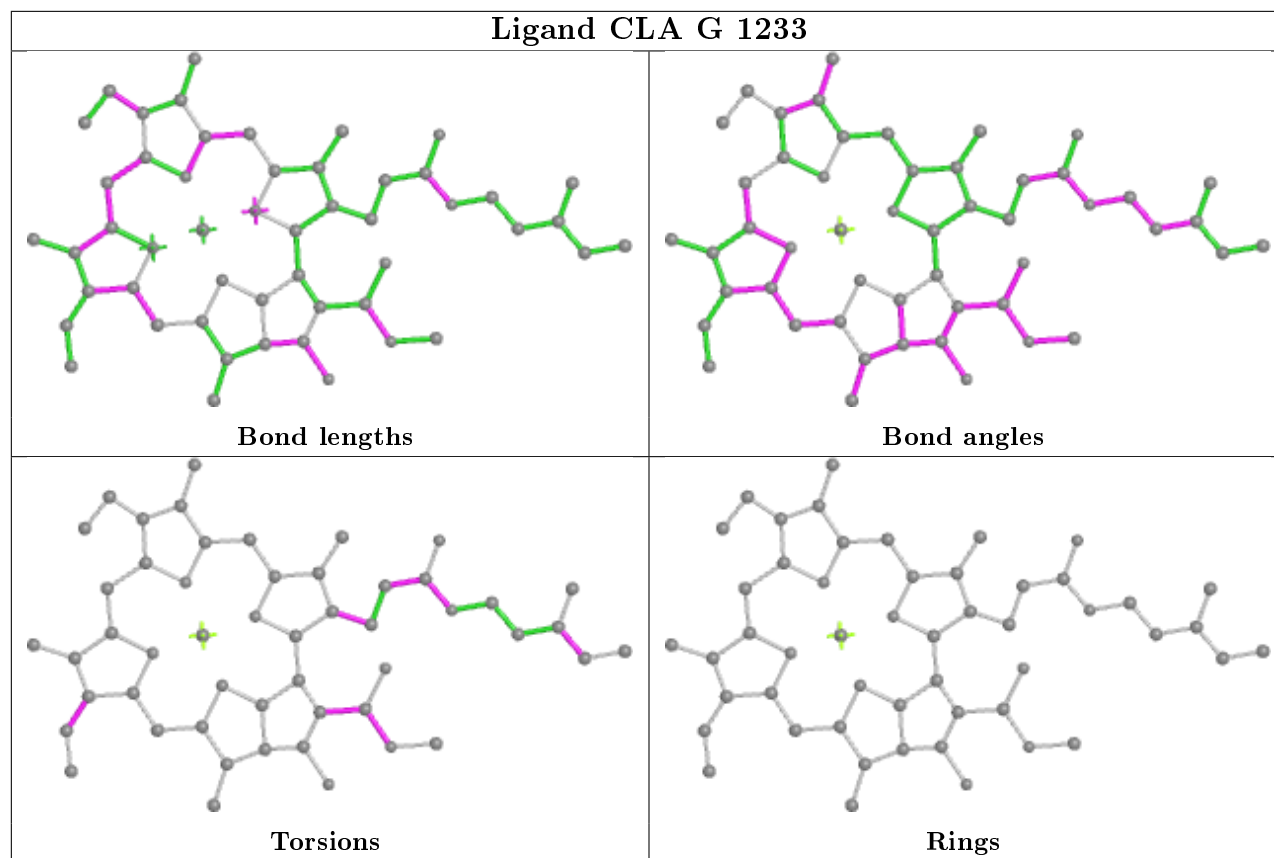


Rings

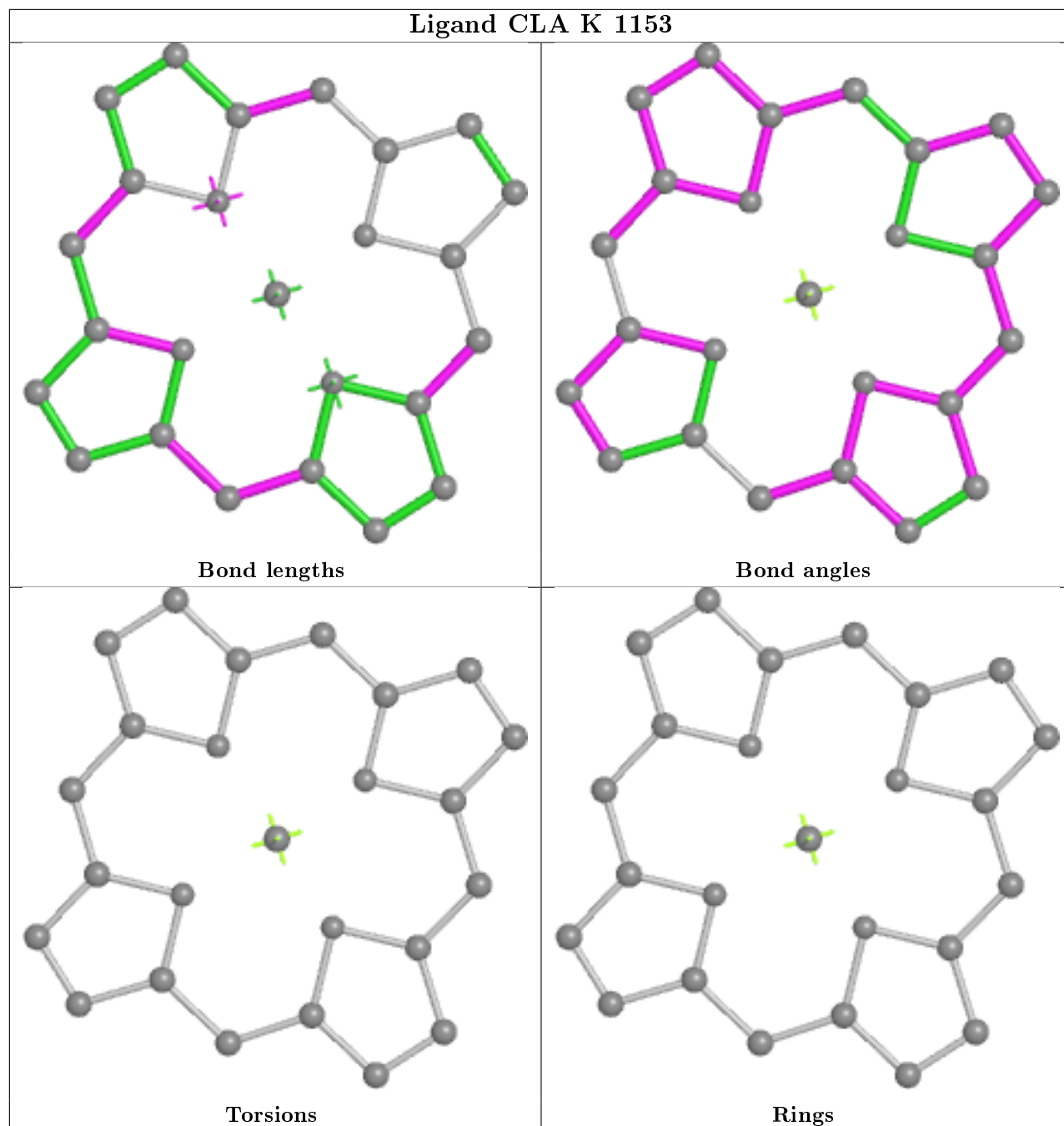
Ligand CLA A 1120

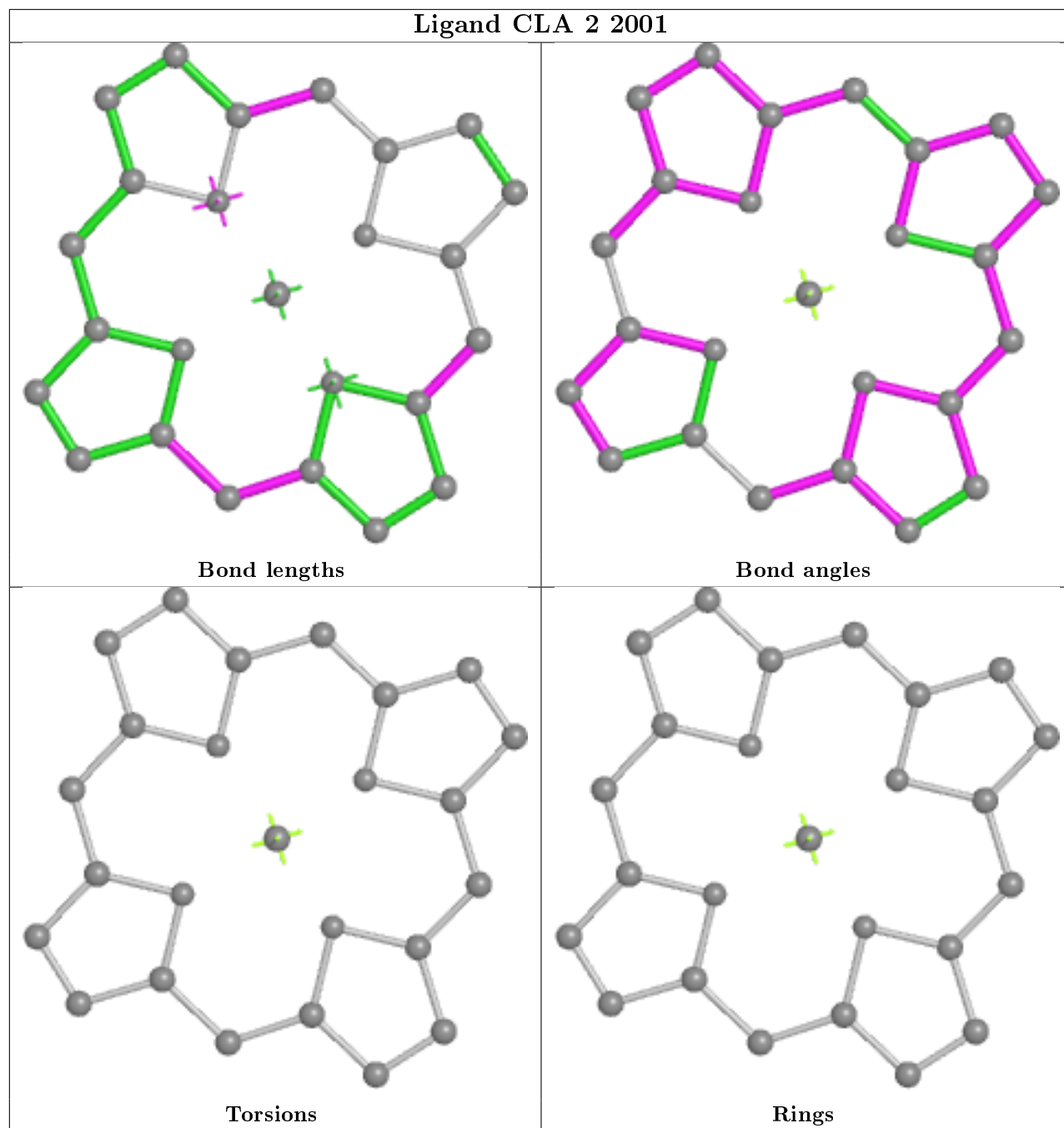




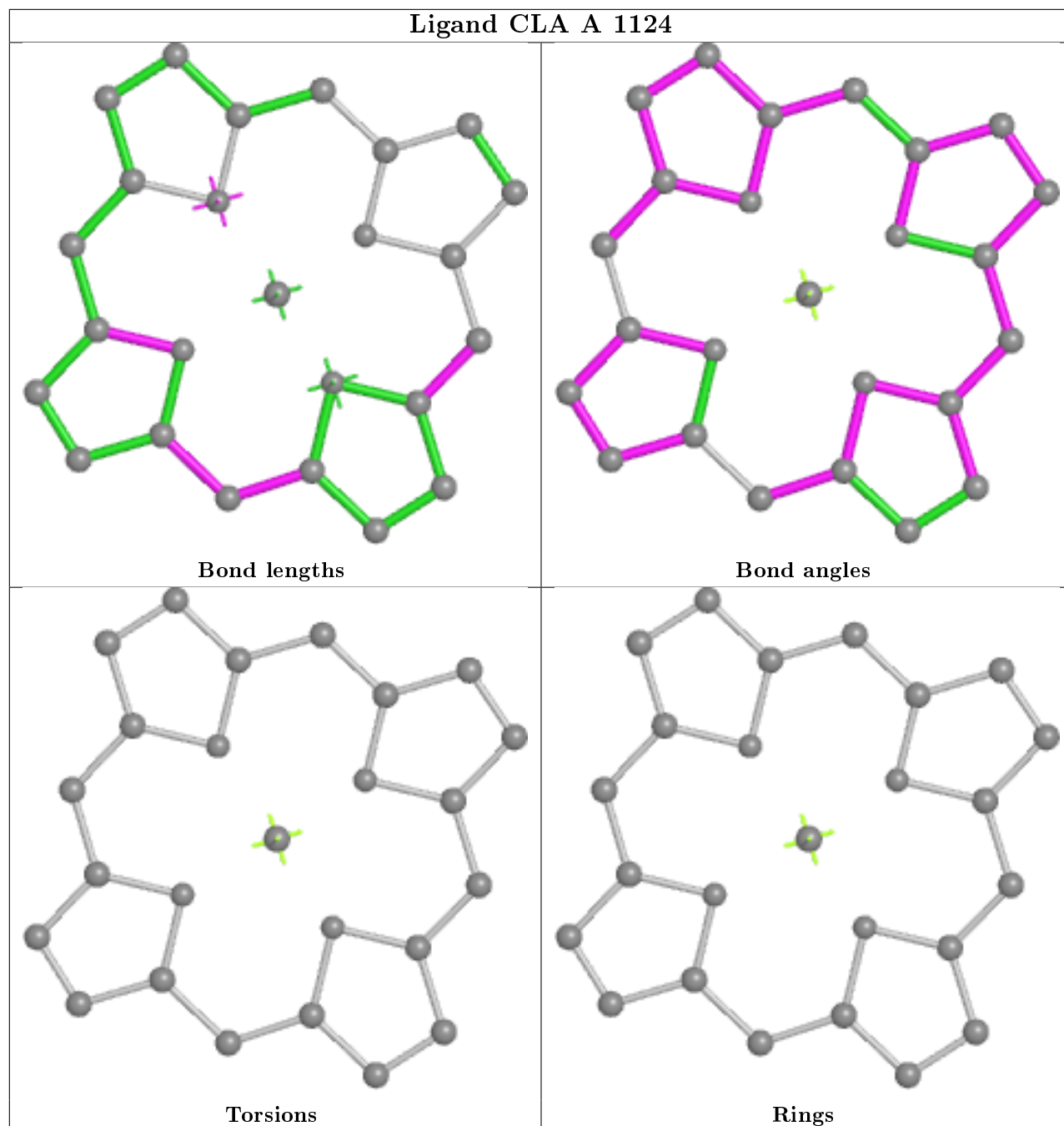


Ligand CLA K 1153

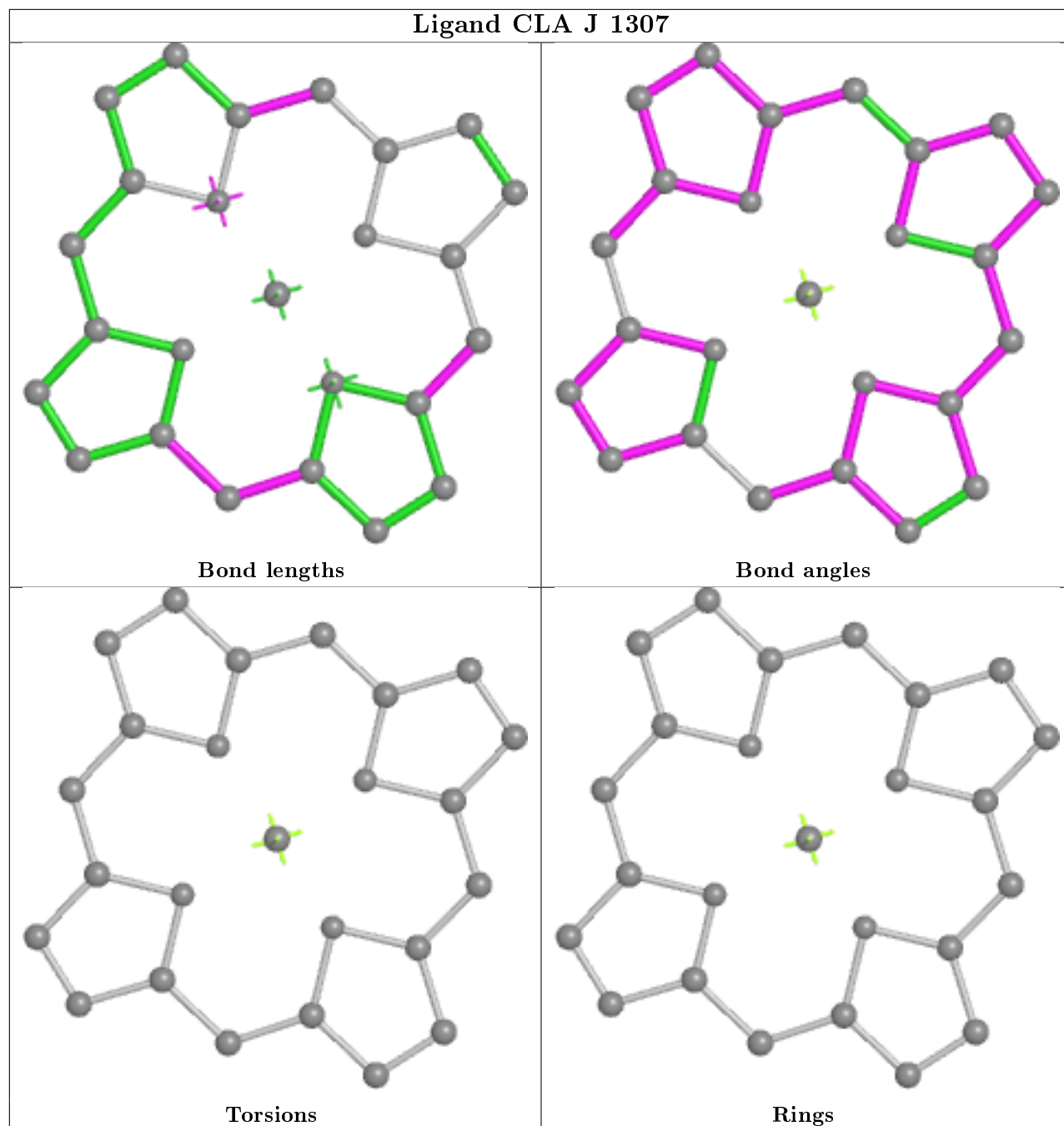




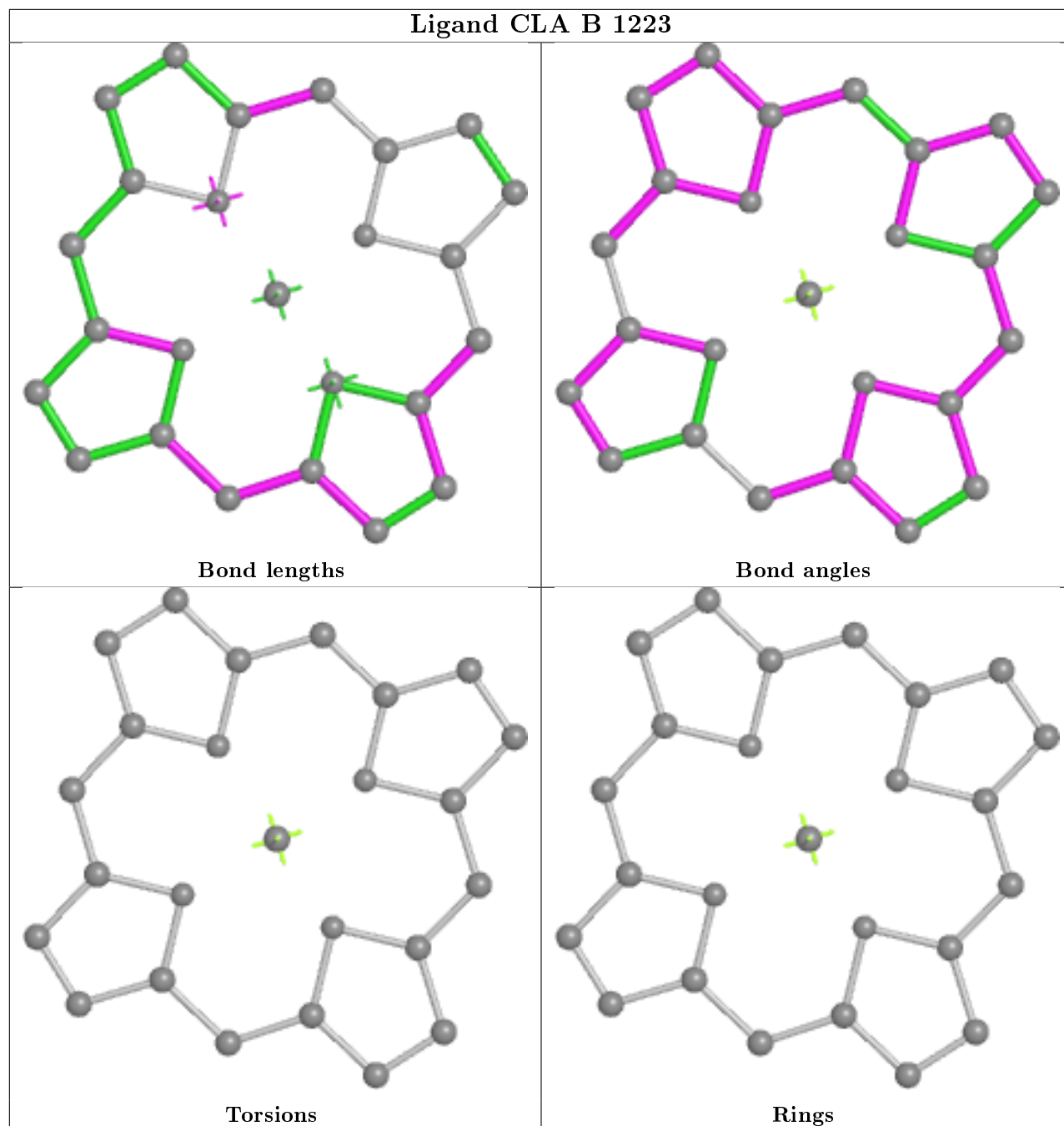
Ligand CLA A 1124



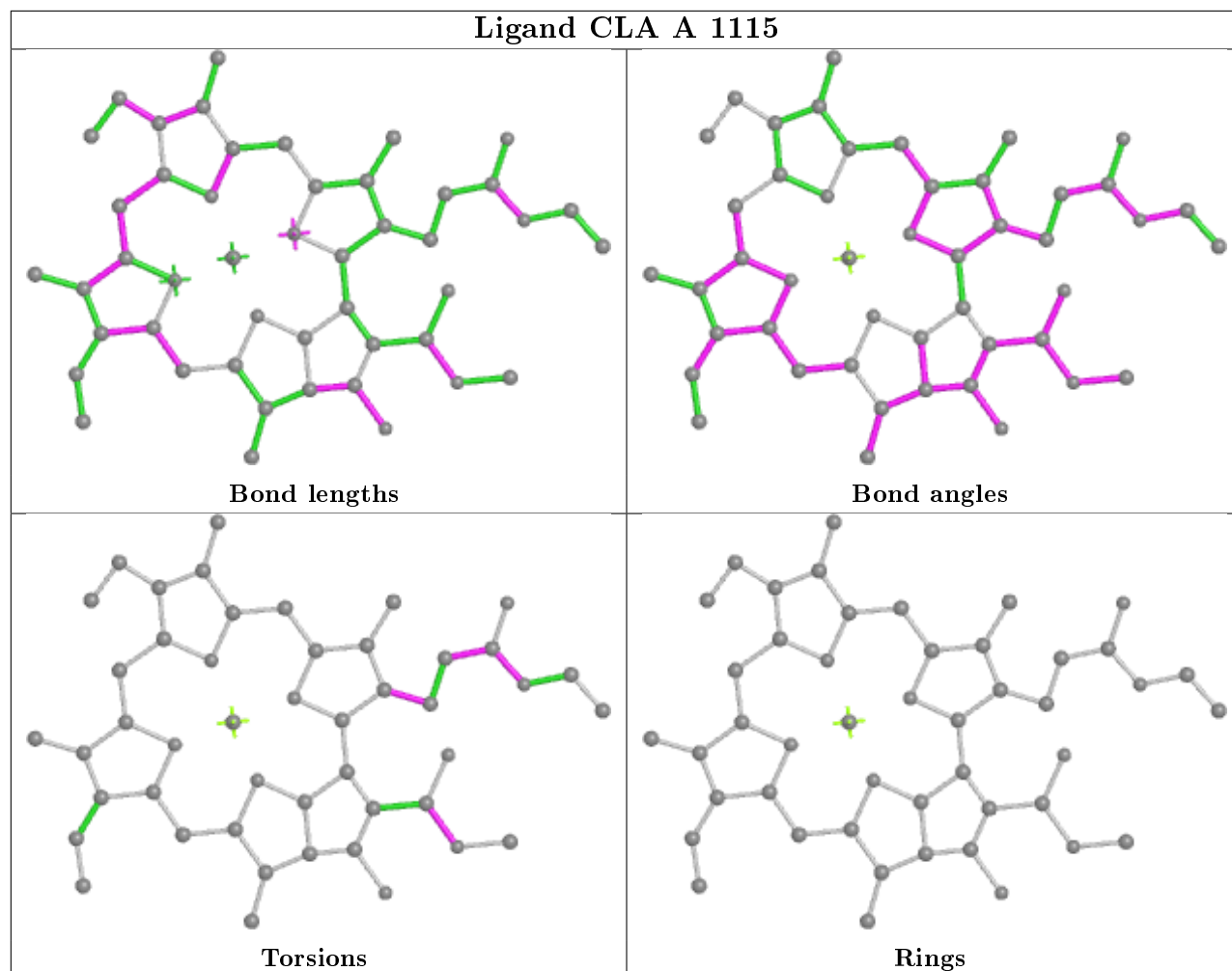
Ligand CLA J 1307



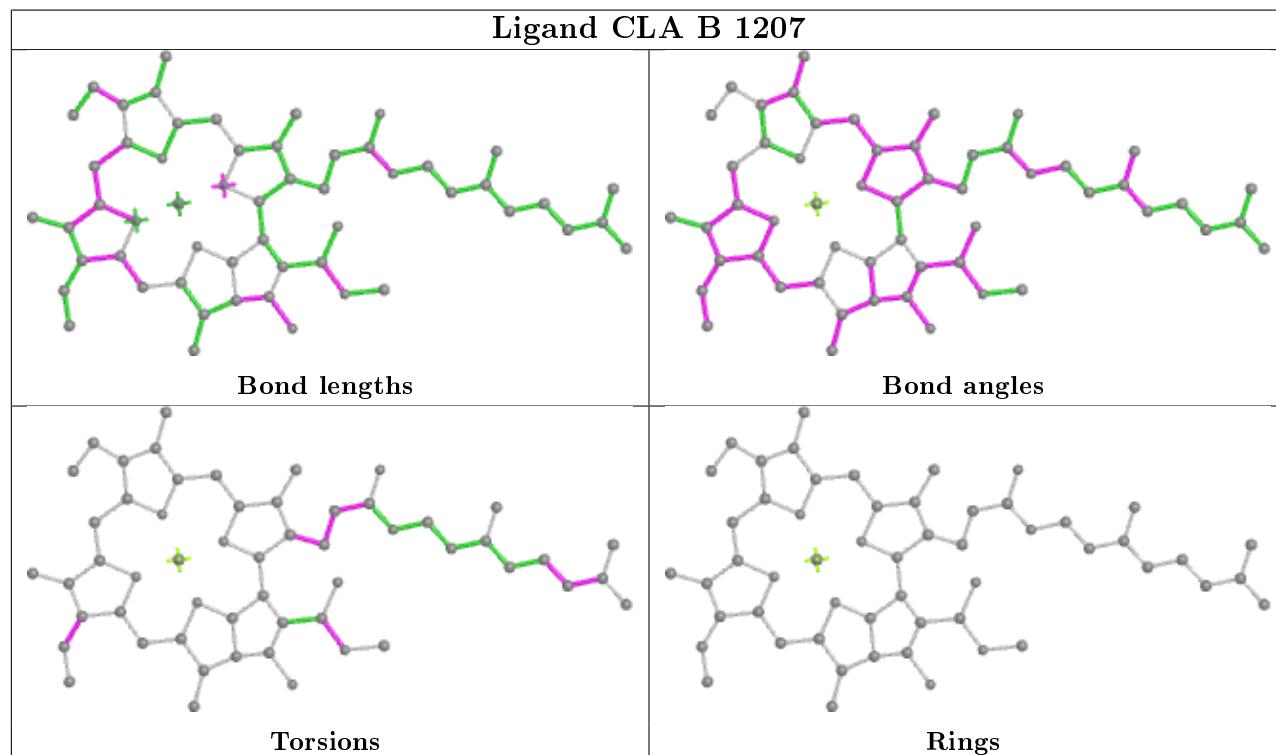
Ligand CLA B 1223

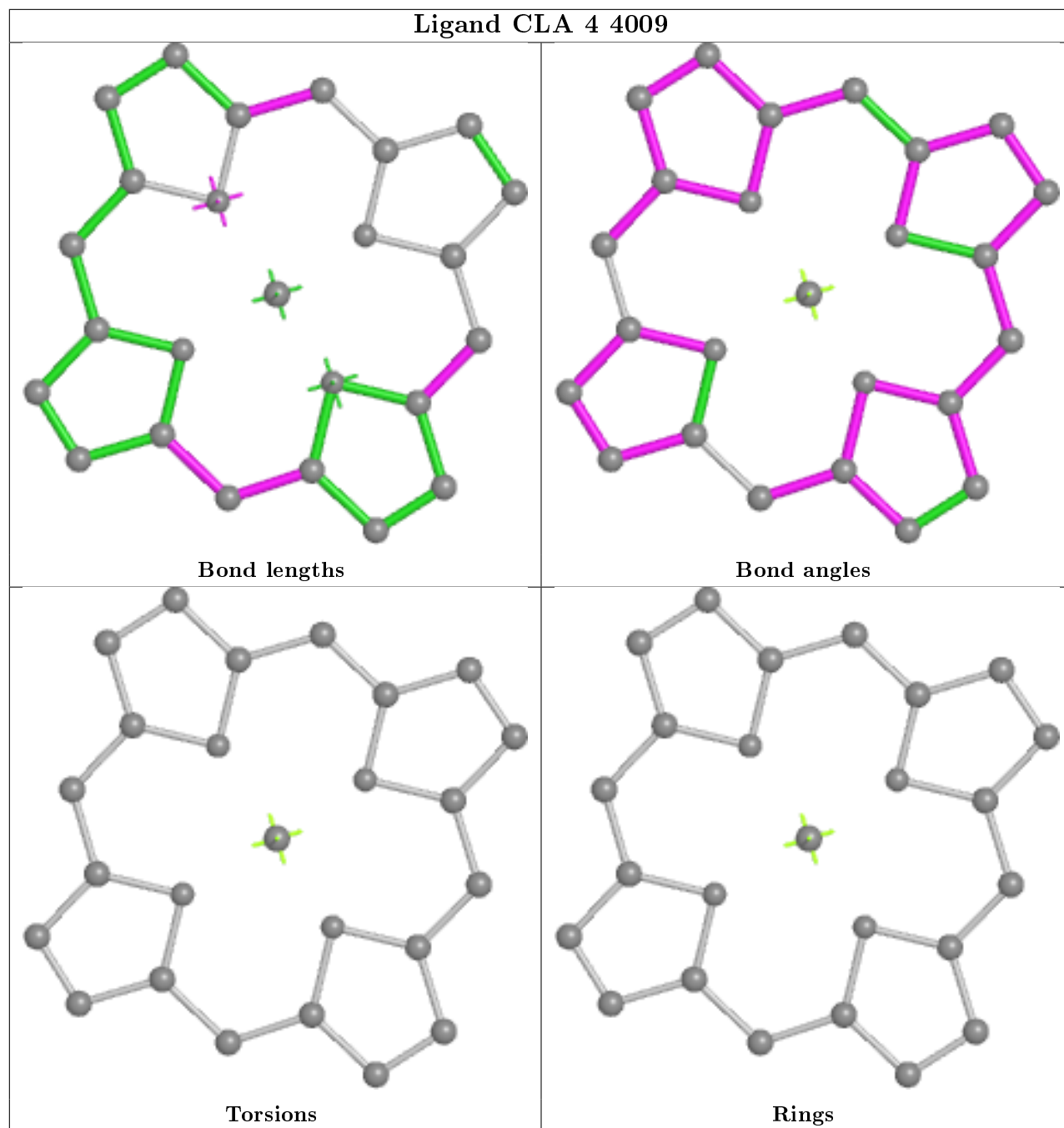


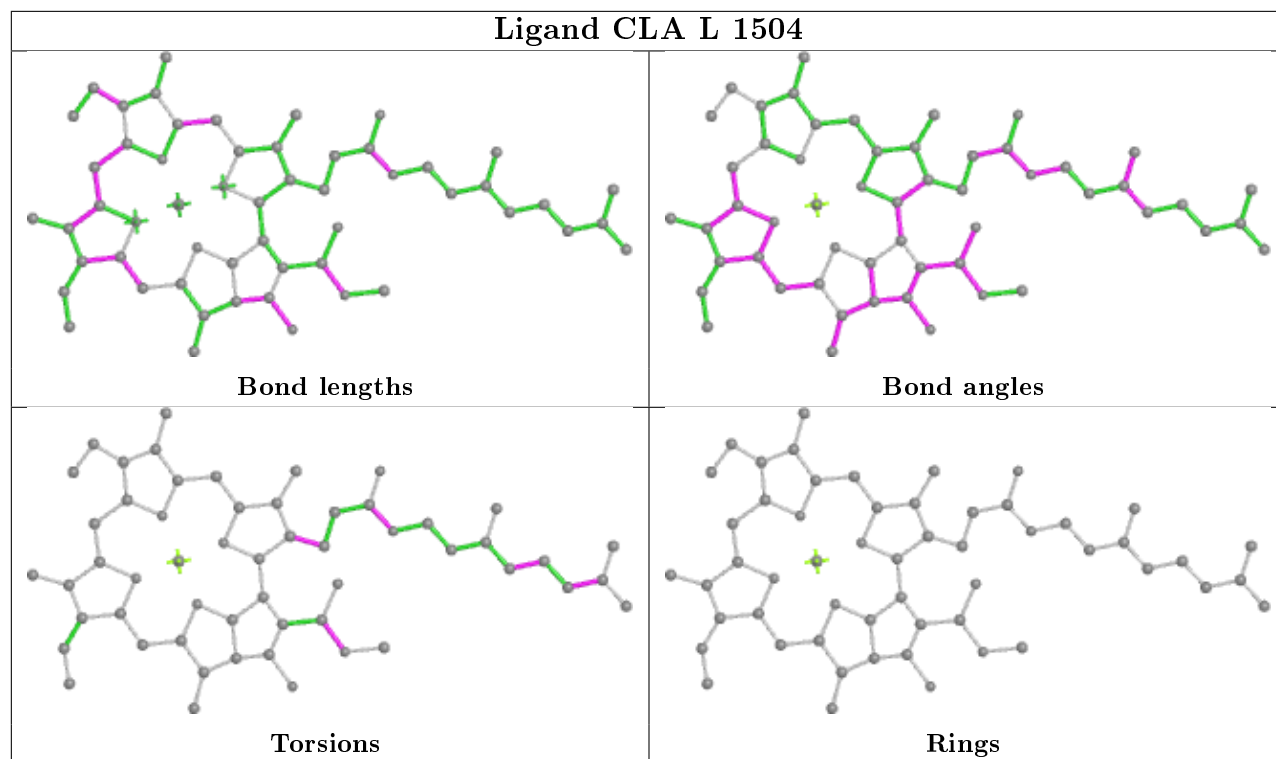
Ligand CLA A 1115



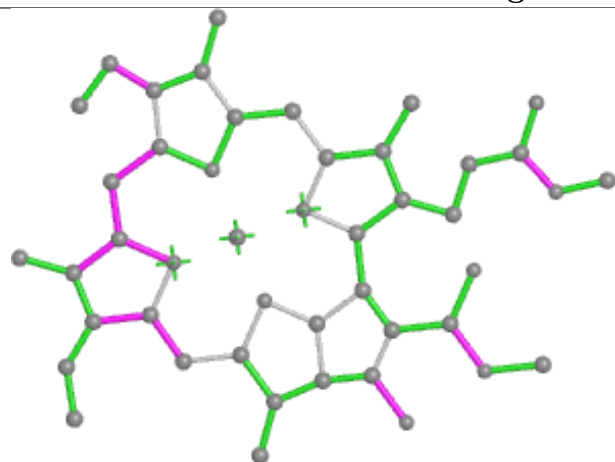
Ligand CLA B 1207



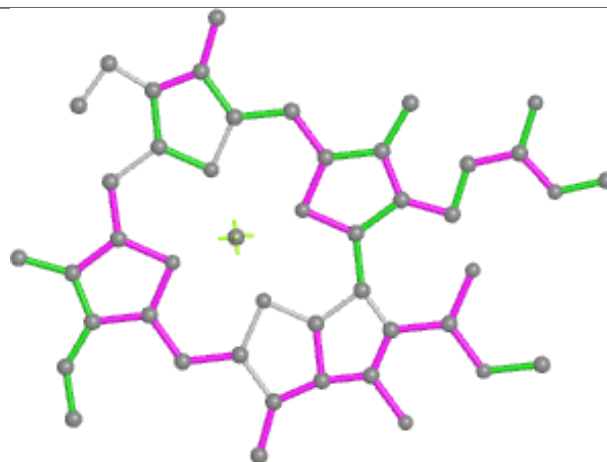




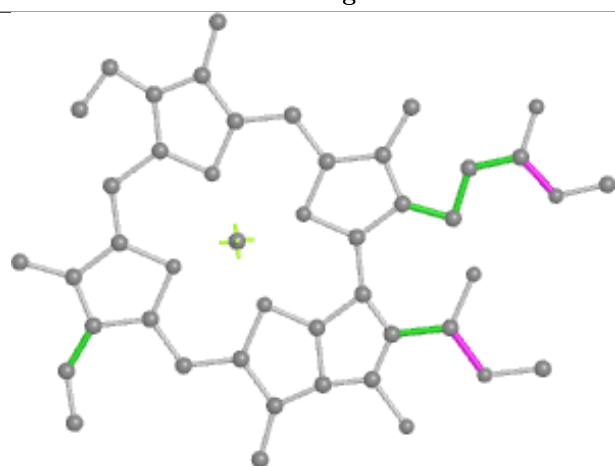
Ligand CLA A 9013



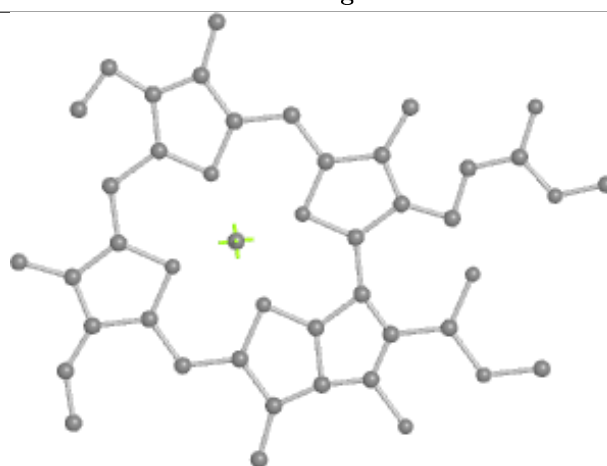
Bond lengths



Bond angles

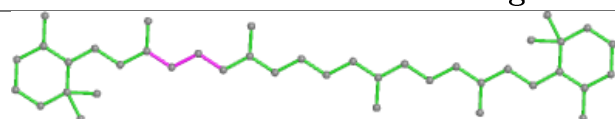


Torsions

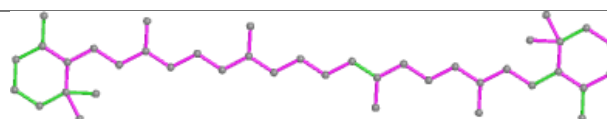


Rings

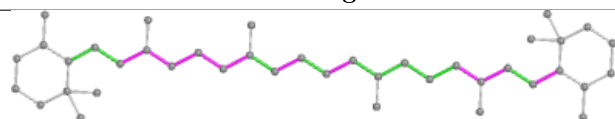
Ligand BCR L 6020



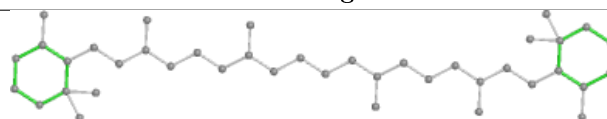
Bond lengths



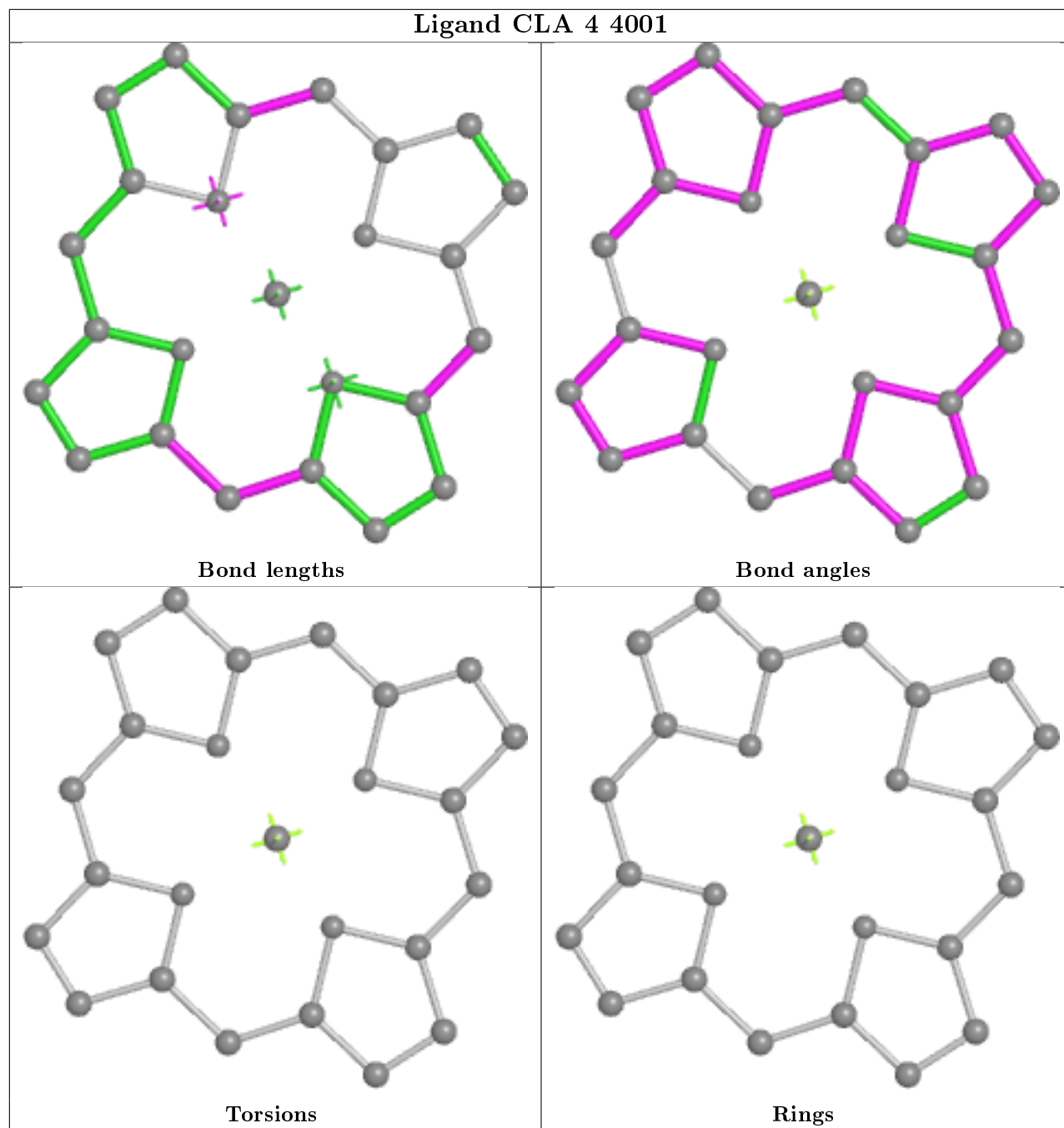
Bond angles



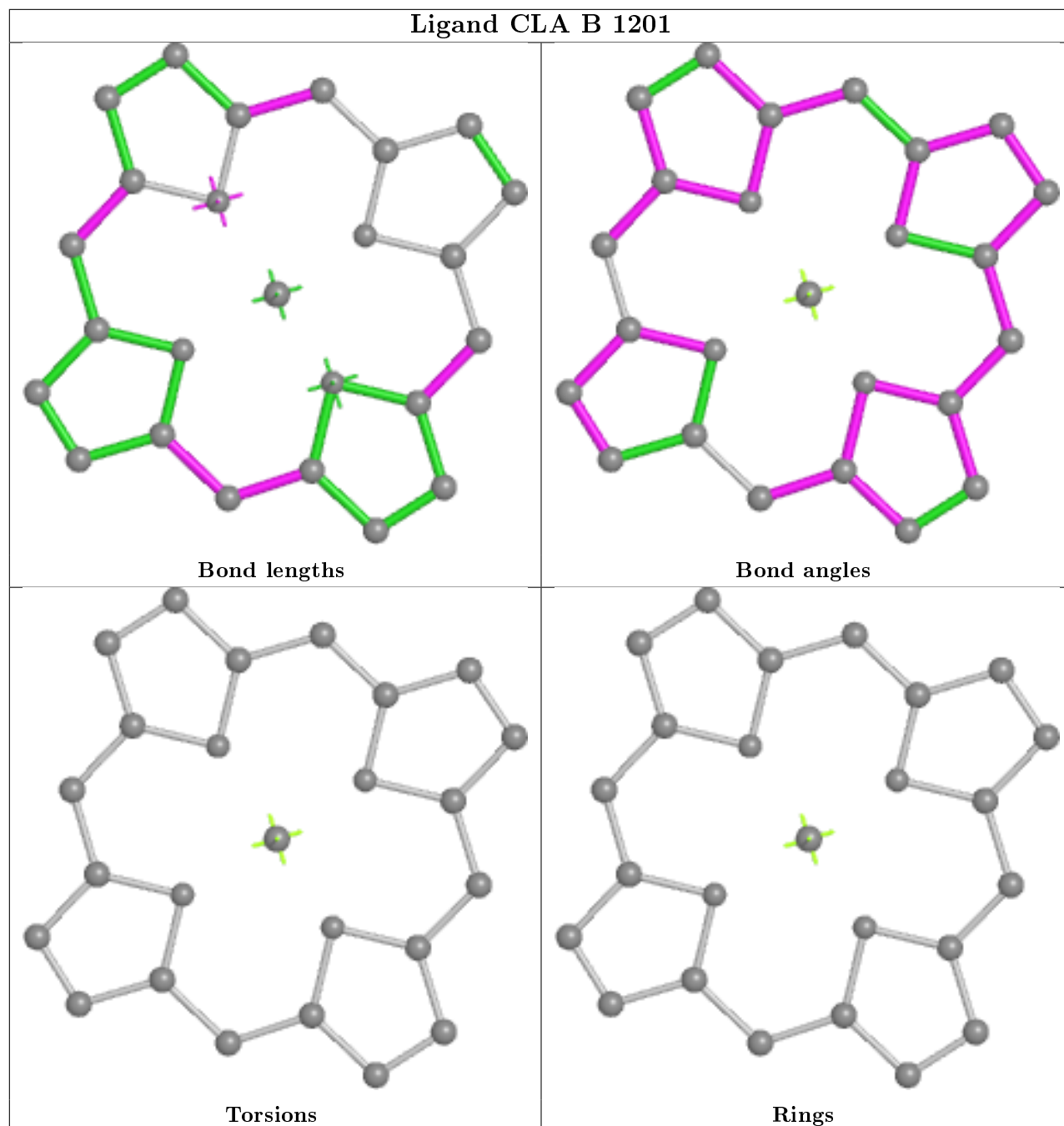
Torsions

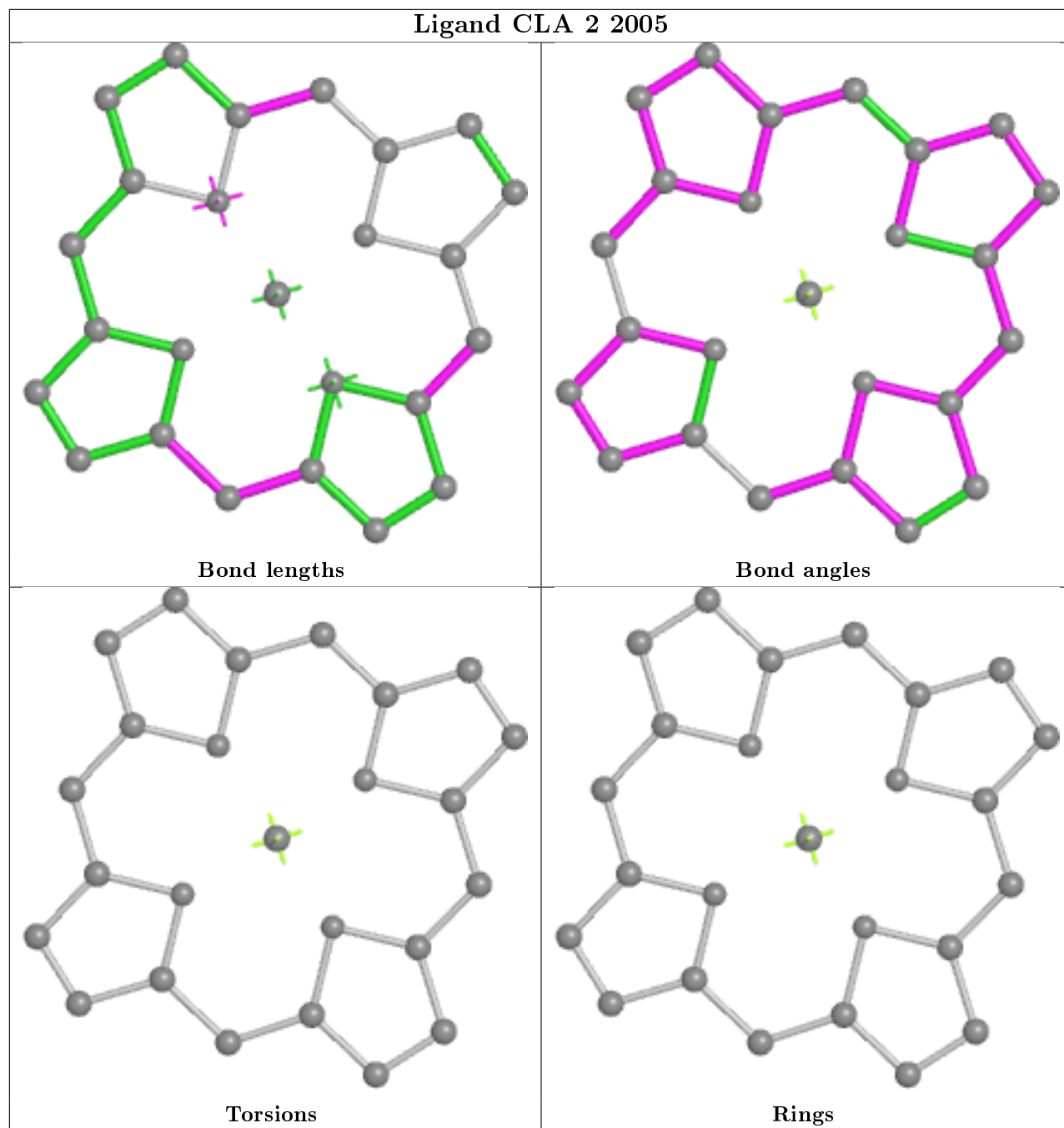


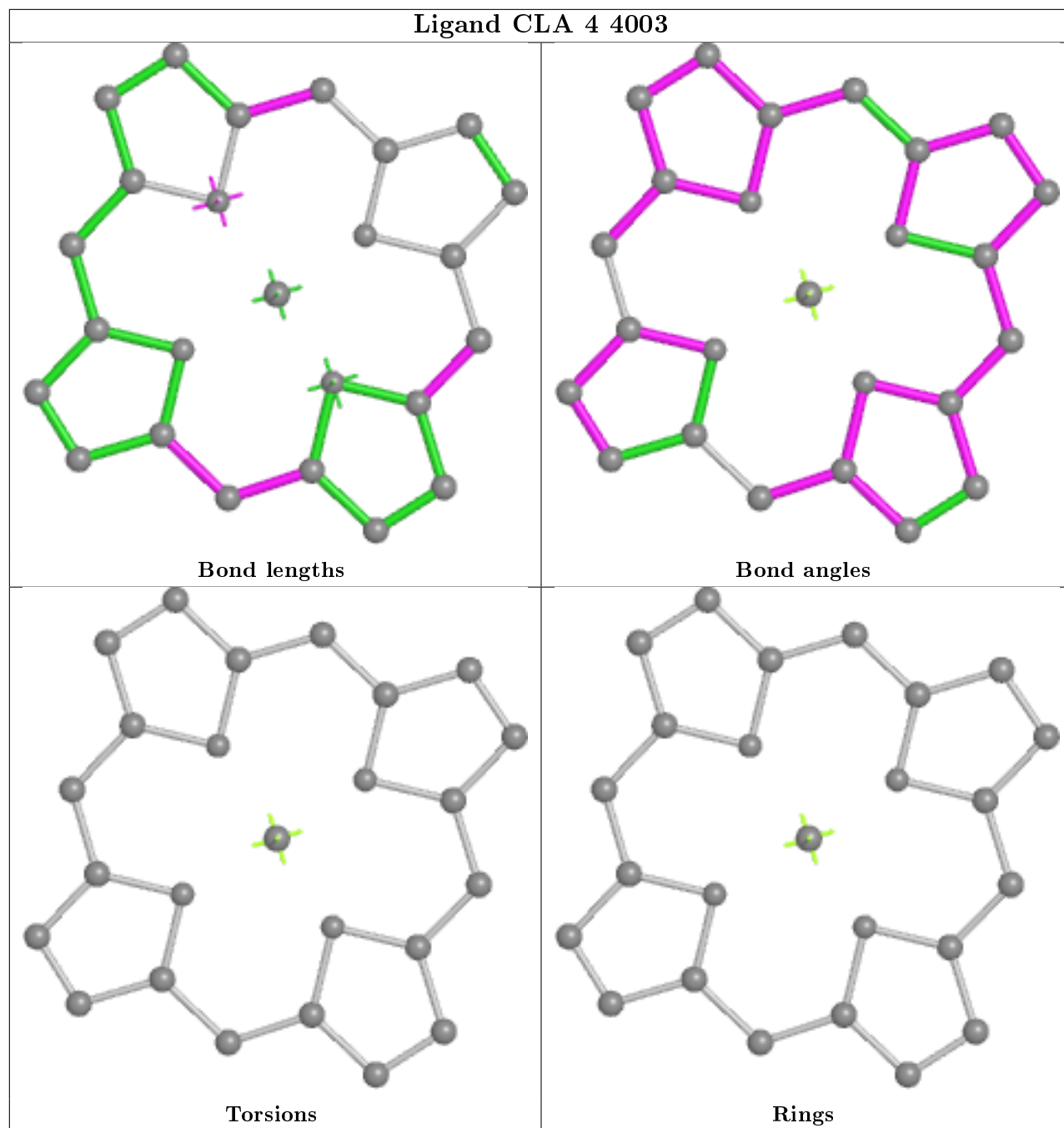
Rings

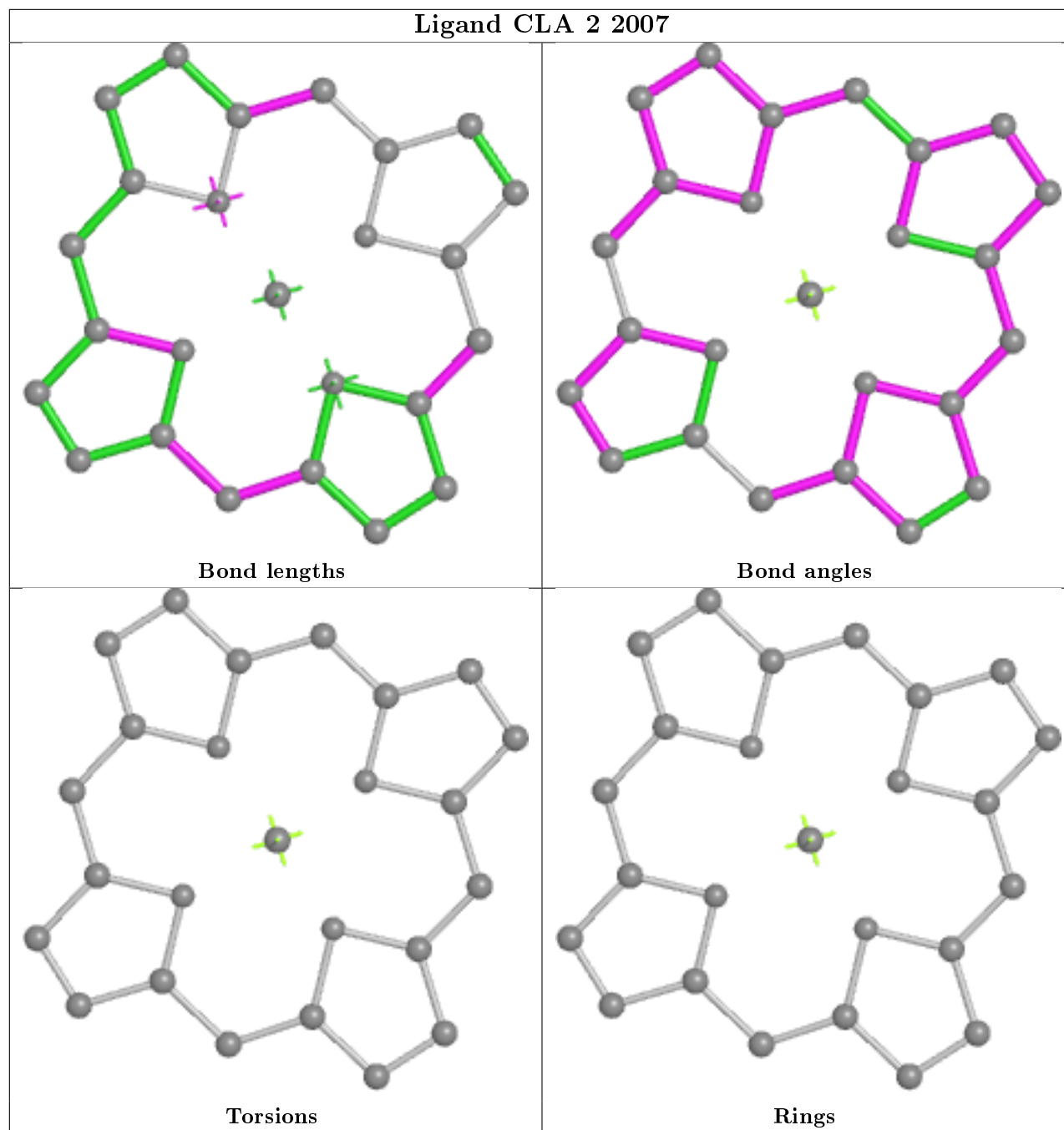


Ligand CLA B 1201

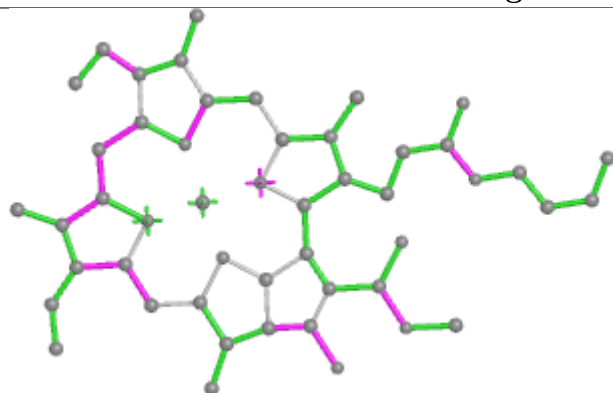




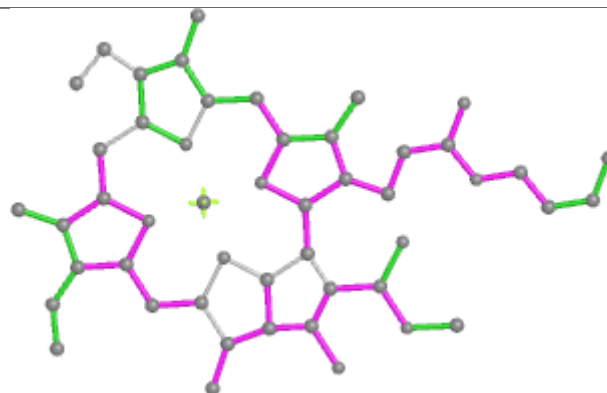




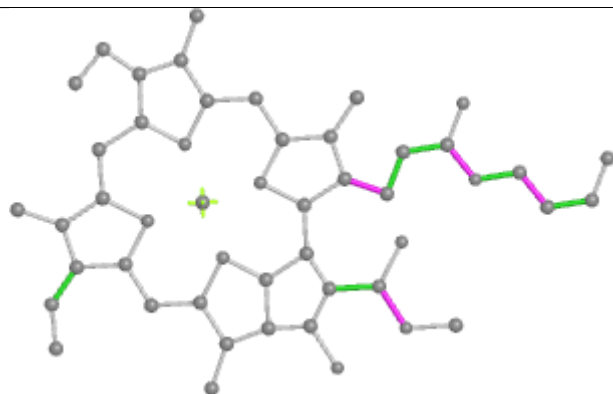
Ligand CLA B 1214



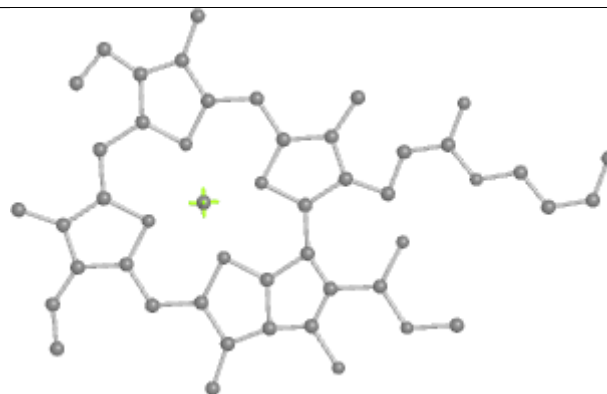
Bond lengths



Bond angles

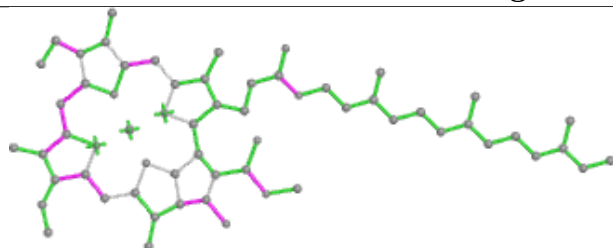


Torsions

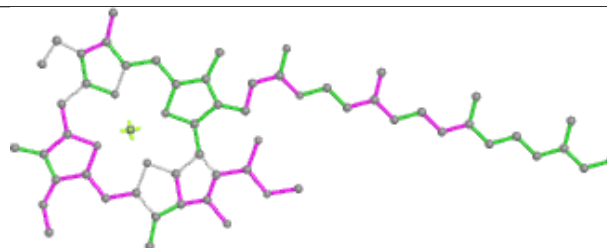


Rings

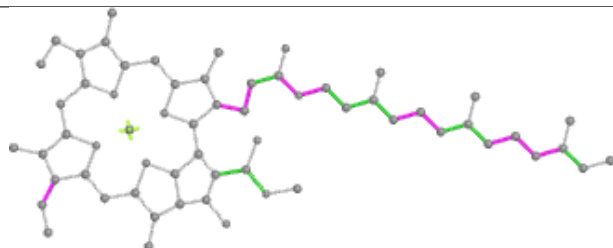
Ligand CLA J 2107



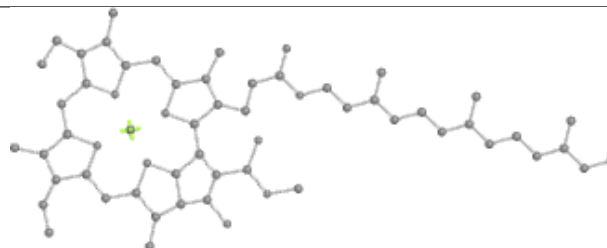
Bond lengths



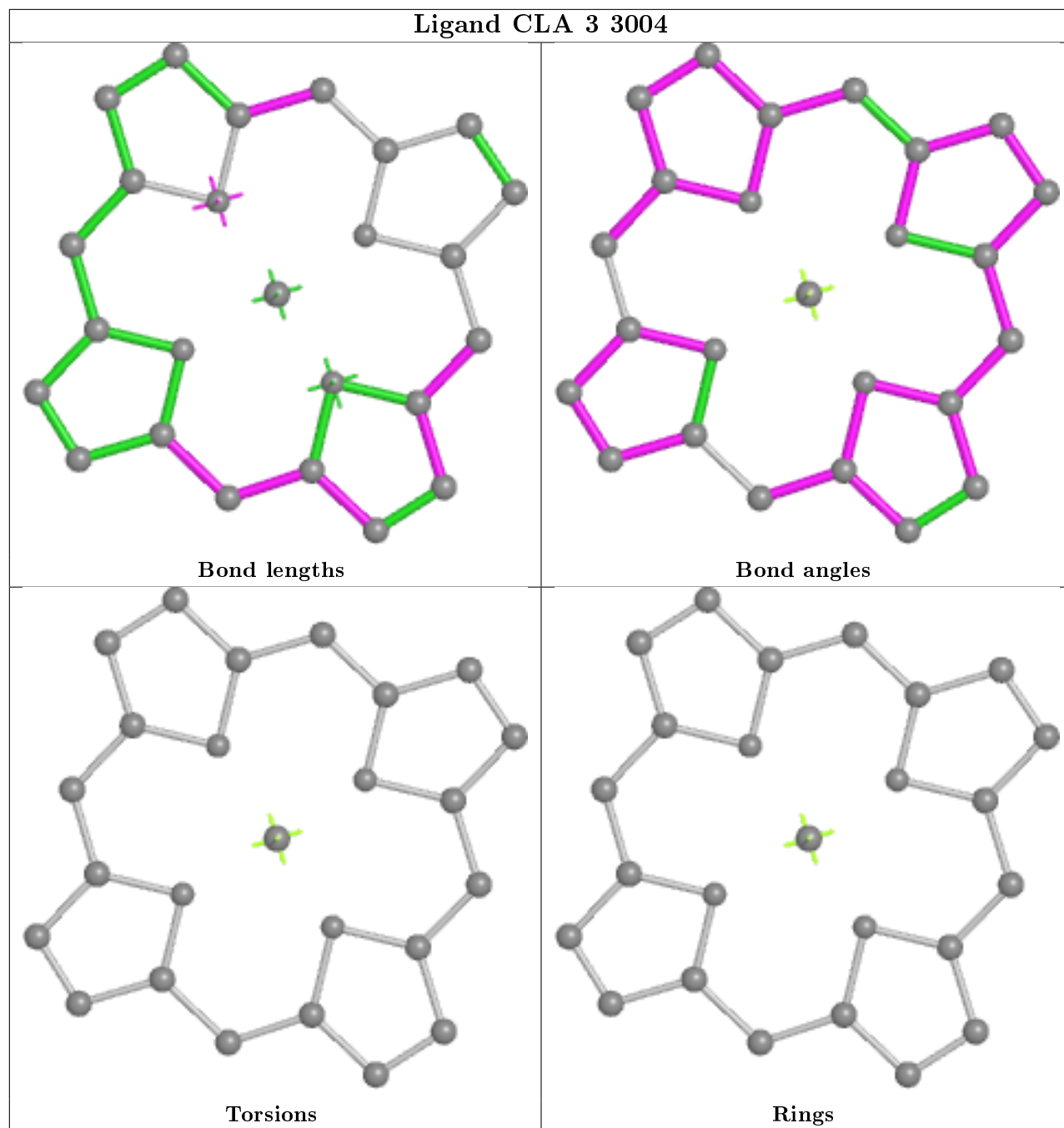
Bond angles

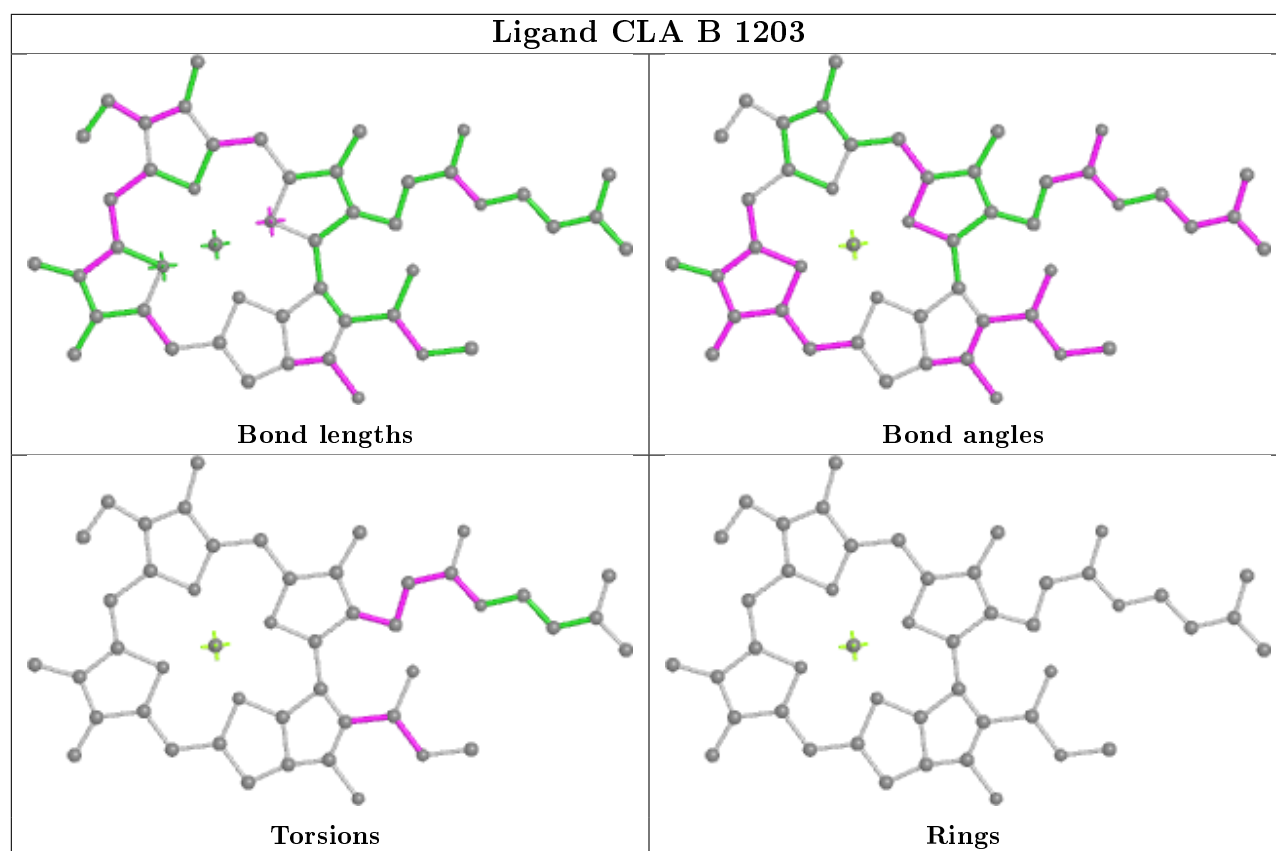


Torsions

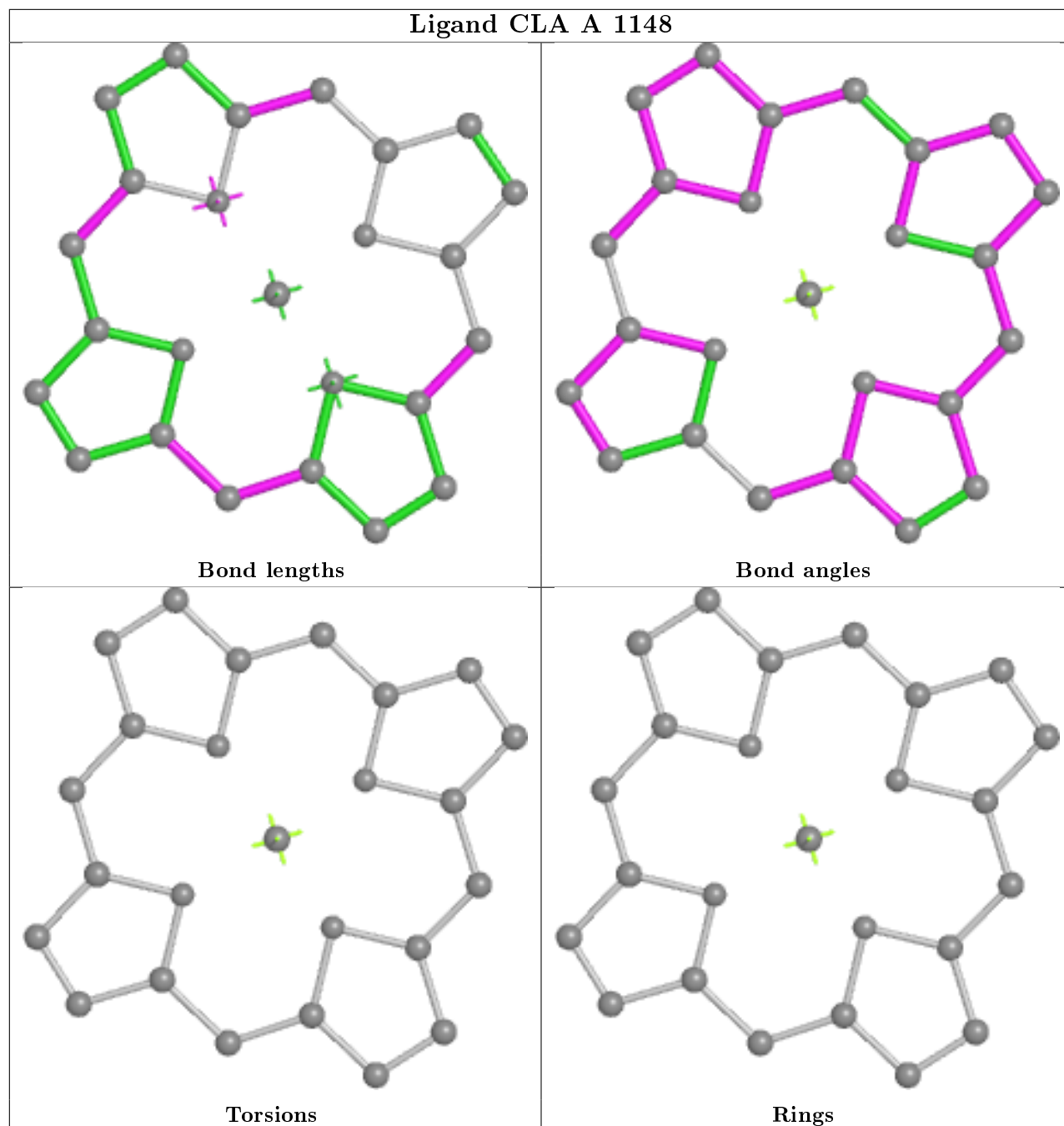


Rings

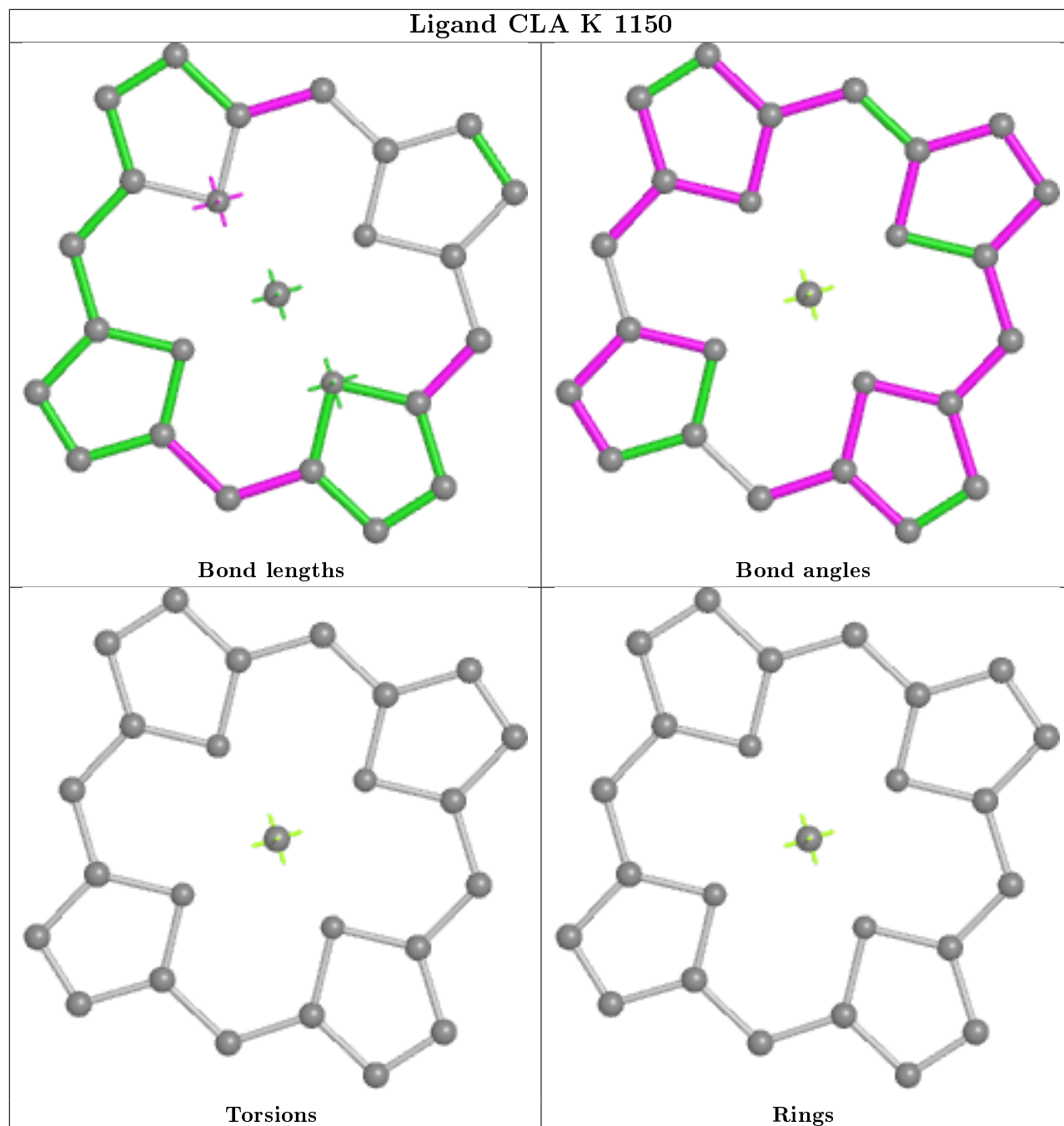


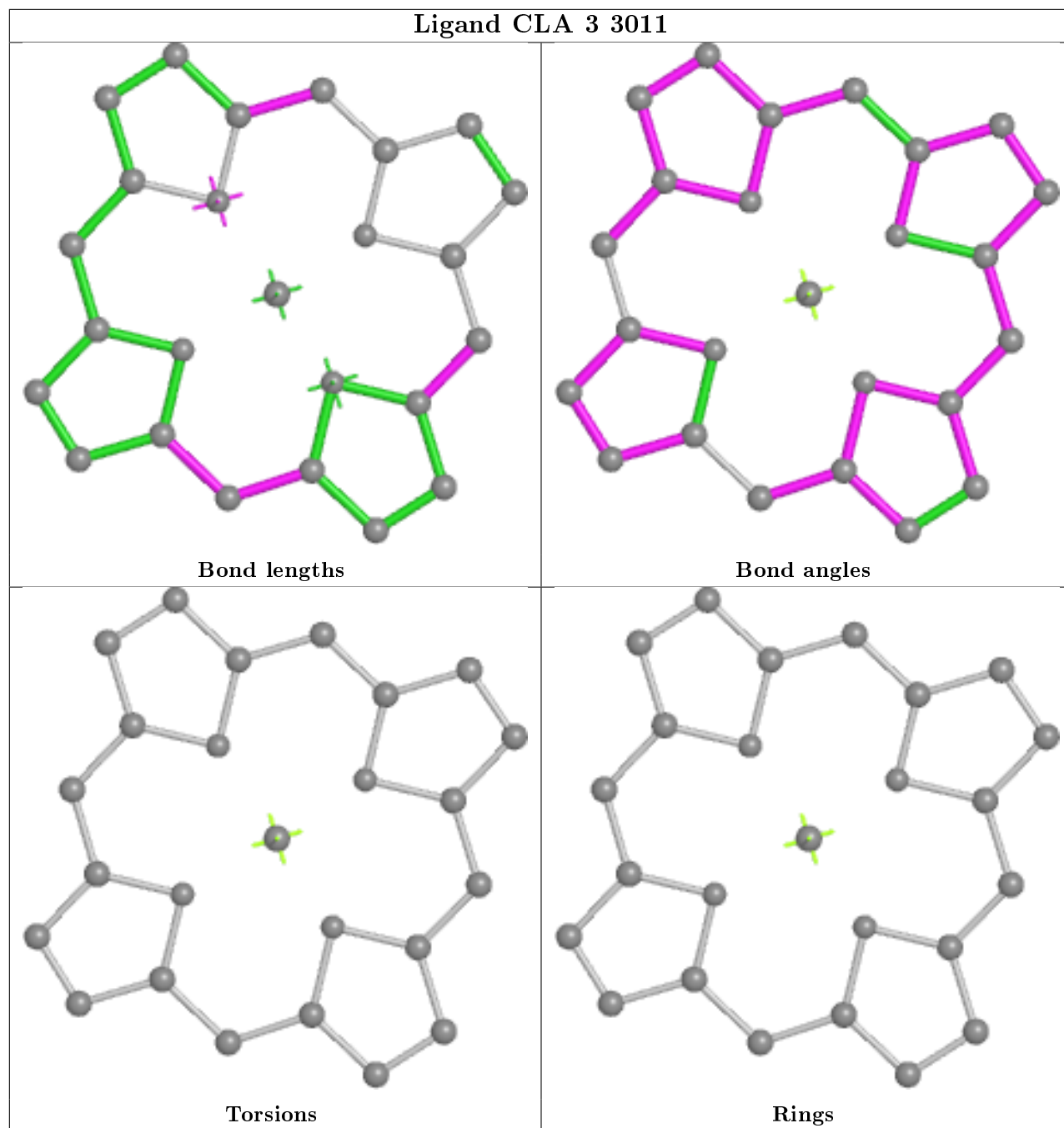


Ligand CLA A 1148

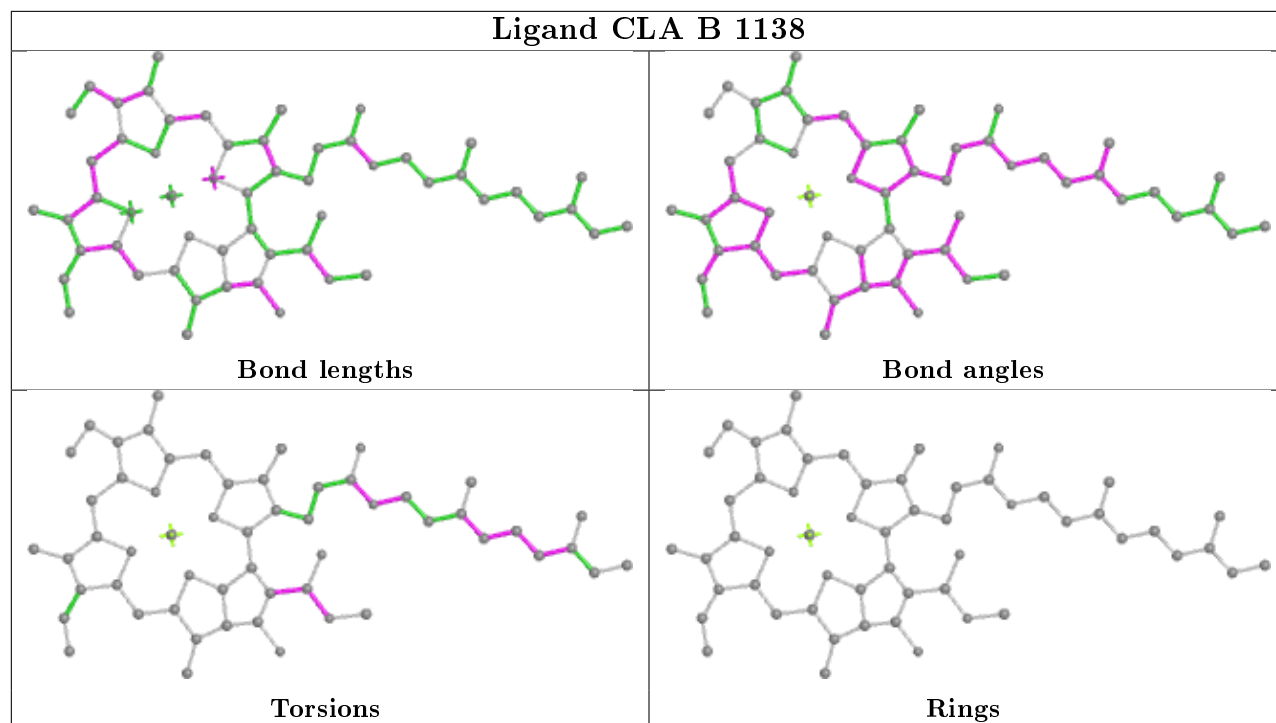


Ligand CLA K 1150

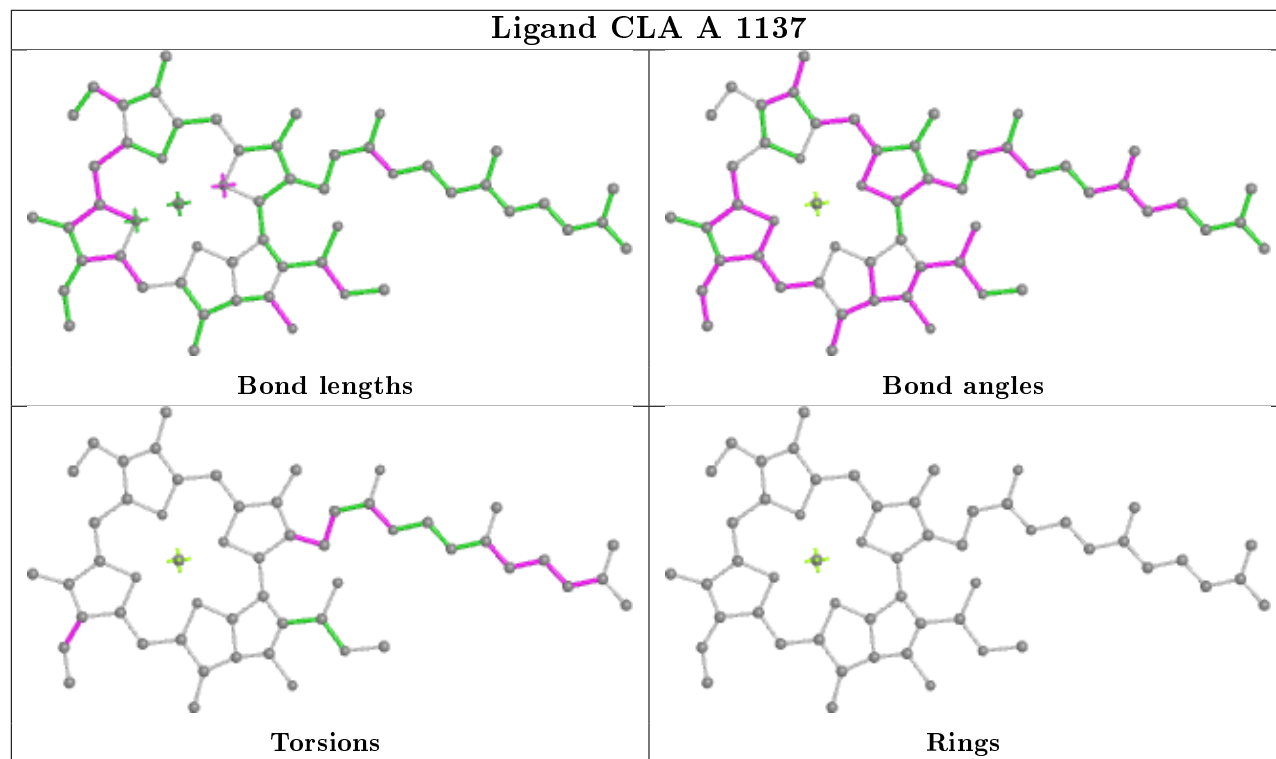


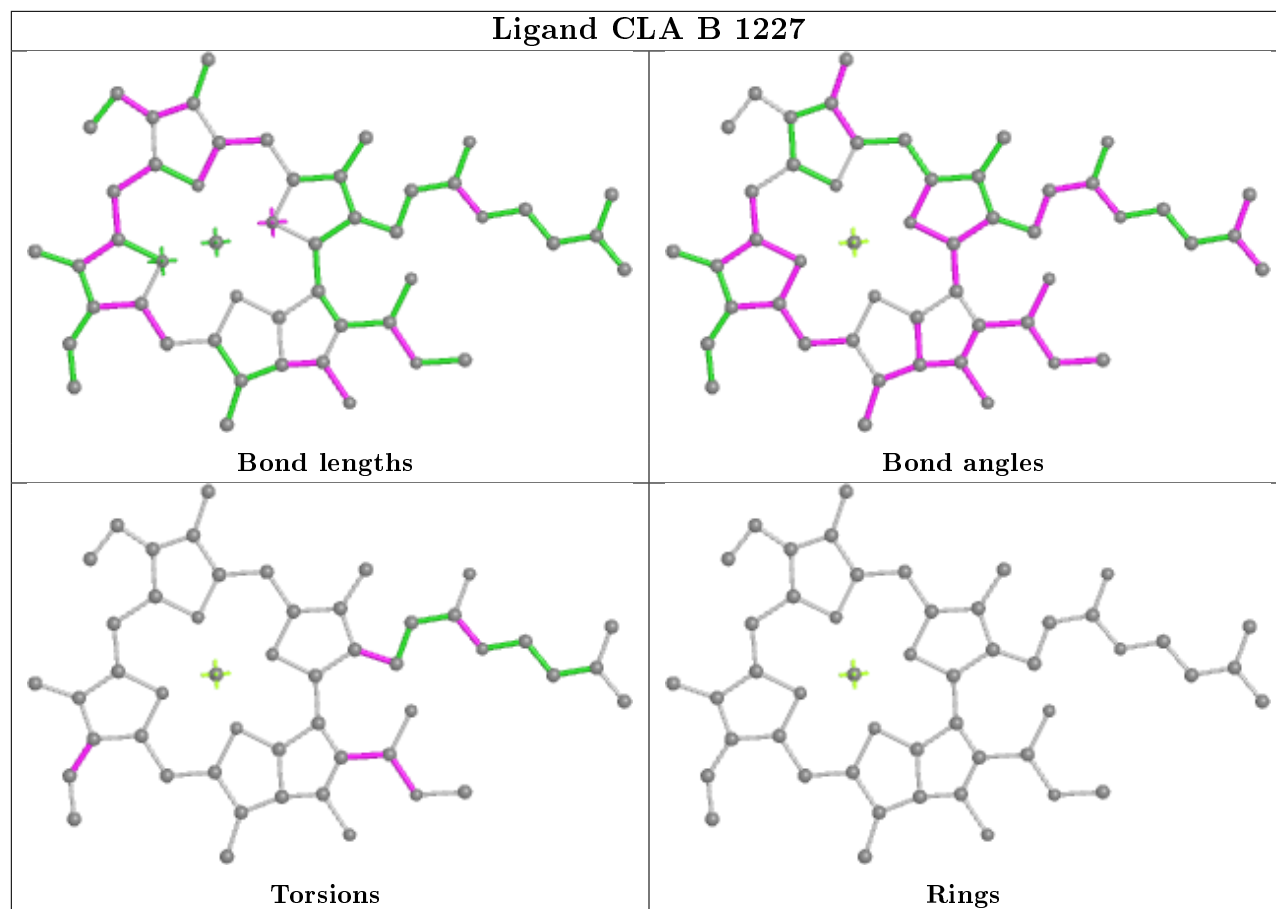


Ligand CLA B 1138

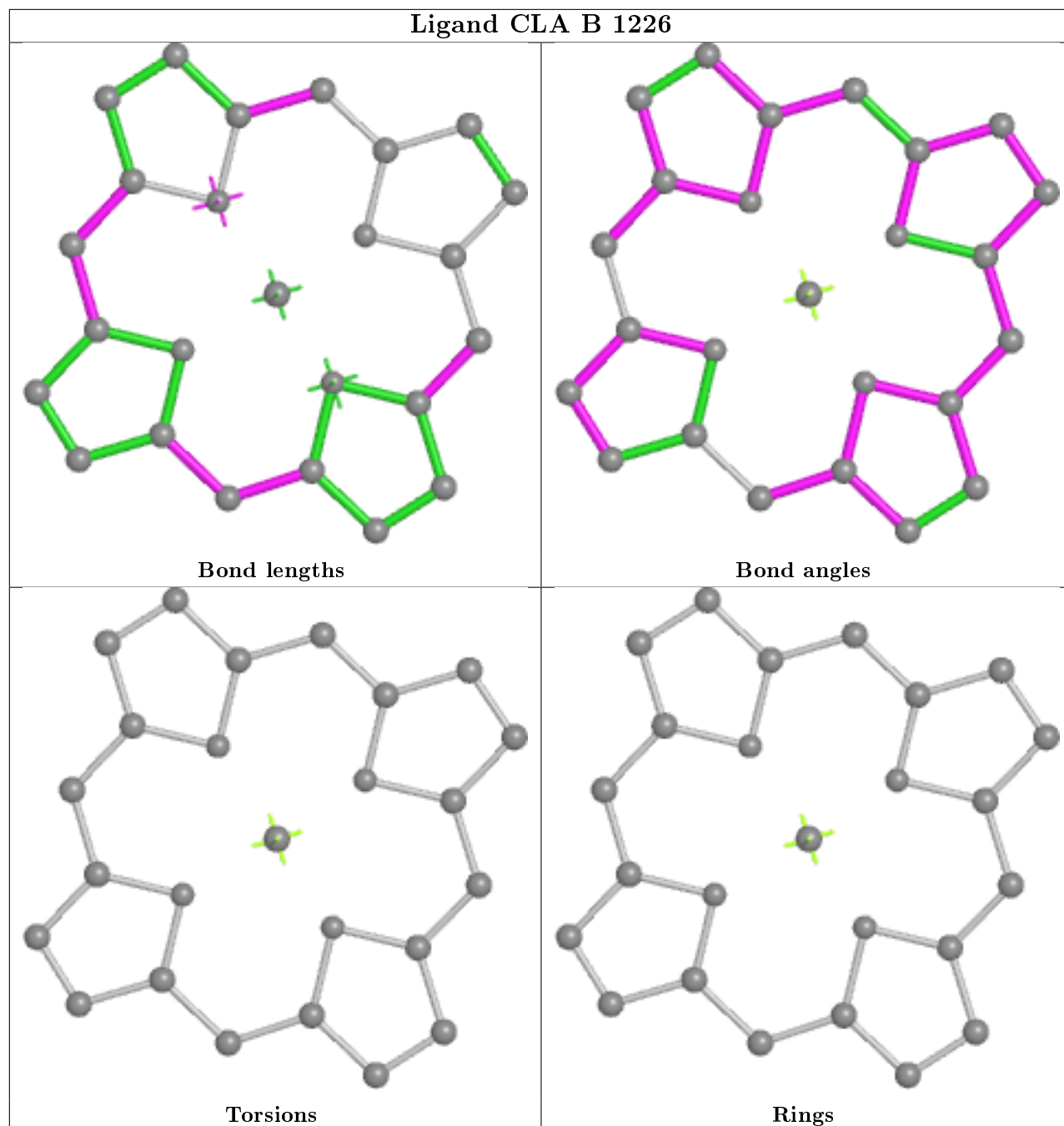


Ligand CLA A 1137

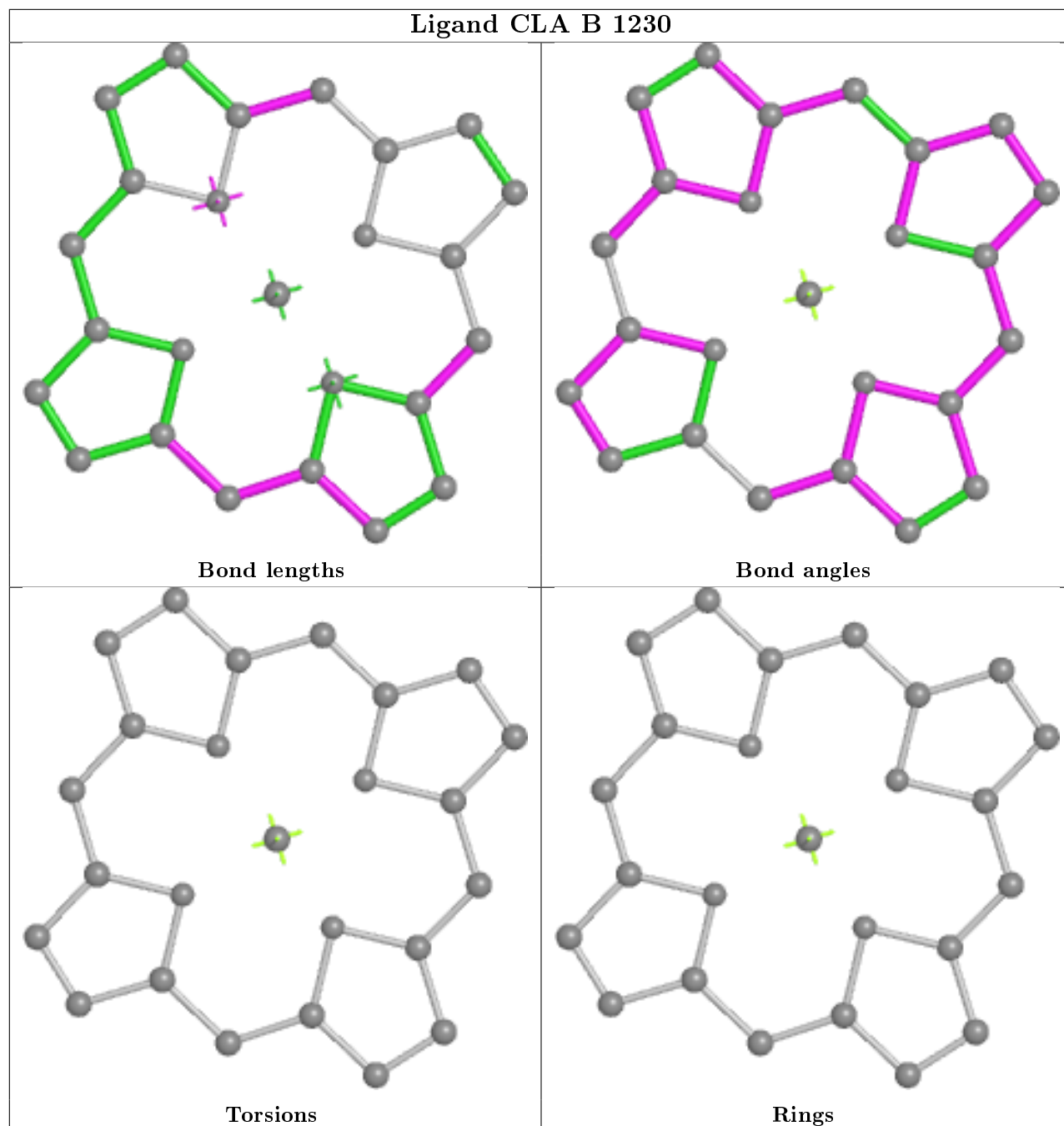




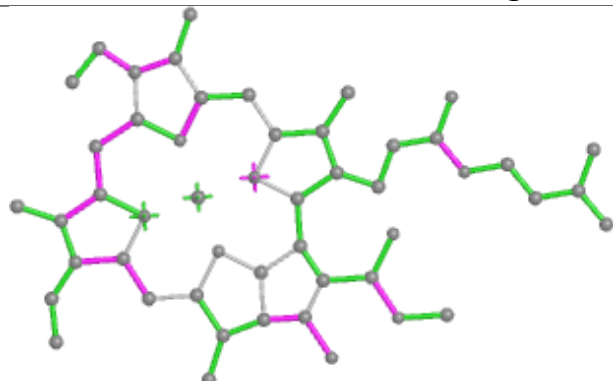
Ligand CLA B 1226



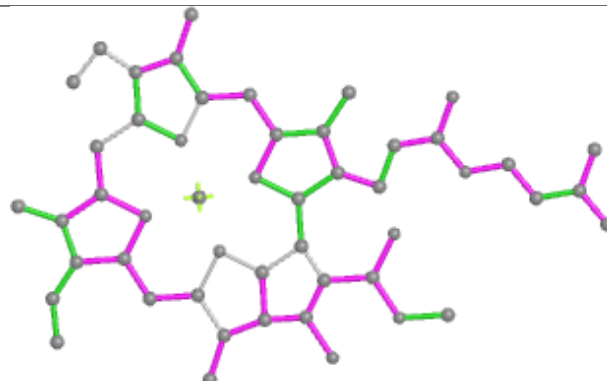
Ligand CLA B 1230



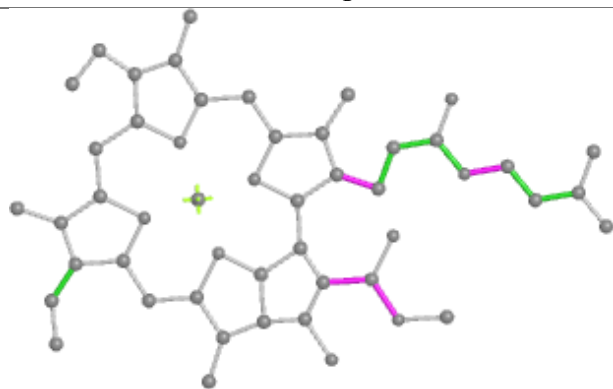
Ligand CLA B 1217



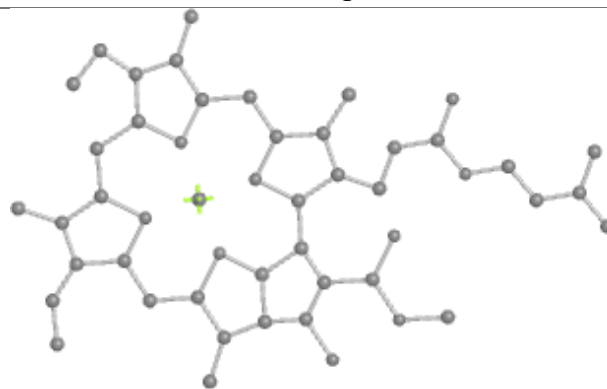
Bond lengths



Bond angles

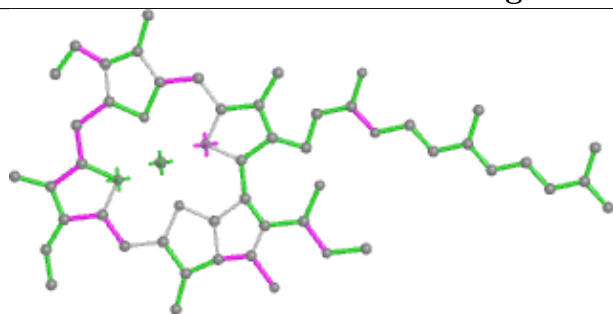


Torsions

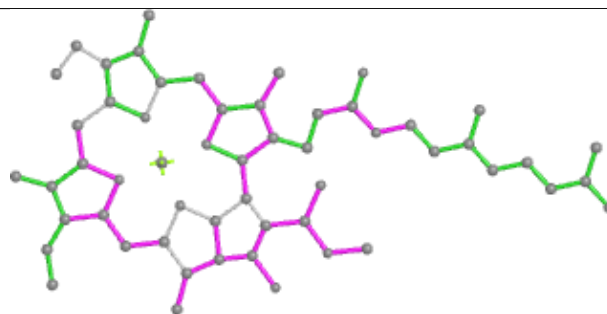


Rings

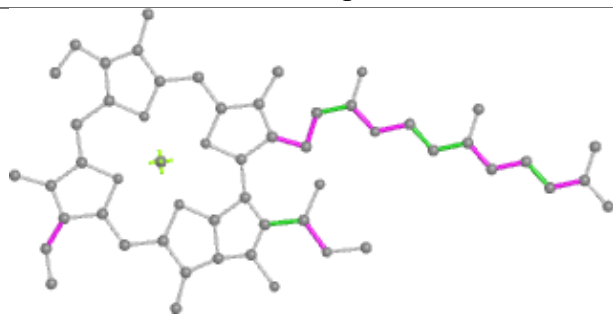
Ligand CLA A 1119



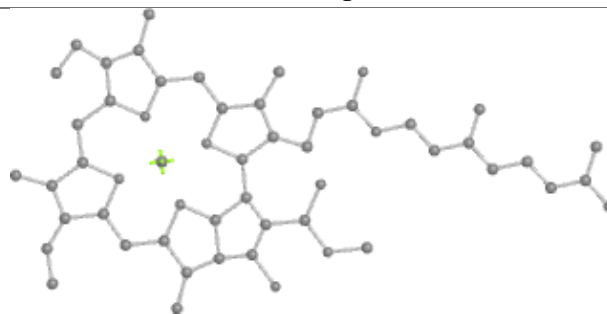
Bond lengths



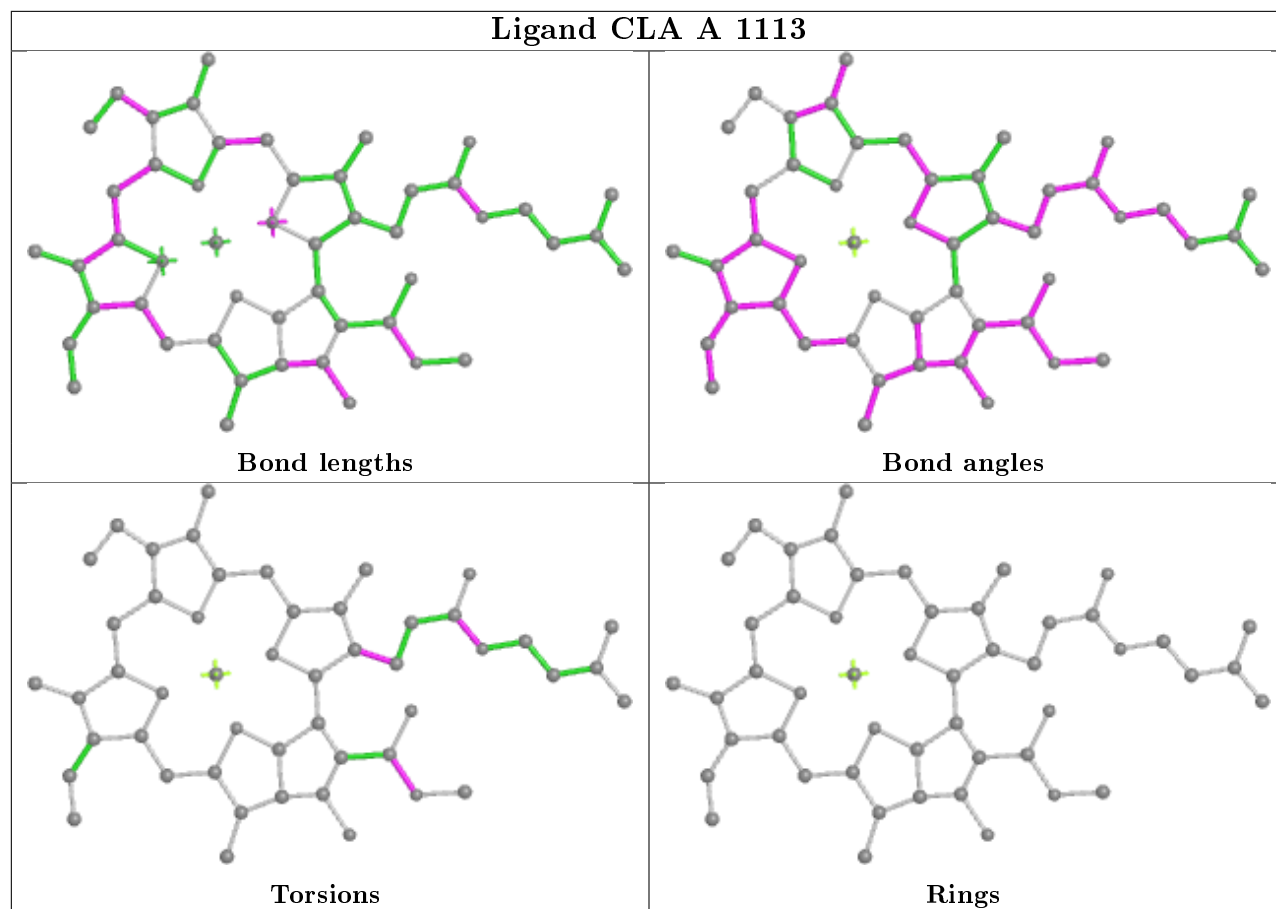
Bond angles

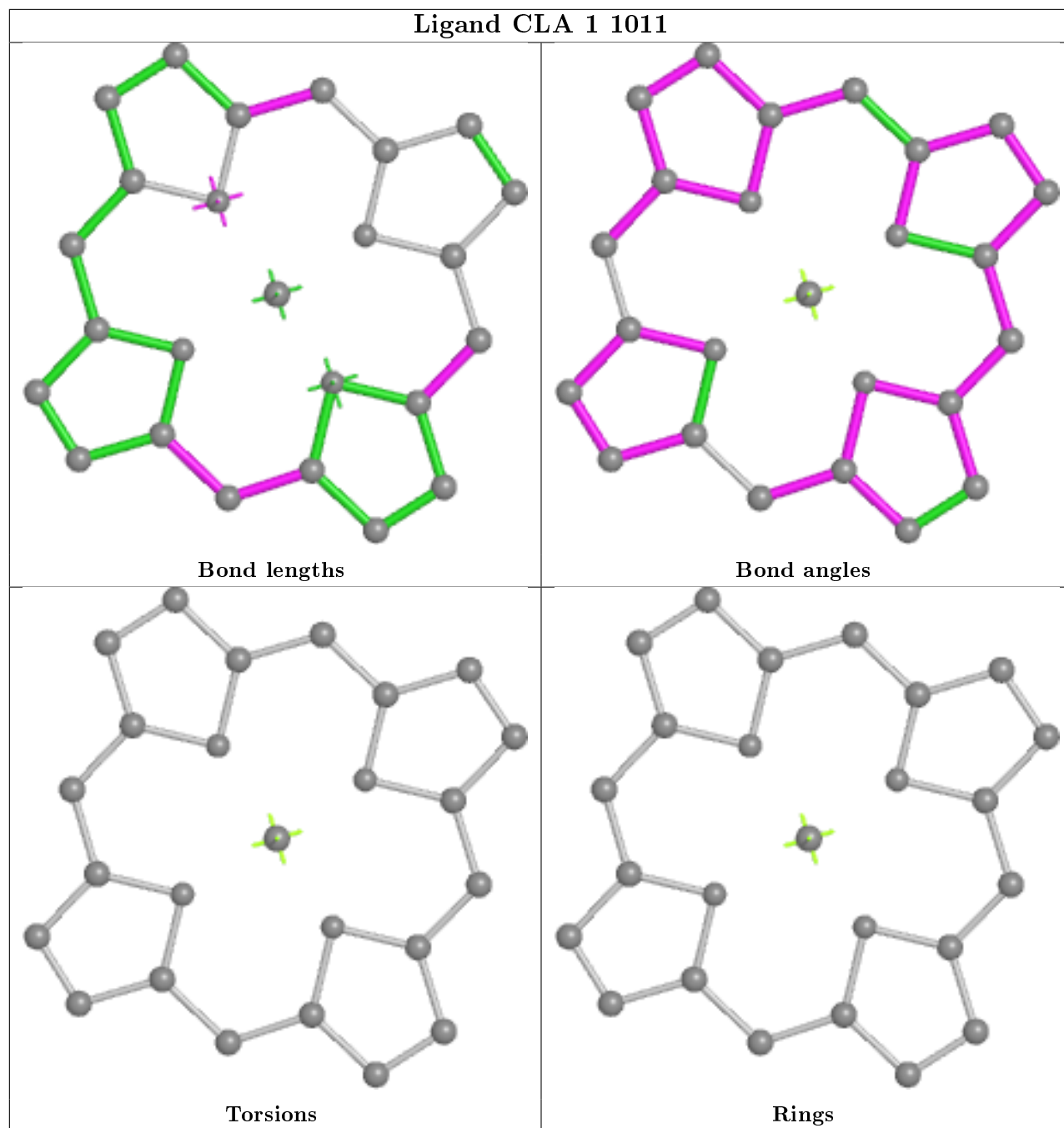


Torsions

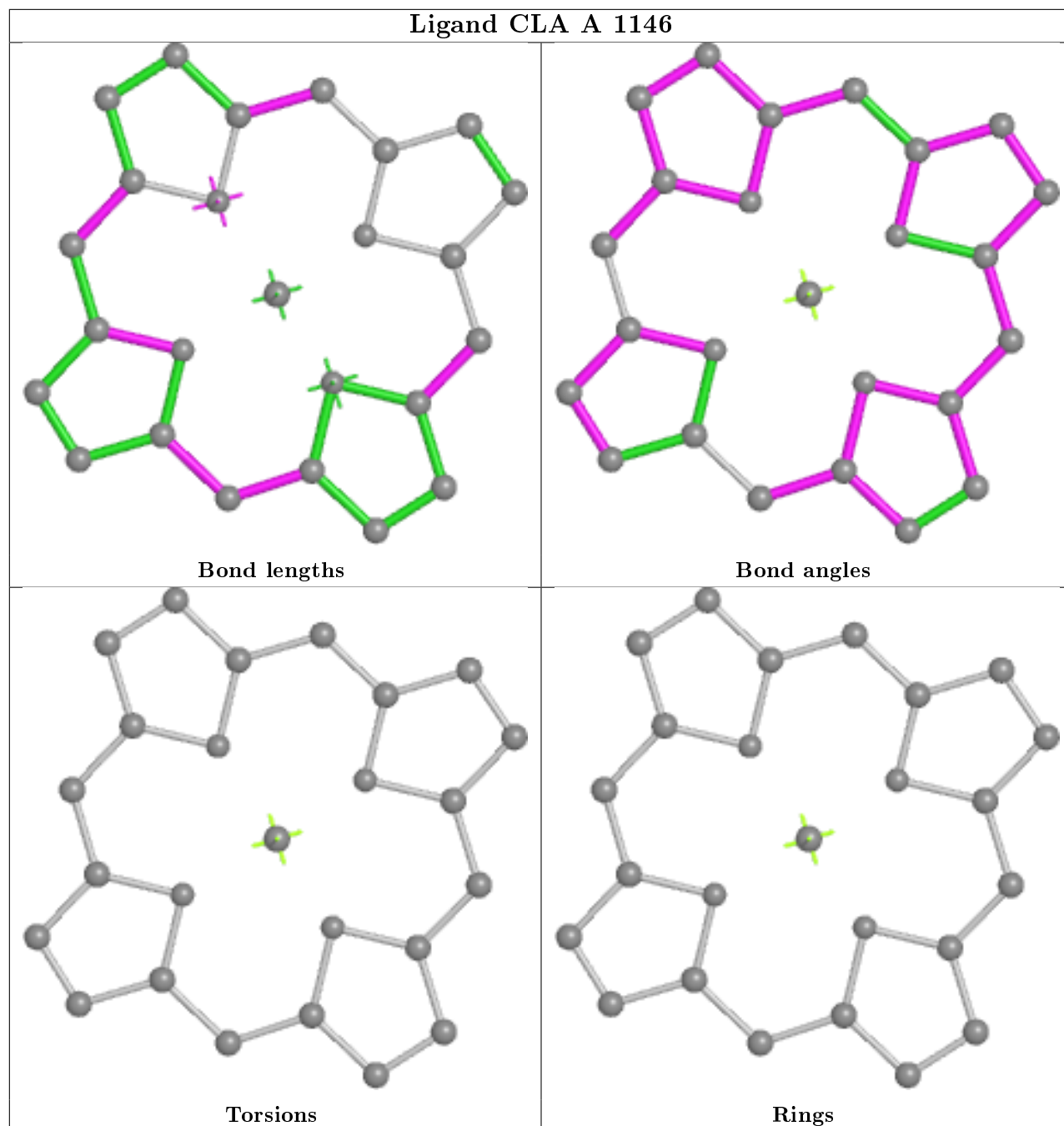


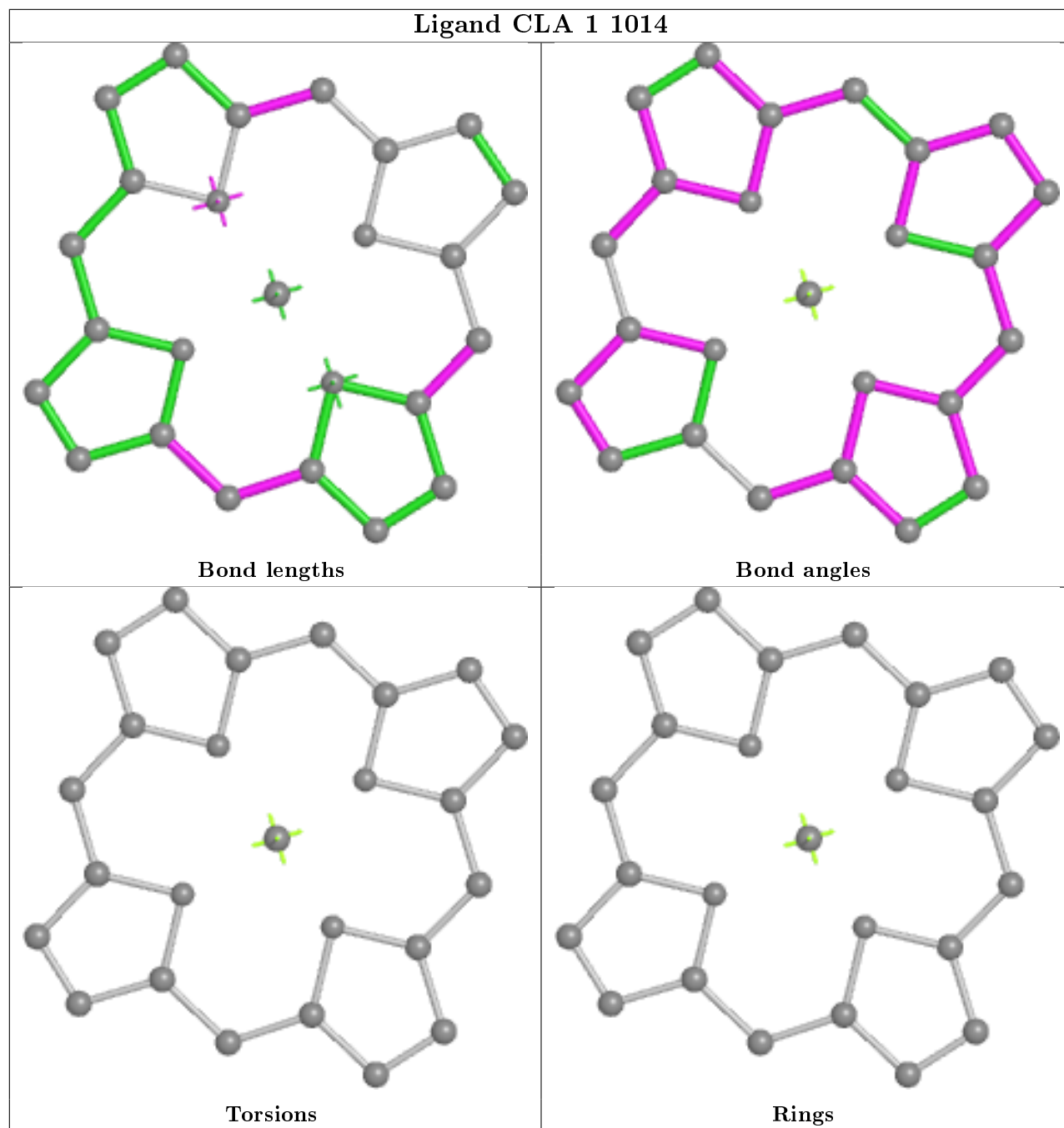
Rings

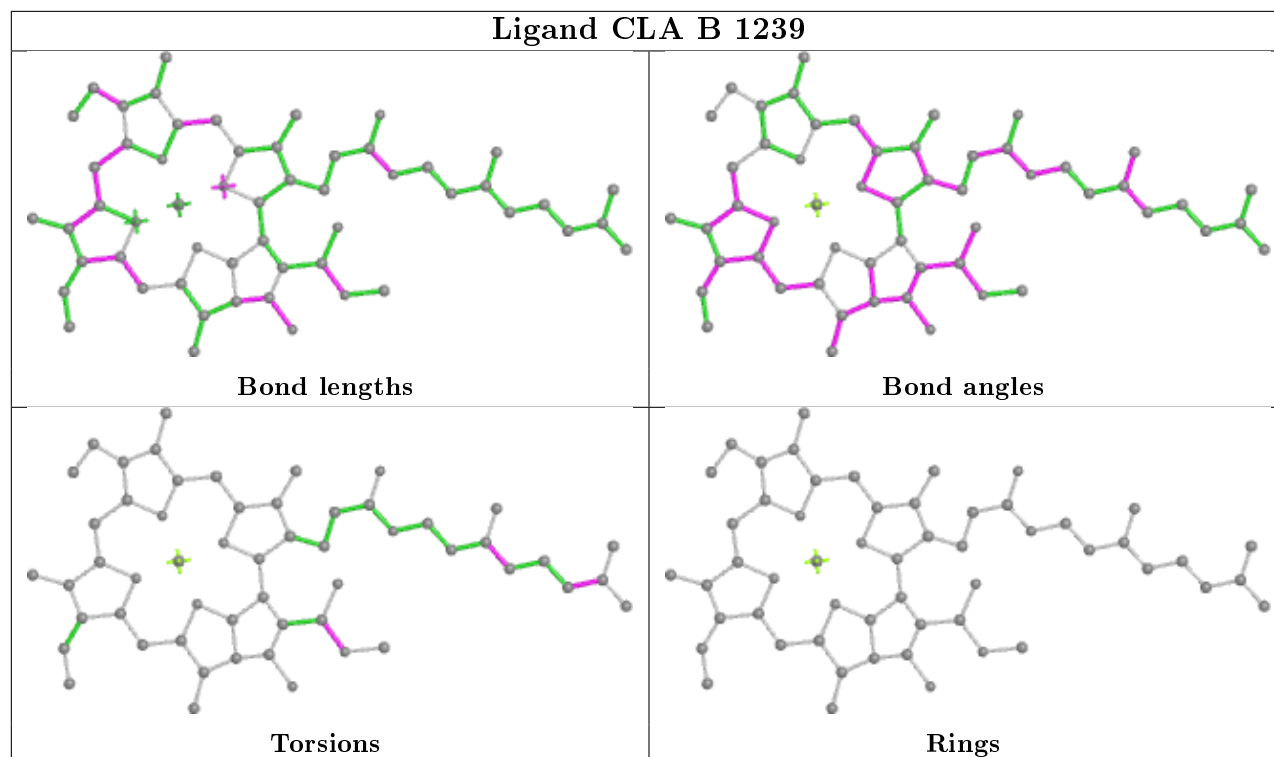
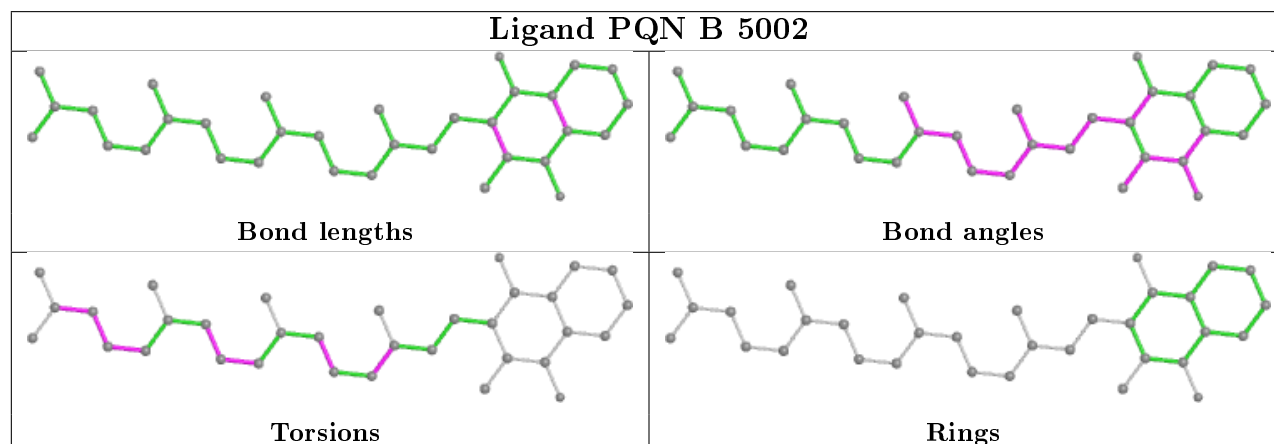




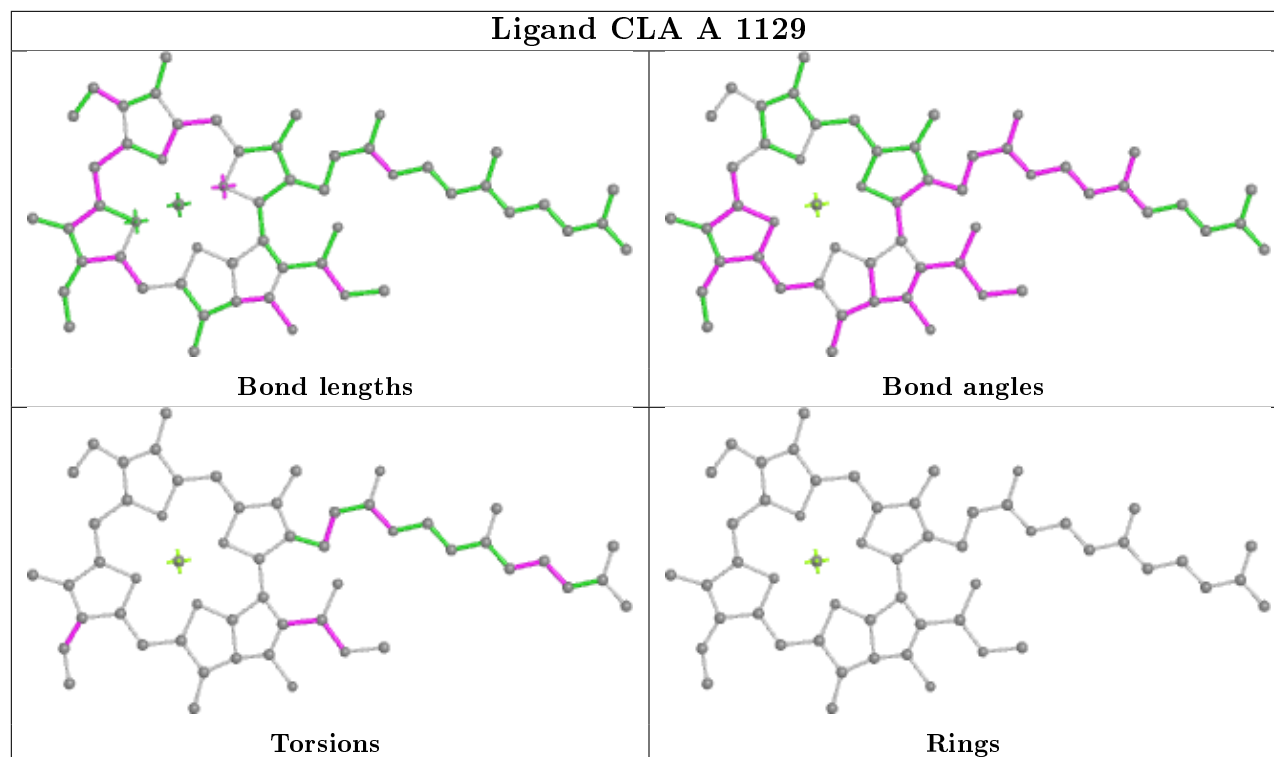
Ligand CLA A 1146



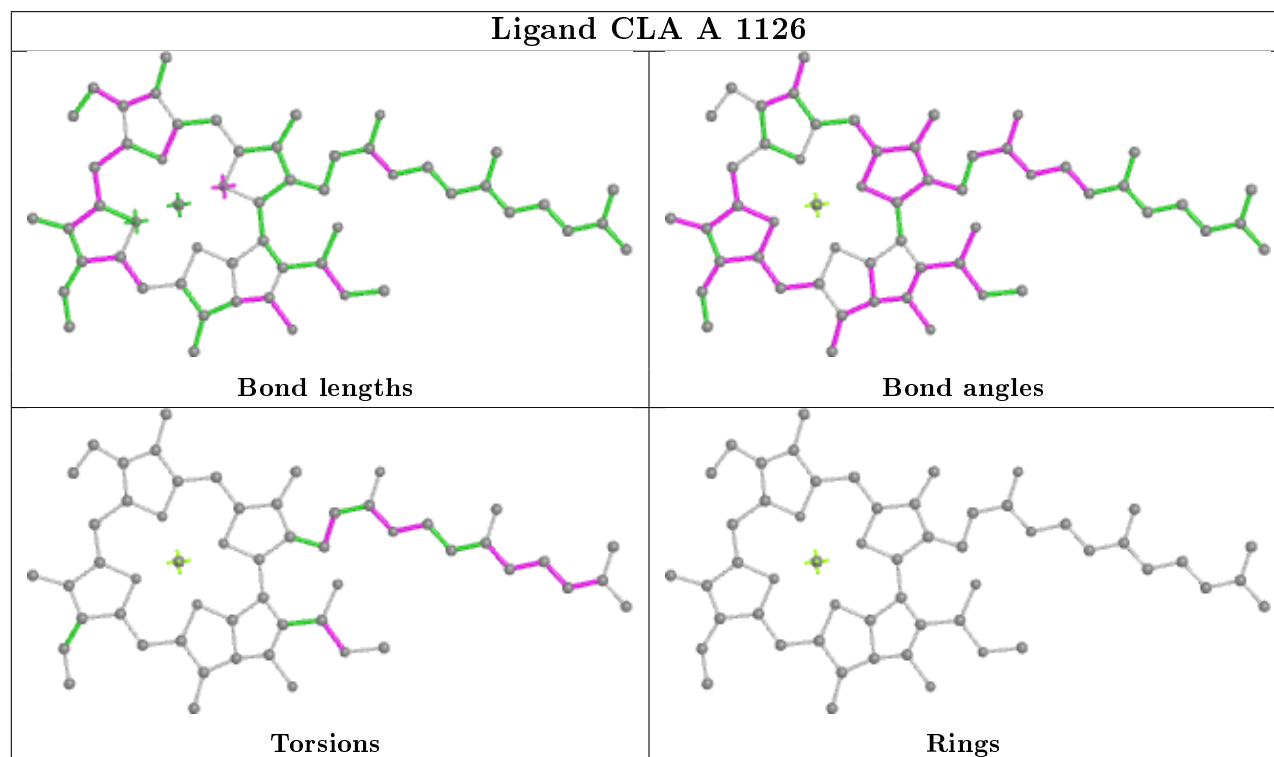


Ligand CLA B 1239**Ligand PQN B 5002**

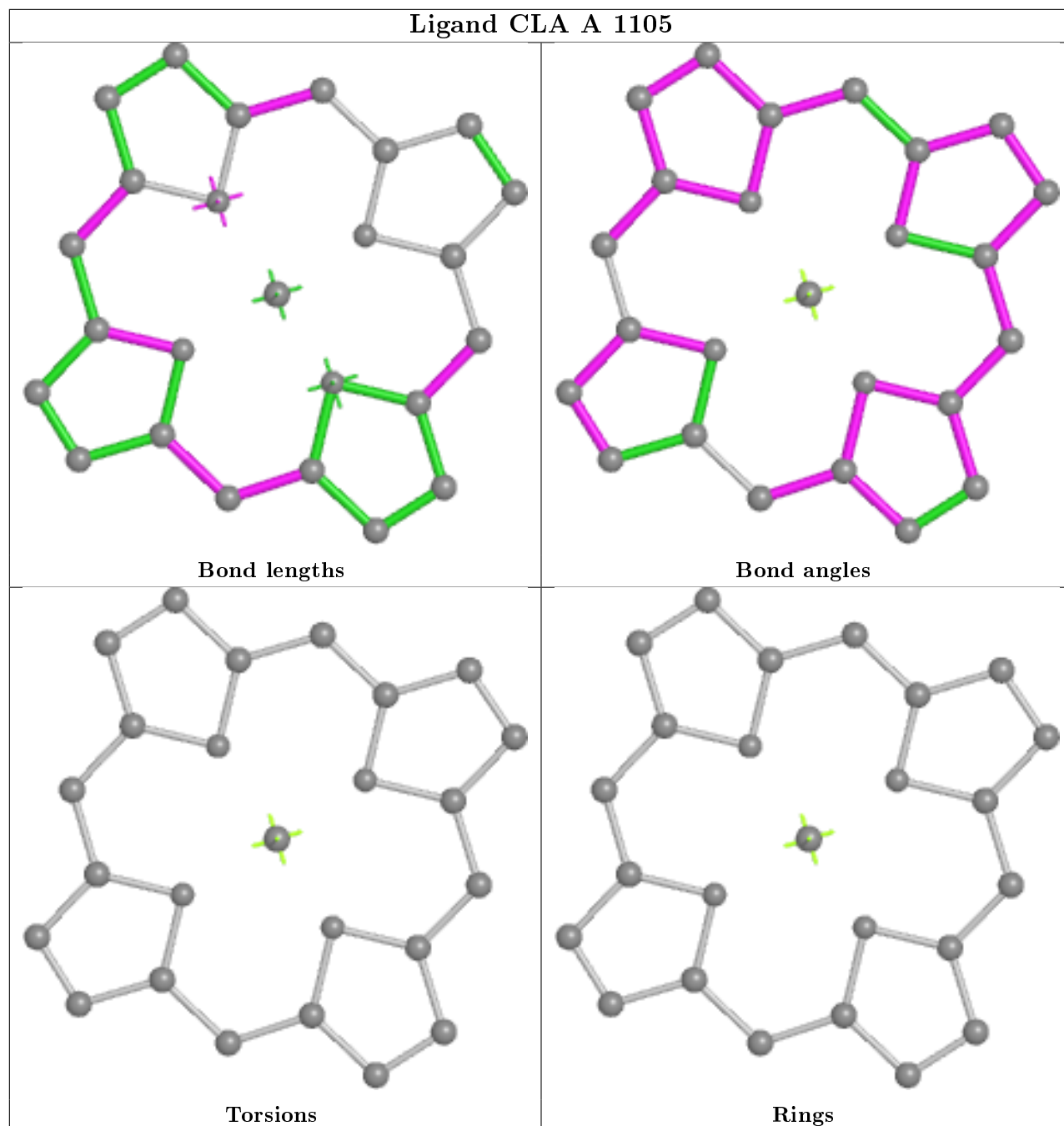
Ligand CLA A 1129



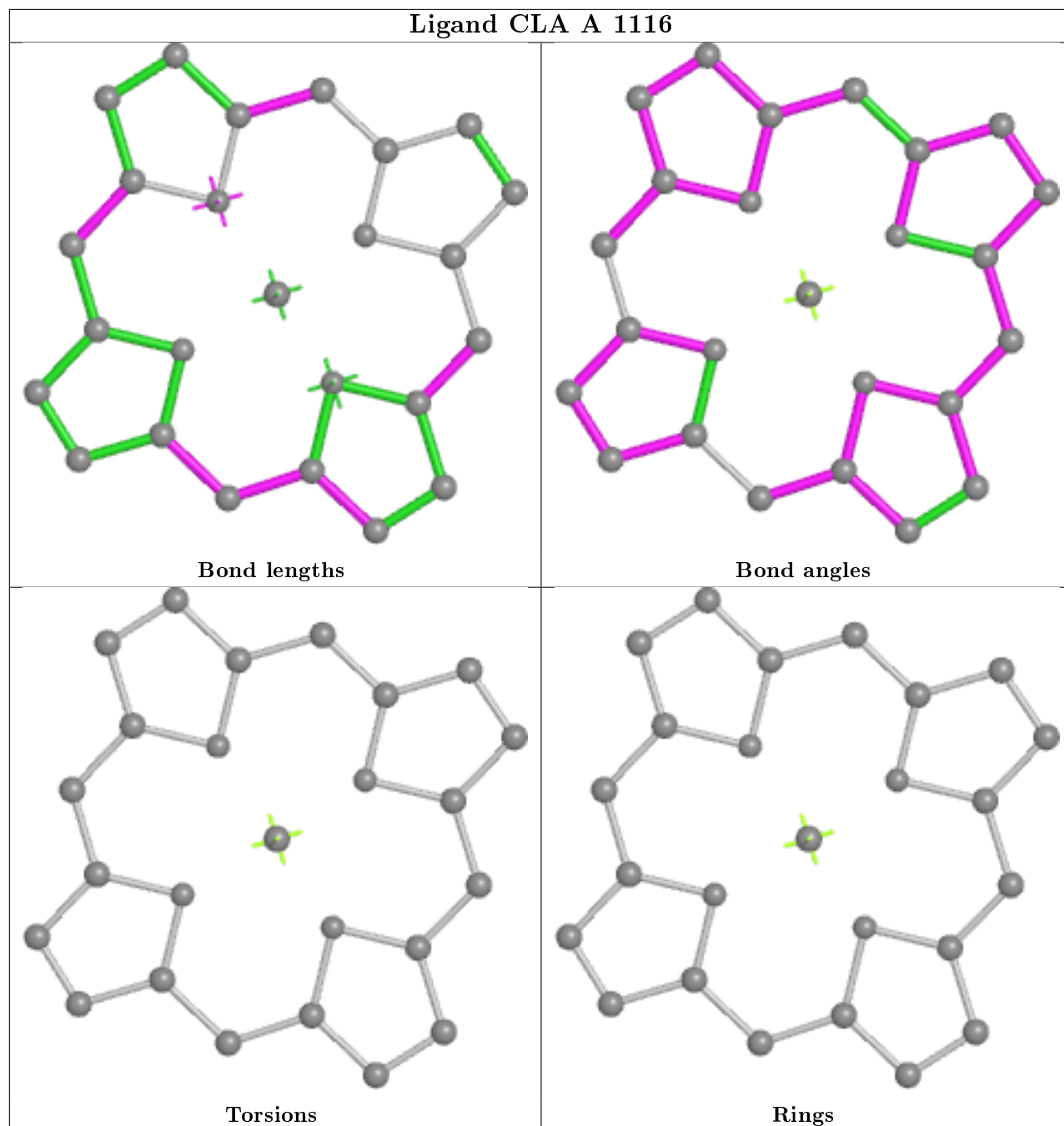
Ligand CLA A 1126



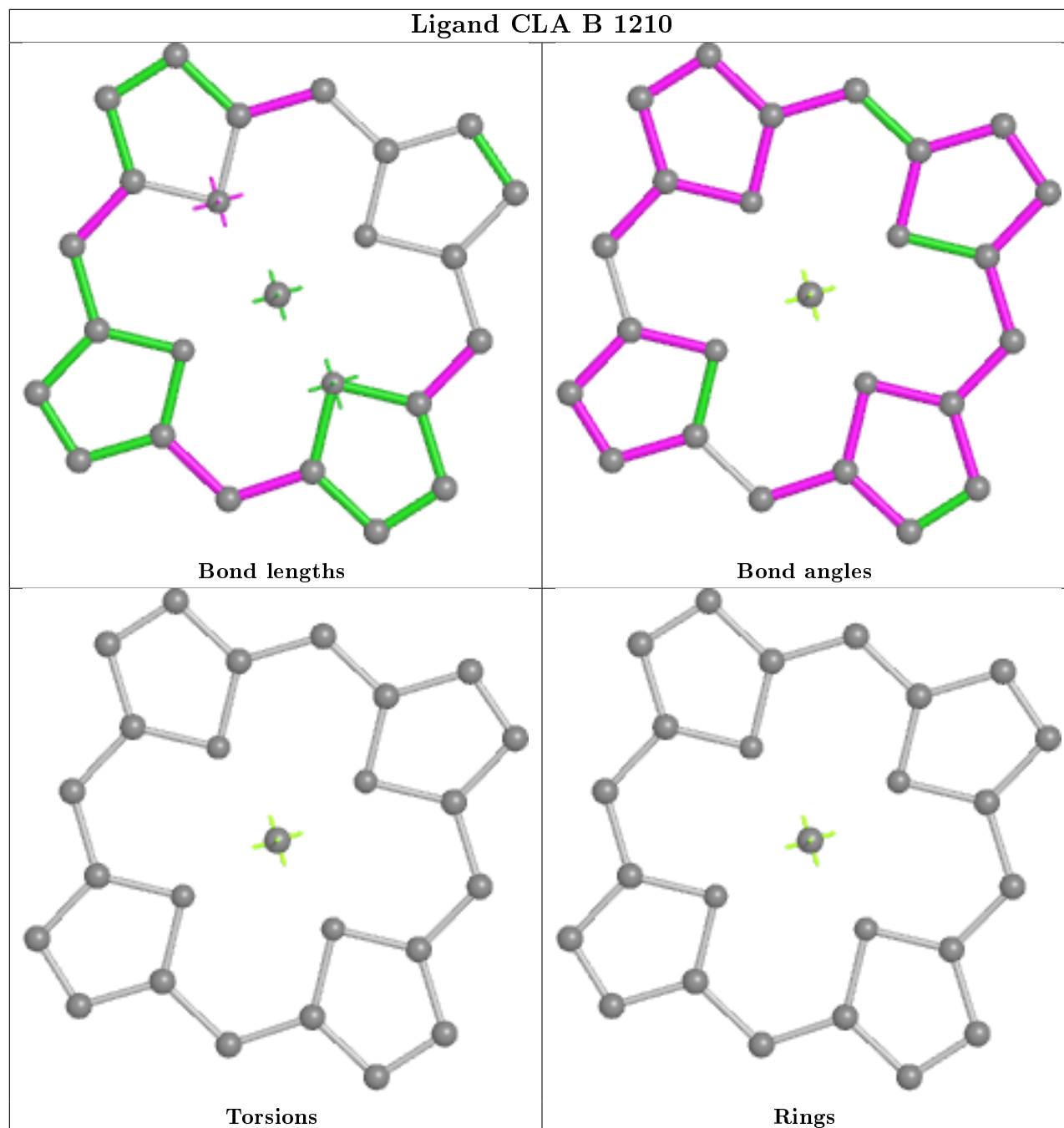
Ligand CLA A 1105



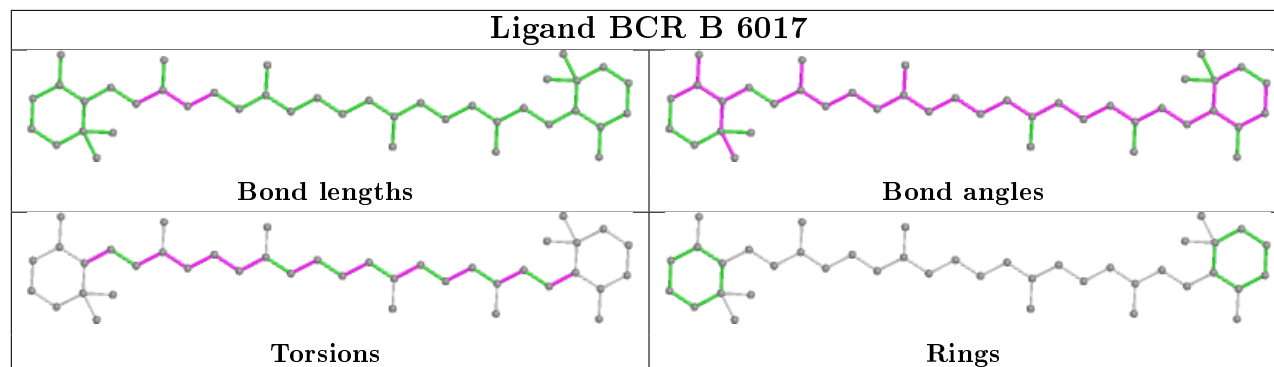
Ligand CLA A 1116



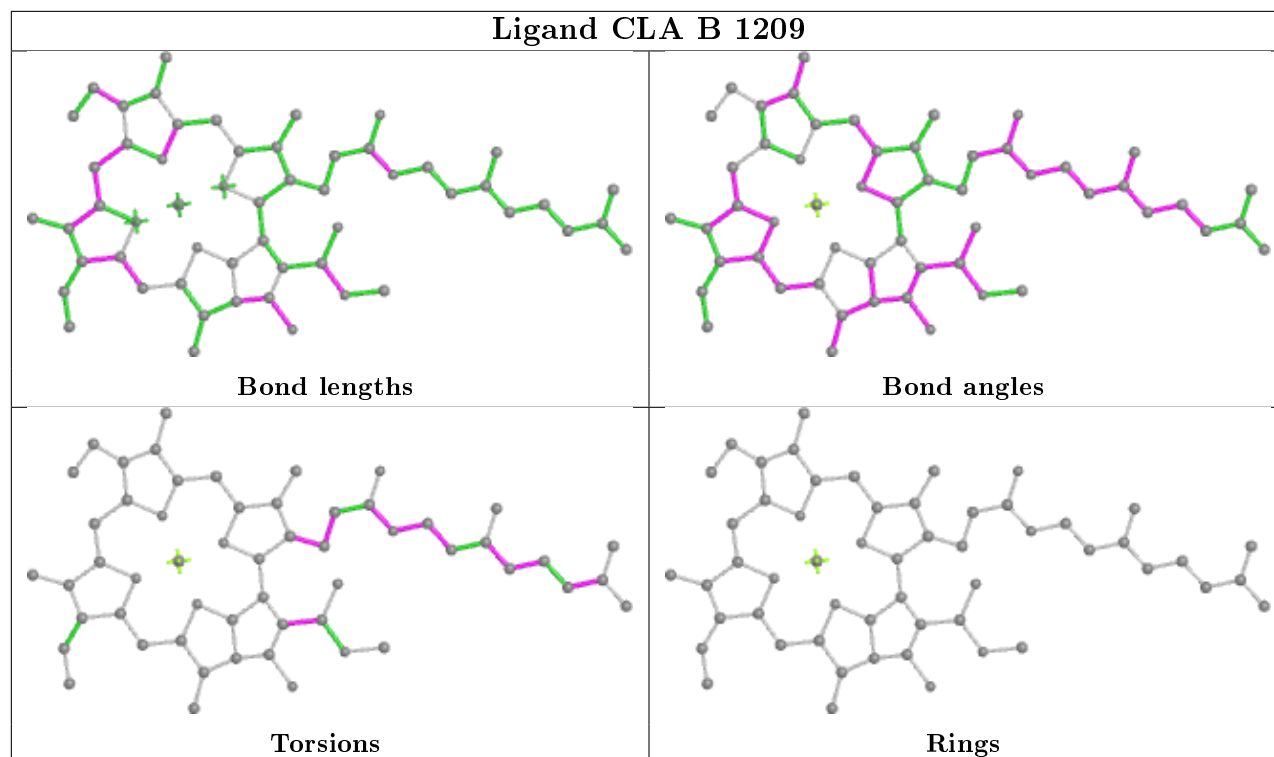
Ligand CLA B 1210



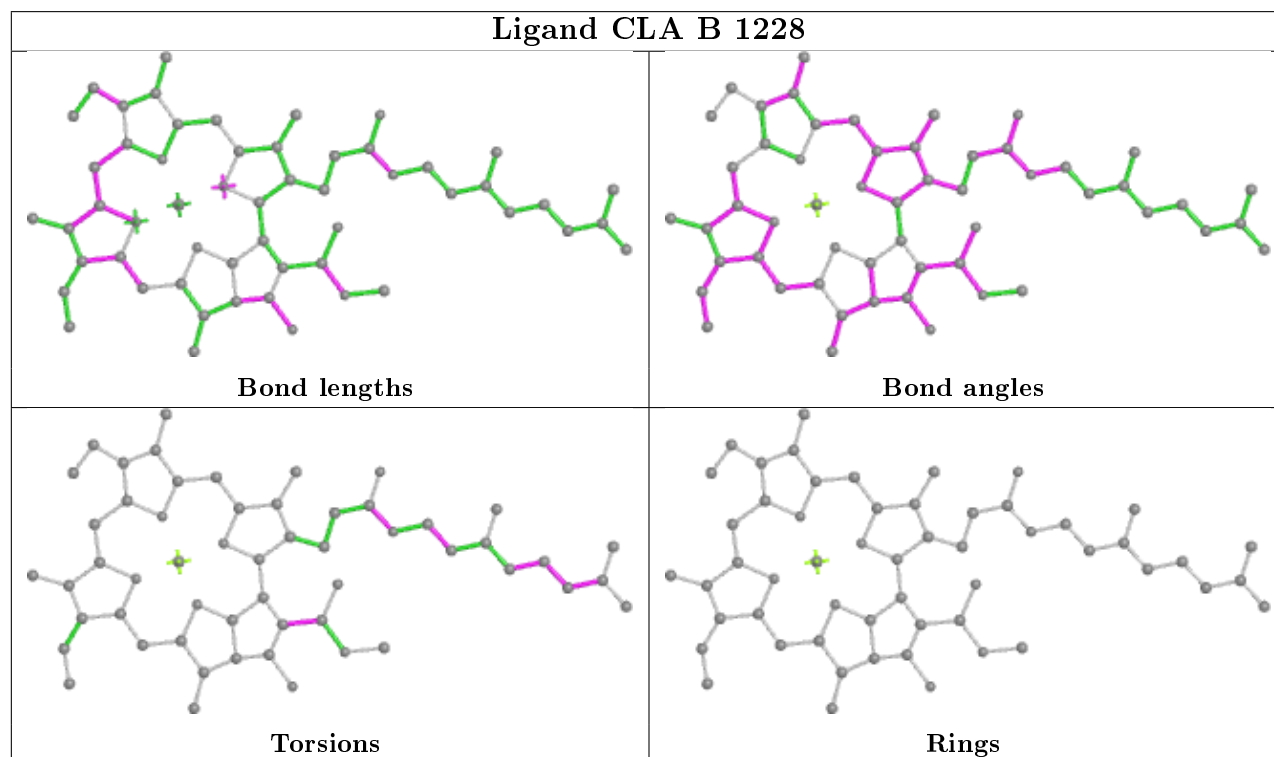
Ligand BCR B 6017

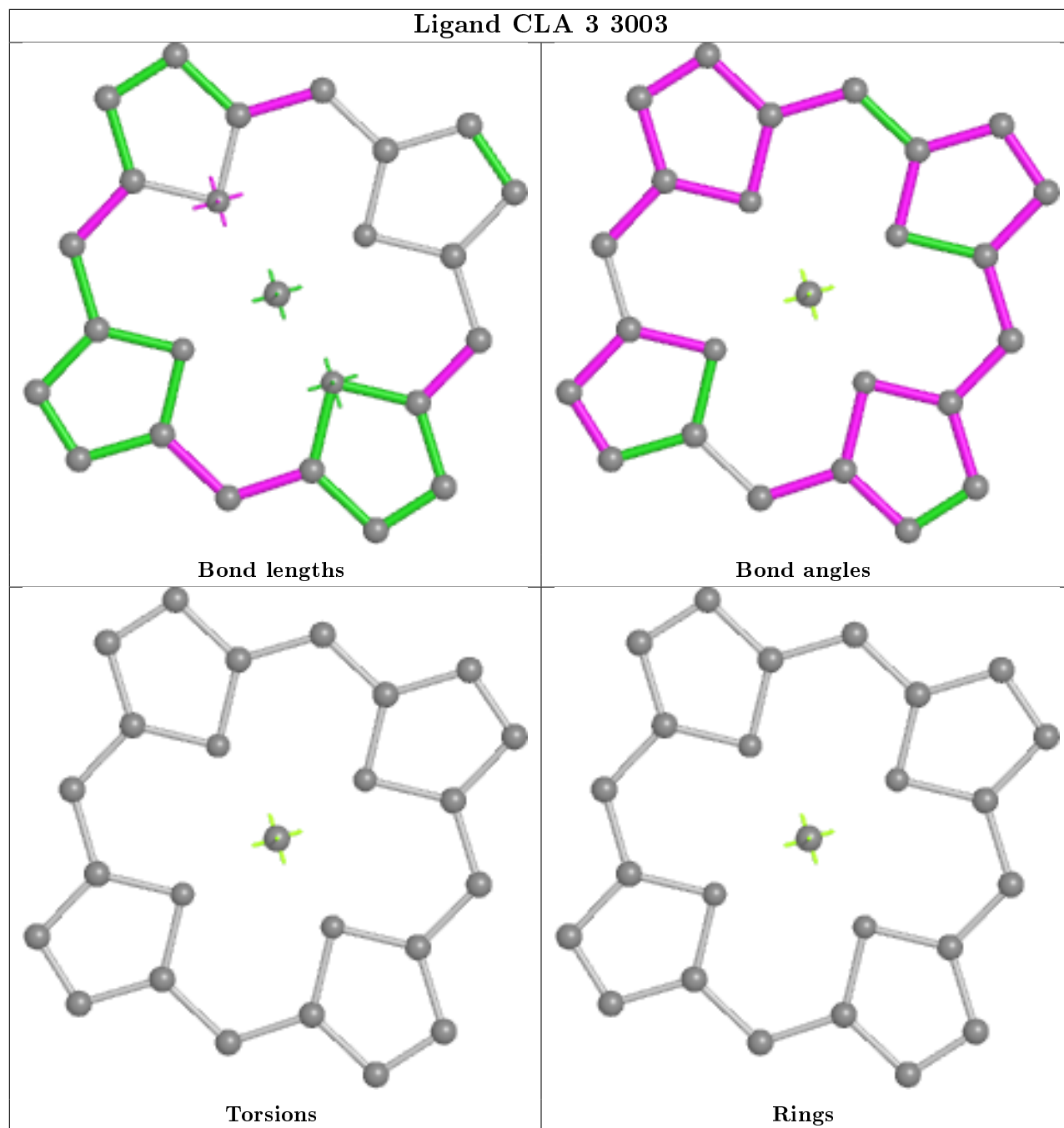


Ligand CLA B 1209

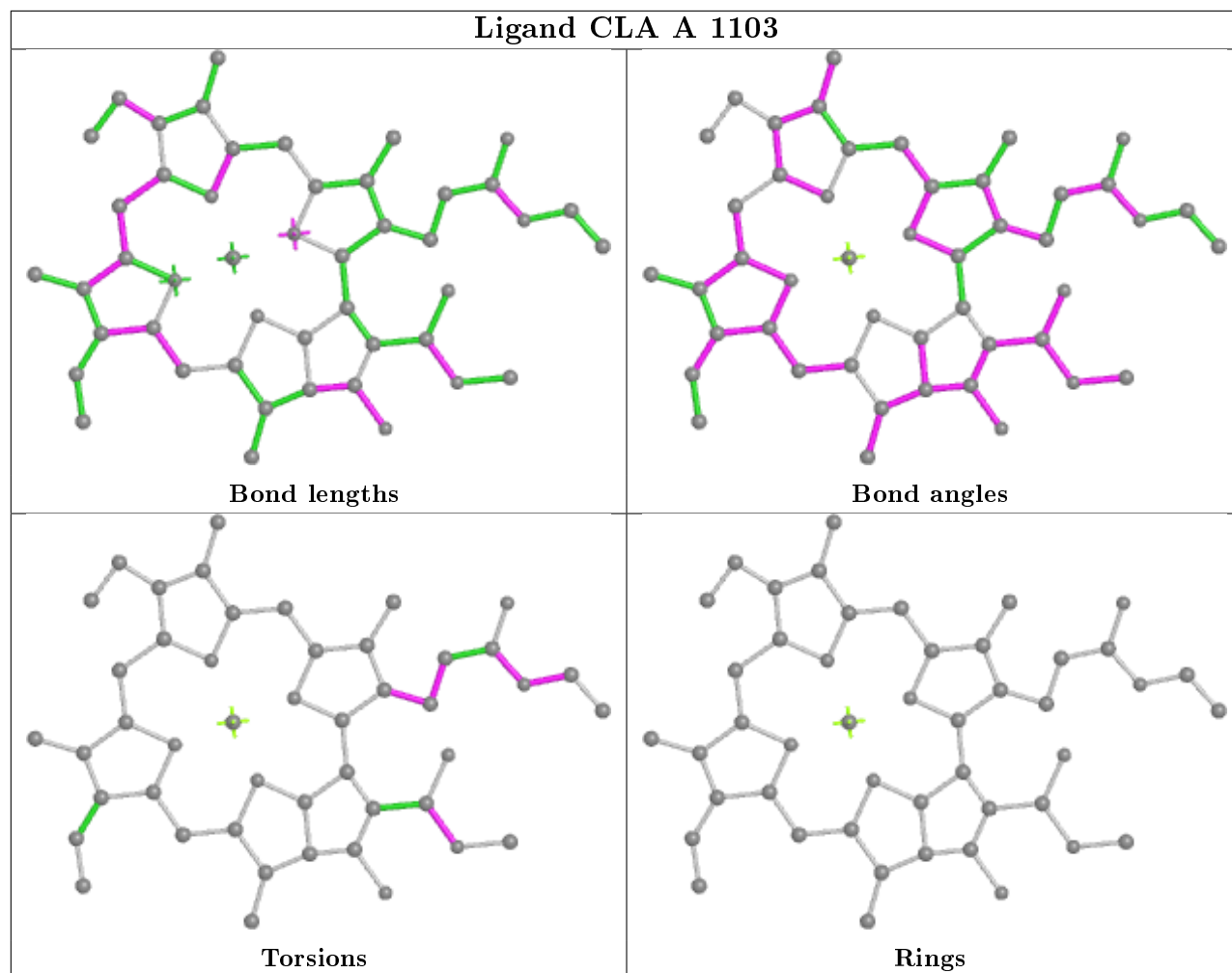


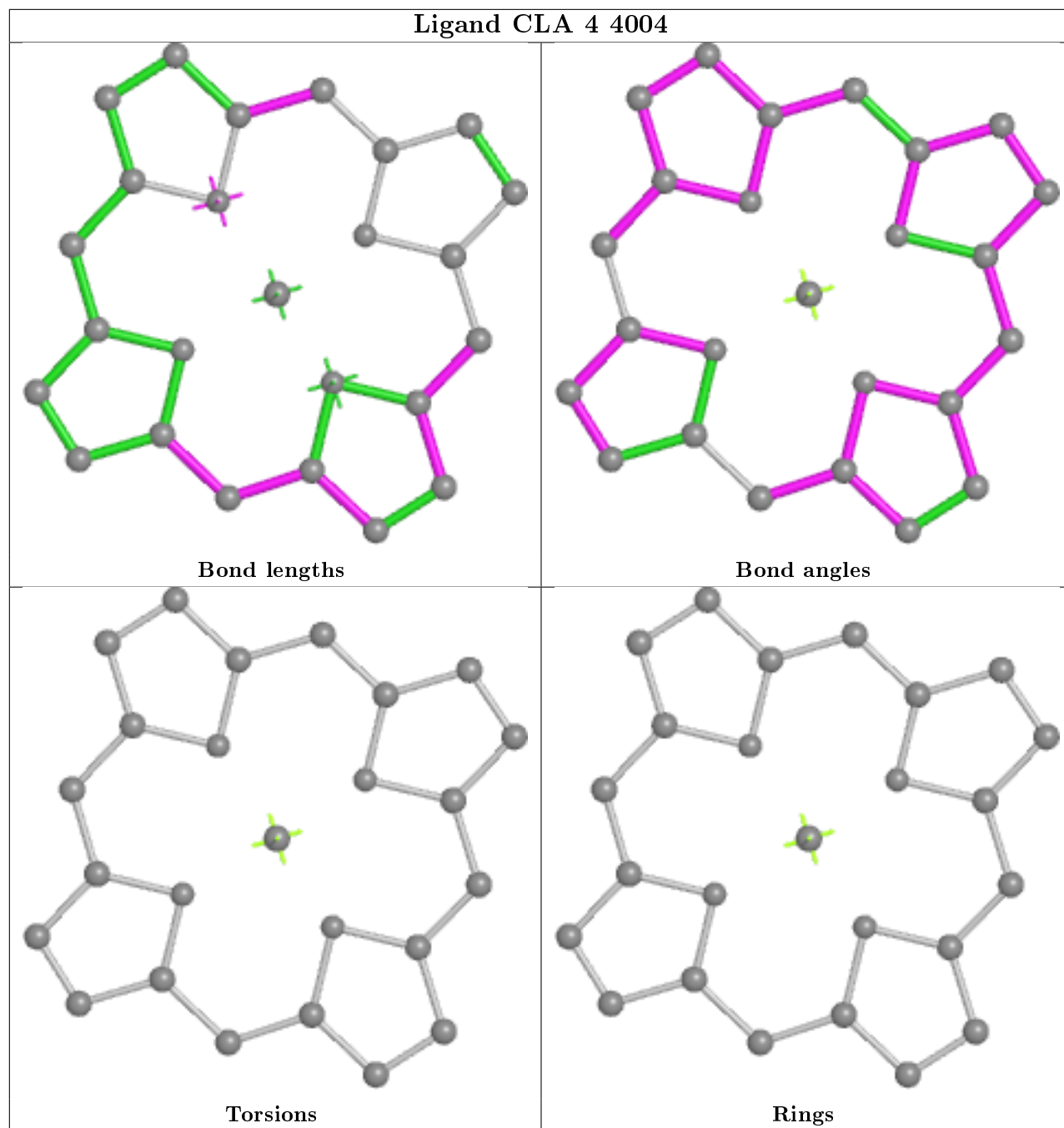
Ligand CLA B 1228

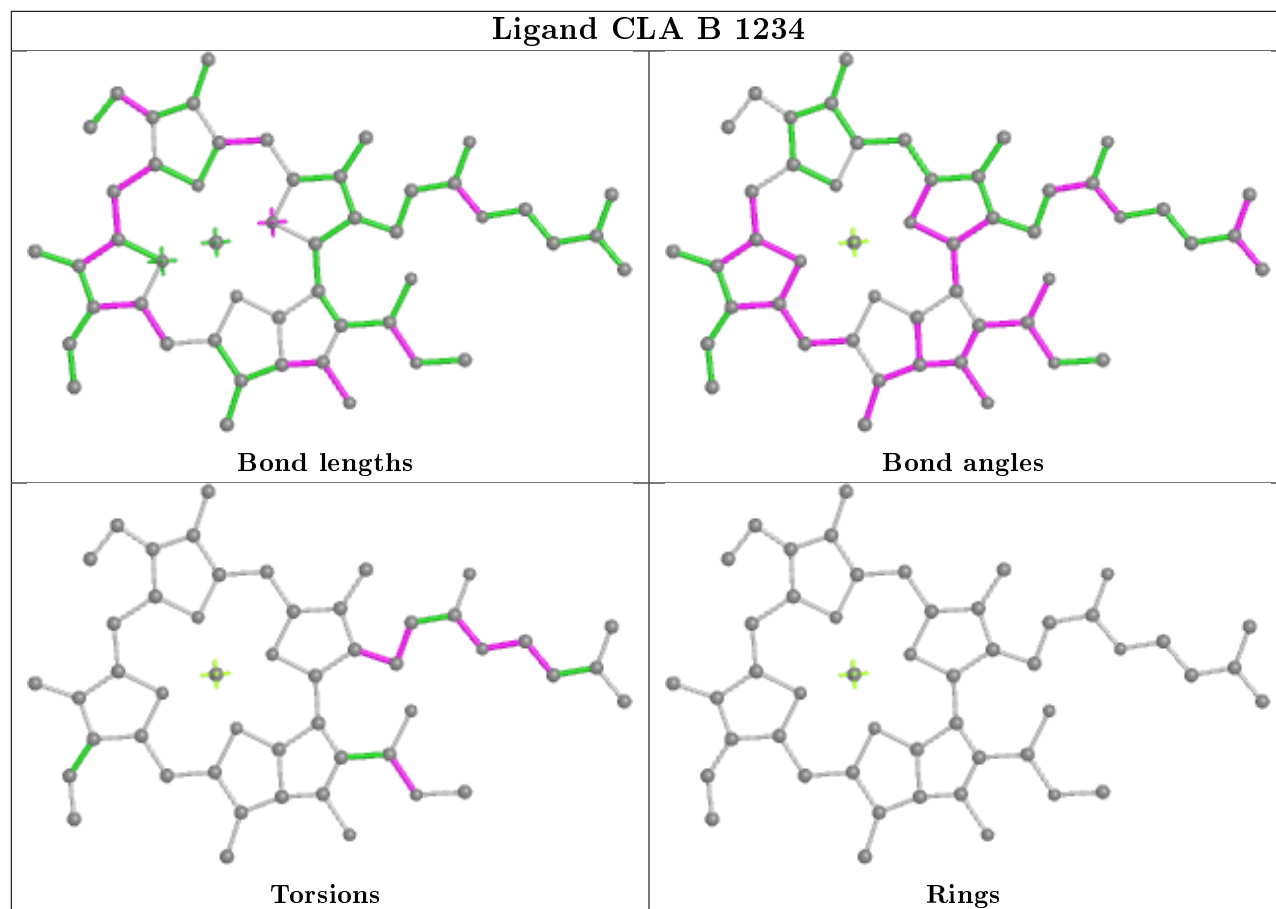


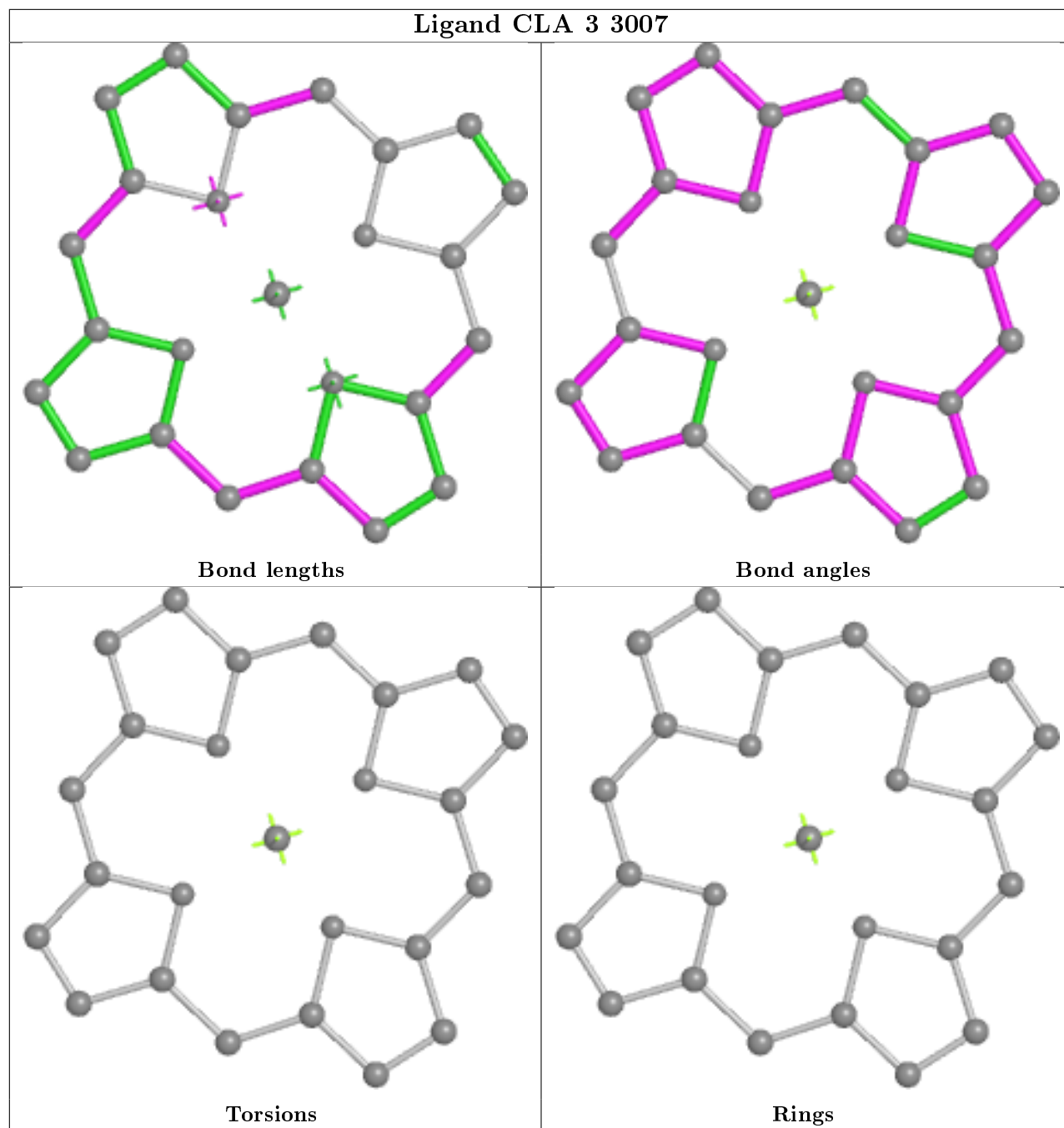


Ligand CLA A 1103

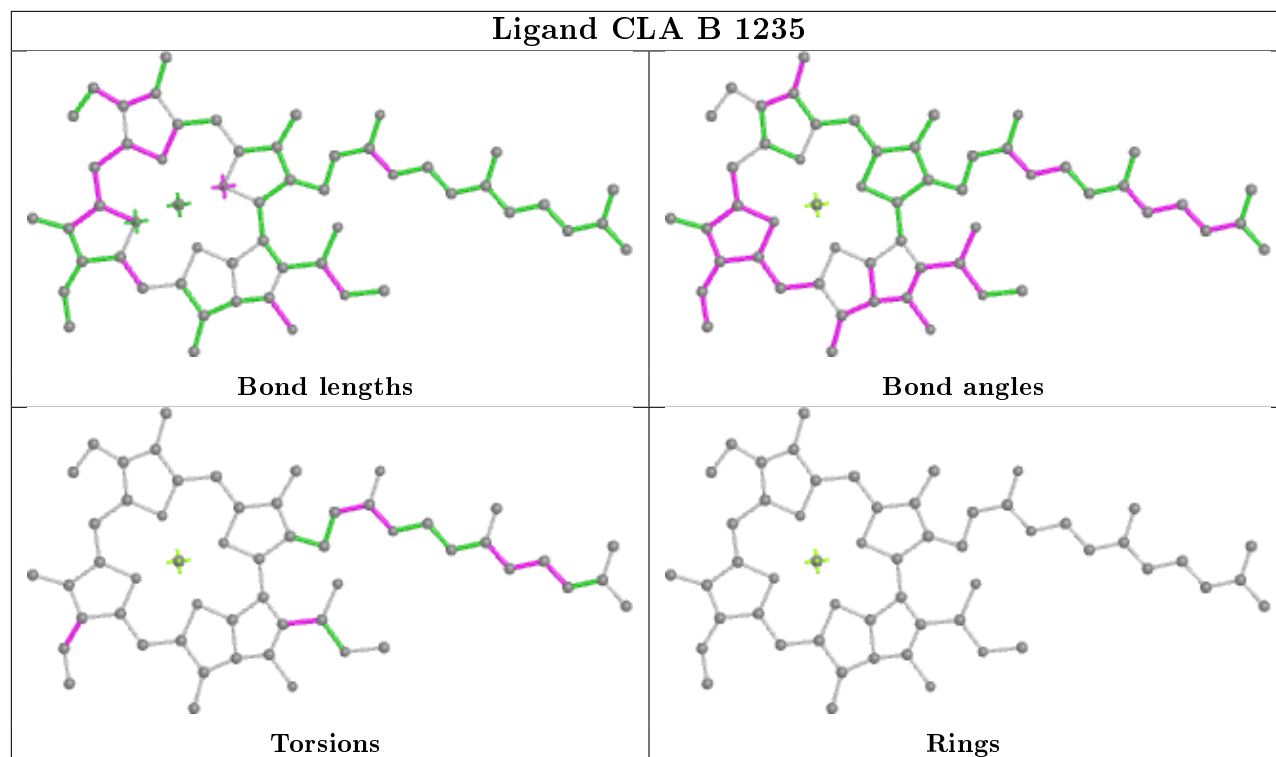




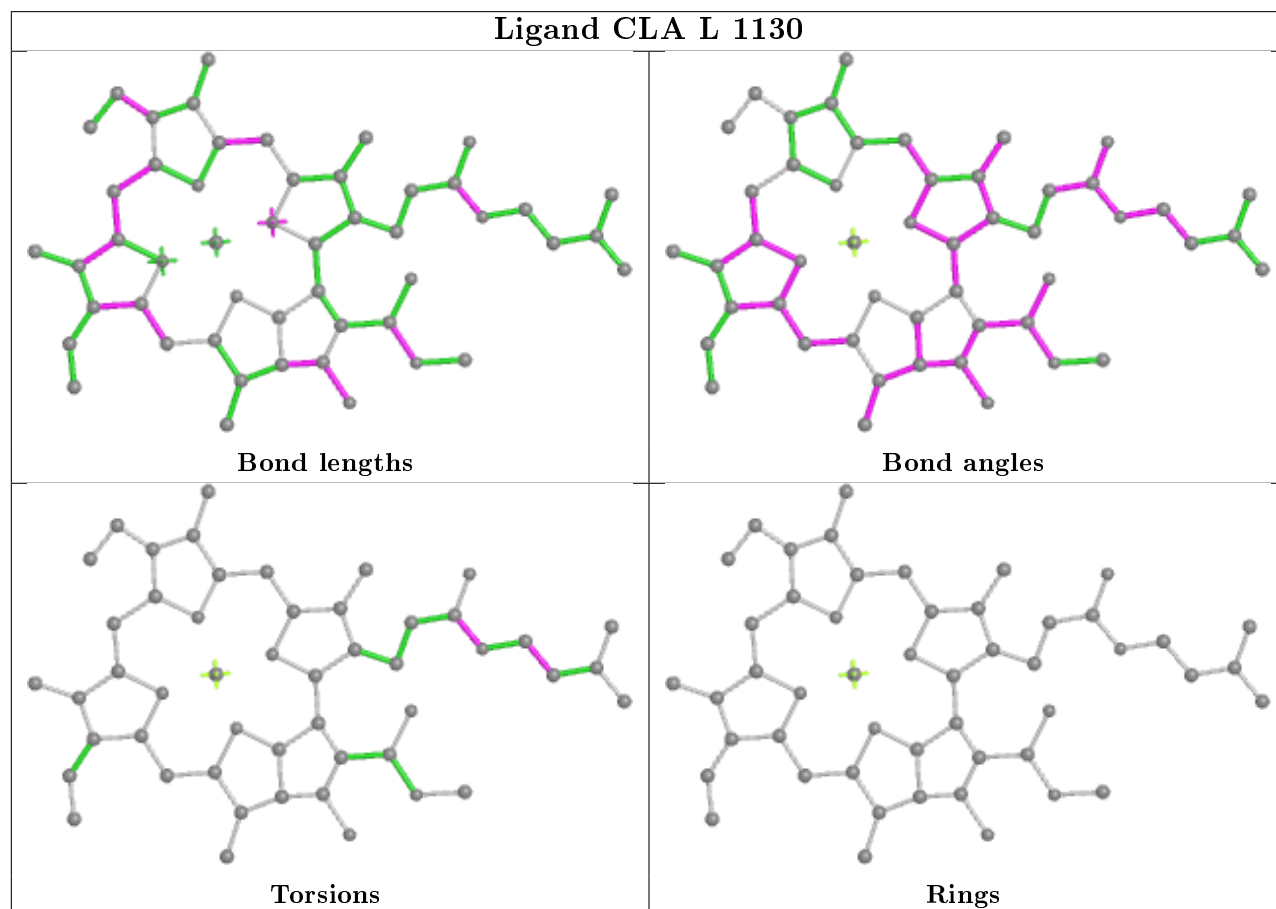


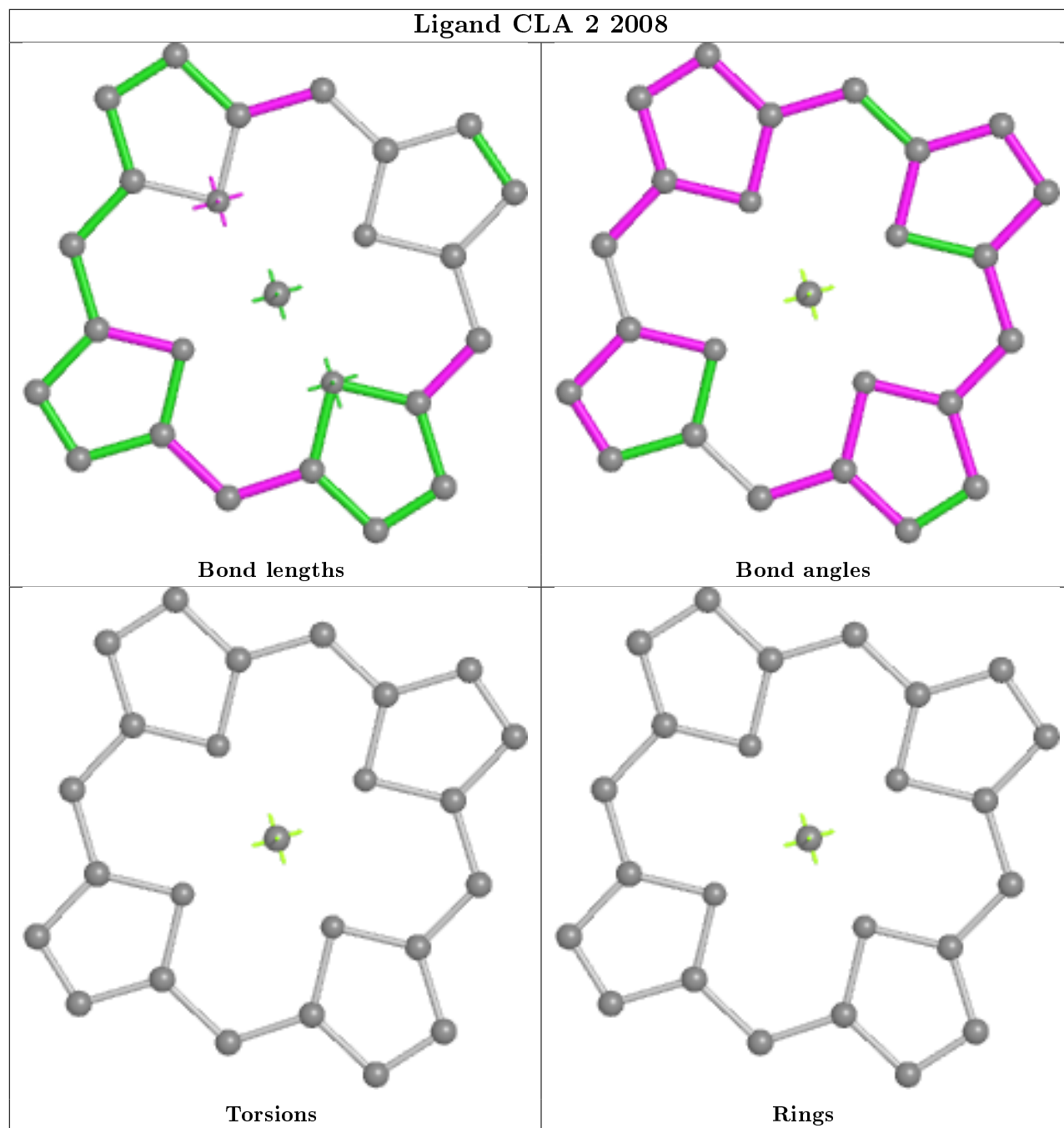


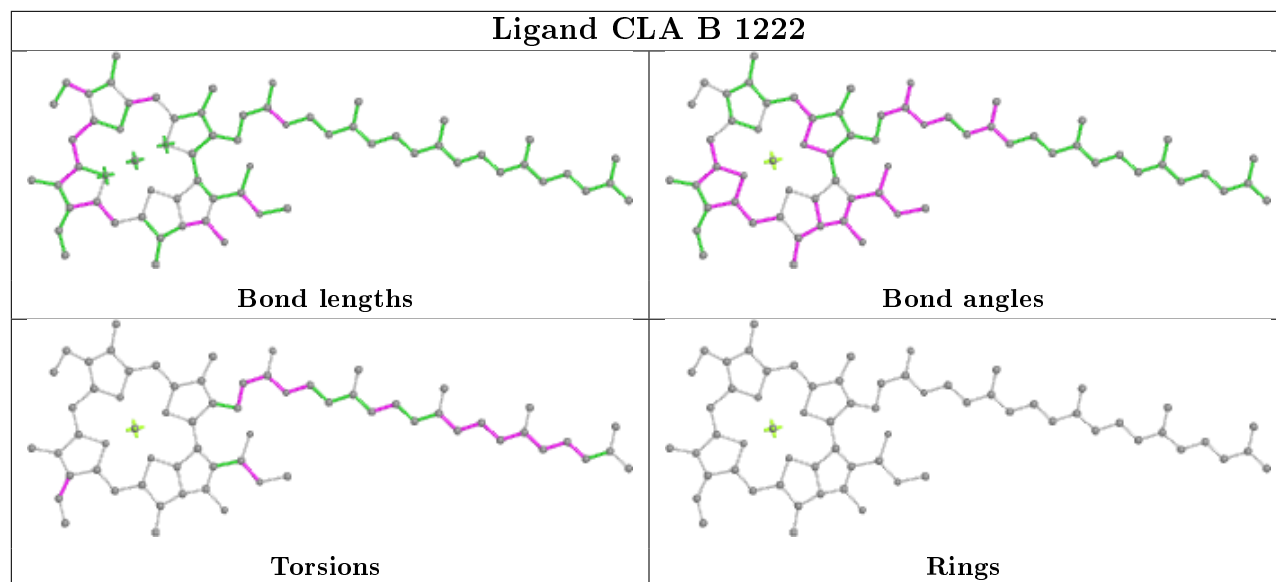
Ligand CLA B 1235



Ligand CLA L 1130







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	728/754 (96%)	0.26	60 (8%) 11 13	12, 39, 59, 72	0
2	B	732/732 (100%)	0.24	40 (5%) 25 25	13, 39, 58, 64	0
3	C	80/80 (100%)	0.42	11 (13%) 2 3	32, 38, 46, 48	0
4	D	138/138 (100%)	0.21	5 (3%) 42 42	25, 45, 53, 55	0
5	E	62/62 (100%)	0.02	1 (1%) 72 70	41, 52, 59, 59	0
6	F	154/154 (100%)	0.25	12 (7%) 13 14	25, 47, 60, 62	0
7	G	95/95 (100%)	0.49	9 (9%) 8 10	50, 61, 68, 73	0
8	H	75/75 (100%)	0.13	1 (1%) 77 76	43, 56, 75, 83	0
9	I	30/30 (100%)	-0.05	1 (3%) 46 45	39, 46, 55, 58	0
10	J	42/42 (100%)	-0.10	0 100 100	28, 55, 65, 67	0
11	K	0/38	-	-	-	-
12	L	164/164 (100%)	0.30	16 (9%) 7 9	24, 49, 62, 69	0
13	N	85/85 (100%)	0.31	6 (7%) 16 18	25, 70, 87, 90	0
14	1	175/187 (93%)	0.22	8 (4%) 32 32	28, 71, 84, 87	0
15	2	166/186 (89%)	0.23	9 (5%) 25 26	25, 71, 86, 91	0
16	3	115/165 (69%)	0.52	14 (12%) 4 5	57, 79, 88, 89	0
17	4	165/165 (100%)	0.37	14 (8%) 10 12	23, 65, 72, 75	0
All	All	3006/3152 (95%)	0.26	207 (6%) 16 18	12, 47, 78, 91	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	10.8
16	3	71	ALA	7.8
1	A	646	SER	7.8
1	A	319	THR	7.6

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Mol	Chain	Res	Type	RSRZ
4	D	75	LEU	7.3
17	4	88	SER	6.4
12	L	116	PRO	6.2
2	B	645	VAL	6.1
14	1	49	TRP	6.1
7	G	87	ALA	6.0
1	A	502	THR	5.8
2	B	267	SER	5.8
2	B	256	THR	5.7
2	B	450	GLU	5.3
15	2	112	ASP	5.3
1	A	325	HIS	5.3
14	1	80	GLY	5.3
7	G	14	LEU	5.2
17	4	132	GLY	5.2
6	F	125	LEU	5.1
17	4	130	GLU	4.9
4	D	60	MET	4.8
3	C	41	SER	4.6
13	N	75	TYR	4.6
1	A	323	ILE	4.6
3	C	40	ALA	4.6
1	A	151	GLN	4.6
17	4	133	TYR	4.5
1	A	487	VAL	4.4
12	L	82	ALA	4.4
12	L	42	ALA	4.4
7	G	36	PRO	4.4
1	A	318	ARG	4.4
12	L	120	LEU	4.3
1	A	653	LEU	4.3
16	3	115	PHE	4.2
2	B	452	GLN	4.2
17	4	85	ALA	4.2
1	A	539	PHE	4.1
1	A	136	VAL	4.1
12	L	45	THR	4.1
2	B	451	LYS	4.1
7	G	37	GLU	4.1
6	F	151	ASP	4.1
6	F	69	PRO	4.1
6	F	70	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	358	TYR	4.0
1	A	101	ALA	4.0
1	A	617	SER	4.0
2	B	137	THR	3.8
2	B	130	ARG	3.8
7	G	90	SER	3.8
1	A	36	LYS	3.8
1	A	200	GLU	3.8
2	B	553	PHE	3.8
16	3	193	LEU	3.7
2	B	118	SER	3.7
1	A	203	LEU	3.7
14	1	32	VAL	3.7
1	A	150	PHE	3.6
1	A	31	PHE	3.6
2	B	610	ASN	3.6
2	B	644	SER	3.6
2	B	302	LYS	3.6
2	B	195	VAL	3.6
15	2	110	TRP	3.5
2	B	234	ALA	3.5
12	L	70	LYS	3.5
17	4	104	ARG	3.4
1	A	249	ILE	3.4
12	L	125	LYS	3.4
1	A	225	VAL	3.4
16	3	192	MET	3.4
16	3	72	GLY	3.4
5	E	48	ASN	3.3
1	A	750	PHE	3.3
2	B	254	ILE	3.3
6	F	42	ILE	3.3
2	B	562	PRO	3.3
3	C	66	ARG	3.3
17	4	131	VAL	3.3
17	4	86	SER	3.3
1	A	570	PRO	3.2
3	C	67	VAL	3.2
2	B	182	LEU	3.2
6	F	126	ALA	3.2
1	A	146	THR	3.2
1	A	74	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	326	ILE	3.2
17	4	116	ASN	3.1
16	3	191	ALA	3.1
1	A	432	LEU	3.1
14	1	79	GLY	3.1
16	3	107	TYR	3.1
1	A	33	GLN	3.0
2	B	136	TYR	3.0
1	A	79	PHE	3.0
1	A	290	LEU	3.0
7	G	40	GLY	3.0
12	L	127	PRO	3.0
16	3	206	GLY	2.9
13	N	50	GLN	2.9
1	A	275	SER	2.9
1	A	161	GLU	2.9
3	C	8	TYR	2.9
1	A	153	TRP	2.9
15	2	61	GLY	2.9
4	D	129	GLY	2.8
2	B	73	ASN	2.8
6	F	72	ILE	2.8
2	B	6	PRO	2.8
1	A	540	LEU	2.8
1	A	242	ILE	2.8
2	B	512	ILE	2.7
2	B	487	ASN	2.7
1	A	191	PRO	2.7
1	A	392	GLN	2.7
13	N	56	LYS	2.7
1	A	224	HIS	2.7
17	4	134	PRO	2.7
1	A	324	GLY	2.7
2	B	687	LEU	2.7
2	B	203	ARG	2.7
1	A	320	ASN	2.7
1	A	650	ASN	2.7
13	N	73	ASP	2.7
1	A	156	SER	2.6
14	1	33	PRO	2.6
7	G	39	ASN	2.6
1	A	296	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	303	TYR	2.5
2	B	132	ASN	2.5
12	L	75	ARG	2.5
1	A	709	TRP	2.5
15	2	167	GLY	2.5
17	4	121	PHE	2.5
14	1	17	SER	2.5
1	A	651	GLY	2.5
6	F	114	PRO	2.5
1	A	127	VAL	2.5
16	3	200	ILE	2.5
15	2	200	GLY	2.5
2	B	578	LEU	2.5
17	4	83	TYR	2.4
16	3	111	ASN	2.4
13	N	74	LYS	2.4
1	A	380	PRO	2.4
6	F	152	ASN	2.4
1	A	34	TRP	2.4
1	A	391	THR	2.4
12	L	112	PRO	2.4
2	B	555	TYR	2.4
1	A	155	ALA	2.4
15	2	113	ILE	2.4
7	G	32	ALA	2.4
3	C	39	ILE	2.4
16	3	74	ILE	2.4
8	H	39	PHE	2.4
14	1	10	ARG	2.4
2	B	233	TYR	2.4
2	B	456	GLU	2.3
1	A	199	VAL	2.3
4	D	27	PRO	2.3
12	L	79	TYR	2.3
2	B	333	GLN	2.3
15	2	195	HIS	2.3
3	C	73	THR	2.3
7	G	50	ARG	2.3
6	F	144	LEU	2.3
15	2	111	ALA	2.3
12	L	78	GLU	2.2
2	B	481	THR	2.2

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Mol	Chain	Res	Type	RSRZ
16	3	121	LEU	2.2
6	F	2	ILE	2.2
15	2	85	GLN	2.2
13	N	24	THR	2.2
1	A	428	TYR	2.2
1	A	143	ILE	2.2
2	B	129	LEU	2.2
16	3	89	THR	2.2
2	B	658	ALA	2.2
16	3	194	ALA	2.2
1	A	614	PHE	2.2
3	C	42	ALA	2.2
12	L	124	LYS	2.2
1	A	698	GLY	2.2
1	A	754	ILE	2.2
17	4	191	HIS	2.2
12	L	81	GLY	2.1
2	B	18	THR	2.1
9	I	2	ILE	2.1
1	A	574	ASN	2.1
14	1	34	ALA	2.1
1	A	187	HIS	2.1
3	C	80	ALA	2.1
4	D	106	SER	2.1
12	L	115	ALA	2.1
1	A	281	LEU	2.1
3	C	62	PHE	2.1
2	B	462	TRP	2.1
3	C	65	VAL	2.0
6	F	128	SER	2.0
1	A	237	VAL	2.0
2	B	117	TYR	2.0
17	4	37	LEU	2.0
12	L	32	LEU	2.0
1	A	122	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	CLA	F	4015	25/65	0.43	0.34	132,133,133,133	0
18	CLA	2	2011	25/65	0.43	0.42	93,94,94,94	0
18	CLA	B	1232	55/65	0.44	0.35	74,91,93,93	0
18	CLA	J	1308	25/65	0.49	0.32	106,107,107,108	0
18	CLA	L	1504	55/65	0.52	0.34	32,67,68,71	0
18	CLA	3	3009	25/65	0.53	0.27	94,94,94,95	0
18	CLA	2	2006	25/65	0.54	0.35	81,82,82,83	0
18	CLA	2	2005	25/65	0.54	0.47	64,65,66,66	0
18	CLA	3	3001	25/65	0.55	0.51	137,137,138,138	0
18	CLA	B	1242	47/65	0.56	0.36	85,91,92,94	0
18	CLA	4	1304	55/65	0.56	0.33	40,77,78,79	0
18	CLA	K	1141	25/65	0.56	0.28	78,79,79,80	0
18	CLA	3	3010	25/65	0.57	0.25	92,93,93,93	0
18	CLA	A	1142	25/65	0.59	0.24	88,89,90,91	0
18	CLA	A	1118	25/65	0.59	0.23	89,90,91,91	0
18	CLA	A	1119	55/65	0.59	0.32	60,66,68,69	0
18	CLA	B	1301	25/65	0.61	0.26	73,74,75,75	0
18	CLA	4	4001	25/65	0.61	0.43	82,83,83,84	0
18	CLA	1	1007	25/65	0.62	0.29	68,68,69,69	0
18	CLA	B	1212	60/65	0.64	0.42	59,73,75,77	0
18	CLA	3	3011	25/65	0.64	0.27	107,107,108,108	0
18	CLA	2	2015	25/65	0.64	0.21	92,93,93,93	0
18	CLA	B	1210	25/65	0.64	0.37	75,76,76,77	0
18	CLA	A	1143	25/65	0.65	0.26	116,118,118,118	0
18	CLA	L	1125	25/65	0.65	0.20	80,80,82,82	0
18	CLA	2	2004	25/65	0.65	0.30	83,84,84,85	0
18	CLA	4	4012	25/65	0.65	0.26	63,65,66,67	0
18	CLA	A	1151	25/65	0.65	0.26	73,76,77,77	0
18	CLA	B	1216	56/65	0.65	0.33	66,72,73,73	0
18	CLA	A	1113	50/65	0.65	0.34	41,60,62,63	0
18	CLA	1	1013	25/65	0.65	0.25	86,87,88,88	0
18	CLA	F	1303	25/65	0.66	0.34	76,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	3	3006	25/65	0.66	0.24	112,113,113,114	0
18	CLA	A	1111	25/65	0.66	0.29	65,66,68,68	0
18	CLA	1	1005	25/65	0.66	0.29	77,78,78,78	0
18	CLA	3	3012	25/65	0.66	0.26	77,79,81,81	0
18	CLA	4	4006	25/65	0.66	0.26	82,83,84,85	0
18	CLA	G	1248	25/65	0.66	0.28	109,110,111,111	0
20	BCR	F	6016	40/40	0.67	0.32	28,33,39,40	0
18	CLA	4	4010	25/65	0.67	0.30	99,99,99,99	0
18	CLA	A	1134	25/65	0.67	0.30	49,51,52,52	0
18	CLA	3	3002	25/65	0.68	0.18	68,70,70,70	0
18	CLA	1	1004	25/65	0.68	0.30	88,89,89,90	0
18	CLA	1	1011	25/65	0.68	0.21	94,95,95,96	0
18	CLA	A	1116	25/65	0.68	0.22	81,82,83,83	0
18	CLA	L	1502	51/65	0.68	0.38	36,63,65,65	0
18	CLA	3	3005	25/65	0.68	0.21	95,96,97,97	0
18	CLA	A	1135	45/65	0.69	0.40	39,54,55,56	0
18	CLA	A	1129	55/65	0.69	0.27	35,58,60,61	0
18	CLA	1	1010	25/65	0.69	0.37	81,81,82,82	0
18	CLA	H	1505	25/65	0.69	0.21	84,85,86,86	0
18	CLA	B	1201	25/65	0.69	0.21	50,51,53,53	0
18	CLA	F	1302	55/65	0.70	0.25	19,75,77,79	0
18	CLA	2	2012	25/65	0.70	0.22	99,100,100,100	0
18	CLA	A	1103	47/65	0.70	0.37	67,77,78,79	0
18	CLA	B	1234	50/65	0.70	0.39	35,53,55,56	0
18	CLA	B	1222	65/65	0.70	0.30	46,69,70,73	0
18	CLA	A	1144	25/65	0.71	0.22	101,101,101,102	0
18	CLA	F	1306	25/65	0.71	0.23	87,88,89,89	0
18	CLA	2	2002	25/65	0.71	0.19	103,103,104,104	0
18	CLA	4	4007	25/65	0.72	0.24	89,91,91,91	0
18	CLA	K	1150	25/65	0.72	0.22	88,90,90,90	0
18	CLA	4	4005	25/65	0.72	0.22	60,62,63,63	0
18	CLA	2	2010	25/65	0.73	0.24	90,90,91,91	0
18	CLA	A	1309	25/65	0.73	0.24	112,112,112,112	0
18	CLA	B	1230	25/65	0.73	0.33	73,75,76,76	0
18	CLA	K	1153	25/65	0.73	0.22	54,55,56,56	0
18	CLA	J	1307	25/65	0.73	0.36	77,78,78,79	0
18	CLA	4	4004	25/65	0.73	0.23	71,72,74,74	0
18	CLA	1	1003	25/65	0.73	0.23	84,85,86,86	0
18	CLA	A	1110	25/65	0.73	0.22	70,71,72,72	0
18	CLA	B	1217	50/65	0.74	0.22	60,66,68,68	0
18	CLA	A	1104	25/65	0.74	0.22	40,42,43,44	0
18	CLA	B	1241	25/65	0.74	0.35	103,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	B	1237	51/65	0.74	0.28	29,59,62,62	0
20	BCR	B	6017	40/40	0.74	0.42	27,33,46,47	0
18	CLA	L	1130	50/65	0.75	0.29	57,66,69,70	0
18	CLA	2	2001	25/65	0.75	0.21	61,63,65,65	0
18	CLA	B	1219	51/65	0.75	0.23	27,47,48,49	0
18	CLA	B	1214	49/65	0.75	0.25	51,69,70,71	0
18	CLA	1	1014	25/65	0.75	0.20	67,68,70,70	0
18	CLA	A	1136	55/65	0.76	0.30	40,45,57,58	0
18	CLA	B	1211	25/65	0.76	0.27	52,54,55,55	0
20	BCR	L	6020	40/40	0.76	0.29	11,24,35,38	0
18	CLA	4	4008	25/65	0.76	0.36	72,74,74,74	0
18	CLA	A	1146	25/65	0.76	0.24	70,72,73,73	0
18	CLA	I	1204	55/65	0.76	0.30	40,44,51,52	0
18	CLA	A	1117	25/65	0.76	0.24	47,48,49,49	0
18	CLA	B	1213	25/65	0.76	0.23	79,81,82,82	0
18	CLA	H	1501	55/65	0.77	0.27	49,68,70,73	0
18	CLA	4	4009	25/65	0.77	0.21	80,81,82,82	0
18	CLA	B	1209	55/65	0.77	0.24	32,50,53,54	0
18	CLA	A	1140	55/65	0.77	0.32	12,39,41,43	0
20	BCR	A	6011	40/40	0.78	0.36	9,12,19,21	0
19	PQN	A	5001	33/33	0.78	0.26	15,23,34,36	0
18	CLA	2	2003	25/65	0.78	0.19	114,114,115,115	0
18	CLA	3	3003	25/65	0.78	0.18	67,68,70,70	0
18	CLA	A	1102	25/65	0.78	0.21	72,73,75,75	0
18	CLA	3	3004	25/65	0.78	0.25	76,77,78,78	0
18	CLA	B	1223	25/65	0.78	0.25	46,48,49,50	0
18	CLA	A	1115	47/65	0.78	0.28	40,44,48,50	0
18	CLA	A	1108	50/65	0.78	0.20	52,74,76,76	0
18	CLA	B	1224	51/65	0.79	0.32	47,55,56,57	0
18	CLA	2	2013	25/65	0.79	0.20	81,82,84,84	0
18	CLA	J	2107	61/65	0.79	0.24	40,62,63,63	0
18	CLA	B	1236	46/65	0.79	0.25	34,44,46,47	0
18	CLA	4	4002	25/65	0.79	0.20	65,66,67,67	0
18	CLA	1	1012	25/65	0.79	0.23	76,77,77,77	0
18	CLA	B	1220	60/65	0.79	0.25	31,39,50,53	0
18	CLA	3	3015	25/65	0.79	0.16	72,73,74,75	0
18	CLA	B	1229	49/65	0.79	0.23	35,48,50,51	0
19	PQN	B	5002	33/33	0.79	0.42	8,18,21,21	0
18	CLA	3	3013	25/65	0.79	0.26	77,78,78,78	0
18	CLA	B	1202	50/65	0.79	0.30	23,37,39,42	0
18	CLA	4	4003	25/65	0.80	0.24	80,81,81,81	0
18	CLA	B	9012	55/65	0.80	0.30	16,47,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	4	4011	25/65	0.80	0.25	51,52,53,54	0
18	CLA	A	9011	55/65	0.80	0.27	2,26,28,29	0
18	CLA	B	1205	55/65	0.80	0.24	17,41,43,46	0
18	CLA	1	1001	25/65	0.80	0.21	63,64,65,66	0
18	CLA	B	1228	55/65	0.80	0.24	42,46,47,49	0
18	CLA	A	1147	25/65	0.80	0.25	66,67,68,69	0
18	CLA	A	1123	55/65	0.80	0.25	37,46,49,50	0
18	CLA	B	1218	51/65	0.80	0.21	20,47,50,51	0
18	CLA	1	1006	25/65	0.80	0.18	60,62,63,63	0
18	CLA	B	1235	55/65	0.80	0.25	31,40,42,44	0
18	CLA	B	1231	46/65	0.80	0.31	36,46,49,51	0
18	CLA	B	1239	55/65	0.80	0.23	27,52,53,55	0
18	CLA	B	1221	48/65	0.81	0.32	20,31,38,42	0
18	CLA	A	1105	25/65	0.81	0.21	83,83,84,84	0
18	CLA	3	3008	25/65	0.81	0.23	90,90,91,91	0
18	CLA	L	1503	46/65	0.81	0.22	19,22,25,28	0
18	CLA	A	1122	55/65	0.81	0.25	18,39,41,43	0
18	CLA	B	1225	45/65	0.81	0.22	34,50,52,52	0
18	CLA	A	1131	44/65	0.81	0.25	35,39,42,44	0
18	CLA	1	1008	25/65	0.82	0.16	79,79,79,80	0
18	CLA	B	1226	25/65	0.82	0.20	50,53,54,54	0
18	CLA	B	1206	25/65	0.82	0.40	50,54,55,56	0
20	BCR	I	6018	40/40	0.82	0.25	6,19,26,28	0
18	CLA	A	9013	46/65	0.82	0.35	11,17,21,24	0
18	CLA	G	1233	51/65	0.82	0.16	61,66,67,67	0
18	CLA	A	1120	25/65	0.82	0.23	76,78,79,80	0
18	CLA	1	1002	25/65	0.82	0.17	86,86,87,88	0
18	CLA	A	1124	25/65	0.82	0.17	48,51,52,53	0
18	CLA	4	4013	25/65	0.82	0.17	86,86,87,87	0
18	CLA	F	1139	44/65	0.82	0.24	36,40,42,43	0
18	CLA	A	1101	25/65	0.82	0.23	61,63,64,64	0
18	CLA	A	1126	55/65	0.82	0.22	15,40,42,44	0
18	CLA	4	1009	25/65	0.83	0.19	78,79,79,79	0
18	CLA	F	1305	25/65	0.83	0.19	78,79,79,79	0
18	CLA	B	1238	54/65	0.83	0.26	13,27,32,33	0
18	CLA	B	1138	56/65	0.83	0.23	18,47,50,53	0
18	CLA	A	1137	55/65	0.83	0.23	20,28,30,32	0
18	CLA	3	2009	25/65	0.83	0.22	94,94,95,95	0
18	CLA	A	1127	25/65	0.83	0.22	58,59,60,60	0
18	CLA	A	1132	25/65	0.83	0.20	27,29,31,32	0
18	CLA	B	1208	55/65	0.83	0.21	36,39,41,42	0
18	CLA	B	9010	47/65	0.83	0.31	23,37,40,41	0

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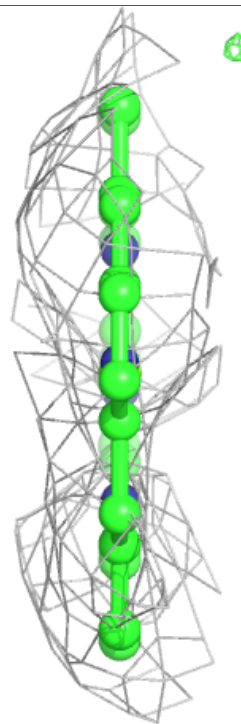
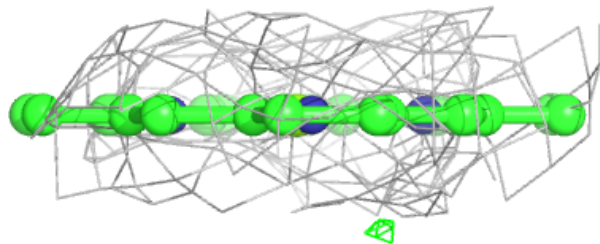
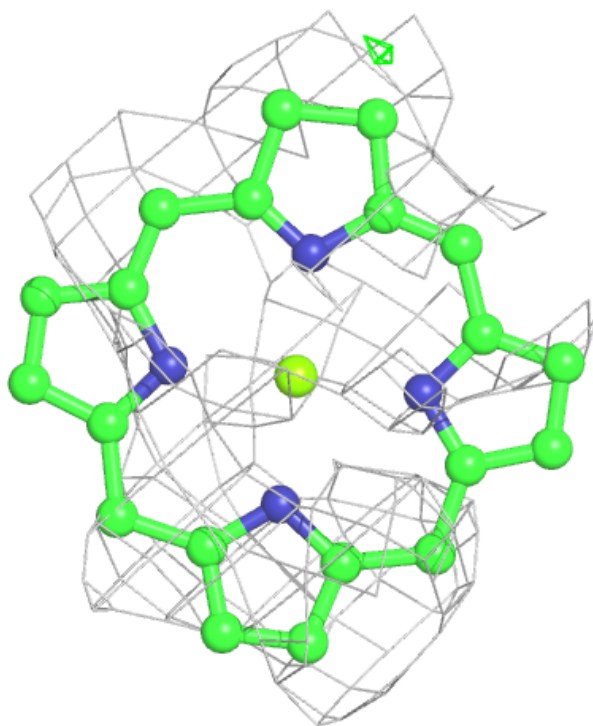
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	A	1133	25/65	0.84	0.22	44,46,47,48	0
18	CLA	A	1109	24/65	0.84	0.20	48,49,50,51	0
18	CLA	3	3007	25/65	0.84	0.23	80,81,82,83	0
18	CLA	2	2008	25/65	0.85	0.19	60,61,62,63	0
18	CLA	B	1207	55/65	0.85	0.24	19,30,35,37	0
18	CLA	A	1148	25/65	0.86	0.26	93,94,95,95	0
18	CLA	B	1203	48/65	0.86	0.18	2,23,24,26	0
18	CLA	A	1152	25/65	0.86	0.19	68,69,70,71	0
18	CLA	B	9023	47/65	0.87	0.21	36,40,41,43	0
18	CLA	A	1107	57/65	0.87	0.19	21,26,30,33	0
18	CLA	B	1227	50/65	0.87	0.22	34,41,44,45	0
18	CLA	B	9022	54/65	0.87	0.27	28,31,41,41	0
18	CLA	A	1106	41/65	0.87	0.23	16,20,22,24	0
18	CLA	A	1128	55/65	0.87	0.19	20,37,39,40	0
18	CLA	B	1215	52/65	0.88	0.20	11,16,27,30	0
18	CLA	F	1240	25/65	0.88	0.18	43,44,45,46	0
18	CLA	2	2007	25/65	0.88	0.27	79,80,81,81	0
21	SF4	C	3102	8/8	0.92	0.15	19,21,24,26	0
21	SF4	C	3103	8/8	0.96	0.09	10,12,15,15	0
21	SF4	B	3101	8/8	0.97	0.12	14,21,22,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

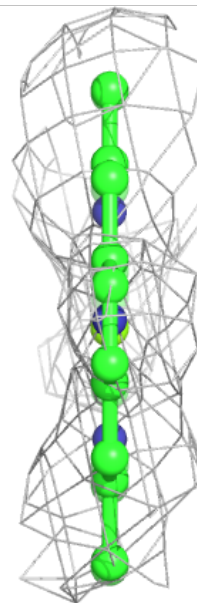
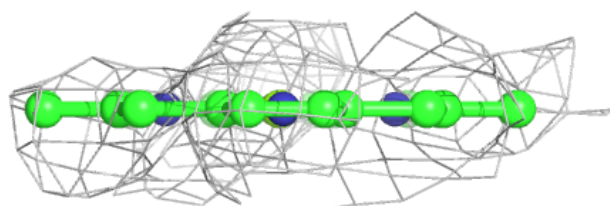
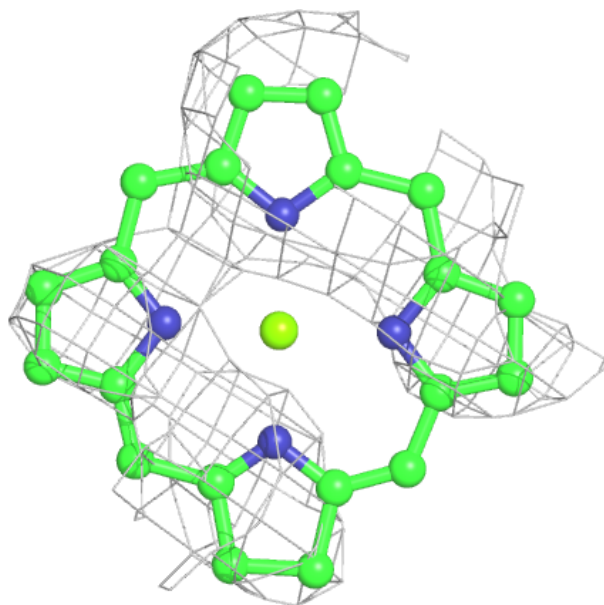
Electron density around CLA F 4015:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



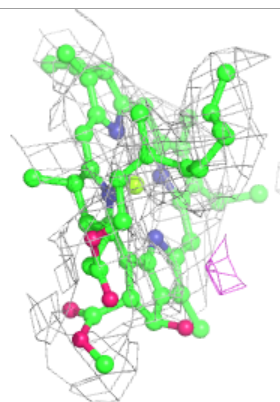
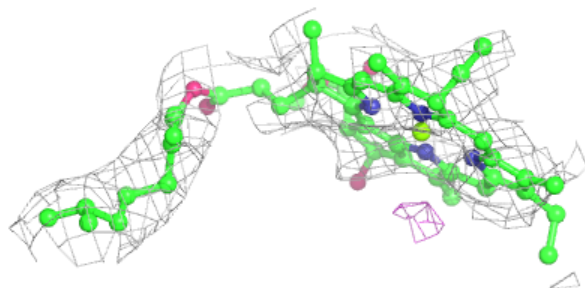
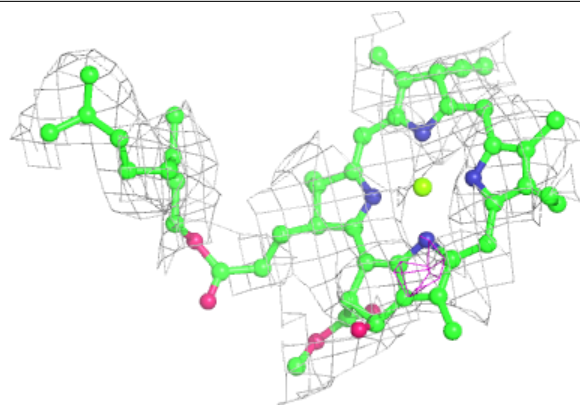
Electron density around CLA 2 2011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



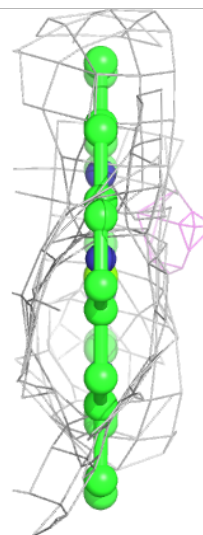
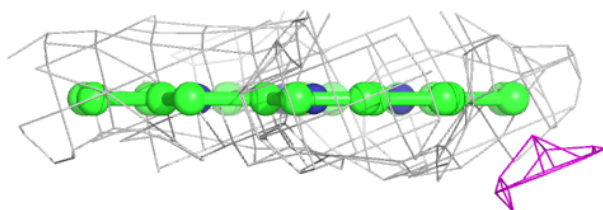
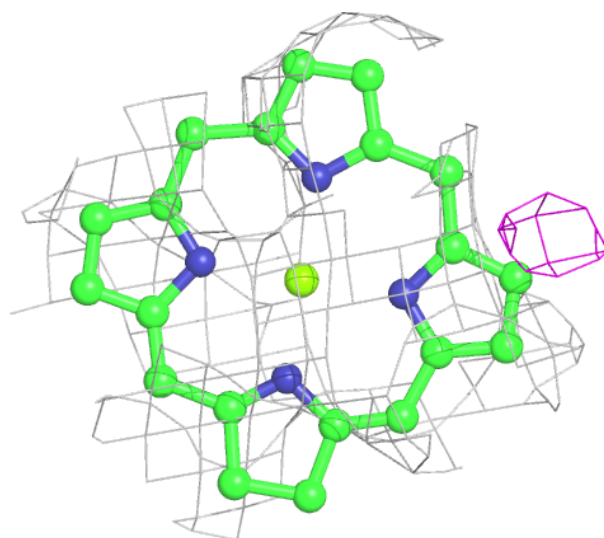
Electron density around CLA B 1232:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



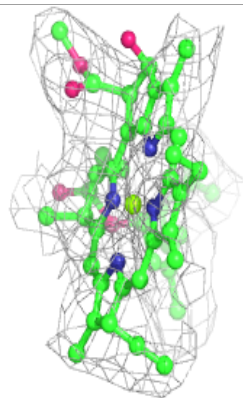
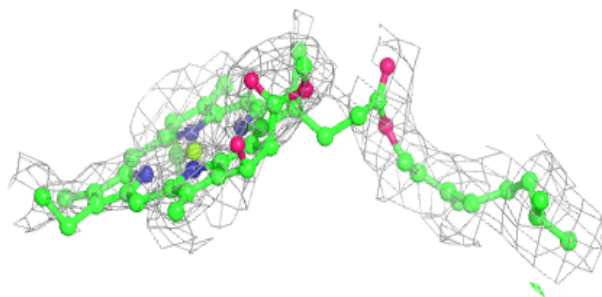
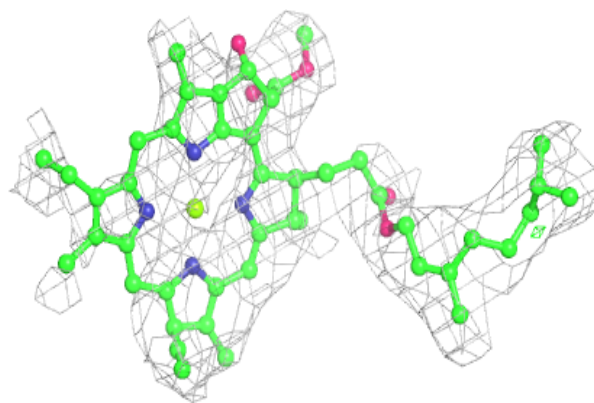
Electron density around CLA J 1308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



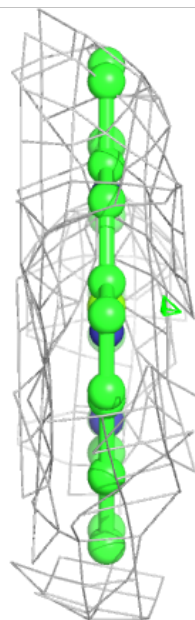
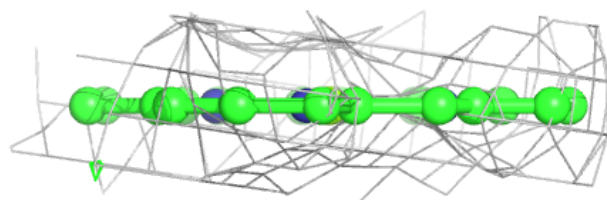
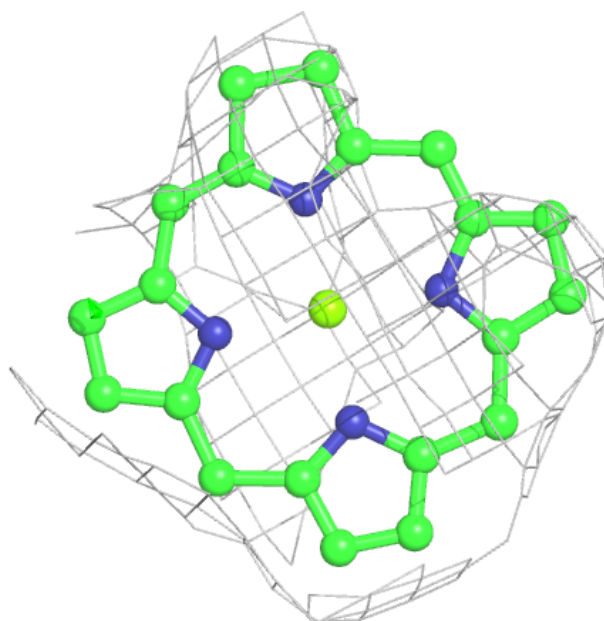
Electron density around CLA L 1504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



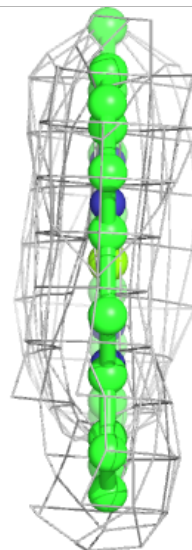
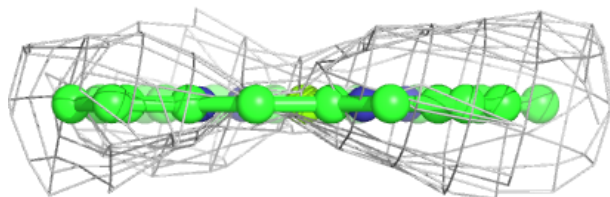
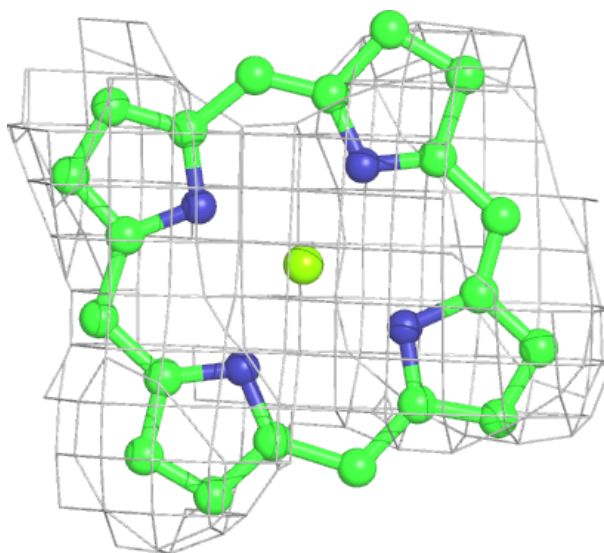
Electron density around CLA 3 3009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



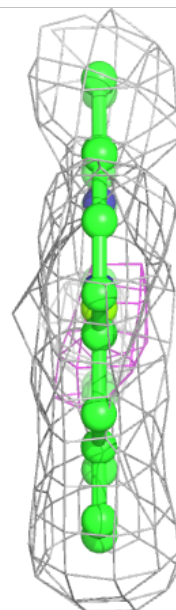
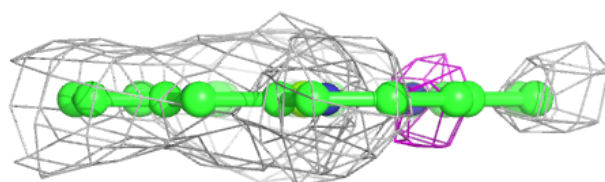
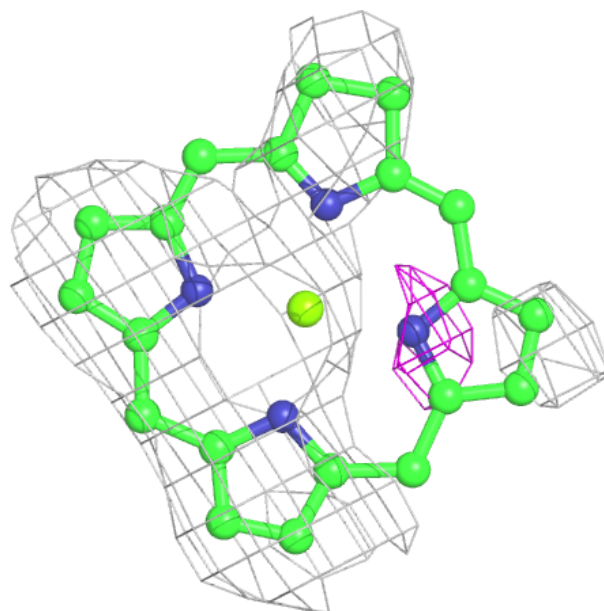
Electron density around CLA 2 2006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



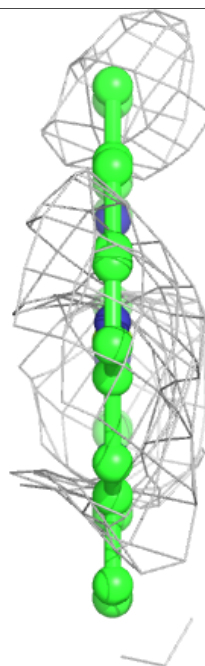
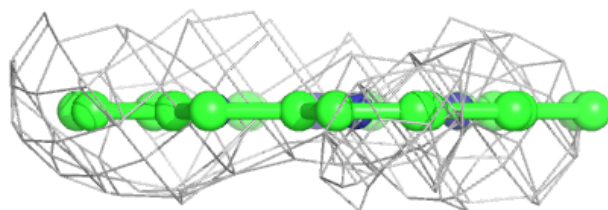
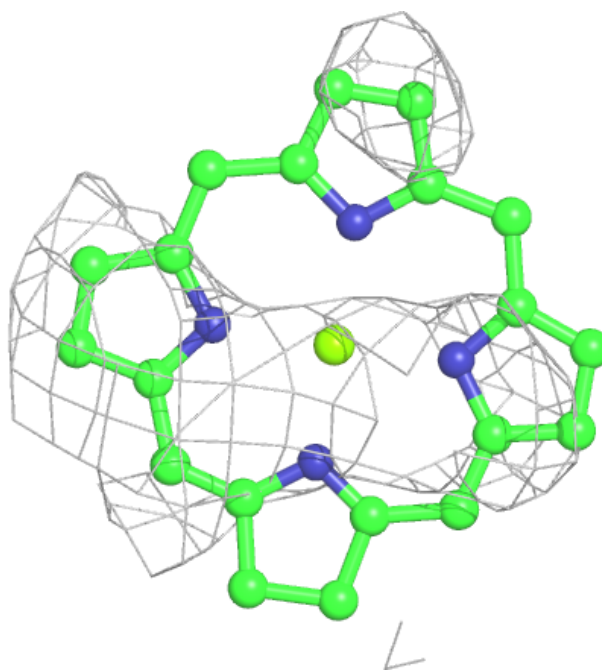
Electron density around CLA 2 2005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



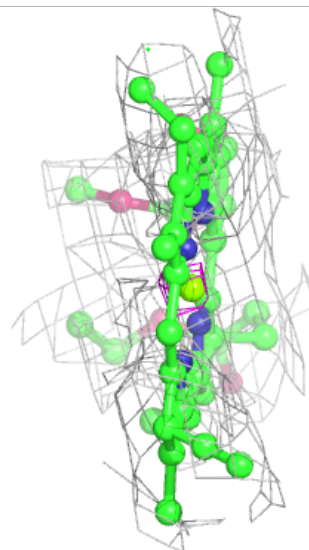
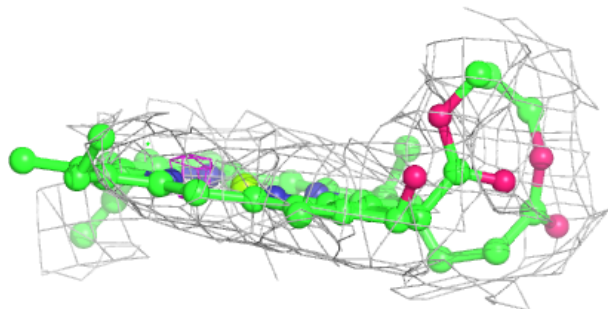
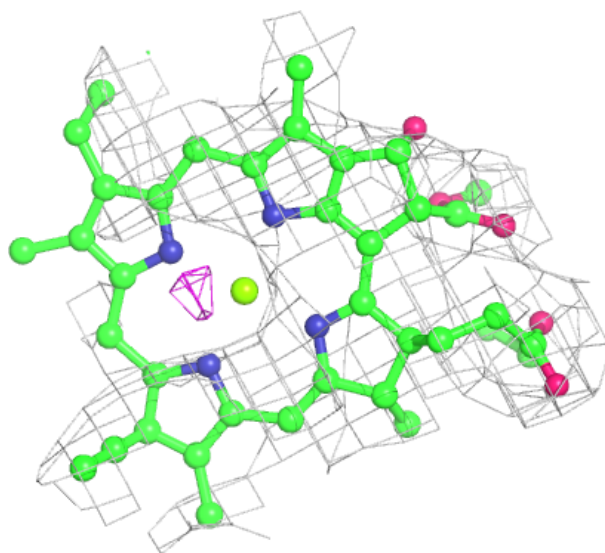
Electron density around CLA 3 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



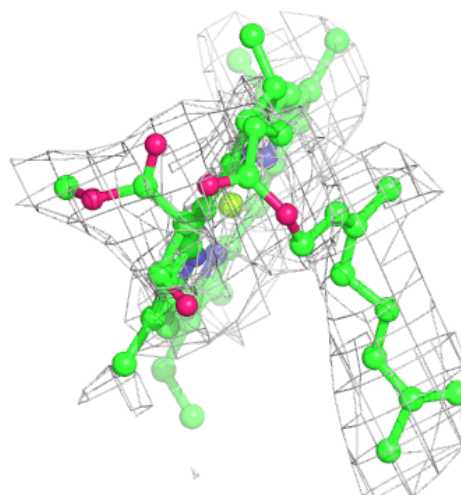
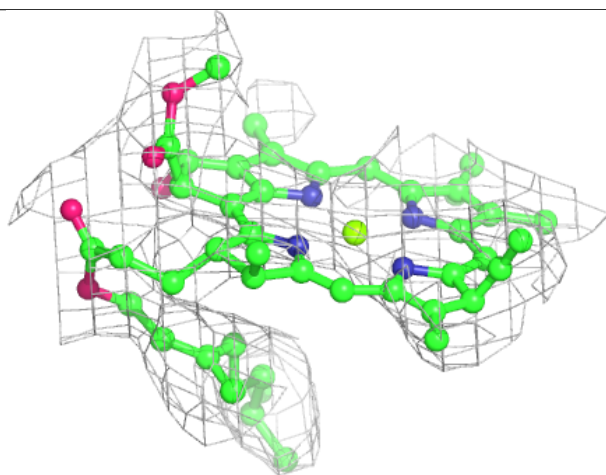
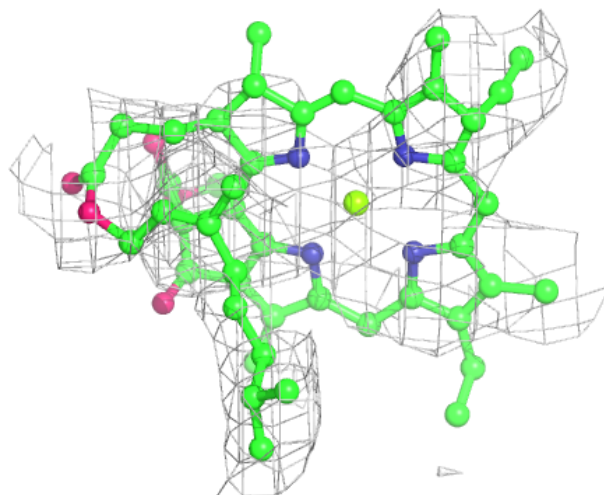
Electron density around CLA B 1242:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



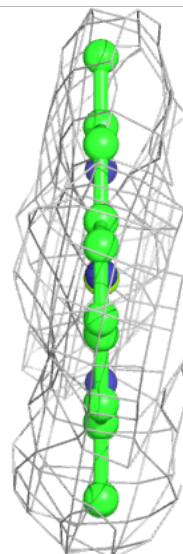
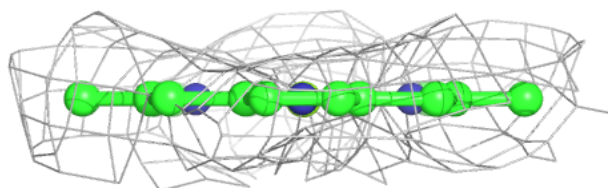
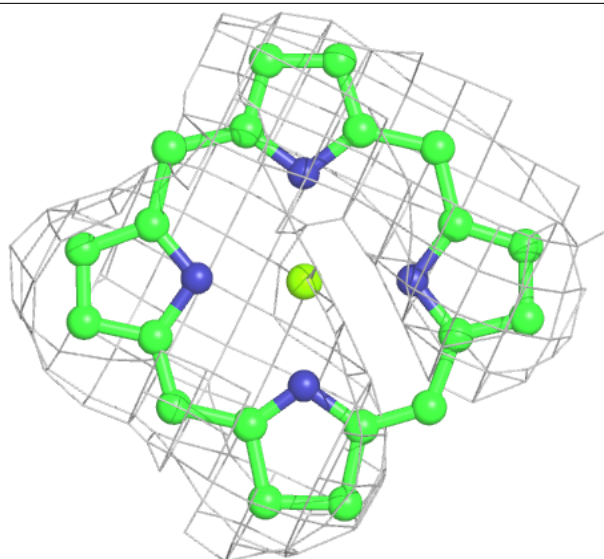
Electron density around CLA 4 1304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



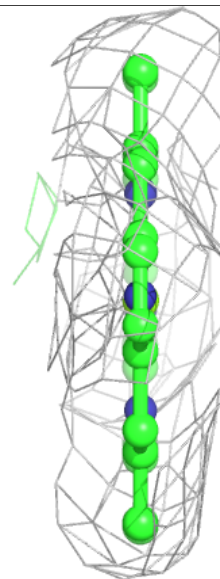
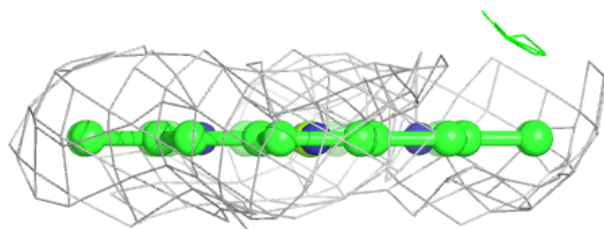
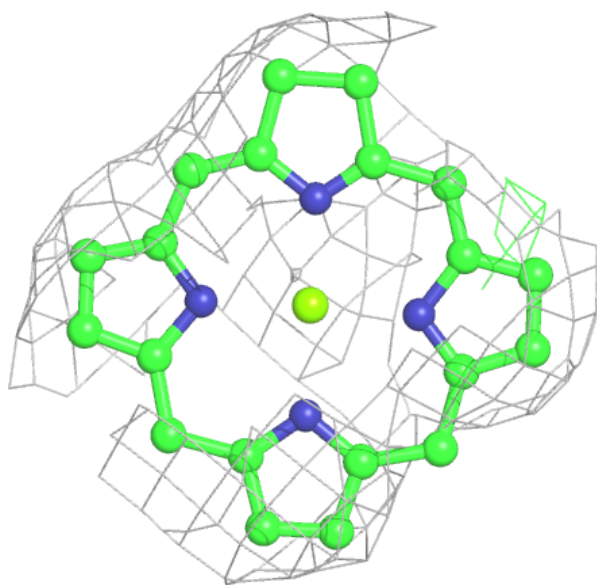
Electron density around CLA K 1141:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



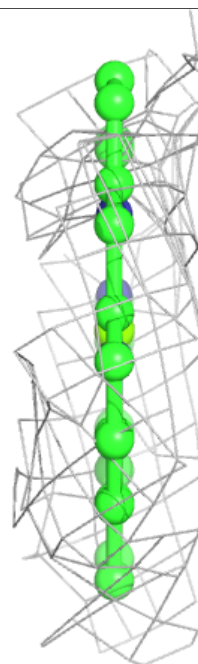
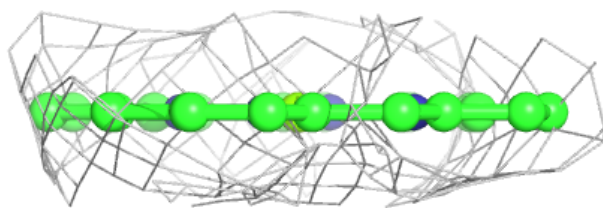
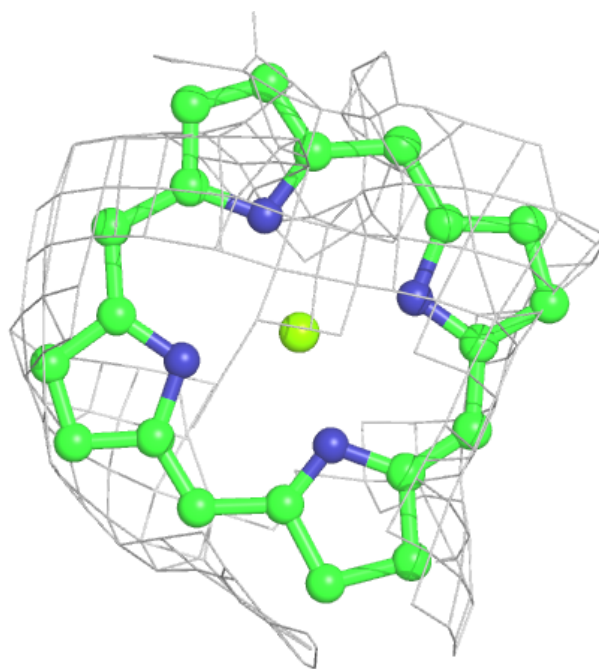
Electron density around CLA 3 3010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



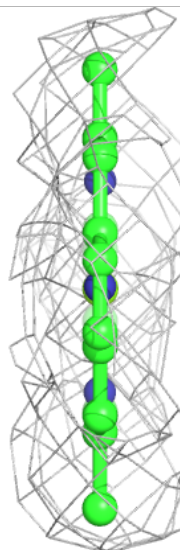
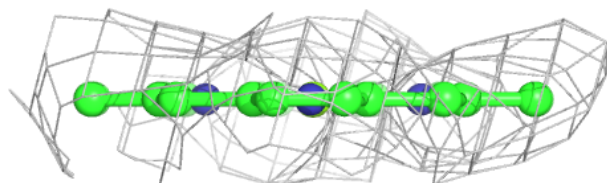
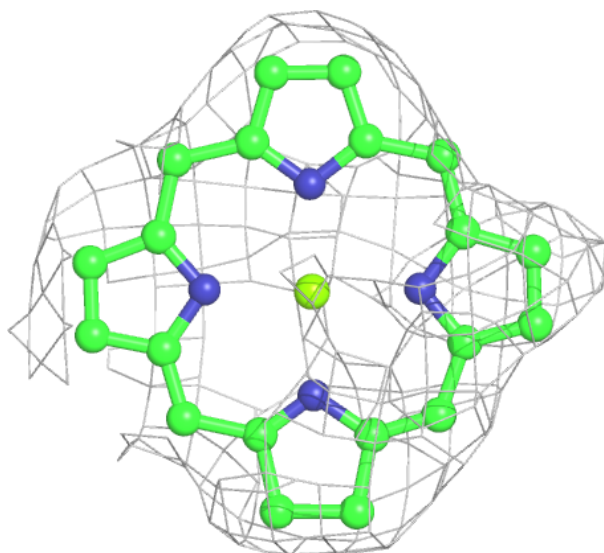
Electron density around CLA A 1142:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



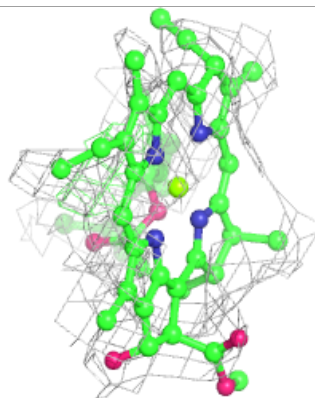
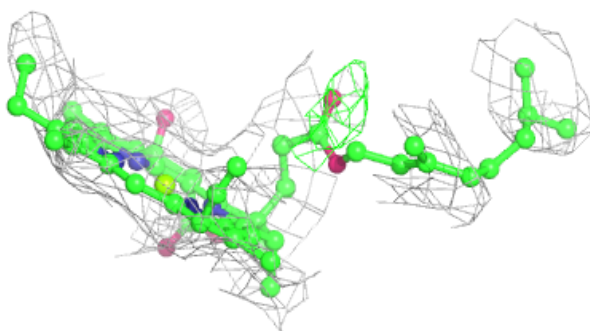
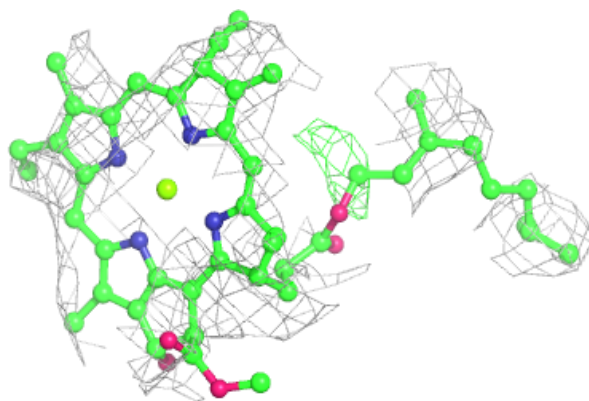
Electron density around CLA A 1118:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



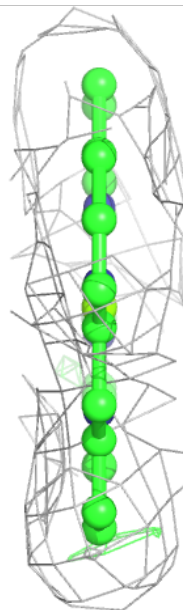
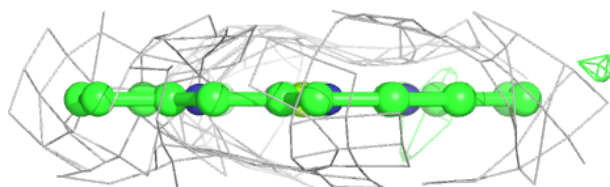
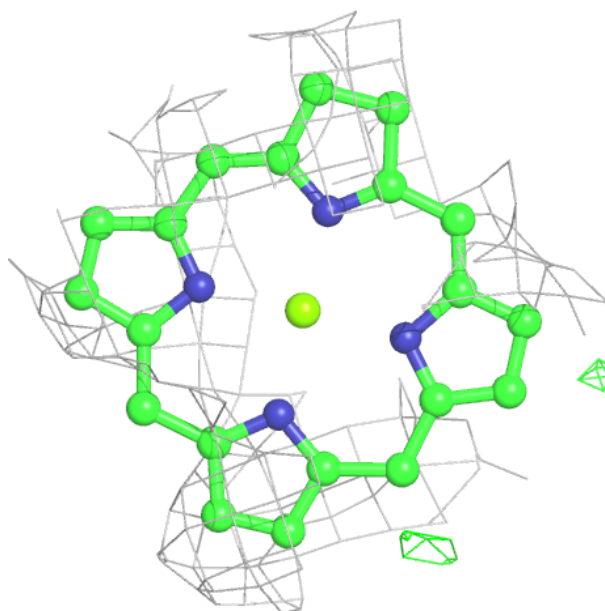
Electron density around CLA A 1119:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



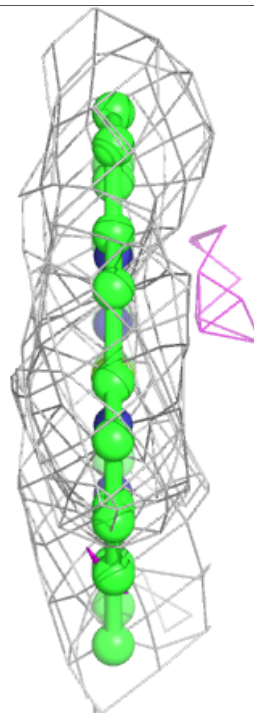
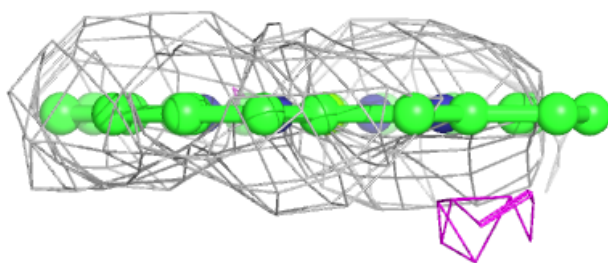
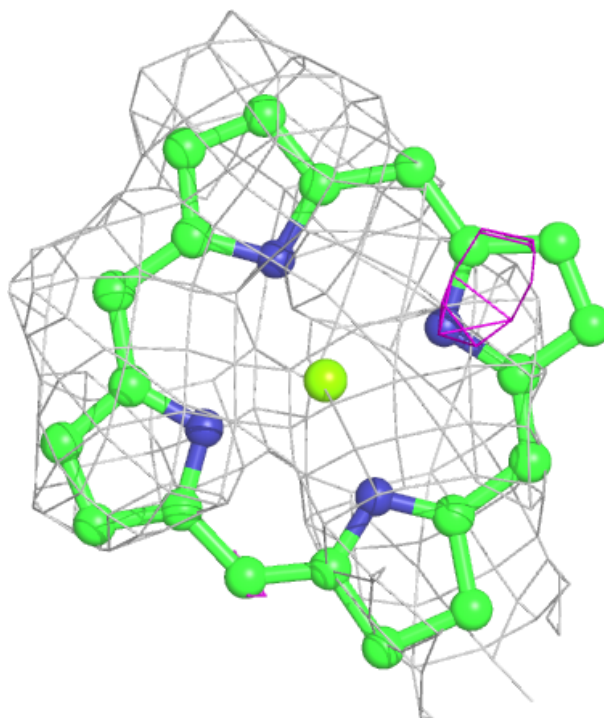
Electron density around CLA B 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



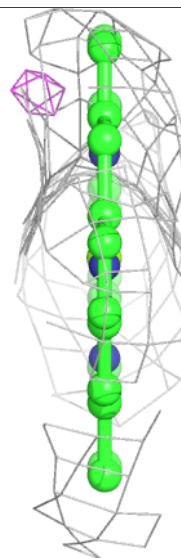
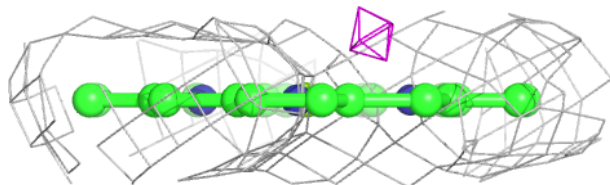
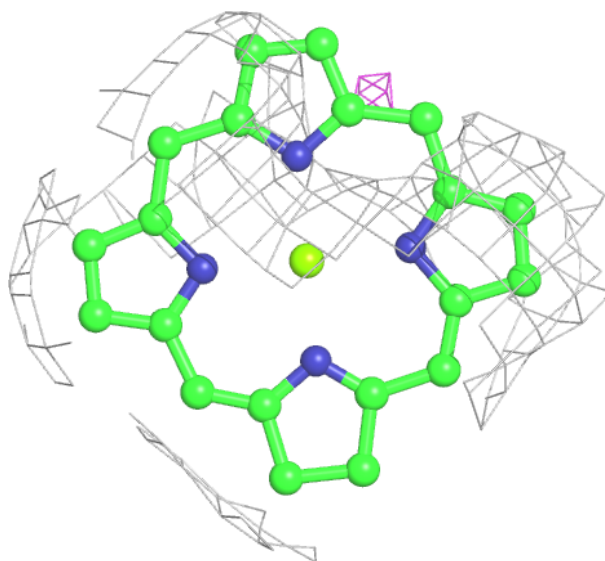
Electron density around CLA 4 4001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



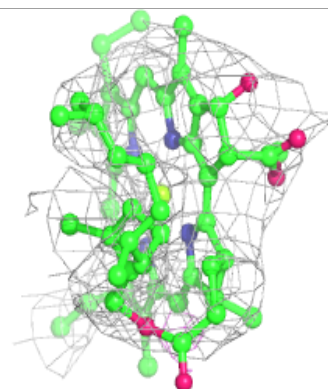
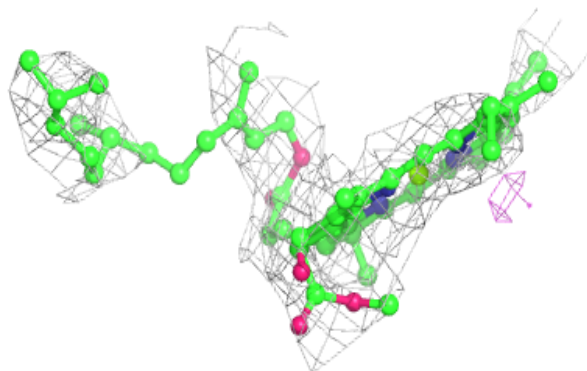
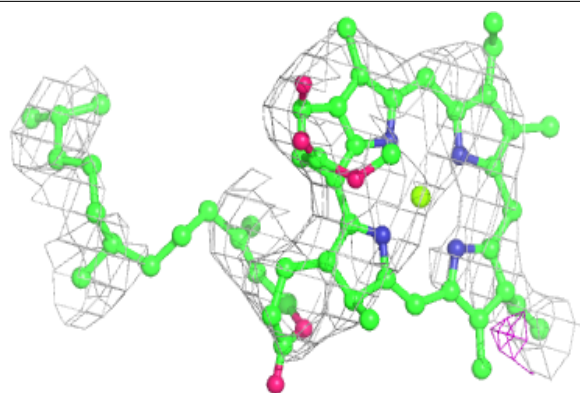
Electron density around CLA 1 1007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



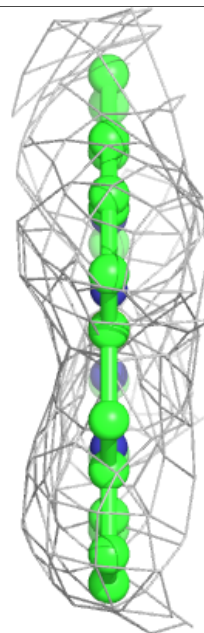
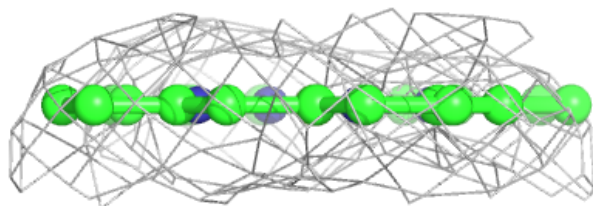
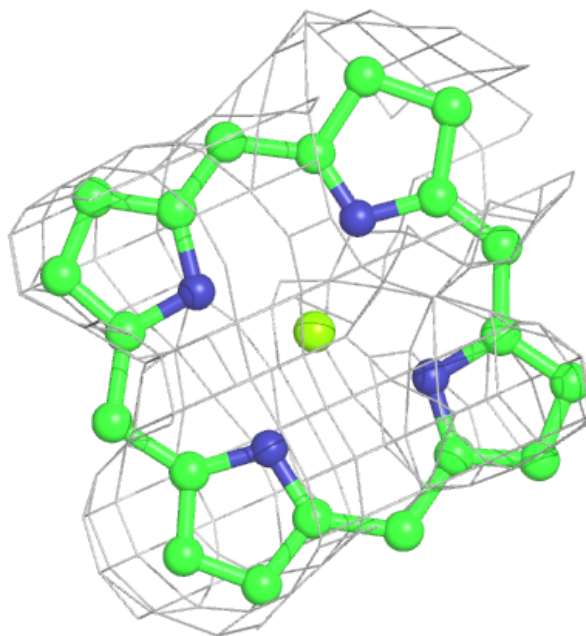
Electron density around CLA B 1212:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



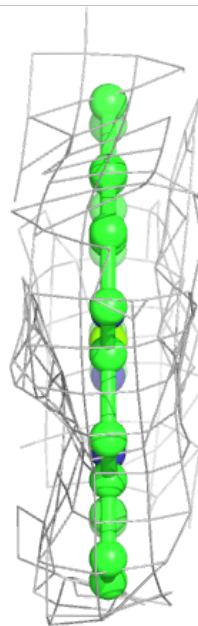
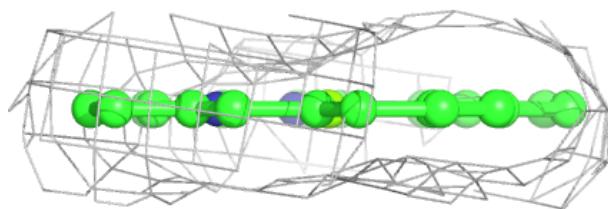
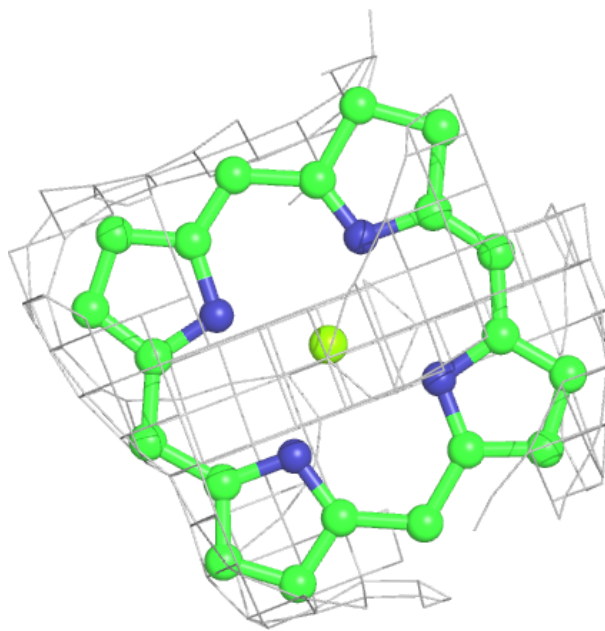
Electron density around CLA 3 3011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



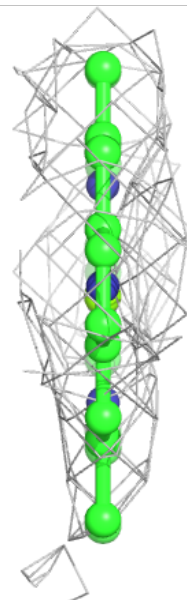
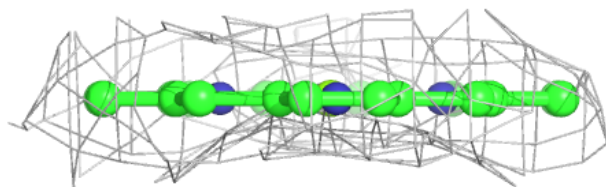
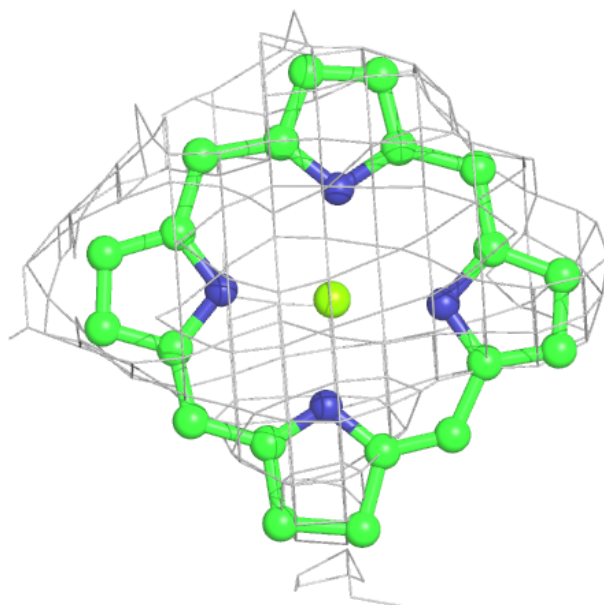
Electron density around CLA 2 2015:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



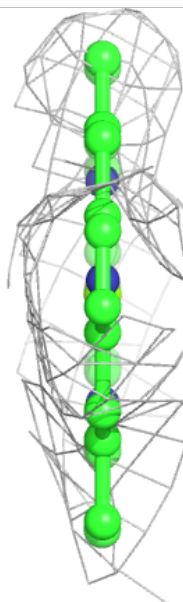
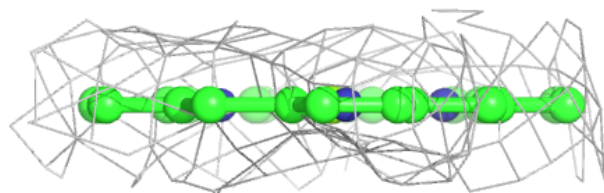
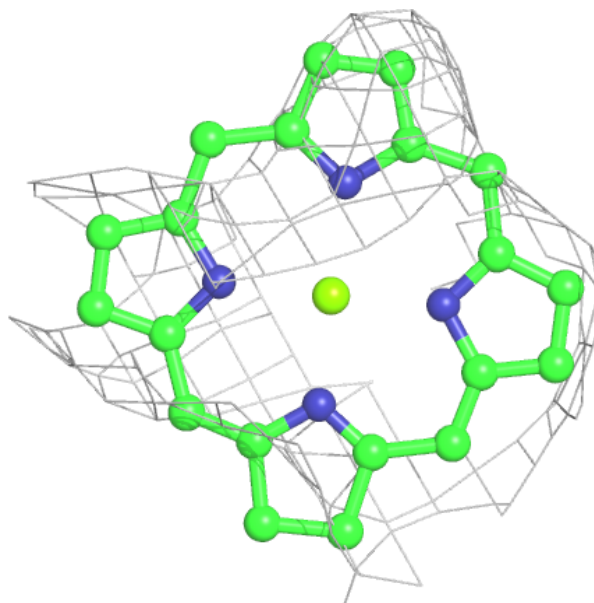
Electron density around CLA B 1210:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



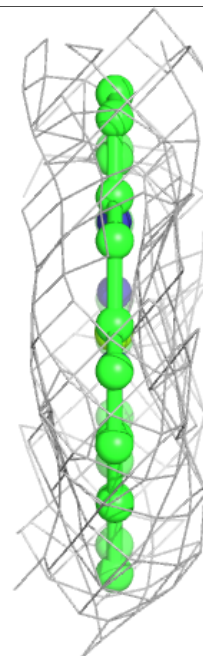
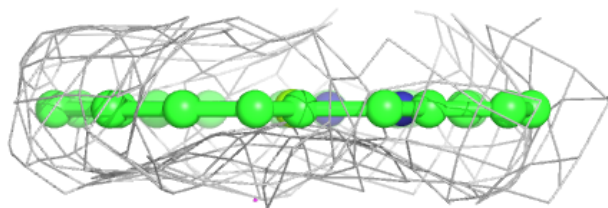
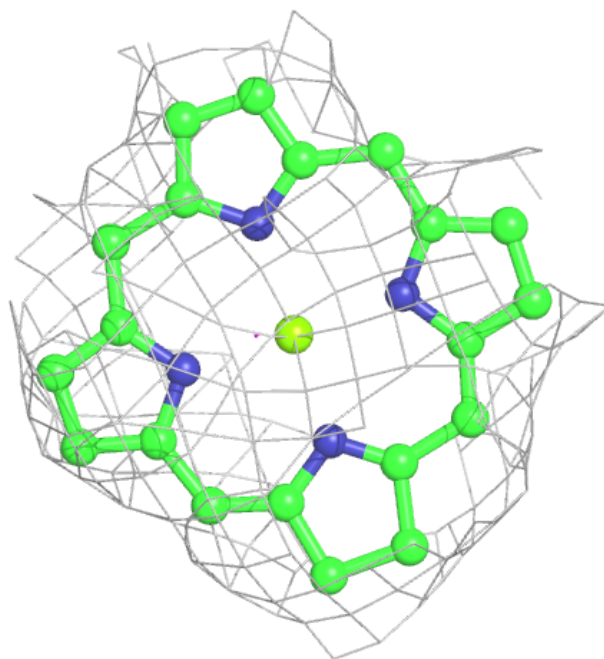
Electron density around CLA A 1143:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



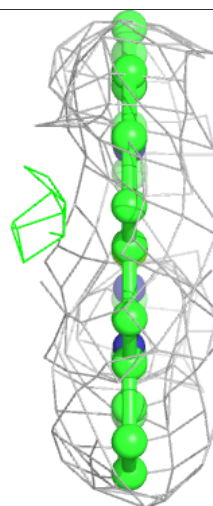
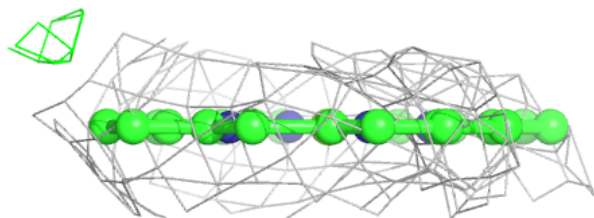
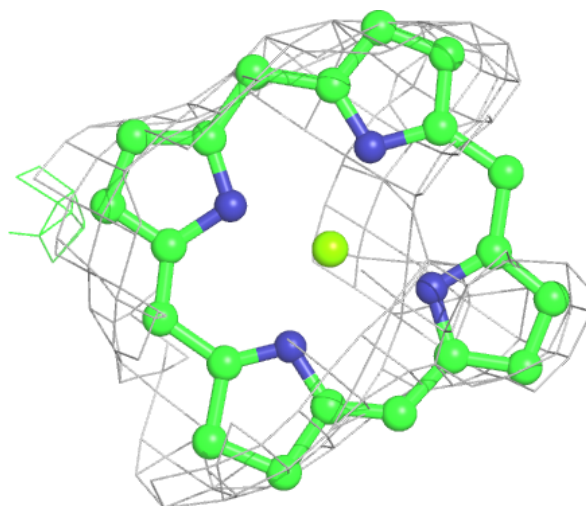
Electron density around CLA L 1125:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



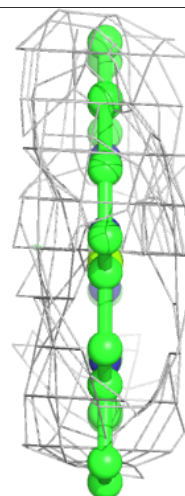
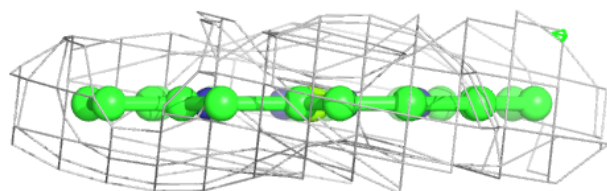
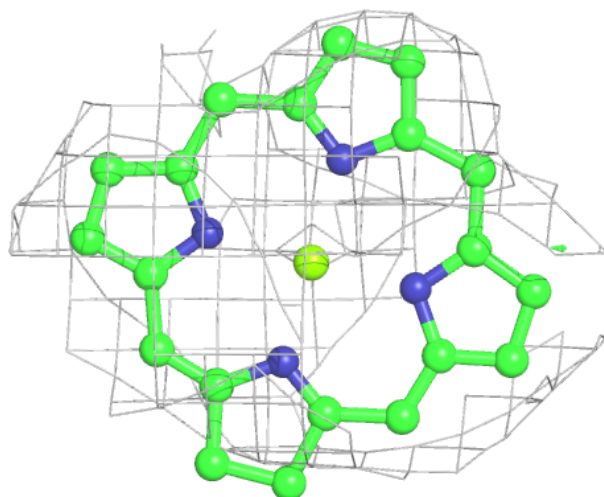
Electron density around CLA 2 2004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



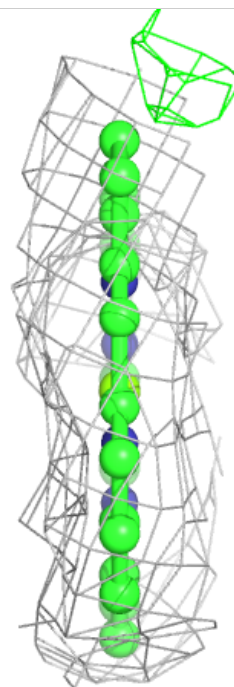
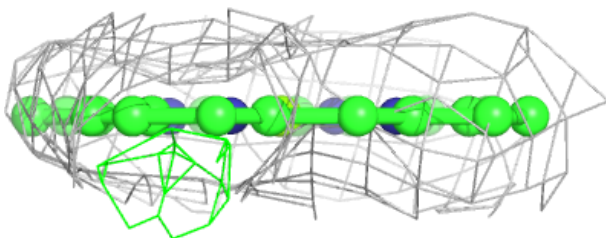
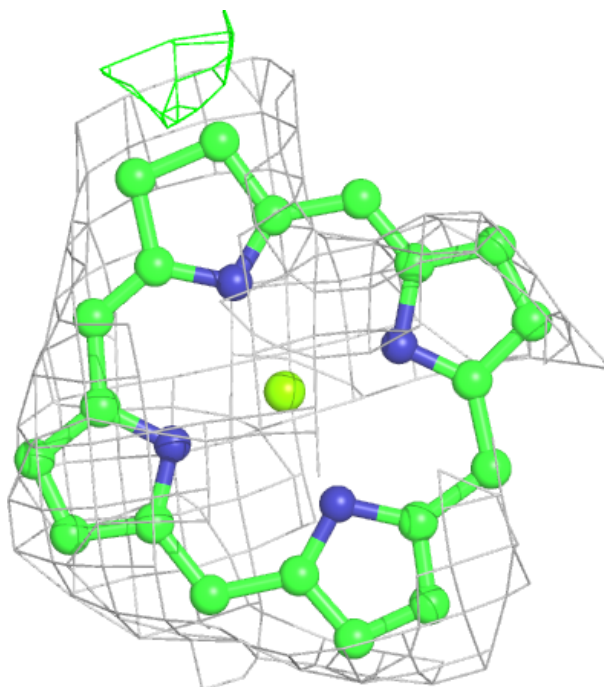
Electron density around CLA 4 4012:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



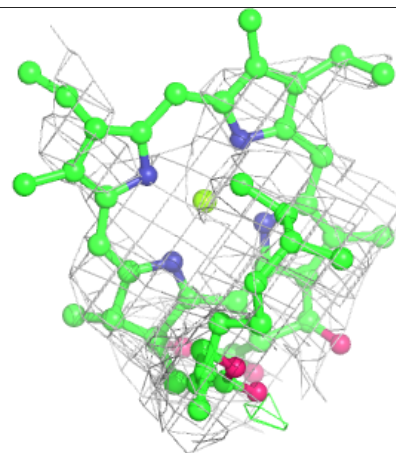
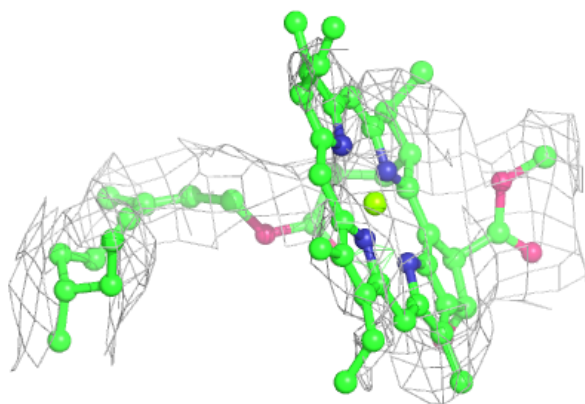
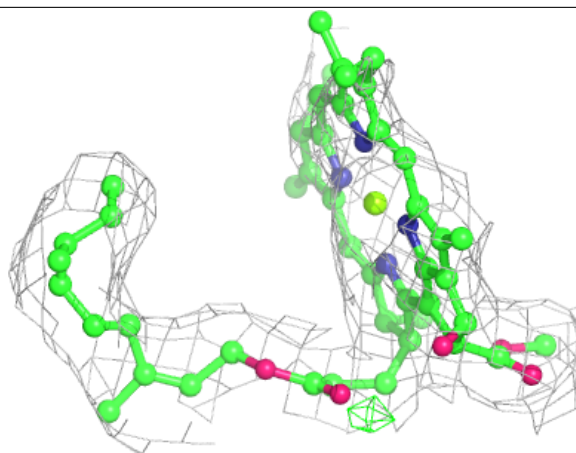
Electron density around CLA A 1151:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



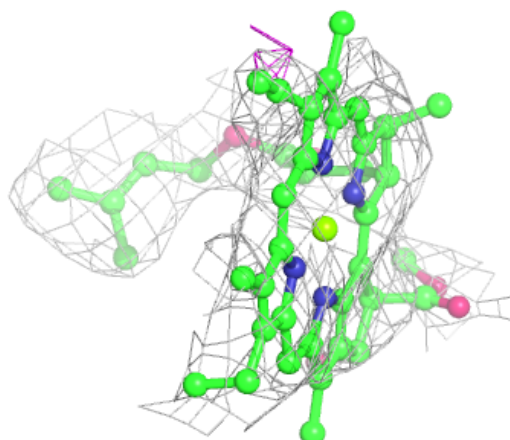
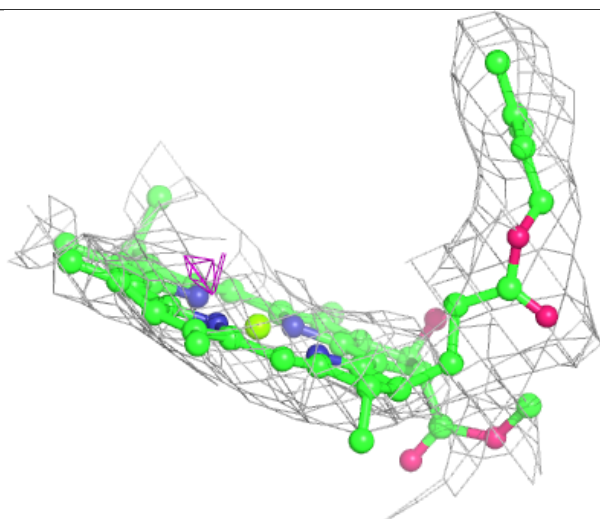
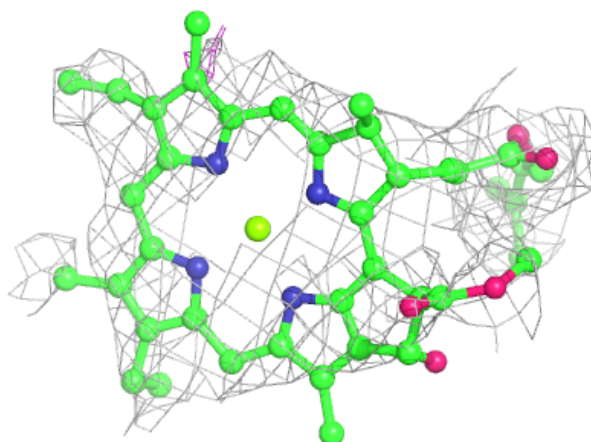
Electron density around CLA B 1216:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



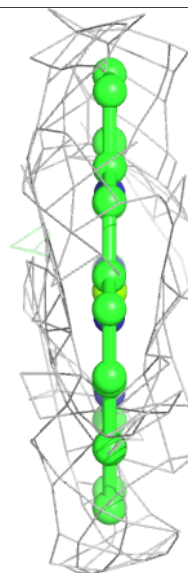
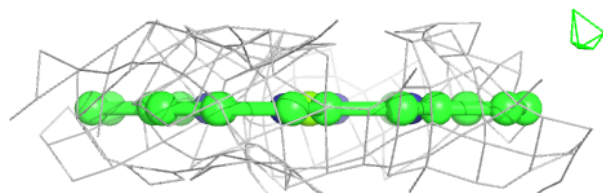
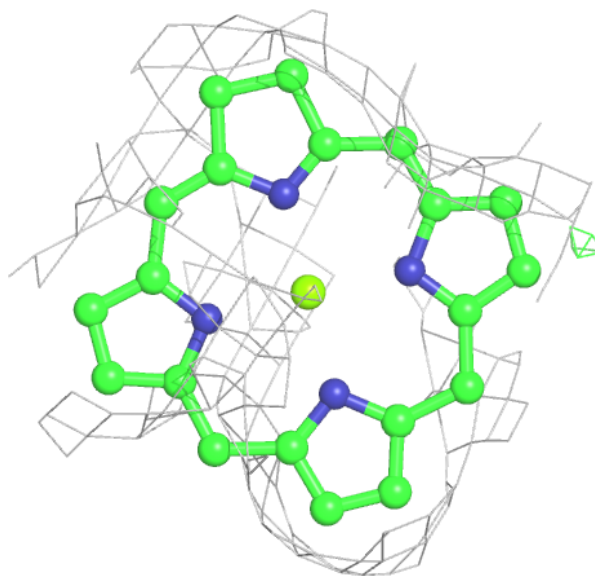
Electron density around CLA A 1113:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



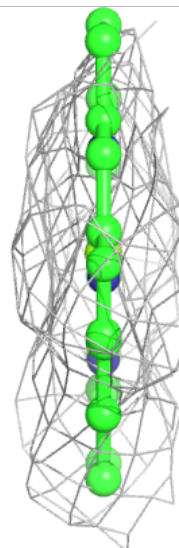
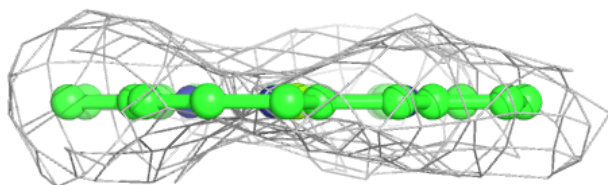
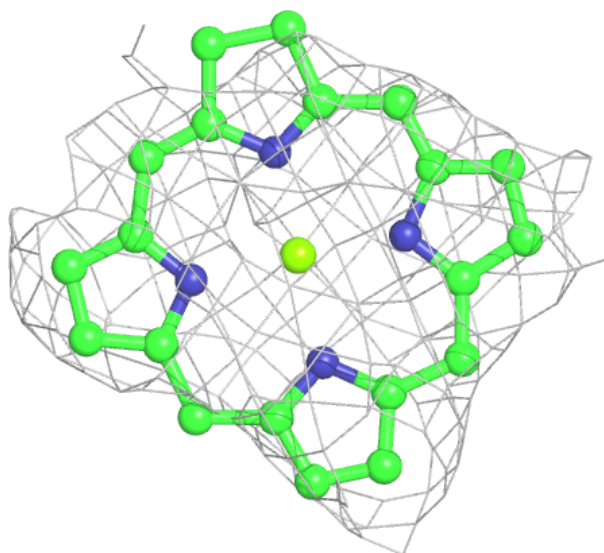
Electron density around CLA 1 1013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



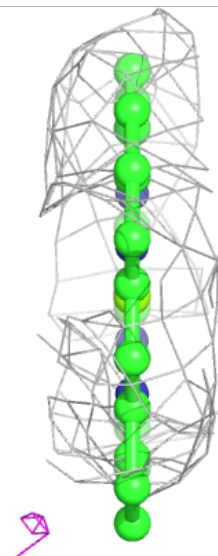
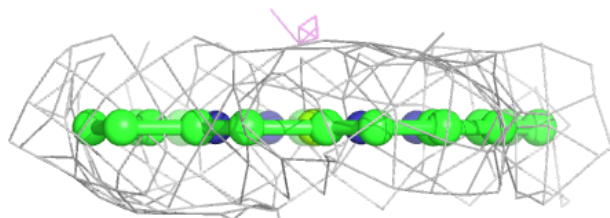
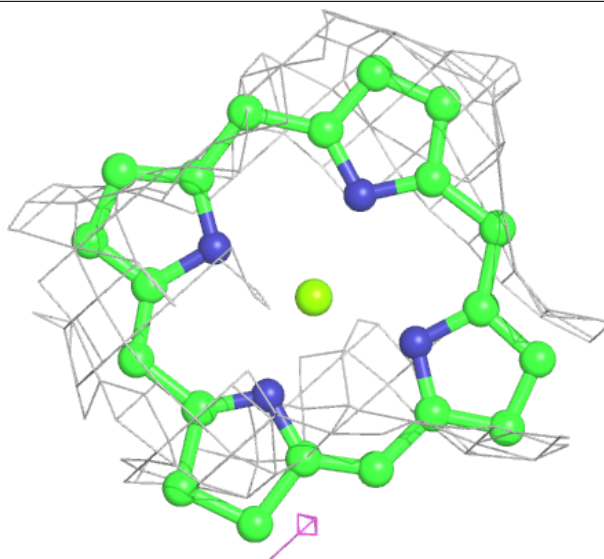
Electron density around CLA F 1303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



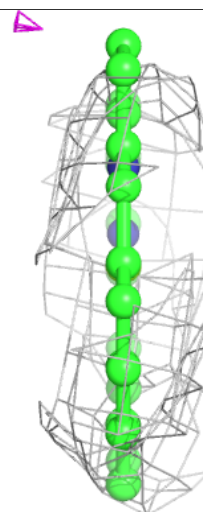
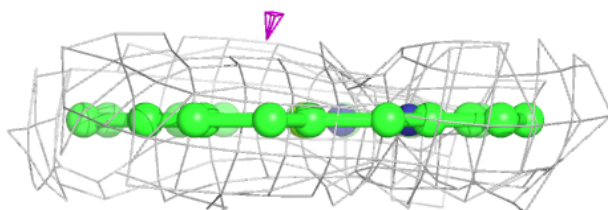
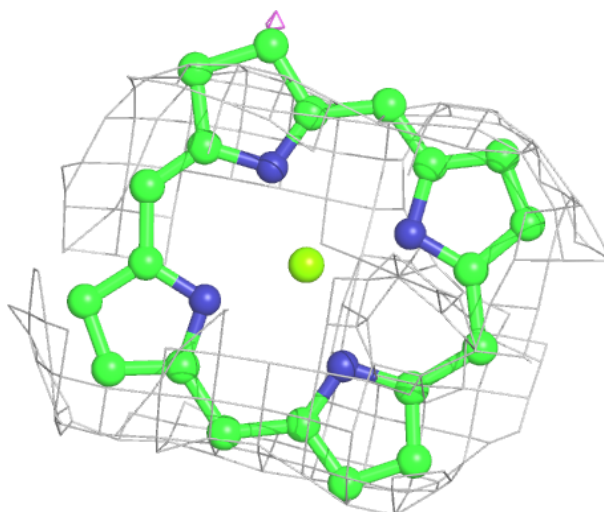
Electron density around CLA 3 3006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



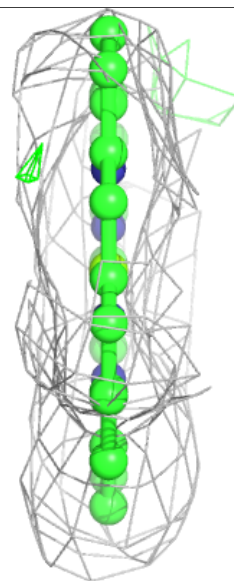
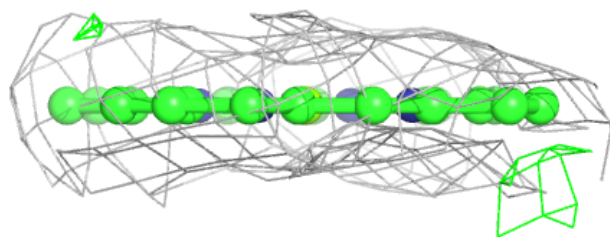
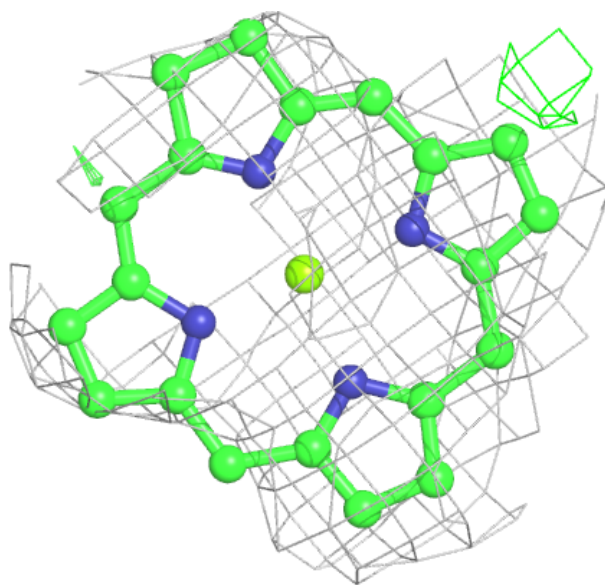
Electron density around CLA A 1111:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



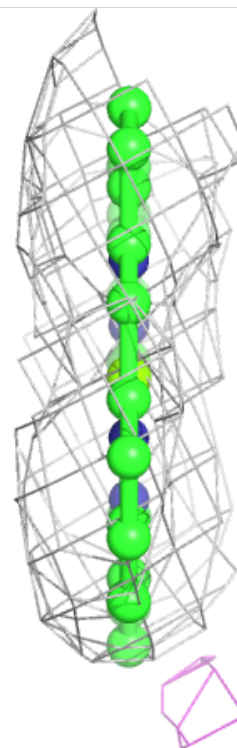
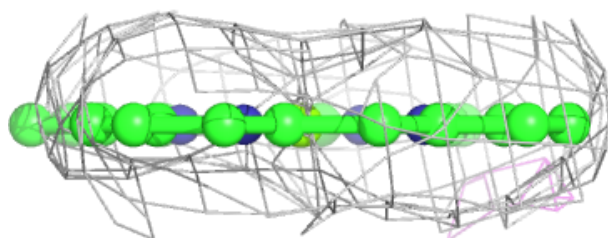
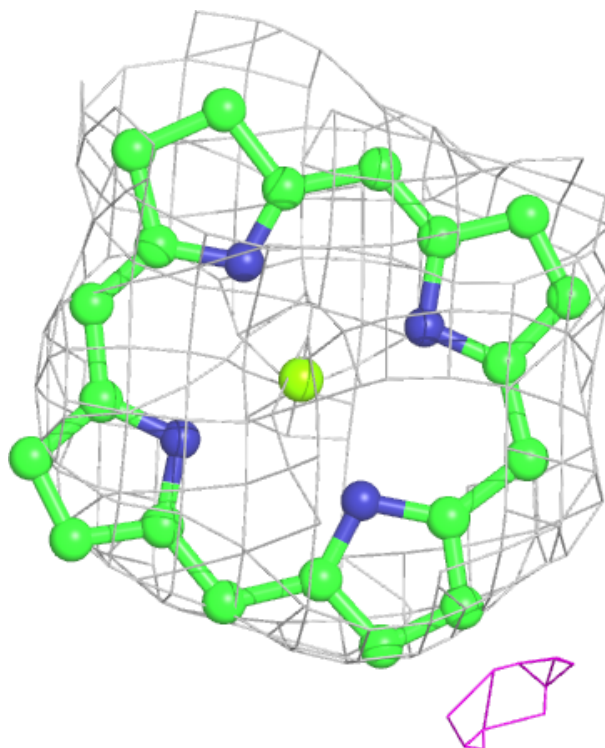
Electron density around CLA 1 1005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



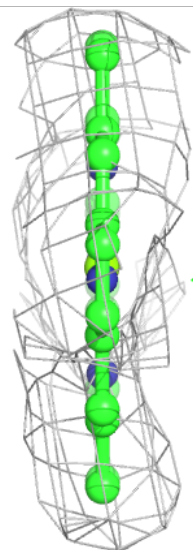
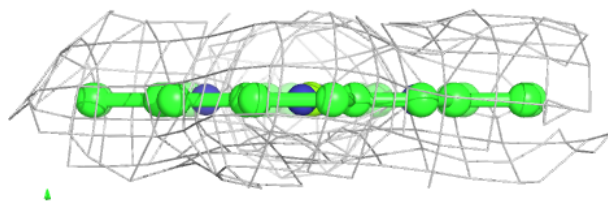
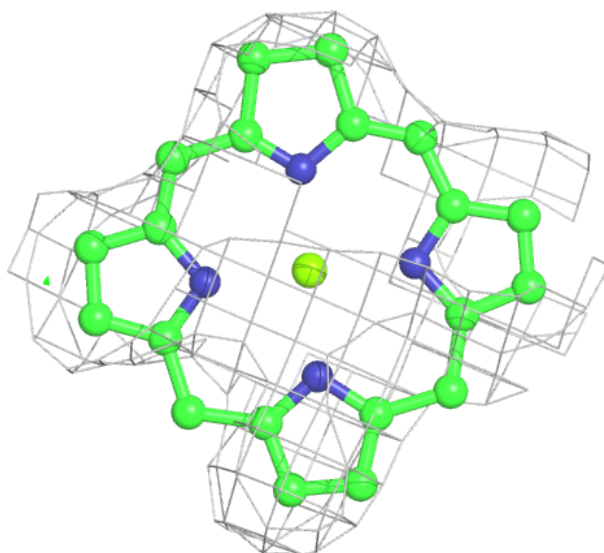
Electron density around CLA 3 3012:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



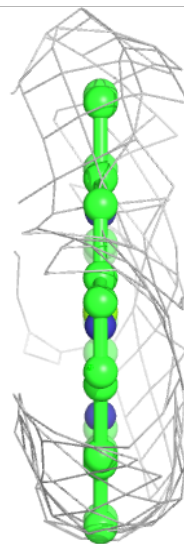
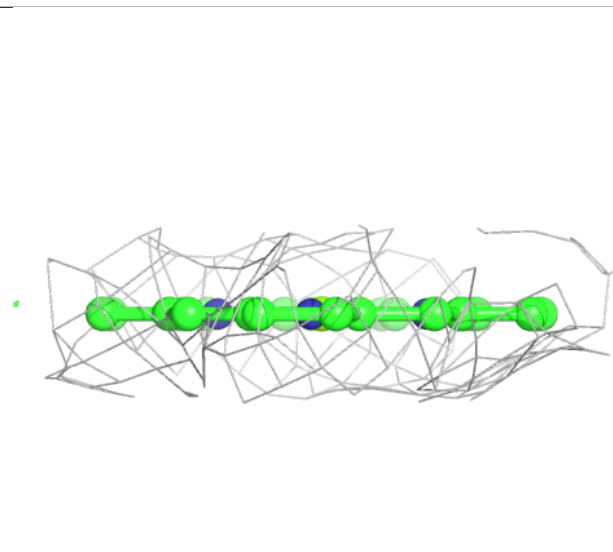
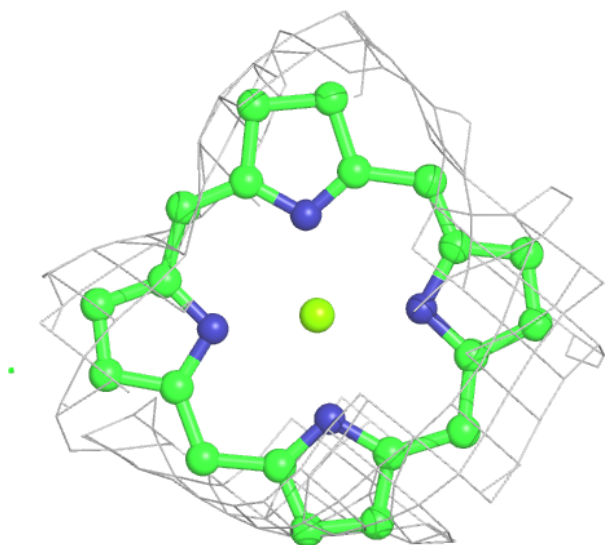
Electron density around CLA 4 4006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



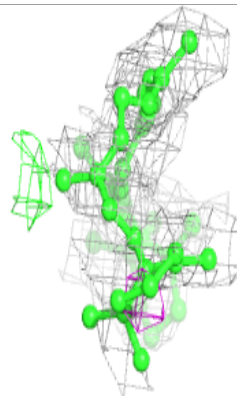
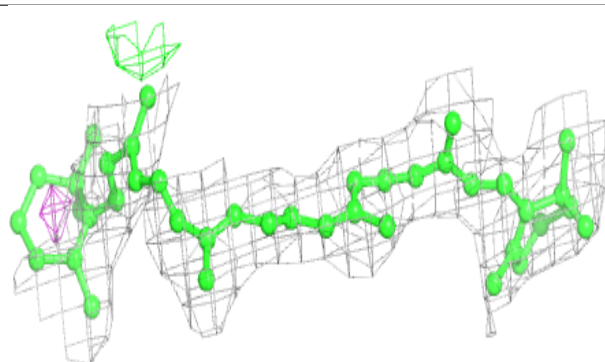
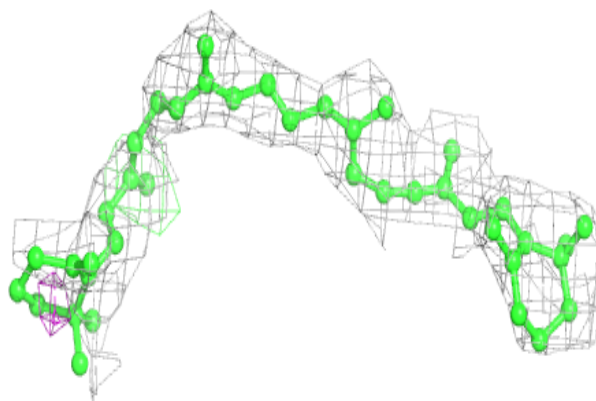
Electron density around CLA G 1248:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



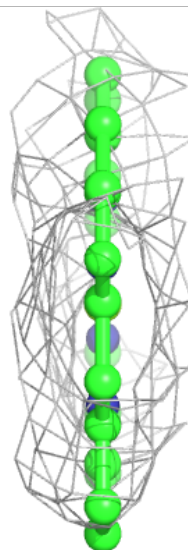
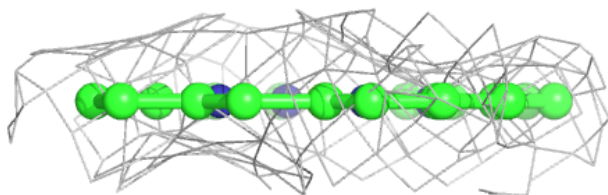
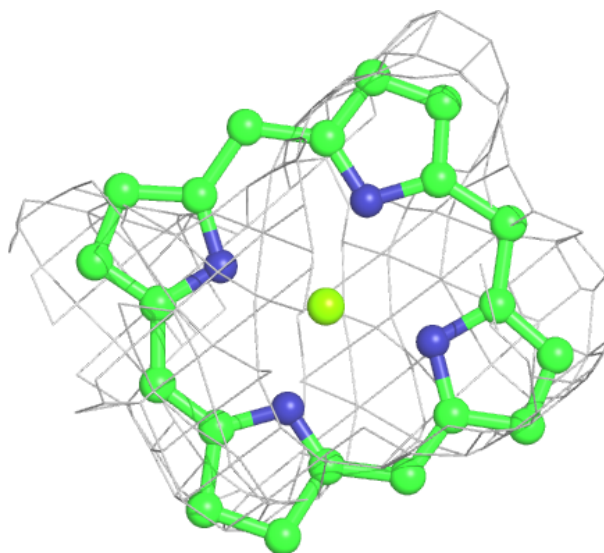
Electron density around BCR F 6016:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



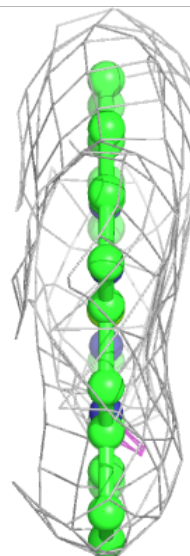
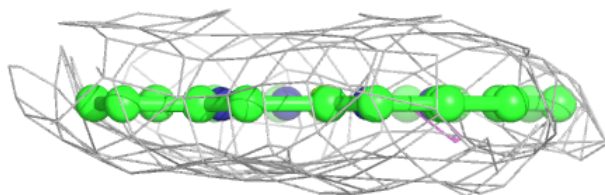
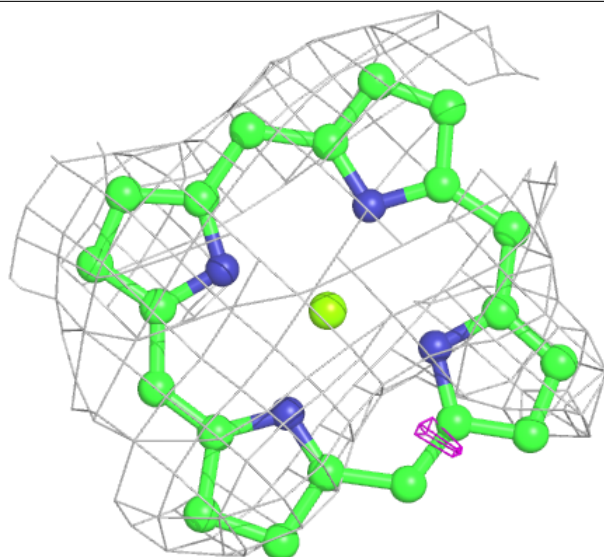
Electron density around CLA 4 4010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



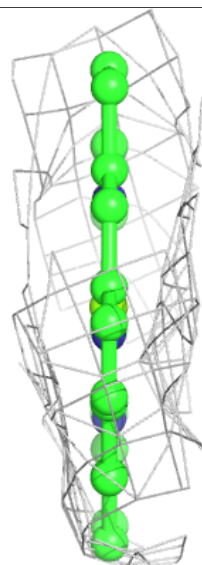
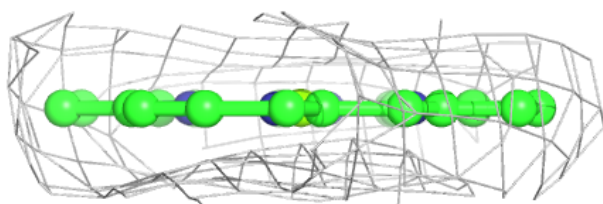
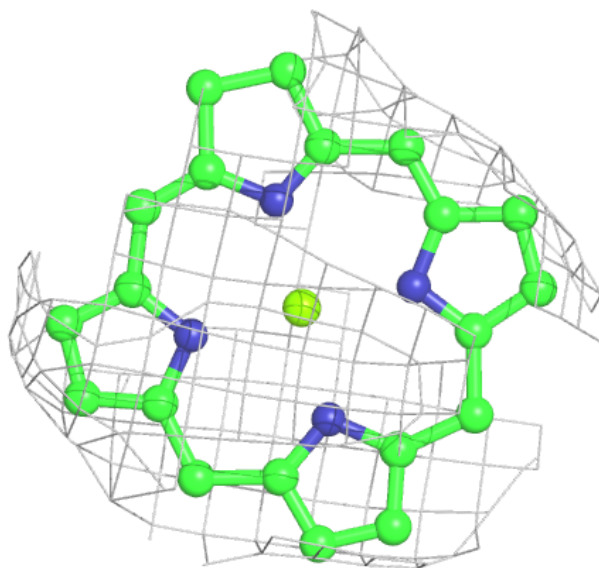
Electron density around CLA A 1134:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



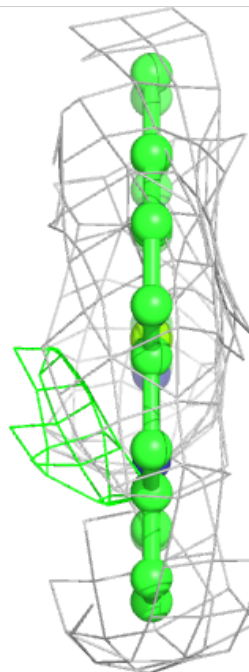
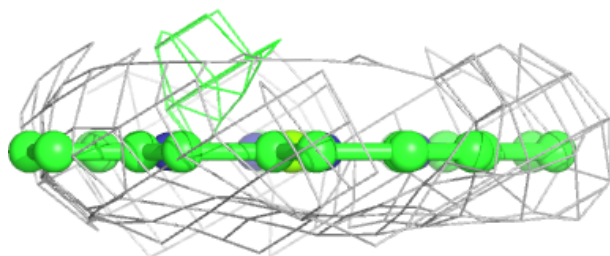
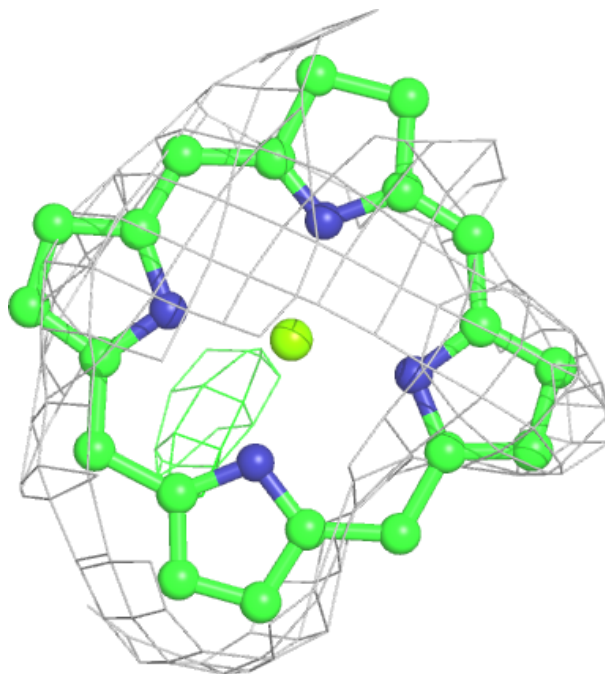
Electron density around CLA 3 3002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



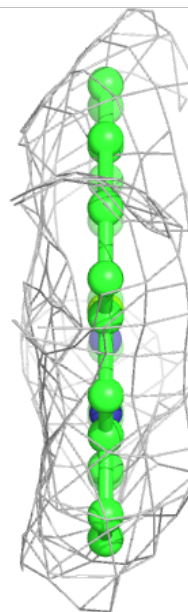
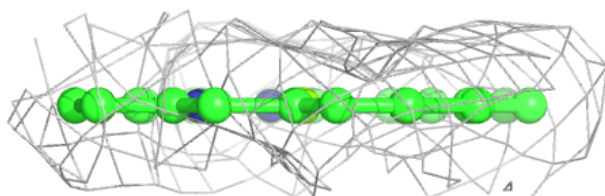
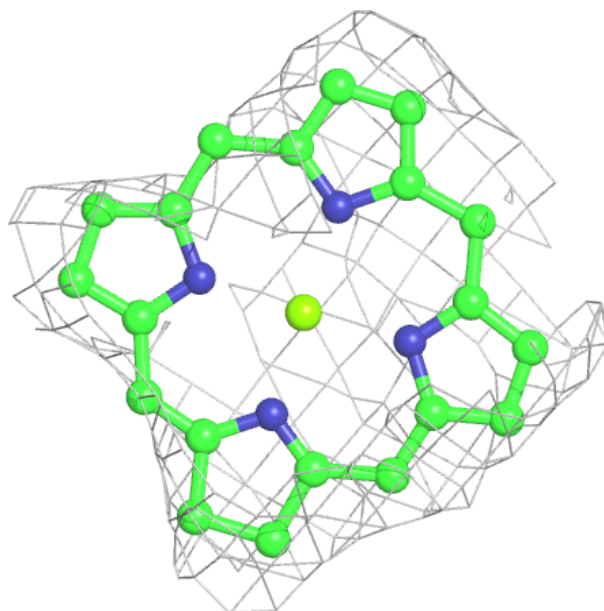
Electron density around CLA 1 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



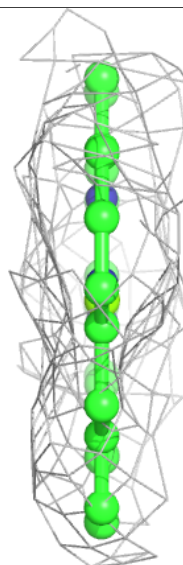
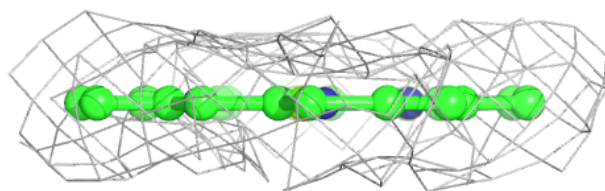
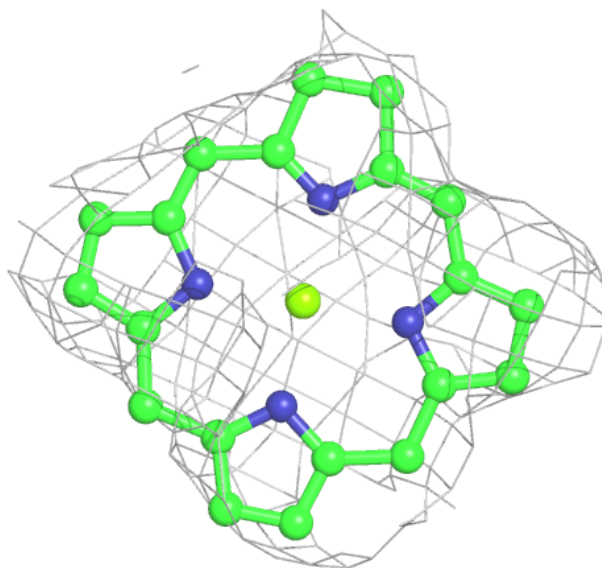
Electron density around CLA 1 1011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



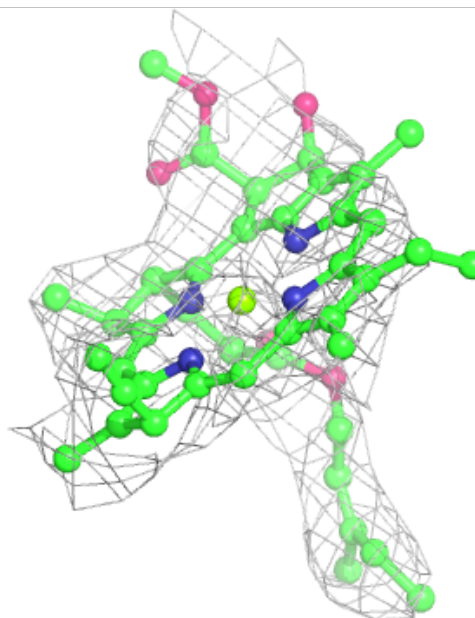
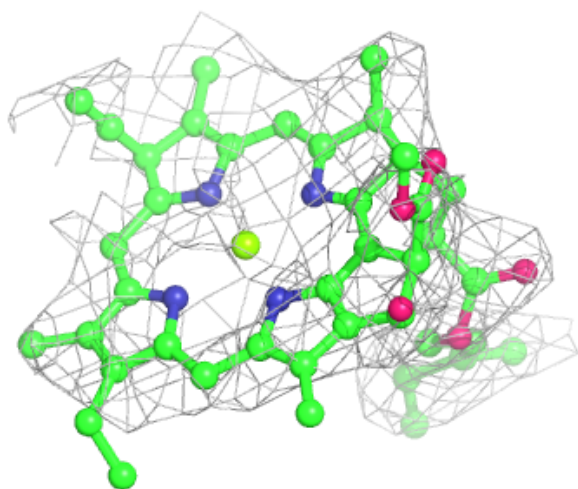
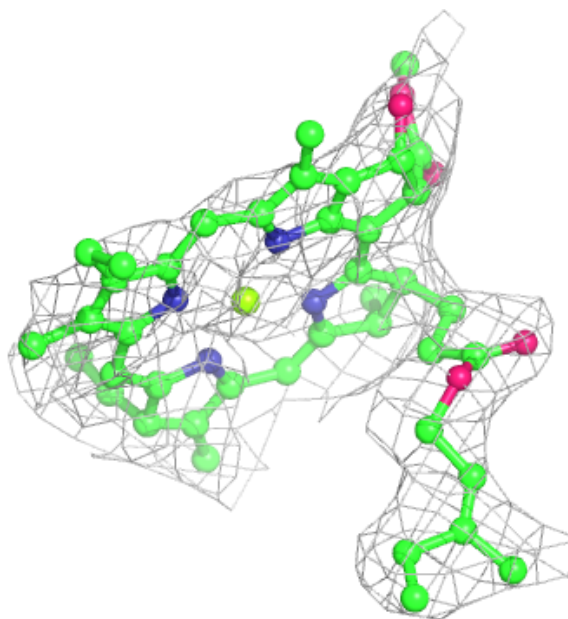
Electron density around CLA A 1116:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



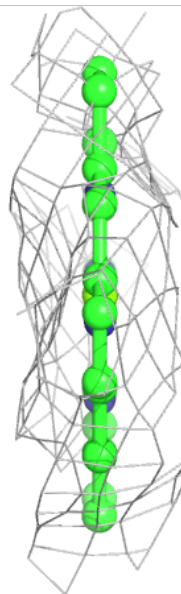
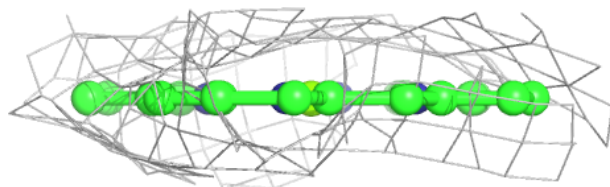
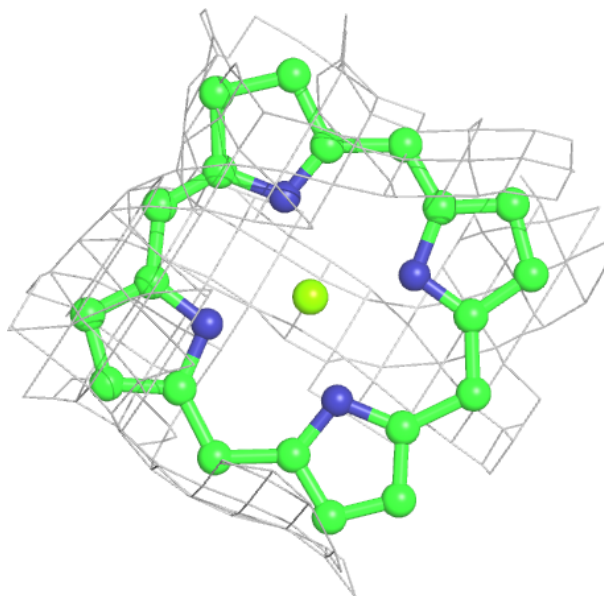
Electron density around CLA L 1502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



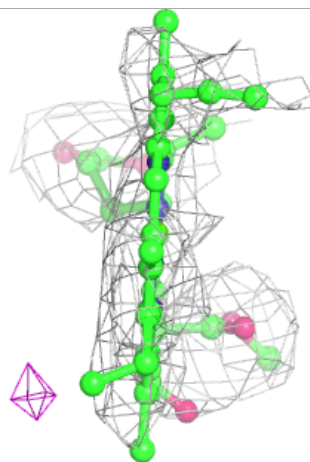
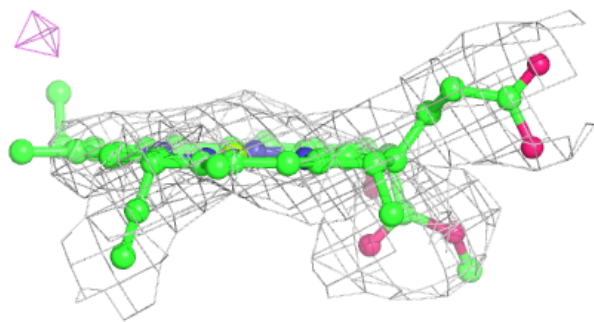
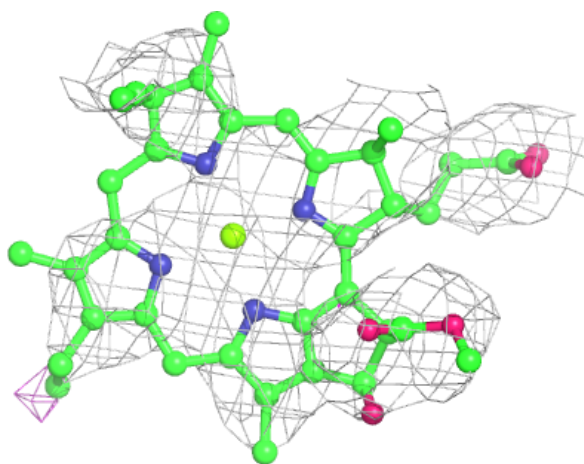
Electron density around CLA 3 3005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



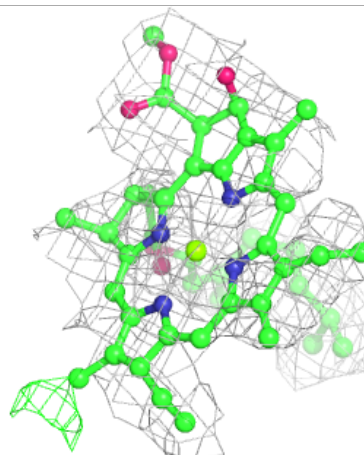
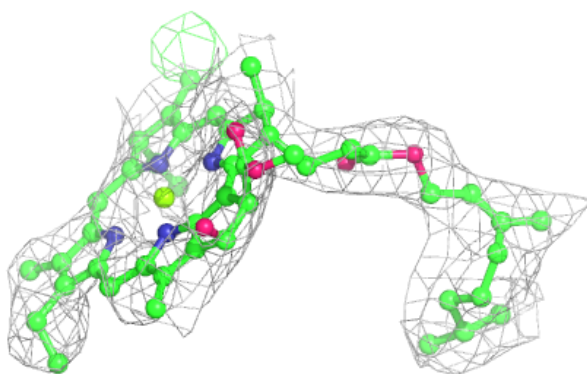
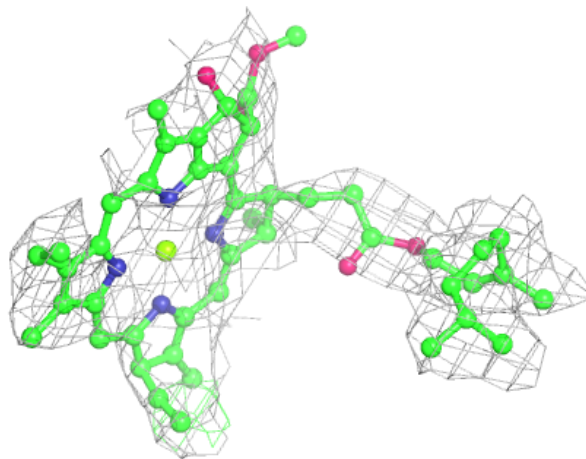
Electron density around CLA A 1135:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



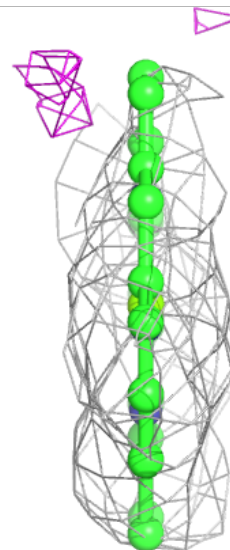
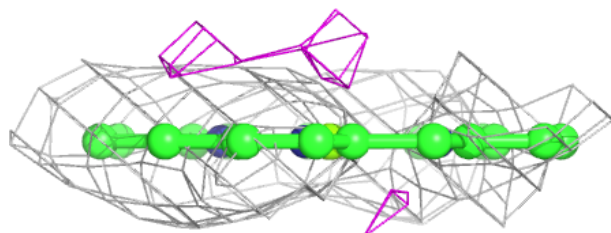
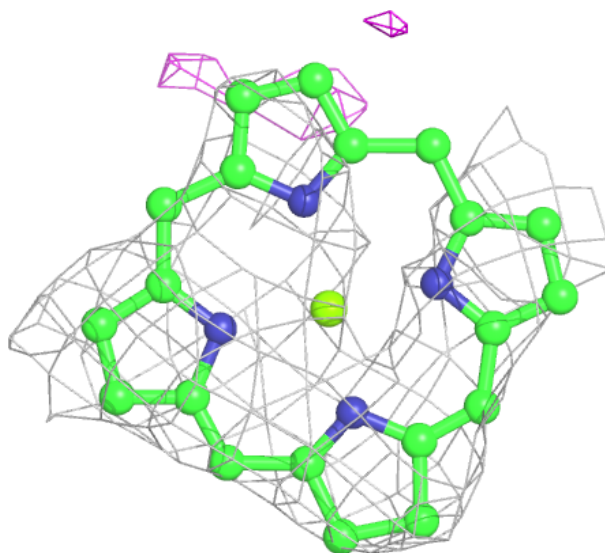
Electron density around CLA A 1129:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



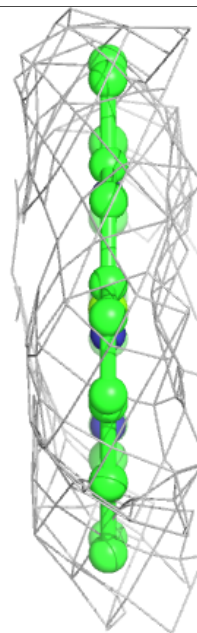
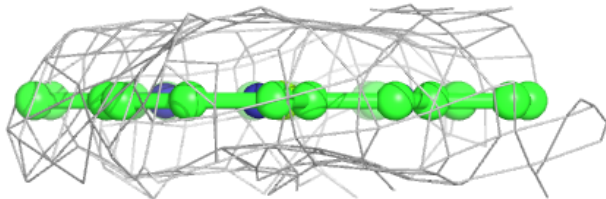
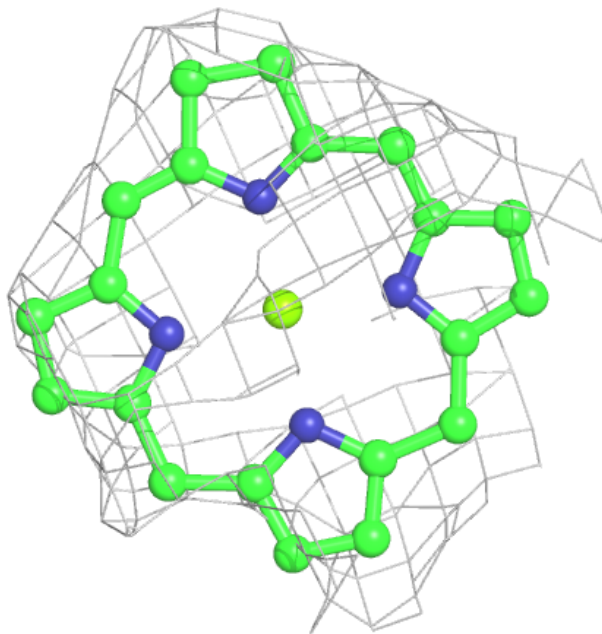
Electron density around CLA 1 1010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



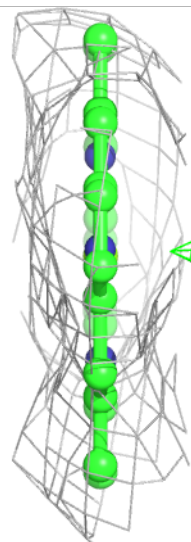
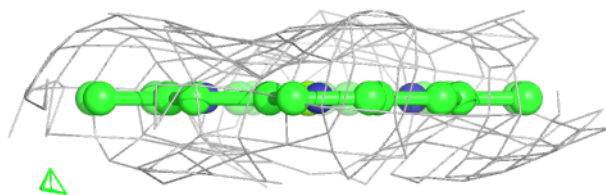
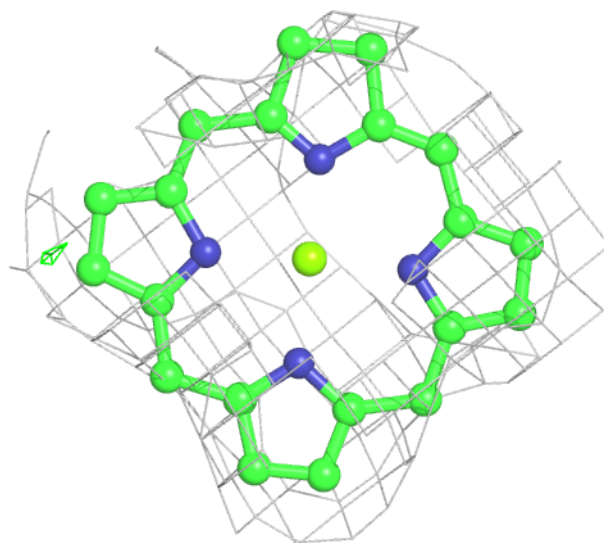
Electron density around CLA H 1505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



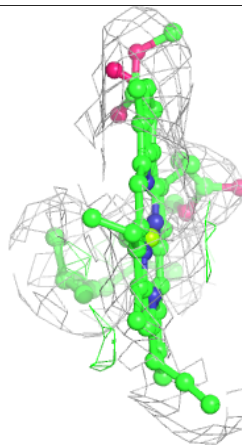
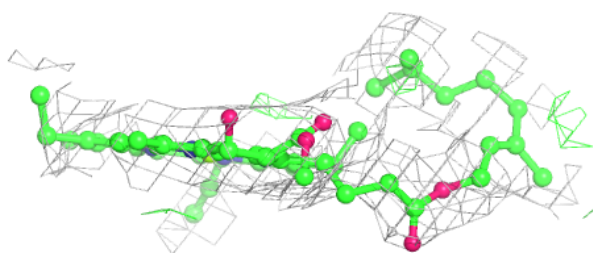
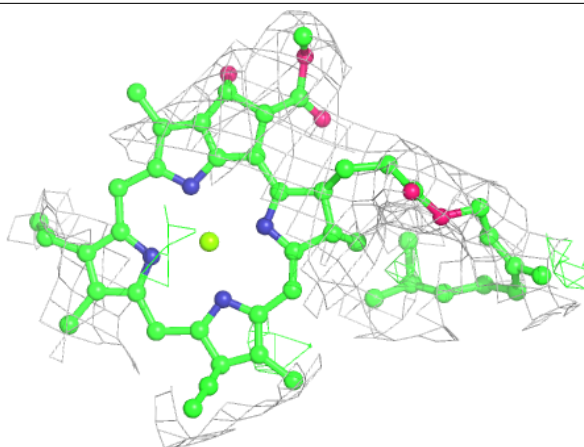
Electron density around CLA B 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



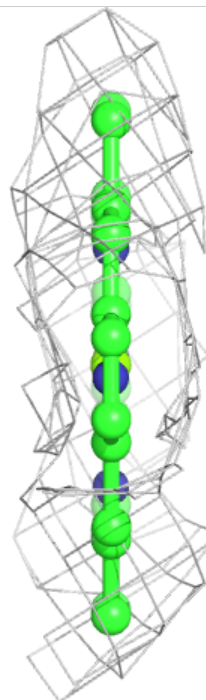
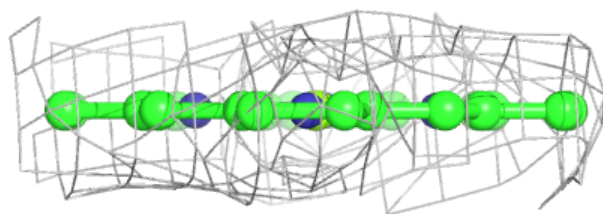
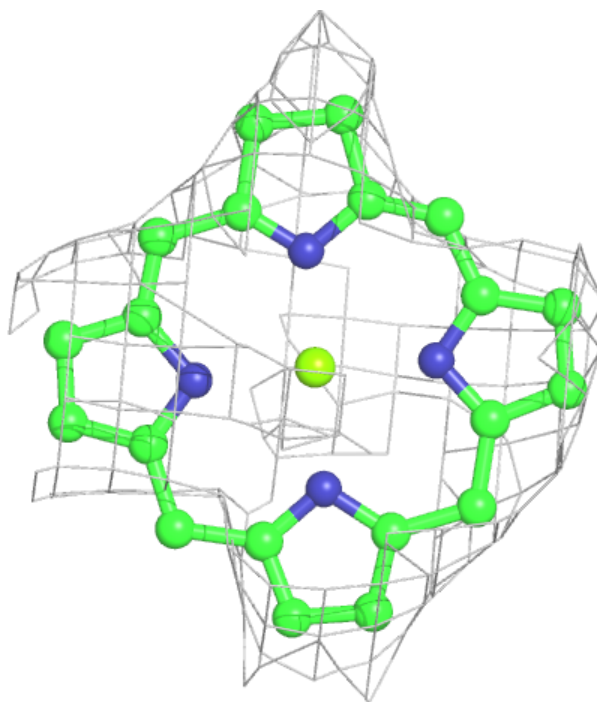
Electron density around CLA F 1302:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



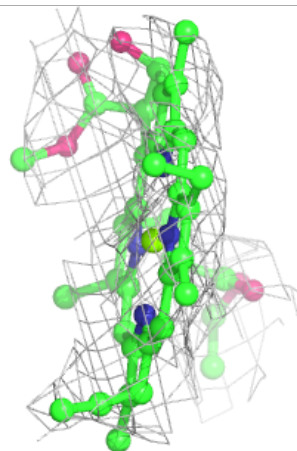
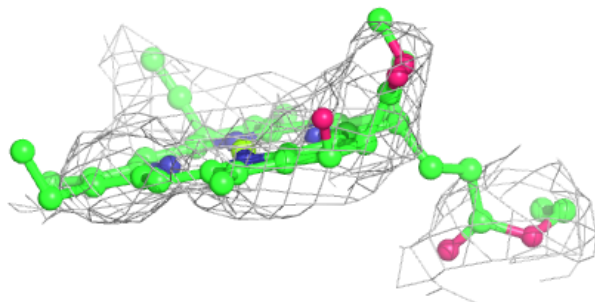
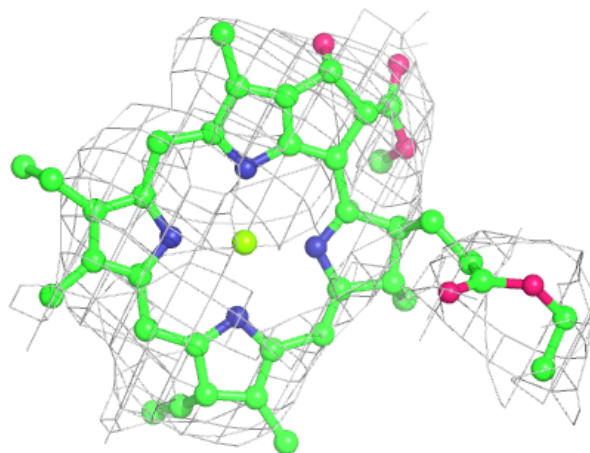
Electron density around CLA 2 2012:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



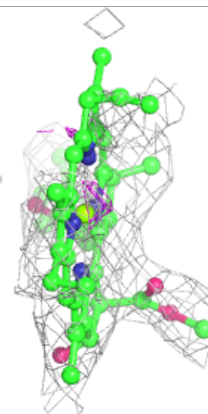
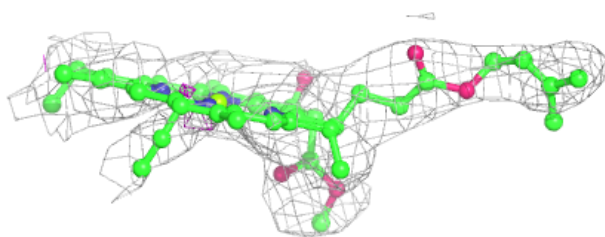
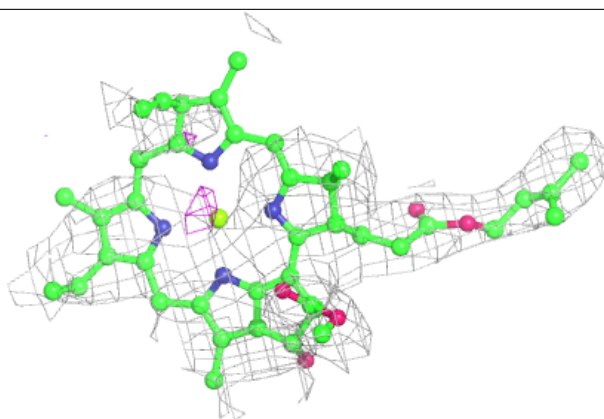
Electron density around CLA A 1103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

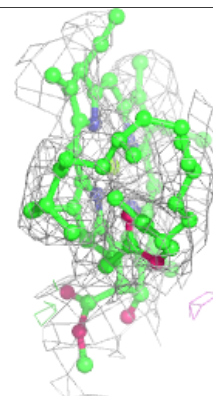
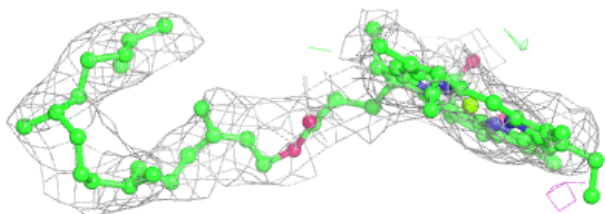
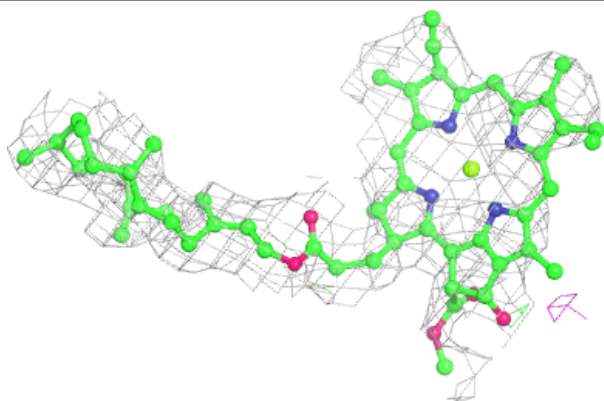


Electron density around CLA B 1234:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

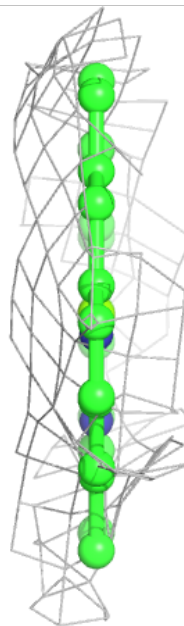
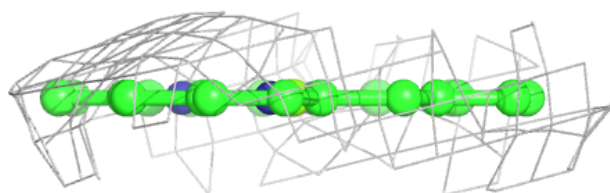
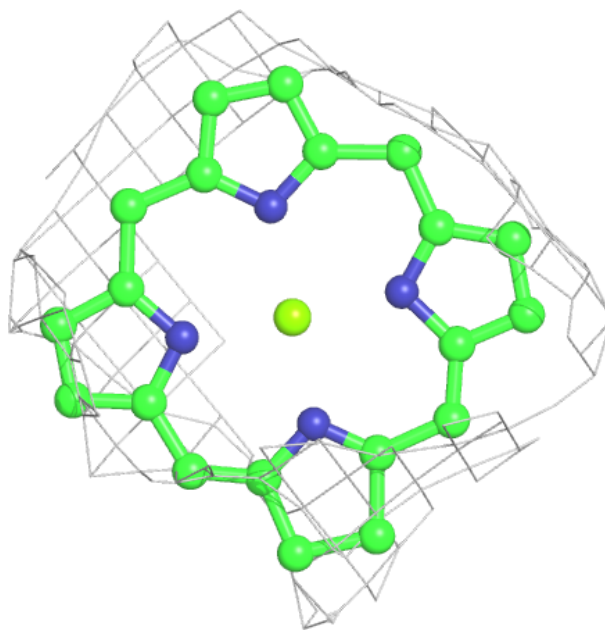
**Electron density around CLA B 1222:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



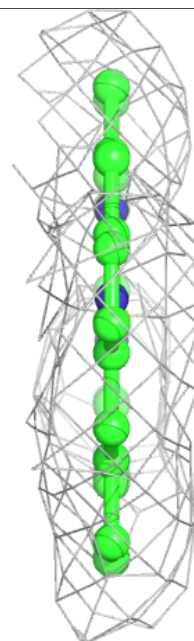
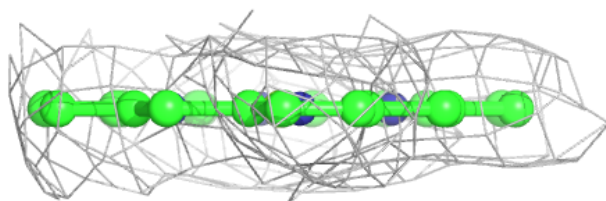
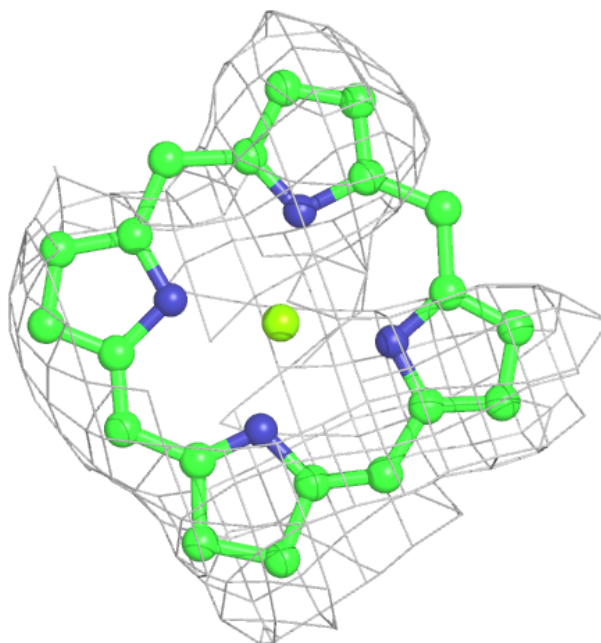
Electron density around CLA A 1144:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



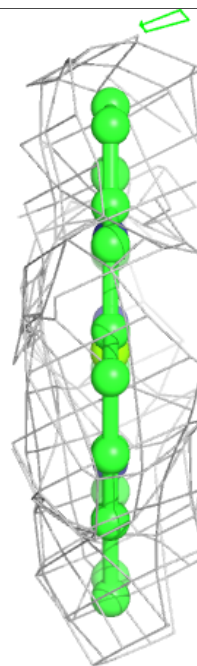
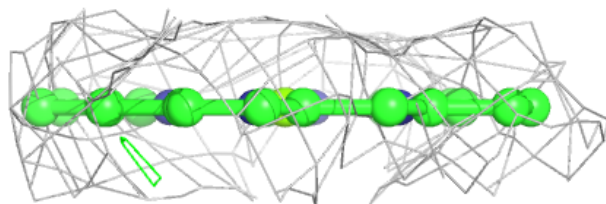
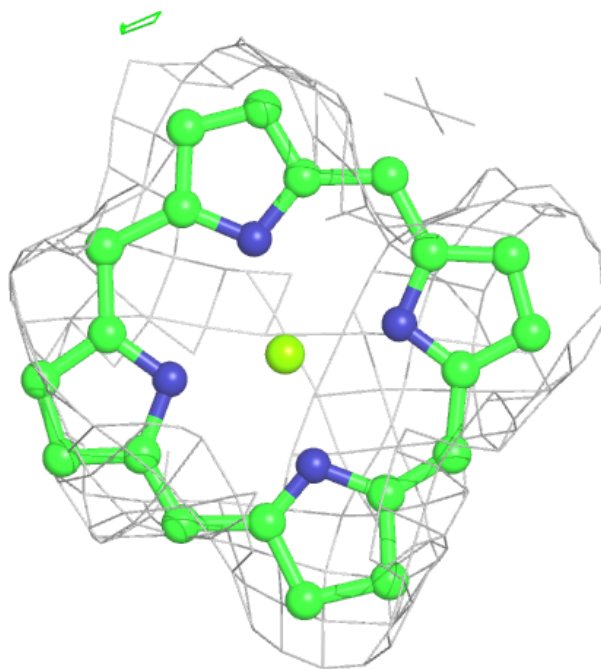
Electron density around CLA F 1306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



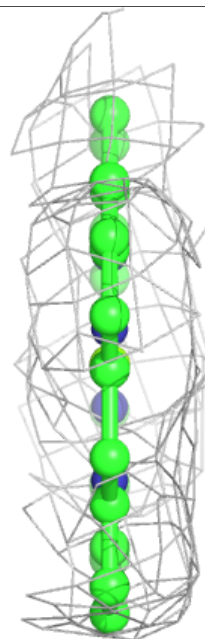
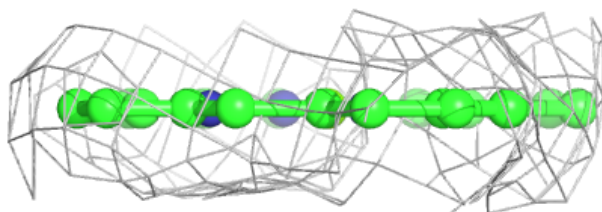
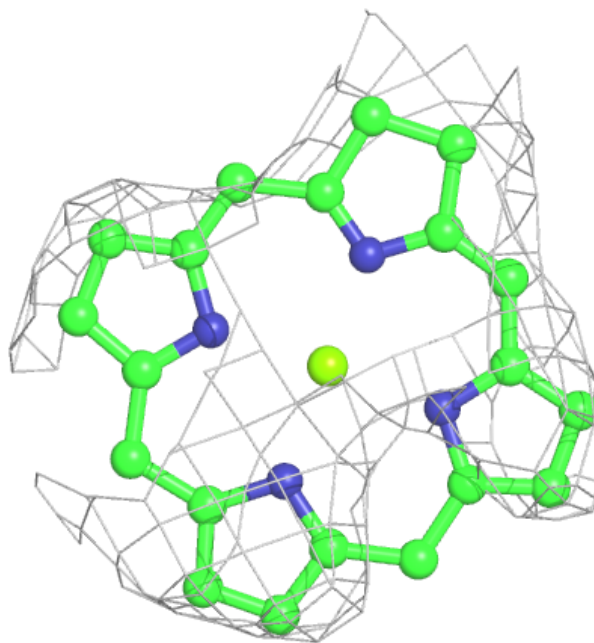
Electron density around CLA 2 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



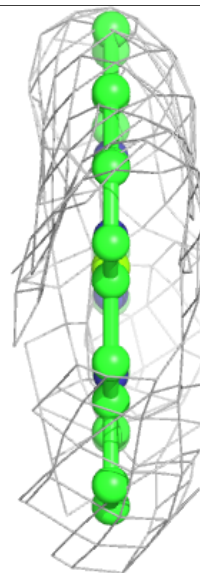
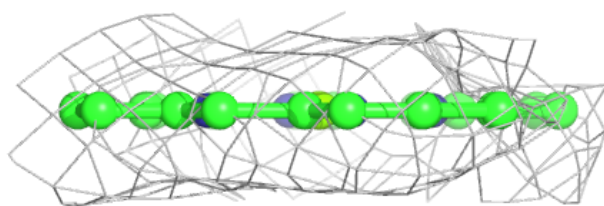
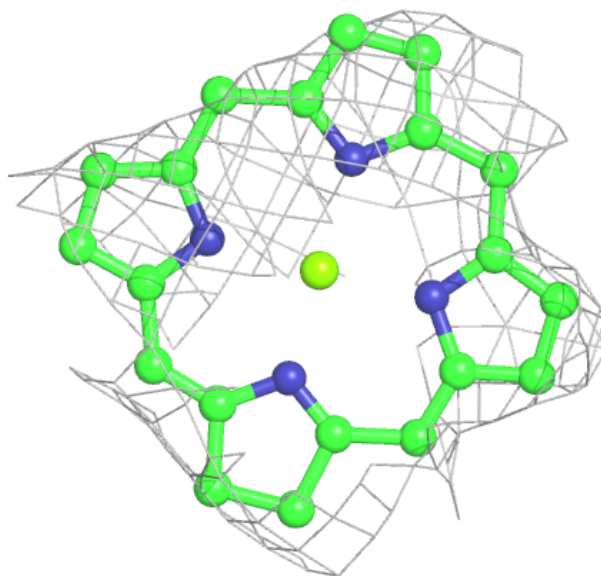
Electron density around CLA 4 4007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



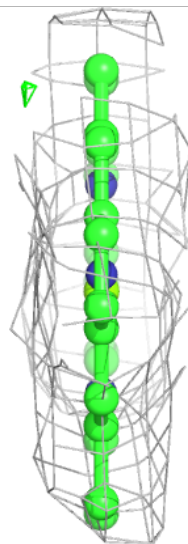
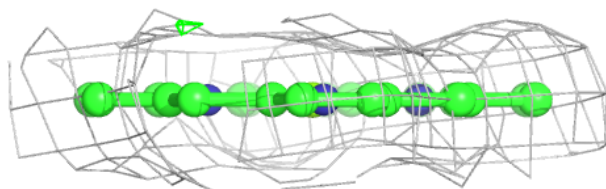
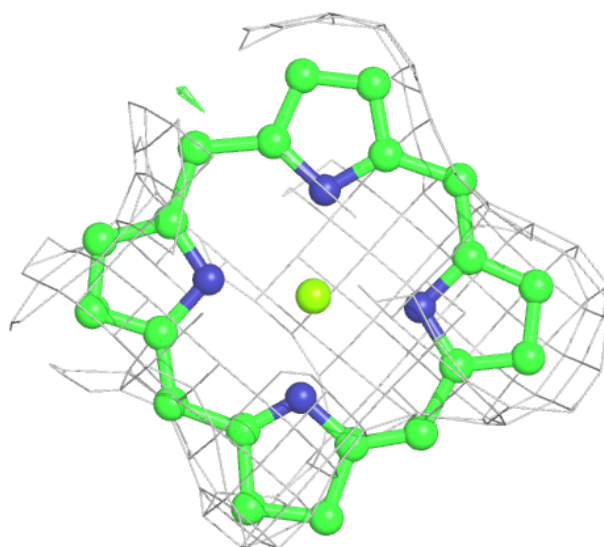
Electron density around CLA K 1150:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



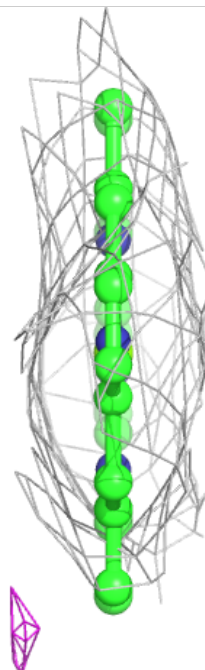
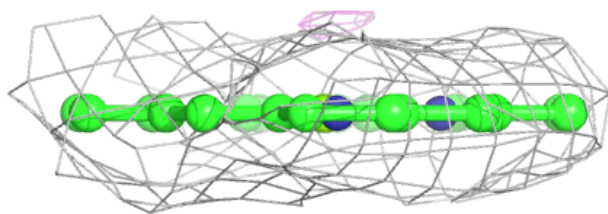
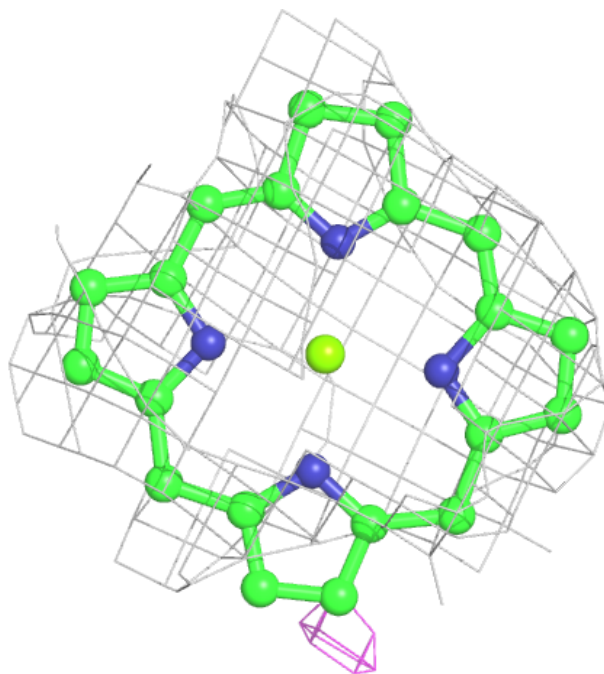
Electron density around CLA 4 4005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



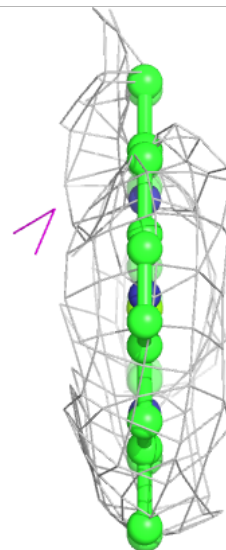
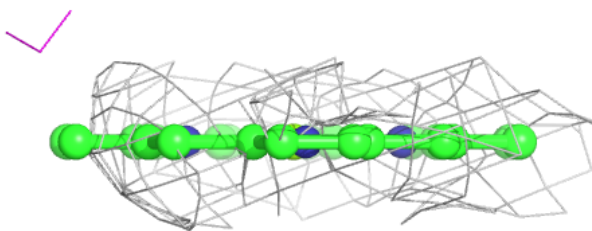
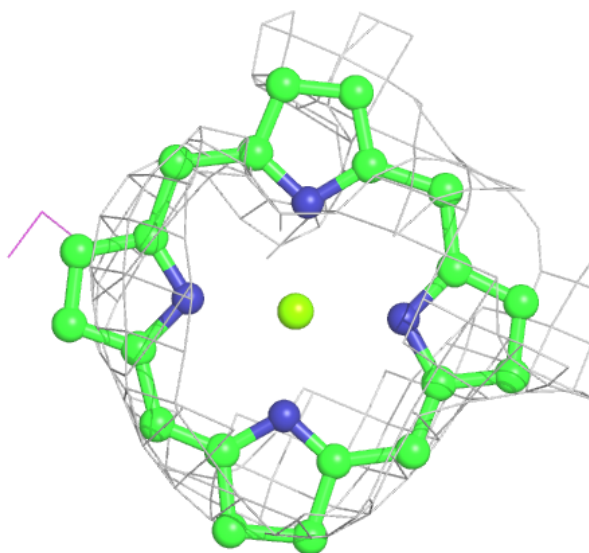
Electron density around CLA 2 2010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



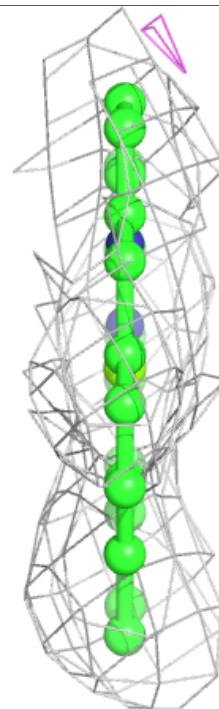
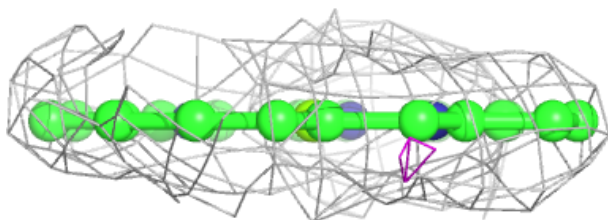
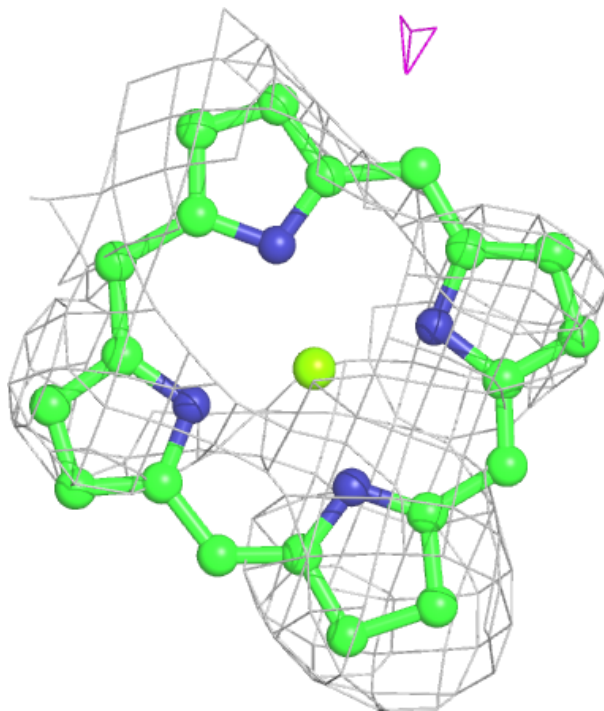
Electron density around CLA A 1309:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



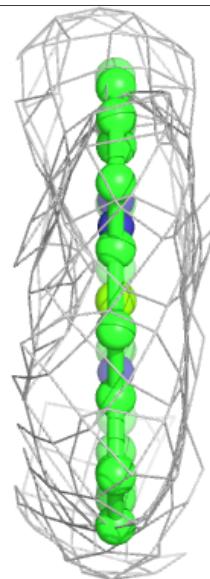
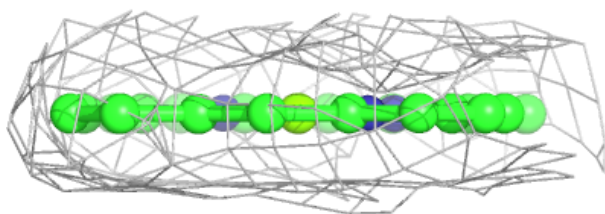
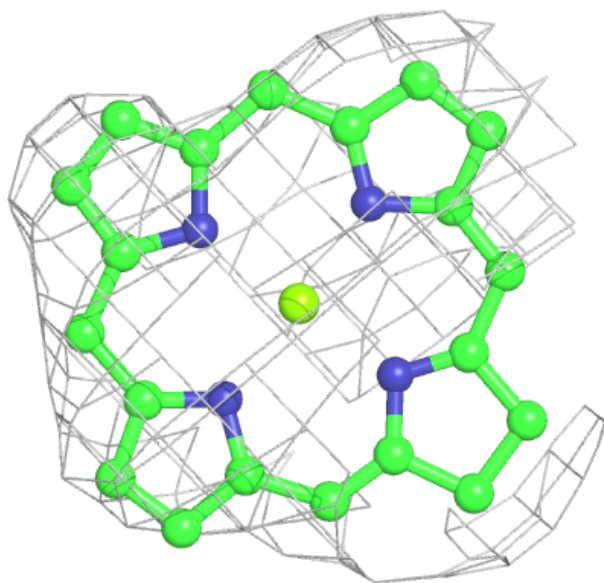
Electron density around CLA B 1230:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



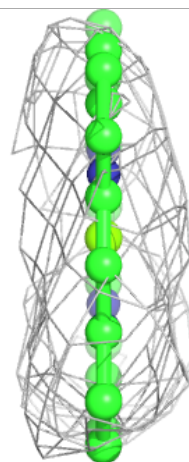
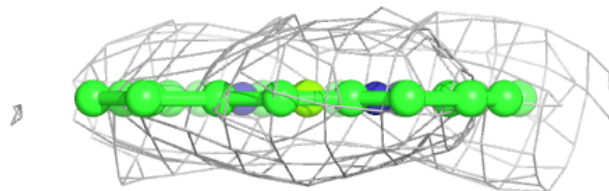
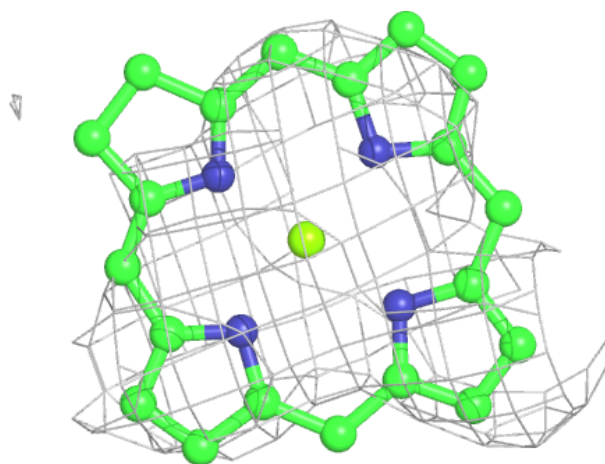
Electron density around CLA K 1153:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



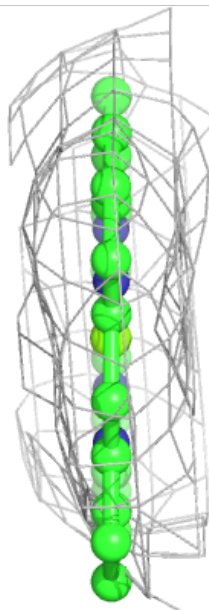
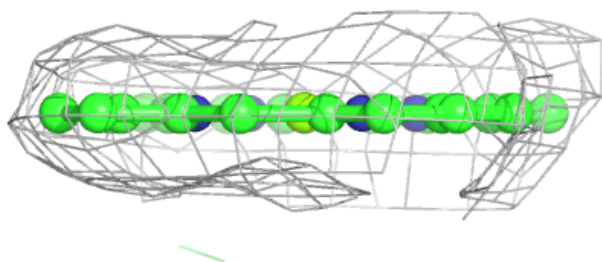
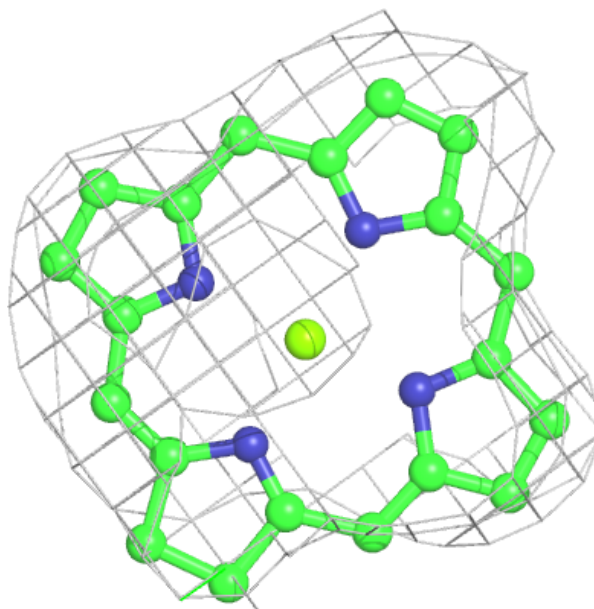
Electron density around CLA J 1307:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



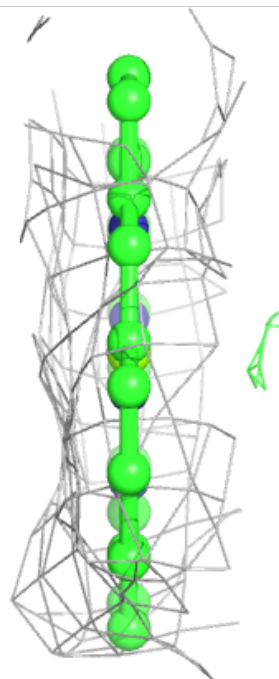
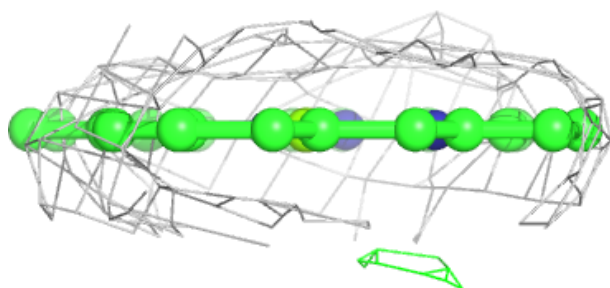
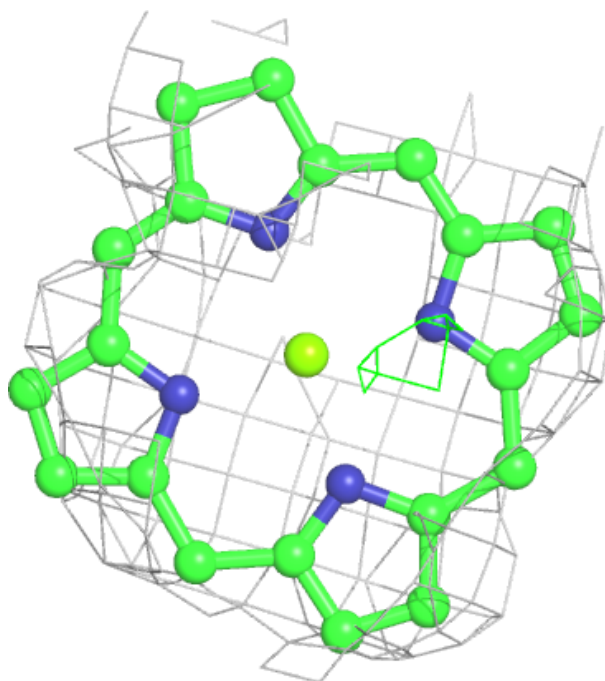
Electron density around CLA 4 4004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



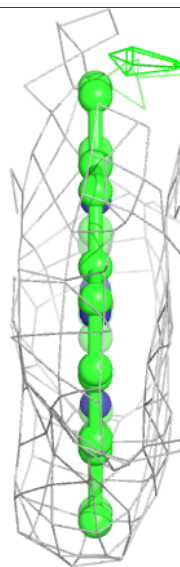
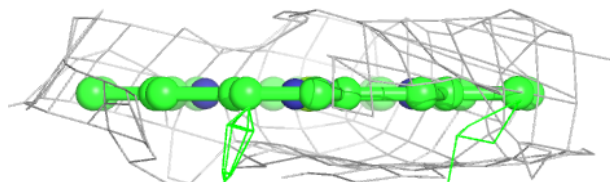
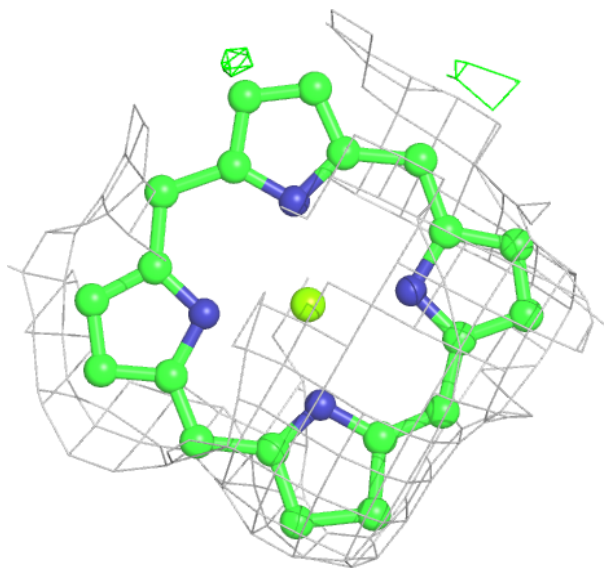
Electron density around CLA 1 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



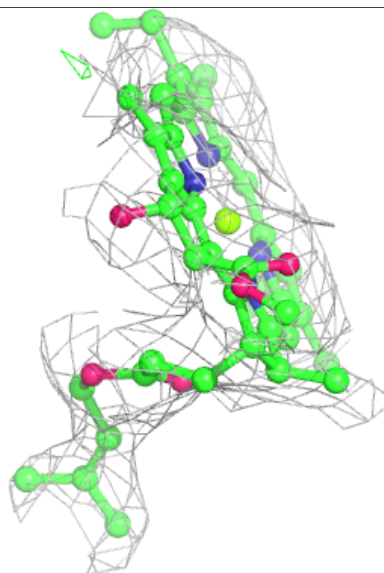
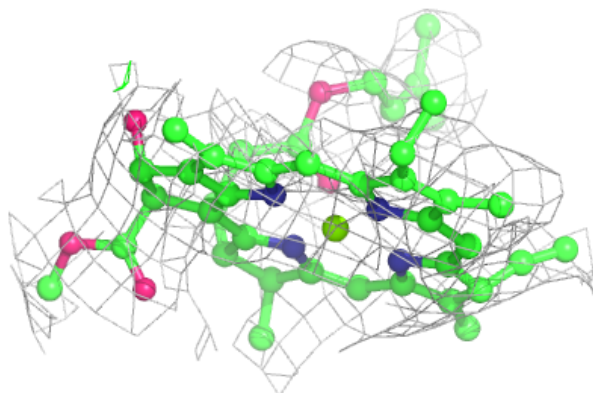
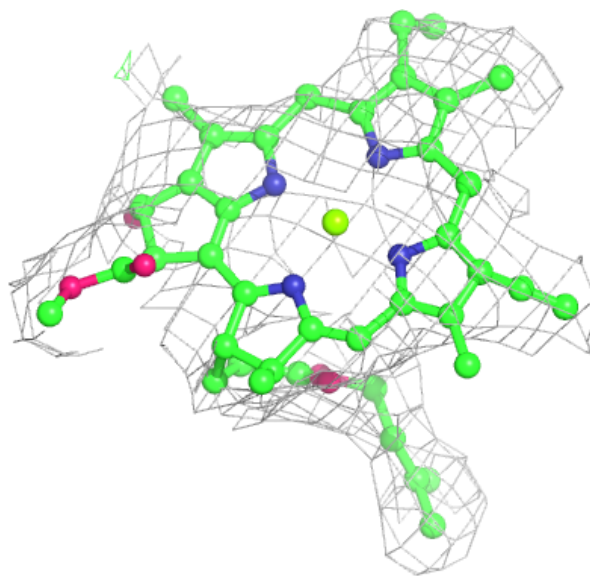
Electron density around CLA A 1110:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



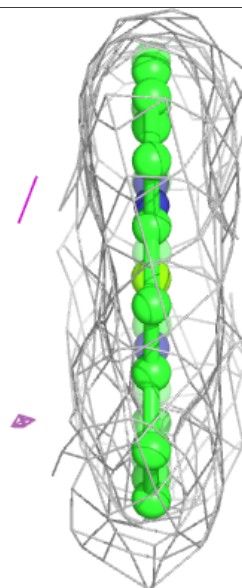
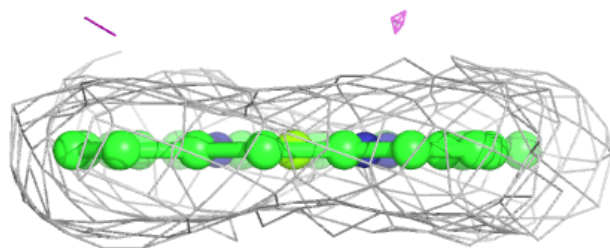
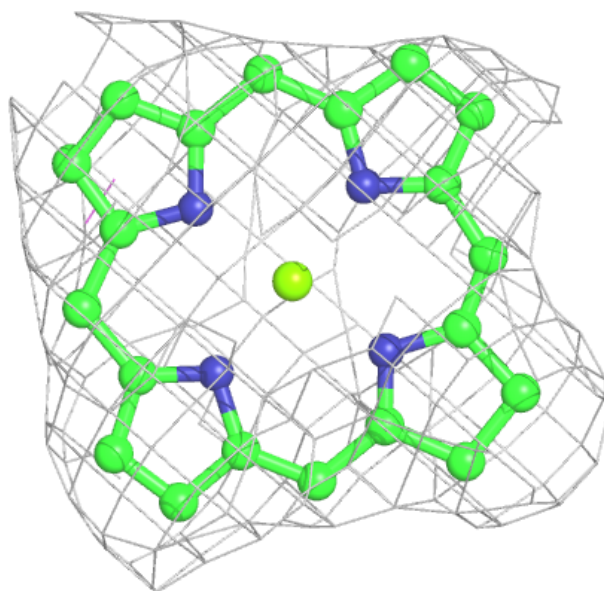
Electron density around CLA B 1217:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



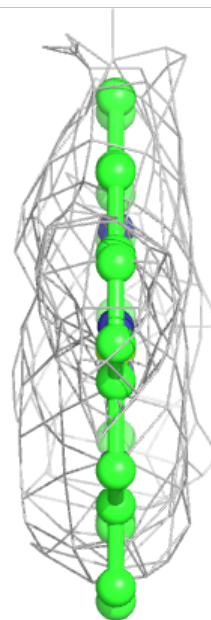
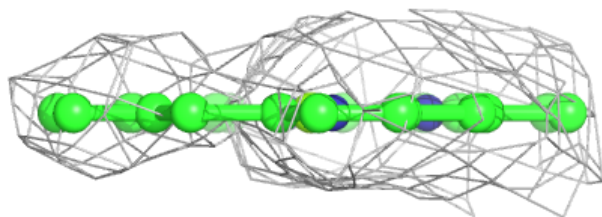
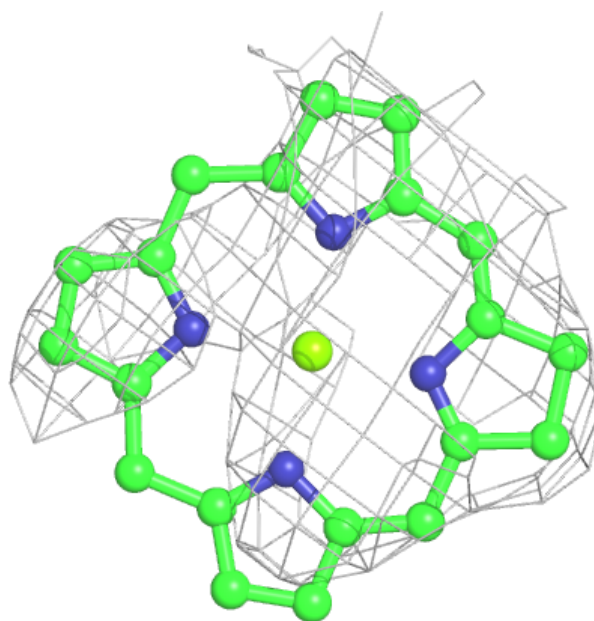
Electron density around CLA A 1104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



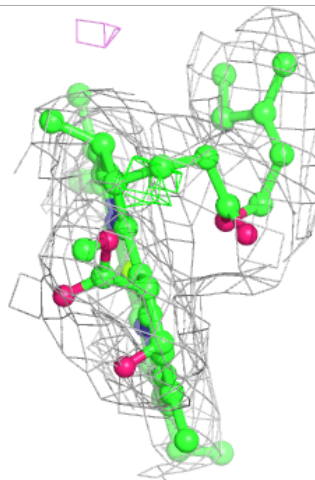
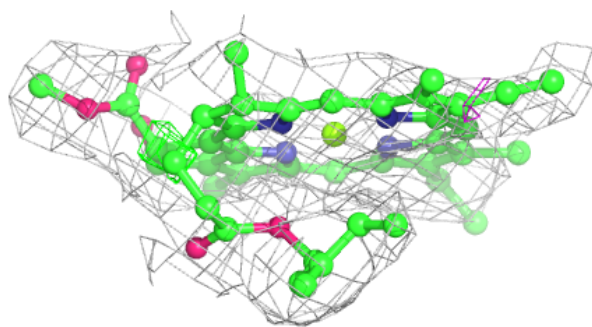
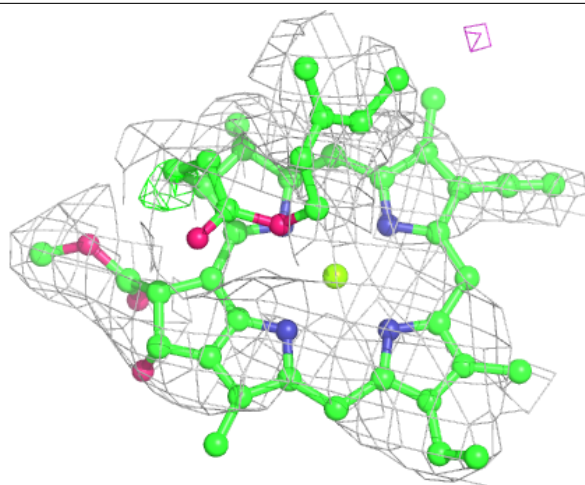
Electron density around CLA B 1241:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



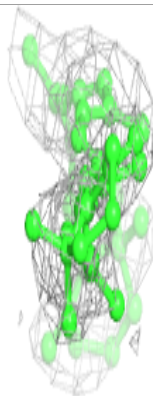
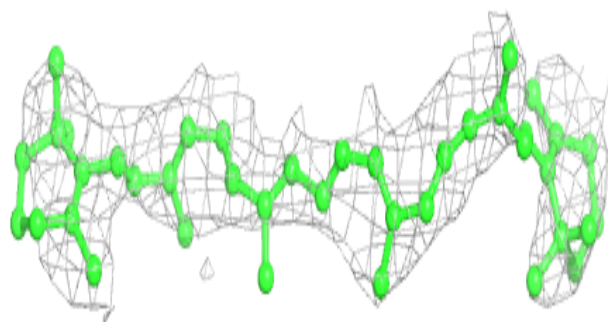
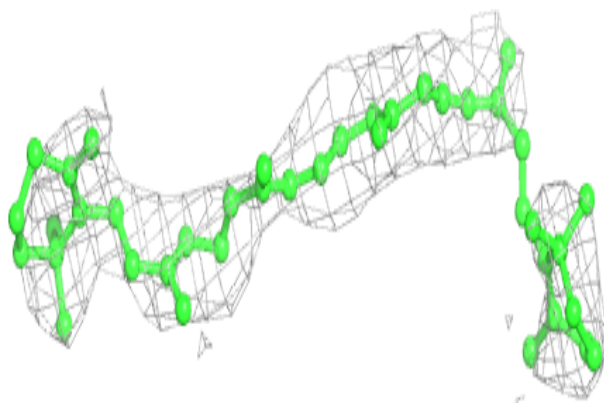
Electron density around CLA B 1237:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



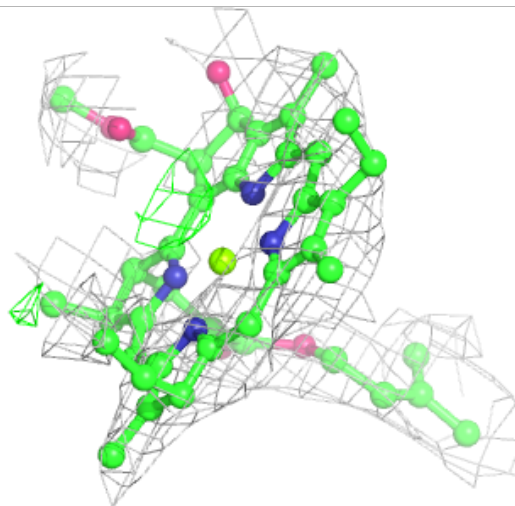
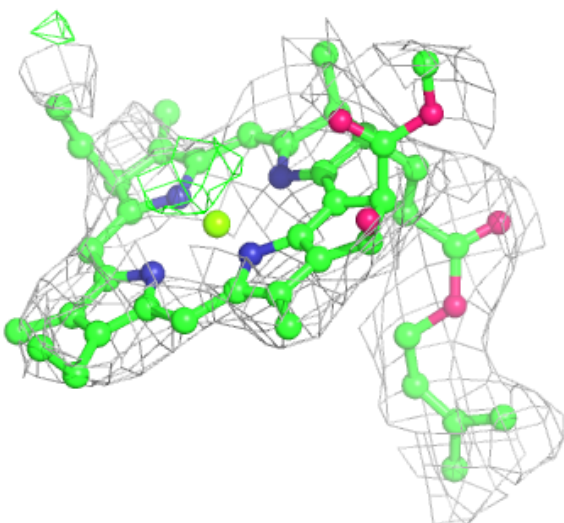
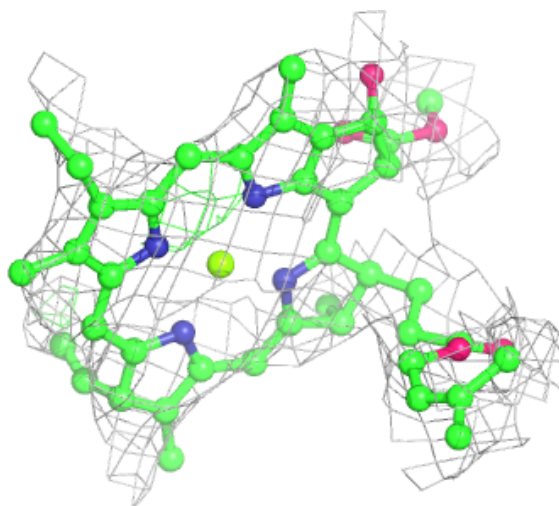
Electron density around BCR B 6017:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



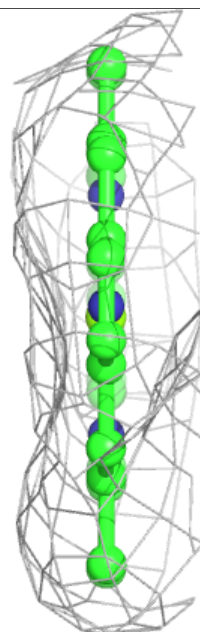
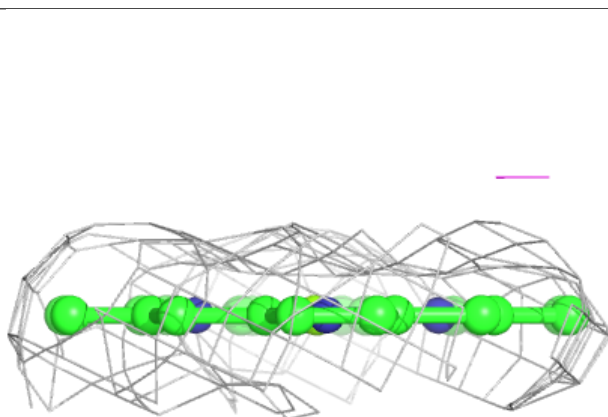
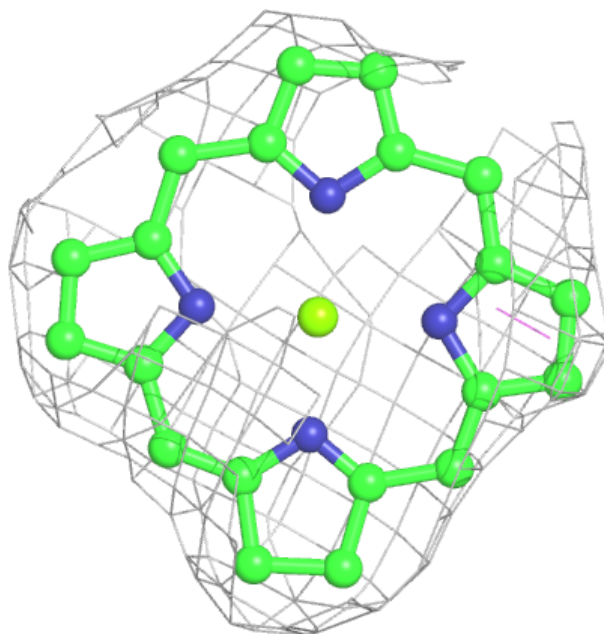
Electron density around CLA L 1130:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



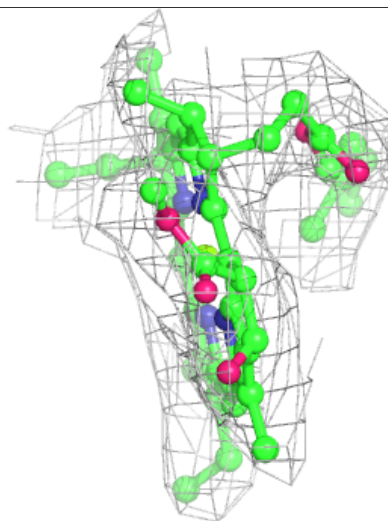
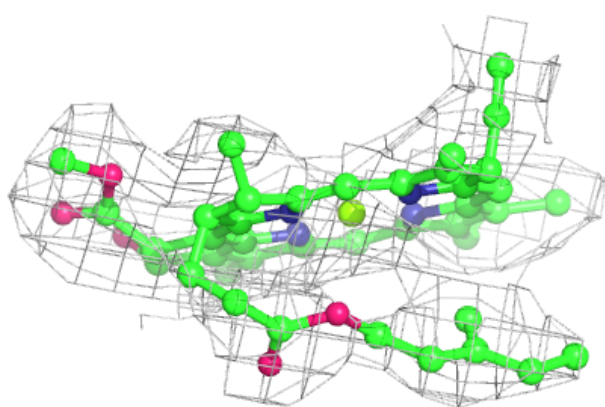
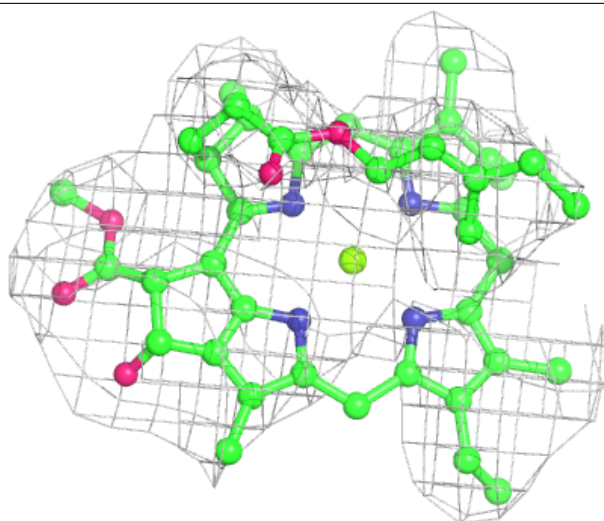
Electron density around CLA 2 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



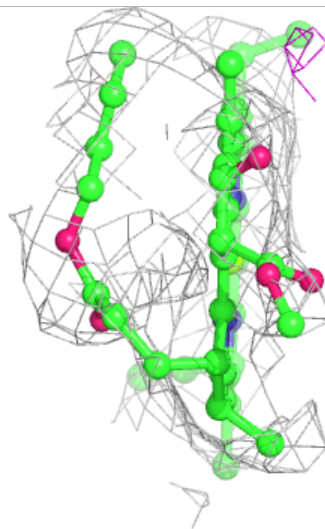
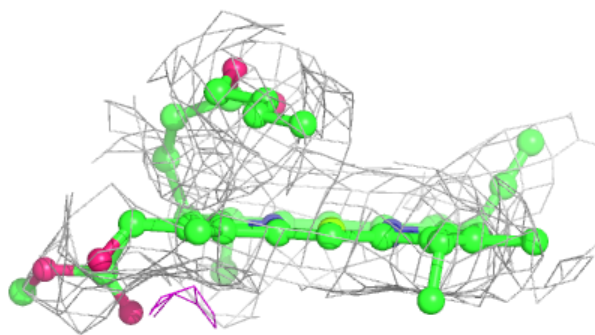
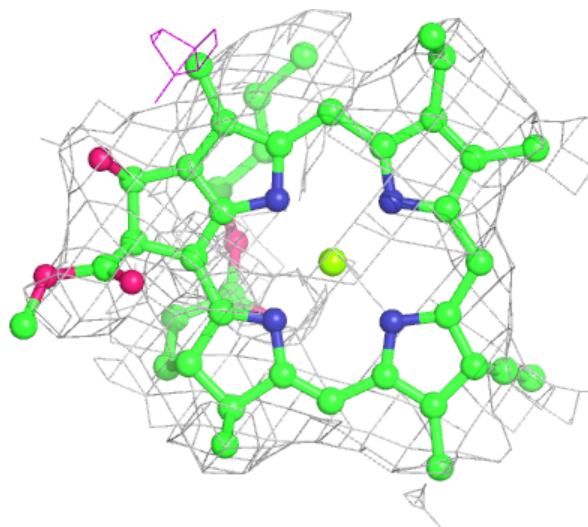
Electron density around CLA B 1219:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



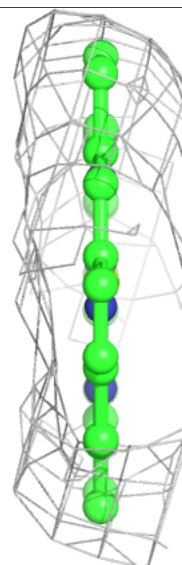
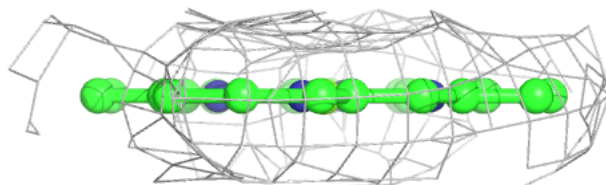
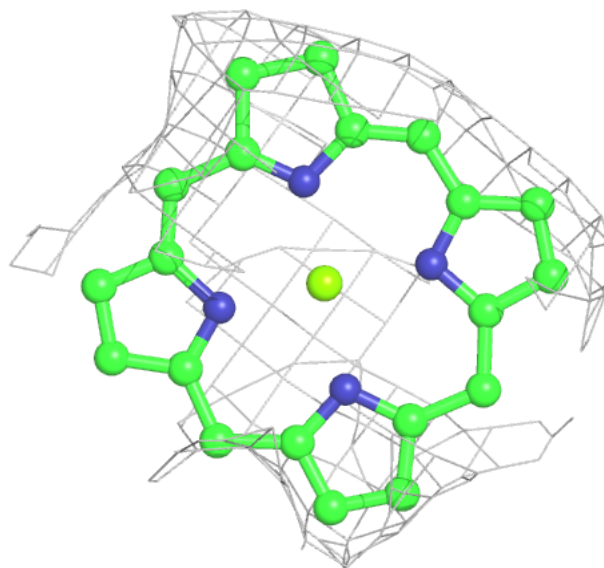
Electron density around CLA B 1214:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



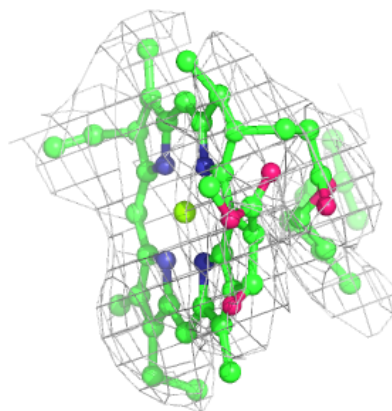
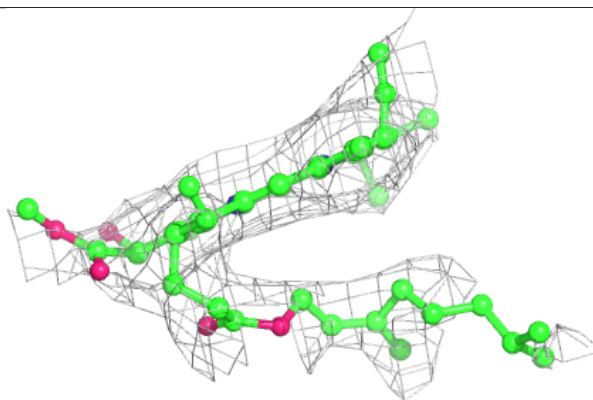
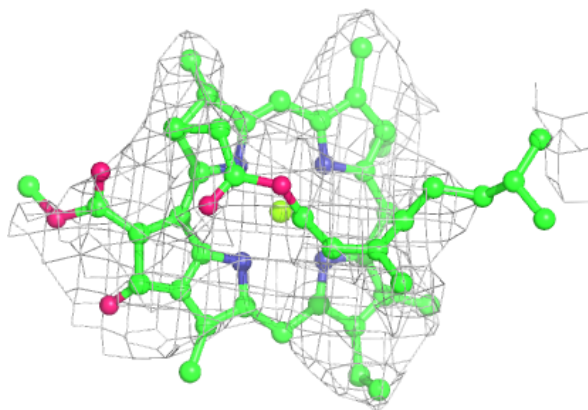
Electron density around CLA 1 1014:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



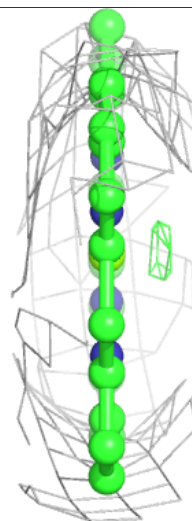
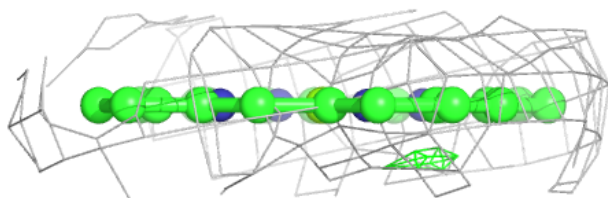
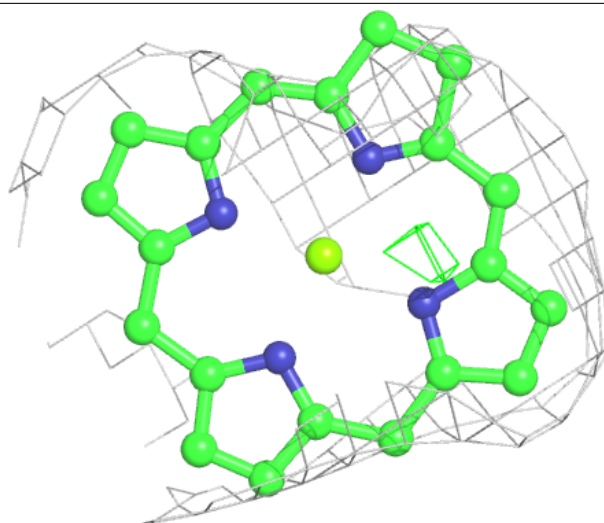
Electron density around CLA A 1136:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



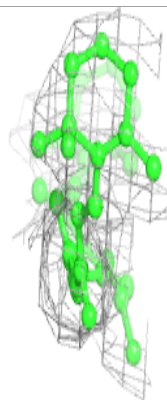
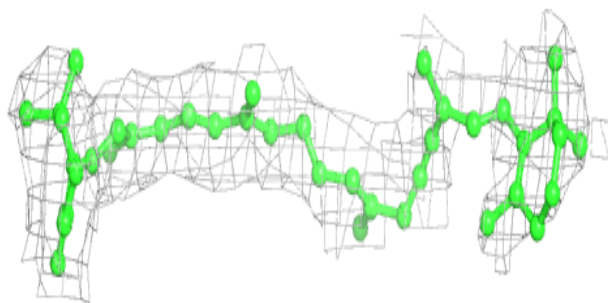
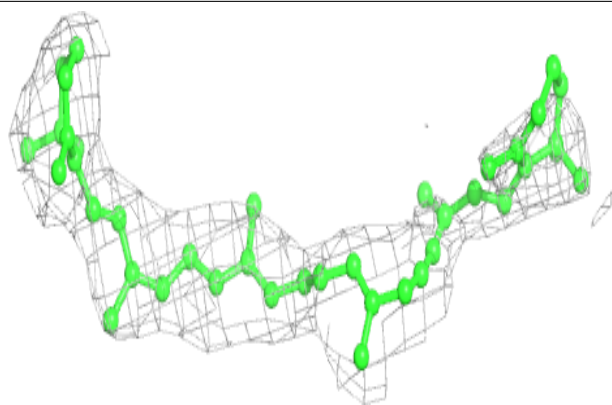
Electron density around CLA B 1211:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



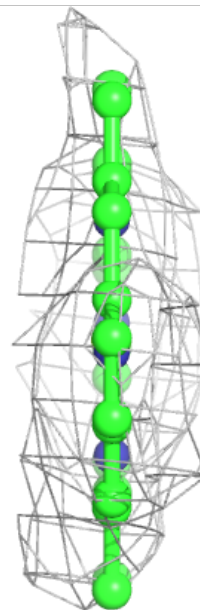
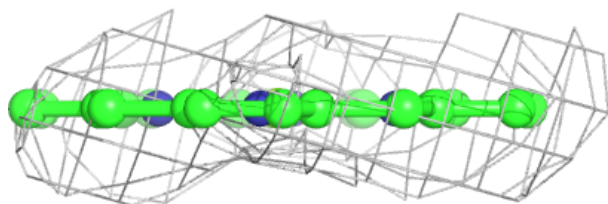
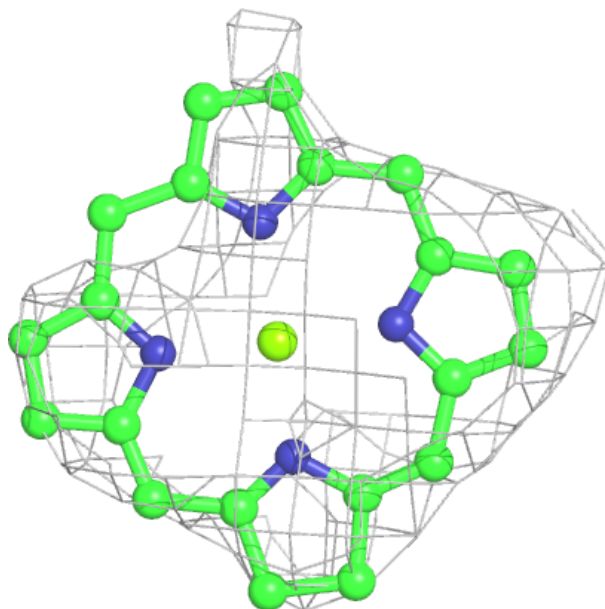
Electron density around BCR L 6020:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



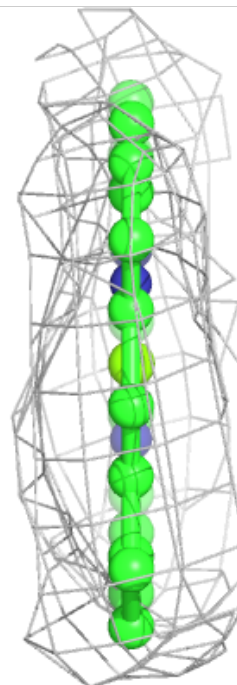
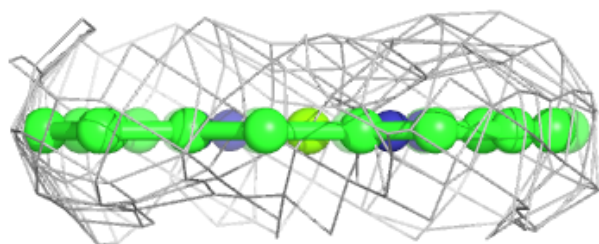
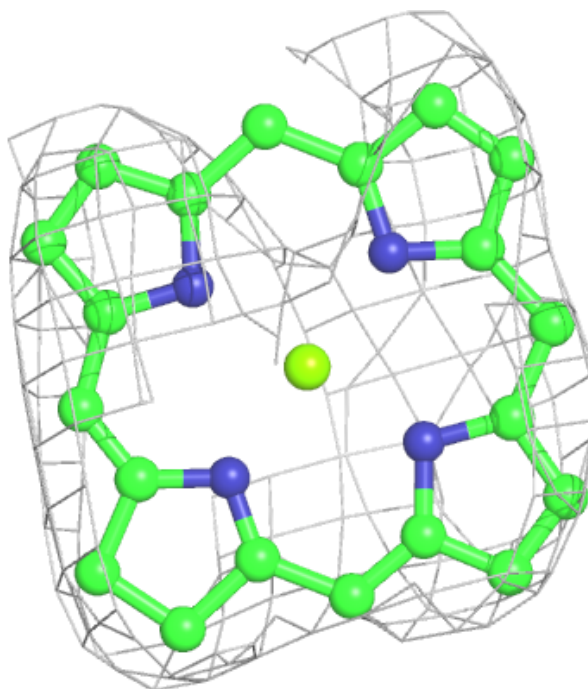
Electron density around CLA 4 4008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



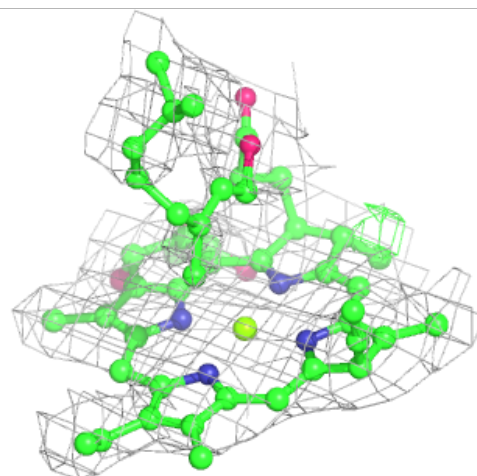
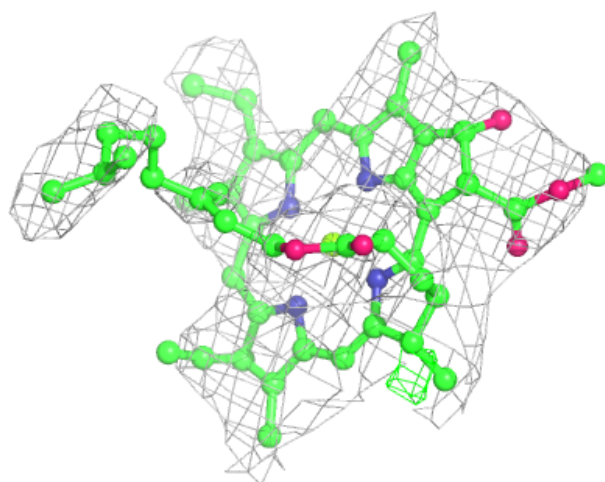
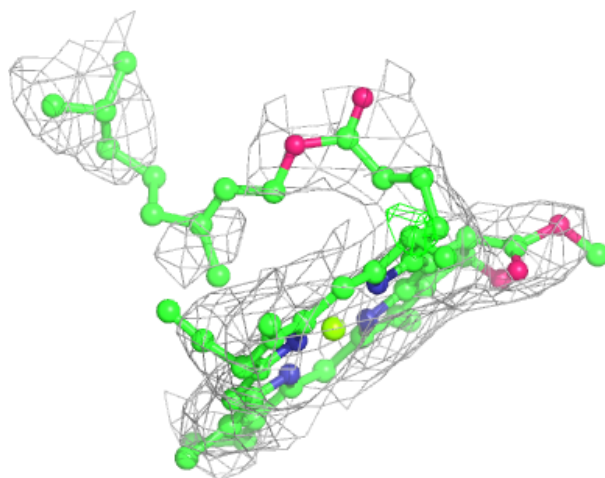
Electron density around CLA A 1146:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



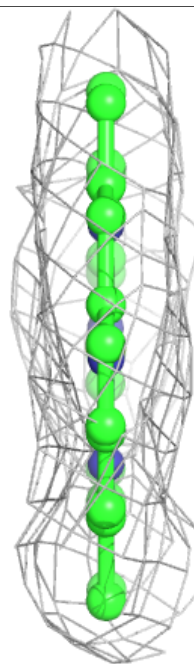
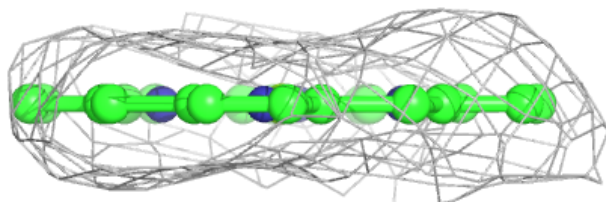
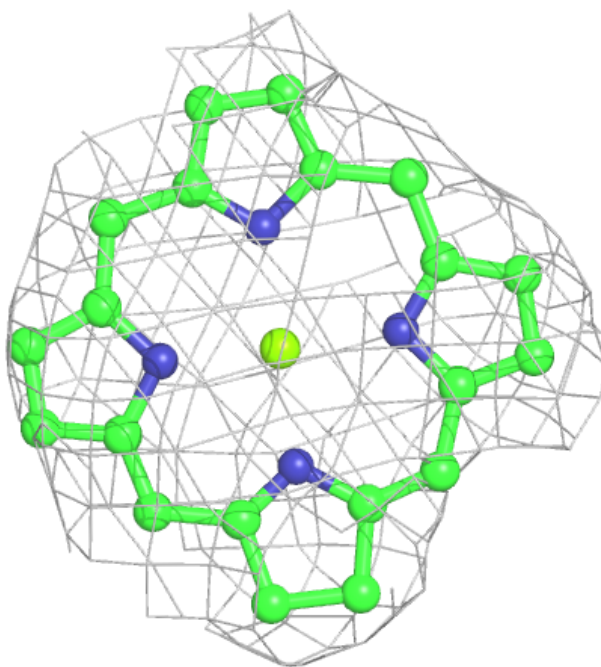
Electron density around CLA I 1204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



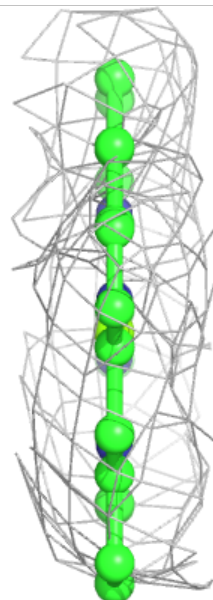
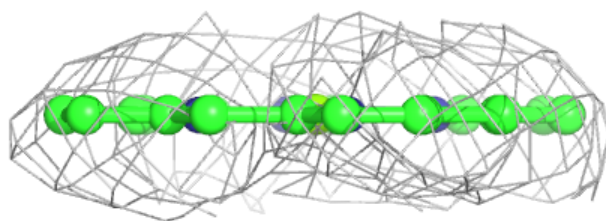
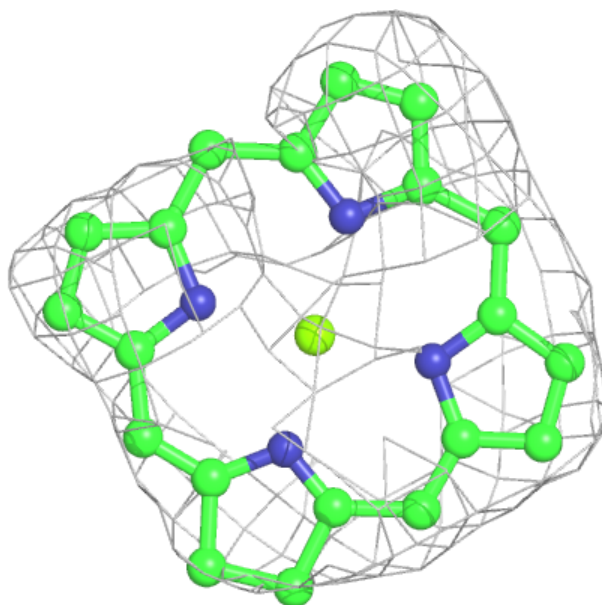
Electron density around CLA A 1117:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



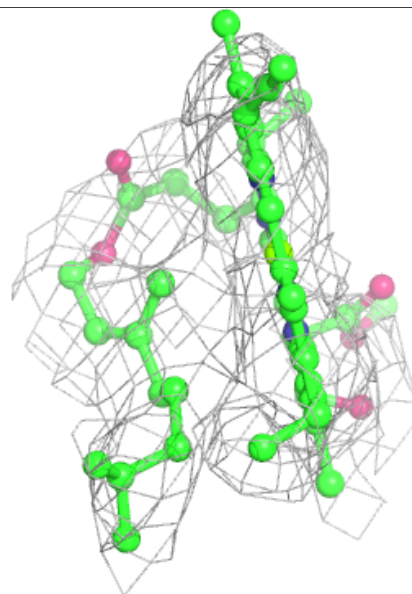
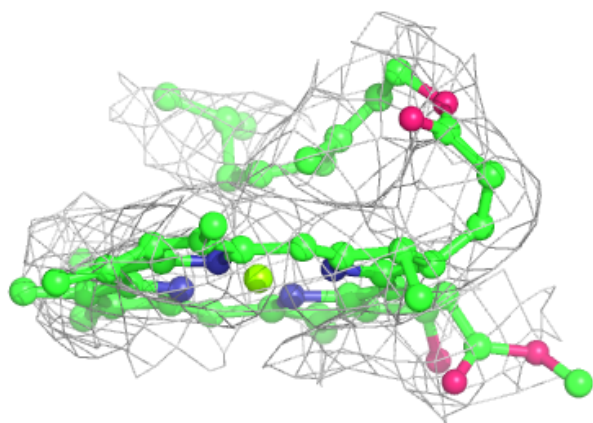
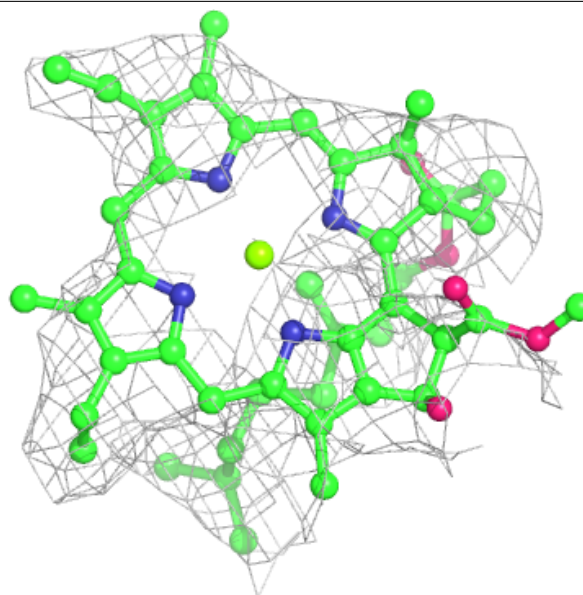
Electron density around CLA B 1213:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



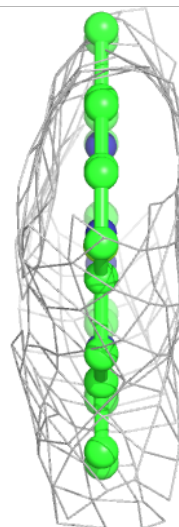
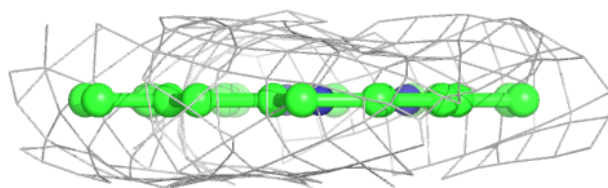
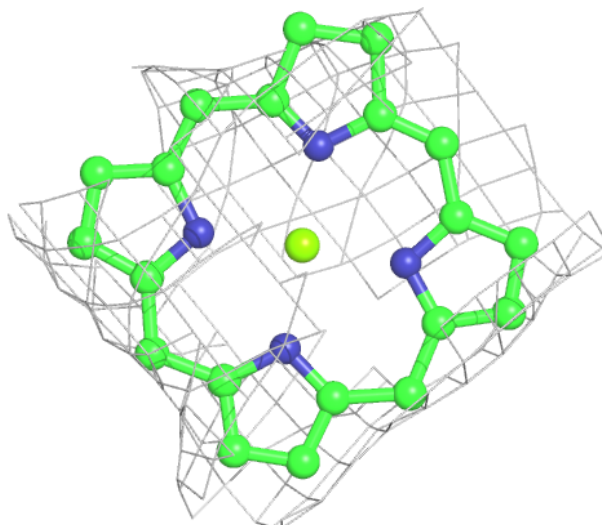
Electron density around CLA H 1501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



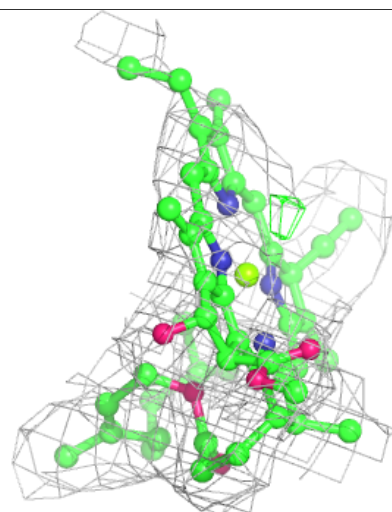
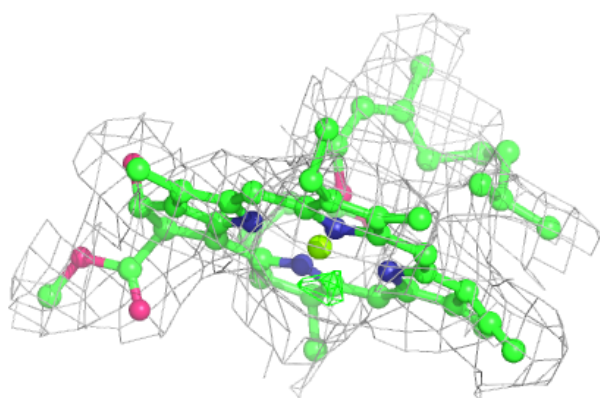
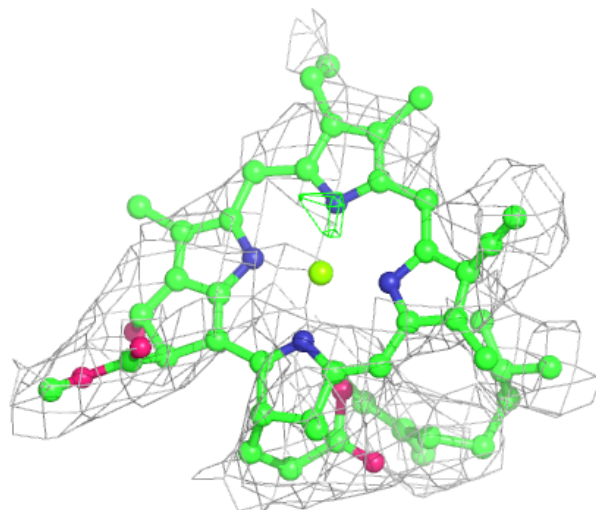
Electron density around CLA 4 4009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



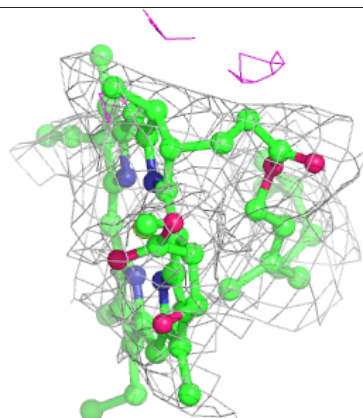
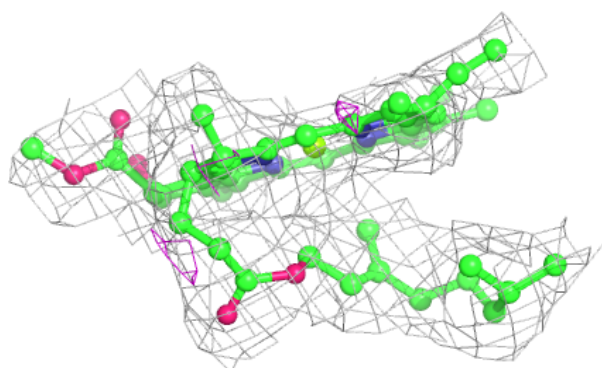
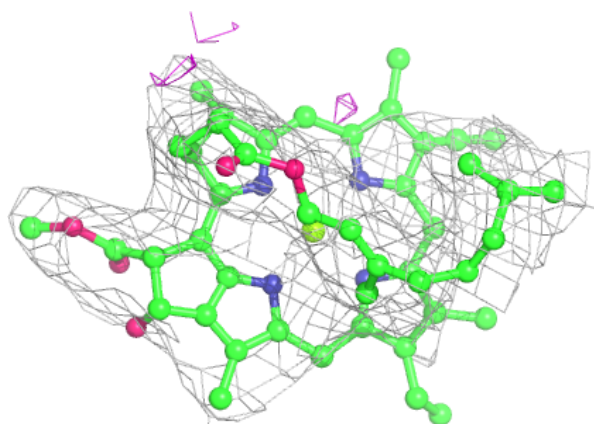
Electron density around CLA B 1209:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

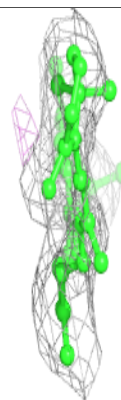
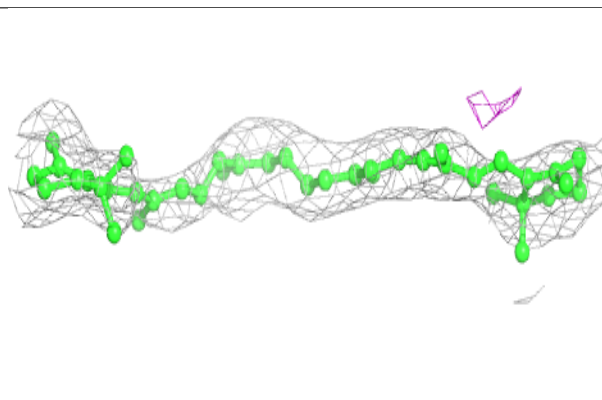
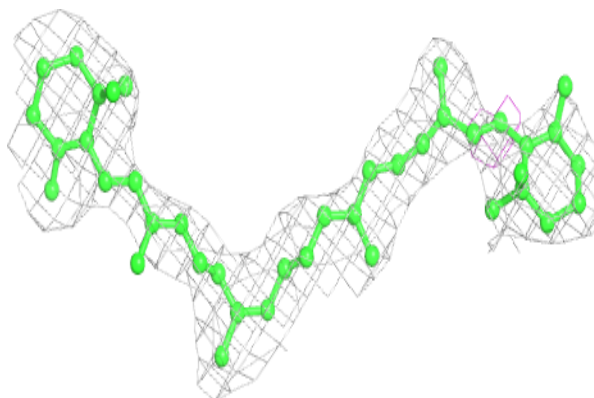


Electron density around CLA A 1140:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

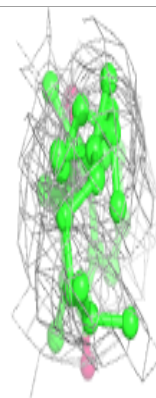
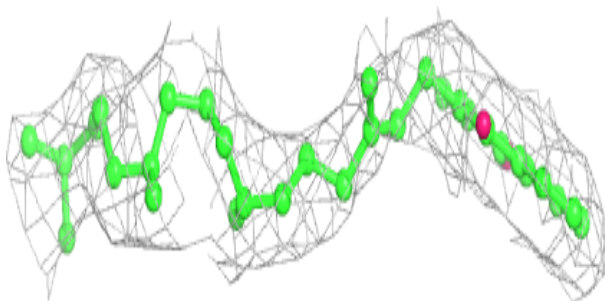
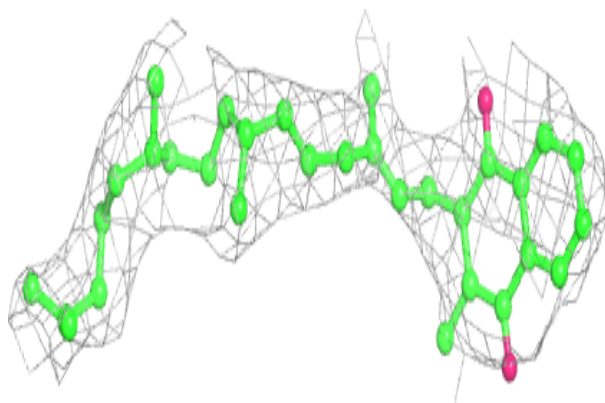
**Electron density around BCR A 6011:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



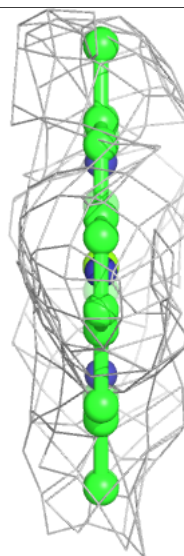
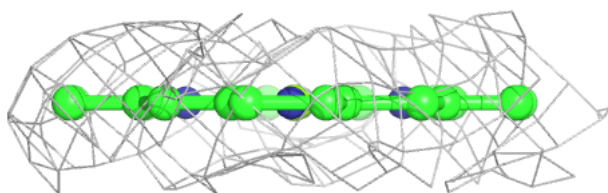
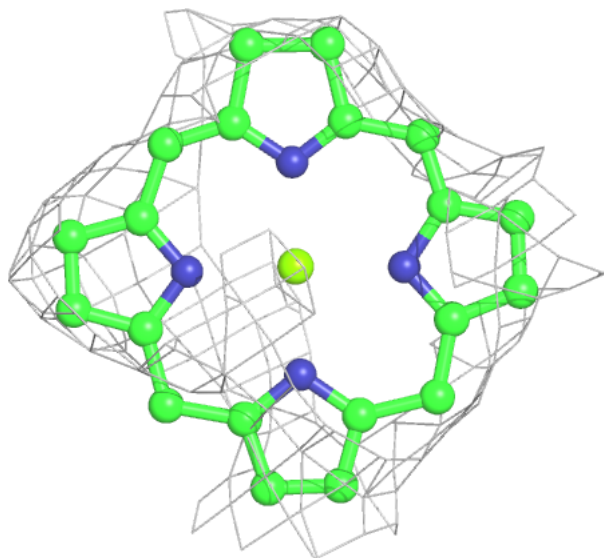
Electron density around PQN A 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



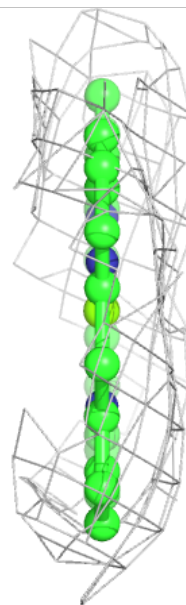
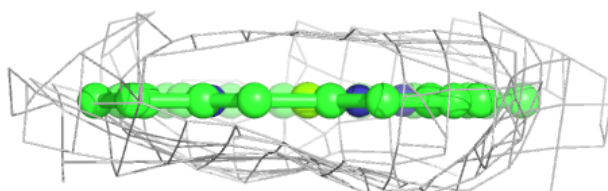
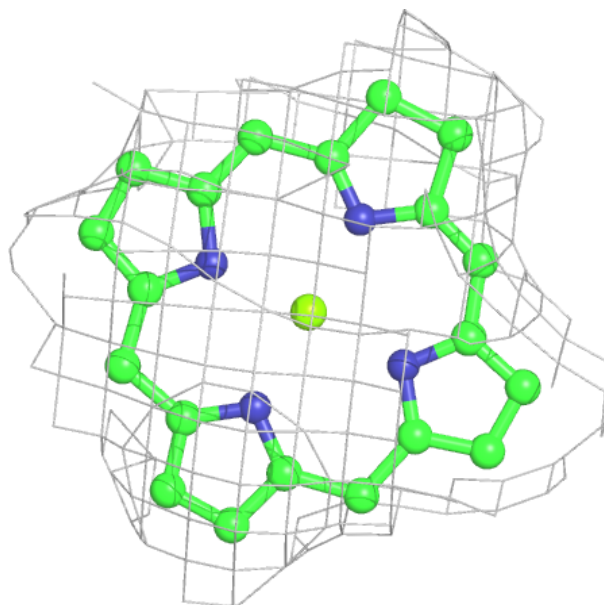
Electron density around CLA 2 2003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



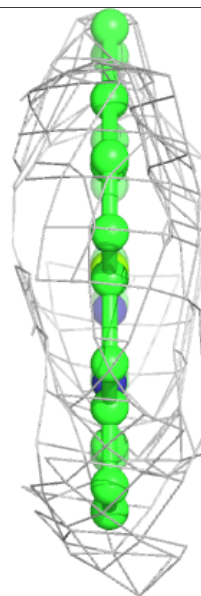
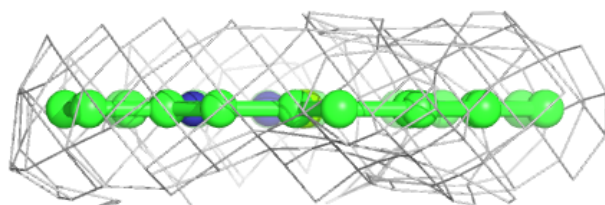
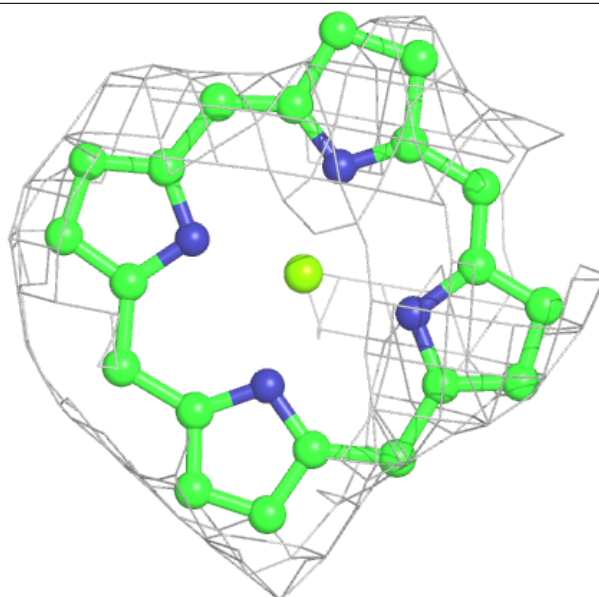
Electron density around CLA 3 3003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



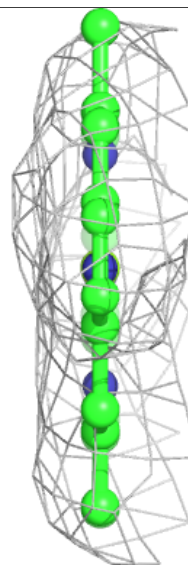
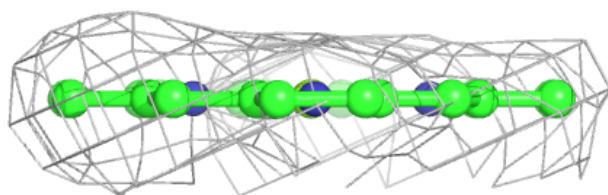
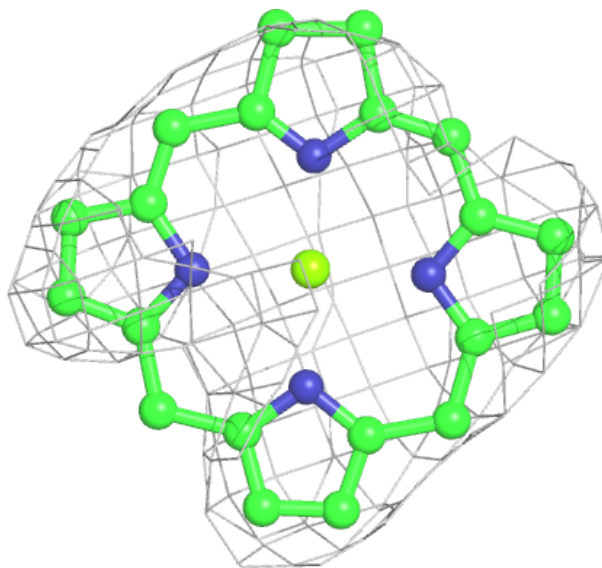
Electron density around CLA A 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



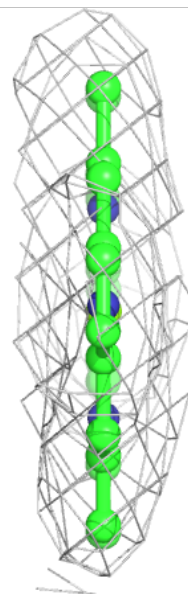
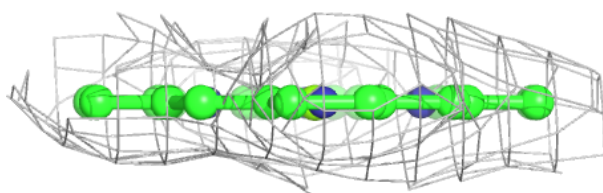
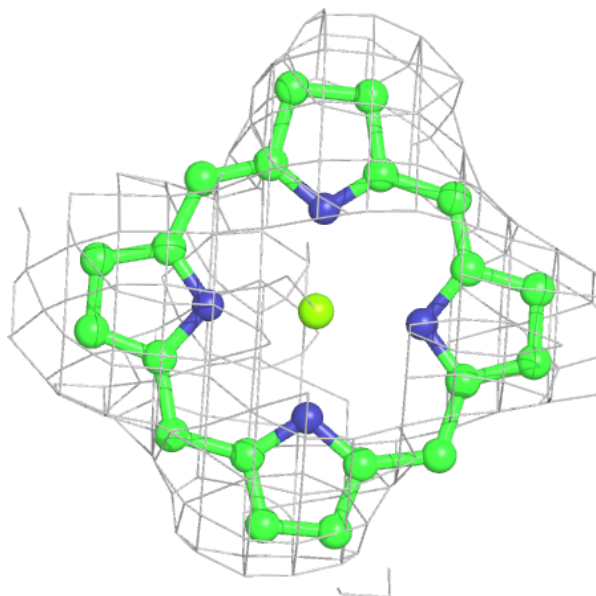
Electron density around CLA 3 3004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



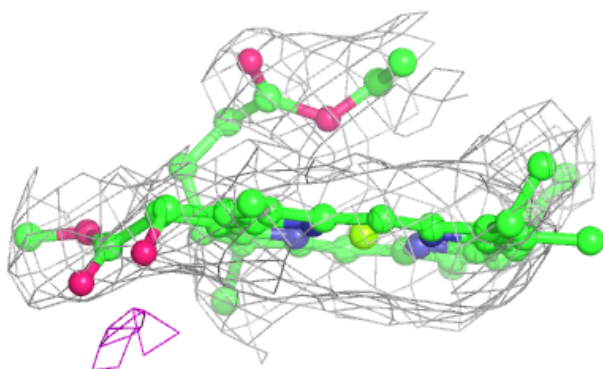
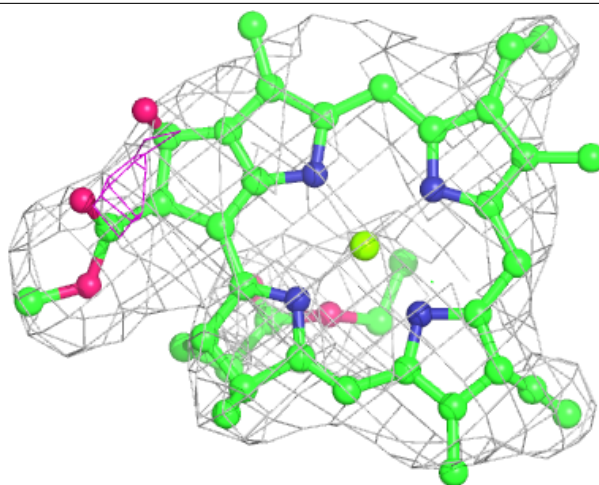
Electron density around CLA B 1223:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



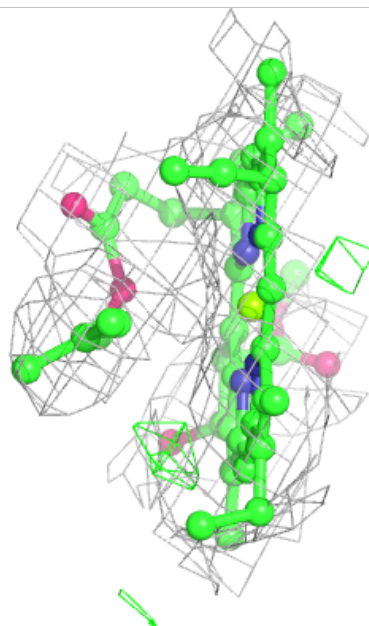
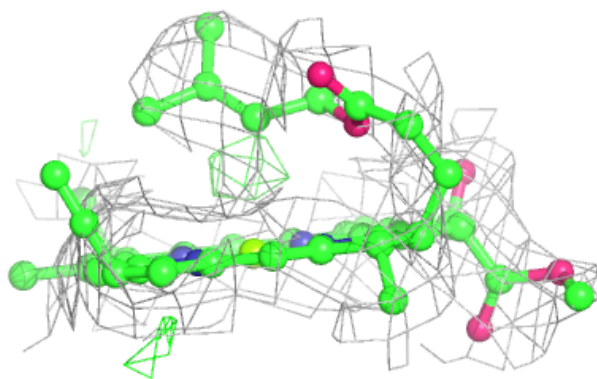
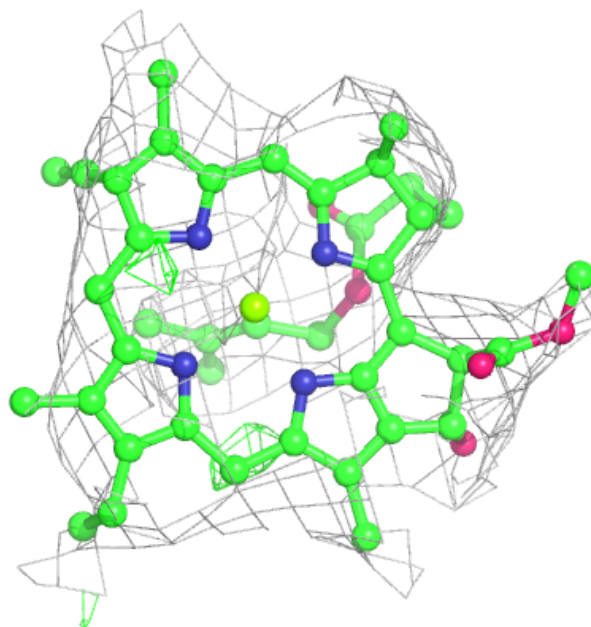
Electron density around CLA A 1115:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



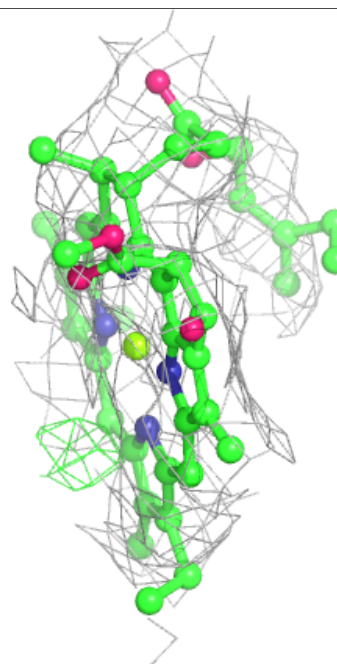
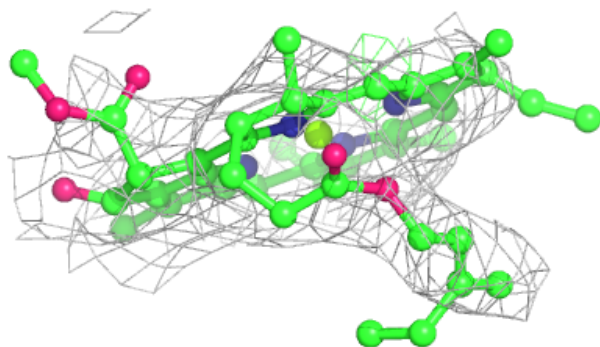
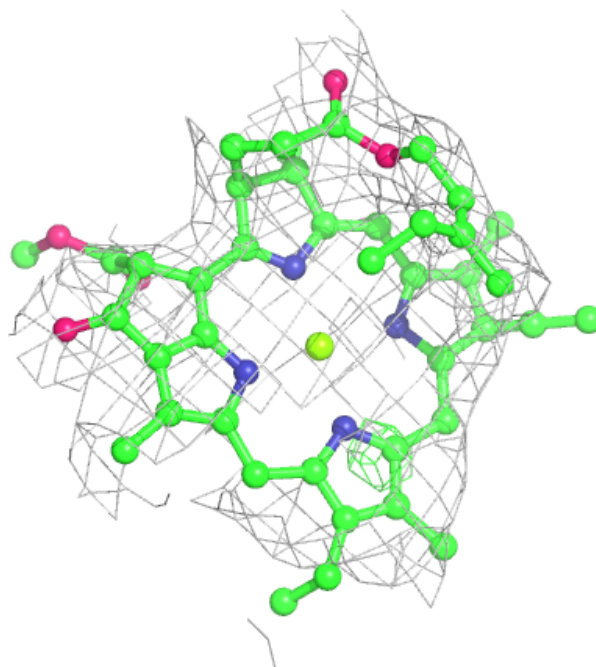
Electron density around CLA A 1108:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



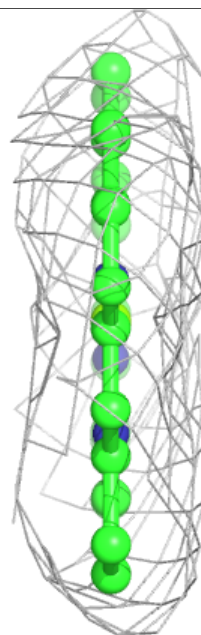
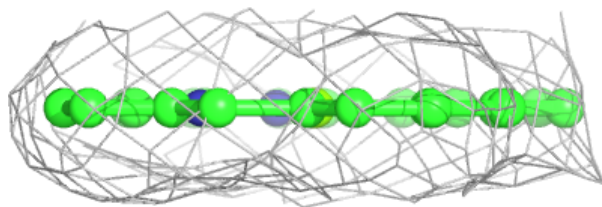
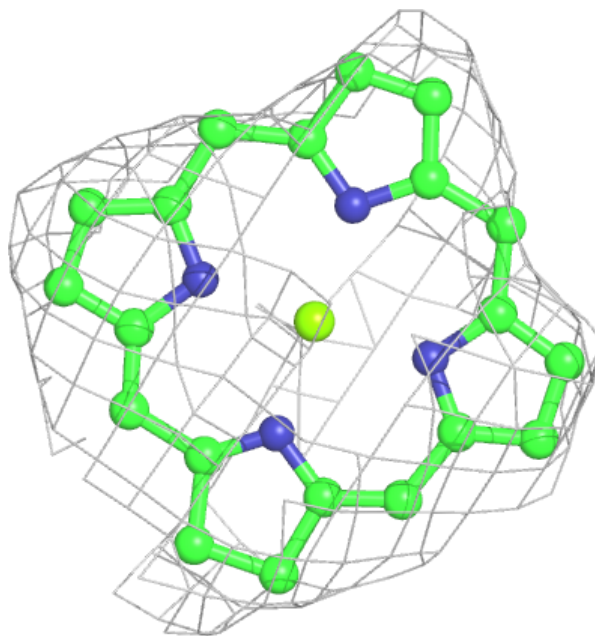
Electron density around CLA B 1224:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



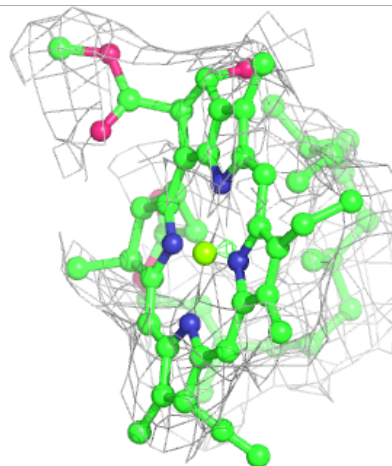
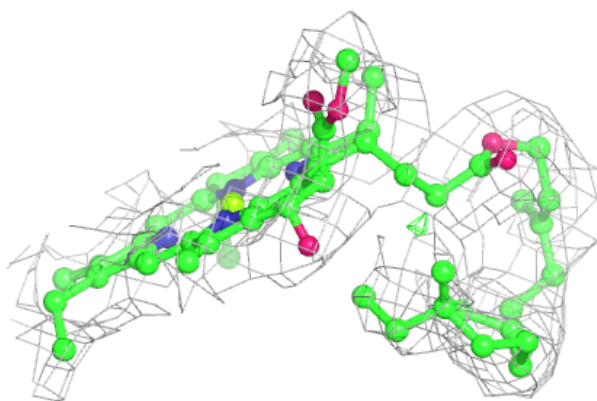
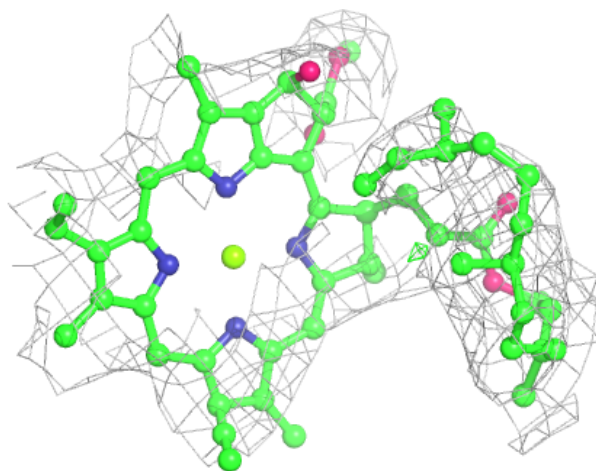
Electron density around CLA 2 2013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



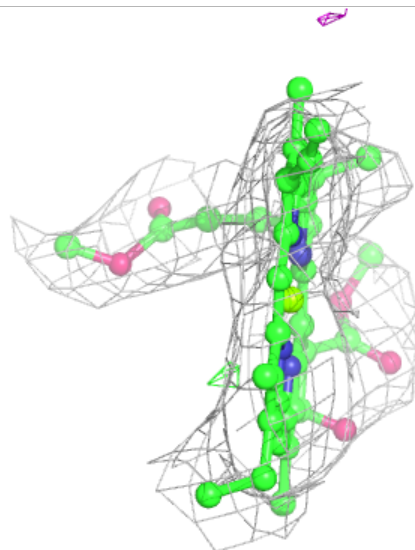
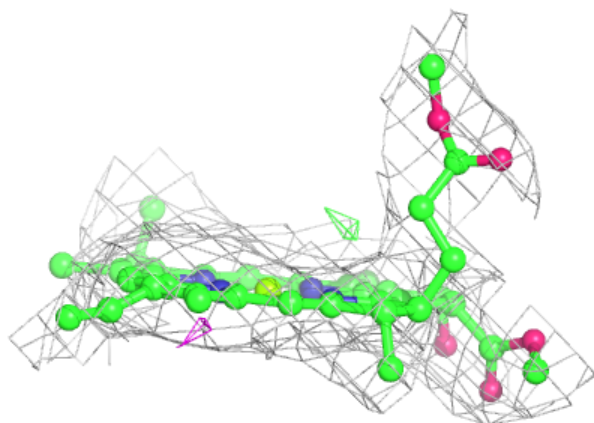
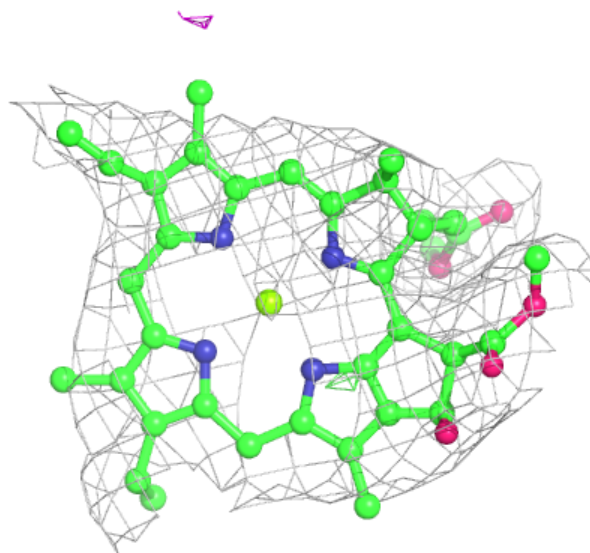
Electron density around CLA J 2107:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



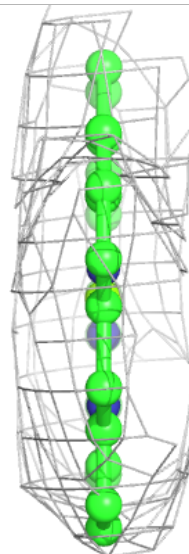
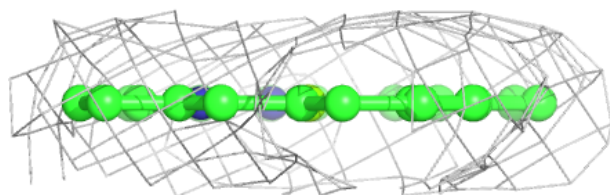
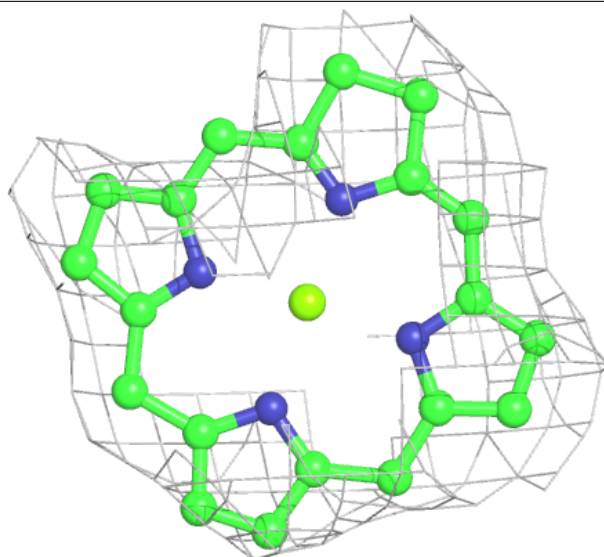
Electron density around CLA B 1236:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



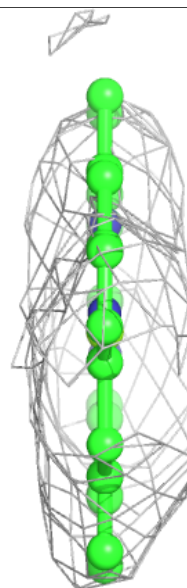
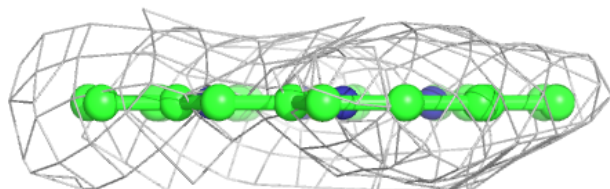
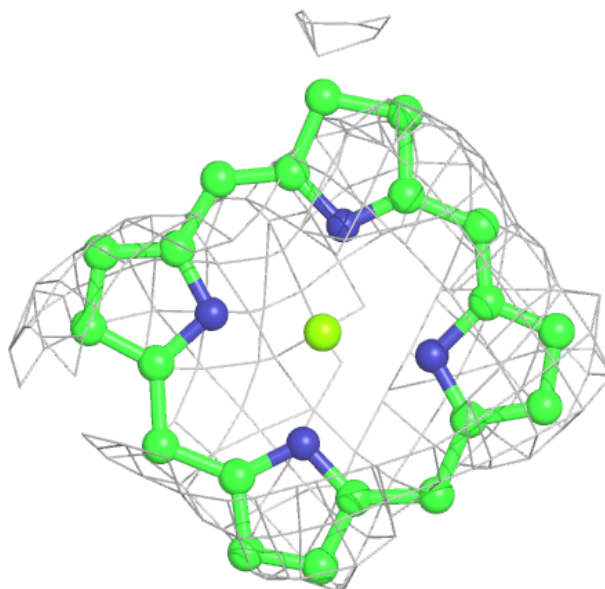
Electron density around CLA 4 4002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



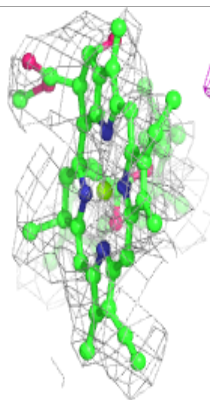
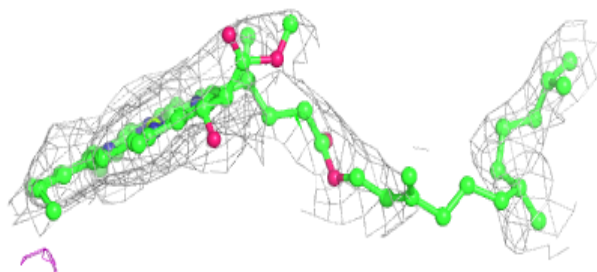
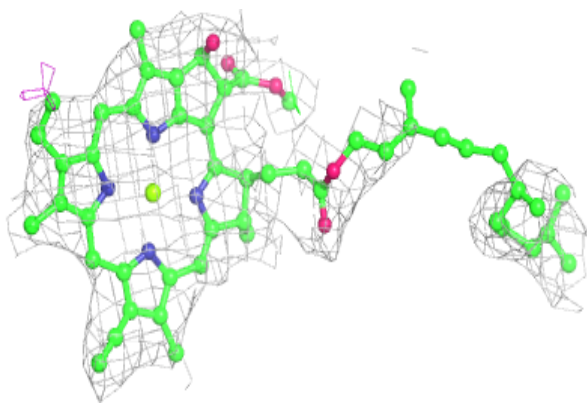
Electron density around CLA 1 1012:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



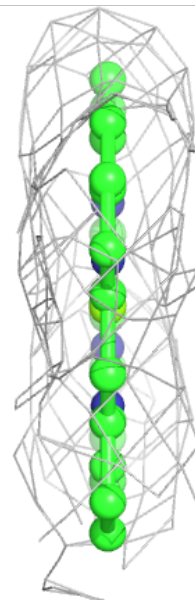
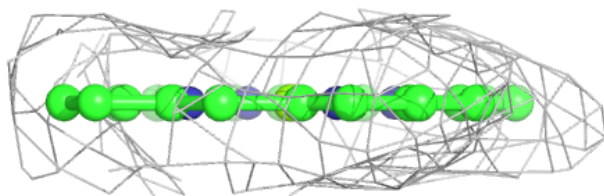
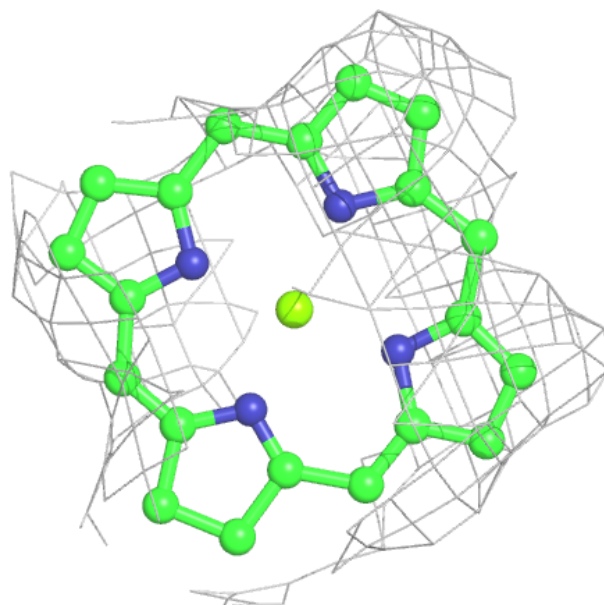
Electron density around CLA B 1220:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



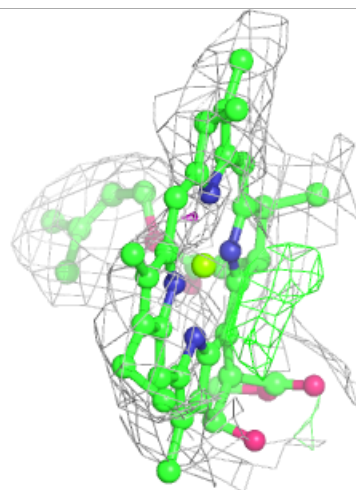
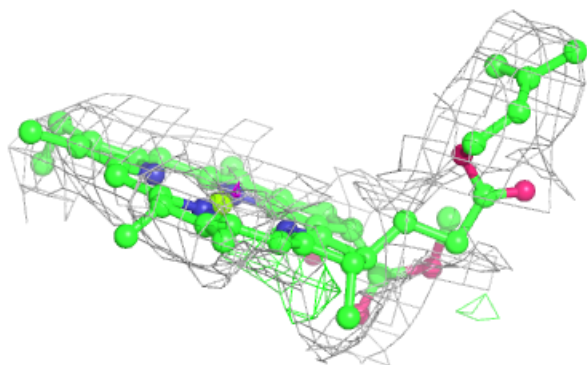
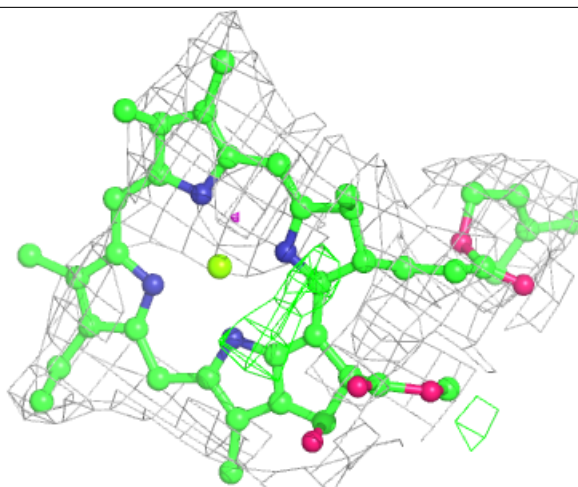
Electron density around CLA 3 3015:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



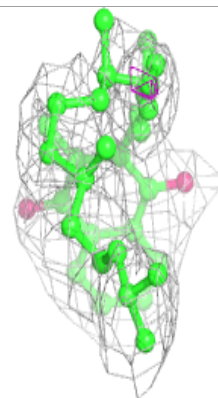
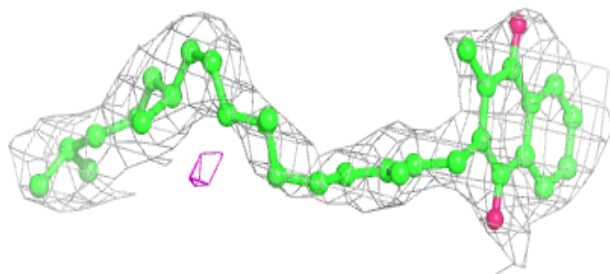
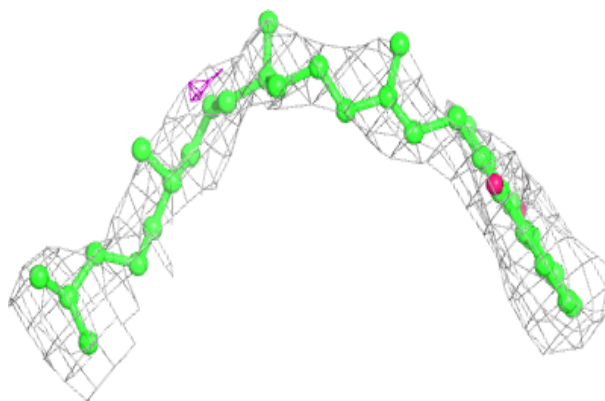
Electron density around CLA B 1229:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



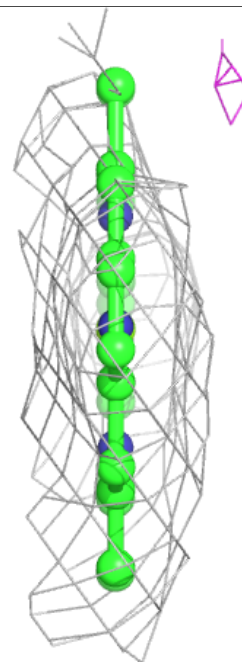
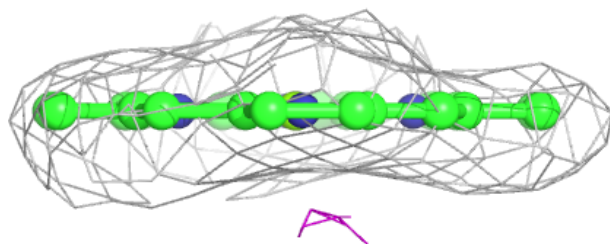
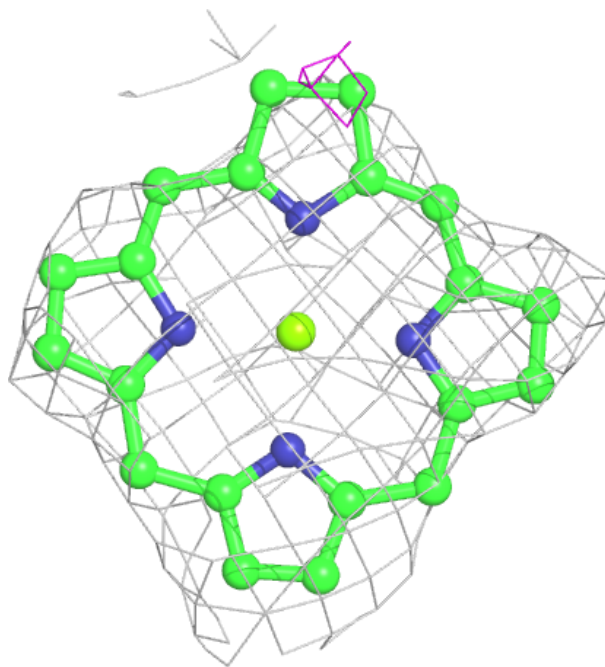
Electron density around PQN B 5002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



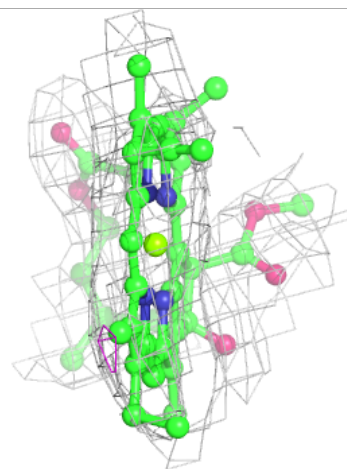
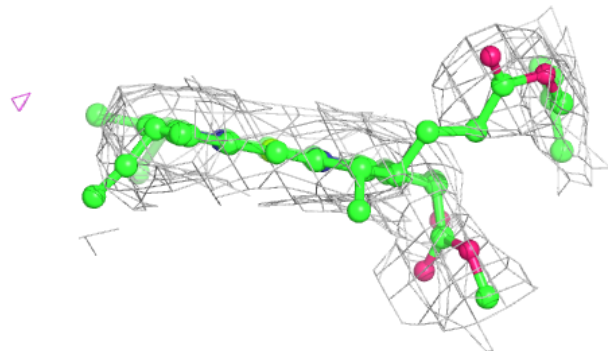
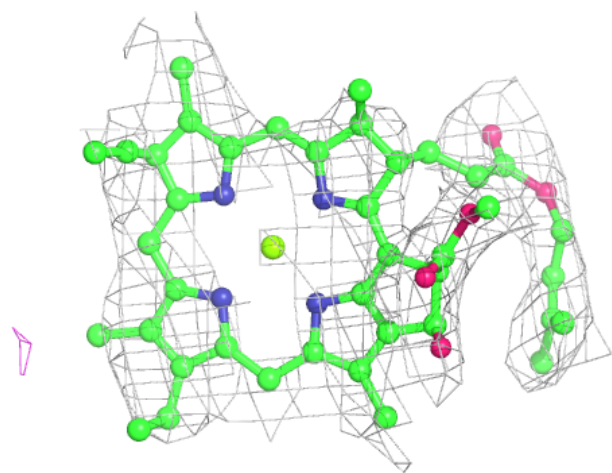
Electron density around CLA 3 3013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



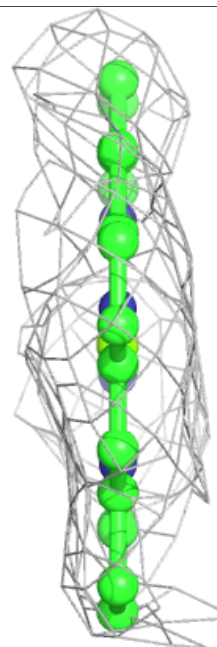
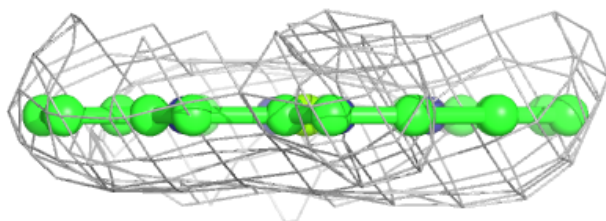
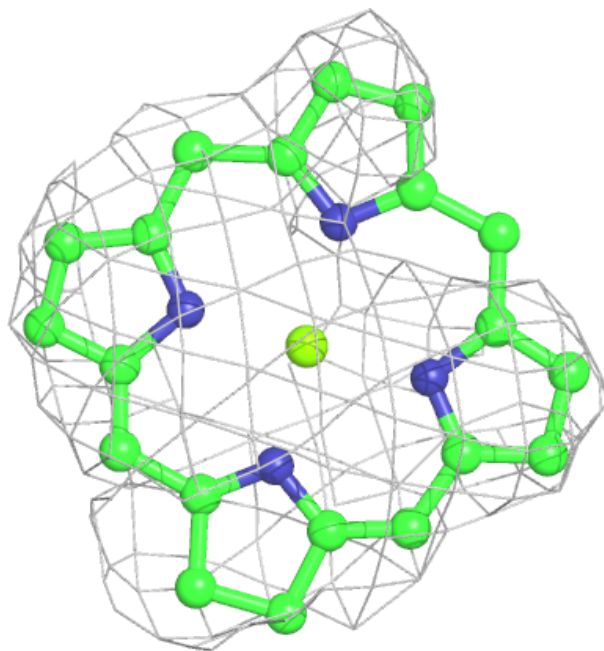
Electron density around CLA B 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



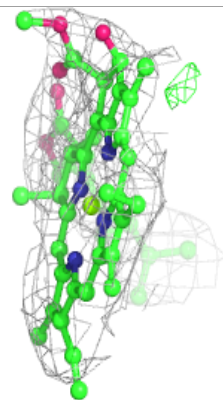
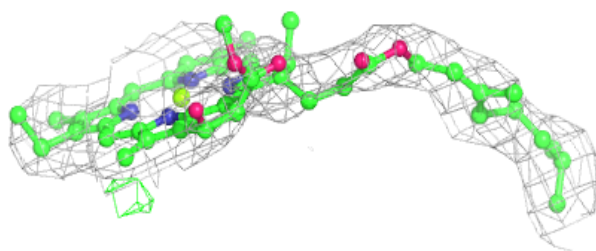
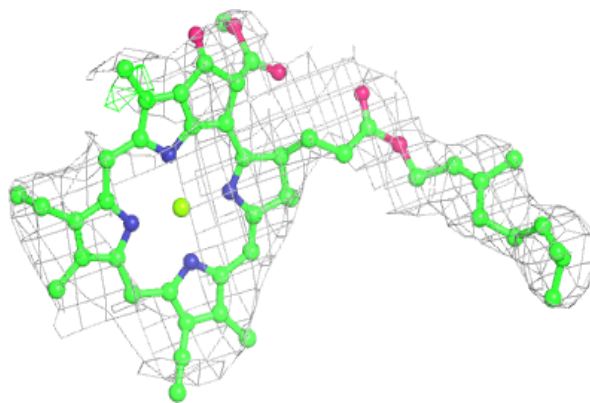
Electron density around CLA 4 4003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



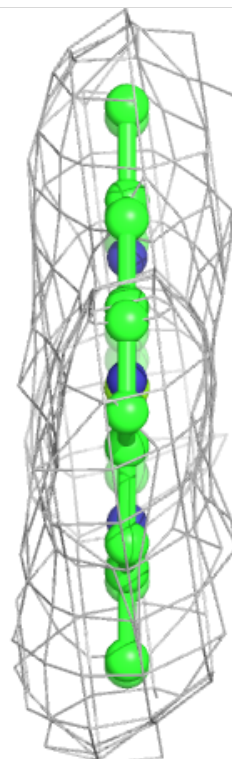
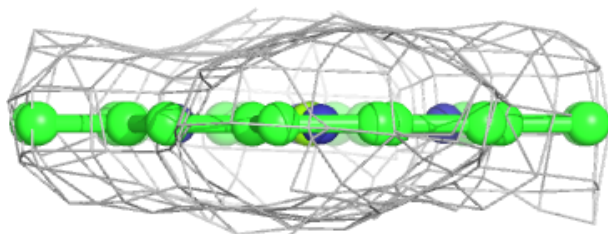
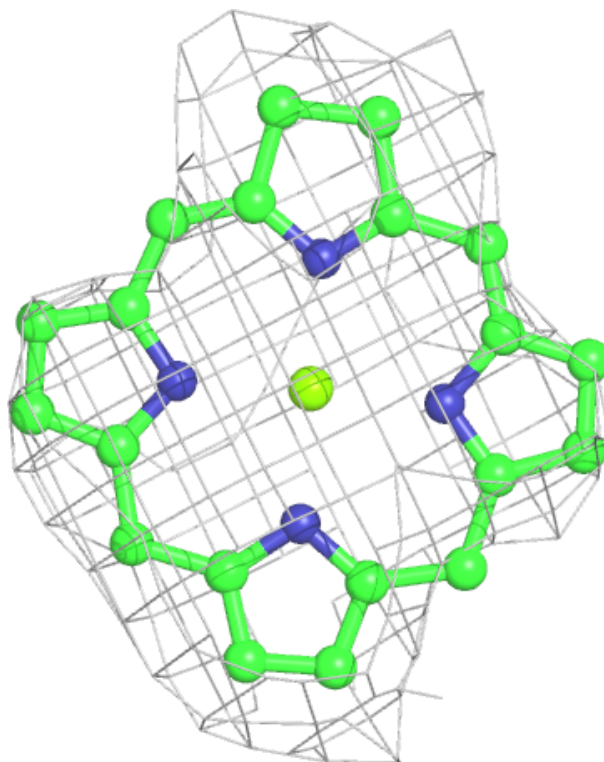
Electron density around CLA B 9012:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



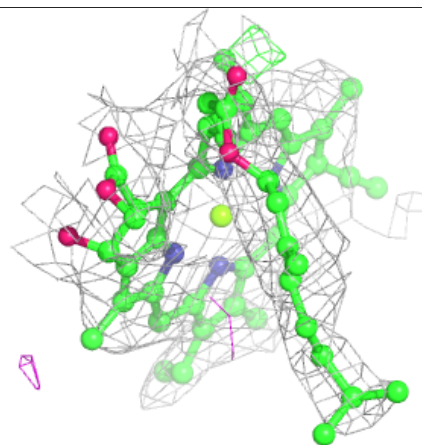
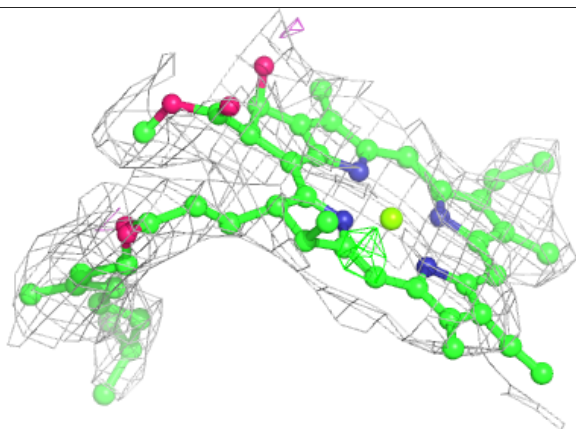
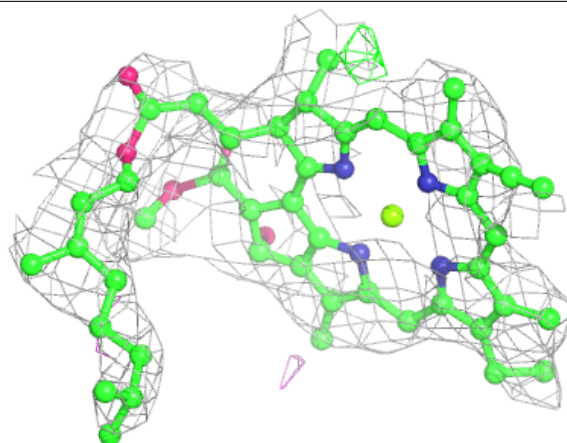
Electron density around CLA 4 4011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



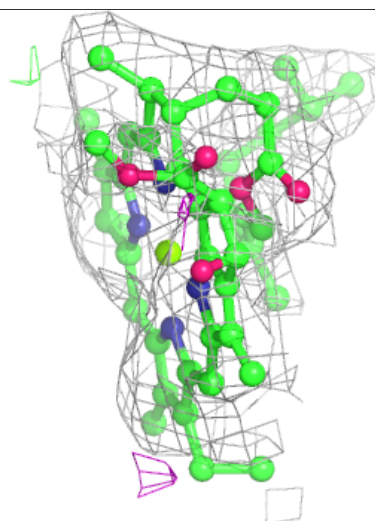
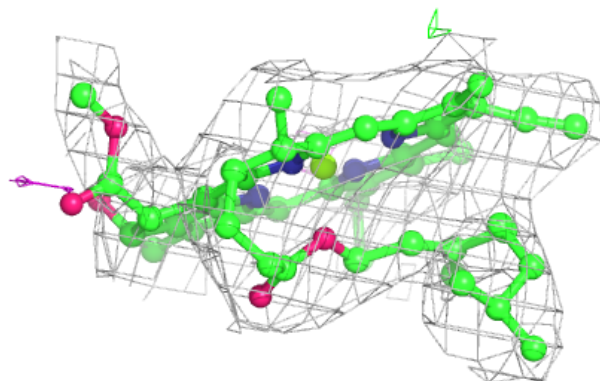
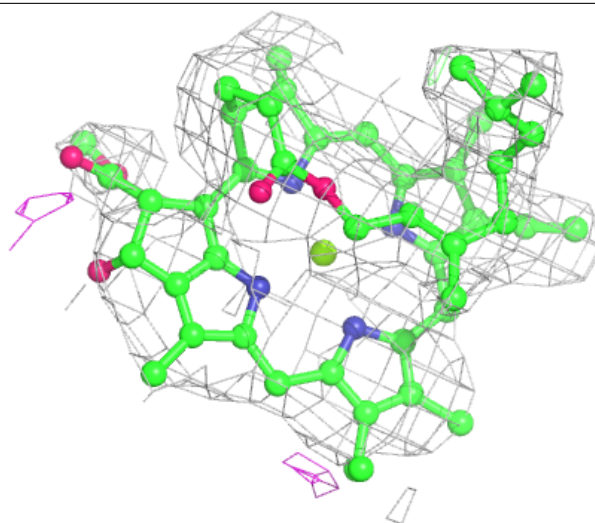
Electron density around CLA A 9011:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



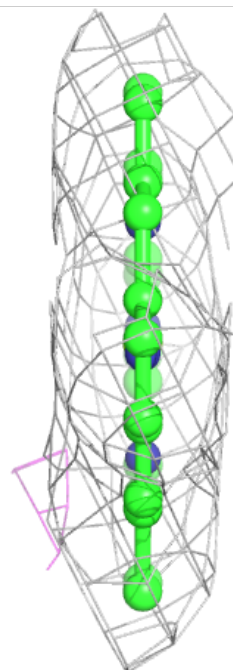
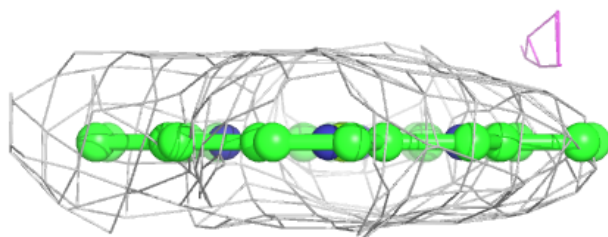
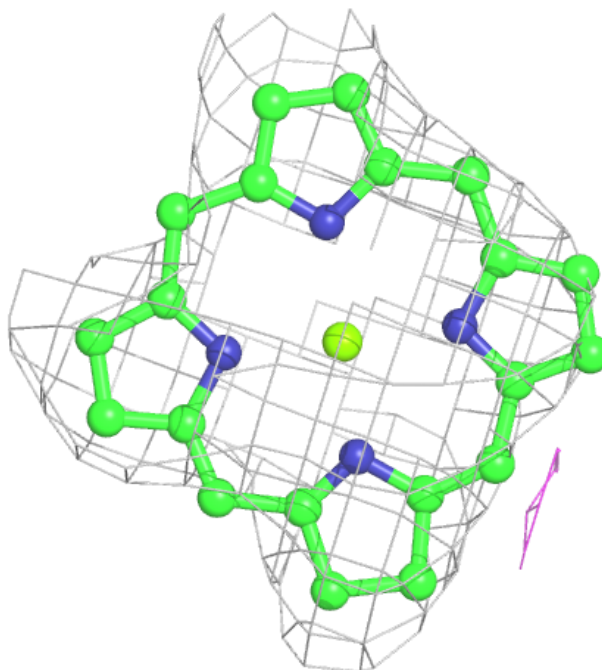
Electron density around CLA B 1205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



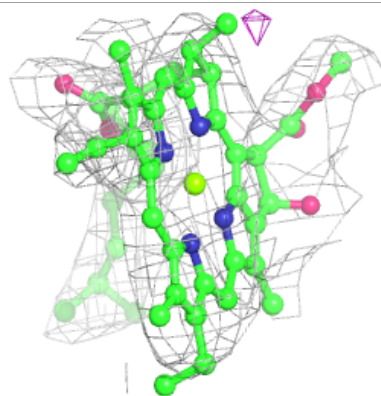
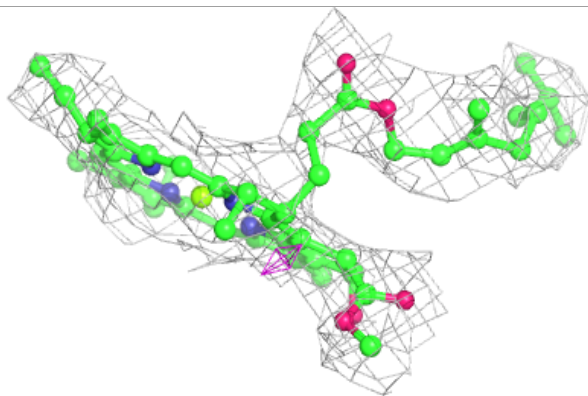
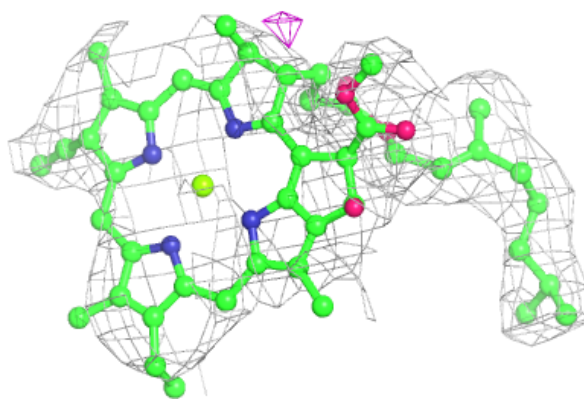
Electron density around CLA 1 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



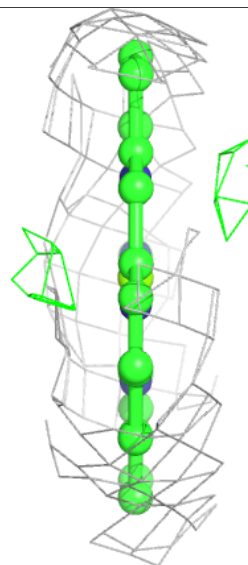
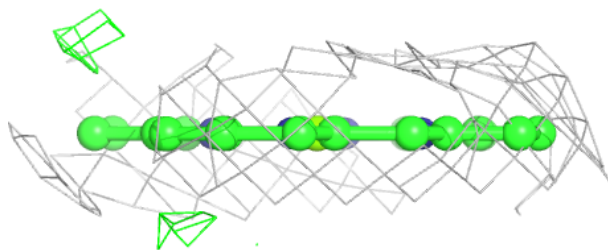
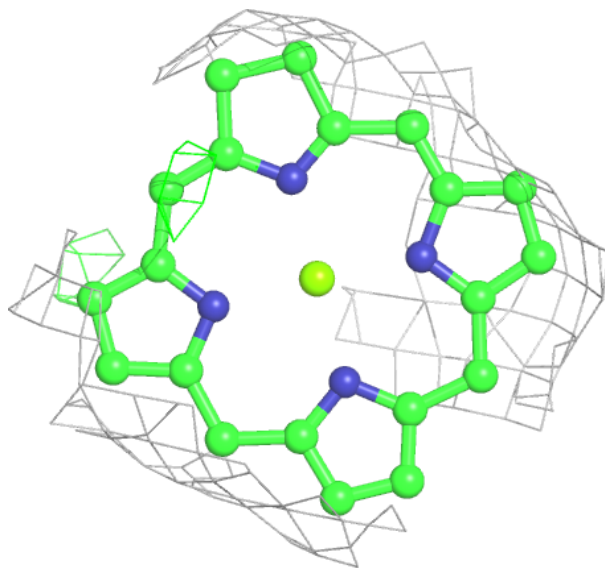
Electron density around CLA B 1228:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



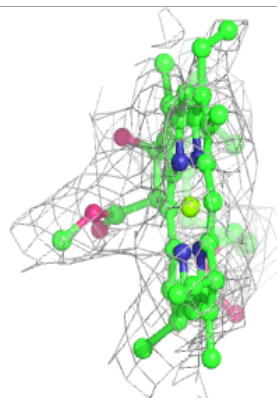
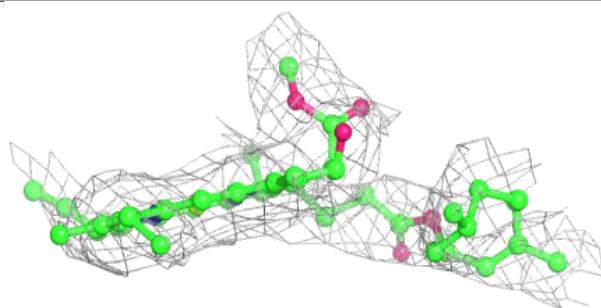
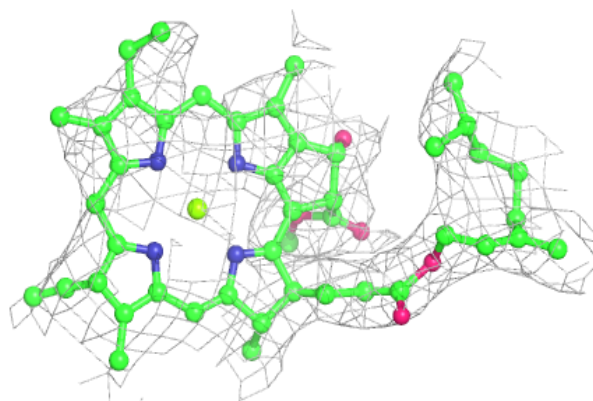
Electron density around CLA A 1147:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

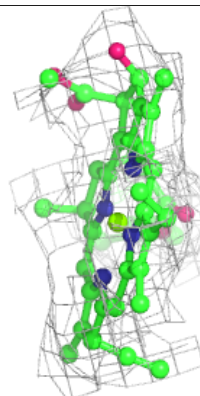
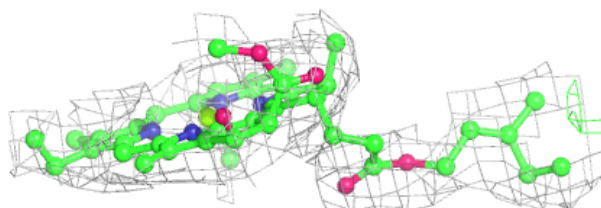
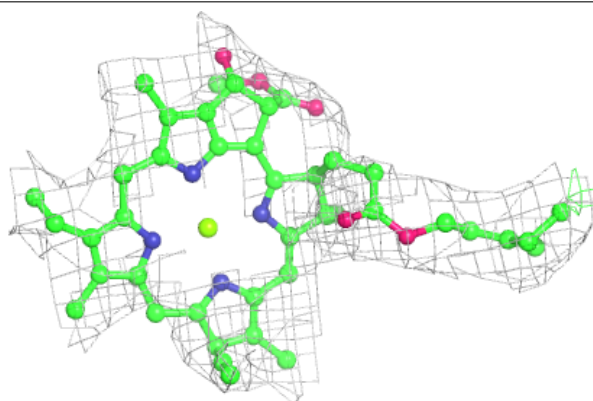


Electron density around CLA A 1123:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

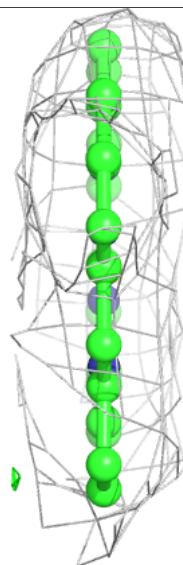
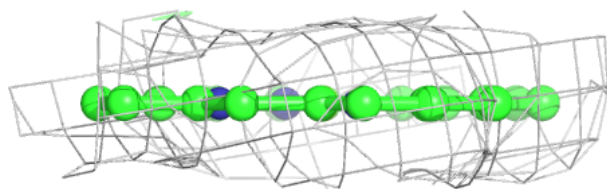
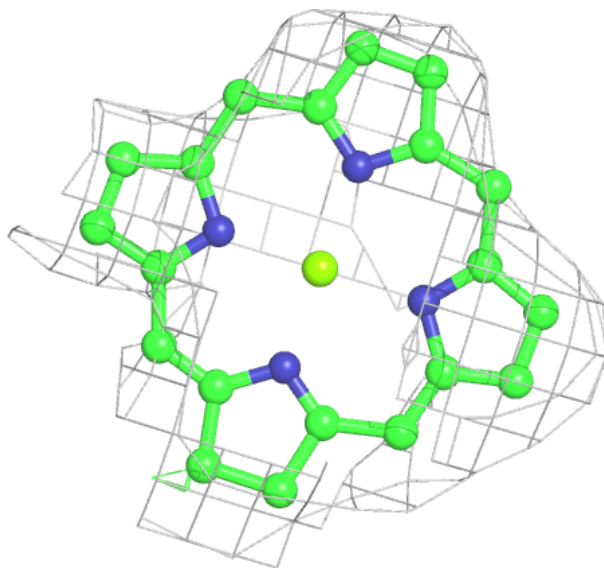
**Electron density around CLA B 1218:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



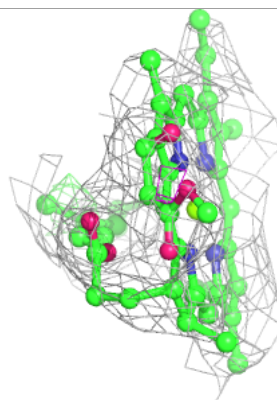
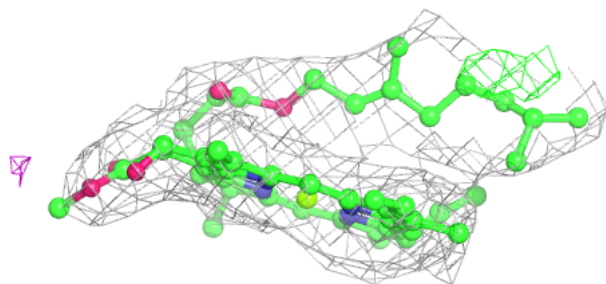
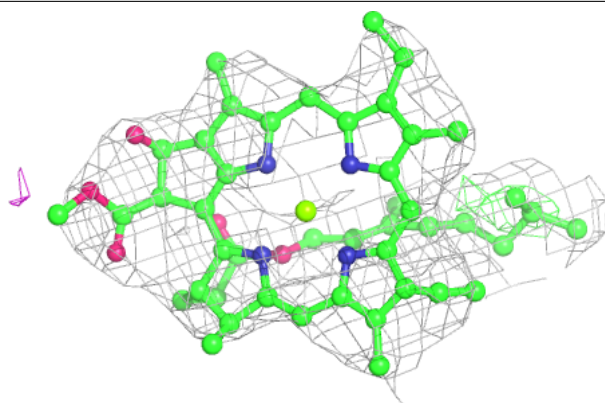
Electron density around CLA 1 1006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



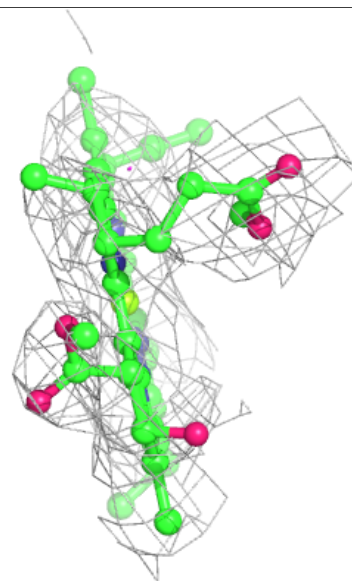
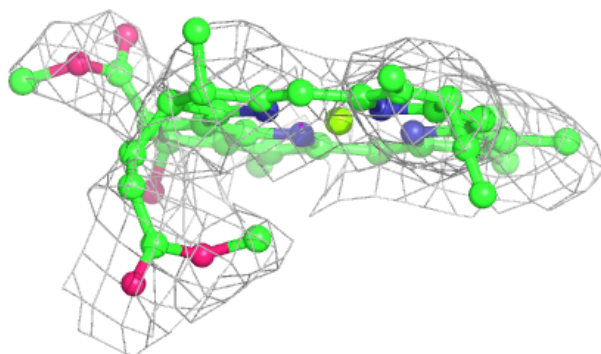
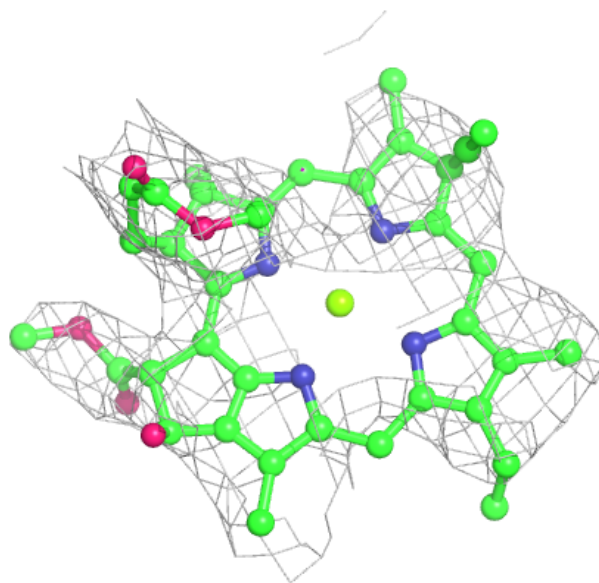
Electron density around CLA B 1235:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



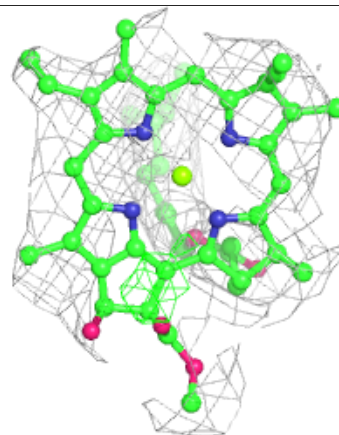
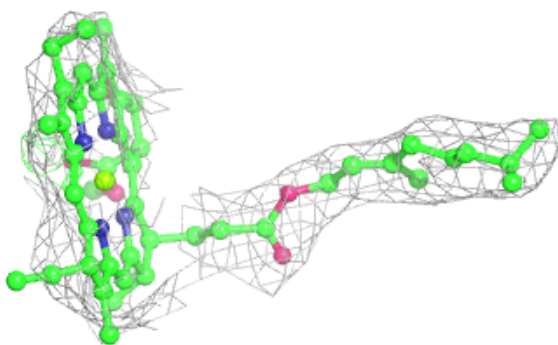
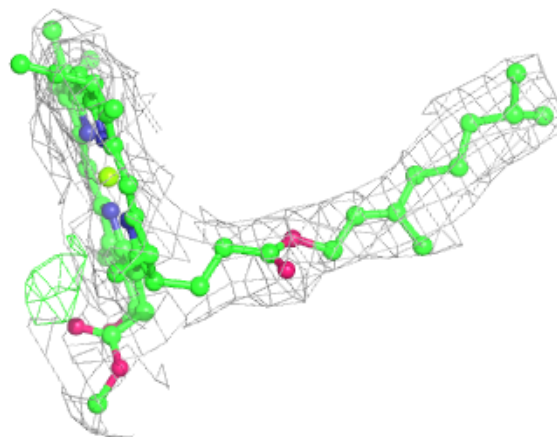
Electron density around CLA B 1231:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



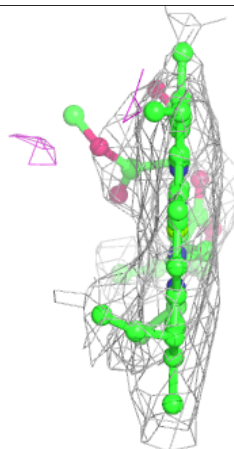
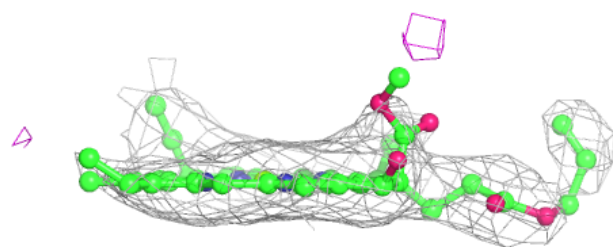
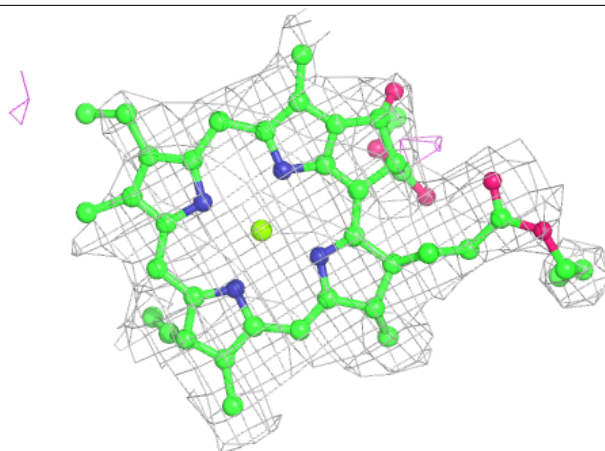
Electron density around CLA B 1239:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



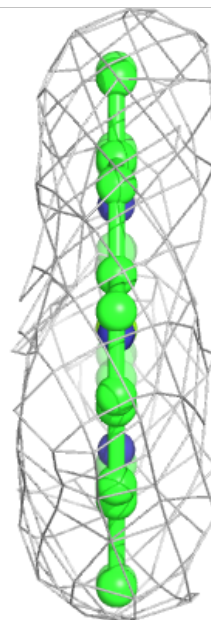
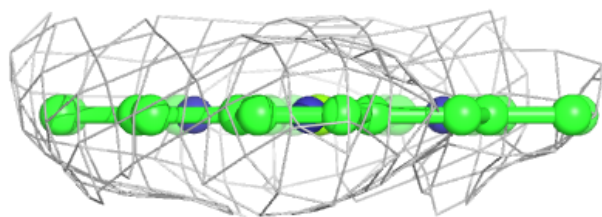
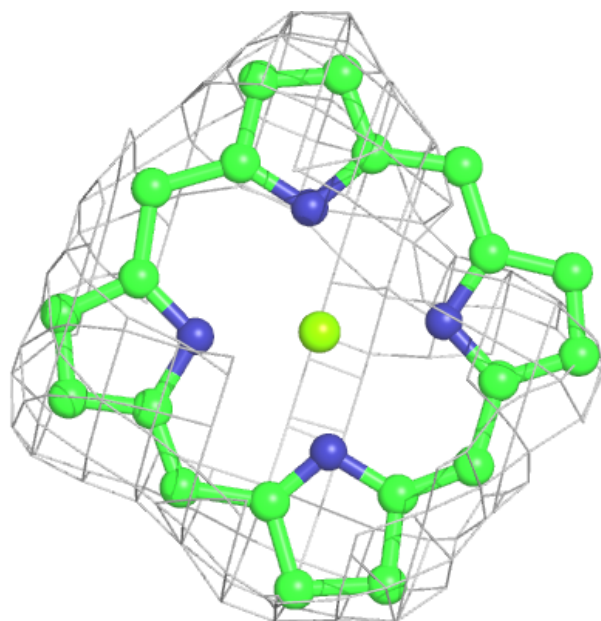
Electron density around CLA B 1221:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



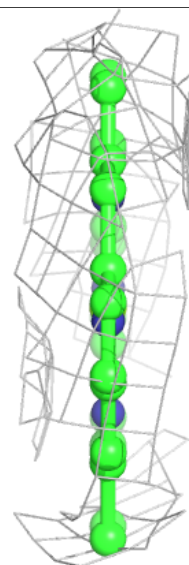
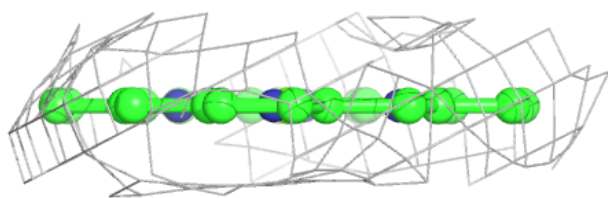
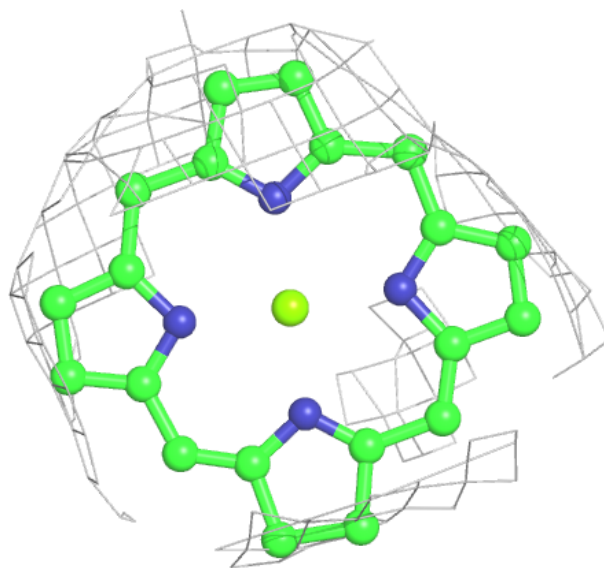
Electron density around CLA A 1105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



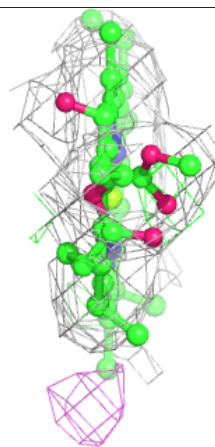
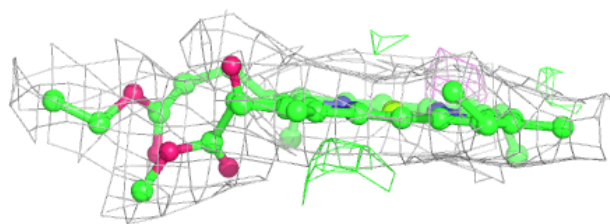
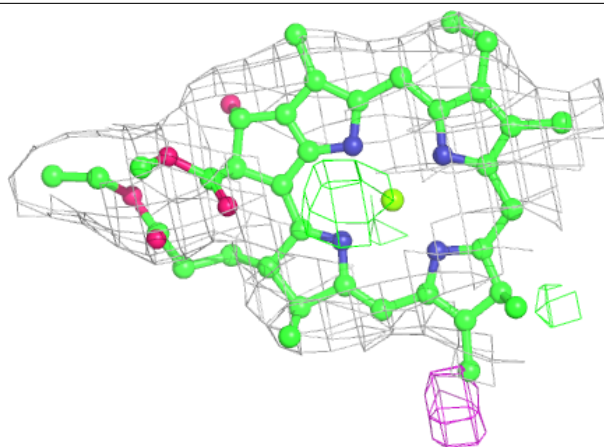
Electron density around CLA 3 3008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



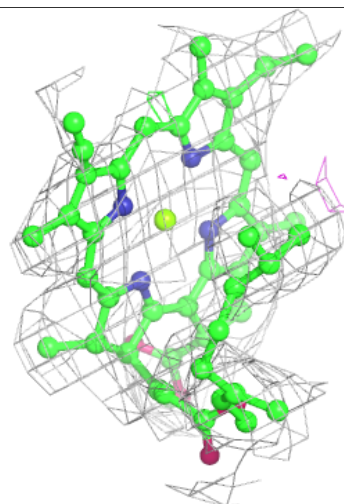
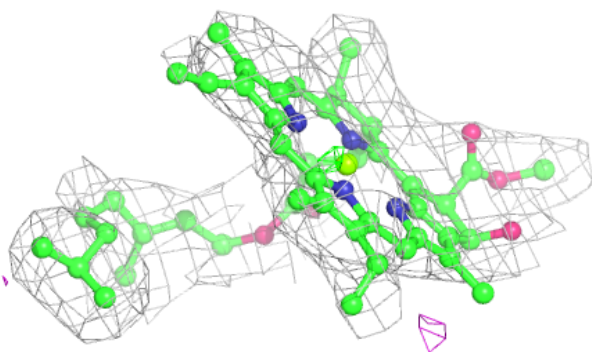
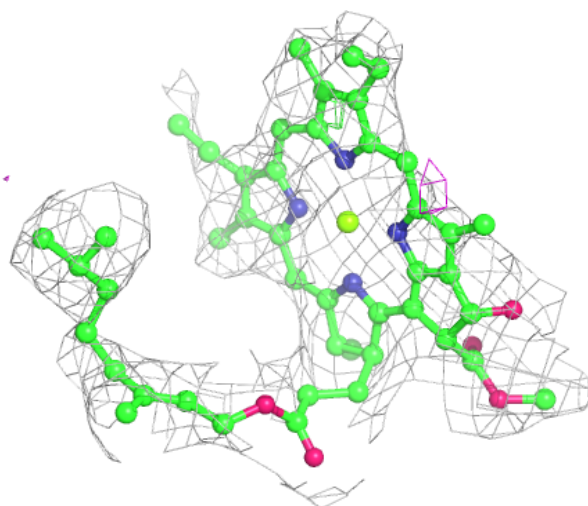
Electron density around CLA L 1503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



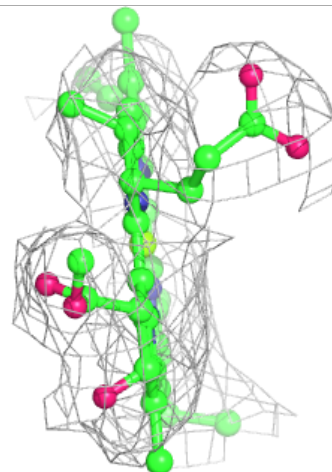
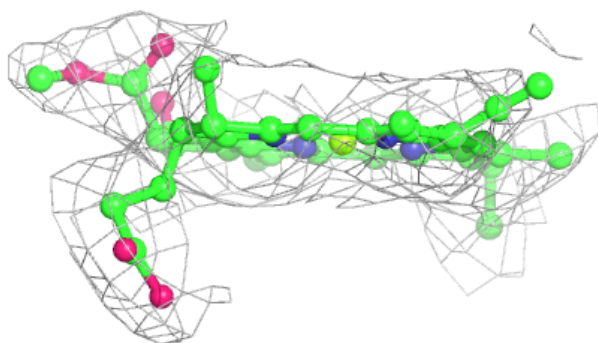
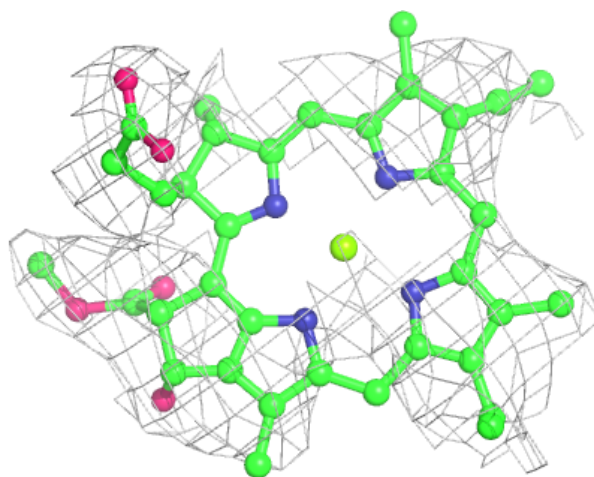
Electron density around CLA A 1122:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



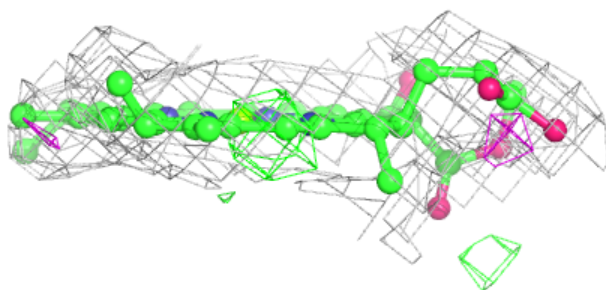
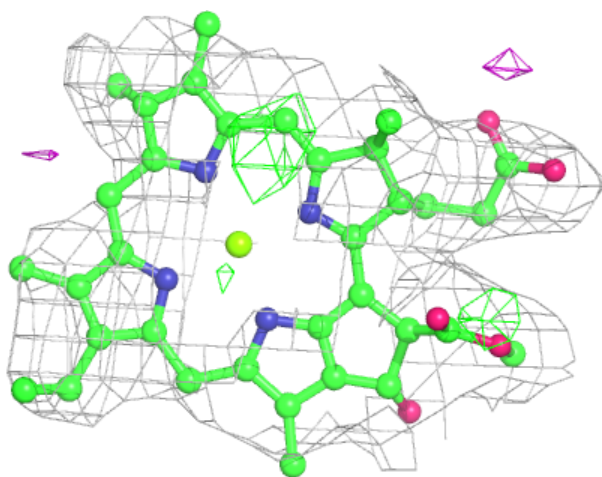
Electron density around CLA B 1225:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



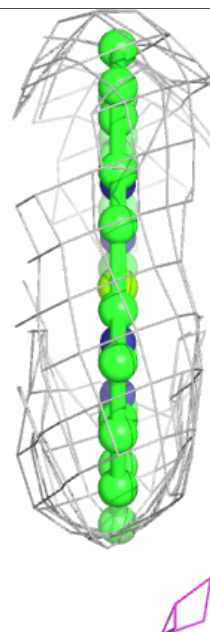
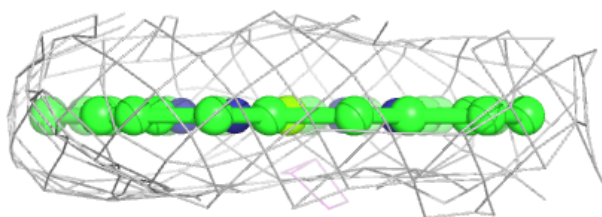
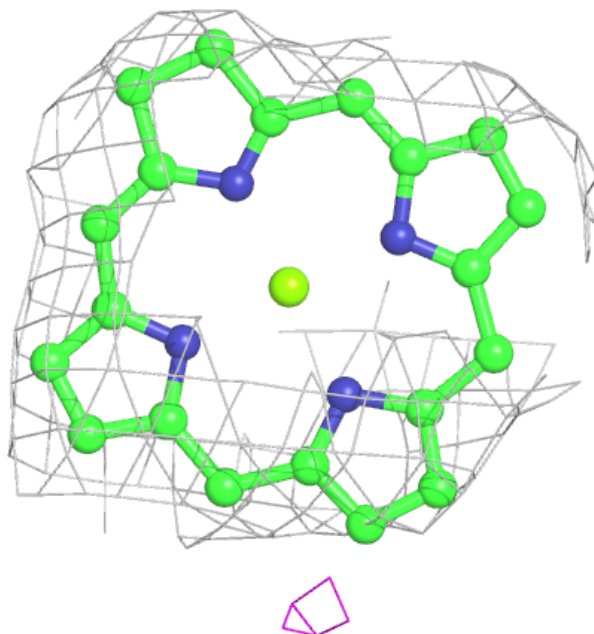
Electron density around CLA A 1131:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



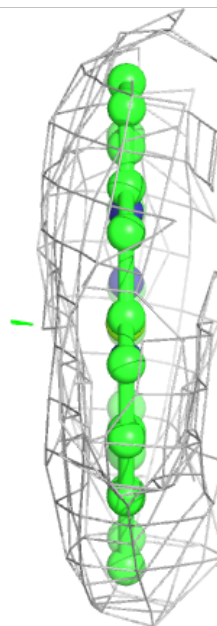
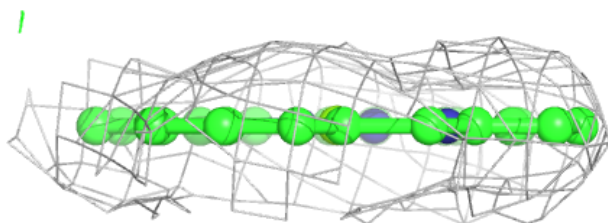
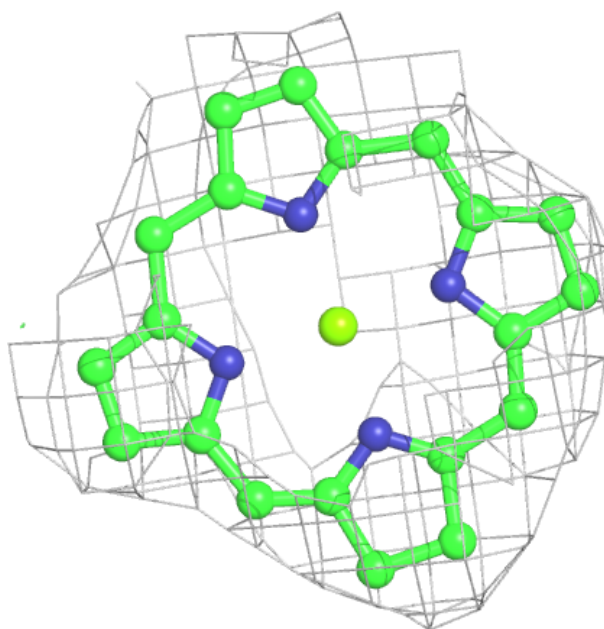
Electron density around CLA 1 1008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



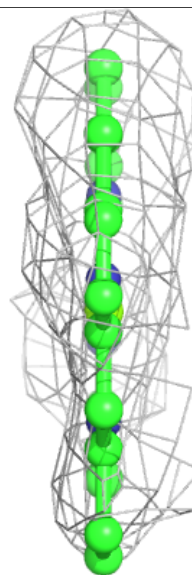
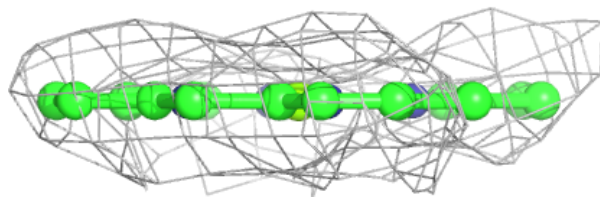
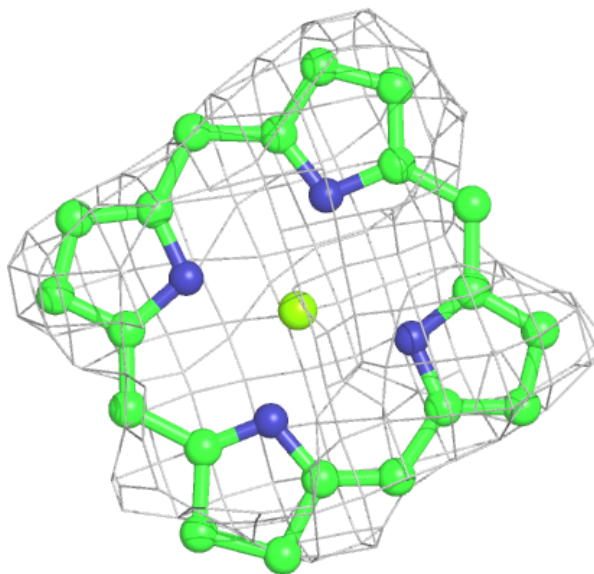
Electron density around CLA B 1226:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



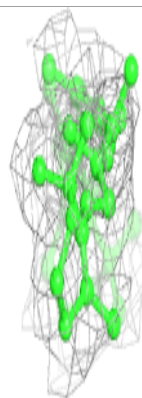
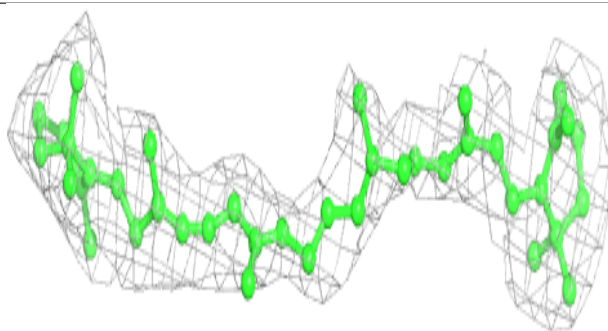
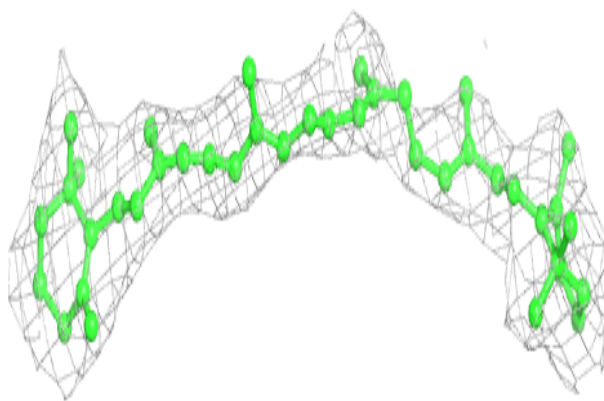
Electron density around CLA B 1206:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



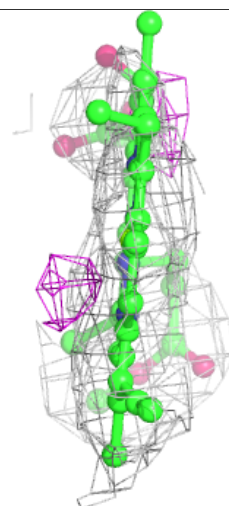
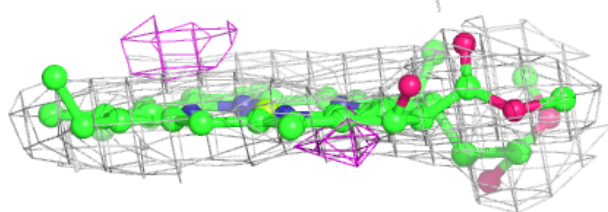
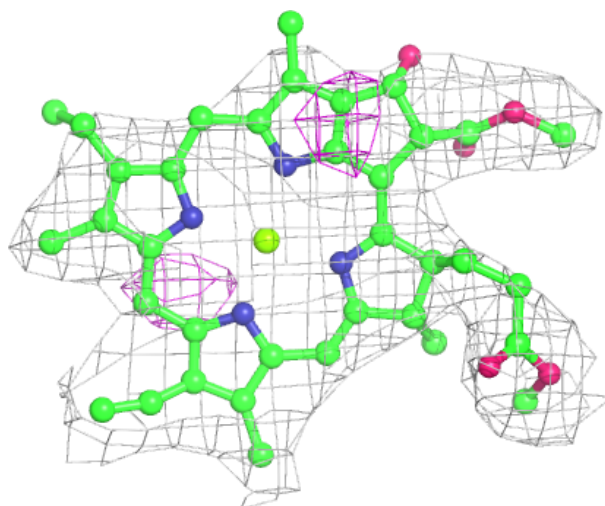
Electron density around BCR I 6018:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



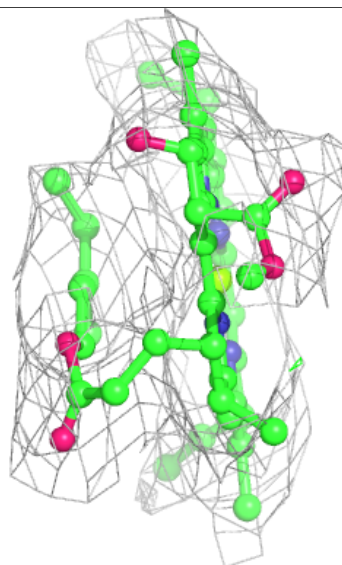
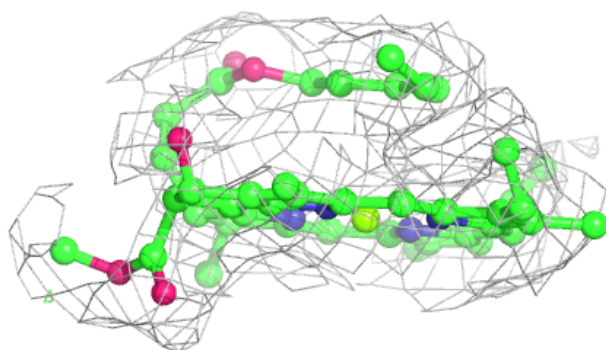
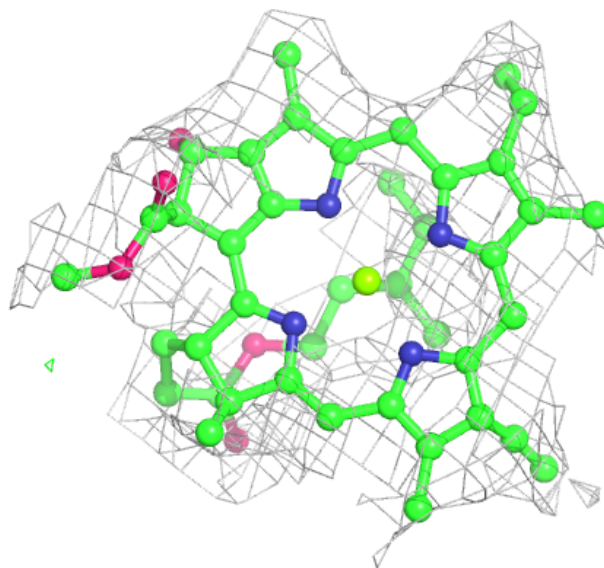
Electron density around CLA A 9013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



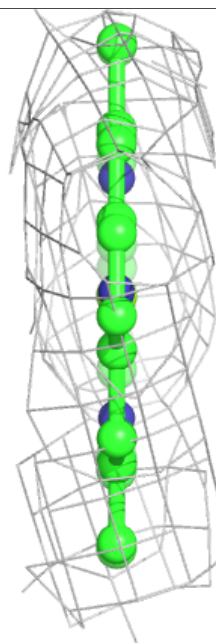
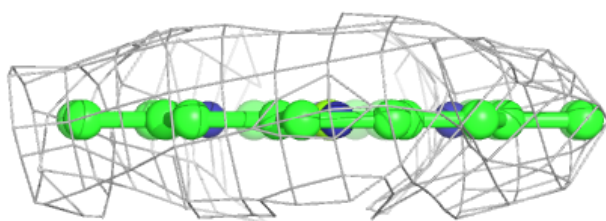
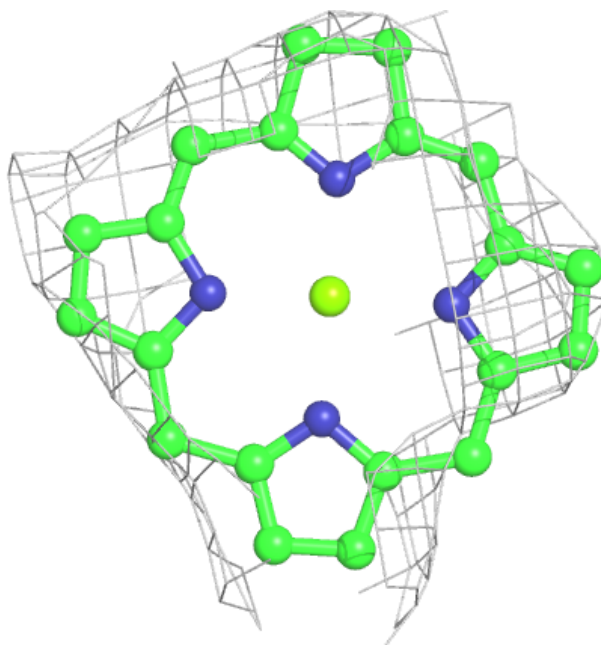
Electron density around CLA G 1233:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



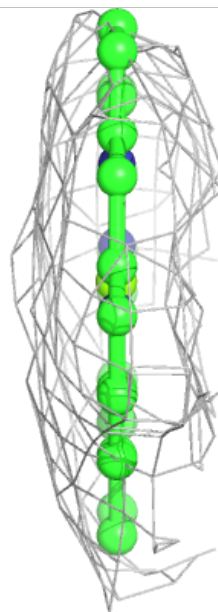
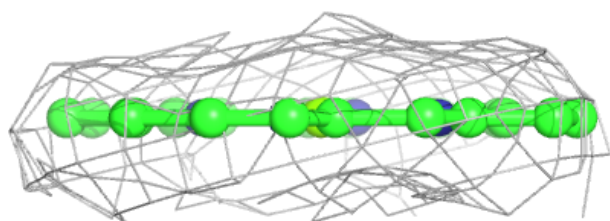
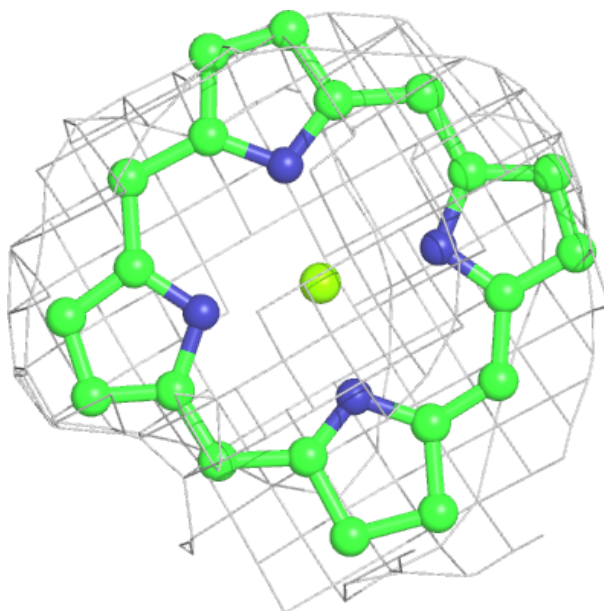
Electron density around CLA A 1120:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



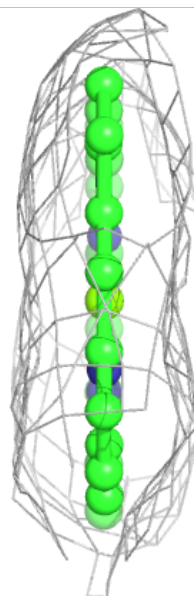
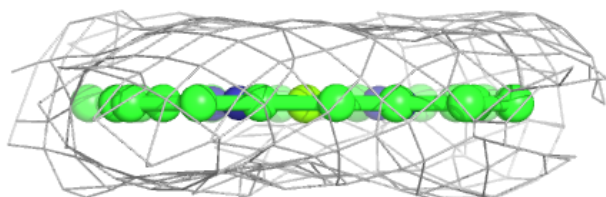
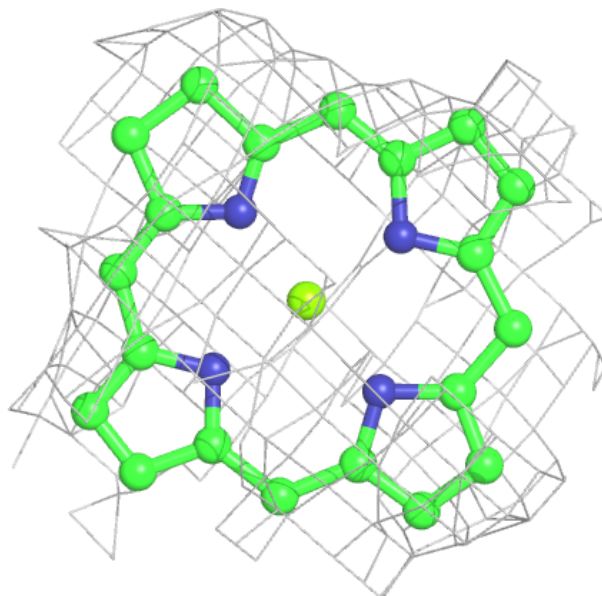
Electron density around CLA 1 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



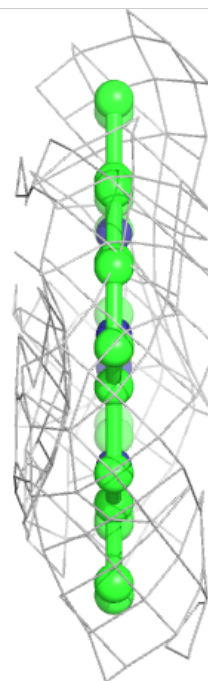
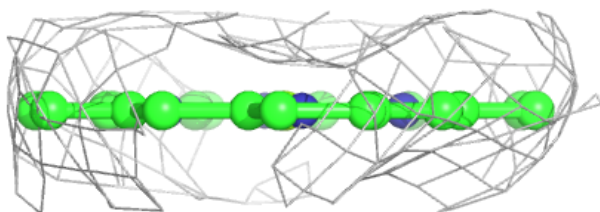
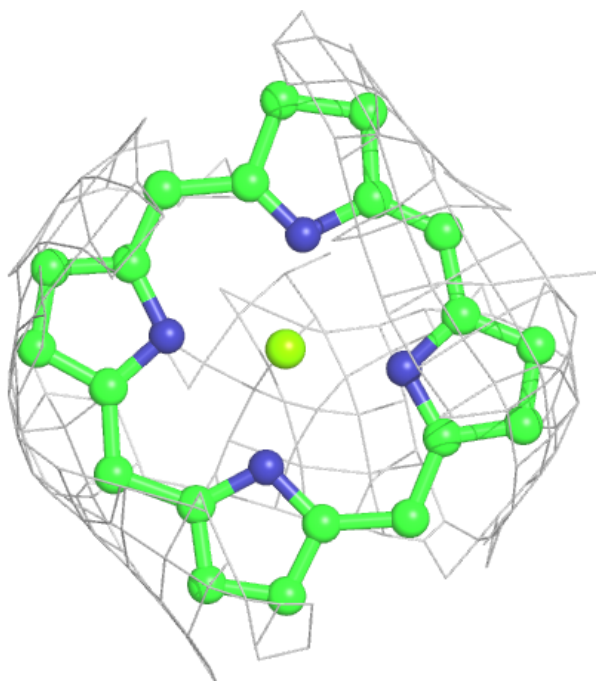
Electron density around CLA A 1124:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



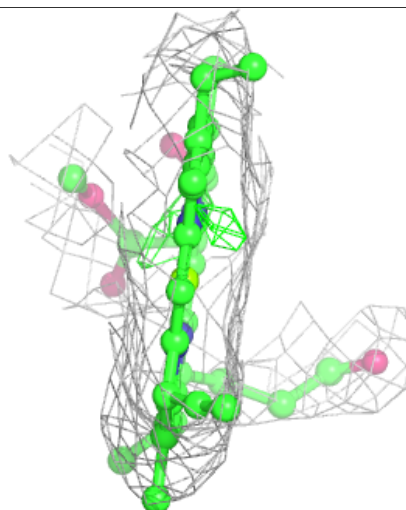
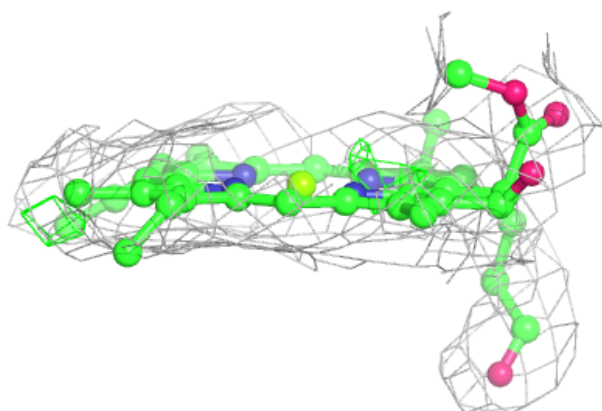
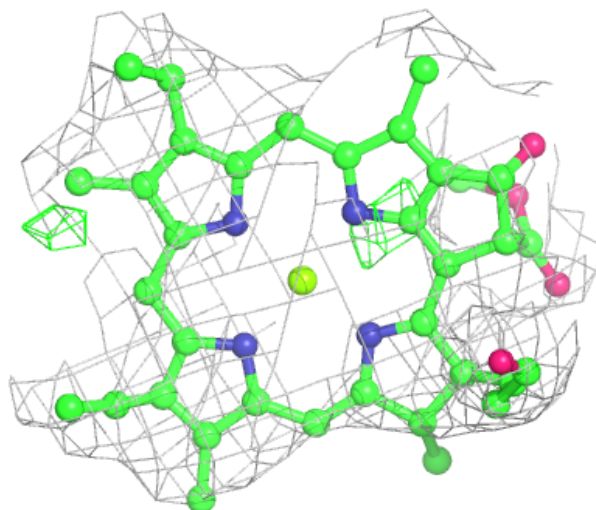
Electron density around CLA 4 4013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



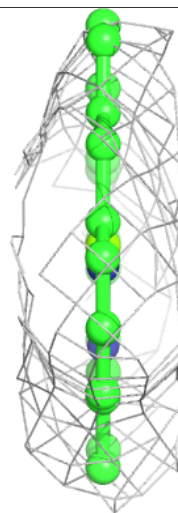
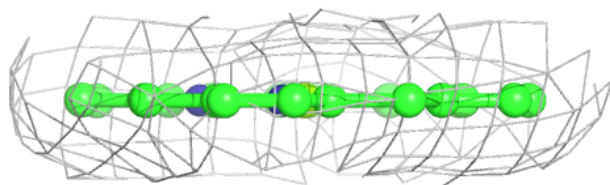
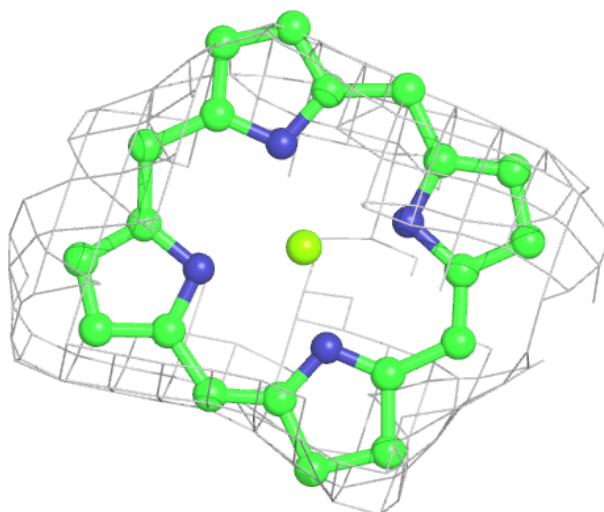
Electron density around CLA F 1139:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



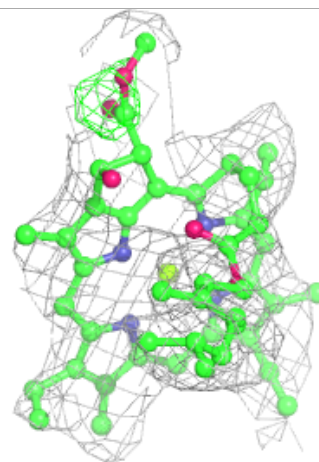
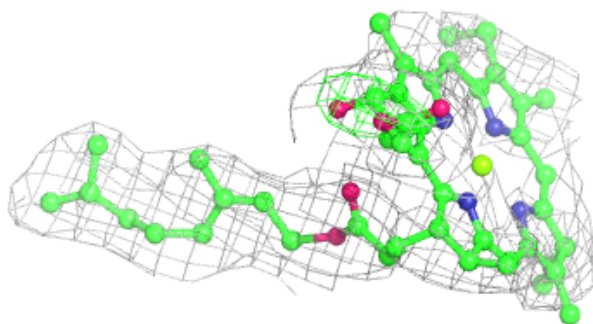
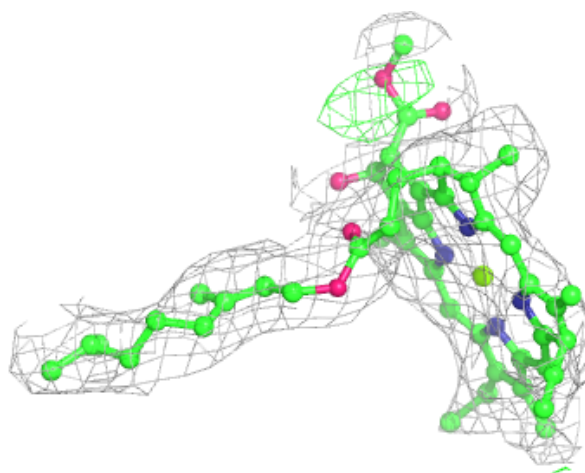
Electron density around CLA A 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



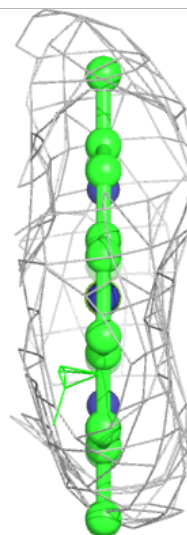
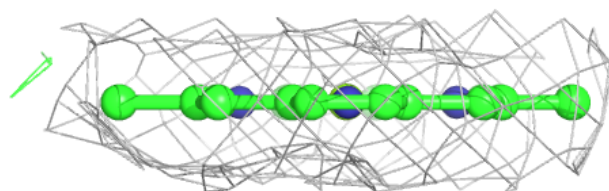
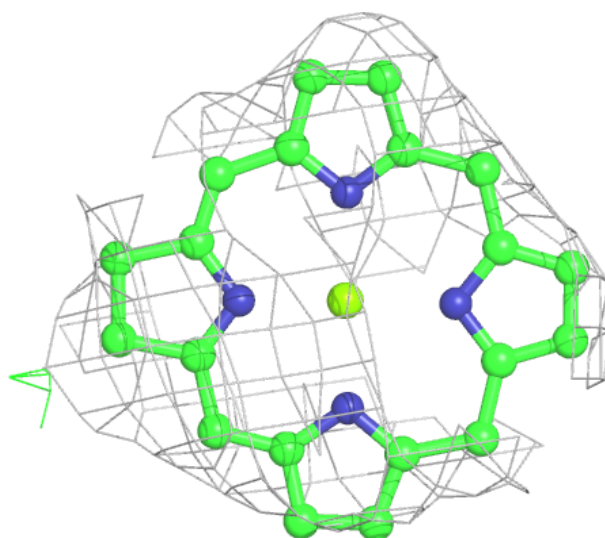
Electron density around CLA A 1126:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



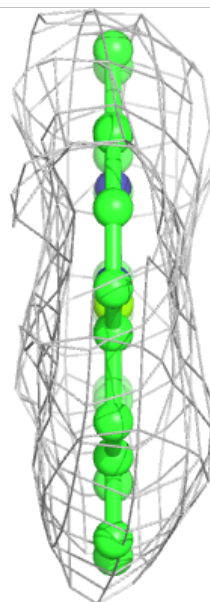
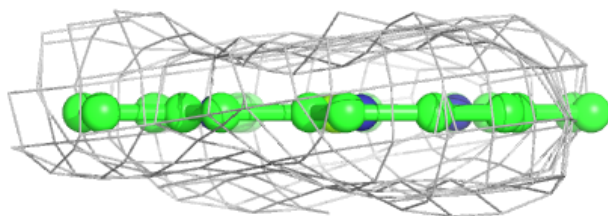
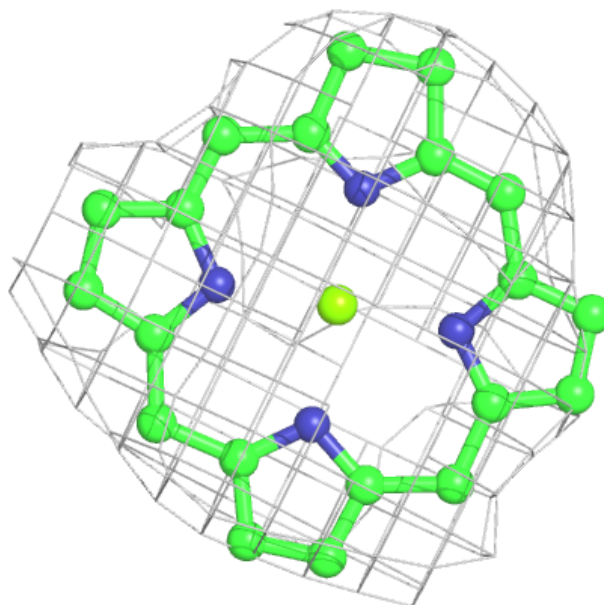
Electron density around CLA 4 1009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



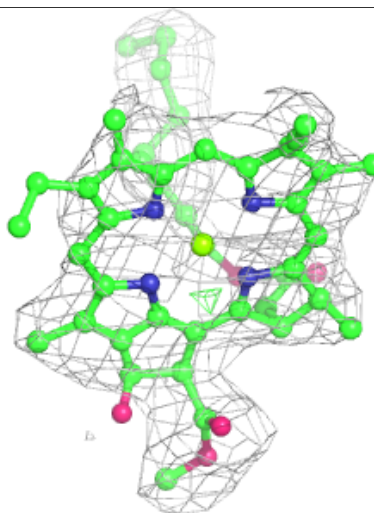
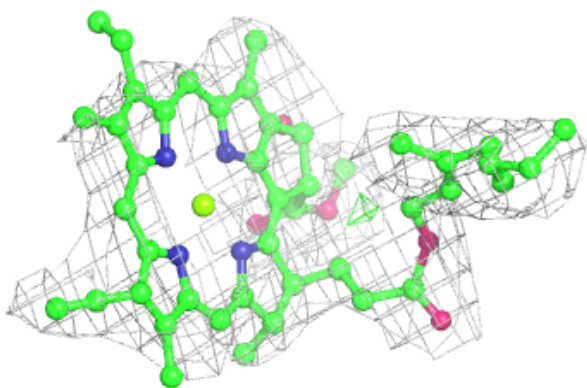
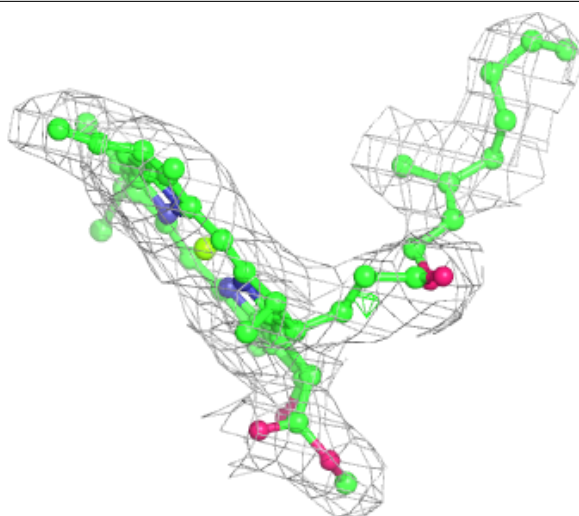
Electron density around CLA F 1305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



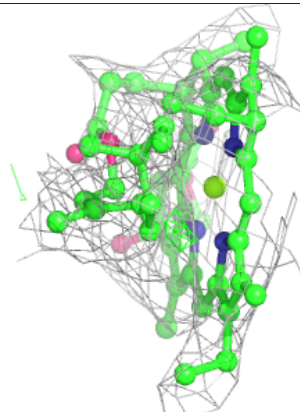
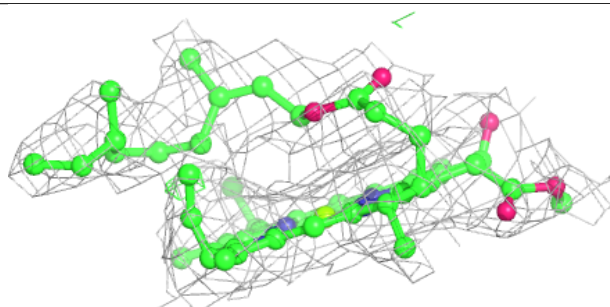
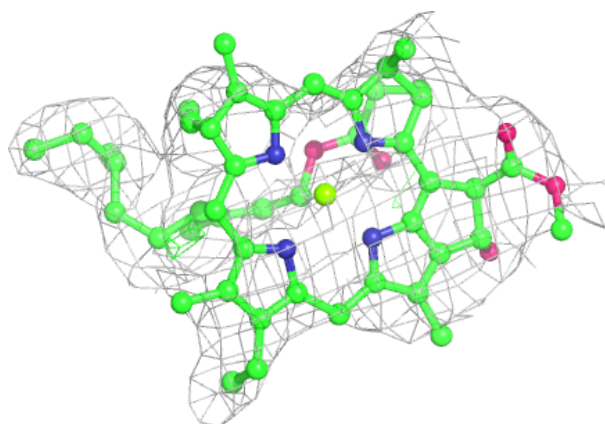
Electron density around CLA B 1238:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

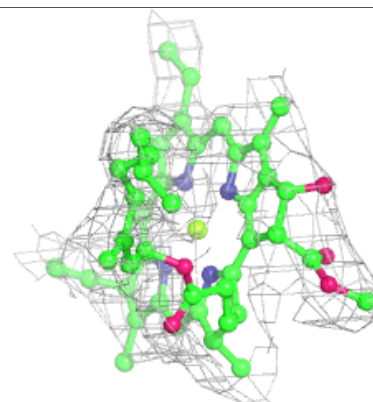
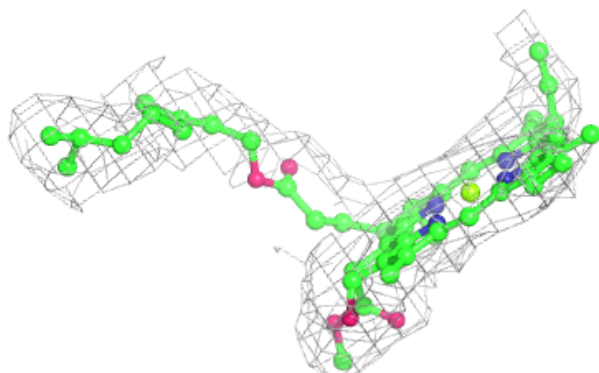
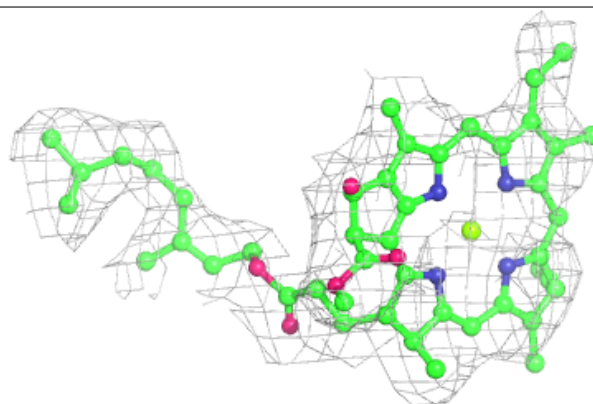


Electron density around CLA B 1138:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

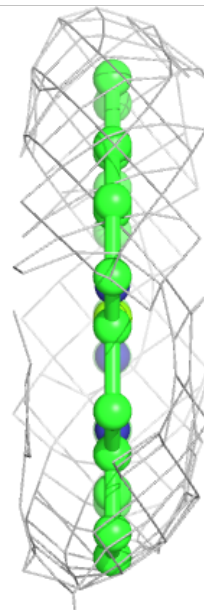
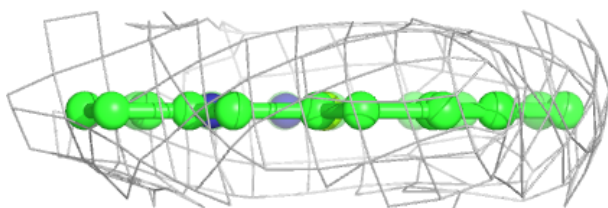
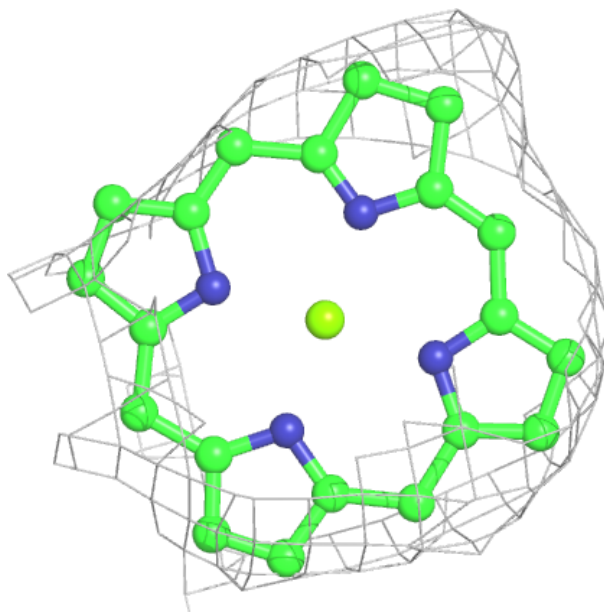
**Electron density around CLA A 1137:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



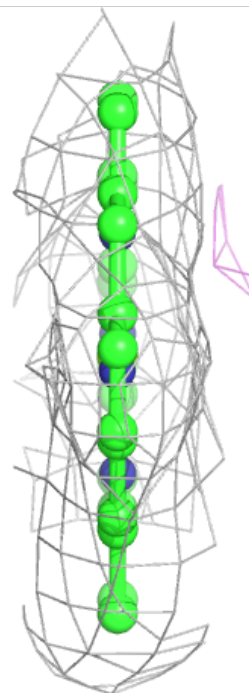
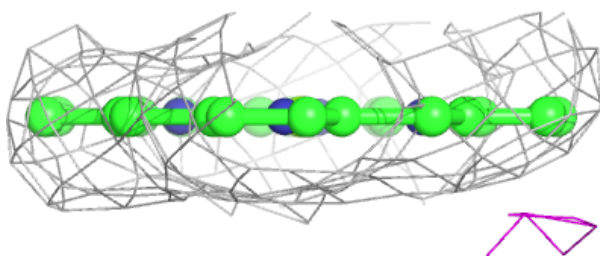
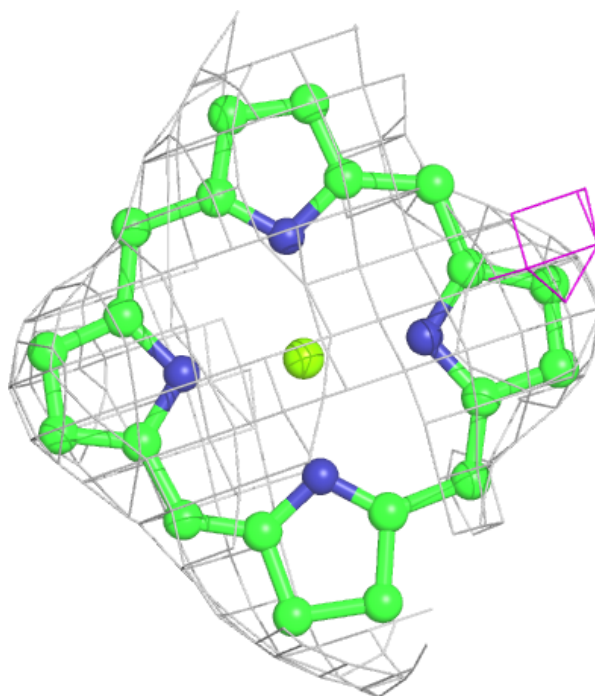
Electron density around CLA 3 2009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



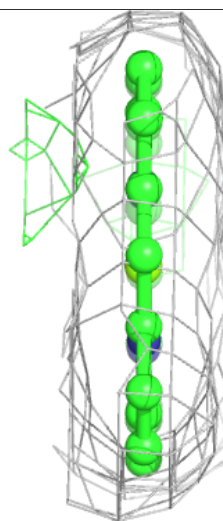
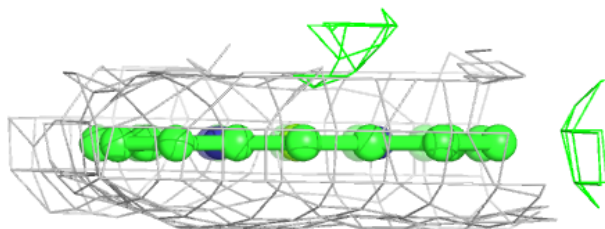
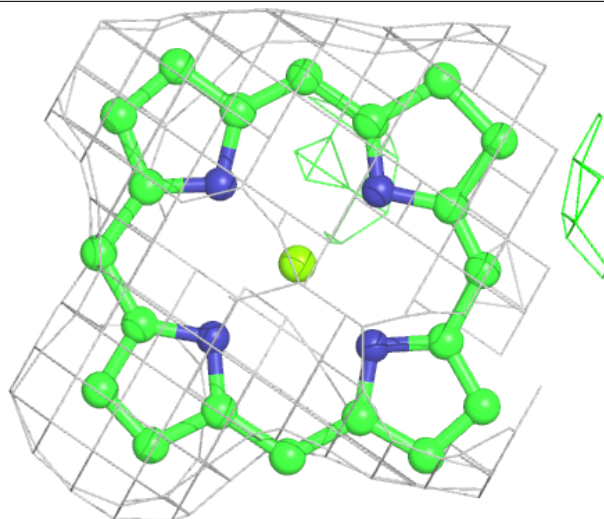
Electron density around CLA A 1127:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



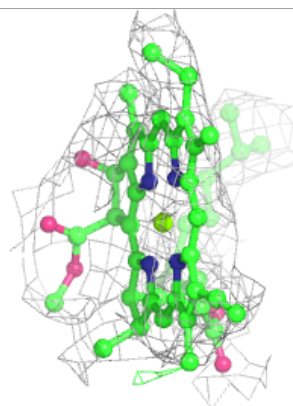
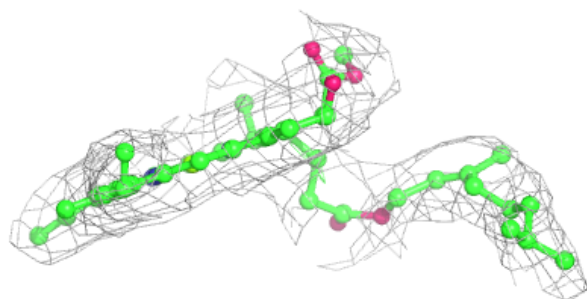
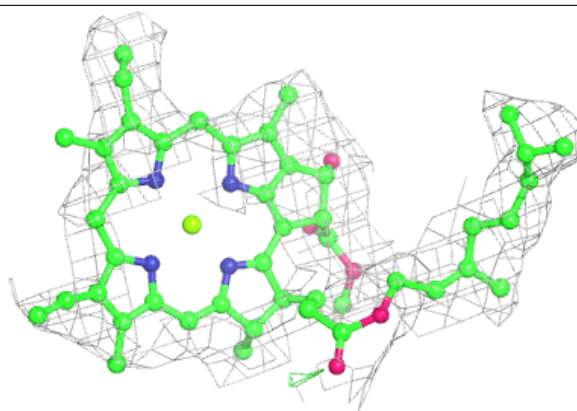
Electron density around CLA A 1132:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



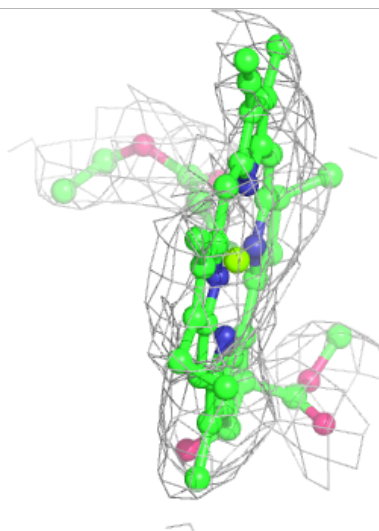
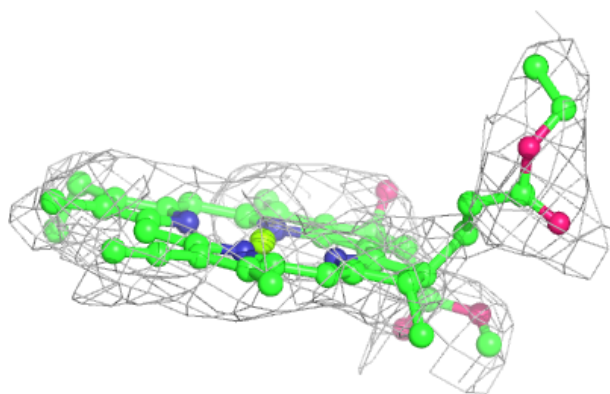
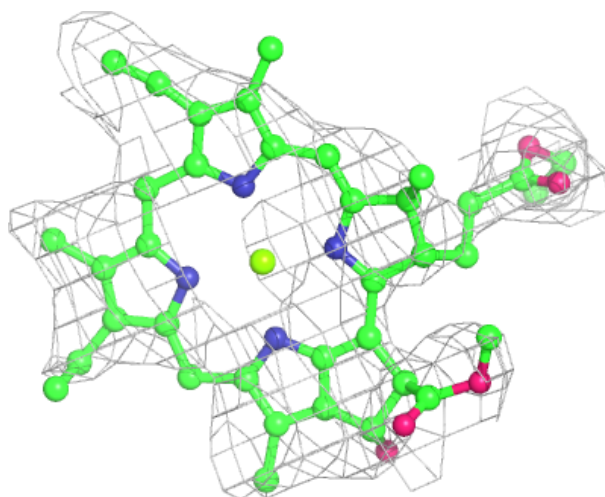
Electron density around CLA B 1208:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



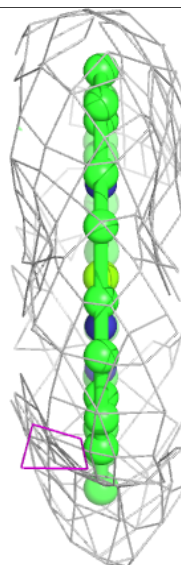
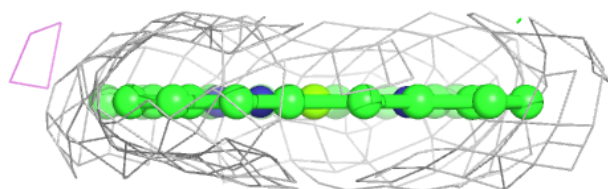
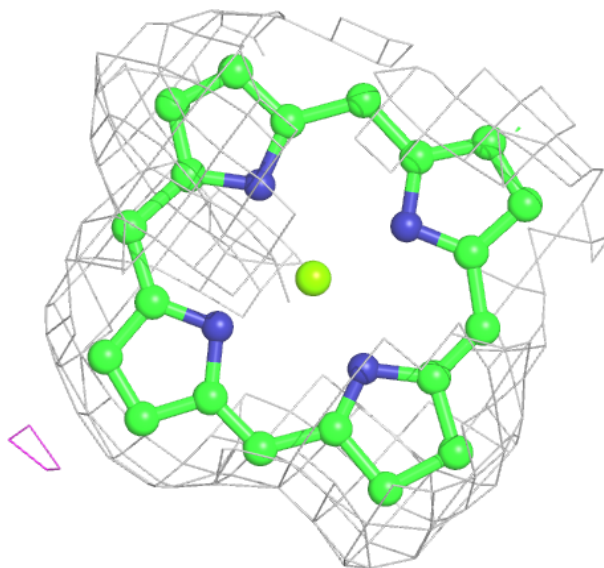
Electron density around CLA B 9010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



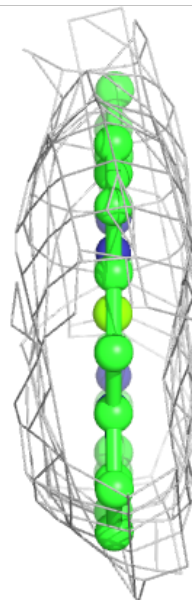
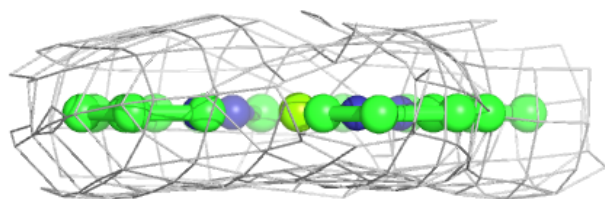
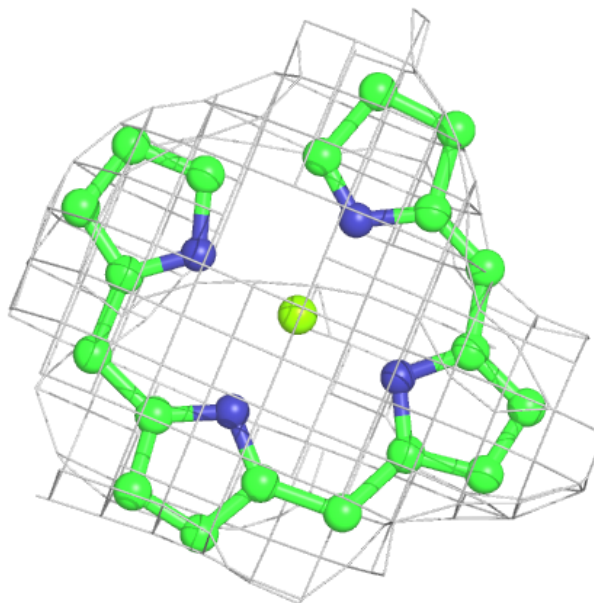
Electron density around CLA A 1133:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



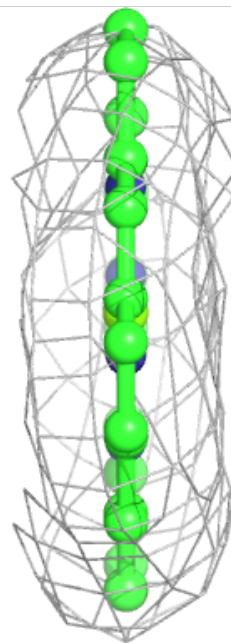
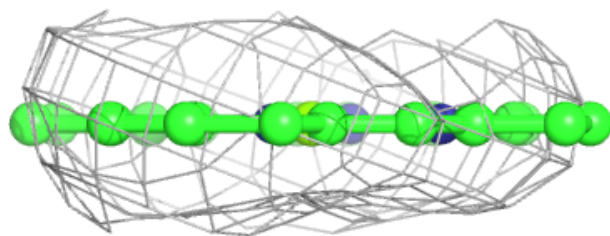
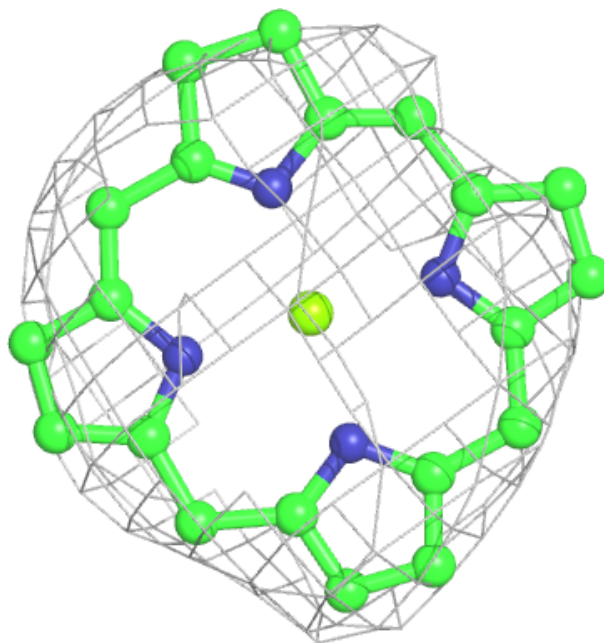
Electron density around CLA A 1109:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



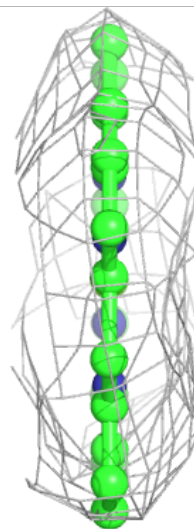
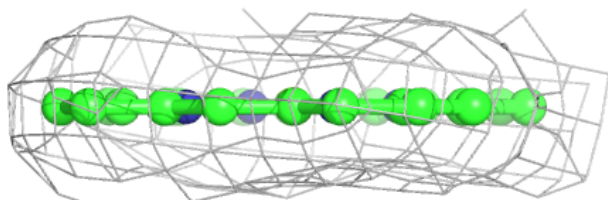
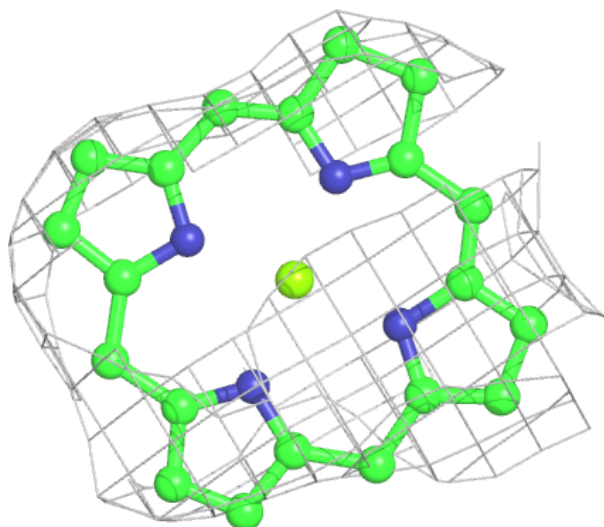
Electron density around CLA 3 3007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



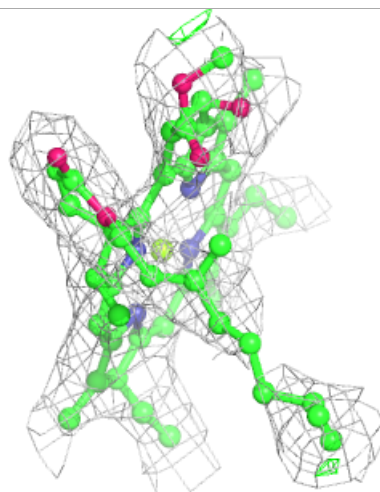
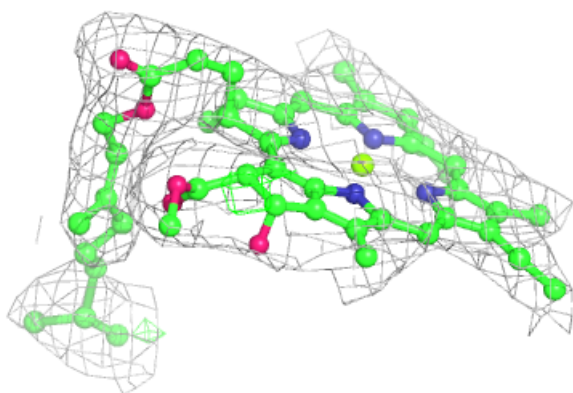
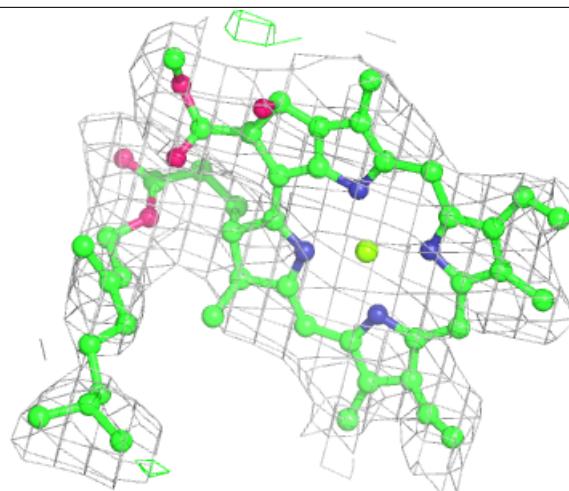
Electron density around CLA 2 2008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



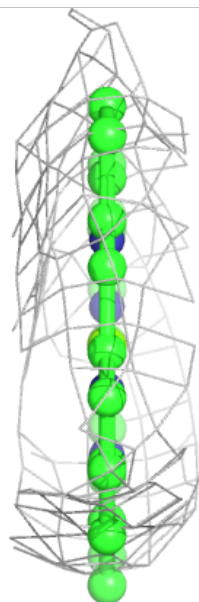
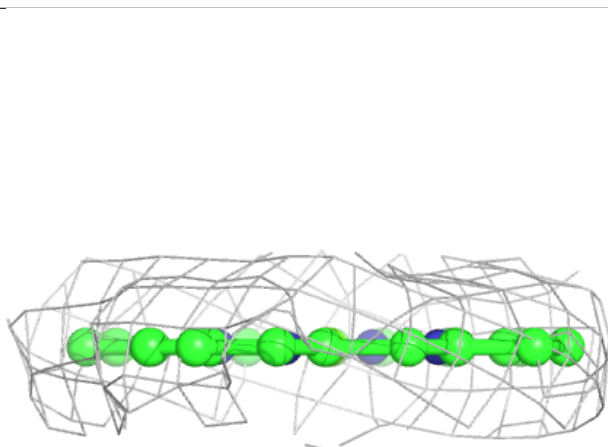
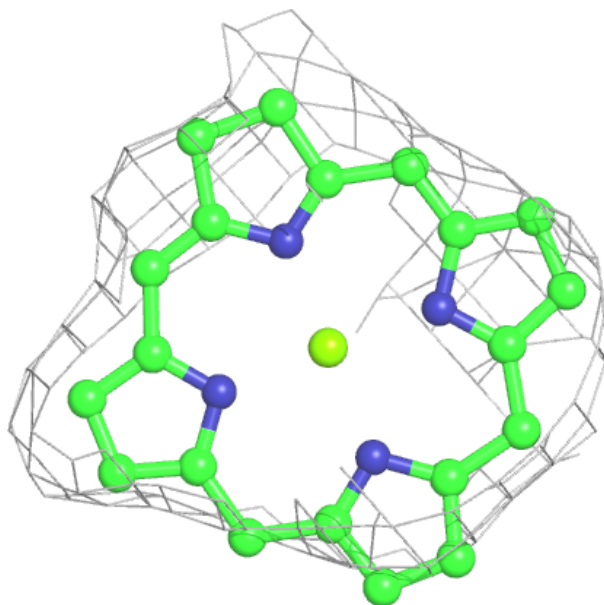
Electron density around CLA B 1207:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



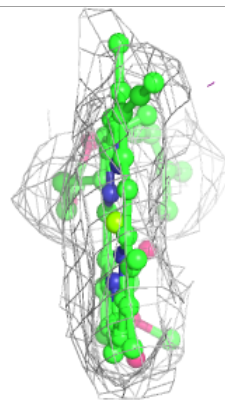
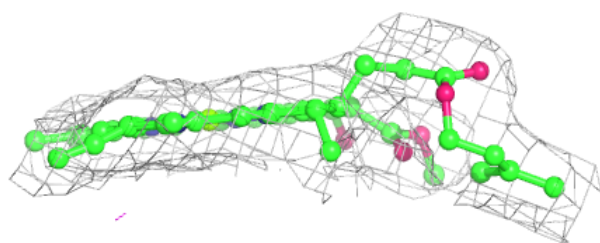
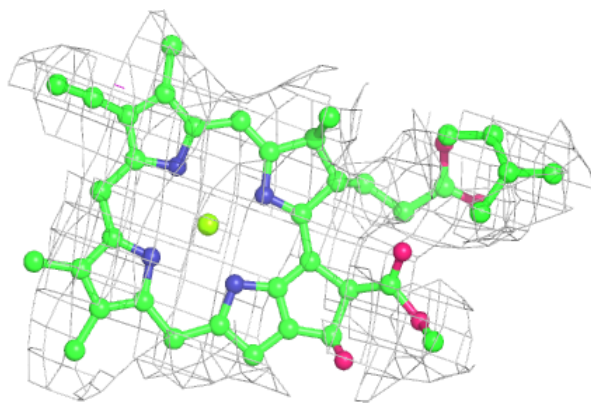
Electron density around CLA A 1148:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



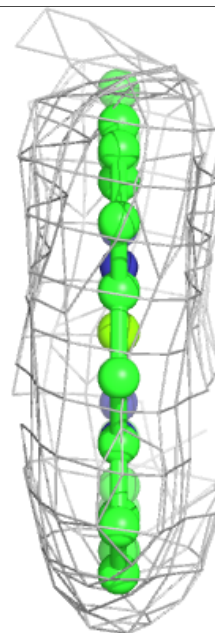
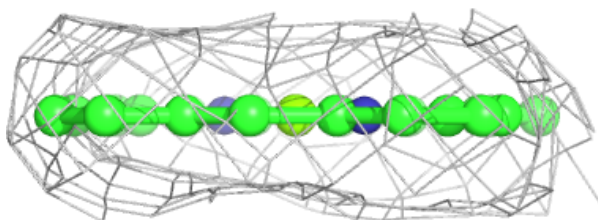
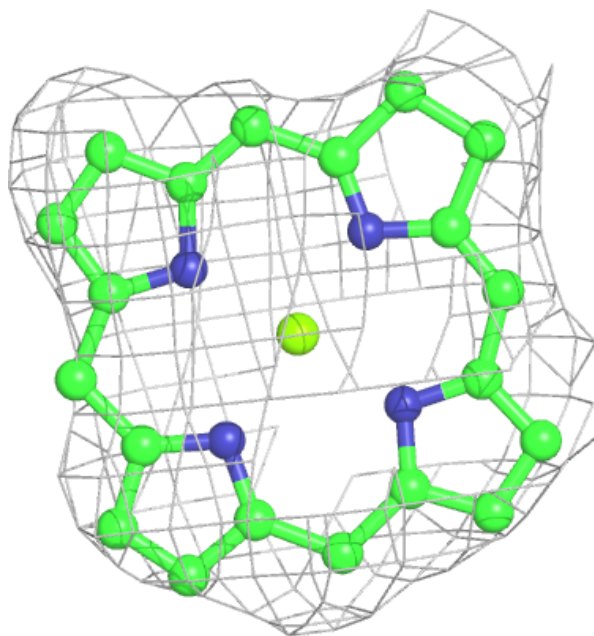
Electron density around CLA B 1203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



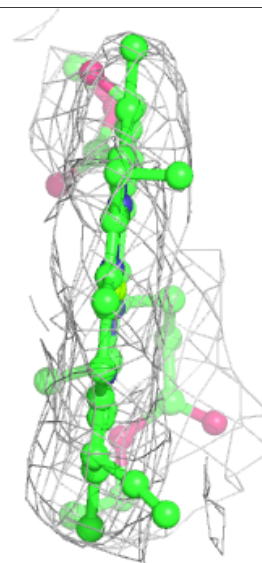
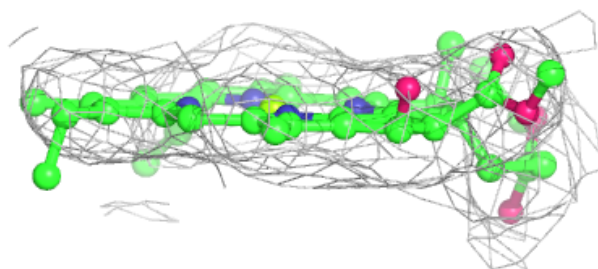
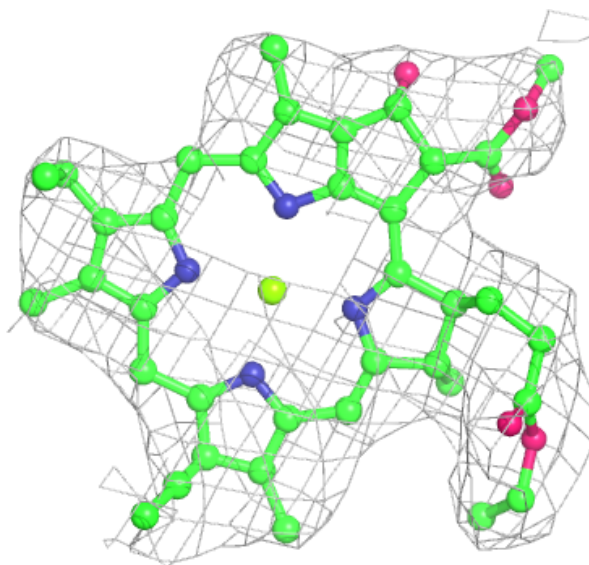
Electron density around CLA A 1152:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



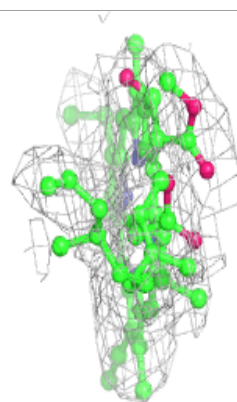
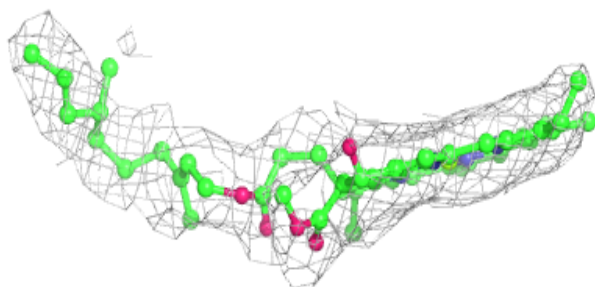
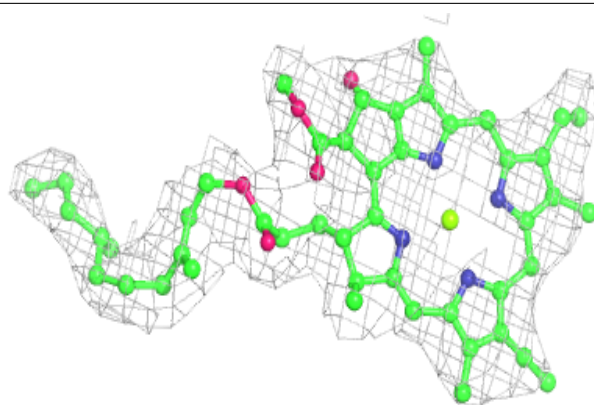
Electron density around CLA B 9023:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



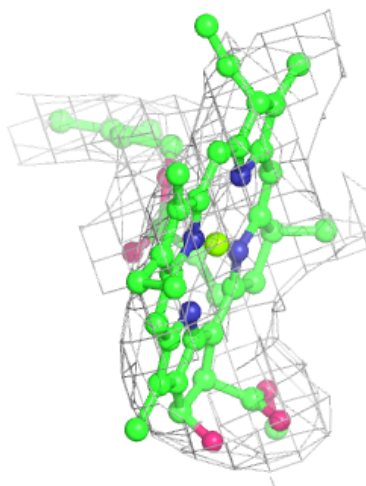
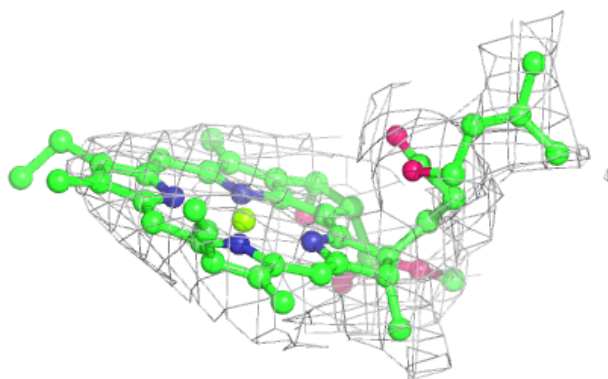
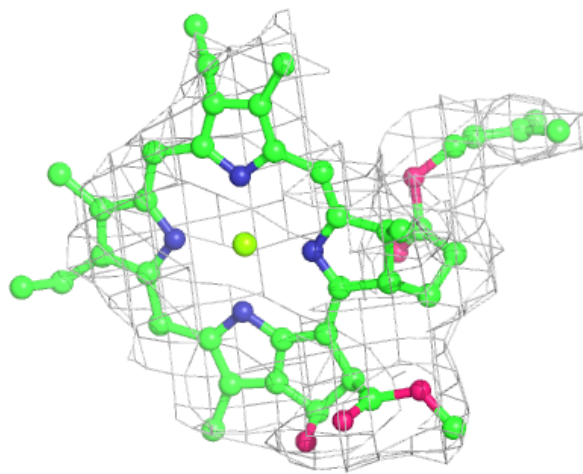
Electron density around CLA A 1107:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



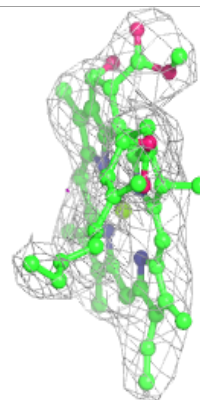
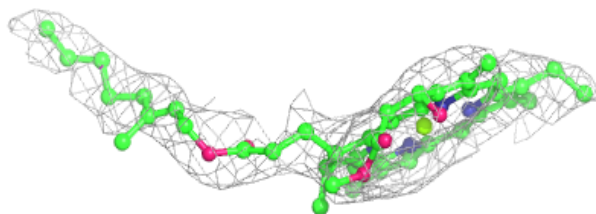
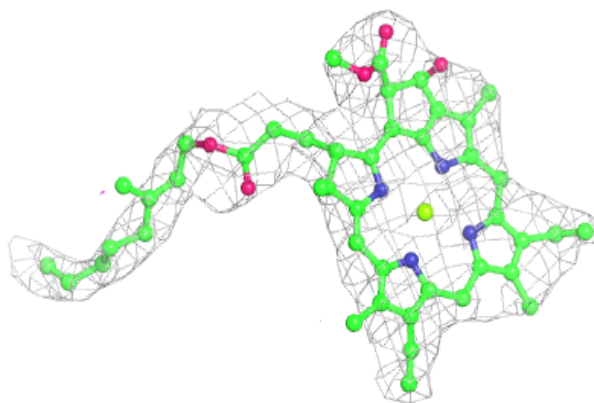
Electron density around CLA B 1227:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



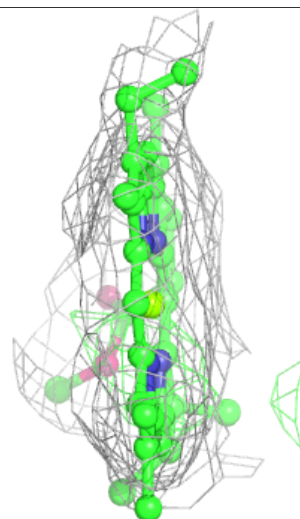
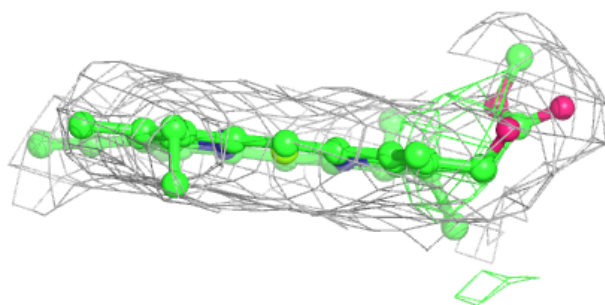
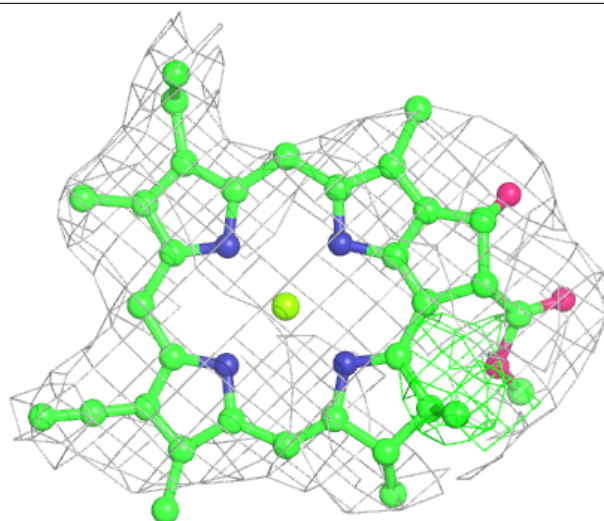
Electron density around CLA B 9022:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



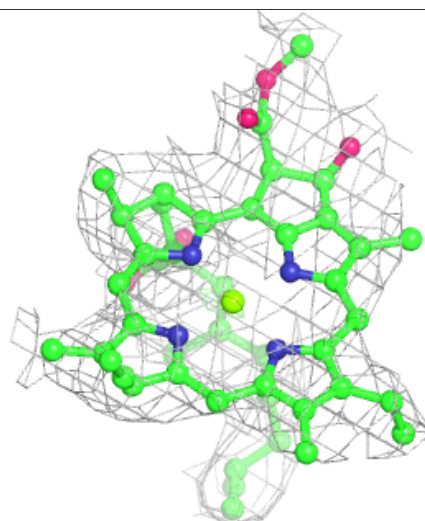
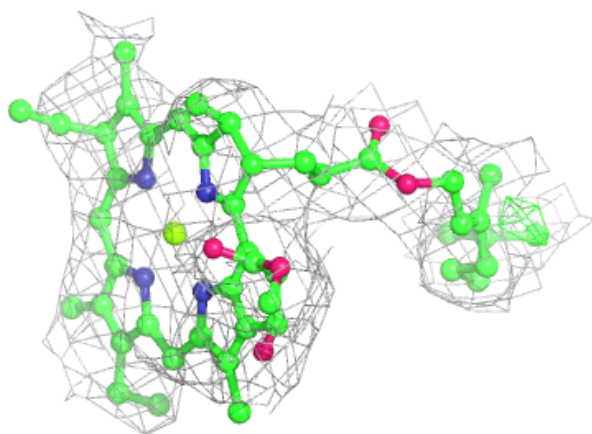
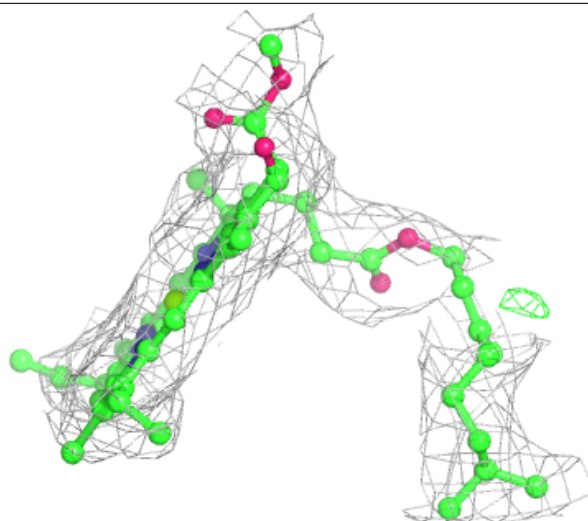
Electron density around CLA A 1106:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



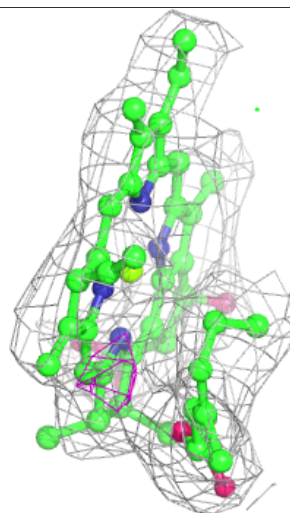
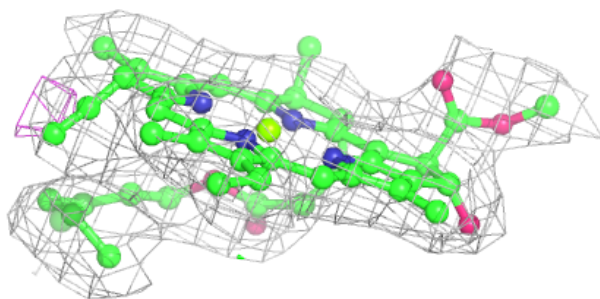
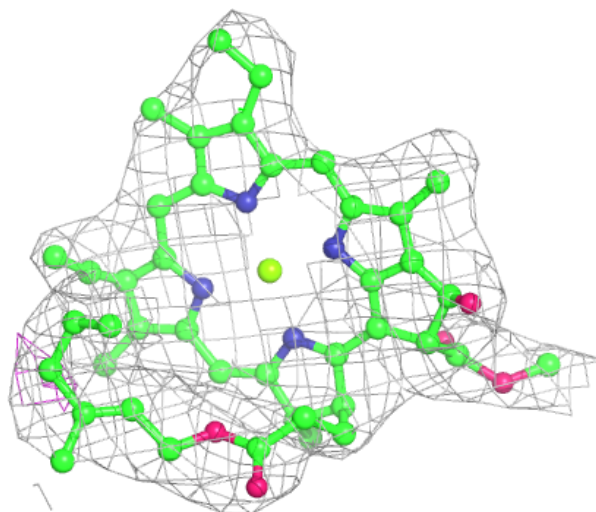
Electron density around CLA A 1128:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



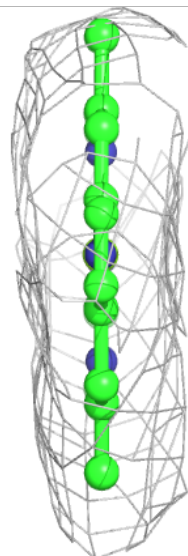
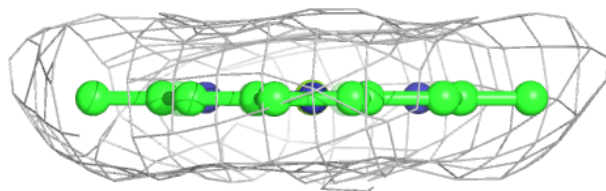
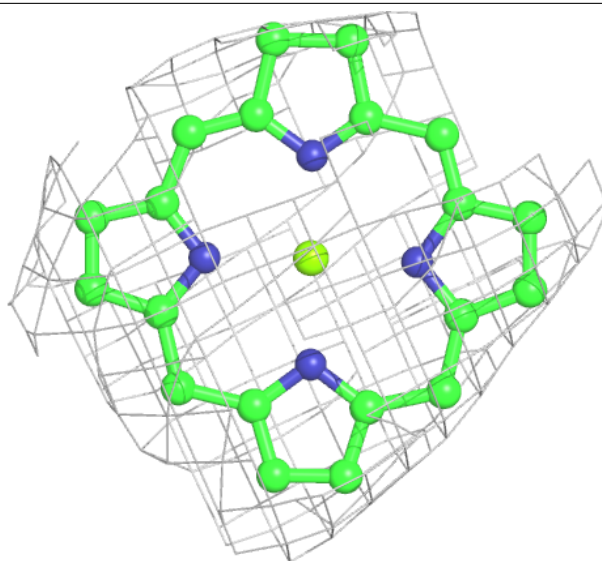
Electron density around CLA B 1215:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



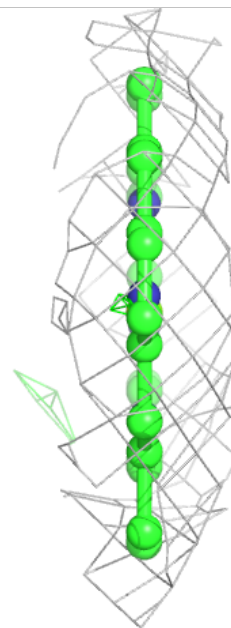
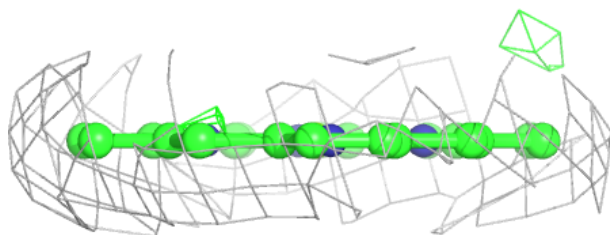
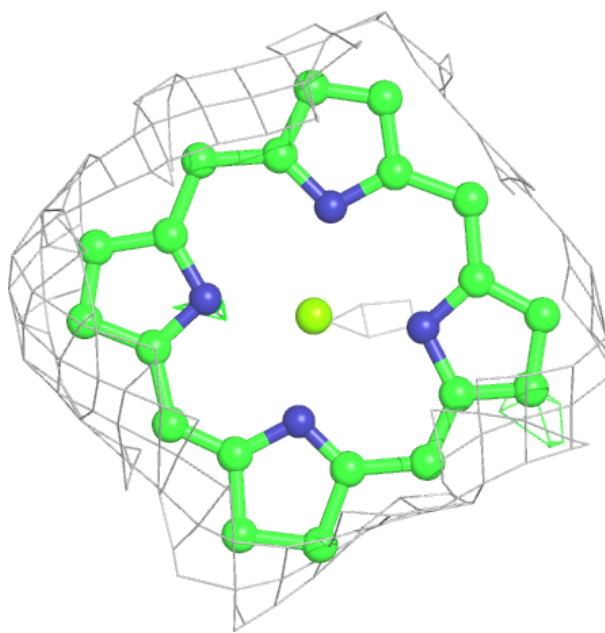
Electron density around CLA F 1240:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 2007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**6.5 Other polymers** ⓘ

There are no such residues in this entry.